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Towards first principles prediction of pK_a : COSMO-RS and the cluster-continuum approach

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Abstract:

The COSMO-RS method, a post quantum chemistry extension of the quantum chemical dielectric continuum solvation model COSMO with a statistical thermodynamics treatment for realistic solvation simulation, has been applied to the prediction of aqueous pK_a of acids and bases. The combination of the COSMO-RS approach to pK_a prediction with the cluster-continuum approach (explicit solvation of the solute compound with one or more solvent molecules) was used on three data sets consisting of 94 acids and 75 bases. Correlation of the calculated free energies of dissociation in water with the experimental aqueous pK_a of the solute acids and bases in their bare state and explicitly solvated by one or two solvent molecules showed an increase of the regression slope with the number of explicit solvent molecules thus showing a regression slope that is closer to the theoretical value than the slope found for bare solutes. It was found that the cluster-continuum approach is limited to a pK_a range of strong to moderately weak acids and bases, because the optimizations of the solvent-solute complexes of the ionic species of very weak acids (such as the anion of *tert*-butanol) did not lead to the desired complexes but yielded dissociation products.

Keywords: pK_a ; acidity; basicity; COSMO; COSMO-RS; explicit solvation; cluster-continuum model;

Introduction

The transfer of protons is one of the central processes in biology, organic, and inorganic chemistry. Consequently, the detailed analysis of the thermodynamics of the proton transfer reaction and the prediction of dissociation constants of acids and bases in different solvents have found substantial interest in many areas of chemistry and biochemistry. Experimental measurement of aqueous phase pK_a values nowadays has become an inexpensive standard application¹. However, there are broad classes of chemicals that are not readily amenable to experimental characterization (e.g. reaction intermediates, very strong and very weak acids or bases with a pK_a outside the pK_a range that can be conveniently measured). Therefore, considerable and ongoing effort has been devoted to the development of first principle prediction methods for pK_a values. The computational prediction of high quality gas phase dissociation constants has become feasible with high level (post-Hartree-Fock) *ab initio* quantum chemistry methods, which nowadays can be as good or even more accurate than the experimentally challenging measurements of this property²⁻⁶. In the liquid phase, which is of much larger practical importance, the situation seems reversed: at least for solvent water there is a large number of reliable experimental dissociation constant data available, but the theoretical prediction from first principles is extremely challenging because of the strong solvation effects of the neutral and ionic species involved in the proton transfer reaction. Thus the prediction of dissociation constants can be seen as the ultimate challenge for quantum chemistry (QC) based solvation models, where the general goal is to improve the reliability of the computational approach so as to have a realistic comparison with the available experimental data. A large number of attempts in this direction have been reported, but a consistent and generally applicable method is still lacking. Nevertheless, the rapid development of efficient QC methods in recent years has opened new perspectives for the modeling of acid-base equilibria in solution

and the rigorous prediction of the associated pK_a values in the liquid. The effect of the solvent on the proton transfer reaction can be included in quantum chemical computations in two ways: either the solvent molecules are accounted for explicitly, as in the molecular dynamics (MD) simulation framework⁷, or implicitly, using a continuum solvation model. Due to its considerable computational cost, the MD based explicit solvation approach yet remained restricted to a limited number of small systems. Of the different implicit QC methodologies available for the computation of pK_a values the Dielectric Continuum Solvation Methods (DCSMs) have become most popular⁹, because they are able to describe long range electrostatic interactions of solutes with a solvent at moderate computational cost in the context of quantum chemical programs¹⁰⁻¹⁷. Thus QC based DCSM methods may help to shed some light on the particulars of the relationship between molecular structure and pK_a value. In DCSMs the interactions of a solute molecule with the solvent are treated by means of putting the solute in a cavity that is surrounded by a dielectric continuum, which represents the solvent. Solvent-related properties like the size and shape of the cavity are treated as adjustable parameters and obtained from physically motivated modeling procedures. DCSMs are distinguished by the construction of the cavity and how the solute-solvent interactions are treated. Despite the well known deficiencies of DCSM methods, (i.e. the neglect of hydrogen bonding and the inadequate treatment of the short range electrostatics^{10,18-21}, which can be much stronger in ions than in neutrals and thus can introduce a large asymmetry to the solvation energy of an acid compared to its conjugate base) it is possible to correlate the quantum chemical dissociation free energy of a solvated molecule ΔG_{diss} with its pK_a via a linear free energy relationship (LFER)¹⁰:

$$pK_a = c_1 \Delta G_{diss} + c_2 \quad (1)$$

From the basic thermodynamics c_1 is expected to be unity if ΔG_{diss} would be calculated without a systematic error and the LFER axis intercept c_2 is expected to be equal to $-\log[\text{Solvent}]$ ²². Looking in detail into the DCSM studies,¹⁰⁻¹⁷ in the regression of pK_a values versus the calculated dissociation free energy ΔG_{diss} the studies report slopes that are significantly lower than the theoretically expected value

of $1/RT\ln(10)$, which was first noted and discussed by Klamt *et al.*¹⁰. Such a behavior has been reported for aqueous¹⁰⁻¹² and non-aqueous acids^{10,13-15,23} as well as for bases.^{16,17,24} This drawback is common to all simple DCSMs unless considerable effort is taken in the (often physically hardly justifiable) adjustment of numerous additional and often physically doubtful parameters of the DCSM. Atom type or hybridization specific cavity radii and cavity definitions that depend on the charge of the molecule are examples of such parameters²⁵. Although such models became quite popular and successful applications for water and nonaqueous solvents have been reported^{10-17, 22-27}, it remains doubtful if the predictive power of such empirical adjustments persists for more complex chemically multifunctional solutes or for solutes such as free radicals, zwitterions or excited states²³. In particular empirical models are very likely to fail if electron delocalization is important in the anions or cations involved in the proton exchange reaction^{8,28}. Pliego and Riveros²⁹ showed that the error of such DCSM methods in pK_a predictions can become as large as 7 pK_a units when solutes with different functional groups are considered. They proposed that the neglect of specific solute-solvent interactions may cause this significant error²⁹.

A promising approach to the pK_a problem, which does not artificially modify the cavity to try to reproduce hydrogen bonding and short-range solute-solvent interaction behavior that is not accounted for by the DCSM, is the addition of explicit solvent molecules to the solute ions²⁹⁻³⁴, which in the context of pK_a prediction by DCSM's has been reported in the literature as "Cluster-Continuum"^{29,30,33}, "Supermolecule"^{32,34}, or "Implicit-Explicit Solvation"³¹ approach. The solute and its according ionic form are represented by a cluster of the neutral and ionic solute molecule with one or more surrounding solvent molecules that form a partial or full solvation shell around the compound, accounting for local solute-solvent interactions such as Hydrogen Bonding (HB) and electrostatic charge-dipole interactions in a physical way. Compared to simple DCSMs, this approach appears to increase the slope of the aqueous pK_a LFER with each added explicit water²⁹⁻³⁴, but its practical application leads to some ambiguities and problems: there is no natural choice of the number of solvent molecules that represent the solvent shell, retaining some level of arbitrariness involved, where a choice has to be taken.

However, what in practice might turn out to be the much harder problem, is the optimization of the solute-solvent cluster. For complex, multifunctional solutes, as most chemically or biologically interesting drug-like compounds are, it is very difficult and computationally demanding to find the global minimum of the weakly bonded solute-solvent complex³⁴. If the solvent itself is a complex multifunctional compound, or if a mixture of several solvent compounds is used, it easily may become impossible to find and optimize the global minimum of the cluster at all. To avoid the problematic optimization of weakly bound complexes Adam³⁴ suggested to use only one or two explicit solvent molecules only if there are strong hydrogen bonds between the solute and solvent, so that the resulting complex is stable in the gas phase and thus can be observed experimentally³⁴. Unfortunately this criterion does not resolve the problem of getting the right number of explicit solvent molecules, nor does it seem to be applicable to complex multifunctional compounds or compounds with electron delocalization, where it might not be easy to decide if there is strong or weak bonding in the complex.

To be able to overcome the arbitrariness involved in the choice of the number of explicit solvent molecules added to the solute, Ding *et al.*³² proposed for each solute to pick from the set of bare, mono- or di-solvated solutes that species, which minimizes the calculated total free energy of dissociation, thus introducing an additional local descriptor of the chemical nature of the solute-solvent interactions. They argue that the minimum dissociation energy species should be the compound with the highest thermodynamic stability in the framework of the quantum chemical dielectric continuum solvation model used. This approach reflects some known defects of DCSM's for protic and polar solvents, in particular the neglect of Hydrogen Bonding interactions between solute and solute, which are introduced when explicit solvent molecules are added. Thus for protic and polar solvents such as water or dimethylsulfoxide the addition of a solvent sphere may lead to improved correlation of ΔG_{diss} with experimental pK_a , while solvents of low polarity are well represented by the DCSM on the bare solute compound. It must be noted, that while being physically plausible, this criterion is hardly applicable in

practical predictions, because for any solute it involves the conformational search and optimization of bare solutes, *mono-*, *di-* and probably even higher solvated solute-solvent clusters.

A different criterion for the choice of the number of explicit solvent molecules was introduced by Pliego and Riveros²⁹. In their reasoning the cluster with the number of explicit solvent molecules that minimizes the free energy of solvation of the anionic or cationic form of the solute acid or base, respectively, should lead to the best predictions of the property based on the cluster-continuum model, based on the assumption that for a rigid cluster, the complex with minimum free energy of solvation will be closest the *real* free energy of solvation of the ion in solution. They found that for aqueous pK_a typically three explicit water molecules minimize the free energy of solvation of the anions or cations. Apart from the significant theoretical and practical problems that are raised by finding the global minimum of a cluster consisting of four weakly bonded compounds, the free energy of solvation of the ionic form only partly reflects the physics of the dissociation reaction, totally neglecting the solvation of the neutral solute and the influence of the quantum chemical method, both of which are accounted for by the criterion of Ding *et al.*³².

Another set of rather heuristic criteria for explicit solvation of acids was proposed by Kelly *et al.*³¹. In combination with their post-DSCM method SM6³⁵, they proposed to add a single explicit water molecule to the anionic form of a solute acid only (*semi-solvation*), either if the anion consists of less than three atoms, or if the charge of the anionic form of the acid is localized on one or more oxygen atoms in a way that the oxygen(s) bear a more negative partial charge than the oxygen of the solvent water. Obviously, for both criteria a certain amount of arbitrariness remains. In particular, the quite arbitrary partition of the solute anions into species that form a strong hydrogen bond with water (the ones whose oxygens have a more negative partial charge than the water oxygen) and those who do not, is doubtful. If explicit solvation is trying to compensate the shortcomings of the DCSM, which does not account for Hydrogen Bonding interactions at all, the division into strong and weak hydrogen bonds does not seem useful. Neither does this separation make sense if one tries to account for shortcomings of

the underlying quantum chemistry or DFT methods, which have or don't have the same problems for strong and weak Hydrogen Bonds.

The DCSM-based implicit/explicit pK_a models already mentioned use the combination of a gas phase dissociation energy of the cluster compounds (the explicit solvation part) computed by a high-level QC method, with the cluster free energy of solvation³⁶⁻³⁸ computed by a DCSM model (the implicit solvation part), which connects the gas phase to the liquid state. These approaches all rely on explicit solvation to correct the shortcomings of the DCSM method. In this work we chose a different approach: the Conductor-like Screening Model for Real Solvents (COSMO-RS)¹⁸⁻²¹. COSMO-RS goes beyond the DCSM concept in that it combines the electrostatic advantages and the computational efficiency of the DCSM COSMO³⁹ with a statistical thermodynamics method for local interaction of surfaces, which takes into account local deviations from dielectric behavior as well as hydrogen bonding. In this approach all information about solutes and solvents is extracted from initial QC-COSMO calculations, and only very few parameters have been adjusted to experimental values of partition coefficients and vapor pressures of a wide range of neutral organic compounds. COSMO-RS is capable of predicting partition coefficients, vapor pressures, and solvation free energies of neutral compounds with a root mean square error (rmse) of 0.3 log-units and better and a lot of experience has been gathered during the past years about its surprising ability to predict mixture thermodynamics¹⁸⁻²⁰. Although COSMO-RS could successfully be applied to the first principles prediction of aqueous acidity¹⁰ and basicity²⁴ as well as acid and base pK_a in non-aqueous solvents^{10,28}, there remained some problematic aspects: most prominently, the correlation of COSMO-RS predicted free energy of dissociation with experimental pK_a showed a slope that is lower than the one expected from thermodynamic theory^{10,24}. I.e. COSMO-RS was not able to solve the slope problem of the underlying DCSM COSMO. In addition it was found that the systematic deviations known from DCSMs for aliphatic amine compounds were also present in COSMO-RS predictions of aqueous base pK_a ²⁴. This study tries to assess if the combination of the COSMO-RS method for predicting pK_a with the explicit solvation approach is able to resolve these issues. In addition, the performance and stability of different criteria for the choice of the number of

explicit solvent molecules is tested. We decided to perform this study on the data sets for aqueous acids and base pK_a already published^{10,24}. The standard COSMO-RS method implemented in the COSMOtherm program⁴⁰ based on Turbomole DFT/COSMO calculations⁴¹⁻⁴⁶ was used for this purpose.

Theoretical calculations

Our theoretical calculations of ΔG_{diss} of aqueous acids are based on the reaction model

The theoretical calculations of ΔG_{diss} of aqueous bases are based on the reaction model

Unlike the DCSM methods mentioned, COSMO-RS is able to directly calculate the free energy of each species in aqueous solution. Thus no gas phase energies were computed. We applied our standard procedure for COSMO-RS calculations to all four species appearing in eqs. 2 and 3, which consists of two steps:

1) Full DFT geometry optimization with the Turbomole program package⁴³ using B-P density functional^{44,45} with TZVP quality basis set using the RI approximation.⁴⁶ During these calculations the COSMO continuum solvation model was applied in the conductor limit ($\epsilon = \infty$). Optimized element-specific radii from the COSMO-RS parameterizations^{19,20} have been used for the COSMO cavity construction. Such calculations end up with the self-consistent state of the solute in the presence of a virtual conductor that surrounds the solute outside the cavity.

2) COSMO-RS calculations have been done using the COSMOtherm program³⁶. In these calculations the deviations of the real solvent, in this case water, compared to an ideal conductor are taken into account in a model of pair-wise interacting molecular surfaces. For this purpose, electrostatic energy differences and hydrogen bonding energies are quantified as functions of the local COSMO polarization

charge densities σ and σ' of the two interacting surface pieces. The chemical potential differences arising from these interactions are evaluated using an exact statistical thermodynamics algorithm for independently pair-wise interacting surfaces, which is implemented in COSMOtherm. More detailed descriptions of the COSMO-RS method are given elsewhere¹⁸⁻²¹.

If more than one cluster conformation or different deprotonation or protonation sites were considered to be potentially relevant for the neutral, anionic, or cationic form of the acids AH and bases B, several conformations were calculated in step 1 and a thermodynamic Boltzmann average over the total Gibbs free energies of the conformers was consistently calculated by the COSMOtherm program in step 2. For this study the geometries of all molecules taken from refs. 10 and 24 have been re-optimized on BP/TZVP/COSMO level. In addition all compounds have been carefully rechecked for possible conformations, and if necessary, additional conformations have been added to the COSMOtherm calculations in step 2.

To avoid the human bias and ambiguity involved in the construction of the clusters of the solute with one or two explicit water molecules, their geometries were created with a novel COSMO-RS based procedure: starting from the optimized BP/TZVP/COSMO geometries of the bare solute molecule and the water molecule, the pair-interaction energies of all possible contacts of the cavities of the two molecules are scanned and the minimum energy contact, which for both molecules is the site where the contact probability between the molecule is largest and thus the site where a cluster is most likely to be formed, will be identified. Along the bond defined by this contact site, the solvent molecule is arranged at different torsional angles between 0° and 360°, in steps of 45° and the resulting cluster geometries were optimized independently at BP/TZVP/COSMO level of theory. Of the cluster conformer thus found, the minimum energy cluster is used in the COSMO-RS computation of step 2. The clusters with two explicit water molecules are created the same way, using the *mono*-solvated solute cluster as starting structure instead of the bare solute. This procedure is applicable in the same manner to neutral and ionic species, and to any solvent or solute (which itself can be a cluster). Thus it can be automated quite

1 easily. Although the cluster generation procedure via COSMO-RS created cluster geometries is not a
 2 global optimization procedure and thus can not guarantee that the optimized clusters are the absolute
 3 minimum energy structures of the phase space spanned by the atomic coordinates of the complexes, it
 4 provides a reliable, consistent - and what is even more important for practical application: simple,
 5 automatic, and unbiased - procedure for finding cluster geometries that are very likely to be the best (and
 6 minimum energy) structures in the framework of the QC/COSMO-RS approach used. For a small subset
 7 of the clusters, a global approach to finding the minimum energy conformations of the clusters was
 8 tested: *ab initio* MD simulated annealing of the geometries on BP/TZVP/COSMO level of theory, as
 9 provided by Turbomole⁴³. For the compounds tested (*tert*-butanol, oxalic acid, indole, melamine) the
 10 MD procedure was not able to find lower energy cluster conformations than the COSMO-RS contact
 11 probability based method, which is strong indicator for the soundness of the COSMO-RS provided
 12 geometries. The optimized geometries of all the acids, bases, ions and explicitly solvated cluster-
 13 compounds are given in the Supplementary Material section of this journal.

14 For all acids AH, the Gibbs free energy of dissociation (ΔG_{diss}) has been calculated as the difference of
 15 the total free energy of the anion A^- and the neutral acid AH. The free energy difference of H_3O^+ and
 16 H_2O is a constant additional contribution:

$$\Delta G_{\text{diss}} = G_{\text{tot}}(A^-) - G_{\text{tot}}(AH) + [G_{\text{tot}}(H_3O^+) - G_{\text{tot}}(H_2O)] \quad (4)$$

17 For all bases B, the Gibbs free energy of dissociation (ΔG_{diss}) has been calculated as the difference of the
 18 total free energy of the protonated cation BH^+ and the base B. To this free energy difference the free
 19 energy difference of H_3O^+ and H_2O is a constant additional contribution:

$$\Delta G_{\text{diss}} = G_{\text{tot}}(B) - G_{\text{tot}}(BH^+) + [G_{\text{tot}}(H_3O^+) - G_{\text{tot}}(H_2O)] \quad (5)$$

20 From the calculation procedure described above, we get $G_{\text{tot}}(H_3O^+) - G_{\text{tot}}(H_2O) = 1124.47$ kJ/mol. This
 21 value is in good agreement with literature estimates²³. Zero point vibrational energies are not taken into
 22 account. Consequently, the geometries optimized in step 1 were not analyzed for the nature of the
 23 stationary point of the optimized geometry. We make the common assumption that the difference in zero

point energy between the neutral and the deprotonated acid or protonated base is small and systematic¹⁰.

All regressions of the dissociation free energy vs. experimental pKa have been cross-validated by a “leave-one-out” cross-validation procedure. The cross-validated regression coefficients g^2 are given together with the regression coefficients r^2 .

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Aqueous Acids

For the purpose of finding the LFER coefficients of eq. 1, a data set of 94 acids in solvent water was used. The data set consists of the reference data set of 5 alcohols, 23 carboxylic acids, 8 inorganic acids, 16 phenols, and 12 heterocyclic compounds as reported in ref. 10. A set of 30 multifunctional substituted benzoic acids⁵¹ has been added to the initial data set, to be able to assess the performance of the explicit solvation on more challenging solutes. The acids experimental pKa values range from 0 to 19. No compound has been removed from the data set for any reason during the study.

FIGURE 1: Calculated Gibbs free energy of dissociation vs. experimental acids pK_a in solvent water. Open rhombus: bare acids and anions. Dotted line: regression line (eq. 4) for bare acids ($r^2 = 0.978$, $q^2 = 0.976$, $c_1 = 0.107$, $c_2 = 1.94$). Filled squares: acids and anions with one explicit water molecule. Striped line: regression line (eq. 5) for *mono*-solvated compounds ($r^2 = 0.935$, $q^2 = 0.932$, $c_1 = 0.164$, $c_2 = -1.56$). Filled triangles: acids and anions with two explicit water molecules, respectively. Solid line: regression line (eq. 6) for *di*-solvated compounds ($r^2 = 0.899$, $q^2 = 0.893$, $c_1 = 0.190$, $c_2 = -2.94$).

The results for all 94 acids are shown in Table 1 and Figure 1. The free energies of all individual species are given in the Supplementary Material section of this journal. The regression of the calculated aqueous Gibbs free energy of dissociation (ΔG_{diss}) vs. experimental pK_a for the bare neutral and ionic compounds results in a correlation coefficient of $r^2 = 0.978$ ($q^2 = 0.976$). The regression equation for the bare acids pK_a in aqueous solution reads

$$pK_a = 0.107(\pm 0.01)\Delta G_{\text{diss}} + 1.94(\pm 0.1) \quad (4)$$

If we would have omitted the free energy difference of H_3O^+ and H_2O , which we calculate as

-1124.47 kJ/mol, in the definition of ΔG_{diss} we would have got a regression constant of $\hat{c}_2 = -118.75$.

Including this energy difference, the calculated axis intercept of 1.9 is reasonably close to the theoretical value of $c_2 = -\log[H_2O] = -1.74$. In accordance with previous work¹⁰ on aqueous acidity of bare compounds we found that the slope of the regression is lower than the theoretical value of $1/RT\ln(10) = 0.1759$.

The regression equation for the *mono*-solvated neutral and ionic compounds ($r^2 = 0.935$, $q^2 = 0.932$) reads

$$pK_a = 0.164(\pm 0.01)\Delta G_{\text{diss}} - 1.56(\pm 0.1) \quad (5)$$

which omitting the free energy difference of H_3O^+ and H_2O , yields a regression constant of $\hat{c}_2 = -185.42$.

Thus, in comparison with the bare compound regression, the slope of the *mono*-solvated solutes is closer to the theoretical value. Yet the slope remains to be somewhat smaller than the theoretical value.

Moreover, the correlation of ΔG_{diss} with the experimental pK_a data is worse than for the bare compounds. If the explicit solvation is applied to the ionic form of the compound set only (*semi*-solvation, as proposed by Kelly *et al.*³¹) the slope of the regression (with $r^2 = 0.929$, $q^2 = 0.926$) decreases to $c_1 = 0.139$ and the regression constant is $c_2 = 27875.09$, which omitting the free energy difference of H_3O^+ and H_2O , yields $\hat{c}_2 = -317.98$. Thus the *semi*-solvation expectably yields to a regression that is somewhat in between the regression of the bare and the *mono*-solvated solutes.

The regression equation for the *di*-solvated neutral and ionic compounds ($r^2 = 0.899$, $q^2 = 0.893$) reads

$$pK_a = 0.190(\pm 0.01) \frac{\Delta G_{\text{diss}}}{RT \ln(10)} - 2.94(\pm 0.1) \quad (6)$$

which omitting the free energy difference of H_3O^+ and H_2O , yields a regression constant of $\hat{c}_2 = -216.54$. Both slope and regression constant are closer to the theoretical values for the *di*-solvated compounds compared to the bare compounds or the *mono*-solvated compounds, the slope is even higher than the theoretical value. Again, the correlation of ΔG_{diss} with the experimental pK_a data for *di*-solvated compounds is worse than for the *mono*-solvated and bare compounds.

These results corroborate the claims given in the literature²⁹⁻³⁴ that the explicit solvation approach is able to solve the *slope problem*¹⁰ of the quantum chemical DCSM's. However, they lead to new problems: First, even when quite careful choice of the minimum energy structure of the solvent-solute cluster is applied, the overall correlation deteriorates with increasing number of explicit solvent molecules. Second, even though the slope of the ΔG_{diss} vs. pK_a correlations is closer to the theoretical slope for the *mono*- or *di*-solvated solutes, it is still somewhat different, and for the *di*-solvated solutes even overshoots the theoretical value. A convergence of the slope appears to be reached at *di*-solvation, because the change in slope from *mono*- to *di*-solvation is much smaller than from bare solutes to *mono*-solvation.

If, following Ding *et al.*³², we introduce the additional solute specific category of minimal ΔG_{diss} in the choice of the cluster or bare solute for the correlation with $\text{p}K_{\text{a}}$, a look at the ΔG_{diss} values in Table 1 reveals an important trend: while for strong and medium acids with $\text{p}K_{\text{a}} < 10$ the bare solute is preferred, weak acids show minimum dissociation free energy if they are solvated with one or, for very weak acids with $\text{p}K_{\text{a}} > 12$, two explicit water molecules. When looking at dissociation energy as computed on the DCSM level only (i.e. BP/TZVP/COSMO without COSMO-RS), the doubly solvated solute is preferred throughout the entire $\text{p}K_{\text{a}}$ range. This implies that a major portion of the interaction effects that are missing in the DCSM already is taken into account by COSMO-RS, which however has problems with very weak acids. This flaw can be explained quite well in the framework of COSMO-RS theory: as yet, non-local long range electrostatic effects and strong hydrogen bonding are not explicitly taken into account by COSMO-RS⁴⁷. Now, the dissociation of very weak acids leads to anions where the charge is very concentrated and often localized on only one atom. It is exactly this type of ions where the COSMO-RS neglect of non-local electrostatic effects and strong hydrogen bonding may lead to increased errors – and, in turn, explicit solvation captures some of these neglected interactions. Thus the combination of COSMO-RS computed free energies of dissociation with the approach of Ding *et al.*³², does not seem to be very promising: the overall correlation of the minimum ΔG_{diss} with $\text{p}K_{\text{a}}$ is worse than the one for the bare solutes ($r^2 = 0.915$, $q^2 = 0.912$) and it leads to a slope that is significantly lower than the theoretical: $c_1 = 0.127$ and the regression constant is $c_2 = 1.54$, which omitting the free energy difference of H_3O^+ and H_2O , yields $\hat{c}_2 = -141.58$.

FIGURE 2: Optimized geometries for $(\text{CH}_3)_3\text{C-O}^{(-)}\cdots\text{H-O-H}$ and $(\text{CH}_3)_3\text{C-OH}\cdots\text{O}^{(-)}\text{-H}$.

Critical inspection of Table 1 and Figure 1 shows that there is one significant outlier in the regression of the mono- and di-solvated compounds, but not in the regression of the bare ions. It is *tert*-butanol, the weakest acid in the data set. A closer look at the optimized geometries of the explicitly solvated *tert*-butanol and *tert*-butoxy-anion revealed that the quantum chemical optimization of the *tert*-butoxy-anion - water and di-water clusters yielded an unexpected structure: Instead of the anion - water cluster $(\text{CH}_3)_3\text{C-O}^{(-)}\cdots\text{H-O-H}$, a complex of *tert*-butanol with an hydroxy-anion $(\text{CH}_3)_3\text{C-OH}\cdots\text{O}^{(-)}\text{-H}$, or in the case of two explicit water molecules the anion $(\text{CH}_3)_3\text{C-OH}\cdots\text{O}^{(-)}\text{-H}\cdots\text{H-O-H}$, was optimized (see Figure 2). The exact same artifact can also be observed in the data published by Kelly *et al.*³¹. A deeper investigation of the configurational space of the *tert*-butoxy-anion cluster showed that any free optimization of the *tert*-butoxy-anion - water cluster always yielded in a *tert*-butanol - hydroxy-anion cluster. A constrained optimization of the *tert*-butoxy-anion - water complex with the contacting hydrogen atom of the water molecule fixed at the equilibrium bond distance of the isolated water molecule with a subsequent potential energy surface scan along the $\text{O}^{(-)}\cdots\text{H-O-H}$ bond resulted in a minimum energy structure with the expected $(\text{CH}_3)_3\text{C-O}^{(-)}\cdots\text{H-O-H}$ geometry, which however was 73 kJ/mol higher in energy than the $(\text{CH}_3)_3\text{C-OH}\cdots\text{O}^{(-)}\text{-H}$ structure and thus lead to an even worse regression with the experimental $\text{p}K_a$. Obviously, for the anions of very weak acids like *tert*-butanol, which have their negative charge sharply localized on one atom, the hydrogen-transfer of a hydrogen atom from the water to the anionic site leads to an energetically much favoured structure, compared to the hydrogen bonded anion - water cluster expected from the explicit solvation model - at least on the quantum chemical level of theory employed in this study. This implies that the cluster-continuum model can not be applied to very weak acids like *tert*-butanol. Thus the applicability range of the cluster-continuum model seems to be restricted to acids of medium strength, (again that is, for the quantum chemical BP//TZVP//COSMO level of theory used in this study). As a consequence, *tert*-butanol was

removed from the regression. The new correlation for 93 acids leads to the following regression

equations: The regression equation for the bare solutes ($r^2 = 0.975$, $q^2 = 0.973$) reads

$$\text{p}K_{\text{a}} = 0.105(\pm 0.01)\Delta G_{\text{diss}} + 1.99(\pm 0.1) \quad (7)$$

which omitting the free energy difference of H_3O^+ and H_2O , yields a regression constant of $\hat{c}_2 = -116.40$.

The regression equation for the *mono*-solvated neutral and ionic compounds ($r^2 = 0.934$, $q^2 = 0.929$) reads

$$\text{p}K_{\text{a}} = 0.157(\pm 0.01)\Delta G_{\text{diss}} - 1.32(\pm 0.1) \quad (8)$$

which omitting the free energy difference of H_3O^+ and H_2O , yields a regression constant of $\hat{c}_2 = -177.83$.

The regression equation for the *di*-solvated neutral and ionic compounds ($r^2 = 0.907$, $q^2 = 0.901$) reads

$$\text{p}K_{\text{a}} = 0.180(\pm 0.01)\Delta G_{\text{diss}} - 2.56(\pm 0.1) \quad (9)$$

which omitting the free energy difference of H_3O^+ and H_2O , yields a regression constant of $\hat{c}_2 = -205.20$.

Thus even if the problematic compound is removed from the data set, the general trends of decreasing correlation quality and non-theoretical slope with increasing number of explicit solvent molecules remained.

Aqueous Bases

For the purpose of finding the eq. 1 LFER correlations of the base protonation reaction, a data set of 43 bases was taken from ref. 24. Experimental base $\text{p}K_{\text{a}}$ values range between -5 and 14. This set consists of 35 bases that are protonated at a nitrogen atom, namely five anilines, four amidines, six benzodiazepines, four guanidines, and 16 five- or six-ring heterocyclic compounds, and eight bases that

are protonated at a carbon atom, namely four pyrroles and four indoles. For the pyrroles and indoles we considered all possible protonation sites in the conformer equilibrium calculations of the cations.

FIGURE 3: Calculated Gibbs free energy of dissociation vs. experimental bases pK_a in solvent water. Open rhombus: bare bases and cations. Dotted line: regression line (eq. 10) for bare bases ($r^2 = 0.981$, $q^2 = 0.979$, $c_1 = 0.130$, $c_2 = -1.57$). Filled squares: bases and cations with one explicit water molecule. Striped line: regression line (eq. 11) for mono-solvated compounds ($r^2 = 0.973$, $q^2 = 0.970$, $c_1 = 0.153$, $c_2 = -2.48$).

The results for all 43 bases are shown in Table 2 and Figure 3. The free energies of all the individual species are given in the Supplementary Material section of this journal. The regression of the calculated

aqueous Gibbs free energy of dissociation (ΔG_{diss}) vs. experimental base $\text{p}K_{\text{a}}$ for the bare neutral and cationic compounds results in a correlation coefficient of $r^2 = 0.981$ ($q^2 = 0.979$). The regression equation for the bare bases $\text{p}K_{\text{a}}$ in aqueous solution reads

$$\text{p}K_{\text{a}} = 0.130(\pm 0.01) \frac{\Delta G_{\text{diss}}}{RT \ln(10)} - 1.57(\pm 0.1) \quad (10)$$

If we would have omitted the free energy difference of H_3O^+ and H_2O in the definition of ΔG_{diss} we would have got a regression constant of $\hat{c}_2 = -147.96$. Including this energy difference, the calculated axis intercept of 1.9 is very close to the theoretical value of $c_2 = -\log[\text{H}_2\text{O}] = -1.74$. In accordance with previous work²⁴ on aqueous basicity of bare compounds we found that the slope of the regression is lower than the theoretical value of $1/RT \ln(10) = 0.1759$.

The regression equation for the *mono*-solvated base compounds ($r^2 = 0.973$, $q^2 = 0.970$) reads

$$\text{p}K_{\text{a}} = 0.153(\pm 0.01) \frac{\Delta G_{\text{diss}}}{RT \ln(10)} - 2.47(\pm 0.1) \quad (11)$$

which omitting the free energy difference of H_3O^+ and H_2O , yields a regression constant of $\hat{c}_2 = -174.24$. Thus, in comparison with the bare compound regression, the slope of the *mono*-solvated solutes is closer to the theoretical value. Yet the slope remains to be significantly smaller than the theoretical value. Moreover, the correlation of ΔG_{diss} with the experimental $\text{p}K_{\text{a}}$ data is worse than for the bare compounds.

If, again following Ding *et al.*³², we introduce the additional solute specific category of minimal ΔG_{diss} in the choice of the cluster or bare solute for the correlation with $\text{p}K_{\text{a}}$, the ΔG_{diss} values in Table 2 follow the same trend that was spotted for the acidic solutes: for strong bases with base $\text{p}K_{\text{a}} < 5$ the bare solute is preferred, while weak bases show minimum dissociation free energy for the solvated molecules, which is essentially the same behavior as recognized for acids. The overall correlation of the minimum

ΔG_{diss} with base $\text{p}K_{\text{a}}$ is worse than the one for the bare solutes ($r^2 = 0.974$, $q^2 = 0.972$) and it leads to a

slope that is significantly lower than the theoretical: $c_1 = 0.140$ and the regression constant is $c_2 = -1.61$, which omitting the free energy difference of H_3O^+ and H_2O , yields $\hat{c}_2 = -159.17$.

Another important aspect of the base $\text{p}K_{\text{a}}$ prediction using DCSM's is the systematic deviation that is found for aliphatic amines²⁴. This group of compounds is known to cause considerable problems in most quantum chemical continuum solvation models^{21,48-50}, which also has consequences in the COSMO-RS prediction of $\text{p}K_{\text{a}}$, namely a systematic deviation for *secondary* and *tertiary* aliphatic amines. COSMO-RS computations of ΔG_{diss} of bare and mono-solvated bases is given in Table 3 for 32 *primary*, *secondary* and *tertiary* aliphatic amines. The $\text{p}K_{\text{a}}$ values for these compounds have been calculated using eq. 10 for bare solutes and eq. 11 for mono-solvated solutes, respectively. The root mean square error (RMSE) is 1.38 for bare amine solutes and 1.76 for mono-solvated amines. The systematic deviation of the *secondary* and *tertiary* aliphatic amines is more pronounced for the mono-solvated amines than for the bare amines. Thus it must be concluded that the explicit solvation approach is not capable of curing the flaws that DCSM's and COSMO-RS show for aliphatic amines.

Conclusions

Linear relations between $\text{p}K_{\text{a}}$ and the free energy of dissociation in aqueous solution ΔG_{diss} , as computed by the post-DCSM method COSMO-RS on the basis of quantum chemical DFT/COSMO calculations, have been obtained for the deprotonation and protonation reactions of acids and bases, respectively. Without any special adjustments of radii or other parameters this led to a prediction model for acid and base $\text{p}K_{\text{a}}$ values in water. This allows for prediction of absolute aqueous acid and base $\text{p}K_{\text{a}}$ values with an average error of typically less than 0.6 $\text{p}K_{\text{a}}$ units. From the observation that the slope of the experimental $\text{p}K_{\text{a}}$ versus theoretical ΔG_{diss} was found to be significantly lower than the theoretical value $1/RT\ln(10)$ if bare solutes and their respective ionic species were used in the COSMO-RS computation, the explicit solvation approach, as first proposed by Pliego and Riveros^{29,38}, was used to comprise local

interaction effects that play an important role in the protonation reaction, but are not, or not sufficiently accounted for by the COSMO-RS method. The application of the COSMO-RS method to the calculation of acids pK_a in acetonitrile²⁸ showed a better performance of the COSMO-RS model on acids that produced anions with delocalized charges, as they are less affected by solvation, while acids that formed localized anions showed a systematic deviation. This observation is corroborated by a recent study, which used multipole derived charge analysis to assess the degree of charge delocalization in anion species formed from aqueous dissociation reactions⁸. Both findings are, at least in part, related to the capability of the solvent to solvate and thus stabilize the anions or cations. Apparently this effect is not captured sufficiently by COSMO-RS and its underlying QC/DCSM method DFT/COSMO if there are short-range interactions in the solvation of ions with localized charges. In this study it was found that the explicit solvation approach in combination with COSMO-RS was able to remove these deficits in parts: while the slope of the pK_a versus ΔG_{diss} correlation was closer to the theoretical slope when the number of explicit solvent atoms in the calculations was increased, the correlation decreased, which may have been expected due to the increasing number of ambiguities with increasing number of explicit solvent molecules. Moreover, it was found that for weak acids, such as *tert*-butanol, the quantum chemical geometry optimization of the solvent-solute complex of the according *tert*-butoxy anion was not possible, which makes the explicit solvation approach inapplicable for such compounds. In addition, the systematic deviation found for aliphatic amines was not resolved by the cluster method. Application of only *mono*- or only *di*-solvated clusters of neutral and ionic solute species lead to an improved, yet not fully theoretical slope of the pK_a versus ΔG_{diss} correlation. Other criteria proposed for the choice of the number of explicit solvent molecules used, such as *semi*-solvation of only ions³¹, or from a list of bare, *mono*- or *di*-solvated solutes, choice of the species that minimizes the free energy of dissociation³² performed worse than the simple decision to use one or two explicit solvent molecule for all solutes involved. Thus the choice of the explicit solvent molecules remains ambiguous and must be considered an unsolved issue. From a practical standpoint it remains difficult or even impossible to find the global minimum energy cluster geometries for weakly bonded clusters with more than one explicit solvent

1 molecules. Even for the medium number of compounds used in this study it was impossible to apply
2 global conformational search procedures for finding the cluster geometries of each solute and ion. To
3 avoid this general problem, an automatic procedure, based on COSMO-RS contact interaction energies
4 was proposed, creating “good” or at least sufficiently low energy cluster geometries, without aguarantee
5 of obtaining the actual global minimum, however. Thus it can be concluded that the combination of
6 COSMO-RS with the explicit solvation methodology leads to a *theoretical* improvement in the slope of
7 the correlation of the free energy of dissociation with pK_a and thus a better understanding of the physics
8 of the protonation reaction in solution, but suffers from serious disadvantages that – at least for now -
9 prevent it from being a *practical* prediction method for everyday production work: the simple linear
10 relation between pK_a and the dissociation free energies of the bare solutes and ions proved to be the
11 more robust approach for pK_a prediction.
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25 **Supplementary Material**

26 Free energies of all species involved in the computation of the dissociation energies (Tables S1, S2, and
27 S3). List of optimized geometries used in the free energy calculations (Table S4).
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TABLE 1: Experimental pK_a and Gibbs free energies of dissociation of bare, mono-solvated and di-solvated aqueous acids.

Compound	$pK_a(\text{exp})^a$	$G_{\text{diss}}(\text{bare})^b$	$\Delta G_{\text{diss}}(\text{H}_2\text{O})^b$	$\Delta G_{\text{diss}}(2\text{H}_2\text{O})^b$
Ethanol	15.9	136.08	105.94	93.53
2,2,2-trichloroethanol	12.2	92.04	83.43	74.74
formic acid	3.77	12.43	29.97	34.06
acetic acid	4.75	24.83	39.69	42.86
Nitromethane	10.2	73.69	71.03	72.31
dichloroacetic acid	1.3	-0.81	21.69	23.47
trichloroacetic acid	0.89	-9.46	15.42	18.86
n-pentanoic acid	4.84	27.56	42.44	44.66
2,2-dimethylpropanoic acid	5.05	30.50	44.45	46.77
benzoic acid	4.27	23.53	39.46	40.93
oxalic acid	1.23	-3.61	18.30	34.47
maleic acid	1.83	-7.35	15.52	19.36
fumaric acid	3.03	14.59	33.21	33.91
acrylic acid	4.26	22.85	38.68	42.33
bromoacetic acid	2.87	8.51	28.40	30.93
chloroacetic acid	2.81	8.07	28.65	31.53
cyanoacetic acid	2.44	5.88	26.08	30.29
fluoroacetic acid	2.66	8.52	28.07	30.84
iodoacetic acid	3.13	7.22	28.64	32.52
2-hydroxypropanoic acid	3.87	9.23	28.01	30.36
2-chloropropanoic acid	2.8	12.58	29.71	32.95
3-chloropropanoic acid	4.1	19.76	36.88	38.34
nitroacetic acid	1.32	-2.75	19.99	24.66
2-acetylbutanedioic acid	2.86	8.81	16.73	23.54
carbonic acid	3.58	10.60	31.62	41.37
hypochlorous acid	7.43	57.75	58.25	56.35
hypobromous acid	8.7	67.41	64.64	59.08
hypoiodous acid	10.64	71.94	68.28	61.87
nitrous acid	3.3	2.04	16.80	30.42
sulfurous acid	1.92	-9.09	6.22	7.57
phosphoric acid	1.97	-1.03	5.92	12.89
boric acid	9.12	70.92	71.10	72.38
pentachlorophenol	4.9	29.41	34.67	36.55
2,3,4,6-tetrachlorophenol	5.62	35.52	38.96	38.19
2,3,4-trichlorophenol	7.1	51.03	53.73	55.52
2,3-dichlorophenol	7.76	55.05	56.73	58.24
2,4,5-trichlorophenol	7.07	48.73	52.22	55.17
2,4,6-trichlorophenol	6.21	41.62	42.76	43.19
2,4-dichlorophenol	8.09	56.88	57.71	59.56
2,5-dichlorophenol	7.51	53.01	55.10	57.45
2,6-dichlorophenol	6.79	47.36	47.81	49.47
2-chlorophenol	8.29	60.88	60.80	63.71
3,4-dichlorophenol	8.68	62.51	62.24	61.19
3,5-dichlorophenol	8.27	57.87	58.91	58.01
3-chlorophenol	8.78	65.41	64.91	63.21

	4-chlorophenol	9.14	69.57	67.63	65.17
1	phenol	9.82	70.87	68.82	66.57
2	5-nitouracil	5.3	34.18	36.17	36.53
3	cis-5-formyluracil	6.84	46.20	46.58	43.60
4	thymine	9.75	68.64	67.21	67.64
5	trans-5-formyluracil	6.84	45.61	45.64	45.44
6	uracil	9.42	64.78	64.13	64.79
7	fluorouracil	8	54.99	58.34	57.85
8	methylthiouracil	8.2	51.60	53.38	57.35
9	phenytoin	8.3	56.53	59.71	56.83
10	3,3-methylphenylglutarimide	9.2	64.17	67.65	65.55
11	3,3-dimethylsuccinimide	9.5	57.89	62.08	59.80
12	dimethadione	6.1	35.86	42.26	44.33
13	phthalimide	8.3	58.09	61.04	60.47
14	succinimide	9.6	57.76	61.20	62.62
15	phthalic acid	2.76	-0.61	19.06	18.70
16	methanol	15.5	137.22	105.05	91.27
17	hypophosphorous acid	2.23	1.72	21.44	22.11
18	4-methylbenzoic acid	4.47	25.56	40.87	42.31
19	4-ethylbenzoic acid	4.47	25.40	41.26	42.49
20	4-propylbenzoic acid	4.47	25.51	41.08	42.11
21	4-(1-methylethyl)-benzoic acid	4.47	25.44	40.40	43.60
22	4-butylbenzoic acid	4.47	25.52	41.27	41.64
23	4-(1,1-dimethylethyl)-benzoic acid	4.4	25.51	41.39	42.06
24	4-phenylbenzoic acid	4.07	23.99	40.19	41.02
25	4-fluorobenzoic acid	4.07	23.17	39.27	40.84
26	4-chlorobenzoic acid	4.07	21.50	38.01	39.74
27	4-bromobenzoic acid	4.47	21.52	38.14	40.56
28	4-iodobenzoic acid	4.47	20.68	37.66	39.99
29	4-methoxybenzoic acid	4.5	27.33	42.67	44.36
30	4-hydroxybenzoic acid	4.58	28.58	42.70	43.75
31	4-nitrobenzoic acid	3.4	14.92	34.05	35.39
32	4-hydroxymethylbenzoic acid	4.27	22.68	38.95	40.09
33	4-cyanobenzoic acid	3.47	16.19	34.72	36.76
34	4-aminobenzoic acid	4.92	36.24	46.32	50.17
35	4-methylaminobenzoic acid	5.04	36.15	49.09	49.67
36	4-dimethylaminobenzoic acid	5.07	35.04	48.01	50.23
37	4-trifluoromethylbenzoic acid	3.67	19.09	36.47	38.60
38	4-sulfamoylbenzoic acid	3.67	17.14	35.17	36.75
39	4-carbamoylbenzoic acid	3.87	20.01	37.27	39.77
40	salicylic acid	2.97	13.13	31.28	32.75
41	2,4-dihydroxybenzoic acid	3.11	18.08	34.85	35.57
42	5-iodo-2-hydroxybenzoic acid	2.89	6.91	29.06	31.52
43	3-hydroxybenzoic acid	4.08	24.19	38.86	41.19
44	mandelic acid	3.41	7.04	26.43	30.56
45	3-hydroxy-2-naphtoic acid	2.97	11.16	30.58	33.13
46	anthracene-9-carboxylic acid	3.65	12.65	28.61	31.41
47	pamoic acid	2.47	4.01	29.28	30.03
48	tert-butanol	19.2	148.88	107.60	91.32
49	^a pK_a^{Exp} : Experimental aqueous pKa value of acids, taken from refs. 10, 51..				

^b ΔG_{diss} : Gibbs free energies of dissociation calculated from eq. 4 in [kJ·mol⁻¹].

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TABLE 2: Experimental base pK_a and Gibbs free energies of dissociation of bare and mono-solvated aqueous bases.

Compound	$pK_a(\text{Exp})^a$	$\Delta G_{\text{diss}}(\text{bare})^b$	$\Delta G_{\text{diss}}(\text{H}_2\text{O})^b$
hydroxyimidazo(2,3-a)isoindole	8.6	84.03	81.42
imidazo[2,3-b]thioxazole	8	70.10	67.38
tetrahydrozoline	10.5	85.97	79.31
tolazoline	10.3	83.64	76.58
4-chloroaniline	4	47.44	44.78
4-methoxyaniline	5.2	57.04	54.43
4-nitroaniline	1	17.79	14.03
aniline	4.6	49.04	48.42
p-toluidine	5.1	55.31	49.08
1,3-dihydro-1-methyl-5-phenyl-1,4-benzodiazepin-2-one	3.3	44.14	44.16
1,3-dihydro-3-hydroxy-1-methyl-5-phenyl-1,4-benzodiazepin-2-one	1.6	24.12	30.42
1,3-dihydro-3-hydroxy-5-phenyl-1,4-benzodiazepin-2-one	1.7	27.01	32.37
1,3-dihydro-5-phenyl-1,4-benzodiazepin-2-one	3.5	46.25	45.91
2,3-dihydro-1-methyl-5-phenyl-1,4-benzodiazepine	6.2	67.59	62.62
3-hydro-2-methylamine-4-oxy-5-phenyl-1,4-benzodiazepine	4.8	50.84	52.73
clonidine	8.1	64.95	59.94
debrisoquin	11.9	104.81	96.56
guanidine	13.8	115.78	104.87
methylguanidine	13.4	109.68	99.79
2-aminopyridine	6.71	67.69	58.98
2-aminothiazole	5.4	55.09	48.11
2-methylimidazole	8	66.68	62.94
3-aminopyridine	6	65.51	60.04
4-aminopyridine	9.23	81.02	72.89
4-methylpyridine	6	56.34	52.25
benzimidazole	5.8	52.15	50.55
imidazole	7	62.51	59.27
isoquinoline	5.4	52.84	49.51
melamine	5	58.94	54.44
pyrazine	0.7	21.47	25.39
pyrazole	2.5	35.36	36.96
pyridine	5.14	51.55	48.55
pyrimidine	1.3	23.74	27.33
quinoline	4.8	46.99	46.62
thiazole	2.8	28.25	31.32
1-methylindole	-2.3	-9.71	-8.02
1-methylpyrrole	-2.9	-16.56	-10.76
2-methylindole	-0.3	6.96	14.10
2-methylpyrrole	-0.2	2.42	14.66
3-methylindole	-4.6	-24.06	-13.34
3-methylpyrrole	-1	7.11	15.84
indole	-3.6	-14.37	-4.23
pyrrole	-3.8	-13.64	-6.38

^a pK_a^{Exp} : Experimental aqueous base pKa value taken from ref. 24.

^b ΔG_{diss} : Gibbs free energies of dissociation calculated from eq. 5 in [kJ·mol⁻¹].

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TABLE 3: Experimental aqueous base pK_a and Gibbs free energies of dissociation of bare and mono-solvated aliphatic amine bases.

Compound	Base-Type	$pK_a(\text{Exp})^a$	$\Delta G_{\text{diss}}(\text{bare})^b$	$\Delta G_{\text{diss}}(\text{H}_2\text{O})^b$	$pK_a^{\text{calc}}(\text{bare})^c$	$pK_a^{\text{calc}}(\text{H}_2\text{O})^d$	$\Delta pK_a(\text{bare})$	$\Delta pK_a(\text{H}_2\text{O})$
methylamine	primary	10.6	104.07	88.78	11.97	11.09	-1.37	-0.49
ethylamine	primary	10.9	100.39	86.62	11.50	10.76	-0.60	0.14
n-propylamine	primary	10.7	99.45	85.81	11.37	10.64	-0.67	0.06
n-butylamine	primary	10.8	99.17	85.81	11.34	10.64	-0.54	0.16
n-pentylamine	primary	10.6	98.93	85.84	11.31	10.64	-0.71	-0.04
n-hexylamine	primary	10.6	98.92	85.18	11.30	10.54	-0.70	0.06
n-heptylamine	primary	10.7	98.84	85.08	11.29	10.53	-0.59	0.17
n-octylamine	primary	10.7	98.76	85.15	11.28	10.54	-0.58	0.16
iso-propylamine	primary	10.6	95.54	83.76	10.86	10.32	-0.26	0.28
sec-butylamine	primary	10.56	91.95	81.99	10.40	10.05	0.16	0.51
tert-butylamine	primary	10.7	93.11	81.53	10.55	9.98	0.15	0.72
neo-pentylamine	primary	10.21	94.59	80.82	10.74	9.87	-0.53	0.34
cyclohexylamine	primary	10.6	95.11	82.76	10.81	10.17	-0.21	0.43
dimethylamine	secondary	10.7	96.12	79.30	10.94	9.64	-0.24	1.06
diethylamine	secondary	11.1	88.89	78.44	10.00	9.51	1.10	1.59
di-n-propylamine	secondary	11	87.51	76.91	9.82	9.28	1.18	1.72
di-iso-propylamine	secondary	11.1	85.10	76.66	9.50	9.24	1.60	1.86
di-n-butylamine	secondary	11.4	87.21	76.31	9.78	9.19	1.62	2.21
di-iso-butylamine	secondary	10.5	77.93	64.94	8.57	7.45	1.93	3.05
di-sec-butylamine	secondary	11.01	80.87	75.10	8.95	9.00	2.06	2.01
tert-butylcyclohexylamine	secondary	11.23	81.90	73.15	9.09	8.70	2.14	2.53
trimethylamine	tertiary	9.8	80.69	66.81	8.93	7.73	0.87	2.07
dimethylethylamine	tertiary	10.2	78.60	67.65	8.66	7.86	1.54	2.34
dimethyl-n-propylamine	tertiary	9.99	77.48	66.97	8.51	7.76	1.48	2.23
dimethyl-iso-propylamine	tertiary	10.3	77.00	68.84	8.45	8.04	1.85	2.26
dimethyl-n-butylamine	tertiary	10.02	77.22	66.78	8.48	7.73	1.54	2.29
dimethyl-iso-butylamine	tertiary	9.91	74.43	65.50	8.11	7.53	1.80	2.38
dimethyl-sec-butylamine	tertiary	10.4	77.84	68.69	8.56	8.02	1.84	2.38
dimethyl-tert-butylamine	tertiary	10.52	80.82	71.46	8.95	8.45	1.57	2.07
triethylamine	tertiary	10.8	78.65	71.56	8.66	8.46	2.14	2.34
tri-n-propylamine	tertiary	10.7	78.96	69.69	8.71	8.17	1.99	2.53
tri-n-butylamine	tertiary	10.89	78.47	69.36	8.64	8.12	2.25	2.77

^a pK_a^{Exp} : Experimental aqueous base pK_a value taken from ref. 24.
^b ΔG_{diss} : Gibbs free energies of dissociation calculated from eq. 5 in [kJ·mol⁻¹].
^c $pK_a^{\text{calc}}(\text{bare})$: pK_a of bare amine bases calculated from eq. 10.
^d $pK_a^{\text{calc}}(\text{H}_2\text{O})$: pK_a of mono-solvated amine bases calculated from eq. 11.

Supplementary Material to:

First principles prediction of pK_a:
COSMO-RS and the cluster-continuum approach

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KEYWORDS: pK_a; acidity; basicity; COSMO; COSMO-RS; density functional theory;

TABLE S1: Experimental pK_a and Gibbs free energies of bare, mono-solvated and di-solvated aqueous acids.

Compound	$pK_a(\text{Exp})^a$	$G(\text{AH})^b$	$G(\text{A}^-)^b$	$G(\text{AH}\cdot\text{H}_2\text{O})^b$	$G(\text{A}^-\cdot\text{H}_2\text{O})^b$	$G(\text{AH}\cdot 2\text{H}_2\text{O})^b$	$G(\text{A}^-\cdot 2\text{H}_2\text{O})^b$
ethanol	15.9	-407192.75	-405932.1933	-607976.05	-606745.64	-808761.49	-807543.49
2,2,2-trichloroethanol	12.2	-4027063.85	-4025847.339	-4227856.50	-4226648.60	-4428641.71	-4427442.50
formic acid	3.77	-498419.13	-497282.2218	-699210.35	-698055.91	-899997.73	-898839.19
acetic acid	4.75	-601684.32	-600535.0143	-802473.84	-801309.68	-1003259.56	-1002092.23
nitromethane	10.2	-643528.89	-642330.7273	-844302.27	-843106.77	-1045086.79	-1043890.01
dichloroacetic acid	1.3	-3014912.86	-3013789.195	-3215708.21	-3214562.05	-3416493.77	-3415345.82
trichloroacetic acid	0.89	-4221505.27	-4220390.258	-4422303.25	-4421163.36	-4623090.73	-4621947.40
n-pentanoic acid	4.84	-911383.95	-910231.9169	-1112173.20	-1111006.29	-1312958.43	-1311789.29
2,2-dimethylpropanoic acid	5.05	-911379.72	-910224.755	-1112168.43	-1110999.50	-1312954.03	-1311782.78
benzoic acid	4.27	-1105183.13	-1104035.132	-1305972.59	-1304808.66	-1506757.71	-1505592.30
oxalic acid	1.23	-993682.13	-992561.2674	-1194476.68	-1193333.90	-1395275.89	-1394116.95
maleic acid	1.83	-1196956.99	-1195839.864	-1397753.04	-1396613.05	-1598539.50	-1597395.67
fumaric acid	3.03	-1196967.63	-1195828.574	-1397758.39	-1396600.71	-1598553.49	-1597395.11
acrylic acid	4.26	-701679.58	-700532.255	-902469.38	-901306.23	-1103254.40	-1102087.59
bromoacetic acid	2.87	-7358183.68	-7357050.701	-7558976.50	-7557823.62	-7759760.56	-7758605.15
chloroacetic acid	2.81	-1808304.94	-1807172.396	-2009097.83	-2007944.70	-2209882.06	-2208726.05
cyanoacetic acid	2.44	-843914.94	-842784.5871	-1044708.49	-1043557.94	-1245493.73	-1244338.97
fluoroacetic acid	2.66	-862284.69	-861151.695	-1063077.34	-1061924.80	-1263861.99	-1262706.68
iodoacetic acid	3.13	-630170.59	-629038.8935	-830964.67	-829811.56	-1031750.65	-1030593.65
2-hydroxypropanoic acid	3.87	-902477.35	-901343.6465	-1103269.20	-1102116.71	-1304053.44	-1302898.61
2-chloropropanoic acid	2.8	-1911547.21	-1910410.158	-2112338.93	-2111184.75	-2313123.36	-2311965.94
3-chloropropanoic acid	4.1	-1911557.21	-1910412.972	-2112347.78	-2111186.43	-2313131.32	-2311968.50
nitroacetic acid	1.32	-1138790.10	-1137668.378	-1339585.59	-1338441.12	-1540370.81	-1539221.67
2-acetylbutanedioic acid	2.86	-1601062.73	-1599929.447	-1801854.80	-1800713.60	-2002637.00	-2001488.99
carbonic acid	3.58	-696063.66	-694928.5828	-896855.56	-895699.46	-1097648.86	-1096483.02
hypochlorous acid	7.43	-1407217.85	-1406035.623	-1608010.03	-1606827.30	-1808796.91	-1807616.09
hypobromous acid	8.7	-6957132.58	-6955940.694	-7157923.29	-7156734.17	-7358708.79	-7357525.24
hypoiodous acid	10.64	-229155.38	-227958.9666	-429946.84	-428754.09	-630733.26	-629546.92
nitrous acid	3.3	-540300.54	-539174.0233	-741089.51	-739948.23	-941886.43	-940731.54
sulfurous acid	1.92	-1641240.08	-1640124.693	-1842029.71	-1840899.02	-2042817.45	-2041685.41
phosphoric acid	1.97	-1691557.18	-1690433.734	-1892350.57	-1891220.18	-2093144.26	-2092006.90
boric acid	9.12	-663171.83	-661976.44	-863958.05	-862762.47	-1064744.19	-1063547.34
pentachlorophenol	4.9	-6840598.39	-6839444.506	-7041383.83	-7040224.69	-7242169.77	-7241008.74
2,3,4,6-tetrachlorophenol	5.62	-5633988.50	-5632828.508	-5834773.01	-5833609.58	-6035558.82	-6034396.15
2,3,4-trichlorophenol	7.1	-4427367.41	-4426191.903	-4628156.05	-4626977.85	-4828942.19	-4827762.20
2,3-dichlorophenol	7.76	-3220743.41	-3219563.891	-3421531.41	-3420350.20	-3622317.22	-3621134.50
2,4,5-trichlorophenol	7.07	-4427376.94	-4426203.737	-4628166.28	-4626989.59	-4828952.12	-4827772.48
2,4,6-trichlorophenol	6.21	-4427374.18	-4426208.085	-4628158.50	-4626991.26	-4828944.52	-4827776.86
2,4-dichlorophenol	8.09	-3220750.81	-3219569.449	-3421538.79	-3420356.61	-3622324.86	-3621140.83
2,5-dichlorophenol	7.51	-3220753.12	-3219575.638	-3421541.64	-3420362.07	-3622327.12	-3621145.20
2,6-dichlorophenol	6.79	-3220742.78	-3219570.947	-3421526.15	-3420353.87	-3622311.80	-3621137.85
2-chlorophenol	8.29	-2014114.41	-2012929.057	-2214901.51	-2213716.24	-2415687.32	-2414499.14
3,4-dichlorophenol	8.68	-3220747.30	-3219560.318	-3421535.27	-3420348.56	-3622321.71	-3621136.04
3,5-dichlorophenol	8.27	-3220756.86	-3219574.512	-3421545.42	-3420362.03	-3622331.64	-3621149.16
3-chlorophenol	8.78	-2014119.59	-2012929.705	-2214907.33	-2213717.95	-2415693.09	-2414505.40
4-chlorophenol	9.14	-2014118.05	-2012924.008	-2214905.55	-2213713.45	-2415690.81	-2414501.17
phenol	9.82	-807476.99	-806281.6423	-1008263.81	-1007070.52	-1209049.16	-1207858.12
5-nitrouracil	5.3	-1626604.26	-1625445.605	-1827385.29	-1826224.65	-2028170.63	-2027009.62
cis-5-formyluracil	6.84	-1387126.03	-1385955.365	-1587905.80	-1586734.75	-1788690.61	-1787522.54
thymine	9.75	-1192743.49	-1191550.382	-1393523.03	-1392331.35	-1594308.61	-1593116.50
trans-5-formyluracil	6.84	-1387126.80	-1385956.72	-1587906.25	-1586736.14	-1788690.49	-1787520.58

uracil	9.42	-1089497.97	-1088308.718	-1290277.91	-1289089.31	-1491063.39	-1489874.12
fluorouracil	8	-1350092.82	-1348913.347	-1550873.31	-1549690.50	-1751657.53	-1750475.21
methylthiouracil	8.2	-2040569.26	-2039393.19	-2241345.72	-2240167.86	-2442134.11	-2440952.29
phenytoin	8.3	-2202875.30	-2201694.294	-2403655.06	-2402470.88	-2604440.43	-2603259.12
3,3-methylphenylglutarimide	9.2	-1760440.91	-1759252.26	-1961218.09	-1960025.97	-2162001.52	-2160811.49
3,3-dimethylsuccinimide	9.5	-1153722.82	-1152540.452	-1354502.51	-1353315.96	-1555287.70	-1554103.43
dimethadione	6.1	-1248067.53	-1246907.195	-1448849.90	-1447683.17	-1649635.83	-1648467.03
phthalimide	8.3	-1347506.31	-1346323.738	-1548286.07	-1547100.56	-1749071.94	-1747887.00
succinimide	9.6	-947253.37	-946071.131	-1148032.98	-1146847.30	-1348818.45	-1347631.36
phthalic acid	2.76	-1600451.16	-1599327.289	-1801244.53	-1800101.00	-2002026.77	-2000883.60
methanol	15.5	-303944.85	-302683.1629	-504728.69	-503499.17	-705514.01	-704298.27
hypophosphorous acid	2.23	-1296181.52	-1295055.33	-1496980.74	-1495834.83	-1697768.92	-1696622.33
4-methylbenzoic acid	4.47	-1208429.73	-1207279.699	-1409219.11	-1408053.76	-1610003.58	-1608836.79
4-ethylbenzoic acid	4.47	-1311661.86	-1310511.979	-1512451.32	-1511285.58	-1713236.34	-1712069.38
4-propylbenzoic acid	4.47	-1414896.30	-1413746.319	-1615685.65	-1614520.09	-1816470.40	-1815303.82
4-(1-methylethyl)-benzoic acid	4.47	-1414894.16	-1413744.25	-1615682.93	-1614518.05	-1816469.17	-1815301.09
4-butylbenzoic acid	4.47	-1518129.79	-1516979.803	-1718919.20	-1717753.46	-1919703.85	-1918537.73
4-(1,1-dimethylethyl)-benzoic acid	4.4	-1518120.53	-1516970.554	-1718910.22	-1717744.36	-1919694.43	-1918527.90
4-phenylbenzoic acid	4.07	-1711933.61	-1710785.145	-1912723.38	-1911558.71	-2113508.03	-2112342.53
4-fluorobenzoic acid	4.07	-1365814.05	-1364666.409	-1566603.79	-1565440.04	-1767388.73	-1766223.42
4-chlorobenzoic acid	4.07	-2311823.82	-2310677.843	-2512613.70	-2511451.22	-2713399.04	-2712234.83
4-bromobenzoic acid	4.47	-7861698.99	-7860552.997	-8062488.85	-8061326.24	-8263274.78	-8262109.75
4-iodobenzoic acid	4.47	-1133680.18	-1132535.028	-1334470.31	-1333308.18	-1535256.61	-1534092.14
4-methoxybenzoic acid	4.5	-1405956.62	-1404804.816	-1606745.65	-1605578.51	-1807530.40	-1806361.57
4-hydroxybenzoic acid	4.58	-1302780.78	-1301627.725	-1503568.82	-1502401.65	-1704361.16	-1703192.94
4-nitrobenzoic acid	3.4	-1642310.23	-1641170.834	-1843101.90	-1841943.38	-2043886.92	-2042727.05
4-hydroxymethylbenzoic acid	4.27	-1405982.04	-1404834.881	-1606771.60	-1605608.18	-1807556.39	-1806391.84
4-cyanobenzoic acid	3.47	-1347430.97	-1346290.307	-1548222.28	-1547063.09	-1749007.41	-1747846.18
4-aminobenzoic acid	4.92	-1250609.21	-1249448.504	-1451396.14	-1450225.35	-1652183.29	-1651008.64
4-methylaminobenzoic acid	5.04	-1353813.87	-1352653.242	-1554600.86	-1553427.29	-1755385.15	-1754211.00
4-dimethylaminobenzoic acid	5.07	-1457011.07	-1455851.555	-1657798.34	-1656625.86	-1858582.64	-1857407.94
4-trifluoromethylbenzoic acid	3.67	-1990349.42	-1989205.856	-2191139.87	-2189978.93	-2391925.76	-2390762.68
4-sulfamoylbenzoic acid	3.67	-2691002.97	-2689861.36	-2891793.37	-2890633.73	-3092578.83	-3091417.61
4-carbamoylbenzoic acid	3.87	-1548296.73	-1547152.255	-1749086.91	-1747925.16	-1949872.98	-1948708.74
salicylic acid	2.97	-1302781.05	-1301643.449	-1503572.26	-1502416.50	-1704357.38	-1703200.15
2,4-dihydroxybenzoic acid	3.11	-1500379.49	-1499236.936	-1701169.59	-1700010.27	-1901962.21	-1900802.17
5-iodo-2-hydroxybenzoic acid	2.89	-1331275.18	-1330143.798	-1532067.89	-1530914.36	-1732854.39	-1731698.40
3-hydroxybenzoic acid	4.08	-1302772.24	-1301623.573	-1503560.22	-1502396.89	-1704353.11	-1703187.44
mandelic acid	3.41	-1405965.98	-1404834.467	-1606758.61	-1605607.71	-1807544.47	-1806389.44
3-hydroxy-2-naphtic acid	2.97	-1706239.82	-1705104.186	-1907031.97	-1905876.92	-2107818.67	-2106661.06
anthracene-9-carboxylic acid	3.65	-1912066.61	-1910929.486	-2112858.36	-2111705.28	-2313643.82	-2312487.94
pamoic acid	2.47	-3512537.22	-3511408.744	-3713327.51	-3712173.75	-3914119.46	-3912964.95
tert-butanol	19.2	-613681.06	-612407.7033	-814465.54	-813233.47	-1015246.84	-1014031.04

^a pK_a^{Exp} : Experimental pK_a value of acids in water..

^b G : Gibbs free energies in [kJ·mol⁻¹].

TABLE S2: Experimental base pK_a and Gibbs free energies of bare and mono-solvated aqueous bases.

Compound	$pK_a(Exp)^a$	$G(B)^b$	$G(BH^+)^b$	$G(B-H_2O)^b$	$G(BH^+-H_2O)^b$
hydroxyimidazo(2,3-a)isoindole	8.6	-1747137.48	-1748345.98	-1947921.18	-1949127.07
imidazo[2,3-b]thioxazole	8	-2088269.45	-2089464.03	-2289054.14	-2290245.99
tetrahydrozoline	10.5	-1613792.59	-1615003.04	-1814578.71	-1815782.50
tolazoline	10.3	-1307246.76	-1308454.87	-1508033.01	-1509234.06
4-chloroaniline	4	-1961939.83	-1963111.75	-2162726.60	-2163895.85
4-methoxyaniline	5.2	-1056058.83	-1057240.34	-1256843.90	-1258022.80
4-nitroaniline	1	-1292458.99	-1293601.26	-1493249.66	-1494388.17
aniline	4.6	-755300.38	-756473.89	-956084.38	-957257.27
p-toluidine	5.1	-858541.01	-859720.79	-1059327.74	-1060501.29
1,3-dihydro-1-methyl-5-phenyl-1,4-benzodiazepin-2-one	3.3	-2108407.13	-2109575.74	-2309189.75	-2310358.39
1,3-dihydro-3-hydroxy-1-methyl-5-phenyl-1,4-benzodiazepin-2-one	1.6	-2305987.13	-2307135.73	-2506764.53	-2507919.42
1,3-dihydro-3-hydroxy-5-phenyl-1,4-benzodiazepin-2-one	1.7	-2202786.39	-2203937.88	-2403564.50	-2404721.34
1,3-dihydro-5-phenyl-1,4-benzodiazepin-2-one	3.5	-2005206.89	-2006377.61	-2205989.94	-2207160.32
2,3-dihydro-1-methyl-5-phenyl-1,4-benzodiazepine	6.2	-1913920.45	-1915112.51	-2114706.02	-2115893.12
3-hydro-2-methylamine-4-oxy-5-phenyl-1,4-benzodiazepine	4.8	-2253639.16	-2254814.48	-2454417.22	-2455594.42
clonidine	8.1	-3762692.20	-3763881.63	-3963474.07	-3964658.48
debrisoquin	11.9	-1452665.25	-1453894.53	-1653451.72	-1654672.75
guanidine	13.8	-539448.31	-540688.56	-740232.78	-741462.12
methylguanidine	13.4	-642651.50	-643885.65	-843437.72	-844661.98
2-aminopyridine	6.71	-797461.96	-798654.13	-998245.68	-999429.14
2-aminothiazole	5.4	-1639571.03	-1640750.59	-1840353.64	-1841526.22
2-methylimidazole	8	-697390.05	-698581.20	-898175.66	-899363.08
3-aminopyridine	6	-797438.34	-798628.33	-998225.57	-999410.08
4-aminopyridine	9.23	-797457.41	-798662.91	-998245.21	-999442.57
4-methylpyridine	6	-755276.85	-756457.67	-956063.31	-957240.03
benzimidazole	5.8	-997614.32	-998790.94	-1198398.63	-1199573.66
imidazole	7	-594137.28	-595324.27	-794922.61	-796106.36
isoquinoline	5.4	-1055491.82	-1056669.13	-1256277.98	-1257451.97
melamine	5	-1172700.67	-1173884.09	-1373479.11	-1374658.03
pyrazine	0.7	-694144.42	-695290.37	-894927.94	-896077.80
pyrazole	2.5	-594086.49	-595246.32	-794869.01	-796030.45
pyridine	5.14	-652027.79	-653203.81	-852813.94	-853986.95
pyrimidine	1.3	-694163.24	-695311.45	-894946.47	-896098.28
quinoline	4.8	-1055495.90	-1056667.36	-1256280.84	-1257451.93
thiazole	2.8	-1494148.96	-1495301.69	-1694932.21	-1696088.00
1-methylindole	-2.3	-1058643.42	-1059758.17	-1259414.79	-1260531.24
1-methylpyrrole	-2.9	-655168.18	-656276.09	-855937.98	-857051.70
2-methylindole	-0.3	-1058683.99	-1059815.42	-1259462.09	-1260600.66
2-methylpyrrole	-0.2	-655207.87	-656334.76	-855980.94	-857120.07
3-methylindole	-4.6	-1058679.73	-1059780.14	-1259454.52	-1260565.65
3-methylpyrrole	-1	-655199.67	-656331.26	-855973.02	-857113.34
indole	-3.6	-955437.39	-956547.49	-1156212.31	-1157332.55
pyrrole	-3.8	-551960.55	-553071.38	-752735.34	-753853.44

^a pK_a^{Exp} : Experimental pK_a value of bases in water..

^b G : Gibbs free energies in [kJ·mol⁻¹].

TABLE S3: Experimental aqueous base pK_a and Gibbs free energies of bare and mono-solvated aliphatic amines.

Compound	Base-Type	pK_a (Exp)	G(B)	G(BH ⁺)	G(B-H ₂ O)	G(BH ⁺ -H ₂ O)
methylamine	primary	10.6	-251766.85	-252993.48	-452559.44	-453772.6972
ethylamine	primary	10.9	-355007.93	-356230.91	-555799.60	-557010.6987
n-propylamine	primary	10.7	-458241.12	-459463.14	-659032.76	-660243.044
n-butylamine	primary	10.8	-561474.48	-562696.40	-762266.01	-763476.2888
n-pentylamine	primary	10.6	-664708.10	-665929.85	-865499.55	-866709.865
n-hexylamine	primary	10.6	-767941.75	-769163.33	-968733.09	-969942.734
n-heptylamine	primary	10.7	-871175.29	-872396.82	-1071966.63	-1073176.187
n-octylamine	primary	10.7	-974408.94	-975630.37	-1175200.31	-1176409.932
iso-propylamine	primary	10.6	-458250.20	-459468.87	-659040.90	-660249.1431
sec-butylamine	primary	10.56	-561481.27	-562696.14	-762271.30	-763477.7667
tert-butylamine	primary	10.7	-561489.55	-562705.66	-762279.98	-763485.9896
neo-pentylamine	primary	10.21	-664705.68	-665923.02	-865496.88	-866702.1767
cyclohexylamine	primary	10.6	-764791.27	-766009.29	-965581.98	-966789.2147
dimethylamine	secondary	10.7	-354980.45	-356191.32	-555765.71	-556969.4821
diethylamine	secondary	11.1	-561460.56	-562665.28	-762244.69	-763447.601
di-n-propylamine	secondary	11	-767926.45	-769129.86	-968710.65	-969912.0297
di-iso-propylamine	secondary	11.1	-767930.46	-769133.70	-968715.06	-969916.1912
di-n-butylamine	secondary	11.4	-974393.18	-975596.37	-1175177.28	-1176378.07
di-iso-butylamine	secondary	10.5	-974392.56	-975588.00	-1175175.99	-1176365.403
di-sec-butylamine	secondary	11.01	-974390.37	-975589.42	-1175174.33	-1176373.912
tert-butylcyclohexylamine	secondary	11.23	-1177699.78	-1178900.20	-1378483.85	-1379681.473
trimethylamine	tertiary	9.8	-458196.12	-459387.58	-658976.61	-660167.8995
dimethylethylamine	tertiary	10.2	-561431.11	-562621.17	-762211.64	-763403.7712
dimethyl-n-propylamine	tertiary	9.99	-664663.97	-665853.12	-865444.01	-866635.4592
dimethyl-iso-propylamine	tertiary	10.3	-664661.48	-665849.88	-865440.42	-866633.729
dimethyl-n-butylamine	tertiary	10.02	-767897.33	-769086.03	-968677.40	-969868.6602
dimethyl-iso-butylamine	tertiary	9.91	-767890.97	-769081.87	-968674.39	-969864.3698
dimethyl-sec-butylamine	tertiary	10.4	-767887.91	-769077.14	-968667.41	-969860.5798
dimethyl-tert-butylamine	tertiary	10.52	-767884.44	-769080.15	-968668.05	-969863.9856
triethylamine	tertiary	10.8	-767892.51	-769088.86	-968675.78	-969871.8192
tri-n-propylamine	tertiary	10.7	-1077590.04	-1078783.91	-1278373.11	-1279567.279
tri-n-butylamine	tertiary	10.89	-1387289.99	-1388483.44	-1588073.28	-1589267.115

^a pK_a^{Exp} : Experimental pK_a value of bases in water..^b G: Gibbs free energies in [kJ·mol⁻¹].

TABLE S4: Optimized Geometries (sdf-format). Different conformers of one compound are denoted by subsequent index numbers 0,1,2,...

S4 a) Bare Acids & Anions

2,2,2-trichloroethanol-anion.sdf									
COSMOTHERM 3D 0									
8	7	0	0	0	0	0	0	0	0
0.0396	0.0000	0.1453	C	0	0	0	0	0	0
-0.8770	-0.0003	1.4201	C	0	0	0	0	0	0
1.8278	-0.0010	0.6248	Cl	0	0	0	0	0	0
-0.2665	-1.4765	-0.8967	Cl	0	0	0	0	0	0
-0.2652	1.4777	-0.8953	Cl	0	0	0	0	0	0
-2.1831	-0.0002	1.1619	O	0	0	0	0	0	0
-0.4788	0.8952	1.9772	H	0	0	0	0	0	0
-0.4790	-0.8965	1.9764	H	0	0	0	0	0	0
2	1	0	0	0	0	0	0	0	0
3	1	0	0	0	0	0	0	0	0
4	1	0	0	0	0	0	0	0	0
5	1	0	0	0	0	0	0	0	0
6	2	0	0	0	0	0	0	0	0
7	2	0	0	0	0	0	0	0	0
2	8	0	0	0	0	0	0	0	0
M END									
\$\$\$\$									
2,2,2-trichloroethanol.sdf									
COSMOTHERM 3D 0									
9	8	0	0	0	0	0	0	0	0
0.0772	0.0000	0.1214	C	0	0	0	0	0	0
-0.7613	-0.0001	1.3971	C	0	0	0	0	0	0
1.8242	-0.0012	0.6046	Cl	0	0	0	0	0	0
-0.2636	-1.4739	-0.8799	Cl	0	0	0	0	0	0
-0.2619	1.4751	-0.8787	Cl	0	0	0	0	0	0
-2.1374	0.0001	1.0499	O	0	0	0	0	0	0
-0.4782	0.8969	1.9727	H	0	0	0	0	0	0
-0.4784	-0.8972	1.9725	H	0	0	0	0	0	0
-2.6437	-0.0011	1.8826	H	0	0	0	0	0	0
2	1	0	0	0	0	0	0	0	0
3	1	0	0	0	0	0	0	0	0
4	1	0	0	0	0	0	0	0	0
5	1	0	0	0	0	0	0	0	0
6	2	0	0	0	0	0	0	0	0
7	2	0	0	0	0	0	0	0	0
8	2	0	0	0	0	0	0	0	0
6	9	0	0	0	0	0	0	0	0
M END									
\$\$\$\$									
2,2-dimethylpropanoicacid-anion.sdf									
COSMOTHERM 3D 0									
16	15	0	0	0	0	0	0	0	0
-1.2058	1.4324	-0.0165	C	0	0	0	0	0	0
-0.6276	0.0101	-0.0004	C	0	0	0	0	0	0
-1.1112	-0.7589	-1.2473	C	0	0	0	0	0	0
-1.1065	-0.7280	1.2672	C	0	0	0	0	0	0
0.9409	0.0213	-0.0014	C	0	0	0	0	0	0
1.5389	1.1426	-0.0011	O	0	0	0	0	0	0
1.5182	-1.1119	-0.0009	O	0	0	0	0	0	0
-2.3077	1.3964	-0.0136	H	0	0	0	0	0	0
-0.8782	2.0055	0.8628	H	0	0	0	0	0	0
-0.8828	1.9836	-0.9116	H	0	0	0	0	0	0
-2.2109	-0.8315	-1.2536	H	0	0	0	0	0	0
-0.6936	-1.7751	-1.2589	H	0	0	0	0	0	0
-0.8014	-0.2499	-2.1740	H	0	0	0	0	0	0
-2.2062	-0.7988	1.2803	H	0	0	0	0	0	0
-0.6905	-1.7445	1.3014	H	0	0	0	0	0	0
-0.7918	-0.1973	2.1800	H	0	0	0	0	0	0
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8	1	0	0	0	0	0	0	0	0
9	1	0	0	0	0	0	0	0	0
10	1	0	0	0	0	0	0	0	0
3	2	0	0	0	0	0	0	0	0
4	2	0	0	0	0	0	0	0	0
5	2	0	0	0	0	0	0	0	0
11	3	0	0	0	0	0	0	0	0
12	3	0	0	0	0	0	0	0	0
13	3	0	0	0	0	0	0	0	0
14	4	0	0	0	0	0	0	0	0
15	4	0	0	0	0	0	0	0	0
6	5	0	0	0	0	0	0	0	0
7	5	0	0	0	0	0	0	0	0
4	16	0	0	0	0	0	0	0	0
M END									
\$\$\$\$									
2,2-dimethylpropanoicacid.sdf									
COSMOTHERM 3D 0									
17	16	0	0	0	0	0	0	0	0
-1.2851	1.3985	-0.0097	C	0	0	0	0	0	0
-0.6520	-0.0010	-0.0002	C	0	0	0	0	0	0
-1.0861	-0.7871	-1.2599	C	0	0	0	0	0	0
-1.0841	-0.7689	1.2716	C	0	0	0	0	0	0
0.8733	0.1326	-0.0009	C	0	0	0	0	0	0
1.4998	1.1843	-0.0007	O	0	0	0	0	0	0
1.5025	-1.0722	-0.0006	O	0	0	0	0	0	0
-2.3800	1.3008	-0.0088	H	0	0	0	0	0	0
-0.9899	1.9783	0.8760	H	0	0	0	0	0	0
-0.9904	1.9660	-0.9036	H	0	0	0	0	0	0

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-0.6557 -1.7793 1.2957 H 0 0 0 0 0 0 0 0 0 0 15
-0.7748 -0.2361 2.1830 H 0 0 0 0 0 0 0 0 0 0 16
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16 4 0 0 0 0
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1.0361 0.0939 0.0000 C 0 0 0 0 0 0 0 0 0 0 5
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1.8185 -2.5703 0.0002 Cl 0 0 0 0 0 0 0 0 0 0 10
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11 2 0 0 0 0
4 3 0 0 0 0
7 3 0 0 0 0
5 4 0 0 0 0
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0.6807 -1.2464 0.0001 C 0 0 0 0 0 0 0 0 0 0 3
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  9  1  0  0  0  0
  3  2  0  0  0  0
10  2  0  0  0  0
  4  3  0  0  0  0
  7  3  0  0  0  0
  5  4  0  0  0  0
11  4  0  0  0  0
  6  5  0  0  0  0
  8  6  0  0  0  0
  5 12  0  0  0  0
M  END
$$$$
2,3,4-trichlorophenol0.sdf
COSMOTHERM      3D      0

13 13  0  0  0  0  0  0  0  0  0  0 V2000
  0.8250 -2.0251  0.0001 C  0  0  0  0  0  0  0  0  0  0  1
 -0.5332 -2.3241  0.0001 C  0  0  0  0  0  0  0  0  0  0  2
 -1.4857 -1.2973  0.0000 C  0  0  0  0  0  0  0  0  0  0  3
 -1.0457  0.0406  0.0001 C  0  0  0  0  0  0  0  0  0  0  4
  0.3245  0.3500  0.0000 C  0  0  0  0  0  0  0  0  0  0  5
  1.2589 -0.6971  0.0000 C  0  0  0  0  0  0  0  0  0  0  6
 -2.8016 -1.6378 -0.0001 O  0  0  0  0  0  0  0  0  0  0  7
 -2.2701  1.3015  0.0000 Cl  0  0  0  0  0  0  0  0  0  0  8
  0.8448  2.0193  0.0000 Cl  0  0  0  0  0  0  0  0  0  0  9
  2.9876 -0.3655 -0.0001 Cl  0  0  0  0  0  0  0  0  0  0 10
  1.5599 -2.8292  0.0001 H  0  0  0  0  0  0  0  0  0  0 11
 -0.8729 -3.3597  0.0000 H  0  0  0  0  0  0  0  0  0  0 12
 -3.3484 -0.8228 -0.0009 H  0  0  0  0  0  0  0  0  0  0 13
  2  1  0  0  0  0
  6  1  0  0  0  0
11  1  0  0  0  0
  3  2  0  0  0  0
12  2  0  0  0  0
  4  3  0  0  0  0
  7  3  0  0  0  0
  5  4  0  0  0  0
  8  4  0  0  0  0
  6  5  0  0  0  0
  9  5  0  0  0  0
10  6  0  0  0  0
  7 13  0  0  0  0
M  END
$$$$
2,3,4-trichlorophenol1-anion.sdf
COSMOTHERM      3D      0

12 12  0  0  0  0  0  0  0  0  0  0 V2000
  2.3427  0.5287 -0.0007 C  0  0  0  0  0  0  0  0  0  0  1
  2.0277 -0.8240 -0.0004 C  0  0  0  0  0  0  0  0  0  0  2
  0.6953 -1.2514 -0.0002 C  0  0  0  0  0  0  0  0  0  0  3
 -0.3328 -0.2935 -0.0001 C  0  0  0  0  0  0  0  0  0  0  4
 -0.0142  1.0694 -0.0002 C  0  0  0  0  0  0  0  0  0  0  5
  1.3495  1.5676  0.0002 C  0  0  0  0  0  0  0  0  0  0  6
  0.3444 -2.9889  0.0003 Cl  0  0  0  0  0  0  0  0  0  0  7
  1.6345  2.8151  0.0008 O  0  0  0  0  0  0  0  0  0  0  8
  3.3897  0.8397 -0.0006 H  0  0  0  0  0  0  0  0  0  0  9
  2.8232 -1.5710 -0.0007 H  0  0  0  0  0  0  0  0  0  0 10
 -2.0208 -0.8188  0.0000 Cl  0  0  0  0  0  0  0  0  0  0 11
 -1.2936  2.2882 -0.0002 Cl  0  0  0  0  0  0  0  0  0  0 12
  2  1  0  0  0  0
  6  1  0  0  0  0
  9  1  0  0  0  0
  3  2  0  0  0  0
10  2  0  0  0  0
  4  3  0  0  0  0
  7  3  0  0  0  0
  5  4  0  0  0  0
11  4  0  0  0  0
  6  5  0  0  0  0
  8  6  0  0  0  0
  5 12  0  0  0  0
M  END
$$$$
2,3,4-trichlorophenol1.sdf
COSMOTHERM      3D      0

13 13  0  0  0  0  0  0  0  0  0  0 V2000
 -2.0276 -0.8247 -0.0001 C  0  0  0  0  0  0  0  0  0  0  1
 -2.3238  0.5354 -0.0005 C  0  0  0  0  0  0  0  0  0  0  2
 -1.2975  1.4888  0.0001 C  0  0  0  0  0  0  0  0  0  0  3
  0.0422  1.0531 -0.0001 C  0  0  0  0  0  0  0  0  0  0  4
  0.3455 -0.3192  0.0001 C  0  0  0  0  0  0  0  0  0  0  5
 -0.7007 -1.2562  0.0000 C  0  0  0  0  0  0  0  0  0  0  6
 -1.5327  2.8290  0.0002 O  0  0  0  0  0  0  0  0  0  0  7
  1.3126  2.2600  0.0001 Cl  0  0  0  0  0  0  0  0  0  0  8
  2.0135 -0.8463 -0.0002 Cl  0  0  0  0  0  0  0  0  0  0  9
 -0.3675 -2.9851  0.0002 Cl  0  0  0  0  0  0  0  0  0  0 10
 -2.8328 -1.5583 -0.0002 H  0  0  0  0  0  0  0  0  0  0 11
 -3.3639  0.8661 -0.0006 H  0  0  0  0  0  0  0  0  0  0 12
 -2.4968  2.9864 -0.0002 H  0  0  0  0  0  0  0  0  0  0 13
  2  1  0  0  0  0
  6  1  0  0  0  0
11  1  0  0  0  0
  3  2  0  0  0  0
12  2  0  0  0  0
  4  3  0  0  0  0
  7  3  0  0  0  0
  5  4  0  0  0  0
  8  4  0  0  0  0
  6  5  0  0  0  0
  9  5  0  0  0  0
10  6  0  0  0  0
  7 13  0  0  0  0
M  END
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$$$$
2,3-dichlorophenol0-anion.sdf
COSMOTHERM      3D      0

12 12 0 0 0 0 0 0 0 0 0 V2000
  1.2943 2.0425 -0.0001 C 0 0 0 0 0 0 0 0 0 0 0 1
  2.3072 1.0896 -0.0002 C 0 0 0 0 0 0 0 0 0 0 0 2
  2.0246 -0.2854 -0.0001 C 0 0 0 0 0 0 0 0 0 0 0 3
  0.6795 -0.6709 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 4
  -0.3549 0.2662 -0.0001 C 0 0 0 0 0 0 0 0 0 0 0 5
  -0.1030 1.6974 0.0001 C 0 0 0 0 0 0 0 0 0 0 0 6
  2.8137 -1.0356 -0.0002 H 0 0 0 0 0 0 0 0 0 0 0 7
  -1.0446 2.5669 0.0003 O 0 0 0 0 0 0 0 0 0 0 0 8
  1.5370 3.1082 0.0000 H 0 0 0 0 0 0 0 0 0 0 0 9
  3.3512 1.4124 -0.0003 H 0 0 0 0 0 0 0 0 0 0 0 10
  0.3219 -2.4184 0.0001 Cl 0 0 0 0 0 0 0 0 0 0 0 11
  -2.0506 -0.2415 -0.0002 Cl 0 0 0 0 0 0 0 0 0 0 0 12
  2 1 0 0 0 0 0
  6 1 0 0 0 0 0
  9 1 0 0 0 0 0
  3 2 0 0 0 0 0
  10 2 0 0 0 0 0
  4 3 0 0 0 0 0
  7 3 0 0 0 0 0
  5 4 0 0 0 0 0
  11 4 0 0 0 0 0
  6 5 0 0 0 0 0
  8 6 0 0 0 0 0
  5 12 0 0 0 0 0
M  END
$$$$
2,3-dichlorophenol0.sdf
COSMOTHERM      3D      0

13 13 0 0 0 0 0 0 0 0 0 V2000
  2.3527 0.9874 -0.0001 C 0 0 0 0 0 0 0 0 0 0 0 1
  1.3697 1.9752 -0.0005 C 0 0 0 0 0 0 0 0 0 0 0 2
  0.0146 1.6169 0.0002 C 0 0 0 0 0 0 0 0 0 0 0 3
  -0.3376 0.2512 -0.0002 C 0 0 0 0 0 0 0 0 0 0 0 4
  0.6637 -0.7291 0.0001 C 0 0 0 0 0 0 0 0 0 0 0 5
  2.0125 -0.3695 -0.0003 C 0 0 0 0 0 0 0 0 0 0 0 6
  -0.9164 2.6107 0.0007 O 0 0 0 0 0 0 0 0 0 0 0 7
  -2.0495 -0.1580 -0.0004 Cl 0 0 0 0 0 0 0 0 0 0 0 8
  0.2341 -2.4376 0.0003 Cl 0 0 0 0 0 0 0 0 0 0 0 9
  -1.8137 2.2133 0.0013 H 0 0 0 0 0 0 0 0 0 0 0 10
  3.4047 1.2742 -0.0003 H 0 0 0 0 0 0 0 0 0 0 0 11
  1.6297 3.0340 -0.0002 H 0 0 0 0 0 0 0 0 0 0 0 12
  2.7795 -1.1427 -0.0002 H 0 0 0 0 0 0 0 0 0 0 0 13
  2 1 0 0 0 0 0
  6 1 0 0 0 0 0
  11 1 0 0 0 0 0
  3 2 0 0 0 0 0
  12 2 0 0 0 0 0
  4 3 0 0 0 0 0
  7 3 0 0 0 0 0
  5 4 0 0 0 0 0
  8 4 0 0 0 0 0
  6 5 0 0 0 0 0
  9 5 0 0 0 0 0
  10 7 0 0 0 0 0
  6 13 0 0 0 0 0
M  END
$$$$
2,3-dichlorophenol1-anion.sdf
COSMOTHERM      3D      0

12 12 0 0 0 0 0 0 0 0 0 V2000
  1.2944 2.0425 -0.0004 C 0 0 0 0 0 0 0 0 0 0 0 1
  2.3072 1.0895 -0.0001 C 0 0 0 0 0 0 0 0 0 0 0 2
  2.0245 -0.2855 -0.0001 C 0 0 0 0 0 0 0 0 0 0 0 3
  0.6795 -0.6710 -0.0001 C 0 0 0 0 0 0 0 0 0 0 0 4
  -0.3549 0.2662 -0.0001 C 0 0 0 0 0 0 0 0 0 0 0 5
  -0.1029 1.6974 0.0002 C 0 0 0 0 0 0 0 0 0 0 0 6
  2.8136 -1.0357 0.0000 H 0 0 0 0 0 0 0 0 0 0 0 7
  -1.0444 2.5670 0.0007 O 0 0 0 0 0 0 0 0 0 0 0 8
  1.5372 3.1081 -0.0003 H 0 0 0 0 0 0 0 0 0 0 0 9
  3.3513 1.4122 -0.0002 H 0 0 0 0 0 0 0 0 0 0 0 10
  0.3218 -2.4185 0.0002 Cl 0 0 0 0 0 0 0 0 0 0 0 11
  -2.0507 -0.2413 -0.0003 Cl 0 0 0 0 0 0 0 0 0 0 0 12
  2 1 0 0 0 0 0
  6 1 0 0 0 0 0
  9 1 0 0 0 0 0
  3 2 0 0 0 0 0
  10 2 0 0 0 0 0
  4 3 0 0 0 0 0
  7 3 0 0 0 0 0
  5 4 0 0 0 0 0
  11 4 0 0 0 0 0
  6 5 0 0 0 0 0
  8 6 0 0 0 0 0
  5 12 0 0 0 0 0
M  END
$$$$
2,3-dichlorophenol1.sdf
COSMOTHERM      3D      0

13 13 0 0 0 0 0 0 0 0 0 V2000
  2.3457 1.0082 -0.0003 C 0 0 0 0 0 0 0 0 0 0 0 1
  1.3521 1.9870 -0.0014 C 0 0 0 0 0 0 0 0 0 0 0 2
  -0.0009 1.6192 -0.0001 C 0 0 0 0 0 0 0 0 0 0 0 3
  -0.3475 0.2519 -0.0006 C 0 0 0 0 0 0 0 0 0 0 0 4
  0.6664 -0.7164 0.0002 C 0 0 0 0 0 0 0 0 0 0 0 5
  2.0141 -0.3491 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 6
  -1.0137 2.5312 0.0022 O 0 0 0 0 0 0 0 0 0 0 0 7
  -2.0462 -0.1888 -0.0009 Cl 0 0 0 0 0 0 0 0 0 0 0 8
```



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0.2572 -2.4307 0.0006 Cl 0 0 0 0 0 0 0 0 0 0 9
-0.6334 3.4310 0.0018 H 0 0 0 0 0 0 0 0 0 0 10
3.3950 1.3045 -0.0008 H 0 0 0 0 0 0 0 0 0 0 11
1.6140 3.0470 -0.0015 H 0 0 0 0 0 0 0 0 0 0 12
2.7852 -1.1181 0.0005 H 0 0 0 0 0 0 0 0 0 0 13
2 1 0 0 0 0
6 1 0 0 0 0
11 1 0 0 0 0
3 2 0 0 0 0
12 2 0 0 0 0
4 3 0 0 0 0
7 3 0 0 0 0
5 4 0 0 0 0
8 4 0 0 0 0
6 5 0 0 0 0
9 5 0 0 0 0
10 7 0 0 0 0
6 13 0 0 0 0
M END
$$$$
2,4,5-trichlorophenol0-anion.sdf
COSMOtherm 3D 0
12 12 0 0 0 0 0 0 0 0 0 V2000
1.6002 -0.0041 0.0002 C 0 0 0 0 0 0 0 0 0 0 1
0.6877 -1.0511 0.0000 C 0 0 0 0 0 0 0 0 0 0 2
-0.6946 -0.8120 0.0001 C 0 0 0 0 0 0 0 0 0 0 3
-1.1425 0.5150 0.0001 C 0 0 0 0 0 0 0 0 0 0 4
-0.2288 1.5603 0.0000 C 0 0 0 0 0 0 0 0 0 0 5
1.2053 1.3837 -0.0001 C 0 0 0 0 0 0 0 0 0 0 6
-1.8841 -2.1227 -0.0001 Cl 0 0 0 0 0 0 0 0 0 0 7
2.0480 2.3454 -0.0002 O 0 0 0 0 0 0 0 0 0 0 8
2.6695 -0.2198 0.0001 H 0 0 0 0 0 0 0 0 0 0 9
1.3102 -2.7174 0.0000 Cl 0 0 0 0 0 0 0 0 0 0 10
-2.2128 0.7214 0.0001 H 0 0 0 0 0 0 0 0 0 0 11
-0.8468 3.2281 0.0000 Cl 0 0 0 0 0 0 0 0 0 0 12
2 1 0 0 0 0
6 1 0 0 0 0
9 1 0 0 0 0
3 2 0 0 0 0
10 2 0 0 0 0
4 3 0 0 0 0
7 3 0 0 0 0
5 4 0 0 0 0
11 4 0 0 0 0
6 5 0 0 0 0
8 6 0 0 0 0
5 12 0 0 0 0
M END
$$$$
2,4,5-trichlorophenol0.sdf
COSMOtherm 3D 0
13 13 0 0 0 0 0 0 0 0 0 V2000
-0.6838 -1.0646 0.0000 C 0 0 0 0 0 0 0 0 0 0 1
-1.5817 0.0011 0.0002 C 0 0 0 0 0 0 0 0 0 0 2
-1.1163 1.3219 0.0000 C 0 0 0 0 0 0 0 0 0 0 3
0.2738 1.5416 0.0000 C 0 0 0 0 0 0 0 0 0 0 4
1.1763 0.4829 -0.0002 C 0 0 0 0 0 0 0 0 0 0 5
0.7000 -0.8301 0.0000 C 0 0 0 0 0 0 0 0 0 0 6
-2.0328 2.3248 0.0000 O 0 0 0 0 0 0 0 0 0 0 7
0.8581 3.2060 0.0000 Cl 0 0 0 0 0 0 0 0 0 0 8
1.8595 -2.1517 0.0000 Cl 0 0 0 0 0 0 0 0 0 0 9
-1.3269 -2.7003 0.0000 Cl 0 0 0 0 0 0 0 0 0 0 10
-2.6557 -0.1818 0.0001 H 0 0 0 0 0 0 0 0 0 0 11
2.2481 0.6749 -0.0001 H 0 0 0 0 0 0 0 0 0 0 12
-1.5656 3.1878 -0.0012 H 0 0 0 0 0 0 0 0 0 0 13
2 1 0 0 0 0
6 1 0 0 0 0
10 1 0 0 0 0
3 2 0 0 0 0
11 2 0 0 0 0
4 3 0 0 0 0
7 3 0 0 0 0
5 4 0 0 0 0
8 4 0 0 0 0
6 5 0 0 0 0
12 5 0 0 0 0
9 6 0 0 0 0
7 13 0 0 0 0
M END
$$$$
2,4,5-trichlorophenol1-anion.sdf
COSMOtherm 3D 0
12 12 0 0 0 0 0 0 0 0 0 V2000
1.6002 -0.0041 -0.0002 C 0 0 0 0 0 0 0 0 0 0 1
0.6877 -1.0511 -0.0001 C 0 0 0 0 0 0 0 0 0 0 2
-0.6946 -0.8120 0.0001 C 0 0 0 0 0 0 0 0 0 0 3
-1.1425 0.5150 -0.0001 C 0 0 0 0 0 0 0 0 0 0 4
-0.2288 1.5603 -0.0001 C 0 0 0 0 0 0 0 0 0 0 5
1.2053 1.3837 -0.0001 C 0 0 0 0 0 0 0 0 0 0 6
-1.8841 -2.1227 0.0000 Cl 0 0 0 0 0 0 0 0 0 0 7
2.0480 2.3454 0.0000 O 0 0 0 0 0 0 0 0 0 0 8
2.6695 -0.2198 -0.0003 H 0 0 0 0 0 0 0 0 0 0 9
1.3102 -2.7174 0.0001 Cl 0 0 0 0 0 0 0 0 0 0 10
-2.2128 0.7214 -0.0002 H 0 0 0 0 0 0 0 0 0 0 11
-0.8468 3.2281 0.0001 Cl 0 0 0 0 0 0 0 0 0 0 12
2 1 0 0 0 0
6 1 0 0 0 0
9 1 0 0 0 0
3 2 0 0 0 0
10 2 0 0 0 0
4 3 0 0 0 0
7 3 0 0 0 0
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5 4 0 0 0 0
11 4 0 0 0 0
6 5 0 0 0 0
8 6 0 0 0 0
5 12 0 0 0 0
M END
$$$$
2,4,5-trichlorophenol1.sdf
COSMOTHERM 3D 0

13 13 0 0 0 0 0 0 0 0 0 V2000
-0.6829 0.0001 -1.0691 C 0 0 0 0 0 0 0 0 0 0 1
-1.5849 -0.0012 -0.0047 C 0 0 0 0 0 0 0 0 0 0 2
-1.1269 0.0006 1.3195 C 0 0 0 0 0 0 0 0 0 0 3
0.2620 -0.0004 1.5492 C 0 0 0 0 0 0 0 0 0 0 4
1.1646 0.0003 0.4902 C 0 0 0 0 0 0 0 0 0 0 5
0.6974 -0.0002 -0.8266 C 0 0 0 0 0 0 0 0 0 0 6
-1.9647 0.0014 2.3895 O 0 0 0 0 0 0 0 0 0 0 7
0.8651 -0.0005 3.2023 Cl 0 0 0 0 0 0 0 0 0 0 8
1.8662 0.0004 -2.1405 Cl 0 0 0 0 0 0 0 0 0 0 9
-1.3199 -0.0003 -2.7072 Cl 0 0 0 0 0 0 0 0 0 0 10
-2.6574 -0.0016 -0.2038 H 0 0 0 0 0 0 0 0 0 0 11
2.2355 -0.0002 0.6872 H 0 0 0 0 0 0 0 0 0 0 12
-2.8920 0.0006 2.0823 H 0 0 0 0 0 0 0 0 0 0 13
2 1 0 0 0 0
6 1 0 0 0 0
10 1 0 0 0 0
3 2 0 0 0 0
11 2 0 0 0 0
4 3 0 0 0 0
7 3 0 0 0 0
5 4 0 0 0 0
8 4 0 0 0 0
6 5 0 0 0 0
12 5 0 0 0 0
9 6 0 0 0 0
7 13 0 0 0 0
M END
$$$$
2,4,6-trichlorophenol-anion.sdf
COSMOTHERM 3D 0

12 12 0 0 0 0 0 0 0 0 0 V2000
1.2155 -0.9108 0.0002 C 0 0 0 0 0 0 0 0 0 0 1
1.1918 0.4802 0.0000 C 0 0 0 0 0 0 0 0 0 0 2
0.0000 1.2988 0.0001 C 0 0 0 0 0 0 0 0 0 0 3
-1.1918 0.4802 0.0000 C 0 0 0 0 0 0 0 0 0 0 4
-1.2155 -0.9108 -0.0001 C 0 0 0 0 0 0 0 0 0 0 5
0.0000 -1.5987 -0.0001 C 0 0 0 0 0 0 0 0 0 0 6
0.0000 2.5726 0.0001 O 0 0 0 0 0 0 0 0 0 0 7
-2.7450 1.3470 0.0000 Cl 0 0 0 0 0 0 0 0 0 0 8
2.7450 1.3470 -0.0001 Cl 0 0 0 0 0 0 0 0 0 0 9
0.0000 -3.3792 0.0000 Cl 0 0 0 0 0 0 0 0 0 0 10
2.1639 -1.4476 0.0004 H 0 0 0 0 0 0 0 0 0 0 11
-2.1639 -1.4476 -0.0004 H 0 0 0 0 0 0 0 0 0 0 12
2 1 0 0 0 0
6 1 0 0 0 0
11 1 0 0 0 0
3 2 0 0 0 0
9 2 0 0 0 0
4 3 0 0 0 0
7 3 0 0 0 0
5 4 0 0 0 0
8 4 0 0 0 0
6 5 0 0 0 0
10 6 0 0 0 0
5 12 0 0 0 0
M END
$$$$
2,4,6-trichlorophenol.sdf
COSMOTHERM 3D 0

13 13 0 0 0 0 0 0 0 0 0 V2000
1.2068 0.4404 0.0000 C 0 0 0 0 0 0 0 0 0 0 1
1.1983 -0.9531 -0.0002 C 0 0 0 0 0 0 0 0 0 0 2
-0.0301 -1.6143 0.0000 C 0 0 0 0 0 0 0 0 0 0 3
-1.2381 -0.9175 0.0000 C 0 0 0 0 0 0 0 0 0 0 4
-1.1914 0.4743 0.0000 C 0 0 0 0 0 0 0 0 0 0 5
0.0186 1.1943 -0.0001 C 0 0 0 0 0 0 0 0 0 0 6
-0.0559 -3.3814 0.0000 Cl 0 0 0 0 0 0 0 0 0 0 7
0.0860 2.5466 -0.0002 O 0 0 0 0 0 0 0 0 0 0 8
2.7452 1.2941 0.0001 Cl 0 0 0 0 0 0 0 0 0 0 9
2.1362 -1.5056 -0.0003 H 0 0 0 0 0 0 0 0 0 0 10
-2.1938 -1.4385 0.0000 H 0 0 0 0 0 0 0 0 0 0 11
-2.6908 1.4051 0.0000 Cl 0 0 0 0 0 0 0 0 0 0 12
-0.8263 2.9098 0.0013 H 0 0 0 0 0 0 0 0 0 0 13
2 1 0 0 0 0
6 1 0 0 0 0
9 1 0 0 0 0
3 2 0 0 0 0
10 2 0 0 0 0
4 3 0 0 0 0
7 3 0 0 0 0
5 4 0 0 0 0
11 4 0 0 0 0
6 5 0 0 0 0
12 5 0 0 0 0
8 6 0 0 0 0
8 13 0 0 0 0
M END
$$$$
2,4-dichlorophenol0-anion.sdf
COSMOTHERM 3D 0

12 12 0 0 0 0 0 0 0 0 0 V2000
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1.9556 0.0851 0.0001 C 0 0 0 0 0 0 0 0 0 0 0 0 1
1.4643 -1.2190 0.0001 C 0 0 0 0 0 0 0 0 0 0 0 0 2
0.0827 -1.4332 0.0001 C 0 0 0 0 0 0 0 0 0 0 0 0 3
-0.8072 -0.3557 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 4
-0.2903 0.9372 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 5
1.1181 1.2583 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 6
-0.5628 -3.0984 -0.0001 Cl 0 0 0 0 0 0 0 0 0 0 0 0 7
1.5806 2.4556 -0.0002 O 0 0 0 0 0 0 0 0 0 0 0 0 8
3.0360 0.2519 0.0001 H 0 0 0 0 0 0 0 0 0 0 0 0 9
2.1532 -2.0657 0.0001 H 0 0 0 0 0 0 0 0 0 0 0 0 10
-1.8850 -0.5198 -0.0001 H 0 0 0 0 0 0 0 0 0 0 0 0 11
-1.4380 2.3030 0.0000 Cl 0 0 0 0 0 0 0 0 0 0 0 0 12
2 1 0 0 0 0
6 1 0 0 0 0
9 1 0 0 0 0
3 2 0 0 0 0
10 2 0 0 0 0
4 3 0 0 0 0
7 3 0 0 0 0
5 4 0 0 0 0
11 4 0 0 0 0
6 5 0 0 0 0
8 6 0 0 0 0
5 12 0 0 0 0
M END
$$$$
2,4-dichlorophenol0.sdf
COSMOtherm 3D 0
13 13 0 0 0 0 0 0 0 0 0 V2000
-1.4557 -1.2285 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 1
-1.9390 0.0795 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 2
-1.0605 1.1725 0.0001 C 0 0 0 0 0 0 0 0 0 0 0 0 3
0.3222 0.9132 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 4
0.8291 -0.3856 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 5
-0.0761 -1.4469 -0.0001 C 0 0 0 0 0 0 0 0 0 0 0 0 6
-1.5848 2.4296 -0.0001 O 0 0 0 0 0 0 0 0 0 0 0 0 7
1.4300 2.2920 0.0000 Cl 0 0 0 0 0 0 0 0 0 0 0 0 8
0.5472 -3.1057 0.0000 Cl 0 0 0 0 0 0 0 0 0 0 0 0 9
-2.1509 -2.0674 0.0000 H 0 0 0 0 0 0 0 0 0 0 0 0 10
-3.0129 0.2701 0.0000 H 0 0 0 0 0 0 0 0 0 0 0 0 11
1.9042 -0.5580 0.0000 H 0 0 0 0 0 0 0 0 0 0 0 0 12
-0.8529 3.0827 0.0006 H 0 0 0 0 0 0 0 0 0 0 0 0 13
2 1 0 0 0 0
6 1 0 0 0 0
10 1 0 0 0 0
3 2 0 0 0 0
11 2 0 0 0 0
4 3 0 0 0 0
7 3 0 0 0 0
5 4 0 0 0 0
8 4 0 0 0 0
6 5 0 0 0 0
12 5 0 0 0 0
9 6 0 0 0 0
7 13 0 0 0 0
M END
$$$$
2,4-dichlorophenol1-anion.sdf
COSMOtherm 3D 0
12 12 0 0 0 0 0 0 0 0 0 V2000
1.9555 0.0851 -0.0008 C 0 0 0 0 0 0 0 0 0 0 0 0 1
1.4643 -1.2191 -0.0002 C 0 0 0 0 0 0 0 0 0 0 0 0 2
0.0827 -1.4332 -0.0003 C 0 0 0 0 0 0 0 0 0 0 0 0 3
-0.8073 -0.3557 -0.0002 C 0 0 0 0 0 0 0 0 0 0 0 0 4
-0.2903 0.9372 -0.0004 C 0 0 0 0 0 0 0 0 0 0 0 0 5
1.1181 1.2582 0.0001 C 0 0 0 0 0 0 0 0 0 0 0 0 6
-0.5629 -3.0983 0.0003 Cl 0 0 0 0 0 0 0 0 0 0 0 0 7
1.5807 2.4555 0.0009 O 0 0 0 0 0 0 0 0 0 0 0 0 8
3.0359 0.2519 -0.0005 H 0 0 0 0 0 0 0 0 0 0 0 0 9
2.1531 -2.0658 -0.0006 H 0 0 0 0 0 0 0 0 0 0 0 0 10
-1.8850 -0.5198 -0.0003 H 0 0 0 0 0 0 0 0 0 0 0 0 11
-1.4380 2.3030 -0.0001 Cl 0 0 0 0 0 0 0 0 0 0 0 0 12
2 1 0 0 0 0
6 1 0 0 0 0
9 1 0 0 0 0
3 2 0 0 0 0
10 2 0 0 0 0
4 3 0 0 0 0
7 3 0 0 0 0
5 4 0 0 0 0
11 4 0 0 0 0
6 5 0 0 0 0
8 6 0 0 0 0
5 12 0 0 0 0
M END
$$$$
2,4-dichlorophenol1.sdf
COSMOtherm 3D 0
13 13 0 0 0 0 0 0 0 0 0 V2000
-1.4604 -1.2291 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 1
-1.9420 0.0809 -0.0001 C 0 0 0 0 0 0 0 0 0 0 0 0 2
-1.0650 1.1759 0.0001 C 0 0 0 0 0 0 0 0 0 0 0 0 3
0.3189 0.9217 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 4
0.8202 -0.3796 0.0001 C 0 0 0 0 0 0 0 0 0 0 0 0 5
-0.0819 -1.4442 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 6
-1.4913 2.4704 0.0000 O 0 0 0 0 0 0 0 0 0 0 0 0 7
1.4451 2.2790 0.0000 Cl 0 0 0 0 0 0 0 0 0 0 0 0 8
0.5467 -3.1014 0.0000 Cl 0 0 0 0 0 0 0 0 0 0 0 0 9
-2.1563 -2.0673 -0.0001 H 0 0 0 0 0 0 0 0 0 0 0 0 10
-3.0191 0.2619 0.0000 H 0 0 0 0 0 0 0 0 0 0 0 0 11
1.8955 -0.5513 0.0002 H 0 0 0 0 0 0 0 0 0 0 0 0 12
-2.4678 2.4888 0.0005 H 0 0 0 0 0 0 0 0 0 0 0 0 13
```

```
2 1 0 0 0 0
6 1 0 0 0 0
10 1 0 0 0 0
3 2 0 0 0 0
11 2 0 0 0 0
4 3 0 0 0 0
7 3 0 0 0 0
5 4 0 0 0 0
8 4 0 0 0 0
6 5 0 0 0 0
12 5 0 0 0 0
9 6 0 0 0 0
7 13 0 0 0 0
M END
$$$$
2,4-dihydroxybenzoicacid-anion0.sdf
COSMOTHERM 3D 0

16 17 0 0 0 0 0 0 0 0 0 V2000
1.5941 -1.3908 -0.0014 C 0 0 0 0 0 0 0 0 0 0 0 1
0.2041 -1.4553 -0.0016 C 0 0 0 0 0 0 0 0 0 0 0 2
-0.5977 -0.3016 -0.0003 C 0 0 0 0 0 0 0 0 0 0 0 3
0.0492 0.9685 0.0005 C 0 0 0 0 0 0 0 0 0 0 0 4
1.4535 1.0466 0.0016 C 0 0 0 0 0 0 0 0 0 0 0 5
2.2138 -0.1263 0.0001 C 0 0 0 0 0 0 0 0 0 0 0 6
-2.0980 -0.3895 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 7
-2.6725 -1.5067 0.0033 O 0 0 0 0 0 0 0 0 0 0 0 8
-2.7328 0.7507 -0.0030 O 0 0 0 0 0 0 0 0 0 0 0 9
-0.6803 2.1049 0.0006 O 0 0 0 0 0 0 0 0 0 0 0 10
3.5875 -0.1022 0.0001 O 0 0 0 0 0 0 0 0 0 0 0 11
-1.6808 1.7205 -0.0016 H 0 0 0 0 0 0 0 0 0 0 0 12
3.8955 0.8242 0.0020 H 0 0 0 0 0 0 0 0 0 0 0 13
2.2073 -2.2927 -0.0026 H 0 0 0 0 0 0 0 0 0 0 0 14
-0.2976 -2.4250 -0.0024 H 0 0 0 0 0 0 0 0 0 0 0 15
1.9366 2.0268 0.0026 H 0 0 0 0 0 0 0 0 0 0 0 16
2 1 0 0 0 0
6 1 0 0 0 0
14 1 0 0 0 0
3 2 0 0 0 0
15 2 0 0 0 0
4 3 0 0 0 0
7 3 0 0 0 0
5 4 0 0 0 0
10 4 0 0 0 0
6 5 0 0 0 0
11 6 0 0 0 0
8 7 0 0 0 0
9 7 0 0 0 0
12 9 0 0 0 0
12 10 0 0 0 0
13 11 0 0 0 0
5 16 0 0 0 0
M END
$$$$
2,4-dihydroxybenzoicacid-anion1.sdf
COSMOTHERM 3D 0

16 16 0 0 0 0 0 0 0 0 0 V2000
1.5302 -1.4156 -0.0202 C 0 0 0 0 0 0 0 0 0 0 0 1
0.1374 -1.4040 -0.0164 C 0 0 0 0 0 0 0 0 0 0 0 2
-0.6334 -0.2259 -0.0025 C 0 0 0 0 0 0 0 0 0 0 0 3
0.0842 0.9983 0.0122 C 0 0 0 0 0 0 0 0 0 0 0 4
1.4889 1.0087 0.0118 C 0 0 0 0 0 0 0 0 0 0 0 5
2.2099 -0.1879 -0.0047 C 0 0 0 0 0 0 0 0 0 0 0 6
-2.1577 -0.3607 -0.0039 C 0 0 0 0 0 0 0 0 0 0 0 7
-2.6195 -1.5465 0.0645 O 0 0 0 0 0 0 0 0 0 0 0 8
-2.8609 0.6924 -0.0757 O 0 0 0 0 0 0 0 0 0 0 0 9
-0.5844 2.1967 0.0325 O 0 0 0 0 0 0 0 0 0 0 0 10
3.5805 -0.0989 -0.0040 O 0 0 0 0 0 0 0 0 0 0 0 11
0.0828 2.9108 0.0505 H 0 0 0 0 0 0 0 0 0 0 0 12
3.9595 -0.9985 -0.0143 H 0 0 0 0 0 0 0 0 0 0 0 13
2.0857 -2.3562 -0.0300 H 0 0 0 0 0 0 0 0 0 0 0 14
-0.4149 -2.3449 -0.0242 H 0 0 0 0 0 0 0 0 0 0 0 15
2.0280 1.9595 0.0263 H 0 0 0 0 0 0 0 0 0 0 0 16
2 1 0 0 0 0
6 1 0 0 0 0
14 1 0 0 0 0
3 2 0 0 0 0
15 2 0 0 0 0
4 3 0 0 0 0
7 3 0 0 0 0
5 4 0 0 0 0
10 4 0 0 0 0
6 5 0 0 0 0
11 6 0 0 0 0
8 7 0 0 0 0
9 7 0 0 0 0
12 10 0 0 0 0
13 11 0 0 0 0
5 16 0 0 0 0
M END
$$$$
2,4-dihydroxybenzoicacid0.sdf
COSMOTHERM 3D 0

17 17 0 0 0 0 0 0 0 0 0 V2000
1.5723 -1.4046 -0.0008 C 0 0 0 0 0 0 0 0 0 0 0 1
0.1901 -1.4473 -0.0009 C 0 0 0 0 0 0 0 0 0 0 0 2
-0.5868 -0.2655 0.0001 C 0 0 0 0 0 0 0 0 0 0 0 3
0.0868 0.9926 0.0002 C 0 0 0 0 0 0 0 0 0 0 0 4
1.4864 1.0397 0.0013 C 0 0 0 0 0 0 0 0 0 0 0 5
2.2204 -0.1495 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 6
-2.0428 -0.2854 -0.0001 C 0 0 0 0 0 0 0 0 0 0 0 7
-2.6034 -1.5138 0.0018 O 0 0 0 0 0 0 0 0 0 0 0 8
-2.7494 0.7444 -0.0016 O 0 0 0 0 0 0 0 0 0 0 0 9
```

URL: <http://mc.manuscriptcentral.com/tandf/tmph>

	2.9875	-0.4694	0.0001	C1	0	0	0	0	0	0	0	0	0	0	8
	-3.2949	0.0150	-0.0001	C1	0	0	0	0	0	0	0	0	0	0	9
	-1.2392	2.0179	0.0004	H	0	0	0	0	0	0	0	0	0	0	10
	0.9267	-2.4671	-0.0001	H	0	0	0	0	0	0	0	0	0	0	11
	-1.5614	-2.2994	-0.0005	H	0	0	0	0	0	0	0	0	0	0	12
	0.8976	2.8452	0.0010	H	0	0	0	0	0	0	0	0	0	0	13
2	1	0	0	0											
6	1	0	0	0											
9	1	0	0	0											
3	2	0	0	0											
10	2	0	0	0											
4	3	0	0	0											
7	3	0	0	0											
5	4	0	0	0											
8	4	0	0	0											
6	5	0	0	0											
11	5	0	0	0											
12	6	0	0	0											
7	13	0	0	0											
M	END														
\$\$\$\$															
2,6-dichlorophenol-anion.sdf															
COSMOtherm			3D										0		
13	12	0	0	0	0	0	0	0	0	V2000					
	1.2079	-1.6352	-0.0002	C	0	0	0	0	0	0	0	0	0	0	1
	1.1906	-0.2449	0.0000	C	0	0	0	0	0	0	0	0	0	0	2
	0.0000	0.5750	-0.0004	C	0	0	0	0	0	0	0	0	0	0	3
	-1.1906	-0.2449	0.0000	C	0	0	0	0	0	0	0	0	0	0	4
	-1.2079	-1.6352	-0.0002	C	0	0	0	0	0	0	0	0	0	0	5
	0.0000	-2.3471	-0.0001	C	0	0	0	0	0	0	0	0	0	0	6
	-0.0001	1.8509	-0.0009	O	0	0	0	0	0	0	0	0	0	0	7
	-2.7476	0.6299	0.0004	C1	0	0	0	0	0	0	0	0	0	0	8
	2.7476	0.6299	0.0004	C1	0	0	0	0	0	0	0	0	0	0	9
	2.1627	-2.1639	0.0000	H	0	0	0	0	0	0	0	0	0	0	10
	-2.1627	-2.1639	-0.0004	H	0	0	0	0	0	0	0	0	0	0	11
	0.0000	-3.4371	-0.0003	H	0	0	0	0	0	0	0	0	0	0	12
2	1	0	0	0											
6	1	0	0	0											
10	1	0	0	0											
3	2	0	0	0											
9	2	0	0	0											
4	3	0	0	0											
7	3	0	0	0											
5	4	0	0	0											
8	4	0	0												

```
2 1 0 0 0 0
10 1 0 0 0 0
11 1 0 0 0 0
3 2 0 0 0 0
12 2 0 0 0 0
13 2 0 0 0 0
4 3 0 0 0 0
7 3 0 0 0 0
14 3 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
15 6 0 0 0 0
16 6 0 0 0 0
17 6 0 0 0 0
8 7 0 0 0 0
9 7 0 0 0 0
8 18 0 0 0 0
M END
$$$$
2-acetylbutanedioicacid0.sdf
COSMOtherm 3D 0
19 18 0 0 0 0 0 0 0 0 0 V2000
2.1182 0.2652 0.2160 C 0 0 0 0 0 0 0 0 0 0 1
0.8190 0.8846 -0.2428 C 0 0 0 0 0 0 0 0 0 0 2
-0.4119 0.1673 0.3022 C 0 0 0 0 0 0 0 0 0 0 3
-1.6943 1.0309 0.1293 C 0 0 0 0 0 0 0 0 0 0 4
-1.5952 2.2153 -0.1614 O 0 0 0 0 0 0 0 0 0 0 5
-3.0218 0.3685 0.3709 C 0 0 0 0 0 0 0 0 0 0 6
-0.5729 -1.2158 -0.3164 C 0 0 0 0 0 0 0 0 0 0 7
-1.0632 -2.1156 0.5642 O 0 0 0 0 0 0 0 0 0 0 8
-0.3037 -1.4879 -1.4767 O 0 0 0 0 0 0 0 0 0 0 9
3.1783 0.8193 -0.4200 O 0 0 0 0 0 0 0 0 0 0 10
2.2332 -0.6124 1.0597 O 0 0 0 0 0 0 0 0 0 0 11
0.8055 0.9116 -1.3414 H 0 0 0 0 0 0 0 0 0 0 12
0.8083 1.9337 0.0887 H 0 0 0 0 0 0 0 0 0 0 13
-0.3183 0.0267 1.3922 H 0 0 0 0 0 0 0 0 0 0 14
-3.8153 1.1228 0.4116 H 0 0 0 0 0 0 0 0 0 0 15
-3.2368 -0.3319 -0.4527 H 0 0 0 0 0 0 0 0 0 0 16
-3.0061 -0.2246 1.2961 H 0 0 0 0 0 0 0 0 0 0 17
-1.1795 -2.9730 0.0980 H 0 0 0 0 0 0 0 0 0 0 18
3.9963 0.4024 -0.0712 H 0 0 0 0 0 0 0 0 0 0 19
2 1 0 0 0 0
10 1 0 0 0 0
11 1 0 0 0 0
3 2 0 0 0 0
12 2 0 0 0 0
13 2 0 0 0 0
4 3 0 0 0 0
7 3 0 0 0 0
14 3 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
15 6 0 0 0 0
16 6 0 0 0 0
17 6 0 0 0 0
8 7 0 0 0 0
9 7 0 0 0 0
18 8 0 0 0 0
10 19 0 0 0 0
M END
$$$$
2-acetylbutanedioicacid0a-anion.sdf
COSMOtherm 3D 0
18 17 0 0 0 0 0 0 0 0 0 V2000
2.1110 0.2524 -0.2723 C 0 0 0 0 0 0 0 0 0 0 1
0.7944 0.9168 0.0530 C 0 0 0 0 0 0 0 0 0 0 2
-0.4231 0.1126 -0.3838 C 0 0 0 0 0 0 0 0 0 0 3
-0.5558 -1.1962 0.3766 C 0 0 0 0 0 0 0 0 0 0 4
-0.0692 -1.3381 1.5023 O 0 0 0 0 0 0 0 0 0 0 5
-1.3304 -2.2988 -0.2997 C 0 0 0 0 0 0 0 0 0 0 6
-1.7793 0.9239 -0.1608 C 0 0 0 0 0 0 0 0 0 0 7
-2.7525 0.5756 -0.8853 O 0 0 0 0 0 0 0 0 0 0 8
-1.7555 1.8239 0.7215 O 0 0 0 0 0 0 0 0 0 0 9
3.1595 0.9487 0.2445 O 0 0 0 0 0 0 0 0 0 0 10
2.2660 -0.7701 -0.9259 O 0 0 0 0 0 0 0 0 0 0 11
0.7942 1.9048 -0.4328 H 0 0 0 0 0 0 0 0 0 0 12
0.7596 1.1140 1.1329 H 0 0 0 0 0 0 0 0 0 0 13
-0.3842 -0.1153 -1.4577 H 0 0 0 0 0 0 0 0 0 0 14
-1.6086 -3.0795 0.4186 H 0 0 0 0 0 0 0 0 0 0 15
-2.2176 -1.8857 -0.8007 H 0 0 0 0 0 0 0 0 0 0 16
-0.6959 -2.7425 -1.0847 H 0 0 0 0 0 0 0 0 0 0 17
3.9862 0.4877 -0.0172 H 0 0 0 0 0 0 0 0 0 0 18
2 1 0 0 0 0
10 1 0 0 0 0
11 1 0 0 0 0
3 2 0 0 0 0
12 2 0 0 0 0
13 2 0 0 0 0
4 3 0 0 0 0
7 3 0 0 0 0
14 3 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
15 6 0 0 0 0
16 6 0 0 0 0
17 6 0 0 0 0
8 7 0 0 0 0
9 7 0 0 0 0
10 18 0 0 0 0
M END
$$$$
2-acetylbutanedioicacid1.sdf
COSMOtherm 3D 0
```


[illegible]

```
0.0520 -3.5717 0.9294 H 0 0 0 0 0 0 0 0 0 0 0 19
2 1 0 0 0 0
10 1 0 0 0 0
11 1 0 0 0 0
3 2 0 0 0 0
12 2 0 0 0 0
13 2 0 0 0 0
4 3 0 0 0 0
7 3 0 0 0 0
14 3 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
15 6 0 0 0 0
16 6 0 0 0 0
17 6 0 0 0 0
8 7 0 0 0 0
9 7 0 0 0 0
18 8 0 0 0 0
10 19 0 0 0 0
M END
$$$$
2-acetylbutanedioicacid2a-anion.sdf
COSMOTHERM 3D 0
18 18 0 0 0 0 0 0 0 0 0 V2000
0.3217 -0.1268 1.9017 C 0 0 0 0 0 0 0 0 0 0 0 1
0.0297 -1.2086 0.8580 C 0 0 0 0 0 0 0 0 0 0 0 2
-0.2316 -0.7694 -0.6141 C 0 0 0 0 0 0 0 0 0 0 0 3
-1.4577 0.1650 -0.6804 C 0 0 0 0 0 0 0 0 0 0 0 4
-2.5826 -0.3246 -0.6119 O 0 0 0 0 0 0 0 0 0 0 0 5
-1.2441 1.6497 -0.8079 C 0 0 0 0 0 0 0 0 0 0 0 6
0.9919 -0.2280 -1.3925 C 0 0 0 0 0 0 0 0 0 0 0 7
1.0370 -0.4309 -2.6221 O 0 0 0 0 0 0 0 0 0 0 0 8
1.9062 0.4142 -0.7323 O 0 0 0 0 0 0 0 0 0 0 0 9
1.2282 0.7802 1.5856 O 0 0 0 0 0 0 0 0 0 0 0 10
-0.2417 -0.1330 3.0027 O 0 0 0 0 0 0 0 0 0 0 0 11
-0.8377 -1.7812 1.2082 H 0 0 0 0 0 0 0 0 0 0 0 12
0.8920 -1.8954 0.8549 H 0 0 0 0 0 0 0 0 0 0 0 13
-0.5471 -1.6788 -1.1447 H 0 0 0 0 0 0 0 0 0 0 0 14
-2.2003 2.1807 -0.7445 H 0 0 0 0 0 0 0 0 0 0 0 15
-0.5547 2.0135 -0.0309 H 0 0 0 0 0 0 0 0 0 0 0 16
-0.7655 1.8692 -1.7760 H 0 0 0 0 0 0 0 0 0 0 0 17
1.5795 0.6114 0.5228 H 0 0 0 0 0 0 0 0 0 0 0 18
2 1 0 0 0 0
10 1 0 0 0 0
11 1 0 0 0 0
3 2 0 0 0 0
12 2 0 0 0 0
13 2 0 0 0 0
4 3 0 0 0 0
7 3 0 0 0 0
14 3 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
15 6 0 0 0 0
16 6 0 0 0 0
17 6 0 0 0 0
8 7 0 0 0 0
9 7 0 0 0 0
9 18 0 0 0 0
10 18 0 0 0 0
M END
$$$$
2-acetylbutanedioicacid4.sdf
COSMOTHERM 3D 0
19 18 0 0 0 0 0 0 0 0 0 V2000
0.0350 1.9702 0.0466 C 0 0 0 0 0 0 0 0 0 0 0 1
0.1428 0.9714 -1.1028 C 0 0 0 0 0 0 0 0 0 0 0 2
0.0832 -0.5287 -0.7368 C 0 0 0 0 0 0 0 0 0 0 0 3
1.2980 -1.1205 0.0023 C 0 0 0 0 0 0 0 0 0 0 0 4
1.1892 -2.2279 0.5455 O 0 0 0 0 0 0 0 0 0 0 0 5
2.5997 -0.3924 -0.0267 C 0 0 0 0 0 0 0 0 0 0 0 6
-1.2695 -0.9704 -0.1519 C 0 0 0 0 0 0 0 0 0 0 0 7
-1.3372 -2.2013 0.3341 O 0 0 0 0 0 0 0 0 0 0 0 8
-2.2619 -0.2391 -0.1695 O 0 0 0 0 0 0 0 0 0 0 0 9
-1.1598 2.0471 0.6665 O 0 0 0 0 0 0 0 0 0 0 0 10
0.9497 2.7061 0.3894 O 0 0 0 0 0 0 0 0 0 0 0 11
1.0789 1.1757 -1.6325 H 0 0 0 0 0 0 0 0 0 0 0 12
-0.6773 1.1751 -1.8060 H 0 0 0 0 0 0 0 0 0 0 0 13
0.1258 -1.0683 -1.7045 H 0 0 0 0 0 0 0 0 0 0 0 14
3.3622 -0.9676 0.5086 H 0 0 0 0 0 0 0 0 0 0 0 15
2.9138 -0.2384 -1.0714 H 0 0 0 0 0 0 0 0 0 0 0 16
2.4961 0.6095 0.4176 H 0 0 0 0 0 0 0 0 0 0 0 17
-0.3730 -2.5345 0.4277 H 0 0 0 0 0 0 0 0 0 0 0 18
-1.7662 1.3371 0.2991 H 0 0 0 0 0 0 0 0 0 0 0 19
2 1 0 0 0 0
10 1 0 0 0 0
11 1 0 0 0 0
3 2 0 0 0 0
12 2 0 0 0 0
13 2 0 0 0 0
4 3 0 0 0 0
7 3 0 0 0 0
14 3 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
15 6 0 0 0 0
16 6 0 0 0 0
17 6 0 0 0 0
8 7 0 0 0 0
9 7 0 0 0 0
18 8 0 0 0 0
10 19 0 0 0 0
M END
```

```

$$$$
2-chlorophenol0-anion.sdf
COSMOtherm 3D 0

12 12 0 0 0 0 0 0 0 0 0 V2000
1.6501 1.0496 -0.0001 C 0 0 0 0 0 0 0 0 0 0 0 1
2.4322 -0.1044 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 2
1.8425 -1.3791 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 3
0.4417 -1.4679 0.0001 C 0 0 0 0 0 0 0 0 0 0 0 4
-0.3288 -0.3092 -0.0001 C 0 0 0 0 0 0 0 0 0 0 0 5
0.2084 1.0303 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 6
2.4494 -2.2854 0.0002 H 0 0 0 0 0 0 0 0 0 0 0 7
-0.5123 2.0953 0.0001 O 0 0 0 0 0 0 0 0 0 0 0 8
2.1236 2.0360 -0.0001 H 0 0 0 0 0 0 0 0 0 0 0 9
3.5220 -0.0112 0.0000 H 0 0 0 0 0 0 0 0 0 0 0 10
-0.0507 -2.4427 0.0001 H 0 0 0 0 0 0 0 0 0 0 0 11
-2.1137 -0.4687 0.0000 Cl 0 0 0 0 0 0 0 0 0 0 0 12

2 1 0 0 0 0
6 1 0 0 0 0
9 1 0 0 0 0
3 2 0 0 0 0
10 2 0 0 0 0
4 3 0 0 0 0
7 3 0 0 0 0
5 4 0 0 0 0
11 4 0 0 0 0
6 5 0 0 0 0
8 6 0 0 0 0
5 12 0 0 0 0

M END
$$$$
2-chlorophenol10.sdf
COSMOtherm 3D 0

13 13 0 0 0 0 0 0 0 0 0 V2000
0.0588 -2.4380 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 1
-1.0749 -1.6238 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 2
-0.9446 -0.2269 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 3
0.3503 0.3219 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 4
1.4877 -0.4839 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 5
1.3413 -1.8748 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 6
-2.0774 0.5341 0.0001 O 0 0 0 0 0 0 0 0 0 0 0 7
0.5037 2.0904 0.0000 Cl 0 0 0 0 0 0 0 0 0 0 0 8
-1.8234 1.4817 -0.0008 H 0 0 0 0 0 0 0 0 0 0 0 9
-0.0629 -3.5222 0.0000 H 0 0 0 0 0 0 0 0 0 0 0 10
-2.0784 -2.0525 -0.0001 H 0 0 0 0 0 0 0 0 0 0 0 11
2.4764 -0.0243 0.0001 H 0 0 0 0 0 0 0 0 0 0 0 12
2.2275 -2.5098 0.0000 H 0 0 0 0 0 0 0 0 0 0 0 13

2 1 0 0 0 0
6 1 0 0 0 0
10 1 0 0 0 0
3 2 0 0 0 0
11 2 0 0 0 0
4 3 0 0 0 0
7 3 0 0 0 0
5 4 0 0 0 0
8 4 0 0 0 0
6 5 0 0 0 0
12 5 0 0 0 0
9 7 0 0 0 0
6 13 0 0 0 0

M END
$$$$
2-chlorophenol11-anion.sdf
COSMOtherm 3D 0

12 12 0 0 0 0 0 0 0 0 0 V2000
1.6499 1.0498 -0.0004 C 0 0 0 0 0 0 0 0 0 0 0 1
2.4320 -0.1042 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 2
1.8426 -1.3790 0.0001 C 0 0 0 0 0 0 0 0 0 0 0 3
0.4419 -1.4679 0.0001 C 0 0 0 0 0 0 0 0 0 0 0 4
-0.3287 -0.3092 -0.0002 C 0 0 0 0 0 0 0 0 0 0 0 5
0.2082 1.0304 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 6
2.4497 -2.2852 0.0004 H 0 0 0 0 0 0 0 0 0 0 0 7
-0.5126 2.0953 0.0003 O 0 0 0 0 0 0 0 0 0 0 0 8
2.1233 2.0362 -0.0003 H 0 0 0 0 0 0 0 0 0 0 0 9
3.5218 -0.0109 0.0001 H 0 0 0 0 0 0 0 0 0 0 0 10
-0.0505 -2.4427 0.0001 H 0 0 0 0 0 0 0 0 0 0 0 11
-2.1134 -0.4690 0.0000 Cl 0 0 0 0 0 0 0 0 0 0 0 12

2 1 0 0 0 0
6 1 0 0 0 0
9 1 0 0 0 0
3 2 0 0 0 0
10 2 0 0 0 0
4 3 0 0 0 0
7 3 0 0 0 0
5 4 0 0 0 0
11 4 0 0 0 0
6 5 0 0 0 0
8 6 0 0 0 0
5 12 0 0 0 0

M END
$$$$
2-chlorophenol11.sdf
COSMOtherm 3D 0

13 13 0 0 0 0 0 0 0 0 0 V2000
0.0877 -2.4388 -0.0001 C 0 0 0 0 0 0 0 0 0 0 0 1
-1.0563 -1.6375 -0.0004 C 0 0 0 0 0 0 0 0 0 0 0 2
-0.9479 -0.2378 0.0001 C 0 0 0 0 0 0 0 0 0 0 0 3
0.3372 0.3334 -0.0002 C 0 0 0 0 0 0 0 0 0 0 0 4
1.4823 -0.4624 0.0002 C 0 0 0 0 0 0 0 0 0 0 0 5
1.3599 -1.8561 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 6
-2.0342 0.5900 0.0002 O 0 0 0 0 0 0 0 0 0 0 0 7
0.4957 2.0962 -0.0001 Cl 0 0 0 0 0 0 0 0 0 0 0 8

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1
2
3      -2.8473      0.0490      -0.0002 H      0      0      0      0      0      0      0      0      0      9
4      -0.0203      -3.5244      -0.0001 H      0      0      0      0      0      0      0      0      0      10
5      -2.0513      -2.0896      -0.0002 H      0      0      0      0      0      0      0      0      0      11
6      2.4642      0.0116      0.0002 H      0      0      0      0      0      0      0      0      0      12
7      2.2565      -2.4766      0.0002 H      0      0      0      0      0      0      0      0      0      13
8
9      2 1 0 0 0 0
10     6 1 0 0 0 0
11     10 1 0 0 0 0
12     3 2 0 0 0 0
13     11 2 0 0 0 0
14     4 3 0 0 0 0
15     7 3 0 0 0 0
16     5 4 0 0 0 0
17     8 4 0 0 0 0
18     6 5 0 0 0 0
19     12 5 0 0 0 0
20     9 7 0 0 0 0
21     6 13 0 0 0 0
22
23 M END
24
25 $$$$
26 2-chloropropanoicacid0-anion.sdf
27 COSMOTHERM      3D
28
29 10 9 0 0 0 0 0 0 0 0 0 V2000
30 -0.4925      0.2550      -1.8656 C      0      0      0      0      0      0      0      0      0      0      1
31 -0.2022      0.5672      -0.4143 C      0      0      0      0      0      0      0      0      0      0      2
32 1.1425      -0.0138      0.1158 C      0      0      0      0      0      0      0      0      0      0      3
33 1.8505      0.7830      0.8025 O      0      0      0      0      0      0      0      0      0      0      4
34 1.4177      -1.2071      -0.1936 O      0      0      0      0      0      0      0      0      0      0      5
35 -1.5726      -0.1447      0.6547 Cl      0      0      0      0      0      0      0      0      0      0      6
36 -1.4673      0.6527      -2.1785 H      0      0      0      0      0      0      0      0      0      0      7
37 0.2855      0.7259      -2.4884 H      0      0      0      0      0      0      0      0      0      0      8
38 -0.4609      -0.8282      -2.0401 H      0      0      0      0      0      0      0      0      0      0      9
39 -0.2560      1.6387      -0.1977 H      0      0      0      0      0      0      0      0      0      0      10
40
41 2 1 0 0 0 0
42 7 1 0 0 0 0
43 8 1 0 0 0 0
44 9 1 0 0 0 0
45 3 2 0 0 0 0
46 6 2 0 0 0 0
47 4 3 0 0 0 0
48 5 3 0 0 0 0
49 2 10 0 0 0 0
50
51 M END
52
53 $$$$
54 2-chloropropanoicacid0.sdf
55 COSMOTHERM      3D
56
57 11 10 0 0 0 0 0 0 0 0 0 V2000
58 -0.5839      0.3216      -1.8659 C      0      0      0      0      0      0      0      0      0      0      1
59 -0.2561      0.5707      -0.4109 C      0      0      0      0      0      0      0      0      0      0      2
60 1.0691      -0.0519      0.0235 C      0      0      0      0      0      0      0      0      0      0      3
61 1.7426      0.7658      0.8589 O      0      0      0      0      0      0      0      0      0      0      4
62 1.4739      -1.1440      -0.3379 O      0      0      0      0      0      0      0      0      0      0      5
63 -1.5387      -0.1928      0.6912 Cl      0      0      0      0      0      0      0      0      0      0      6
64 -1.5632      0.7486      -2.1145 H      0      0      0      0      0      0      0      0      0      0      7
65 0.1763      0.8169      -2.4896 H      0      0      0      0      0      0      0      0      0      0      8
66 -0.5803      -0.7509      -2.0962 H      0      0      0      0      0      0      0      0      0      0      9
67 -0.2747      1.6331      -0.1526 H      0      0      0      0      0      0      0      0      0      0      10
68 2.5789      0.3218      1.1230 H      0      0      0      0      0      0      0      0      0      0      11
69
70 2 1 0 0 0 0
71 7 1 0 0 0 0
72 8 1 0 0 0 0
73 9 1 0 0 0 0
74 3 2 0 0 0 0
75 6 2 0 0 0 0
76 10 2 0 0 0 0
77 4 3 0 0 0 0
78 5 3 0 0 0 0
79 4 11 0 0 0 0
80
81 M END
82
83 $$$$
84 2-chloropropanoicacid1-anion.sdf
85 COSMOTHERM      3D
86
87 10 9 0 0 0 0 0 0 0 0 0 V2000
88 -0.4852      0.2133      -1.8696 C      0      0      0      0      0      0      0      0      0      0      1
89 -0.1986      0.5580      -0.4244 C      0      0      0      0      0      0      0      0      0      0      2
90 1.1429      -0.0171      0.1190 C      0      0      0      0      0      0      0      0      0      0      3
91 1.3926      -1.2312      -0.1260 O      0      0      0      0      0      0      0      0      0      0      4
92 1.8761      0.8051      0.7464 O      0      0      0      0      0      0      0      0      0      0      5
93 -1.5776      -0.1211      0.6544 Cl      0      0      0      0      0      0      0      0      0      0      6
94 -1.4563      0.6096      -2.1956 H      0      0      0      0      0      0      0      0      0      0      7
95 0.2982      0.6645      -2.5000 H      0      0      0      0      0      0      0      0      0      0      8
96 -0.4606      -0.8740      -2.0186 H      0      0      0      0      0      0      0      0      0      0      9
97 -0.2469      1.6346      -0.2334 H      0      0      0      0      0      0      0      0      0      0      10
98
99 2 1 0 0 0 0
100 7 1 0 0 0 0
101 8 1 0 0 0 0
102 9 1 0 0 0 0
103 3 2 0 0 0 0
104 6 2 0 0 0 0
105 4 3 0 0 0 0
106 5 3 0 0 0 0
107 2 10 0 0 0 0
108
109 M END
110
111 $$$$
112 2-chloropropanoicacid1.sdf
113 COSMOTHERM      3D
114
115 11 10 0 0 0 0 0 0 0 0 0 V2000
116 -0.5144      0.2200      -1.8773 C      0      0      0      0      0      0      0      0      0      0      1
117 -0.2474      0.5766      -0.4287 C      0      0      0      0      0      0      0      0      0      0      2
118 1.0902      0.0912      0.1213 C      0      0      0      0      0      0      0      0      0      0      3
119 1.3392      -1.1976      -0.1814 O      0      0      0      0      0      0      0      0      0      0      4
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1.8527 0.8029 0.7562 O 0 0 0 0 0 0 0 0 0 0 0 0 5
-1.5569 -0.1409 0.6733 Cl 0 0 0 0 0 0 0 0 0 0 0 0 6
-1.4781 0.6359 -2.1965 H 0 0 0 0 0 0 0 0 0 0 0 0 7
0.2753 0.6627 -2.5040 H 0 0 0 0 0 0 0 0 0 0 0 0 8
-0.5164 -0.8657 -2.0316 H 0 0 0 0 0 0 0 0 0 0 0 0 9
-0.3039 1.6536 -0.2492 H 0 0 0 0 0 0 0 0 0 0 0 0 10
2.2055 -1.4462 0.2093 H 0 0 0 0 0 0 0 0 0 0 0 0 11
2 1 0 0 0 0
7 1 0 0 0 0
8 1 0 0 0 0
9 1 0 0 0 0
3 2 0 0 0 0
6 2 0 0 0 0
10 2 0 0 0 0
4 3 0 0 0 0
5 3 0 0 0 0
4 11 0 0 0 0
M END
$$$$
2-hydroxypropanoicacid0-anion.sdf
COSMOTHERM 3D 0
11 10 0 0 0 0 0 0 0 0 0 V2000
1.3699 0.4374 -1.2545 C 0 0 0 0 0 0 0 0 0 0 0 0 1
0.7044 -0.3973 -0.1596 C 0 0 0 0 0 0 0 0 0 0 0 0 2
-0.8025 -0.0481 0.0023 C 0 0 0 0 0 0 0 0 0 0 0 0 3
-1.1337 0.3953 1.1526 O 0 0 0 0 0 0 0 0 0 0 0 0 4
-1.5639 -0.2270 -0.9867 O 0 0 0 0 0 0 0 0 0 0 0 0 5
1.3654 -0.2009 1.1057 O 0 0 0 0 0 0 0 0 0 0 0 0 6
2.4352 0.1777 -1.3398 H 0 0 0 0 0 0 0 0 0 0 0 0 7
0.8878 0.2518 -2.2243 H 0 0 0 0 0 0 0 0 0 0 0 0 8
1.2911 1.5106 -1.0223 H 0 0 0 0 0 0 0 0 0 0 0 0 9
0.7665 -1.4674 -0.4310 H 0 0 0 0 0 0 0 0 0 0 0 0 10
0.6104 0.1402 1.6567 H 0 0 0 0 0 0 0 0 0 0 0 0 11
2 1 0 0 0 0
7 1 0 0 0 0
8 1 0 0 0 0
9 1 0 0 0 0
3 2 0 0 0 0
6 2 0 0 0 0
10 2 0 0 0 0
4 3 0 0 0 0
5 3 0 0 0 0
6 11 0 0 0 0
M END
$$$$
2-hydroxypropanoicacid0.sdf
COSMOTHERM 3D 0
12 11 0 0 0 0 0 0 0 0 0 V2000
1.2591 -1.2440 -0.6320 C 0 0 0 0 0 0 0 0 0 0 0 0 1
0.7077 -0.2273 0.3784 C 0 0 0 0 0 0 0 0 0 0 0 0 2
-0.7342 0.1267 0.0141 C 0 0 0 0 0 0 0 0 0 0 0 0 3
-1.0505 1.1150 -0.6314 O 0 0 0 0 0 0 0 0 0 0 0 0 4
-1.6147 -0.7971 0.4549 O 0 0 0 0 0 0 0 0 0 0 0 0 5
1.5012 0.9589 0.4507 O 0 0 0 0 0 0 0 0 0 0 0 0 6
2.2947 -1.4913 -0.3641 H 0 0 0 0 0 0 0 0 0 0 0 0 7
0.6655 -2.1687 -0.6270 H 0 0 0 0 0 0 0 0 0 0 0 0 8
1.2459 -0.8228 -1.6481 H 0 0 0 0 0 0 0 0 0 0 0 0 9
0.7176 -0.6608 1.3876 H 0 0 0 0 0 0 0 0 0 0 0 0 10
-2.5120 -0.5488 0.1403 H 0 0 0 0 0 0 0 0 0 0 0 0 11
1.3752 1.4474 -0.3865 H 0 0 0 0 0 0 0 0 0 0 0 0 12
2 1 0 0 0 0
7 1 0 0 0 0
8 1 0 0 0 0
9 1 0 0 0 0
3 2 0 0 0 0
6 2 0 0 0 0
10 2 0 0 0 0
4 3 0 0 0 0
5 3 0 0 0 0
11 5 0 0 0 0
6 12 0 0 0 0
M END
$$$$
2-hydroxypropanoicacid1-anion.sdf
COSMOTHERM 3D 0
11 10 0 0 0 0 0 0 0 0 0 V2000
1.3803 0.4201 -1.2530 C 0 0 0 0 0 0 0 0 0 0 0 0 1
0.7068 -0.3977 -0.1509 C 0 0 0 0 0 0 0 0 0 0 0 0 2
-0.8031 -0.0489 -0.0033 C 0 0 0 0 0 0 0 0 0 0 0 0 3
-1.5537 -0.2086 -1.0024 O 0 0 0 0 0 0 0 0 0 0 0 0 4
-1.1470 0.3733 1.1527 O 0 0 0 0 0 0 0 0 0 0 0 0 5
1.3581 -0.1788 1.1160 O 0 0 0 0 0 0 0 0 0 0 0 0 6
2.4508 0.1746 -1.3106 H 0 0 0 0 0 0 0 0 0 0 0 0 7
0.9202 0.2026 -2.2269 H 0 0 0 0 0 0 0 0 0 0 0 0 8
1.2815 1.4976 -1.0508 H 0 0 0 0 0 0 0 0 0 0 0 0 9
0.7715 -1.4720 -0.4060 H 0 0 0 0 0 0 0 0 0 0 0 0 10
0.5887 0.1376 1.6631 H 0 0 0 0 0 0 0 0 0 0 0 0 11
2 1 0 0 0 0
7 1 0 0 0 0
8 1 0 0 0 0
9 1 0 0 0 0
3 2 0 0 0 0
6 2 0 0 0 0
10 2 0 0 0 0
4 3 0 0 0 0
5 3 0 0 0 0
6 11 0 0 0 0
M END
$$$$
2-hydroxypropanoicacid1.sdf
COSMOTHERM 3D 0
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12 11 0 0 0 0 0 0 0 0 0 V2000
-1.3160 1.1794 -0.6690 C 0 0 0 0 0 0 0 0 0 1
-0.7142 0.2399 0.3842 C 0 0 0 0 0 0 0 0 0 2
0.7766 0.0394 0.0960 C 0 0 0 0 0 0 0 0 0 3
1.6518 0.8102 0.4612 O 0 0 0 0 0 0 0 0 0 4
1.0149 -1.0634 -0.6485 O 0 0 0 0 0 0 0 0 0 5
-1.4327 -0.9936 0.4943 O 0 0 0 0 0 0 0 0 0 6
-2.3684 1.3710 -0.4213 H 0 0 0 0 0 0 0 0 0 7
-0.7804 2.1385 -0.6915 H 0 0 0 0 0 0 0 0 0 8
-1.2636 0.7252 -1.6697 H 0 0 0 0 0 0 0 0 0 9
-0.7748 0.7071 1.3761 H 0 0 0 0 0 0 0 0 0 10
1.9785 -1.1119 -0.8334 H 0 0 0 0 0 0 0 0 0 11
-1.4399 -1.4194 -0.3840 H 0 0 0 0 0 0 0 0 0 12
2 1 0 0 0 0
7 1 0 0 0 0
8 1 0 0 0 0
9 1 0 0 0 0
3 2 0 0 0 0
6 2 0 0 0 0
10 2 0 0 0 0
4 3 0 0 0 0
5 3 0 0 0 0
11 5 0 0 0 0
6 12 0 0 0 0
M END
$$$$
2-hydroxypropanoicacid2-anion.sdf
COSMOTHERM 3D 0
11 10 0 0 0 0 0 0 0 0 V2000
1.3659 0.4451 -1.2546 C 0 0 0 0 0 0 0 0 0 1
0.7036 -0.3980 -0.1638 C 0 0 0 0 0 0 0 0 0 2
-0.8024 -0.0481 0.0042 C 0 0 0 0 0 0 0 0 0 3
-1.1275 0.4050 1.1525 O 0 0 0 0 0 0 0 0 0 4
-1.5688 -0.2346 -0.9796 O 0 0 0 0 0 0 0 0 0 5
1.3681 -0.2104 1.1014 O 0 0 0 0 0 0 0 0 0 6
2.4306 0.1851 -1.3459 H 0 0 0 0 0 0 0 0 0 7
0.8803 0.2680 -2.2244 H 0 0 0 0 0 0 0 0 0 8
1.2890 1.5164 -1.0135 H 0 0 0 0 0 0 0 0 0 9
0.7652 -1.4659 -0.4425 H 0 0 0 0 0 0 0 0 0 10
0.6187 0.1418 1.6530 H 0 0 0 0 0 0 0 0 0 11
2 1 0 0 0 0
7 1 0 0 0 0
8 1 0 0 0 0
9 1 0 0 0 0
3 2 0 0 0 0
6 2 0 0 0 0
10 2 0 0 0 0
4 3 0 0 0 0
5 3 0 0 0 0
6 11 0 0 0 0
M END
$$$$
2-hydroxypropanoicacid2.sdf
COSMOTHERM 3D 0
12 11 0 0 0 0 0 0 0 0 V2000
1.2563 0.6166 -1.2558 C 0 0 0 0 0 0 0 0 0 1
0.7093 -0.3794 -0.2225 C 0 0 0 0 0 0 0 0 0 2
-0.7338 -0.0184 0.1282 C 0 0 0 0 0 0 0 0 0 3
-1.0542 0.6067 1.1283 O 0 0 0 0 0 0 0 0 0 4
-1.6085 -0.4351 -0.8112 O 0 0 0 0 0 0 0 0 0 5
1.5027 -0.4273 0.9651 O 0 0 0 0 0 0 0 0 0 6
2.2932 0.3492 -1.4979 H 0 0 0 0 0 0 0 0 0 7
0.6632 0.5931 -2.1805 H 0 0 0 0 0 0 0 0 0 8
1.2386 1.6395 -0.8518 H 0 0 0 0 0 0 0 0 0 9
0.7236 -1.3951 -0.6413 H 0 0 0 0 0 0 0 0 0 10
-2.5076 -0.1267 -0.5614 H 0 0 0 0 0 0 0 0 0 11
1.3237 0.3915 1.4685 H 0 0 0 0 0 0 0 0 0 12
2 1 0 0 0 0
7 1 0 0 0 0
8 1 0 0 0 0
9 1 0 0 0 0
3 2 0 0 0 0
6 2 0 0 0 0
10 2 0 0 0 0
4 3 0 0 0 0
5 3 0 0 0 0
11 5 0 0 0 0
6 12 0 0 0 0
M END
$$$$
3,3-dimethylsuccinimide0-anion.sdf
COSMOTHERM 3D 0
17 17 0 0 0 0 0 0 0 0 V2000
-0.8095 -0.5649 0.0000 C 0 0 0 0 0 0 0 0 0 1
0.5722 -1.2426 -0.0001 C 0 0 0 0 0 0 0 0 0 2
-0.4141 0.9411 -0.0001 C 0 0 0 0 0 0 0 0 0 3
0.9388 1.1404 0.0004 N 0 0 0 0 0 0 0 0 0 4
1.5653 -0.0734 0.0000 C 0 0 0 0 0 0 0 0 0 5
-1.6317 -0.8790 1.2624 C 0 0 0 0 0 0 0 0 0 6
-1.6321 -0.8795 -1.2621 C 0 0 0 0 0 0 0 0 0 7
2.8062 -0.2310 -0.0002 O 0 0 0 0 0 0 0 0 0 8
-1.2619 1.8575 -0.0004 O 0 0 0 0 0 0 0 0 0 9
0.7483 -1.8731 -0.8849 H 0 0 0 0 0 0 0 0 0 10
0.7483 -1.8732 0.8846 H 0 0 0 0 0 0 0 0 0 11
-1.0532 -0.6780 2.1773 H 0 0 0 0 0 0 0 0 0 12
-2.5432 -0.2645 1.2905 H 0 0 0 0 0 0 0 0 0 13
-1.9291 -1.9389 1.2731 H 0 0 0 0 0 0 0 0 0 14
-1.0540 -0.6781 -2.1771 H 0 0 0 0 0 0 0 0 0 15
-2.5439 -0.2656 -1.2898 H 0 0 0 0 0 0 0 0 0 16
-1.9288 -1.9396 -1.2726 H 0 0 0 0 0 0 0 0 0 17
2 1 0 0 0 0
3 1 0 0 0 0
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6 1 0 0 0 0
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8 5 0 0 0 0
12 6 0 0 0 0
13 6 0 0 0 0
14 6 0 0 0 0
15 7 0 0 0 0
16 7 0 0 0 0
7 17 0 0 0 0
M END
$$$$
3,3-dimethylsuccinimide0.sdf
COSMOTHERM 3D 0

18 18 0 0 0 0 0 0 0 0 0 V2000
-0.8230 -0.5670 0.0000 C 0 0 0 0 0 0 0 0 0 0 1
0.5684 -1.2495 0.0005 C 0 0 0 0 0 0 0 0 0 0 2
-0.4835 0.9348 0.0001 C 0 0 0 0 0 0 0 0 0 0 3
0.8988 1.0718 -0.0007 N 0 0 0 0 0 0 0 0 0 0 4
1.5945 -0.1316 0.0001 C 0 0 0 0 0 0 0 0 0 0 5
-1.6377 -0.8941 1.2663 C 0 0 0 0 0 0 0 0 0 0 6
-1.6365 -0.8939 -1.2671 C 0 0 0 0 0 0 0 0 0 0 7
2.8166 -0.2259 0.0004 O 0 0 0 0 0 0 0 0 0 0 8
-1.2703 1.8741 0.0005 O 0 0 0 0 0 0 0 0 0 0 9
1.3649 1.9807 -0.0009 H 0 0 0 0 0 0 0 0 0 0 10
0.7355 -1.8818 -0.8830 H 0 0 0 0 0 0 0 0 0 0 11
0.7353 -1.8808 0.8848 H 0 0 0 0 0 0 0 0 0 0 12
-1.0681 -0.6693 2.1800 H 0 0 0 0 0 0 0 0 0 0 13
-2.5703 -0.3141 1.2850 H 0 0 0 0 0 0 0 0 0 0 14
-1.8927 -1.9634 1.2738 H 0 0 0 0 0 0 0 0 0 0 15
-1.0663 -0.6687 -2.1803 H 0 0 0 0 0 0 0 0 0 0 16
-2.5693 -0.3141 -1.2865 H 0 0 0 0 0 0 0 0 0 0 17
-1.8914 -1.9633 -1.2752 H 0 0 0 0 0 0 0 0 0 0 18

2 1 0 0 0 0
3 1 0 0 0 0
6 1 0 0 0 0
7 1 0 0 0 0
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13 6 0 0 0 0
14 6 0 0 0 0
15 6 0 0 0 0
16 7 0 0 0 0
17 7 0 0 0 0
7 18 0 0 0 0
M END
$$$$
3,3-dimethylsuccinimide1-anion.sdf
COSMOTHERM 3D 0

17 17 0 0 0 0 0 0 0 0 0 V2000
-0.8095 -0.5649 0.0000 C 0 0 0 0 0 0 0 0 0 0 1
0.5722 -1.2426 -0.0001 C 0 0 0 0 0 0 0 0 0 0 2
-0.4141 0.9411 -0.0001 C 0 0 0 0 0 0 0 0 0 0 3
0.9388 1.1404 0.0004 N 0 0 0 0 0 0 0 0 0 0 4
1.5653 -0.0734 0.0000 C 0 0 0 0 0 0 0 0 0 0 5
-1.6317 -0.8790 1.2624 C 0 0 0 0 0 0 0 0 0 0 6
-1.6321 -0.8795 -1.2621 C 0 0 0 0 0 0 0 0 0 0 7
2.8062 -0.2310 -0.0002 O 0 0 0 0 0 0 0 0 0 0 8
-1.2619 1.8575 -0.0004 O 0 0 0 0 0 0 0 0 0 0 9
0.7483 -1.8731 -0.8849 H 0 0 0 0 0 0 0 0 0 0 10
0.7483 -1.8732 0.8846 H 0 0 0 0 0 0 0 0 0 0 11
-1.0532 -0.6780 2.1773 H 0 0 0 0 0 0 0 0 0 0 12
-2.5432 -0.2645 1.2905 H 0 0 0 0 0 0 0 0 0 0 13
-1.9291 -1.9389 1.2731 H 0 0 0 0 0 0 0 0 0 0 14
-1.0540 -0.6781 -2.1771 H 0 0 0 0 0 0 0 0 0 0 15
-2.5439 -0.2656 -1.2898 H 0 0 0 0 0 0 0 0 0 0 16
-1.9288 -1.9396 -1.2726 H 0 0 0 0 0 0 0 0 0 0 17

2 1 0 0 0 0
3 1 0 0 0 0
6 1 0 0 0 0
7 1 0 0 0 0
5 2 0 0 0 0
10 2 0 0 0 0
11 2 0 0 0 0
4 3 0 0 0 0
9 3 0 0 0 0
5 4 0 0 0 0
8 5 0 0 0 0
12 6 0 0 0 0
13 6 0 0 0 0
14 6 0 0 0 0
15 7 0 0 0 0
16 7 0 0 0 0
7 17 0 0 0 0
M END
$$$$
3,3-dimethylsuccinimide1.sdf
COSMOTHERM 3D 0

18 18 0 0 0 0 0 0 0 0 0 V2000
-0.8436 -0.5574 -0.0001 C 0 0 0 0 0 0 0 0 0 0 1
0.5415 -1.2443 -0.0013 C 0 0 0 0 0 0 0 0 0 0 2
```

-0.4528	0.9440	-0.0002	C	0	0	0	0	0	0	0	0
0.9469	1.1222	0.0000	N	0	0	0	0	0	0	0	0
1.4738	-0.0726	-0.0004	C	0	0	0	0	0	0	0	0
-1.6592	-0.8731	1.2669	C	0	0	0	0	0	0	0	0
-1.6619	-0.8731	-1.2652	C	0	0	0	0	0	0	0	0
2.7813	-0.2912	0.0000	O	0	0	0	0	0	0	0	0
-1.2462	1.8795	0.0000	O	0	0	0	0	0	0	0	0
0.7211	-1.8719	-0.8867	H	0	0	0	0	0	0	0	0
0.7218	-1.8738	0.8826	H	0	0	0	0	0	0	0	0
-1.0844	-0.6589	2.1801	H	0	0	0	0	0	0	0	0
-2.5790	-0.2725	1.2872	H	0	0	0	0	0	0	0	0
-1.9386	-1.9367	1.2775	H	0	0	0	0	0	0	0	0
-1.0888	-0.6597	-2.1797	H	0	0	0	0	0	0	0	0
-2.5814	-0.2720	-1.2839	H	0	0	0	0	0	0	0	0
-1.9421	-1.9365	-1.2749	H	0	0	0	0	0	0	0	0
3.2550	0.5702	0.0015	H	0	0	0	0	0	0	0	0
2	1	0	0	0	0	0	0	0	0	0	0
3	1	0	0	0	0	0	0	0	0	0	0
6	1	0	0	0	0	0	0	0	0	0	0
7	1	0	0	0	0	0	0	0	0	0	0
5	2	0	0	0	0	0	0	0	0	0	0
10	2	0	0	0	0	0	0	0	0	0	0
11	2	0	0	0	0	0	0	0	0	0	0
4	3	0	0	0	0	0	0	0	0	0	0
9	3	0	0	0	0	0	0	0	0	0	0
5	4	0	0	0	0	0	0	0	0	0	0
8	5	0	0	0	0	0	0	0	0	0	0
12	6	0	0	0	0	0	0	0	0	0	0
13	6	0	0	0	0	0	0	0	0	0	0
14	6	0	0	0	0	0	0	0	0	0	0
15	7	0	0	0	0	0	0	0	0	0	0
16	7	0	0	0	0	0	0	0	0	0	0
17	7	0	0	0	0	0	0	0	0	0	0
8	18	0	0	0	0	0	0	0	0	0	0
M	END										
\$\$\$\$											
3,3-dimethylsuccinimide2-anion.sdf											
COSMOtherm		3D								0	
17	17	0	0	0	0	0	0	0	V2000		
-0.8095	-0.5649	0.0000	C	0	0	0	0	0	0	0	0
0.5722	-1.2426	-0.0001	C	0	0	0	0	0	0	0	0
-0.4141	0.9411	-0.0001	C	0	0	0	0	0	0	0	0
0.9388	1.1404	0.0004	N	0	0	0	0	0	0	0	0
1.5653	-0.0734	0.0000	C	0	0	0	0	0	0	0	0
-1.6317	-0.8790	1.2624	C	0	0	0	0	0	0	0	0
-1.6321	-0.8795	-1.2621	C	0	0	0	0	0	0	0	0
2.8062	-0.2310	-0.0002	O	0	0	0	0	0	0	0	0
-1.2619	1.8575	-0.0004	O	0	0	0	0	0	0	0	0
0.7483	-1.8731	-0.8849	H	0	0	0	0	0	0	0	0
0.7483	-1.8732	0.8846	H	0	0	0	0				

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4 3 0 0 0 0
9 3 0 0 0 0
5 4 0 0 0 0
8 5 0 0 0 0
12 6 0 0 0 0
13 6 0 0 0 0
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15 7 0 0 0 0
16 7 0 0 0 0
17 7 0 0 0 0
9 18 0 0 0 0
M END
$$$$
3,3-methylphenylglutarimide0-anion.sdf
COSMOtherm 3D 0

27 28 0 0 0 0 0 0 0 0 0 V2000
2.2998 -0.2222 1.1824 C 0 0 0 0 0 0 0 0 0 1
2.9743 -0.2331 0.0011 N 0 0 0 0 0 0 0 0 0 2
2.3027 -0.2092 -1.1818 C 0 0 0 0 0 0 0 0 0 3
0.7730 -0.1887 -1.2395 C 0 0 0 0 0 0 0 0 0 4
0.1033 0.4480 0.0008 C 0 0 0 0 0 0 0 0 0 5
0.7699 -0.2019 1.2358 C 0 0 0 0 0 0 0 0 0 6
2.9287 -0.2351 -2.2718 O 0 0 0 0 0 0 0 0 0 7
2.9225 -0.2599 2.2736 O 0 0 0 0 0 0 0 0 0 8
-1.4053 0.1477 -0.0019 C 0 0 0 0 0 0 0 0 0 9
0.3945 1.9607 0.0089 C 0 0 0 0 0 0 0 0 0 10
0.4499 -1.2377 -1.3471 H 0 0 0 0 0 0 0 0 0 11
0.4719 0.3297 -2.1614 H 0 0 0 0 0 0 0 0 0 12
0.4464 -1.2521 1.3308 H 0 0 0 0 0 0 0 0 0 13
0.4663 0.3063 2.1625 H 0 0 0 0 0 0 0 0 0 14
-4.1792 -0.4676 -0.0016 C 0 0 0 0 0 0 0 0 0 15
-3.2250 -1.4932 -0.0162 C 0 0 0 0 0 0 0 0 0 16
-1.8620 -1.1863 -0.0163 C 0 0 0 0 0 0 0 0 0 17
-2.3778 1.1625 0.0125 C 0 0 0 0 0 0 0 0 0 18
-3.7472 0.8609 0.0125 C 0 0 0 0 0 0 0 0 0 19
1.4788 2.1389 0.0099 H 0 0 0 0 0 0 0 0 0 20
-0.0221 2.4462 0.9035 H 0 0 0 0 0 0 0 0 0 21
-0.0226 2.4558 -0.8801 H 0 0 0 0 0 0 0 0 0 22
-5.2449 -0.7040 -0.0015 H 0 0 0 0 0 0 0 0 0 23
-3.5430 -2.5377 -0.0274 H 0 0 0 0 0 0 0 0 0 24
-1.1437 -2.0094 -0.0273 H 0 0 0 0 0 0 0 0 0 25
-2.0768 2.2096 0.0238 H 0 0 0 0 0 0 0 0 0 26
-4.4759 1.6742 0.0239 H 0 0 0 0 0 0 0 0 0 27
2 1 0 0 0 0
6 1 0 0 0 0
8 1 0 0 0 0
3 2 0 0 0 0
4 3 0 0 0 0
7 3 0 0 0 0
5 4 0 0 0 0
11 4 0 0 0 0
12 4 0 0 0 0
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10 5 0 0 0 0
13 6 0 0 0 0
14 6 0 0 0 0
17 9 0 0 0 0
18 9 0 0 0 0
20 10 0 0 0 0
21 10 0 0 0 0
22 10 0 0 0 0
16 15 0 0 0 0
19 15 0 0 0 0
23 15 0 0 0 0
17 16 0 0 0 0
24 16 0 0 0 0
25 17 0 0 0 0
19 18 0 0 0 0
26 18 0 0 0 0
19 27 0 0 0 0
M END
$$$$
3,3-methylphenylglutarimide0.sdf
COSMOtherm 3D 0

28 29 0 0 0 0 0 0 0 0 0 V2000
2.2522 0.2135 -1.2480 C 0 0 0 0 0 0 0 0 0 1
2.8693 0.2514 -0.0002 N 0 0 0 0 0 0 0 0 0 2
2.2516 0.2192 1.2475 C 0 0 0 0 0 0 0 0 0 3
0.7401 0.2137 1.2521 C 0 0 0 0 0 0 0 0 0 4
0.0954 -0.4377 0.0007 C 0 0 0 0 0 0 0 0 0 5
0.7407 0.2080 -1.2533 C 0 0 0 0 0 0 0 0 0 6
2.9356 0.2250 2.2705 O 0 0 0 0 0 0 0 0 0 7
2.9367 0.2144 -2.2707 O 0 0 0 0 0 0 0 0 0 8
-1.4162 -0.1437 0.0001 C 0 0 0 0 0 0 0 0 0 9
0.3978 -1.9483 0.0042 C 0 0 0 0 0 0 0 0 0 10
3.8930 0.2645 0.0001 H 0 0 0 0 0 0 0 0 0 11
0.4335 1.2696 1.3357 H 0 0 0 0 0 0 0 0 0 12
0.4124 -0.2854 2.1738 H 0 0 0 0 0 0 0 0 0 13
0.4341 1.2634 -1.3422 H 0 0 0 0 0 0 0 0 0 14
0.4135 -0.2954 -2.1728 H 0 0 0 0 0 0 0 0 0 15
-4.1878 0.4534 -0.0017 C 0 0 0 0 0 0 0 0 0 16
-3.2414 1.4858 -0.0067 C 0 0 0 0 0 0 0 0 0 17
-1.8766 1.1878 -0.0059 C 0 0 0 0 0 0 0 0 0 18
-2.3783 -1.1667 0.0056 C 0 0 0 0 0 0 0 0 0 19
-3.7489 -0.8727 0.0052 C 0 0 0 0 0 0 0 0 0 20
1.4818 -2.1310 0.0048 H 0 0 0 0 0 0 0 0 0 21
-0.0173 -2.4399 -0.8867 H 0 0 0 0 0 0 0 0 0 22
-0.0174 -2.4358 0.8972 H 0 0 0 0 0 0 0 0 0 23
-5.2549 0.6832 -0.0023 H 0 0 0 0 0 0 0 0 0 24
-3.5660 2.5280 -0.0116 H 0 0 0 0 0 0 0 0 0 25
-1.1644 2.0164 -0.0102 H 0 0 0 0 0 0 0 0 0 26
-2.0707 -2.2117 0.0108 H 0 0 0 0 0 0 0 0 0 27
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URL: <http://mc.manuscriptcentral.com/tandf/tmph>

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-0.8056	-2.6341	-0.0581	C	0	0	0	0	0	0	0	0	0	9
-0.0571	-0.4252	-0.9960	C	0	0	0	0	0	0	0	0	0	10
0.4628	1.9082	2.4082	H	0	0	0	0	0	0	0	0	0	11
0.5522	-1.9127	2.1131	H	0	0	0	0	0	0	0	0	0	12
1.7171	-1.7111	0.8084	H	0	0	0	0	0	0	0	0	0	13
-1.8025	-1.1377	1.9378	H	0	0	0	0	0	0	0	0	0	14
-2.4225	-0.3638	0.4777	H	0	0	0	0	0	0	0	0	0	15
0.4579	0.9241	-3.4356	C	0	0	0	0	0	0	0	0	0	16
1.5030	0.6236	-2.5590	C	0	0	0	0	0	0	0	0	0	17
1.2471	-0.0450	-1.3543	C	0	0	0	0	0	0	0	0	0	18
-1.0980	-0.1181	-1.8941	C	0	0	0	0	0	0	0	0	0	19
-0.8474	0.5470	-3.0970	C	0	0	0	0	0	0	0	0	0	20
-1.0494	-3.2023	0.8521	H	0	0	0	0	0	0	0	0	0	21
-1.6918	-2.6285	-0.7078	H	0	0	0	0	0	0	0	0	0	22
0.0034	-3.1568	-0.5886	H	0	0	0	0	0	0	0	0	0	23
0.6559	1.4458	-4.3736	H	0	0	0	0	0	0	0	0	0	24
2.5272	0.9086	-2.8074	H	0	0	0	0	0	0	0	0	0	25
2.0909	-0.2680	-0.7007	H	0	0	0	0	0	0	0	0	0	26
-2.1252	-0.4051	-1.6601	H	0	0	0	0	0	0	0	0	0	27
-1.6756	0.7714	-3.7721	H	0	0	0	0	0	0	0	0	0	28
2	1	0	0	0	0	0	0	0	0	0	0	0	0
6	1	0	0	0	0	0	0	0	0	0	0	0	0
8	1	0	0	0	0	0	0	0	0	0	0	0	0
3	2	0	0	0	0	0	0	0	0	0	0	0	0
11	2	0	0	0	0	0	0	0	0	0	0	0	0
4	3	0	0	0	0	0	0	0	0	0	0	0	0
7	3	0	0	0	0	0	0	0	0	0	0	0	0
5	4	0	0	0	0	0	0	0	0	0	0	0	0
12	4	0	0	0	0	0	0	0	0	0	0	0	0
13	4	0	0	0	0	0	0	0	0	0	0	0	0
6	5	0	0	0	0	0	0	0	0	0	0	0	0
9	5	0	0	0	0	0	0	0	0	0	0	0	0
10	5	0	0	0	0	0	0	0	0	0	0	0	0
14	6	0	0	0	0	0	0	0	0	0	0	0	0
15	6	0	0	0	0	0	0	0	0	0	0	0	0
21	9	0	0	0	0	0	0	0	0	0	0	0	0
22	9	0	0	0	0	0	0	0	0	0	0	0	0
23	9	0	0	0	0	0	0	0	0	0	0	0	0
18	10	0	0	0	0	0	0	0	0	0	0	0	0
19	10	0	0	0	0	0	0	0	0	0	0	0	0
17	16	0	0	0	0	0	0	0	0	0	0	0	0
20	16	0	0	0	0	0	0	0	0	0	0	0	0
24	16	0	0	0	0	0	0	0	0	0	0	0	0
18	17	0	0	0	0	0	0	0	0	0	0	0	0
25	17	0	0	0	0	0	0	0	0	0	0	0	0
26	18	0	0	0	0	0	0	0	0	0	0	0	0
20	19	0	0	0	0	0	0	0	0	0	0	0	0
27	19	0	0	0	0	0	0	0	0	0	0	0	0
20	28	0	0	0	0	0	0	0	0	0	0	0	0
M END													
\$\$\$\$													
3,3-methylphenylglutarimide2-anion.sdf													
COSMOtherm 3D 0													
27	28	0	0	0	0	0	0	0	0	0	0	0	V2000
2.2986	1.1836	0.2183	C	0	0	0	0	0	0	0	0	0	1
2.9742	0.0031	0.2337	N	0	0	0	0	0	0	0	0	0	2
2.3037	-1.1805	0.2132	C	0	0	0	0	0	0	0	0	0	3
0.7740	-1.2394	0.1929	C	0	0	0	0	0	0	0	0	0	4
0.1033	-0.0022	-0.4487	C	0	0	0	0	0	0	0	0	0	5
0.7687	1.2360	0.1966	C	0	0	0	0	0	0	0	0	0	6
2.9305	-2.2697	0.2424	O	0	0	0	0	0	0	0	0	0	7
2.9203	2.2757	0.2532	O	0	0	0	0	0	0	0	0	0	8
-1.4052	-0.0031	-0.1479	C	0	0	0	0	0	0	0	0	0	9
0.3943	0.0005	-1.9615	C	0	0	0	0	0	0	0	0	0	10
0.4511	-1.3431	1.2423	H	0	0	0	0	0	0	0	0	0	11
0.4737	-2.1636	-0.3218	H	0	0	0	0	0	0	0	0	0	12
0.4445	1.3352	1.2461	H	0	0	0	0	0	0	0	0	0	13
0.4648	2.1604	-0.3155	H	0	0	0	0	0	0	0	0	0	14
-4.1789	0.0004	0.4683	C	0	0	0	0	0	0	0	0	0	15
-3.2244	-0.0085	1.4936	C	0	0	0	0	0	0	0	0	0	16
-1.8615	-0.0102	1.1862	C	0	0	0	0	0	0	0	0	0	17
-2.3780	0.0055	-1.1625	C	0	0	0	0	0	0	0	0	0	18
-3.7474	0.0072	-0.8605	C	0	0	0	0	0	0	0	0	0	19
1.4786	0.0009	-2.1398	H	0	0	0	0	0	0	0	0	0	20
-0.0224	0.8933	-2.4502	H	0	0	0	0	0	0	0	0	0	21
-0.0226	-0.8905	-2.4532	H	0	0	0	0	0	0	0	0	0	22
-5.2445	0.0019	0.7051	H	0	0	0	0	0	0	0	0	0	23
-3.5420	-0.0140	2.5383	H	0	0	0	0	0	0	0	0	0	24
-1.1430	-0.0168	2.0091	H	0	0	0	0	0	0	0	0	0	25
-2.0773	0.0112	-2.2098	H	0	0	0	0	0	0	0	0	0	26
-4.4764	0.0140	-1.6736	H	0	0	0	0	0	0	0	0	0	27
2	1	0	0	0	0	0	0	0	0	0	0	0	0
6	1	0	0	0	0	0	0	0	0	0	0	0	0
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3	2	0	0	0	0	0	0	0	0	0	0	0	0
4	3	0	0	0	0	0	0	0	0	0	0	0	0
7	3	0	0	0	0	0	0	0	0	0	0	0	0
5	4	0	0	0	0	0	0	0	0	0	0	0	0
11	4	0	0	0	0	0	0	0	0	0	0	0	0
12	4	0	0	0	0	0	0	0	0	0	0	0	0
6	5	0	0	0	0	0	0	0	0	0	0	0	0
9	5	0	0	0	0	0	0	0	0	0	0	0	0
10	5	0	0	0	0	0	0	0	0	0	0	0	0
13	6	0	0	0	0	0	0	0	0	0	0	0	0
14	6	0	0	0	0	0	0	0	0	0	0	0	0
17	9	0	0	0	0	0	0	0	0	0	0	0	0
18	9	0	0	0	0	0	0	0	0	0	0	0	0
20	10	0	0	0	0	0	0	0	0	0	0	0	0
21	10	0	0	0	0	0	0	0	0	0	0	0	0
22	10	0	0	0	0	0	0	0	0	0	0	0	0
16	15	0	0	0	0	0	0	0	0	0	0	0	0
19	15	0	0	0	0	0	0	0	0	0	0	0	0
23	15	0	0	0	0	0	0	0	0	0	0	0	0
17	16	0	0	0	0	0	0	0	0	0	0	0	0

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24 16 0 0 0 0
25 17 0 0 0 0
19 18 0 0 0 0
26 18 0 0 0 0
19 27 0 0 0 0
M END
$$$$
3,3-methylphenylglutarimide2.sdf
COSMOTHERM 3D 0

28 29 0 0 0 0 0 0 0 0 0 V2000
2.2410 1.1280 0.0428 C 0 0 0 0 0 0 0 0 0 0 1
2.9404 0.0524 0.2585 N 0 0 0 0 0 0 0 0 0 0 2
2.2688 -1.1678 0.3989 C 0 0 0 0 0 0 0 0 0 0 3
0.7502 -1.1809 0.4671 C 0 0 0 0 0 0 0 0 0 0 4
0.0892 -0.1121 -0.4438 C 0 0 0 0 0 0 0 0 0 0 5
0.7534 1.2456 -0.1032 C 0 0 0 0 0 0 0 0 0 0 6
2.9262 -2.2068 0.5040 O 0 0 0 0 0 0 0 0 0 0 7
2.8766 2.3007 -0.0551 O 0 0 0 0 0 0 0 0 0 0 8
-1.4182 -0.0357 -0.1447 C 0 0 0 0 0 0 0 0 0 0 9
0.3800 -0.4582 -1.9165 C 0 0 0 0 0 0 0 0 0 0 10
0.4818 -0.9993 1.5212 H 0 0 0 0 0 0 0 0 0 0 11
0.3992 -2.1893 0.2111 H 0 0 0 0 0 0 0 0 0 0 12
0.3777 1.6384 0.8556 H 0 0 0 0 0 0 0 0 0 0 13
0.5237 2.0078 -0.8615 H 0 0 0 0 0 0 0 0 0 0 14
-4.1836 0.1181 0.4617 C 0 0 0 0 0 0 0 0 0 0 15
-3.2267 0.3495 1.4577 C 0 0 0 0 0 0 0 0 0 0 16
-1.8649 0.2733 1.1554 C 0 0 0 0 0 0 0 0 0 0 17
-2.3910 -0.2654 -1.1311 C 0 0 0 0 0 0 0 0 0 0 18
-3.7585 -0.1903 -0.8327 C 0 0 0 0 0 0 0 0 0 0 19
1.4631 -0.4907 -2.1015 H 0 0 0 0 0 0 0 0 0 0 20
-0.0468 0.2929 -2.5958 H 0 0 0 0 0 0 0 0 0 0 21
-0.0292 -1.4427 -2.1832 H 0 0 0 0 0 0 0 0 0 0 22
-5.2482 0.1780 0.6949 H 0 0 0 0 0 0 0 0 0 0 23
-3.5410 0.5914 2.4748 H 0 0 0 0 0 0 0 0 0 0 24
-1.1441 0.4583 1.9551 H 0 0 0 0 0 0 0 0 0 0 25
-2.0936 -0.5074 -2.1509 H 0 0 0 0 0 0 0 0 0 0 26
-4.4907 -0.3735 -1.6217 H 0 0 0 0 0 0 0 0 0 0 27
3.8366 2.1430 0.0933 H 0 0 0 0 0 0 0 0 0 0 28

2 1 0 0 0 0
6 1 0 0 0 0
8 1 0 0 0 0
3 2 0 0 0 0
4 3 0 0 0 0
7 3 0 0 0 0
5 4 0 0 0 0
11 4 0 0 0 0
12 4 0 0 0 0
6 5 0 0 0 0
9 5 0 0 0 0
10 5 0 0 0 0
13 6 0 0 0 0
14 6 0 0 0 0
17 9 0 0 0 0
18 9 0 0 0 0
20 10 0 0 0 0
21 10 0 0 0 0
22 10 0 0 0 0
16 15 0 0 0 0
19 15 0 0 0 0
23 15 0 0 0 0
17 16 0 0 0 0
24 16 0 0 0 0
25 17 0 0 0 0
19 18 0 0 0 0
26 18 0 0 0 0
27 19 0 0 0 0
8 28 0 0 0 0
M END
$$$$
3,3-methylphenylglutarimide3-anion.sdf
COSMOTHERM 3D 0

27 28 0 0 0 0 0 0 0 0 0 V2000
0.9051 -1.6836 1.0375 C 0 0 0 0 0 0 0 0 0 0 1
1.0659 -2.0718 -0.2578 N 0 0 0 0 0 0 0 0 0 0 2
0.0554 -1.9165 -1.1567 C 0 0 0 0 0 0 0 0 0 0 3
-1.2703 -1.2643 -0.7573 C 0 0 0 0 0 0 0 0 0 0 4
-1.1651 -0.2885 0.4252 C 0 0 0 0 0 0 0 0 0 0 5
-0.4069 -1.0658 1.5235 C 0 0 0 0 0 0 0 0 0 0 6
0.1793 -2.3316 -2.3372 O 0 0 0 0 0 0 0 0 0 0 7
1.8277 -1.8523 1.8746 O 0 0 0 0 0 0 0 0 0 0 8
-2.5821 0.0770 0.9182 C 0 0 0 0 0 0 0 0 0 0 9
-0.4125 1.0057 0.0673 C 0 0 0 0 0 0 0 0 0 0 10
-1.9501 -2.0824 -0.4602 H 0 0 0 0 0 0 0 0 0 0 11
-1.7186 -0.8043 -1.6486 H 0 0 0 0 0 0 0 0 0 0 12
-1.0505 -1.8931 1.8734 H 0 0 0 0 0 0 0 0 0 0 13
-0.1888 -0.4431 2.4010 H 0 0 0 0 0 0 0 0 0 0 14
0.9041 3.4502 -0.5252 C 0 0 0 0 0 0 0 0 0 0 15
0.6326 2.5273 -1.5386 C 0 0 0 0 0 0 0 0 0 0 16
-0.0182 1.3212 -1.2439 C 0 0 0 0 0 0 0 0 0 0 17
-0.1283 1.9484 1.0757 C 0 0 0 0 0 0 0 0 0 0 18
0.5190 3.1531 0.7881 C 0 0 0 0 0 0 0 0 0 0 19
-3.1383 -0.8330 1.1911 H 0 0 0 0 0 0 0 0 0 0 20
-2.5435 0.7295 1.8026 H 0 0 0 0 0 0 0 0 0 0 21
-3.1454 0.6030 0.1323 H 0 0 0 0 0 0 0 0 0 0 22
1.4096 4.3904 -0.7537 H 0 0 0 0 0 0 0 0 0 0 23
0.9268 2.7415 -2.5683 H 0 0 0 0 0 0 0 0 0 0 24
-0.2125 0.6243 -2.0597 H 0 0 0 0 0 0 0 0 0 0 25
-0.4211 1.7450 2.1081 H 0 0 0 0 0 0 0 0 0 0 26
0.7225 3.8628 1.5929 H 0 0 0 0 0 0 0 0 0 0 27

2 1 0 0 0 0
6 1 0 0 0 0
8 1 0 0 0 0
3 2 0 0 0 0
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4 3 0 0 0 0
7 3 0 0 0 0
5 4 0 0 0 0
11 4 0 0 0 0
12 4 0 0 0 0
6 5 0 0 0 0
9 5 0 0 0 0
10 5 0 0 0 0
13 6 0 0 0 0
14 6 0 0 0 0
20 9 0 0 0 0
21 9 0 0 0 0
22 9 0 0 0 0
17 10 0 0 0 0
18 10 0 0 0 0
16 15 0 0 0 0
19 15 0 0 0 0
23 15 0 0 0 0
17 16 0 0 0 0
24 16 0 0 0 0
25 17 0 0 0 0
19 18 0 0 0 0
26 18 0 0 0 0
19 27 0 0 0 0
M END
$$$$
3,3-methylphenylglutarimide3.sdf
COSMOTHERM 3D 0
28 29 0 0 0 0 0 0 0 0 0 V2000
0.7502 0.9846 1.7241 C 0 0 0 0 0 0 0 0 0 0 0 1
1.0544 -0.2387 2.0498 N 0 0 0 0 0 0 0 0 0 0 0 2
0.1049 -1.2436 1.8253 C 0 0 0 0 0 0 0 0 0 0 0 3
-1.2454 -0.8771 1.2279 C 0 0 0 0 0 0 0 0 0 0 0 4
-1.2038 0.3410 0.2846 C 0 0 0 0 0 0 0 0 0 0 0 5
-0.5254 1.4661 1.1031 C 0 0 0 0 0 0 0 0 0 0 0 6
0.3705 -2.4045 2.1489 O 0 0 0 0 0 0 0 0 0 0 0 7
1.6382 1.9548 1.9611 O 0 0 0 0 0 0 0 0 0 0 0 8
-2.6429 0.7626 -0.0774 C 0 0 0 0 0 0 0 0 0 0 0 9
-0.4173 0.0643 -1.0111 C 0 0 0 0 0 0 0 0 0 0 0 10
-1.9050 -0.6263 2.0777 H 0 0 0 0 0 0 0 0 0 0 0 11
-1.6774 -1.7689 0.7567 H 0 0 0 0 0 0 0 0 0 0 0 12
-1.1956 1.7717 1.9260 H 0 0 0 0 0 0 0 0 0 0 0 13
-0.3262 2.3694 0.5130 H 0 0 0 0 0 0 0 0 0 0 0 14
0.9560 -0.3803 -3.4514 C 0 0 0 0 0 0 0 0 0 0 0 15
0.6538 -1.4494 -2.6044 C 0 0 0 0 0 0 0 0 0 0 0 16
-0.0264 -1.2281 -1.3994 C 0 0 0 0 0 0 0 0 0 0 0 17
-0.1103 1.1290 -1.8805 C 0 0 0 0 0 0 0 0 0 0 0 18
0.5673 0.9135 -3.0834 C 0 0 0 0 0 0 0 0 0 0 0 19
-3.2244 0.9734 0.8327 H 0 0 0 0 0 0 0 0 0 0 0 20
-2.6437 1.6660 -0.7034 H 0 0 0 0 0 0 0 0 0 0 0 21
-3.1486 -0.0389 -0.6349 H 0 0 0 0 0 0 0 0 0 0 0 22
1.4873 -0.5512 -4.3894 H 0 0 0 0 0 0 0 0 0 0 0 23
0.9471 -2.4652 -2.8767 H 0 0 0 0 0 0 0 0 0 0 0 24
-0.2485 -2.0883 -0.7674 H 0 0 0 0 0 0 0 0 0 0 0 25
-0.4074 2.1482 -1.6243 H 0 0 0 0 0 0 0 0 0 0 0 26
0.7921 1.7600 -3.7353 H 0 0 0 0 0 0 0 0 0 0 0 27
2.4228 1.5530 2.3993 H 0 0 0 0 0 0 0 0 0 0 0 28
2 1 0 0 0 0
6 1 0 0 0 0
8 1 0 0 0 0
3 2 0 0 0 0
4 3 0 0 0 0
7 3 0 0 0 0
5 4 0 0 0 0
11 4 0 0 0 0
12 4 0 0 0 0
6 5 0 0 0 0
9 5 0 0 0 0
10 5 0 0 0 0
13 6 0 0 0 0
14 6 0 0 0 0
20 9 0 0 0 0
21 9 0 0 0 0
22 9 0 0 0 0
17 10 0 0 0 0
18 10 0 0 0 0
16 15 0 0 0 0
19 15 0 0 0 0
23 15 0 0 0 0
17 16 0 0 0 0
24 16 0 0 0 0
25 17 0 0 0 0
19 18 0 0 0 0
26 18 0 0 0 0
27 19 0 0 0 0
8 28 0 0 0 0
M END
$$$$
3,4-dichlorophenol-anion.sdf
COSMOTHERM 3D 0
12 12 0 0 0 0 0 0 0 0 0 V2000
-0.5191 -1.7123 0.0002 C 0 0 0 0 0 0 0 0 0 0 0 1
-1.8648 -1.3605 0.0003 C 0 0 0 0 0 0 0 0 0 0 0 2
-2.3003 0.0124 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 3
-1.2363 0.9879 0.0002 C 0 0 0 0 0 0 0 0 0 0 0 4
0.1019 0.6136 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 5
0.4872 -0.7354 0.0002 C 0 0 0 0 0 0 0 0 0 0 0 6
-3.5428 0.3554 -0.0004 O 0 0 0 0 0 0 0 0 0 0 0 7
1.3394 1.8991 0.0000 Cl 0 0 0 0 0 0 0 0 0 0 0 8
2.1895 -1.2346 -0.0002 Cl 0 0 0 0 0 0 0 0 0 0 0 9
-0.2299 -2.7651 0.0003 H 0 0 0 0 0 0 0 0 0 0 0 10
-2.6264 -2.1442 0.0002 H 0 0 0 0 0 0 0 0 0 0 0 11
-1.5013 2.0464 0.0000 H 0 0 0 0 0 0 0 0 0 0 0 12
```

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2 1 0 0 0 0
6 1 0 0 0 0
10 1 0 0 0 0
3 2 0 0 0 0
11 2 0 0 0 0
4 3 0 0 0 0
7 3 0 0 0 0
5 4 0 0 0 0
6 5 0 0 0 0
8 5 0 0 0 0
9 6 0 0 0 0
4 12 0 0 0 0
M END
$$$$
3,4-dichlorophenol.sdf
COSMOTHERM 3D 0
13 13 0 0 0 0 0 0 0 0 0 V2000
-0.1348 0.6171 0.0000 C 0 0 0 0 0 0 0 0 0 1
-0.5079 -0.7337 0.0000 C 0 0 0 0 0 0 0 0 0 2
0.4871 -1.7173 -0.0001 C 0 0 0 0 0 0 0 0 0 3
1.8344 -1.3656 -0.0001 C 0 0 0 0 0 0 0 0 0 4
2.2006 -0.0111 -0.0001 C 0 0 0 0 0 0 0 0 0 5
1.2131 0.9835 0.0001 C 0 0 0 0 0 0 0 0 0 6
-2.2007 -1.2241 0.0001 Cl 0 0 0 0 0 0 0 0 0 7
0.1995 -2.7686 -0.0001 H 0 0 0 0 0 0 0 0 0 8
2.6059 -2.1358 -0.0001 H 0 0 0 0 0 0 0 0 0 9
3.5361 0.2849 0.0000 O 0 0 0 0 0 0 0 0 0 10
1.4875 2.0392 0.0003 H 0 0 0 0 0 0 0 0 0 11
-1.3466 1.8959 -0.0001 Cl 0 0 0 0 0 0 0 0 0 12
3.6624 1.2530 0.0008 H 0 0 0 0 0 0 0 0 0 13
2 1 0 0 0 0
6 1 0 0 0 0
12 1 0 0 0 0
3 2 0 0 0 0
7 2 0 0 0 0
4 3 0 0 0 0
8 3 0 0 0 0
5 4 0 0 0 0
9 4 0 0 0 0
6 5 0 0 0 0
10 5 0 0 0 0
11 6 0 0 0 0
10 13 0 0 0 0
M END
$$$$
3,5-dichlorophenol-anion.sdf
COSMOTHERM 3D 0
12 12 0 0 0 0 0 0 0 0 0 V2000
0.2651 -1.1813 -0.0001 C 0 0 0 0 0 0 0 0 0 1
-1.1191 -1.2230 0.0002 C 0 0 0 0 0 0 0 0 0 2
-1.8893 -0.0001 0.0000 C 0 0 0 0 0 0 0 0 0 3
-1.1192 1.2229 0.0003 C 0 0 0 0 0 0 0 0 0 4
0.2650 1.1814 -0.0001 C 0 0 0 0 0 0 0 0 0 5
1.0176 0.0000 0.0000 C 0 0 0 0 0 0 0 0 0 6
-3.1750 -0.0001 -0.0002 O 0 0 0 0 0 0 0 0 0 7
1.1705 2.7296 0.0000 Cl 0 0 0 0 0 0 0 0 0 8
1.1705 -2.7296 0.0000 Cl 0 0 0 0 0 0 0 0 0 9
-1.6517 -2.1748 -0.0001 H 0 0 0 0 0 0 0 0 0 10
-1.6518 2.1747 0.0002 H 0 0 0 0 0 0 0 0 0 11
2.1046 0.0000 -0.0004 H 0 0 0 0 0 0 0 0 0 12
2 1 0 0 0 0
6 1 0 0 0 0
9 1 0 0 0 0
3 2 0 0 0 0
10 2 0 0 0 0
4 3 0 0 0 0
7 3 0 0 0 0
5 4 0 0 0 0
11 4 0 0 0 0
6 5 0 0 0 0
8 5 0 0 0 0
6 12 0 0 0 0
M END
$$$$
3,5-dichlorophenol.sdf
COSMOTHERM 3D 0
13 13 0 0 0 0 0 0 0 0 0 V2000
-3.1543 0.0674 -0.0001 O 0 0 0 0 0 0 0 0 0 1
-1.7903 0.0017 0.0000 C 0 0 0 0 0 0 0 0 0 2
-1.0947 1.2213 0.0000 C 0 0 0 0 0 0 0 0 0 3
0.2961 1.1876 -0.0001 C 0 0 0 0 0 0 0 0 0 4
1.1828 2.7203 0.0000 Cl 0 0 0 0 0 0 0 0 0 5
1.0278 -0.0028 -0.0001 C 0 0 0 0 0 0 0 0 0 6
0.2943 -1.1902 0.0000 C 0 0 0 0 0 0 0 0 0 7
1.1757 -2.7259 0.0000 Cl 0 0 0 0 0 0 0 0 0 8
-1.0989 -1.2201 0.0001 C 0 0 0 0 0 0 0 0 0 9
-3.5298 -0.8341 0.0006 H 0 0 0 0 0 0 0 0 0 10
-1.6429 2.1623 0.0000 H 0 0 0 0 0 0 0 0 0 11
2.1156 -0.0040 -0.0001 H 0 0 0 0 0 0 0 0 0 12
-1.6403 -2.1666 0.0004 H 0 0 0 0 0 0 0 0 0 13
2 1 0 0 0 0
10 1 0 0 0 0
3 2 0 0 0 0
9 2 0 0 0 0
4 3 0 0 0 0
11 3 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
7 6 0 0 0 0
12 6 0 0 0 0
8 7 0 0 0 0
9 7 0 0 0 0
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9 13 0 0 0 0
M END
$$$$
3-chlorophenol-anion.sdf
COSMOtherm 3D 0

12 12 0 0 0 0 0 0 0 0 0 V2000
-0.9068 0.0000 -1.8240 C 0 0 0 0 0 0 0 0 0 0 0 1
-1.9260 0.0000 -0.8751 C 0 0 0 0 0 0 0 0 0 0 0 2
-1.6532 -0.0001 0.5399 C 0 0 0 0 0 0 0 0 0 0 0 3
-0.2522 -0.0001 0.8965 C 0 0 0 0 0 0 0 0 0 0 0 4
0.7257 0.0000 -0.0875 C 0 0 0 0 0 0 0 0 0 0 0 5
0.4525 0.0000 -1.4586 C 0 0 0 0 0 0 0 0 0 0 0 6
-2.5837 0.0001 1.4353 O 0 0 0 0 0 0 0 0 0 0 0 7
2.4537 0.0000 0.4269 Cl 0 0 0 0 0 0 0 0 0 0 0 8
-1.1626 -0.0001 -2.8872 H 0 0 0 0 0 0 0 0 0 0 0 9
-2.9726 0.0002 -1.1917 H 0 0 0 0 0 0 0 0 0 0 0 10
0.0165 -0.0001 1.9543 H 0 0 0 0 0 0 0 0 0 0 0 11
1.2488 0.0002 -2.2012 H 0 0 0 0 0 0 0 0 0 0 0 12
2 1 0 0 0 0
6 1 0 0 0 0
9 1 0 0 0 0
3 2 0 0 0 0
10 2 0 0 0 0
4 3 0 0 0 0
7 3 0 0 0 0
5 4 0 0 0 0
11 4 0 0 0 0
6 5 0 0 0 0
8 5 0 0 0 0
6 12 0 0 0 0
M END
$$$$
3-chlorophenol.sdf
COSMOtherm 3D 0

13 13 0 0 0 0 0 0 0 0 0 V2000
-0.2407 0.8828 -0.0004 C 0 0 0 0 0 0 0 0 0 0 0 1
0.7584 -0.0877 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 2
0.4796 -1.4560 -0.0002 C 0 0 0 0 0 0 0 0 0 0 0 3
-0.8642 -1.8488 0.0002 C 0 0 0 0 0 0 0 0 0 0 0 4
-1.8954 -0.9061 -0.0002 C 0 0 0 0 0 0 0 0 0 0 0 5
-1.5800 0.4614 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 6
1.2825 -2.1918 0.0001 H 0 0 0 0 0 0 0 0 0 0 0 7
-2.5372 1.4423 0.0001 O 0 0 0 0 0 0 0 0 0 0 0 8
-0.0029 1.9460 -0.0003 H 0 0 0 0 0 0 0 0 0 0 0 9
2.4534 0.4453 0.0001 Cl 0 0 0 0 0 0 0 0 0 0 0 10
-1.1093 -2.9119 0.0002 H 0 0 0 0 0 0 0 0 0 0 0 11
-2.9395 -1.2257 0.0002 H 0 0 0 0 0 0 0 0 0 0 0 12
-3.4228 1.0313 0.0011 H 0 0 0 0 0 0 0 0 0 0 0 13
2 1 0 0 0 0
6 1 0 0 0 0
9 1 0 0 0 0
3 2 0 0 0 0
10 2 0 0 0 0
4 3 0 0 0 0
7 3 0 0 0 0
5 4 0 0 0 0
11 4 0 0 0 0
6 5 0 0 0 0
12 5 0 0 0 0
8 6 0 0 0 0
8 13 0 0 0 0
M END
$$$$
3-chloropropanoicacid0-anion.sdf
COSMOtherm 3D 0

10 9 0 0 0 0 0 0 0 0 0 V2000
-0.7343 -0.5148 -0.2079 C 0 0 0 0 0 0 0 0 0 0 0 1
0.2837 0.5534 0.1273 C 0 0 0 0 0 0 0 0 0 0 0 2
1.7454 0.0307 0.0239 C 0 0 0 0 0 0 0 0 0 0 0 3
2.6470 0.9137 -0.0889 O 0 0 0 0 0 0 0 0 0 0 0 4
1.9260 -1.2239 0.0852 O 0 0 0 0 0 0 0 0 0 0 0 5
0.1364 0.9052 1.1615 H 0 0 0 0 0 0 0 0 0 0 0 6
-2.4728 0.1131 0.0260 Cl 0 0 0 0 0 0 0 0 0 0 0 7
-0.6935 -0.8257 -1.2564 H 0 0 0 0 0 0 0 0 0 0 0 8
-0.6542 -1.3883 0.4436 H 0 0 0 0 0 0 0 0 0 0 0 9
0.1711 1.4271 -0.5297 H 0 0 0 0 0 0 0 0 0 0 0 10
2 1 0 0 0 0
7 1 0 0 0 0
8 1 0 0 0 0
9 1 0 0 0 0
3 2 0 0 0 0
6 2 0 0 0 0
4 3 0 0 0 0
5 3 0 0 0 0
2 10 0 0 0 0
M END
$$$$
3-chloropropanoicacid0.sdf
COSMOtherm 3D 0

11 10 0 0 0 0 0 0 0 0 0 V2000
-0.7923 -0.5857 -0.0217 C 0 0 0 0 0 0 0 0 0 0 0 1
0.2456 0.5226 0.0172 C 0 0 0 0 0 0 0 0 0 0 0 2
1.6531 -0.0326 0.0040 C 0 0 0 0 0 0 0 0 0 0 0 3
2.5754 0.9591 -0.0115 O 0 0 0 0 0 0 0 0 0 0 0 4
1.9487 -1.2190 0.0089 O 0 0 0 0 0 0 0 0 0 0 0 5
0.1318 1.1389 0.9219 H 0 0 0 0 0 0 0 0 0 0 0 6
-2.4809 0.1364 0.0019 Cl 0 0 0 0 0 0 0 0 0 0 0 7
-0.7342 -1.1790 -0.9385 H 0 0 0 0 0 0 0 0 0 0 0 8
-0.7353 -1.2411 0.8518 H 0 0 0 0 0 0 0 0 0 0 0 9
0.1343 1.2009 -0.8417 H 0 0 0 0 0 0 0 0 0 0 0 10
3.4673 0.5474 -0.0132 H 0 0 0 0 0 0 0 0 0 0 0 11
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2 1 0 0 0 0
7 1 0 0 0 0
8 1 0 0 0 0
9 1 0 0 0 0
3 2 0 0 0 0
6 2 0 0 0 0
10 2 0 0 0 0
4 3 0 0 0 0
5 3 0 0 0 0
4 11 0 0 0 0
M END
$$$$
3-chloropropanoicacid1-anion.sdf
COSMOTHERM 3D 0
10 9 0 0 0 0 0 0 0 0 0 V2000
-0.7349 -0.5338 -0.1532 C 0 0 0 0 0 0 0 0 0 0 1
0.2838 0.5566 0.0966 C 0 0 0 0 0 0 0 0 0 0 2
1.7457 0.0321 0.0174 C 0 0 0 0 0 0 0 0 0 0 3
1.9232 -1.2237 0.0646 O 0 0 0 0 0 0 0 0 0 0 4
2.6501 0.9153 -0.0684 O 0 0 0 0 0 0 0 0 0 0 5
0.1428 0.9866 1.1014 H 0 0 0 0 0 0 0 0 0 0 6
-0.6893 -0.9325 -1.1710 H 0 0 0 0 0 0 0 0 0 0 7
-0.6641 -1.3500 0.5701 H 0 0 0 0 0 0 0 0 0 0 8
-2.4727 0.1182 0.0185 Cl 0 0 0 0 0 0 0 0 0 0 9
0.1653 1.3793 -0.6230 H 0 0 0 0 0 0 0 0 0 0 10
2 1 0 0 0 0
7 1 0 0 0 0
8 1 0 0 0 0
9 1 0 0 0 0
3 2 0 0 0 0
6 2 0 0 0 0
4 3 0 0 0 0
5 3 0 0 0 0
2 10 0 0 0 0
M END
$$$$
3-chloropropanoicacid1.sdf
COSMOTHERM 3D 0
11 10 0 0 0 0 0 0 0 0 0 V2000
-0.9512 1.0698 0.0607 C 0 0 0 0 0 0 0 0 0 0 1
0.3671 0.8780 0.7875 C 0 0 0 0 0 0 0 0 0 0 2
1.3722 -0.0169 0.0920 C 0 0 0 0 0 0 0 0 0 0 3
1.4481 0.2246 -1.2376 O 0 0 0 0 0 0 0 0 0 0 4
2.0693 -0.8466 0.6579 O 0 0 0 0 0 0 0 0 0 0 5
0.2126 0.4914 1.8019 H 0 0 0 0 0 0 0 0 0 0 6
-1.6099 1.7445 0.6141 H 0 0 0 0 0 0 0 0 0 0 7
-0.8209 1.4242 -0.9652 H 0 0 0 0 0 0 0 0 0 0 8
-1.8755 -0.5202 -0.0773 Cl 0 0 0 0 0 0 0 0 0 0 9
0.8332 1.8748 0.8841 H 0 0 0 0 0 0 0 0 0 0 10
2.1272 -0.3734 -1.6196 H 0 0 0 0 0 0 0 0 0 0 11
2 1 0 0 0 0
7 1 0 0 0 0
8 1 0 0 0 0
9 1 0 0 0 0
3 2 0 0 0 0
6 2 0 0 0 0
10 2 0 0 0 0
4 3 0 0 0 0
5 3 0 0 0 0
4 11 0 0 0 0
M END
$$$$
3-hydroxy-2-naphtoicacid-anion0.sdf
COSMOTHERM 3D 0
21 23 0 0 0 0 0 0 0 0 0 V2000
3.8273 0.2954 -0.0003 C 0 0 0 0 0 0 0 0 0 0 1
3.5764 -1.1026 -0.0005 C 0 0 0 0 0 0 0 0 0 0 2
2.2758 -1.5704 -0.0002 C 0 0 0 0 0 0 0 0 0 0 3
1.1745 -0.6679 0.0001 C 0 0 0 0 0 0 0 0 0 0 4
1.4276 0.7531 0.0005 C 0 0 0 0 0 0 0 0 0 0 5
2.7822 1.1999 0.0003 C 0 0 0 0 0 0 0 0 0 0 6
-0.1714 -1.1142 0.0001 C 0 0 0 0 0 0 0 0 0 0 7
-1.2401 -0.2332 0.0001 C 0 0 0 0 0 0 0 0 0 0 8
-0.9780 1.1859 0.0002 C 0 0 0 0 0 0 0 0 0 0 9
0.3323 1.6516 0.0005 C 0 0 0 0 0 0 0 0 0 0 10
-2.6662 -0.7481 0.0000 C 0 0 0 0 0 0 0 0 0 0 11
-2.8864 -1.9828 0.0006 O 0 0 0 0 0 0 0 0 0 0 12
-3.5939 0.1607 -0.0008 O 0 0 0 0 0 0 0 0 0 0 13
-2.0135 2.0576 -0.0003 O 0 0 0 0 0 0 0 0 0 0 14
-2.8543 1.4117 -0.0006 H 0 0 0 0 0 0 0 0 0 0 15
4.8577 0.6565 -0.0005 H 0 0 0 0 0 0 0 0 0 0 16
4.4135 -1.8030 -0.0009 H 0 0 0 0 0 0 0 0 0 0 17
2.0737 -2.6445 -0.0004 H 0 0 0 0 0 0 0 0 0 0 18
2.9827 2.2740 0.0005 H 0 0 0 0 0 0 0 0 0 0 19
-0.3838 -2.1860 0.0000 H 0 0 0 0 0 0 0 0 0 0 20
0.5136 2.7290 0.0005 H 0 0 0 0 0 0 0 0 0 0 21
2 1 0 0 0 0
6 1 0 0 0 0
16 1 0 0 0 0
3 2 0 0 0 0
17 2 0 0 0 0
4 3 0 0 0 0
18 3 0 0 0 0
5 4 0 0 0 0
7 4 0 0 0 0
6 5 0 0 0 0
10 5 0 0 0 0
19 6 0 0 0 0
8 7 0 0 0 0
20 7 0 0 0 0
9 8 0 0 0 0
11 8 0 0 0 0
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10 9 0 0 0 0
14 9 0 0 0 0
12 11 0 0 0 0
13 11 0 0 0 0
15 13 0 0 0 0
15 14 0 0 0 0
10 21 0 0 0 0
M END
$$$$
3-hydroxy-2-naphtoicacid-anion1.sdf
COSMOtherm 3D 0

21 22 0 0 0 0 0 0 0 0 0 V2000
3.8241 0.2396 0.0002 C 0 0 0 0 0 0 0 0 0 0 1
3.5381 -1.1515 -0.0037 C 0 0 0 0 0 0 0 0 0 0 2
2.2266 -1.5890 -0.0048 C 0 0 0 0 0 0 0 0 0 0 3
1.1491 -0.6584 -0.0023 C 0 0 0 0 0 0 0 0 0 0 4
1.4396 0.7504 0.0011 C 0 0 0 0 0 0 0 0 0 0 5
2.8014 1.1699 0.0026 C 0 0 0 0 0 0 0 0 0 0 6
-0.2090 -1.0632 -0.0021 C 0 0 0 0 0 0 0 0 0 0 7
-1.2771 -0.1760 -0.0004 C 0 0 0 0 0 0 0 0 0 0 8
-0.9661 1.2277 0.0021 C 0 0 0 0 0 0 0 0 0 0 9
0.3551 1.6607 0.0034 C 0 0 0 0 0 0 0 0 0 0 10
-2.7009 -0.7650 -0.0006 C 0 0 0 0 0 0 0 0 0 0 11
-2.7797 -2.0344 0.0179 O 0 0 0 0 0 0 0 0 0 0 12
-3.6838 0.0323 -0.0194 O 0 0 0 0 0 0 0 0 0 0 13
-1.9847 2.1470 0.0045 O 0 0 0 0 0 0 0 0 0 0 14
-1.5800 3.0371 0.0086 H 0 0 0 0 0 0 0 0 0 0 15
4.8633 0.5744 0.0014 H 0 0 0 0 0 0 0 0 0 0 16
4.3581 -1.8718 -0.0057 H 0 0 0 0 0 0 0 0 0 0 17
1.9988 -2.6578 -0.0077 H 0 0 0 0 0 0 0 0 0 0 18
3.0268 2.2390 0.0057 H 0 0 0 0 0 0 0 0 0 0 19
-0.4519 -2.1277 -0.0029 H 0 0 0 0 0 0 0 0 0 0 20
0.5635 2.7353 0.0064 H 0 0 0 0 0 0 0 0 0 0 21

2 1 0 0 0 0
6 1 0 0 0 0
16 1 0 0 0 0
3 2 0 0 0 0
17 2 0 0 0 0
4 3 0 0 0 0
18 3 0 0 0 0
5 4 0 0 0 0
7 4 0 0 0 0
6 5 0 0 0 0
10 5 0 0 0 0
19 6 0 0 0 0
8 7 0 0 0 0
20 7 0 0 0 0
9 8 0 0 0 0
11 8 0 0 0 0
10 9 0 0 0 0
14 9 0 0 0 0
12 11 0 0 0 0
13 11 0 0 0 0
15 14 0 0 0 0
10 21 0 0 0 0
M END
$$$$
3-hydroxy-2-naphtoicacid0.sdf
COSMOtherm 3D 0

22 23 0 0 0 0 0 0 0 0 0 V2000
3.8316 0.2671 -0.0020 C 0 0 0 0 0 0 0 0 0 0 1
3.5657 -1.1293 -0.0012 C 0 0 0 0 0 0 0 0 0 0 2
2.2634 -1.5845 0.0005 C 0 0 0 0 0 0 0 0 0 0 3
1.1735 -0.6654 0.0017 C 0 0 0 0 0 0 0 0 0 0 4
1.4420 0.7529 0.0007 C 0 0 0 0 0 0 0 0 0 0 5
2.8000 1.1855 -0.0005 C 0 0 0 0 0 0 0 0 0 0 6
-0.1693 -1.0991 0.0018 C 0 0 0 0 0 0 0 0 0 0 7
-1.2292 -0.1949 0.0012 C 0 0 0 0 0 0 0 0 0 0 8
-0.9536 1.2204 0.0010 C 0 0 0 0 0 0 0 0 0 0 9
0.3597 1.6651 0.0009 C 0 0 0 0 0 0 0 0 0 0 10
-2.6276 -0.6489 -0.0004 C 0 0 0 0 0 0 0 0 0 0 11
-2.7910 -1.9852 -0.0001 O 0 0 0 0 0 0 0 0 0 0 12
-3.6004 0.1250 -0.0025 O 0 0 0 0 0 0 0 0 0 0 13
-1.9577 2.1354 0.0002 O 0 0 0 0 0 0 0 0 0 0 14
-3.7543 -2.1743 -0.0033 H 0 0 0 0 0 0 0 0 0 0 15
-2.8145 1.6135 -0.0007 H 0 0 0 0 0 0 0 0 0 0 16
4.8663 0.6148 -0.0034 H 0 0 0 0 0 0 0 0 0 0 17
4.3960 -1.8371 -0.0024 H 0 0 0 0 0 0 0 0 0 0 18
2.0477 -2.6554 0.0011 H 0 0 0 0 0 0 0 0 0 0 19
3.0131 2.2565 -0.0013 H 0 0 0 0 0 0 0 0 0 0 20
-0.3804 -2.1691 0.0017 H 0 0 0 0 0 0 0 0 0 0 21
0.5527 2.7395 0.0003 H 0 0 0 0 0 0 0 0 0 0 22

2 1 0 0 0 0
6 1 0 0 0 0
17 1 0 0 0 0
3 2 0 0 0 0
18 2 0 0 0 0
4 3 0 0 0 0
19 3 0 0 0 0
5 4 0 0 0 0
7 4 0 0 0 0
6 5 0 0 0 0
10 5 0 0 0 0
20 6 0 0 0 0
8 7 0 0 0 0
21 7 0 0 0 0
9 8 0 0 0 0
11 8 0 0 0 0
10 9 0 0 0 0
14 9 0 0 0 0
12 11 0 0 0 0
13 11 0 0 0 0
15 12 0 0 0 0
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16 14 0 0 0 0
10 22 0 0 0 0
M END
$$$$
3-hydroxy-2-naphtoicacid1.sdf
COSMOtherm 3D 0
22 23 0 0 0 0 0 0 0 0 V2000
3.8356 0.2787 -0.0012 C 0 0 0 0 0 0 0 0 0 0 0 1
3.5773 -1.1192 -0.0062 C 0 0 0 0 0 0 0 0 0 0 0 2
2.2776 -1.5827 -0.0070 C 0 0 0 0 0 0 0 0 0 0 0 3
1.1830 -0.6693 -0.0025 C 0 0 0 0 0 0 0 0 0 0 0 4
1.4442 0.7488 0.0024 C 0 0 0 0 0 0 0 0 0 0 0 5
2.7989 1.1912 0.0032 C 0 0 0 0 0 0 0 0 0 0 0 6
-0.1585 -1.1036 -0.0030 C 0 0 0 0 0 0 0 0 0 0 0 7
-1.2304 -0.2128 -0.0002 C 0 0 0 0 0 0 0 0 0 0 0 8
-0.9596 1.2035 0.0045 C 0 0 0 0 0 0 0 0 0 0 0 9
0.3542 1.6496 0.0069 C 0 0 0 0 0 0 0 0 0 0 0 10
-2.5892 -0.8050 0.0010 C 0 0 0 0 0 0 0 0 0 0 0 11
-3.5823 0.1383 -0.0346 O 0 0 0 0 0 0 0 0 0 0 0 12
-2.8459 -2.0007 0.0283 O 0 0 0 0 0 0 0 0 0 0 0 13
-1.9358 2.1548 0.0097 O 0 0 0 0 0 0 0 0 0 0 0 14
-4.4569 -0.3067 -0.0216 H 0 0 0 0 0 0 0 0 0 0 0 15
-2.8155 1.7071 0.0014 H 0 0 0 0 0 0 0 0 0 0 0 16
4.8685 0.6321 -0.0008 H 0 0 0 0 0 0 0 0 0 0 0 17
4.4119 -1.8219 -0.0096 H 0 0 0 0 0 0 0 0 0 0 0 18
2.0687 -2.6549 -0.0109 H 0 0 0 0 0 0 0 0 0 0 0 19
3.0052 2.2636 0.0070 H 0 0 0 0 0 0 0 0 0 0 0 20
-0.3762 -2.1732 -0.0057 H 0 0 0 0 0 0 0 0 0 0 0 21
0.5392 2.7255 0.0115 H 0 0 0 0 0 0 0 0 0 0 0 22
2 1 0 0 0 0
6 1 0 0 0 0
17 1 0 0 0 0
3 2 0 0 0 0
18 2 0 0 0 0
4 3 0 0 0 0
19 3 0 0 0 0
5 4 0 0 0 0
7 4 0 0 0 0
6 5 0 0 0 0
10 5 0 0 0 0
20 6 0 0 0 0
8 7 0 0 0 0
21 7 0 0 0 0
9 8 0 0 0 0
11 8 0 0 0 0
10 9 0 0 0 0
14 9 0 0 0 0
12 11 0 0 0 0
13 11 0 0 0 0
15 12 0 0 0 0
16 14 0 0 0 0
10 22 0 0 0 0
M END
$$$$
3-hydroxy-2-naphtoicacid2.sdf
COSMOtherm 3D 0
22 23 0 0 0 0 0 0 0 0 V2000
3.8371 0.2528 -0.0041 C 0 0 0 0 0 0 0 0 0 0 0 1
3.5617 -1.1412 -0.0070 C 0 0 0 0 0 0 0 0 0 0 0 2
2.2558 -1.5887 -0.0058 C 0 0 0 0 0 0 0 0 0 0 0 3
1.1735 -0.6620 -0.0016 C 0 0 0 0 0 0 0 0 0 0 0 4
1.4526 0.7504 0.0015 C 0 0 0 0 0 0 0 0 0 0 0 5
2.8109 1.1781 0.0003 C 0 0 0 0 0 0 0 0 0 0 0 6
-0.1748 -1.0788 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 7
-1.2421 -0.1836 0.0017 C 0 0 0 0 0 0 0 0 0 0 0 8
-0.9507 1.2252 0.0069 C 0 0 0 0 0 0 0 0 0 0 0 9
0.3675 1.6589 0.0062 C 0 0 0 0 0 0 0 0 0 0 0 10
-2.6008 -0.7955 0.0002 C 0 0 0 0 0 0 0 0 0 0 0 11
-3.6285 0.0846 -0.0445 O 0 0 0 0 0 0 0 0 0 0 0 12
-2.7966 -2.0095 0.0329 O 0 0 0 0 0 0 0 0 0 0 0 13
-1.9818 2.1197 0.0152 O 0 0 0 0 0 0 0 0 0 0 0 14
-4.4538 -0.4486 -0.0412 H 0 0 0 0 0 0 0 0 0 0 0 15
-1.6071 3.0224 0.0192 H 0 0 0 0 0 0 0 0 0 0 0 16
4.8741 0.5936 -0.0052 H 0 0 0 0 0 0 0 0 0 0 0 17
4.3874 -1.8544 -0.0102 H 0 0 0 0 0 0 0 0 0 0 0 18
2.0336 -2.6583 -0.0082 H 0 0 0 0 0 0 0 0 0 0 0 19
3.0302 2.2479 0.0027 H 0 0 0 0 0 0 0 0 0 0 0 20
-0.4035 -2.1457 -0.0029 H 0 0 0 0 0 0 0 0 0 0 0 21
0.5718 2.7333 0.0106 H 0 0 0 0 0 0 0 0 0 0 0 22
2 1 0 0 0 0
6 1 0 0 0 0
17 1 0 0 0 0
3 2 0 0 0 0
18 2 0 0 0 0
4 3 0 0 0 0
19 3 0 0 0 0
5 4 0 0 0 0
7 4 0 0 0 0
6 5 0 0 0 0
10 5 0 0 0 0
20 6 0 0 0 0
8 7 0 0 0 0
21 7 0 0 0 0
9 8 0 0 0 0
11 8 0 0 0 0
10 9 0 0 0 0
14 9 0 0 0 0
12 11 0 0 0 0
13 11 0 0 0 0
15 12 0 0 0 0
16 14 0 0 0 0
10 22 0 0 0 0
M END
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$$$$
3-hydroxybenzoicacid-anion.sdf
COSMOTHERM      3D      0

15 15 0 0 0 0 0 0 0 0 0 V2000
  1.1373 -1.8685 0.0015 C 0 0 0 0 0 0 0 0 0 0 1
 -0.2128 -1.4995 0.0010 C 0 0 0 0 0 0 0 0 0 0 2
 -0.5718 -0.1417 0.0003 C 0 0 0 0 0 0 0 0 0 0 3
  0.4364 0.8343 -0.0004 C 0 0 0 0 0 0 0 0 0 0 4
  1.7858 0.4590 -0.0003 C 0 0 0 0 0 0 0 0 0 0 5
  2.1433 -0.8978 0.0003 C 0 0 0 0 0 0 0 0 0 0 6
 -2.0464 0.2811 -0.0001 C 0 0 0 0 0 0 0 0 0 0 7
  2.8078 1.3840 -0.0015 O 0 0 0 0 0 0 0 0 0 0 8
 -2.2906 1.5276 0.0029 O 0 0 0 0 0 0 0 0 0 0 9
 -2.9127 -0.6472 -0.0034 O 0 0 0 0 0 0 0 0 0 0 10
  1.4154 -2.9246 0.0021 H 0 0 0 0 0 0 0 0 0 0 11
 -1.0019 -2.2520 0.0016 H 0 0 0 0 0 0 0 0 0 0 12
  0.1502 1.8890 -0.0006 H 0 0 0 0 0 0 0 0 0 0 13
  3.1984 -1.1768 0.0004 H 0 0 0 0 0 0 0 0 0 0 14
  2.4256 2.2821 -0.0002 H 0 0 0 0 0 0 0 0 0 0 15

  2 1 0 0 0 0
  6 1 0 0 0 0
 11 1 0 0 0 0
  3 2 0 0 0 0
 12 2 0 0 0 0
  4 3 0 0 0 0
  7 3 0 0 0 0
  5 4 0 0 0 0
 13 4 0 0 0 0
  6 5 0 0 0 0
  8 5 0 0 0 0
 14 6 0 0 0 0
  9 7 0 0 0 0
 10 7 0 0 0 0
  8 15 0 0 0 0
M  END
$$$$
3-hydroxybenzoicacid.sdf
COSMOTHERM      3D      0

16 16 0 0 0 0 0 0 0 0 0 V2000
  1.1774 -1.8678 0.0016 C 0 0 0 0 0 0 0 0 0 0 1
 -0.1768 -1.5251 0.0010 C 0 0 0 0 0 0 0 0 0 0 2
 -0.5459 -0.1696 0.0001 C 0 0 0 0 0 0 0 0 0 0 3
  0.4386 0.8340 -0.0004 C 0 0 0 0 0 0 0 0 0 0 4
  1.7917 0.4753 -0.0004 C 0 0 0 0 0 0 0 0 0 0 5
  2.1635 -0.8788 0.0005 C 0 0 0 0 0 0 0 0 0 0 6
 -1.9959 0.1697 -0.0003 C 0 0 0 0 0 0 0 0 0 0 7
  2.7992 1.4055 -0.0016 O 0 0 0 0 0 0 0 0 0 0 8
 -2.2324 1.5068 0.0032 O 0 0 0 0 0 0 0 0 0 0 9
 -2.9043 -0.6553 -0.0035 O 0 0 0 0 0 0 0 0 0 0 10
  1.4729 -2.9179 0.0025 H 0 0 0 0 0 0 0 0 0 0 11
 -0.9497 -2.2932 0.0016 H 0 0 0 0 0 0 0 0 0 0 12
  0.1535 1.8869 -0.0010 H 0 0 0 0 0 0 0 0 0 0 13
  3.2225 -1.1414 0.0009 H 0 0 0 0 0 0 0 0 0 0 14
  2.4160 2.3035 -0.0007 H 0 0 0 0 0 0 0 0 0 0 15
 -3.2051 1.6365 0.0030 H 0 0 0 0 0 0 0 0 0 0 16

  2 1 0 0 0 0
  6 1 0 0 0 0
 11 1 0 0 0 0
  3 2 0 0 0 0
 12 2 0 0 0 0
  4 3 0 0 0 0
  7 3 0 0 0 0
  5 4 0 0 0 0
 13 4 0 0 0 0
  6 5 0 0 0 0
  8 5 0 0 0 0
 14 6 0 0 0 0
  9 7 0 0 0 0
 10 7 0 0 0 0
 15 8 0 0 0 0
  9 16 0 0 0 0
M  END
$$$$
4-(1,1-dimethylethyl)-benzoicacid-anion.sdf
COSMOTHERM      3D      0

26 26 0 0 0 0 0 0 0 0 0 V2000
 -0.4275 0.0017 -1.2251 C 0 0 0 0 0 0 0 0 0 0 1
  0.9727 0.0015 -1.2132 C 0 0 0 0 0 0 0 0 0 0 2
  1.6878 0.0003 -0.0077 C 0 0 0 0 0 0 0 0 0 0 3
  0.9530 -0.0007 1.1901 C 0 0 0 0 0 0 0 0 0 0 4
 -0.4426 -0.0010 1.1774 C 0 0 0 0 0 0 0 0 0 0 5
 -1.1698 0.0004 -0.0311 C 0 0 0 0 0 0 0 0 0 0 6
  3.2171 -0.0001 0.0047 C 0 0 0 0 0 0 0 0 0 0 7
 -2.7081 -0.0001 -0.0038 C 0 0 0 0 0 0 0 0 0 0 8
 -3.2062 -1.2638 0.7384 C 0 0 0 0 0 0 0 0 0 0 9
 -3.3201 0.0039 -1.4169 C 0 0 0 0 0 0 0 0 0 0 10
 -3.2070 1.2588 0.7459 C 0 0 0 0 0 0 0 0 0 0 11
  3.8074 -0.0027 -1.1209 O 0 0 0 0 0 0 0 0 0 0 12
  3.7879 0.0021 1.1407 O 0 0 0 0 0 0 0 0 0 0 13
 -0.9408 0.0029 -2.1873 H 0 0 0 0 0 0 0 0 0 0 14
  1.5307 0.0022 -2.1516 H 0 0 0 0 0 0 0 0 0 0 15
  1.4972 -0.0015 2.1366 H 0 0 0 0 0 0 0 0 0 0 16
 -0.9754 -0.0020 2.1312 H 0 0 0 0 0 0 0 0 0 0 17
 -4.3066 -1.2735 0.7706 H 0 0 0 0 0 0 0 0 0 0 18
 -2.8379 -1.2981 1.7736 H 0 0 0 0 0 0 0 0 0 0 19
 -2.8704 -2.1783 0.2263 H 0 0 0 0 0 0 0 0 0 0 20
 -4.4172 0.0033 -1.3390 H 0 0 0 0 0 0 0 0 0 0 21
 -3.0268 0.8976 -1.9880 H 0 0 0 0 0 0 0 0 0 0 22
 -3.0262 -0.8861 -1.9935 H 0 0 0 0 0 0 0 0 0 0 23
 -4.3076 1.2703 0.7734 H 0 0 0 0 0 0 0 0 0 0 24
 -2.8674 2.1766 0.2423 H 0 0 0 0 0 0 0 0 0 0 25
 -2.8433 1.2846 1.7829 H 0 0 0 0 0 0 0 0 0 0 26
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2 1 0 0 0 0
6 1 0 0 0 0
14 1 0 0 0 0
3 2 0 0 0 0
15 2 0 0 0 0
4 3 0 0 0 0
7 3 0 0 0 0
5 4 0 0 0 0
16 4 0 0 0 0
6 5 0 0 0 0
17 5 0 0 0 0
8 6 0 0 0 0
12 7 0 0 0 0
13 7 0 0 0 0
9 8 0 0 0 0
10 8 0 0 0 0
11 8 0 0 0 0
18 9 0 0 0 0
19 9 0 0 0 0
20 9 0 0 0 0
21 10 0 0 0 0
22 10 0 0 0 0
23 10 0 0 0 0
24 11 0 0 0 0
25 11 0 0 0 0
11 26 0 0 0 0
M END
$$$$
4-(1,1-dimethylethyl)-benzoicacid.sdf
COSMOtherm 3D 0

27 27 0 0 0 0 0 0 0 0 0 V2000
-0.4569 0.0007 -1.2386 C 0 0 0 0 0 0 0 0 0 1
0.9388 0.0003 -1.2411 C 0 0 0 0 0 0 0 0 0 2
1.6538 -0.0007 -0.0334 C 0 0 0 0 0 0 0 0 0 3
0.9380 -0.0018 1.1787 C 0 0 0 0 0 0 0 0 0 4
-0.4542 -0.0020 1.1693 C 0 0 0 0 0 0 0 0 0 5
-1.1872 -0.0003 -0.0361 C 0 0 0 0 0 0 0 0 0 6
3.1369 -0.0001 -0.0787 C 0 0 0 0 0 0 0 0 0 7
-2.7230 0.0003 0.0039 C 0 0 0 0 0 0 0 0 0 8
-3.2116 -1.2637 0.7529 C 0 0 0 0 0 0 0 0 0 9
-3.3465 0.0036 -1.4041 C 0 0 0 0 0 0 0 0 0 10
-3.2104 1.2615 0.7583 C 0 0 0 0 0 0 0 0 0 11
3.8072 -0.0016 -1.1080 O 0 0 0 0 0 0 0 0 0 12
3.7106 0.0028 1.1542 O 0 0 0 0 0 0 0 0 0 13
-0.9775 0.0019 -2.1957 H 0 0 0 0 0 0 0 0 0 14
1.4854 0.0009 -2.1853 H 0 0 0 0 0 0 0 0 0 15
1.4734 -0.0027 2.1282 H 0 0 0 0 0 0 0 0 0 16
-0.9800 -0.0030 2.1256 H 0 0 0 0 0 0 0 0 0 17
-4.3114 -1.2718 0.7924 H 0 0 0 0 0 0 0 0 0 18
-2.8365 -1.2958 1.7854 H 0 0 0 0 0 0 0 0 0 19
-2.8801 -2.1786 0.2393 H 0 0 0 0 0 0 0 0 0 20
-4.4425 0.0034 -1.3151 H 0 0 0 0 0 0 0 0 0 21
-3.0591 0.8973 -1.9780 H 0 0 0 0 0 0 0 0 0 22
-3.0590 -0.8872 -1.9824 H 0 0 0 0 0 0 0 0 0 23
-4.3103 1.2736 0.7927 H 0 0 0 0 0 0 0 0 0 24
-2.8729 2.1783 0.2520 H 0 0 0 0 0 0 0 0 0 25
-2.8401 1.2860 1.7928 H 0 0 0 0 0 0 0 0 0 26
4.6835 0.0038 1.0262 H 0 0 0 0 0 0 0 0 0 27

2 1 0 0 0 0
6 1 0 0 0 0
14 1 0 0 0 0
3 2 0 0 0 0
15 2 0 0 0 0
4 3 0 0 0 0
7 3 0 0 0 0
5 4 0 0 0 0
16 4 0 0 0 0
6 5 0 0 0 0
17 5 0 0 0 0
8 6 0 0 0 0
12 7 0 0 0 0
13 7 0 0 0 0
9 8 0 0 0 0
10 8 0 0 0 0
11 8 0 0 0 0
18 9 0 0 0 0
19 9 0 0 0 0
20 9 0 0 0 0
21 10 0 0 0 0
22 10 0 0 0 0
23 10 0 0 0 0
24 11 0 0 0 0
25 11 0 0 0 0
26 11 0 0 0 0
13 27 0 0 0 0
M END
$$$$
4-(1-methylethyl)-benzoicacid-anion.sdf
COSMOtherm 3D 0

23 23 0 0 0 0 0 0 0 0 0 V2000
-0.6182 0.0021 1.3698 C 0 0 0 0 0 0 0 0 0 1
0.7769 0.0016 1.2700 C 0 0 0 0 0 0 0 0 0 2
1.4086 0.0000 0.0170 C 0 0 0 0 0 0 0 0 0 3
0.5995 -0.0009 -1.1322 C 0 0 0 0 0 0 0 0 0 4
-0.7936 -0.0007 -1.0316 C 0 0 0 0 0 0 0 0 0 5
-1.4309 0.0011 0.2233 C 0 0 0 0 0 0 0 0 0 6
2.9342 -0.0003 -0.0963 C 0 0 0 0 0 0 0 0 0 7
-2.9479 0.0012 0.3453 C 0 0 0 0 0 0 0 0 0 8
-3.5713 1.2676 -0.2730 C 0 0 0 0 0 0 0 0 0 9
-3.5698 -1.2703 -0.2642 C 0 0 0 0 0 0 0 0 0 10
3.5974 0.0011 0.9879 O 0 0 0 0 0 0 0 0 0 11
3.4288 -0.0018 -1.2674 O 0 0 0 0 0 0 0 0 0 12
-1.0897 0.0035 2.3566 H 0 0 0 0 0 0 0 0 0 13
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1.3974      0.0023      2.1683 H      0      0      0      0      0      0      0      0      0      0      14
1.0849     -0.0023     -2.1100 H      0      0      0      0      0      0      0      0      0      0      15
-1.3932     -0.0013     -1.9456 H      0      0      0      0      0      0      0      0      0      0      16
-3.1820      0.0048      1.4229 H      0      0      0      0      0      0      0      0      0      0      17
-4.6618      1.2705     -0.1248 H      0      0      0      0      0      0      0      0      0      0      18
-3.1609      2.1796      0.1849 H      0      0      0      0      0      0      0      0      0      0      19
-3.3796      1.3159     -1.3562 H      0      0      0      0      0      0      0      0      0      0      20
-4.6606     -1.2728     -0.1176 H      0      0      0      0      0      0      0      0      0      0      21
-3.1596     -2.1785      0.2014 H      0      0      0      0      0      0      0      0      0      0      22
-3.3763     -1.3267     -1.3467 H      0      0      0      0      0      0      0      0      0      0      23
2  1  0  0  0  0
6  1  0  0  0  0
13 1  0  0  0  0
3  2  0  0  0  0
14 2  0  0  0  0
4  3  0  0  0  0
7  3  0  0  0  0
5  4  0  0  0  0
15 4  0  0  0  0
6  5  0  0  0  0
16 5  0  0  0  0
8  6  0  0  0  0
11 7  0  0  0  0
12 7  0  0  0  0
9  8  0  0  0  0
10 8  0  0  0  0
17 8  0  0  0  0
18 9  0  0  0  0
19 9  0  0  0  0
20 9  0  0  0  0
21 10 0  0  0  0
22 10 0  0  0  0
10 23 0  0  0  0
M  END
$$$$
4-(1-methylethyl)-benzoicacid.sdf
COSMOtherm      3D      0

24 24  0  0  0  0  0  0  0  0  0  0 V2000
-0.6472      0.0023      1.3838 C      0      0      0      0      0      0      0      0      0      0      1
0.7444      0.0022      1.2982 C      0      0      0      0      0      0      0      0      0      0      2
1.3760      0.0008      0.0430 C      0      0      0      0      0      0      0      0      0      0      3
0.5848     -0.0003     -1.1216 C      0      0      0      0      0      0      0      0      0      0      4
-0.8052      0.0001     -1.0243 C      0      0      0      0      0      0      0      0      0      0      5
-1.4485      0.0013      0.2280 C      0      0      0      0      0      0      0      0      0      0      6
2.8590     -0.0002     -0.0086 C      0      0      0      0      0      0      0      0      0      0      7
-2.9644      0.0009      0.3367 C      0      0      0      0      0      0      0      0      0      0      8
-3.5780      1.2683     -0.2901 C      0      0      0      0      0      0      0      0      0      0      9
-3.5759     -1.2721     -0.2808 C      0      0      0      0      0      0      0      0      0      0      10
3.5947      0.0006      0.9749 O      0      0      0      0      0      0      0      0      0      0      11
3.3511     -0.0024     -1.2762 O      0      0      0      0      0      0      0      0      0      0      12
-1.1256      0.0031      2.3659 H      0      0      0      0      0      0      0      0      0      0      13
1.3538      0.0033      2.2031 H      0      0      0      0      0      0      0      0      0      0      14
1.0604     -0.0013     -2.1022 H      0      0      0      0      0      0      0      0      0      0      15
-1.3979     -0.0009     -1.9414 H      0      0      0      0      0      0      0      0      0      0      16
-3.2090      0.0046      1.4113 H      0      0      0      0      0      0      0      0      0      0      17
-4.6692      1.2708     -0.1499 H      0      0      0      0      0      0      0      0      0      0      18
-3.1709      2.1802      0.1706 H      0      0      0      0      0      0      0      0      0      0      19
-3.3780      1.3142     -1.3716 H      0      0      0      0      0      0      0      0      0      0      20
-4.6674     -1.2743     -0.1427 H      0      0      0      0      0      0      0      0      0      0      21
-3.1691     -2.1797      0.1882 H      0      0      0      0      0      0      0      0      0      0      22
-3.3735     -1.3267     -1.3615 H      0      0      0      0      0      0      0      0      0      0      23
4.3302     -0.0039     -1.2121 H      0      0      0      0      0      0      0      0      0      0      24
2  1  0  0  0  0
6  1  0  0  0  0
13 1  0  0  0  0
3  2  0  0  0  0
14 2  0  0  0  0
4  3  0  0  0  0
7  3  0  0  0  0
5  4  0  0  0  0
15 4  0  0  0  0
6  5  0  0  0  0
16 5  0  0  0  0
8  6  0  0  0  0
11 7  0  0  0  0
12 7  0  0  0  0
9  8  0  0  0  0
10 8  0  0  0  0
17 8  0  0  0  0
18 9  0  0  0  0
19 9  0  0  0  0
20 9  0  0  0  0
21 10 0  0  0  0
22 10 0  0  0  0
23 10 0  0  0  0
12 24 0  0  0  0
M  END
$$$$
4-aminobenzoicacid-anion.sdf
COSMOtherm      3D      0

16 16  0  0  0  0  0  0  0  0  0  0 V2000
1.4503      1.2142     -0.0004 C      0      0      0      0      0      0      0      0      0      0      1
0.0577      1.2023     -0.0006 C      0      0      0      0      0      0      0      0      0      0      2
-0.6743      0.0000     -0.0001 C      0      0      0      0      0      0      0      0      0      0      3
0.0577     -1.2023      0.0002 C      0      0      0      0      0      0      0      0      0      0      4
1.4503     -1.2142      0.0004 C      0      0      0      0      0      0      0      0      0      0      5
2.1809      0.0000      0.0000 C      0      0      0      0      0      0      0      0      0      0      6
-2.1928      0.0000      0.0000 C      0      0      0      0      0      0      0      0      0      0      7
3.5533      0.0000      0.0003 N      0      0      0      0      0      0      0      0      0      0      8
-2.7812      1.1305      0.0009 O      0      0      0      0      0      0      0      0      0      0      9
-2.7812     -1.1305     -0.0007 O      0      0      0      0      0      0      0      0      0      0      10
4.0773     -0.8667     -0.0007 H      0      0      0      0      0      0      0      0      0      0      11
4.0773      0.8666     -0.0008 H      0      0      0      0      0      0      0      0      0      0      12
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[illegible]

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0.8200	0.0057	0.0002	C	0	0	0	0	0	0	0	0	0	0	6
-3.4476	0.0812	0.0001	C	0	0	0	0	0	0	0	0	0	0	7
2.7427	-0.0077	-0.0002	Br	0	0	0	0	0	0	0	0	0	0	8
-4.1036	1.1178	0.0012	O	0	0	0	0	0	0	0	0	0	0	9
-4.0257	-1.1463	-0.0019	O	0	0	0	0	0	0	0	0	0	0	10
0.7021	2.1715	-0.0014	H	0	0	0	0	0	0	0	0	0	0	11
-1.7868	2.1796	-0.0009	H	0	0	0	0	0	0	0	0	0	0	12
-1.8059	-2.1397	0.0017	H	0	0	0	0	0	0	0	0	0	0	13
0.6728	-2.1576	0.0018	H	0	0	0	0	0	0	0	0	0	0	14
-4.9986	-1.0175	-0.0027	H	0	0	0	0	0	0	0	0	0	0	15
2	1	0	0	0	0									
6	1	0	0	0	0									
11	1	0	0	0	0									
3	2	0	0	0	0									
12	2	0	0	0	0									
4	3	0	0	0	0									
7	3	0	0	0	0									
5	4	0	0	0	0									
13	4	0	0	0	0									
6	5	0	0	0	0									
14	5	0	0	0	0									
8	6	0	0	0	0									
9	7	0	0	0	0									
10	7	0	0	0	0									
10	15	0	0	0	0									
M END														
\$\$\$\$														
4-butylbenzoicacid-anion.sdf														
COSMOtherm 3D 0														
26	26	0	0	0	0	0	0	0	0	0	0	0	0	0
-0.0196	-0.4742	1.2350	C	0	0	0	0	0	0	0	0	0	0	1
1.3393	-0.1465	1.2146	C	0	0	0	0	0	0	0	0	0	0	2
2.0317	-0.0154	-0.0004	C	0	0	0	0	0	0	0	0	0	0	3
1.3217	-0.2246	-1.1944	C	0	0	0	0	0	0	0	0	0	0	4
-0.0368	-0.5531	-1.1738	C	0	0	0	0	0	0	0	0	0	0	5
-0.7343	-0.6813	0.0413	C	0	0	0	0	0	0	0	0	0	0	6
3.5194	0.3414	-0.0226	C	0	0	0	0	0	0	0	0	0	0	7
-2.2134	-0.9936	0.0614	C	0	0	0	0	0	0	0	0	0	0	8
-3.0969	0.2704	-0.0137	C	0	0	0	0	0	0	0	0	0	0	9
-4.5981	-0.0437	0.0067	C	0	0	0	0	0	0	0	0	0	0	10
-5.4752	1.2116	-0.0710	C	0	0	0	0	0	0	0	0	0	0	11
4.0948	0.5010	1.0995	O	0	0	0	0	0	0	0	0	0	0	12
4.0726	0.4538	-1.1615	O	0	0	0	0	0	0	0	0	0	0	13
-0.5371	-0.5759	2.1930	H	0	0	0	0	0	0	0	0	0	0	14
1.8869	0.0079	2.1462	H	0	0	0	0	0	0	0	0	0	0	15
1.8558	-0.1308	-2.1418	H	0	0	0	0	0	0	0	0	0	0	16
-0.5674	-0.7176	-2.1158	H	0	0	0	0	0	0	0	0	0	0	17
-2.4605	-1.5469	0.9822	H	0	0	0	0	0	0	0	0	0	0	18
-2.4628	-1.6523	-0.7863	H	0	0	0	0	0	0	0	0	0	0	19
-2.8500	0.8293	-0.9328	H	0	0	0	0	0	0	0	0	0	0	20
-2.8479	0.9353	0.8309	H	0	0	0	0	0	0	0	0	0	0	21
-4.8374	-0.6054	0.9260	H	0	0	0	0	0	0	0	0	0	0	22
-4.8383	-0.7147	-0.8355	H	0	0	0	0	0	0	0	0	0	0	23
-6.5451	0.9555	-0.0546	H	0	0	0	0	0	0	0	0	0	0	24
-5.2798	1.7755	-0.9965	H	0	0	0	0	0	0	0	0	0	0	25
-5.2787	1.8853	0.7773	H	0	0	0	0	0	0	0	0	0	0	26
2	1	0	0	0	0									
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14	1	0	0	0	0									
3	2	0	0	0	0									
15	2	0	0	0	0									
4	3	0	0	0	0									
7	3	0	0	0	0									
5	4	0	0	0	0									
16	4	0	0	0	0									
6	5	0	0	0	0									
17	5	0	0	0	0									
8	6	0	0	0	0									
12	7	0	0	0	0									
13	7	0	0	0	0									
9	8	0	0	0	0									
18	8	0	0	0	0									
19	8	0	0	0	0									
10	9	0	0	0	0									
20	9	0	0	0	0									
21	9	0	0	0	0									
11	10	0	0	0	0									
22	10	0	0	0	0									
23	10	0	0	0	0									
24	11	0	0	0	0									
25	11	0	0	0	0									
11	26	0	0	0	0									
M END														
\$\$\$\$														
4-butylbenzoicacid.sdf														
COSMOtherm 3D 0														
27	27	0	0	0	0	0	0	0	0	0	0	0	0	0
-0.0485	-0.4639	1.2590	C	0	0	0	0	0	0	0	0	0	0	1
1.3059	-0.1365	1.2447	C	0	0	0	0	0	0	0	0	0	0	2
1.9951	-0.0219	0.0239	C	0	0	0	0	0	0	0	0	0	0	3
1.2999	-0.2445	-1.1795	C	0	0	0	0	0	0	0	0	0	0	4
-0.0551	-0.5723	-1.1542	C	0	0	0	0	0	0	0	0	0	0	5
-0.7547	-0.6856	0.0616	C	0	0	0	0	0	0	0	0	0	0	6
3.4375	0.3267	0.0509	C	0	0	0	0	0	0	0	0	0	0	7
-2.2313	-0.9971	0.0774	C	0	0	0	0	0	0	0	0	0	0	8
-3.1070	0.2723	-0.0178	C	0	0	0	0	0	0	0	0	0	0	9
-4.6091	-0.0382	-0.0103	C	0	0	0	0	0	0	0	0	0	0	10
-5.4799	1.2200	-0.1060	C	0	0	0	0	0	0	0	0	0	0	11
4.0920	0.5252	1.0712	O	0	0	0	0	0	0	0	0	0	0	12
3.9916	0.4120	-1.1882	O	0	0	0	0	0	0	0	0	0	0	13
-0.5699	-0.5547	2.2146	H	0	0	0	0	0	0	0	0	0	0	14
1.8447	0.0291	2.1787	H	0	0	0	0	0	0	0	0	0	0	15
1.8223	-0.1660	-2.1328	H	0	0	0	0	0	0	0	0	0	0	16

URL: <http://mc.manuscriptcentral.com/tandf/tmph>

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2 1 0 0 0 0
6 1 0 0 0 0
15 1 0 0 0 0
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16 2 0 0 0 0
4 3 0 0 0 0
7 3 0 0 0 0
5 4 0 0 0 0
17 4 0 0 0 0
6 5 0 0 0 0
18 5 0 0 0 0
8 6 0 0 0 0
11 7 0 0 0 0
12 7 0 0 0 0
9 8 0 0 0 0
10 8 0 0 0 0
13 10 0 0 0 0
14 10 0 0 0 0
12 19 0 0 0 0
M END
$$$$
4-chlorobenzoicacid-anion.sdf
COSMOTHERM 3D 0

14 14 0 0 0 0 0 0 0 0 0 V2000
0.9353 1.2201 -0.0010 C 0 0 0 0 0 0 0 0 0 0 1
-0.4626 1.2070 -0.0007 C 0 0 0 0 0 0 0 0 0 0 2
-1.1796 0.0000 -0.0002 C 0 0 0 0 0 0 0 0 0 0 3
-0.4626 -1.2070 0.0007 C 0 0 0 0 0 0 0 0 0 0 4
0.9353 -1.2201 0.0005 C 0 0 0 0 0 0 0 0 0 0 5
1.6147 0.0000 -0.0001 C 0 0 0 0 0 0 0 0 0 0 6
-2.7120 0.0000 0.0000 C 0 0 0 0 0 0 0 0 0 0 7
3.3914 0.0000 0.0001 Cl 0 0 0 0 0 0 0 0 0 0 8
-3.2874 1.1317 0.0016 O 0 0 0 0 0 0 0 0 0 0 9
-3.2873 -1.1317 -0.0013 O 0 0 0 0 0 0 0 0 0 0 10
1.4865 2.1609 -0.0017 H 0 0 0 0 0 0 0 0 0 0 11
-1.0167 2.1468 -0.0010 H 0 0 0 0 0 0 0 0 0 0 12
-1.0167 -2.1468 0.0011 H 0 0 0 0 0 0 0 0 0 0 13
1.4865 -2.1609 0.0013 H 0 0 0 0 0 0 0 0 0 0 14

2 1 0 0 0 0
6 1 0 0 0 0
11 1 0 0 0 0
3 2 0 0 0 0
12 2 0 0 0 0
4 3 0 0 0 0
7 3 0 0 0 0
5 4 0 0 0 0
13 4 0 0 0 0
6 5 0 0 0 0
8 6 0 0 0 0
9 7 0 0 0 0
10 7 0 0 0 0
5 14 0 0 0 0
M END
$$$$
4-chlorobenzoicacid.sdf
COSMOTHERM 3D 0

15 15 0 0 0 0 0 0 0 0 0 V2000
0.9654 1.2282 -0.0002 C 0 0 0 0 0 0 0 0 0 0 1
-0.4283 1.2316 0.0000 C 0 0 0 0 0 0 0 0 0 0 2
-1.1470 0.0238 0.0004 C 0 0 0 0 0 0 0 0 0 0 3
-0.4500 -1.1974 0.0008 C 0 0 0 0 0 0 0 0 0 0 4
0.9448 -1.2152 0.0007 C 0 0 0 0 0 0 0 0 0 0 5
1.6337 0.0004 0.0001 C 0 0 0 0 0 0 0 0 0 0 6
-2.6331 0.0835 0.0001 C 0 0 0 0 0 0 0 0 0 0 7
3.4008 -0.0150 -0.0003 Cl 0 0 0 0 0 0 0 0 0 0 8
-3.2875 1.1211 0.0005 O 0 0 0 0 0 0 0 0 0 0 9
-3.2139 -1.1430 -0.0012 O 0 0 0 0 0 0 0 0 0 0 10
1.5237 2.1639 -0.0008 H 0 0 0 0 0 0 0 0 0 0 11
-0.9689 2.1786 -0.0002 H 0 0 0 0 0 0 0 0 0 0 12
-0.9955 -2.1404 0.0011 H 0 0 0 0 0 0 0 0 0 0 13
1.4869 -2.1604 0.0012 H 0 0 0 0 0 0 0 0 0 0 14
-4.1864 -1.0119 -0.0022 H 0 0 0 0 0 0 0 0 0 0 15

2 1 0 0 0 0
6 1 0 0 0 0
11 1 0 0 0 0
3 2 0 0 0 0
12 2 0 0 0 0
4 3 0 0 0 0
7 3 0 0 0 0
5 4 0 0 0 0
13 4 0 0 0 0
6 5 0 0 0 0
14 5 0 0 0 0
8 6 0 0 0 0
9 7 0 0 0 0
10 7 0 0 0 0
10 15 0 0 0 0
M END
$$$$
4-chlorophenol-anion.sdf
COSMOTHERM 3D 0

12 12 0 0 0 0 0 0 0 0 0 V2000
0.1684 1.2153 0.0002 C 0 0 0 0 0 0 0 0 0 0 1
-1.2270 1.2140 0.0007 C 0 0 0 0 0 0 0 0 0 0 2
-2.0031 0.0000 -0.0001 C 0 0 0 0 0 0 0 0 0 0 3
-1.2270 -1.2140 0.0006 C 0 0 0 0 0 0 0 0 0 0 4
0.1684 -1.2153 0.0003 C 0 0 0 0 0 0 0 0 0 0 5
0.8606 0.0000 0.0005 C 0 0 0 0 0 0 0 0 0 0 6
-3.2979 0.0000 -0.0009 O 0 0 0 0 0 0 0 0 0 0 7
2.6522 0.0000 -0.0004 Cl 0 0 0 0 0 0 0 0 0 0 8
0.7173 2.1598 0.0005 H 0 0 0 0 0 0 0 0 0 0 9
-1.7646 2.1666 0.0004 H 0 0 0 0 0 0 0 0 0 0 10
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2
3      -1.7646   -2.1666   0.0002 H   0   0   0   0   0   0   0   0   0   0   11
4      0.7173   -2.1598   0.0006 H   0   0   0   0   0   0   0   0   0   0   12
5
6      2   1   0   0   0   0
7      6   1   0   0   0   0
8      9   1   0   0   0   0
9      3   2   0   0   0   0
10     10  2   0   0   0   0
11     4   3   0   0   0   0
12     7   3   0   0   0   0
13     5   4   0   0   0   0
14     11  4   0   0   0   0
15     6   5   0   0   0   0
16     8   6   0   0   0   0
17     5  12   0   0   0   0
18
19 M   END
20 $$$$
21 4-chlorophenol.sdf
22 COSMOTHERM      3D      0
23
24 13 13   0   0   0   0   0   0   0   0   0   0 V2000
25 1.2136   1.1990  -0.0003 C   0   0   0   0   0   0   0   0   0   0   1
26 1.2156  -0.1970   0.0001 C   0   0   0   0   0   0   0   0   0   0   2
27 -0.0015  -0.8823  -0.0001 C   0   0   0   0   0   0   0   0   0   0   3
28 -1.2180  -0.1991  -0.0001 C   0   0   0   0   0   0   0   0   0   0   4
29 -1.2163   1.1989  -0.0001 C   0   0   0   0   0   0   0   0   0   0   5
30 -0.0014   1.9006   0.0001 C   0   0   0   0   0   0   0   0   0   0   6
31 0.0001  -2.6600   0.0001 Cl  0   0   0   0   0   0   0   0   0   0   7
32 0.0597   3.2715   0.0001 O   0   0   0   0   0   0   0   0   0   0   8
33 2.1550   1.7501  -0.0001 H   0   0   0   0   0   0   0   0   0   0   9
34 2.1597  -0.7418   0.0004 H   0   0   0   0   0   0   0   0   0   0   10
35 -2.1622  -0.7437  -0.0003 H   0   0   0   0   0   0   0   0   0   0   11
36 -2.1644   1.7416   0.0000 H   0   0   0   0   0   0   0   0   0   0   12
37 -0.8451   3.6379   0.0012 H   0   0   0   0   0   0   0   0   0   0   13
38
39 2   1   0   0   0   0
40 6   1   0   0   0   0
41 9   1   0   0   0   0
42 3   2   0   0   0   0
43 10  2   0   0   0   0
44 4   3   0   0   0   0
45 7   3   0   0   0   0
46 5   4   0   0   0   0
47 11  4   0   0   0   0
48 6   5   0   0   0   0
49 12  5   0   0   0   0
50 8   6   0   0   0   0
51 8  13   0   0   0   0
52
53 M   END
54 $$$$
55 4-cyanobenzoicacid-anion.sdf
56 COSMOTHERM      3D      0
57
58 15 15   0   0   0   0   0   0   0   0   0   0 V2000
59 1.0942   1.2228  -0.0008 C   0   0   0   0   0   0   0   0   0   0   1
60 -0.2988   1.2104  -0.0009 C   0   0   0   0   0   0   0   0   0   0   2
61 -1.0116   0.0000  -0.0001 C   0   0   0   0   0   0   0   0   0   0   3
62 -0.2989  -1.2105   0.0007 C   0   0   0   0   0   0   0   0   0   0   4
63 1.0941  -1.2230   0.0007 C   0   0   0   0   0   0   0   0   0   0   5
64 1.7976  -0.0001   0.0000 C   0   0   0   0   0   0   0   0   0   0   6
65 -2.5482   0.0000   0.0000 C   0   0   0   0   0   0   0   0   0   0   7
66 3.2248   0.0000   0.0001 C   0   0   0   0   0   0   0   0   0   0   8
67 4.3931   0.0002   0.0001 N   0   0   0   0   0   0   0   0   0   0   9
68 -3.1184   1.1326   0.0017 O   0   0   0   0   0   0   0   0   0   0   10
69 -3.1185  -1.1324  -0.0015 O   0   0   0   0   0   0   0   0   0   0   11
70 1.6426   2.1655  -0.0015 H   0   0   0   0   0   0   0   0   0   0   12
71 -0.8581   2.1467  -0.0015 H   0   0   0   0   0   0   0   0   0   0   13
72 -0.8583  -2.1468  -0.0011 H   0   0   0   0   0   0   0   0   0   0   14
73 1.6425  -2.1657   0.0014 H   0   0   0   0   0   0   0   0   0   0   15
74
75 2   1   0   0   0   0
76 6   1   0   0   0   0
77 12  1   0   0   0   0
78 3   2   0   0   0   0
79 13  2   0   0   0   0
80 4   3   0   0   0   0
81 7   3   0   0   0   0
82 5   4   0   0   0   0
83 14  4   0   0   0   0
84 6   5   0   0   0   0
85 8   6   0   0   0   0
86 10  7   0   0   0   0
87 11  7   0   0   0   0
88 9   8   0   0   0   0
89 5  15   0   0   0   0
90
91 M   END
92 $$$$
93 4-cyanobenzoicacid.sdf
94 COSMOTHERM      3D      0
95
96 16 16   0   0   0   0   0   0   0   0   0   0 V2000
97 1.1235   1.2298  -0.0012 C   0   0   0   0   0   0   0   0   0   0   1
98 -0.2673   1.2329  -0.0008 C   0   0   0   0   0   0   0   0   0   0   2
99 -0.9802   0.0222   0.0003 C   0   0   0   0   0   0   0   0   0   0   3
100 -0.2881  -1.2013   0.0016 C   0   0   0   0   0   0   0   0   0   0   4
101 1.1038  -1.2180   0.0016 C   0   0   0   0   0   0   0   0   0   0   5
102 1.8126  -0.0002   0.0000 C   0   0   0   0   0   0   0   0   0   0   6
103 -2.4728   0.0823   0.0002 C   0   0   0   0   0   0   0   0   0   0   7
104 3.2415  -0.0126  -0.0003 C   0   0   0   0   0   0   0   0   0   0   8
105 4.4086  -0.0224  -0.0004 N   0   0   0   0   0   0   0   0   0   0   9
106 -3.1199   1.1225   0.0023 O   0   0   0   0   0   0   0   0   0   0   10
107 -3.0487  -1.1426  -0.0029 O   0   0   0   0   0   0   0   0   0   0   11
108 1.6784   2.1677  -0.0024 H   0   0   0   0   0   0   0   0   0   0   12
109 -0.8127   2.1767  -0.0016 H   0   0   0   0   0   0   0   0   0   0   13
110 -0.8374  -2.1416   0.0026 H   0   0   0   0   0   0   0   0   0   0   14
111 1.6434  -2.1648   0.0028 H   0   0   0   0   0   0   0   0   0   0   15
112 -4.0224  -1.0180  -0.0035 H   0   0   0   0   0   0   0   0   0   0   16
113
114 2   1   0   0   0   0
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6 1 0 0 0 0
12 1 0 0 0 0
3 2 0 0 0 0
13 2 0 0 0 0
4 3 0 0 0 0
7 3 0 0 0 0
5 4 0 0 0 0
14 4 0 0 0 0
6 5 0 0 0 0
15 5 0 0 0 0
8 6 0 0 0 0
10 7 0 0 0 0
11 7 0 0 0 0
9 8 0 0 0 0
11 16 0 0 0 0
M END
$$$$
4-dimethylaminobenzoicacid-anion.sdf
COSMOtherm 3D 0

22 22 0 0 0 0 0 0 0 0 0 V2000
-0.7029 0.0066 1.2146 C 0 0 0 0 0 0 0 0 0 0 1
0.6897 0.0056 1.1998 C 0 0 0 0 0 0 0 0 0 0 2
1.4242 0.0002 -0.0001 C 0 0 0 0 0 0 0 0 0 0 3
0.6898 -0.0050 -1.1999 C 0 0 0 0 0 0 0 0 0 0 4
-0.7028 -0.0049 -1.2148 C 0 0 0 0 0 0 0 0 0 0 5
-1.4459 0.0010 -0.0001 C 0 0 0 0 0 0 0 0 0 0 6
2.9418 -0.0004 0.0001 C 0 0 0 0 0 0 0 0 0 0 7
-2.8221 0.0019 -0.0001 N 0 0 0 0 0 0 0 0 0 0 8
-3.5580 0.0040 -1.2595 C 0 0 0 0 0 0 0 0 0 0 9
-3.5582 -0.0070 1.2596 C 0 0 0 0 0 0 0 0 0 0 10
3.5306 -0.0057 1.1305 O 0 0 0 0 0 0 0 0 0 0 11
3.5308 0.0046 -1.1304 O 0 0 0 0 0 0 0 0 0 0 12
-1.2221 0.0117 2.1727 H 0 0 0 0 0 0 0 0 0 0 13
1.2385 0.0096 2.1441 H 0 0 0 0 0 0 0 0 0 0 14
1.2385 -0.0097 -2.1442 H 0 0 0 0 0 0 0 0 0 0 15
-1.2220 -0.0104 -2.1728 H 0 0 0 0 0 0 0 0 0 0 16
-4.6309 0.0208 -1.0424 H 0 0 0 0 0 0 0 0 0 0 17
-3.3185 0.8903 -1.8709 H 0 0 0 0 0 0 0 0 0 0 18
-3.3440 -0.8954 -1.8618 H 0 0 0 0 0 0 0 0 0 0 19
-4.6312 -0.0178 1.0424 H 0 0 0 0 0 0 0 0 0 0 20
-3.3221 -0.8985 1.8650 H 0 0 0 0 0 0 0 0 0 0 21
-3.3407 0.8873 1.8680 H 0 0 0 0 0 0 0 0 0 0 22
2 1 0 0 0 0
6 1 0 0 0 0
13 1 0 0 0 0
3 2 0 0 0 0
14 2 0 0 0 0
4 3 0 0 0 0
7 3 0 0 0 0
5 4 0 0 0 0
15 4 0 0 0 0
6 5 0 0 0 0
16 5 0 0 0 0
8 6 0 0 0 0
11 7 0 0 0 0
12 7 0 0 0 0
9 8 0 0 0 0
10 8 0 0 0 0
17 9 0 0 0 0
18 9 0 0 0 0
19 9 0 0 0 0
20 10 0 0 0 0
21 10 0 0 0 0
10 22 0 0 0 0
M END
$$$$
4-dimethylaminobenzoicacid.sdf
COSMOtherm 3D 0

23 23 0 0 0 0 0 0 0 0 0 V2000
-0.7321 0.0039 1.2288 C 0 0 0 0 0 0 0 0 0 0 1
0.6526 0.0039 1.2300 C 0 0 0 0 0 0 0 0 0 0 2
1.3926 0.0006 0.0275 C 0 0 0 0 0 0 0 0 0 0 3
0.6751 -0.0024 -1.1892 C 0 0 0 0 0 0 0 0 0 0 4
-0.7105 -0.0026 -1.2099 C 0 0 0 0 0 0 0 0 0 0 5
-1.4636 0.0006 0.0025 C 0 0 0 0 0 0 0 0 0 0 6
2.8571 -0.0004 0.0853 C 0 0 0 0 0 0 0 0 0 0 7
-2.8295 0.0002 -0.0103 N 0 0 0 0 0 0 0 0 0 0 8
-3.5584 0.0041 -1.2786 C 0 0 0 0 0 0 0 0 0 0 9
-3.5832 -0.0058 1.2432 C 0 0 0 0 0 0 0 0 0 0 10
3.5331 -0.0018 1.1181 O 0 0 0 0 0 0 0 0 0 0 11
3.4536 0.0006 -1.1472 O 0 0 0 0 0 0 0 0 0 0 12
-1.2601 0.0075 2.1810 H 0 0 0 0 0 0 0 0 0 0 13
1.1887 0.0068 2.1807 H 0 0 0 0 0 0 0 0 0 0 14
1.2167 -0.0054 -2.1356 H 0 0 0 0 0 0 0 0 0 0 15
-1.2215 -0.0061 -2.1712 H 0 0 0 0 0 0 0 0 0 0 16
-4.6319 0.0172 -1.0677 H 0 0 0 0 0 0 0 0 0 0 17
-3.3143 0.8936 -1.8812 H 0 0 0 0 0 0 0 0 0 0 18
-3.3348 -0.8941 -1.8766 H 0 0 0 0 0 0 0 0 0 0 19
-4.6523 -0.0203 1.0109 H 0 0 0 0 0 0 0 0 0 0 20
-3.3501 -0.8955 1.8499 H 0 0 0 0 0 0 0 0 0 0 21
-3.3730 0.8922 1.8462 H 0 0 0 0 0 0 0 0 0 0 22
4.4222 -0.0022 -0.9950 H 0 0 0 0 0 0 0 0 0 0 23
2 1 0 0 0 0
6 1 0 0 0 0
13 1 0 0 0 0
3 2 0 0 0 0
14 2 0 0 0 0
4 3 0 0 0 0
7 3 0 0 0 0
5 4 0 0 0 0
15 4 0 0 0 0
6 5 0 0 0 0
16 5 0 0 0 0
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8 6 0 0 0 0
11 7 0 0 0 0
12 7 0 0 0 0
9 8 0 0 0 0
10 8 0 0 0 0
17 9 0 0 0 0
18 9 0 0 0 0
19 9 0 0 0 0
20 10 0 0 0 0
21 10 0 0 0 0
22 10 0 0 0 0
12 23 0 0 0 0
M END
$$$$
4-ethylbenzoicacid-anion.sdf
COSMOtherm 3D 0

20 20 0 0 0 0 0 0 0 0 0 V2000
1.0330 -1.2117 0.2584 C 0 0 0 0 0 0 0 0 0 0 1
-0.3574 -1.2078 0.1141 C 0 0 0 0 0 0 0 0 0 0 2
-1.0720 -0.0007 0.0430 C 0 0 0 0 0 0 0 0 0 0 3
-0.3513 1.2023 0.1238 C 0 0 0 0 0 0 0 0 0 0 4
1.0389 1.1982 0.2683 C 0 0 0 0 0 0 0 0 0 0 5
1.7580 -0.0089 0.3349 C 0 0 0 0 0 0 0 0 0 0 6
-2.5938 0.0037 -0.1151 C 0 0 0 0 0 0 0 0 0 0 7
3.2666 -0.0126 0.4483 C 0 0 0 0 0 0 0 0 0 0 8
3.9678 0.0214 -0.9239 C 0 0 0 0 0 0 0 0 0 0 9
-3.1739 -1.1254 -0.1806 O 0 0 0 0 0 0 0 0 0 0 10
-3.1683 1.1362 -0.1710 O 0 0 0 0 0 0 0 0 0 0 11
1.5679 -2.1639 0.3163 H 0 0 0 0 0 0 0 0 0 0 12
-0.9124 -2.1463 0.0595 H 0 0 0 0 0 0 0 0 0 0 13
-0.9018 2.1439 0.0770 H 0 0 0 0 0 0 0 0 0 0 14
1.5782 2.1475 0.3343 H 0 0 0 0 0 0 0 0 0 0 15
3.5896 -0.9114 0.9967 H 0 0 0 0 0 0 0 0 0 0 16
3.5907 0.8578 1.0402 H 0 0 0 0 0 0 0 0 0 0 17
5.0611 0.0194 -0.8025 H 0 0 0 0 0 0 0 0 0 0 18
3.6892 0.9245 -1.4872 H 0 0 0 0 0 0 0 0 0 0 19
3.6906 -0.8537 -1.5303 H 0 0 0 0 0 0 0 0 0 0 20
2 1 0 0 0 0
6 1 0 0 0 0
12 1 0 0 0 0
3 2 0 0 0 0
13 2 0 0 0 0
4 3 0 0 0 0
7 3 0 0 0 0
5 4 0 0 0 0
14 4 0 0 0 0
6 5 0 0 0 0
15 5 0 0 0 0
8 6 0 0 0 0
10 7 0 0 0 0
11 7 0 0 0 0
9 8 0 0 0 0
16 8 0 0 0 0
17 8 0 0 0 0
18 9 0 0 0 0
19 9 0 0 0 0
9 20 0 0 0 0
M END
$$$$
4-ethylbenzoicacid.sdf
COSMOtherm 3D 0

21 21 0 0 0 0 0 0 0 0 0 V2000
1.0620 -1.2238 0.2495 C 0 0 0 0 0 0 0 0 0 0 1
-0.3239 -1.2345 0.1056 C 0 0 0 0 0 0 0 0 0 0 2
-1.0398 -0.0255 0.0433 C 0 0 0 0 0 0 0 0 0 0 3
-0.3388 1.1918 0.1297 C 0 0 0 0 0 0 0 0 0 0 4
1.0480 1.1914 0.2743 C 0 0 0 0 0 0 0 0 0 0 5
1.7737 -0.0124 0.3346 C 0 0 0 0 0 0 0 0 0 0 6
-2.5153 -0.0788 -0.1066 C 0 0 0 0 0 0 0 0 0 0 7
3.2797 -0.0033 0.4499 C 0 0 0 0 0 0 0 0 0 0 8
3.9758 0.0511 -0.9252 C 0 0 0 0 0 0 0 0 0 0 9
-3.1758 -1.1120 -0.1790 O 0 0 0 0 0 0 0 0 0 0 10
-3.0939 1.1507 -0.1585 O 0 0 0 0 0 0 0 0 0 0 11
1.6045 -2.1706 0.3018 H 0 0 0 0 0 0 0 0 0 0 12
-0.8663 -2.1792 0.0451 H 0 0 0 0 0 0 0 0 0 0 13
-0.8809 2.1365 0.0895 H 0 0 0 0 0 0 0 0 0 0 14
1.5793 2.1433 0.3464 H 0 0 0 0 0 0 0 0 0 0 15
3.6099 -0.9049 0.9882 H 0 0 0 0 0 0 0 0 0 0 16
3.5939 0.8654 1.0487 H 0 0 0 0 0 0 0 0 0 0 17
5.0684 0.0593 -0.8025 H 0 0 0 0 0 0 0 0 0 0 18
3.6874 0.9570 -1.4786 H 0 0 0 0 0 0 0 0 0 0 19
3.7072 -0.8214 -1.5388 H 0 0 0 0 0 0 0 0 0 0 20
-4.0610 1.0172 -0.2561 H 0 0 0 0 0 0 0 0 0 0 21
2 1 0 0 0 0
6 1 0 0 0 0
12 1 0 0 0 0
3 2 0 0 0 0
13 2 0 0 0 0
4 3 0 0 0 0
7 3 0 0 0 0
5 4 0 0 0 0
14 4 0 0 0 0
6 5 0 0 0 0
15 5 0 0 0 0
8 6 0 0 0 0
10 7 0 0 0 0
11 7 0 0 0 0
9 8 0 0 0 0
16 8 0 0 0 0
17 8 0 0 0 0
18 9 0 0 0 0
19 9 0 0 0 0
20 9 0 0 0 0
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11 21 0 0 0 0
M END
$$$$
4-fluorobenzoicacid-anion.sdf
COSMOtherm 3D 0

14 14 0 0 0 0 0 0 0 0 0 V2000
1.3944 1.2219 -0.0006 C 0 0 0 0 0 0 0 0 0 0 0 1
-0.0039 1.2085 -0.0006 C 0 0 0 0 0 0 0 0 0 0 0 2
-0.7202 0.0000 -0.0001 C 0 0 0 0 0 0 0 0 0 0 0 3
-0.0039 -1.2085 0.0003 C 0 0 0 0 0 0 0 0 0 0 0 4
1.3944 -1.2219 0.0005 C 0 0 0 0 0 0 0 0 0 0 0 5
2.0613 0.0000 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 6
-2.2516 0.0000 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 7
3.4334 0.0000 0.0002 F 0 0 0 0 0 0 0 0 0 0 0 8
-2.8287 1.1314 0.0012 O 0 0 0 0 0 0 0 0 0 0 0 9
-2.8287 -1.1314 -0.0009 O 0 0 0 0 0 0 0 0 0 0 0 10
1.9590 2.1553 -0.0011 H 0 0 0 0 0 0 0 0 0 0 0 11
-0.5603 2.1468 -0.0009 H 0 0 0 0 0 0 0 0 0 0 0 12
-0.5602 -2.1468 0.0006 H 0 0 0 0 0 0 0 0 0 0 0 13
1.9590 -2.1553 0.0010 H 0 0 0 0 0 0 0 0 0 0 0 14
2 1 0 0 0 0
6 1 0 0 0 0
11 1 0 0 0 0
3 2 0 0 0 0
12 2 0 0 0 0
4 3 0 0 0 0
7 3 0 0 0 0
5 4 0 0 0 0
13 4 0 0 0 0
6 5 0 0 0 0
8 6 0 0 0 0
9 7 0 0 0 0
10 7 0 0 0 0
5 14 0 0 0 0
M END
$$$$
4-fluorobenzoicacid.sdf
COSMOtherm 3D 0

15 15 0 0 0 0 0 0 0 0 0 V2000
1.4251 1.2249 0.0004 C 0 0 0 0 0 0 0 0 0 0 0 1
0.0317 1.2312 0.0003 C 0 0 0 0 0 0 0 0 0 0 0 2
-0.6896 0.0234 0.0004 C 0 0 0 0 0 0 0 0 0 0 0 3
0.0036 -1.2014 -0.0001 C 0 0 0 0 0 0 0 0 0 0 0 4
1.3980 -1.2235 0.0001 C 0 0 0 0 0 0 0 0 0 0 0 5
2.0767 -0.0070 -0.0001 C 0 0 0 0 0 0 0 0 0 0 0 6
-2.1738 0.0868 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 7
3.4398 -0.0223 -0.0003 F 0 0 0 0 0 0 0 0 0 0 0 8
-2.8276 1.1256 -0.0006 O 0 0 0 0 0 0 0 0 0 0 0 9
-2.7597 -1.1383 0.0002 O 0 0 0 0 0 0 0 0 0 0 0 10
2.0000 2.1509 0.0003 H 0 0 0 0 0 0 0 0 0 0 0 11
-0.5089 2.1779 0.0007 H 0 0 0 0 0 0 0 0 0 0 0 12
-0.5467 -2.1414 -0.0003 H 0 0 0 0 0 0 0 0 0 0 0 13
1.9521 -2.1622 -0.0002 H 0 0 0 0 0 0 0 0 0 0 0 14
-3.7314 -1.0021 -0.0010 H 0 0 0 0 0 0 0 0 0 0 0 15
2 1 0 0 0 0
6 1 0 0 0 0
11 1 0 0 0 0
3 2 0 0 0 0
12 2 0 0 0 0
4 3 0 0 0 0
7 3 0 0 0 0
5 4 0 0 0 0
13 4 0 0 0 0
6 5 0 0 0 0
14 5 0 0 0 0
8 6 0 0 0 0
9 7 0 0 0 0
10 7 0 0 0 0
10 15 0 0 0 0
M END
$$$$
4-hydroxybenzoicacid-anion.sdf
COSMOtherm 3D 0

15 15 0 0 0 0 0 0 0 0 0 V2000
1.4351 1.2150 -0.0003 C 0 0 0 0 0 0 0 0 0 0 0 1
0.0402 1.2041 -0.0004 C 0 0 0 0 0 0 0 0 0 0 0 2
-0.6844 -0.0011 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 3
0.0384 -1.2058 0.0006 C 0 0 0 0 0 0 0 0 0 0 0 4
1.4350 -1.2161 0.0006 C 0 0 0 0 0 0 0 0 0 0 0 5
2.1372 -0.0006 -0.0001 C 0 0 0 0 0 0 0 0 0 0 0 6
-2.2104 -0.0005 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 7
-2.7931 -1.1310 -0.0010 O 0 0 0 0 0 0 0 0 0 0 0 8
-2.7918 1.1308 0.0009 O 0 0 0 0 0 0 0 0 0 0 0 9
3.5103 0.0580 -0.0003 O 0 0 0 0 0 0 0 0 0 0 0 10
3.8721 -0.8488 0.0008 H 0 0 0 0 0 0 0 0 0 0 0 11
1.9918 2.1542 -0.0008 H 0 0 0 0 0 0 0 0 0 0 0 12
-0.5134 2.1447 -0.0006 H 0 0 0 0 0 0 0 0 0 0 0 13
-0.5147 -2.1466 0.0008 H 0 0 0 0 0 0 0 0 0 0 0 14
1.9841 -2.1617 0.0009 H 0 0 0 0 0 0 0 0 0 0 0 15
2 1 0 0 0 0
6 1 0 0 0 0
12 1 0 0 0 0
3 2 0 0 0 0
13 2 0 0 0 0
4 3 0 0 0 0
7 3 0 0 0 0
5 4 0 0 0 0
14 4 0 0 0 0
6 5 0 0 0 0
10 6 0 0 0 0
8 7 0 0 0 0
9 7 0 0 0 0
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11 10 0 0 0 0
5 15 0 0 0 0
M END
$$$$
4-hydroxybenzoicacid.sdf
COSMOtherm 3D 0
16 16 0 0 0 0 0 0 0 0 V2000
1.4658 1.2181 -0.0010 C 0 0 0 0 0 0 0 0 0 0 1
0.0771 1.2279 -0.0007 C 0 0 0 0 0 0 0 0 0 0 2
-0.6544 0.0232 0.0000 C 0 0 0 0 0 0 0 0 0 0 3
0.0455 -1.1992 0.0009 C 0 0 0 0 0 0 0 0 0 0 4
1.4369 -1.2199 0.0005 C 0 0 0 0 0 0 0 0 0 0 5
2.1523 -0.0096 0.0001 C 0 0 0 0 0 0 0 0 0 0 6
-2.1307 0.0873 0.0002 C 0 0 0 0 0 0 0 0 0 0 7
-2.7239 -1.1389 -0.0015 O 0 0 0 0 0 0 0 0 0 0 8
-2.7908 1.1251 0.0015 O 0 0 0 0 0 0 0 0 0 0 9
3.5152 0.0346 0.0000 O 0 0 0 0 0 0 0 0 0 0 10
-3.6940 -0.9936 -0.0020 H 0 0 0 0 0 0 0 0 0 0 11
3.8753 -0.8736 0.0015 H 0 0 0 0 0 0 0 0 0 0 12
2.0342 2.1491 -0.0016 H 0 0 0 0 0 0 0 0 0 0 13
-0.4604 2.1769 -0.0013 H 0 0 0 0 0 0 0 0 0 0 14
-0.5028 -2.1409 0.0013 H 0 0 0 0 0 0 0 0 0 0 15
1.9749 -2.1706 0.0012 H 0 0 0 0 0 0 0 0 0 0 16
2 1 0 0 0 0
6 1 0 0 0 0
13 1 0 0 0 0
3 2 0 0 0 0
14 2 0 0 0 0
4 3 0 0 0 0
7 3 0 0 0 0
5 4 0 0 0 0
15 4 0 0 0 0
6 5 0 0 0 0
10 6 0 0 0 0
8 7 0 0 0 0
9 7 0 0 0 0
11 8 0 0 0 0
12 10 0 0 0 0
5 16 0 0 0 0
M END
$$$$
4-hydroxymethylbenzoicacid-anion.sdf
COSMOtherm 3D 0
18 18 0 0 0 0 0 0 0 0 V2000
-0.9914 -0.2400 1.2259 C 0 0 0 0 0 0 0 0 0 0 1
0.3991 -0.0988 1.2146 C 0 0 0 0 0 0 0 0 0 0 2
1.1054 -0.0419 0.0020 C 0 0 0 0 0 0 0 0 0 0 3
0.3830 -0.1319 -1.1995 C 0 0 0 0 0 0 0 0 0 0 4
-1.0067 -0.2753 -1.1891 C 0 0 0 0 0 0 0 0 0 0 5
-1.7128 -0.3308 0.0243 C 0 0 0 0 0 0 0 0 0 0 6
2.6304 0.1095 -0.0100 C 0 0 0 0 0 0 0 0 0 0 7
-3.2142 -0.4489 0.0344 C 0 0 0 0 0 0 0 0 0 0 8
-3.7822 0.8851 -0.0563 O 0 0 0 0 0 0 0 0 0 0 9
3.2141 0.1711 1.1164 O 0 0 0 0 0 0 0 0 0 0 10
3.1967 0.1631 -1.1458 O 0 0 0 0 0 0 0 0 0 0 11
-4.7517 0.7800 -0.0592 H 0 0 0 0 0 0 0 0 0 0 12
-1.5263 -0.2863 2.1783 H 0 0 0 0 0 0 0 0 0 0 13
0.9600 -0.0346 2.1486 H 0 0 0 0 0 0 0 0 0 0 14
0.9320 -0.0938 -2.1421 H 0 0 0 0 0 0 0 0 0 0 15
-1.5533 -0.3507 -2.1329 H 0 0 0 0 0 0 0 0 0 0 16
-3.5495 -0.9370 0.9651 H 0 0 0 0 0 0 0 0 0 0 17
-3.5527 -1.0577 -0.8211 H 0 0 0 0 0 0 0 0 0 0 18
2 1 0 0 0 0
6 1 0 0 0 0
13 1 0 0 0 0
3 2 0 0 0 0
14 2 0 0 0 0
4 3 0 0 0 0
7 3 0 0 0 0
5 4 0 0 0 0
15 4 0 0 0 0
6 5 0 0 0 0
16 5 0 0 0 0
8 6 0 0 0 0
10 7 0 0 0 0
11 7 0 0 0 0
9 8 0 0 0 0
17 8 0 0 0 0
12 9 0 0 0 0
8 18 0 0 0 0
M END
$$$$
4-hydroxymethylbenzoicacid.sdf
COSMOtherm 3D 0
19 19 0 0 0 0 0 0 0 0 V2000
-1.0217 -0.2358 1.2347 C 0 0 0 0 0 0 0 0 0 0 1
0.3653 -0.0947 1.2394 C 0 0 0 0 0 0 0 0 0 0 2
1.0731 -0.0429 0.0261 C 0 0 0 0 0 0 0 0 0 0 3
0.3718 -0.1339 -1.1901 C 0 0 0 0 0 0 0 0 0 0 4
-1.0156 -0.2771 -1.1847 C 0 0 0 0 0 0 0 0 0 0 5
-1.7283 -0.3292 0.0243 C 0 0 0 0 0 0 0 0 0 0 6
2.5531 0.1014 0.0741 C 0 0 0 0 0 0 0 0 0 0 7
-3.2308 -0.4494 0.0201 C 0 0 0 0 0 0 0 0 0 0 8
-3.7893 0.8852 -0.0743 O 0 0 0 0 0 0 0 0 0 0 9
3.2139 0.1710 1.1058 O 0 0 0 0 0 0 0 0 0 0 10
3.1247 0.1500 -1.1567 O 0 0 0 0 0 0 0 0 0 0 11
-4.7592 0.7853 -0.0874 H 0 0 0 0 0 0 0 0 0 0 12
-1.5648 -0.2785 2.1812 H 0 0 0 0 0 0 0 0 0 0 13
0.9125 -0.0275 2.1805 H 0 0 0 0 0 0 0 0 0 0 14
0.9126 -0.0997 -2.1355 H 0 0 0 0 0 0 0 0 0 0 15
-1.5536 -0.3537 -2.1320 H 0 0 0 0 0 0 0 0 0 0 16
-3.5727 -0.9394 0.9468 H 0 0 0 0 0 0 0 0 0 0 17
```

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-3.5576 -1.0579 -0.8398 H 0 0 0 0 0 0 0 0 0 0 0 18
4.0935 0.2424 -1.0304 H 0 0 0 0 0 0 0 0 0 0 0 19
2 1 0 0 0 0
6 1 0 0 0 0
13 1 0 0 0 0
3 2 0 0 0 0
14 2 0 0 0 0
4 3 0 0 0 0
7 3 0 0 0 0
5 4 0 0 0 0
15 4 0 0 0 0
6 5 0 0 0 0
16 5 0 0 0 0
8 6 0 0 0 0
10 7 0 0 0 0
11 7 0 0 0 0
9 8 0 0 0 0
17 8 0 0 0 0
18 8 0 0 0 0
12 9 0 0 0 0
11 19 0 0 0 0
M END
$$$$
4-iodobenzoicacid-anion.sdf
COSMOTHERM 3D 0
14 13 0 0 0 0 0 0 0 0 0 V2000
-0.5104 1.2197 -0.0009 C 0 0 0 0 0 0 0 0 0 0 0 1
-1.9095 1.2066 -0.0008 C 0 0 0 0 0 0 0 0 0 0 0 2
-2.6263 0.0000 -0.0001 C 0 0 0 0 0 0 0 0 0 0 0 3
-1.9095 -1.2066 0.0006 C 0 0 0 0 0 0 0 0 0 0 0 4
-0.5104 -1.2198 0.0007 C 0 0 0 0 0 0 0 0 0 0 0 5
0.1716 0.0000 -0.0001 C 0 0 0 0 0 0 0 0 0 0 0 6
-4.1592 0.0000 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 7
2.3164 0.0000 0.0000 I 0 0 0 0 0 0 0 0 0 0 0 8
-4.7341 1.1318 0.0016 O 0 0 0 0 0 0 0 0 0 0 0 9
-4.7341 -1.1318 -0.0015 O 0 0 0 0 0 0 0 0 0 0 0 10
0.0305 2.1664 -0.0016 H 0 0 0 0 0 0 0 0 0 0 0 11
-2.4629 2.1471 -0.0012 H 0 0 0 0 0 0 0 0 0 0 0 12
-2.4629 -2.1472 0.0011 H 0 0 0 0 0 0 0 0 0 0 0 13
0.0305 -2.1664 0.0014 H 0 0 0 0 0 0 0 0 0 0 0 14
2 1 0 0 0 0
6 1 0 0 0 0
11 1 0 0 0 0
3 2 0 0 0 0
12 2 0 0 0 0
4 3 0 0 0 0
7 3 0 0 0 0
5 4 0 0 0 0
13 4 0 0 0 0
6 5 0 0 0 0
9 7 0 0 0 0
10 7 0 0 0 0
5 14 0 0 0 0
M END
$$$$
4-iodobenzoicacid.sdf
COSMOTHERM 3D 0
15 14 0 0 0 0 0 0 0 0 0 V2000
-0.4819 1.2336 -0.0007 C 0 0 0 0 0 0 0 0 0 0 0 1
-1.8770 1.2335 -0.0006 C 0 0 0 0 0 0 0 0 0 0 0 2
-2.5923 0.0243 0.0003 C 0 0 0 0 0 0 0 0 0 0 0 3
-1.8921 -1.1946 0.0011 C 0 0 0 0 0 0 0 0 0 0 0 4
-0.4960 -1.2082 0.0011 C 0 0 0 0 0 0 0 0 0 0 0 5
0.1932 0.0084 0.0002 C 0 0 0 0 0 0 0 0 0 0 0 6
-4.0792 0.0799 0.0001 C 0 0 0 0 0 0 0 0 0 0 0 7
2.3290 -0.0051 -0.0001 I 0 0 0 0 0 0 0 0 0 0 0 8
-4.7359 1.1160 0.0014 O 0 0 0 0 0 0 0 0 0 0 0 9
-4.6563 -1.1480 -0.0020 O 0 0 0 0 0 0 0 0 0 0 0 10
0.0635 2.1767 -0.0016 H 0 0 0 0 0 0 0 0 0 0 0 11
-2.4194 2.1796 -0.0011 H 0 0 0 0 0 0 0 0 0 0 0 12
-2.4344 -2.1397 0.0017 H 0 0 0 0 0 0 0 0 0 0 0 13
0.0384 -2.1577 0.0020 H 0 0 0 0 0 0 0 0 0 0 0 14
-5.6293 -1.0201 -0.0026 H 0 0 0 0 0 0 0 0 0 0 0 15
2 1 0 0 0 0
6 1 0 0 0 0
11 1 0 0 0 0
3 2 0 0 0 0
12 2 0 0 0 0
4 3 0 0 0 0
7 3 0 0 0 0
5 4 0 0 0 0
13 4 0 0 0 0
6 5 0 0 0 0
14 5 0 0 0 0
9 7 0 0 0 0
10 7 0 0 0 0
10 15 0 0 0 0
M END
$$$$
4-methoxybenzoicacid-anion.sdf
COSMOTHERM 3D 0
18 18 0 0 0 0 0 0 0 0 0 V2000
-0.9110 1.4046 -0.0032 C 0 0 0 0 0 0 0 0 0 0 0 1
0.4752 1.2773 -0.0023 C 0 0 0 0 0 0 0 0 0 0 0 2
1.0940 0.0126 0.0001 C 0 0 0 0 0 0 0 0 0 0 0 3
0.2696 -1.1215 0.0014 C 0 0 0 0 0 0 0 0 0 0 0 4
-1.1262 -1.0179 0.0011 C 0 0 0 0 0 0 0 0 0 0 0 5
-1.7227 0.2540 -0.0014 C 0 0 0 0 0 0 0 0 0 0 0 6
2.6140 -0.1198 0.0005 C 0 0 0 0 0 0 0 0 0 0 0 7
-3.0765 0.4755 -0.0028 O 0 0 0 0 0 0 0 0 0 0 0 8
-3.9446 -0.6747 0.0045 C 0 0 0 0 0 0 0 0 0 0 0 9
3.2916 0.9567 0.0070 O 0 0 0 0 0 0 0 0 0 0 0 10
```

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1
2
3      3.0964   -1.2966   -0.0057 O   0   0   0   0   0   0   0   0   0   0   11
4     -1.3871    2.3872   -0.0052 H   0   0   0   0   0   0   0   0   0   0   12
5      1.1065    2.1676   -0.0032 H   0   0   0   0   0   0   0   0   0   0   13
6      0.7394   -2.1067    0.0028 H   0   0   0   0   0   0   0   0   0   0   14
7     -1.7333   -1.9227    0.0024 H   0   0   0   0   0   0   0   0   0   0   15
8     -4.9633   -0.2733    0.0048 H   0   0   0   0   0   0   0   0   0   0   16
9     -3.7917   -1.2932   -0.8930 H   0   0   0   0   0   0   0   0   0   0   17
10    -3.7875   -1.2846    0.9071 H   0   0   0   0   0   0   0   0   0   0   18
11
12      2   1   0   0   0   0
13      6   1   0   0   0   0
14     12   1   0   0   0   0
15      3   2   0   0   0   0
16     13   2   0   0   0   0
17      4   3   0   0   0   0
18      7   3   0   0   0   0
19      5   4   0   0   0   0
20     14   4   0   0   0   0
21      6   5   0   0   0   0
22     15   5   0   0   0   0
23      8   6   0   0   0   0
24     10   7   0   0   0   0
25     11   7   0   0   0   0
26      9   8   0   0   0   0
27     16   9   0   0   0   0
28     17   9   0   0   0   0
29     18   9   0   0   0   0
30
31 M   END
32 $$$
33 4-methoxybenzoicacid.sdf
34 COSMOTHERM      3D      0
35
36 19 19   0   0   0   0   0   0   0   0   0   0 V2000
37   -0.9403    1.4156   -0.0022 C   0   0   0   0   0   0   0   0   0   0   1
38    0.4414    1.3055   -0.0020 C   0   0   0   0   0   0   0   0   0   0   2
39    1.0641    0.0394   -0.0006 C   0   0   0   0   0   0   0   0   0   0   3
40    0.2579   -1.1126    0.0000 C   0   0   0   0   0   0   0   0   0   0   4
41   -1.1331   -1.0159   -0.0001 C   0   0   0   0   0   0   0   0   0   0   5
42   -1.7404    0.2534   -0.0013 C   0   0   0   0   0   0   0   0   0   0   6
43    2.5398   -0.0285    0.0008 C   0   0   0   0   0   0   0   0   0   0   7
44   -3.0855    0.4603   -0.0018 O   0   0   0   0   0   0   0   0   0   0   8
45   -3.9526   -0.6957    0.0042 C   0   0   0   0   0   0   0   0   0   0   9
46    3.2895    0.9467    0.0052 O   0   0   0   0   0   0   0   0   0   0   10
47    3.0216   -1.3026   -0.0033 O   0   0   0   0   0   0   0   0   0   0   11
48   -1.4261    2.3923   -0.0032 H   0   0   0   0   0   0   0   0   0   0   12
49    1.0598    2.2040   -0.0025 H   0   0   0   0   0   0   0   0   0   0   13
50    0.7204   -2.0993    0.0011 H   0   0   0   0   0   0   0   0   0   0   14
51   -1.7319   -1.9252    0.0004 H   0   0   0   0   0   0   0   0   0   0   15
52   -4.9706   -0.2943    0.0060 H   0   0   0   0   0   0   0   0   0   0   16
53   -3.7959   -1.3082   -0.8956 H   0   0   0   0   0   0   0   0   0   0   17
54   -3.7904   -1.3028    0.9066 H   0   0   0   0   0   0   0   0   0   0   18
55    4.0008   -1.2446   -0.0002 H   0   0   0   0   0   0   0   0   0   0   19
56
57      2   1   0   0   0   0
58      6   1   0   0   0   0
59     12   1   0   0   0   0
60      3   2   0   0   0   0
61     13   2   0   0   0   0
62      4   3   0   0   0   0
63      7   3   0   0   0   0
64      5   4   0   0   0   0
65     14   4   0   0   0   0
66      6   5   0   0   0   0
67     15   5   0   0   0   0
68      8   6   0   0   0   0
69     10   7   0   0   0   0
70     11   7   0   0   0   0
71      9   8   0   0   0   0
72     16   9   0   0   0   0
73     17   9   0   0   0   0
74     18   9   0   0   0   0
75     11  19   0   0   0   0
76
77 M   END
78 $$$
79 4-methylaminobenzoicacid-anion.sdf
80 COSMOTHERM      3D      0
81
82 19 19   0   0   0   0   0   0   0   0   0   0 V2000
83   -0.9039    1.4182   -0.0037 C   0   0   0   0   0   0   0   0   0   0   1
84    0.4788    1.2800   -0.0025 C   0   0   0   0   0   0   0   0   0   0   2
85    1.0977    0.0129    0.0000 C   0   0   0   0   0   0   0   0   0   0   3
86    0.2586   -1.1142    0.0024 C   0   0   0   0   0   0   0   0   0   0   4
87   -1.1323   -1.0020    0.0021 C   0   0   0   0   0   0   0   0   0   0   5
88   -1.7482    0.2752   -0.0011 C   0   0   0   0   0   0   0   0   0   0   6
89    2.6090   -0.1275    0.0004 C   0   0   0   0   0   0   0   0   0   0   7
90   -3.1113    0.4253   -0.0020 N   0   0   0   0   0   0   0   0   0   0   8
91   -4.0576   -0.6750    0.0030 C   0   0   0   0   0   0   0   0   0   0   9
92    3.2996    0.9439    0.0075 O   0   0   0   0   0   0   0   0   0   0   10
93    3.0913   -1.3073   -0.0068 O   0   0   0   0   0   0   0   0   0   0   11
94   -3.4821    1.3690   -0.0031 H   0   0   0   0   0   0   0   0   0   0   12
95   -1.3579    2.4129   -0.0061 H   0   0   0   0   0   0   0   0   0   0   13
96    1.1140    2.1682   -0.0041 H   0   0   0   0   0   0   0   0   0   0   14
97    0.7212   -2.1034    0.0043 H   0   0   0   0   0   0   0   0   0   0   15
98   -1.7461   -1.9037    0.0046 H   0   0   0   0   0   0   0   0   0   0   16
99   -5.0718   -0.2604    0.0023 H   0   0   0   0   0   0   0   0   0   0   17
100  -3.9476   -1.3174   -0.8874 H   0   0   0   0   0   0   0   0   0   0   18
101  -3.9460   -1.3107    0.8981 H   0   0   0   0   0   0   0   0   0   0   19
102
103      2   1   0   0   0   0
104      6   1   0   0   0   0
105     13   1   0   0   0   0
106      3   2   0   0   0   0
107     14   2   0   0   0   0
108      4   3   0   0   0   0
109      7   3   0   0   0   0
110      5   4   0   0   0   0
111     15   4   0   0   0   0
112      6   5   0   0   0   0
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16 5 0 0 0 0
8 6 0 0 0 0
10 7 0 0 0 0
11 7 0 0 0 0
9 8 0 0 0 0
12 8 0 0 0 0
17 9 0 0 0 0
18 9 0 0 0 0
9 19 0 0 0 0
M END
$$$$
4-methylaminobenzoicacid.sdf
COSMOtherm 3D 0

20 20 0 0 0 0 0 0 0 0 V2000
-0.9334 1.4307 -0.0018 C 0 0 0 0 0 0 0 0 0 0 1
0.4431 1.3104 -0.0015 C 0 0 0 0 0 0 0 0 0 0 2
1.0685 0.0409 -0.0005 C 0 0 0 0 0 0 0 0 0 0 3
0.2459 -1.1058 0.0001 C 0 0 0 0 0 0 0 0 0 0 4
-1.1383 -1.0018 0.0002 C 0 0 0 0 0 0 0 0 0 0 5
-1.7654 0.2739 -0.0006 C 0 0 0 0 0 0 0 0 0 0 6
2.5323 -0.0343 0.0005 C 0 0 0 0 0 0 0 0 0 0 7
-3.1193 0.4097 -0.0002 N 0 0 0 0 0 0 0 0 0 0 8
-4.0629 -0.6965 0.0019 C 0 0 0 0 0 0 0 0 0 0 9
3.2983 0.9335 0.0035 O 0 0 0 0 0 0 0 0 0 0 10
3.0151 -1.3154 -0.0023 O 0 0 0 0 0 0 0 0 0 0 11
-3.4979 1.3514 -0.0007 H 0 0 0 0 0 0 0 0 0 0 12
-1.3984 2.4191 -0.0026 H 0 0 0 0 0 0 0 0 0 0 13
1.0655 2.2068 -0.0022 H 0 0 0 0 0 0 0 0 0 0 14
0.7021 -2.0961 0.0010 H 0 0 0 0 0 0 0 0 0 0 15
-1.7439 -1.9078 0.0008 H 0 0 0 0 0 0 0 0 0 0 16
-5.0772 -0.2837 0.0043 H 0 0 0 0 0 0 0 0 0 0 17
-3.9482 -1.3307 -0.8921 H 0 0 0 0 0 0 0 0 0 0 18
-3.9439 -1.3308 0.8951 H 0 0 0 0 0 0 0 0 0 0 19
3.9935 -1.2516 0.0004 H 0 0 0 0 0 0 0 0 0 0 20
2 1 0 0 0 0
6 1 0 0 0 0
13 1 0 0 0 0
3 2 0 0 0 0
14 2 0 0 0 0
4 3 0 0 0 0
7 3 0 0 0 0
5 4 0 0 0 0
15 4 0 0 0 0
6 5 0 0 0 0
16 5 0 0 0 0
8 6 0 0 0 0
10 7 0 0 0 0
11 7 0 0 0 0
9 8 0 0 0 0
12 8 0 0 0 0
17 9 0 0 0 0
18 9 0 0 0 0
19 9 0 0 0 0
11 20 0 0 0 0
M END
$$$$
4-methylbenzoicacid-anion.sdf
COSMOtherm 3D 0

17 17 0 0 0 0 0 0 0 0 V2000
1.4618 1.2047 -0.0101 C 0 0 0 0 0 0 0 0 0 0 1
0.0640 1.2046 -0.0045 C 0 0 0 0 0 0 0 0 0 0 2
-0.6582 0.0001 -0.0005 C 0 0 0 0 0 0 0 0 0 0 3
0.0643 -1.2044 -0.0050 C 0 0 0 0 0 0 0 0 0 0 4
1.4619 -1.2045 -0.0105 C 0 0 0 0 0 0 0 0 0 0 5
2.1880 0.0003 -0.0095 C 0 0 0 0 0 0 0 0 0 0 6
3.6968 -0.0001 0.0185 C 0 0 0 0 0 0 0 0 0 0 7
-2.1878 -0.0001 0.0033 C 0 0 0 0 0 0 0 0 0 0 8
-2.7686 1.1306 0.0046 O 0 0 0 0 0 0 0 0 0 0 9
-2.7683 -1.1310 0.0056 O 0 0 0 0 0 0 0 0 0 0 10
2.0019 2.1555 -0.0176 H 0 0 0 0 0 0 0 0 0 0 11
-0.4903 2.1450 -0.0067 H 0 0 0 0 0 0 0 0 0 0 12
-0.4899 -2.1449 -0.0076 H 0 0 0 0 0 0 0 0 0 0 13
2.0019 -2.1553 -0.0185 H 0 0 0 0 0 0 0 0 0 0 14
4.0700 -0.0358 1.0553 H 0 0 0 0 0 0 0 0 0 0 15
4.1075 0.9080 -0.4443 H 0 0 0 0 0 0 0 0 0 0 16
4.1082 -0.8750 -0.5043 H 0 0 0 0 0 0 0 0 0 0 17
2 1 0 0 0 0
6 1 0 0 0 0
11 1 0 0 0 0
3 2 0 0 0 0
12 2 0 0 0 0
4 3 0 0 0 0
8 3 0 0 0 0
5 4 0 0 0 0
13 4 0 0 0 0
6 5 0 0 0 0
14 5 0 0 0 0
7 6 0 0 0 0
15 7 0 0 0 0
16 7 0 0 0 0
9 8 0 0 0 0
10 8 0 0 0 0
7 17 0 0 0 0
M END
$$$$
4-methylbenzoicacid.sdf
COSMOtherm 3D 0

18 18 0 0 0 0 0 0 0 0 V2000
1.4921 1.2082 -0.0093 C 0 0 0 0 0 0 0 0 0 0 1
0.0990 1.2280 -0.0040 C 0 0 0 0 0 0 0 0 0 0 2
-0.6281 0.0242 -0.0002 C 0 0 0 0 0 0 0 0 0 0 3
0.0707 -1.1972 -0.0047 C 0 0 0 0 0 0 0 0 0 0 4
```

```
1
2
3      1.4648   -1.2064   -0.0103 C   0   0   0   0   0   0   0   0   0   0   5
4      2.2014   -0.0076   -0.0092 C   0   0   0   0   0   0   0   0   0   0   6
5      3.7072   -0.0262   0.0169 C   0   0   0   0   0   0   0   0   0   0   7
6     -2.1104    0.0868    0.0029 C   0   0   0   0   0   0   0   0   0   0   8
7     -2.7686    1.1239    0.0040 O   0   0   0   0   0   0   0   0   0   0   9
8     -2.6992   -1.1391    0.0051 O   0   0   0   0   0   0   0   0   0   0   10
9      2.0430    2.1513   -0.0164 H   0   0   0   0   0   0   0   0   0   0   11
10     -0.4397    2.1767   -0.0056 H   0   0   0   0   0   0   0   0   0   0   12
11     -0.4783   -2.1388   -0.0072 H   0   0   0   0   0   0   0   0   0   0   13
12      1.9940   -2.1619   -0.0182 H   0   0   0   0   0   0   0   0   0   0   14
13      4.0735   -0.0657    1.0559 H   0   0   0   0   0   0   0   0   0   0   15
14      4.1283    0.8773   -0.4442 H   0   0   0   0   0   0   0   0   0   0   16
15      4.1065   -0.9081   -0.5023 H   0   0   0   0   0   0   0   0   0   0   17
16     -3.6703   -0.9992    0.0065 H   0   0   0   0   0   0   0   0   0   0   18
17
18      2   1   0   0   0   0
19      6   1   0   0   0   0
20     11   1   0   0   0   0
21      3   2   0   0   0   0
22     12   2   0   0   0   0
23      4   3   0   0   0   0
24      8   3   0   0   0   0
25      5   4   0   0   0   0
26     13   4   0   0   0   0
27      6   5   0   0   0   0
28     14   5   0   0   0   0
29      7   6   0   0   0   0
30     15   7   0   0   0   0
31     16   7   0   0   0   0
32     17   7   0   0   0   0
33      9   8   0   0   0   0
34     10   8   0   0   0   0
35     10 18   0   0   0   0
36
37 M   END
38 $$$
39 4-nitrobenzoicacid-anion.sdf
40 COSMOtherm      3D      0
41
42 16 16   0   0   0   0   0   0   0   0   0   0 V2000
43   0.6867    1.2239    0.0015 C   0   0   0   0   0   0   0   0   0   0   1
44   -0.7066    1.2115    0.0007 C   0   0   0   0   0   0   0   0   0   0   2
45   -1.4190   -0.0001    0.0001 C   0   0   0   0   0   0   0   0   0   0   3
46   -0.7065   -1.2117   -0.0003 C   0   0   0   0   0   0   0   0   0   0   4
47   0.6867   -1.2241   -0.0012 C   0   0   0   0   0   0   0   0   0   0   5
48   1.3651   -0.0001    0.0000 C   0   0   0   0   0   0   0   0   0   0   6
49   -2.9566    0.0000   -0.0001 C   0   0   0   0   0   0   0   0   0   0   7
50   2.8380   -0.0001   -0.0001 N   0   0   0   0   0   0   0   0   0   0   8
51   3.4291   -1.0930   -0.0155 O   0   0   0   0   0   0   0   0   0   0   9
52   3.4287    1.0933    0.0153 O   0   0   0   0   0   0   0   0   0   0   10
53   -3.5248    1.1329   -0.0168 O   0   0   0   0   0   0   0   0   0   0   11
54   -3.5251   -1.1327    0.0165 O   0   0   0   0   0   0   0   0   0   0   12
55   1.2446    2.1591    0.0023 H   0   0   0   0   0   0   0   0   0   0   13
56   -1.2654    2.1477    0.0003 H   0   0   0   0   0   0   0   0   0   0   14
57   -1.2654   -2.1479    0.0001 H   0   0   0   0   0   0   0   0   0   0   15
58   1.2447   -2.1594   -0.0022 H   0   0   0   0   0   0   0   0   0   0   16
59
60      2   1   0   0   0   0
61      6   1   0   0   0   0
62     13   1   0   0   0   0
63      3   2   0   0   0   0
64     14   2   0   0   0   0
65      4   3   0   0   0   0
66      7   3   0   0   0   0
67      5   4   0   0   0   0
68     15   4   0   0   0   0
69      6   5   0   0   0   0
70      8   6   0   0   0   0
71     11   7   0   0   0   0
72     12   7   0   0   0   0
73      9   8   0   0   0   0
74     10   8   0   0   0   0
75     5 16   0   0   0   0
76
77 M   END
78 $$$
79 4-nitrobenzoicacid.sdf
80 COSMOtherm      3D      0
81
82 17 17   0   0   0   0   0   0   0   0   0   0 V2000
83   0.7162    1.2326   -0.0001 C   0   0   0   0   0   0   0   0   0   0   1
84   -0.6758    1.2353   -0.0009 C   0   0   0   0   0   0   0   0   0   0   2
85   -1.3872    0.0235    0.0003 C   0   0   0   0   0   0   0   0   0   0   3
86   -0.6954   -1.2005    0.0017 C   0   0   0   0   0   0   0   0   0   0   4
87   0.6975   -1.2165    0.0008 C   0   0   0   0   0   0   0   0   0   0   5
88   1.3790    0.0025    0.0003 C   0   0   0   0   0   0   0   0   0   0   6
89   -2.8815    0.0823   -0.0013 C   0   0   0   0   0   0   0   0   0   0   7
90   2.8610   -0.0097   -0.0001 N   0   0   0   0   0   0   0   0   0   0   8
91   3.4357   -1.1077   -0.0200 O   0   0   0   0   0   0   0   0   0   0   9
92   3.4539    1.0786    0.0193 O   0   0   0   0   0   0   0   0   0   0   10
93   -3.5276    1.1223   -0.0170 O   0   0   0   0   0   0   0   0   0   0   11
94   -3.4543   -1.1427    0.0165 O   0   0   0   0   0   0   0   0   0   0   12
95   1.2808    2.1632   -0.0008 H   0   0   0   0   0   0   0   0   0   0   13
96   -1.2211    2.1788   -0.0026 H   0   0   0   0   0   0   0   0   0   0   14
97   -1.2439   -2.1410    0.0025 H   0   0   0   0   0   0   0   0   0   0   15
98   1.2479   -2.1556    0.0012 H   0   0   0   0   0   0   0   0   0   0   16
99   -4.4286   -1.0222    0.0114 H   0   0   0   0   0   0   0   0   0   0   17
100
101      2   1   0   0   0   0
102      6   1   0   0   0   0
103     13   1   0   0   0   0
104      3   2   0   0   0   0
105     14   2   0   0   0   0
106      4   3   0   0   0   0
107      7   3   0   0   0   0
108      5   4   0   0   0   0
109     15   4   0   0   0   0
110      6   5   0   0   0   0
111     16   5   0   0   0   0
112      8   6   0   0   0   0
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11 7 0 0 0 0
12 7 0 0 0 0
9 8 0 0 0 0
10 8 0 0 0 0
12 17 0 0 0 0
M END
$$$$
4-phenylbenzoicacid-anion.sdf
COSMOtherm 3D 0

24 25 0 0 0 0 0 0 0 0 0 V2000
-0.2565 1.1704 -0.2985 C 0 0 0 0 0 0 0 0 0 0 1
-1.6523 1.1671 -0.2990 C 0 0 0 0 0 0 0 0 0 0 2
-2.3740 -0.0001 -0.0004 C 0 0 0 0 0 0 0 0 0 0 3
-1.6522 -1.1675 0.2976 C 0 0 0 0 0 0 0 0 0 0 4
-0.2563 -1.1707 0.2964 C 0 0 0 0 0 0 0 0 0 0 5
0.4715 -0.0001 -0.0012 C 0 0 0 0 0 0 0 0 0 0 6
1.9563 0.0001 -0.0011 C 0 0 0 0 0 0 0 0 0 0 7
-3.9047 0.0001 0.0006 C 0 0 0 0 0 0 0 0 0 0 8
4.0796 -1.1204 -0.4532 C 0 0 0 0 0 0 0 0 0 0 9
2.6818 -1.1210 -0.4535 C 0 0 0 0 0 0 0 0 0 0 10
2.6810 1.1214 0.4522 C 0 0 0 0 0 0 0 0 0 0 11
4.0788 1.1206 0.4551 C 0 0 0 0 0 0 0 0 0 0 12
4.7854 0.0000 0.0018 C 0 0 0 0 0 0 0 0 0 0 13
-4.4831 1.0967 -0.2762 O 0 0 0 0 0 0 0 0 0 0 14
-4.4831 -1.0967 0.2785 O 0 0 0 0 0 0 0 0 0 0 15
0.2781 2.0875 -0.5549 H 0 0 0 0 0 0 0 0 0 0 16
-2.2066 2.0760 -0.5397 H 0 0 0 0 0 0 0 0 0 0 17
-2.2062 -2.0764 0.5385 H 0 0 0 0 0 0 0 0 0 0 18
0.2784 -2.0878 0.5525 H 0 0 0 0 0 0 0 0 0 0 19
4.6198 -1.9968 -0.8166 H 0 0 0 0 0 0 0 0 0 0 20
2.1459 -1.9944 -0.8300 H 0 0 0 0 0 0 0 0 0 0 21
2.1444 1.9946 0.8281 H 0 0 0 0 0 0 0 0 0 0 22
4.6183 1.9969 0.8199 H 0 0 0 0 0 0 0 0 0 0 23
5.8768 -0.0001 0.0032 H 0 0 0 0 0 0 0 0 0 0 24

2 1 0 0 0 0
6 1 0 0 0 0
16 1 0 0 0 0
3 2 0 0 0 0
17 2 0 0 0 0
4 3 0 0 0 0
8 3 0 0 0 0
5 4 0 0 0 0
18 4 0 0 0 0
6 5 0 0 0 0
19 5 0 0 0 0
7 6 0 0 0 0
10 7 0 0 0 0
11 7 0 0 0 0
14 8 0 0 0 0
15 8 0 0 0 0
10 9 0 0 0 0
13 9 0 0 0 0
20 9 0 0 0 0
21 10 0 0 0 0
12 11 0 0 0 0
22 11 0 0 0 0
13 12 0 0 0 0
23 12 0 0 0 0
13 24 0 0 0 0
M END
$$$$
4-phenylbenzoicacid.sdf
COSMOtherm 3D 0

25 26 0 0 0 0 0 0 0 0 0 V2000
-0.2278 1.1884 -0.2988 C 0 0 0 0 0 0 0 0 0 0 1
-1.6195 1.1954 -0.3017 C 0 0 0 0 0 0 0 0 0 0 2
-2.3382 0.0242 -0.0035 C 0 0 0 0 0 0 0 0 0 0 3
-1.6318 -1.1546 0.2980 C 0 0 0 0 0 0 0 0 0 0 4
-0.2390 -1.1573 0.2976 C 0 0 0 0 0 0 0 0 0 0 5
0.4915 0.0117 -0.0007 C 0 0 0 0 0 0 0 0 0 0 6
1.9745 0.0026 -0.0007 C 0 0 0 0 0 0 0 0 0 0 7
-3.8223 0.0750 -0.0204 C 0 0 0 0 0 0 0 0 0 0 8
4.0860 -1.1273 -0.4702 C 0 0 0 0 0 0 0 0 0 0 9
2.6887 -1.1190 -0.4685 C 0 0 0 0 0 0 0 0 0 0 10
2.7041 1.1139 0.4677 C 0 0 0 0 0 0 0 0 0 0 11
4.1015 1.1016 0.4715 C 0 0 0 0 0 0 0 0 0 0 12
4.7985 -0.0180 0.0013 C 0 0 0 0 0 0 0 0 0 0 13
-4.4844 1.0730 -0.2895 O 0 0 0 0 0 0 0 0 0 0 14
-4.4013 -1.1140 0.2944 O 0 0 0 0 0 0 0 0 0 0 15
0.3112 2.1022 -0.5537 H 0 0 0 0 0 0 0 0 0 0 16
-2.1643 2.1086 -0.5444 H 0 0 0 0 0 0 0 0 0 0 17
-2.1739 -2.0681 0.5411 H 0 0 0 0 0 0 0 0 0 0 18
0.2913 -2.0756 0.5541 H 0 0 0 0 0 0 0 0 0 0 19
4.6202 -2.0011 -0.8478 H 0 0 0 0 0 0 0 0 0 0 20
2.1459 -1.9827 -0.8567 H 0 0 0 0 0 0 0 0 0 0 21
2.1736 1.9855 0.8554 H 0 0 0 0 0 0 0 0 0 0 22
4.6480 1.9674 0.8500 H 0 0 0 0 0 0 0 0 0 0 23
5.8999 -0.0261 0.0024 H 0 0 0 0 0 0 0 0 0 0 24
-5.3738 -0.9881 0.2578 H 0 0 0 0 0 0 0 0 0 0 25

2 1 0 0 0 0
6 1 0 0 0 0
16 1 0 0 0 0
3 2 0 0 0 0
17 2 0 0 0 0
4 3 0 0 0 0
8 3 0 0 0 0
5 4 0 0 0 0
18 4 0 0 0 0
6 5 0 0 0 0
19 5 0 0 0 0
7 6 0 0 0 0
10 7 0 0 0 0
11 7 0 0 0 0
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1
2
3 14 8 0 0 0 0
4 15 8 0 0 0 0
5 10 9 0 0 0 0
6 13 9 0 0 0 0
7 20 9 0 0 0 0
8 21 10 0 0 0 0
9 12 11 0 0 0 0
10 22 11 0 0 0 0
11 13 12 0 0 0 0
12 23 12 0 0 0 0
13 24 13 0 0 0 0
14 15 25 0 0 0 0
15 M END
16 $$$$
17 4-propylbenzoicacid-anion.sdf
18 COSMOTHERM 3D 0
19
20 23 23 0 0 0 0 0 0 0 0 0 V2000
21 -0.5333 -0.3469 1.2153 C 0 0 0 0 0 0 0 0 0 0 1
22 0.8491 -0.1397 1.2089 C 0 0 0 0 0 0 0 0 0 0 2
23 1.5582 -0.0403 0.0005 C 0 0 0 0 0 0 0 0 0 0 3
24 0.8403 -0.1572 -1.2013 C 0 0 0 0 0 0 0 0 0 0 4
25 -0.5419 -0.3649 -1.1947 C 0 0 0 0 0 0 0 0 0 0 5
26 -1.2558 -0.4606 0.0138 C 0 0 0 0 0 0 0 0 0 0 6
27 3.0713 0.1862 -0.0064 C 0 0 0 0 0 0 0 0 0 0 7
28 -2.7565 -0.6415 0.0202 C 0 0 0 0 0 0 0 0 0 0 8
29 -3.5264 0.6968 -0.0205 C 0 0 0 0 0 0 0 0 0 0 9
30 -5.0463 0.5036 -0.0115 C 0 0 0 0 0 0 0 0 0 0 10
31 3.6499 0.2768 1.1217 O 0 0 0 0 0 0 0 0 0 0 11
32 3.6406 0.2690 -1.1399 O 0 0 0 0 0 0 0 0 0 0 12
33 -1.0639 -0.4263 2.1684 H 0 0 0 0 0 0 0 0 0 0 13
34 1.4022 -0.0569 2.1464 H 0 0 0 0 0 0 0 0 0 0 14
35 1.3867 -0.0879 -2.1438 H 0 0 0 0 0 0 0 0 0 0 15
36 -1.0789 -0.4589 -2.1428 H 0 0 0 0 0 0 0 0 0 0 16
37 -3.0574 -1.1972 0.9236 H 0 0 0 0 0 0 0 0 0 0 17
38 -3.0590 -1.2510 -0.8472 H 0 0 0 0 0 0 0 0 0 0 18
39 -3.2257 1.2562 -0.9219 H 0 0 0 0 0 0 0 0 0 0 19
40 -3.2222 1.3114 0.8428 H 0 0 0 0 0 0 0 0 0 0 20
41 -5.5715 1.4696 -0.0411 H 0 0 0 0 0 0 0 0 0 0 21
42 -5.3732 -0.0287 0.8953 H 0 0 0 0 0 0 0 0 0 0 22
43 -5.3763 -0.0852 -0.8816 H 0 0 0 0 0 0 0 0 0 0 23
44
45 2 1 0 0 0 0
46 6 1 0 0 0 0
47 13 1 0 0 0 0
48 3 2 0 0 0 0
49 14 2 0 0 0 0
50 4 3 0 0 0 0
51 7 3 0 0 0 0
52 5 4 0 0 0 0
53 15 4 0 0 0 0
54 6 5 0 0 0 0
55 16 5 0 0 0 0
56 8 6 0 0 0 0
57 11 7 0 0 0 0
58 12 7 0 0 0 0
59 9 8 0 0 0 0
60 17 8 0 0 0 0
18 8 0 0 0 0
10 9 0 0 0 0
19 9 0 0 0 0
20 9 0 0 0 0
21 10 0 0 0 0
22 10 0 0 0 0
10 23 0 0 0 0
M END
$$$$
4-propylbenzoicacid.sdf
COSMOTHERM 3D 0
24 24 0 0 0 0 0 0 0 0 0 V2000
-0.5616 -0.3352 1.2343 C 0 0 0 0 0 0 0 0 0 0 1
0.8165 -0.1288 1.2377 C 0 0 0 0 0 0 0 0 0 0 2
1.5237 -0.0422 0.0250 C 0 0 0 0 0 0 0 0 0 0 3
0.8222 -0.1684 -1.1885 C 0 0 0 0 0 0 0 0 0 0 4
-0.5566 -0.3759 -1.1810 C 0 0 0 0 0 0 0 0 0 0 5
-1.2739 -0.4613 0.0267 C 0 0 0 0 0 0 0 0 0 0 6
2.9912 0.1743 0.0709 C 0 0 0 0 0 0 0 0 0 0 7
-2.7719 -0.6435 0.0250 C 0 0 0 0 0 0 0 0 0 0 8
-3.5364 0.6985 -0.0369 C 0 0 0 0 0 0 0 0 0 0 9
-5.0561 0.5066 -0.0412 C 0 0 0 0 0 0 0 0 0 0 10
3.6528 0.2779 1.1008 O 0 0 0 0 0 0 0 0 0 0 11
3.5608 0.2512 -1.1615 O 0 0 0 0 0 0 0 0 0 0 12
-1.0972 -0.4056 2.1838 H 0 0 0 0 0 0 0 0 0 0 13
1.3595 -0.0370 2.1794 H 0 0 0 0 0 0 0 0 0 0 14
1.3578 -0.1099 -2.1360 H 0 0 0 0 0 0 0 0 0 0 15
-1.0882 -0.4790 -2.1298 H 0 0 0 0 0 0 0 0 0 0 16
-3.0781 -1.1872 0.9331 H 0 0 0 0 0 0 0 0 0 0 17
-3.0668 -1.2609 -0.8387 H 0 0 0 0 0 0 0 0 0 0 18
-3.2255 1.2472 -0.9411 H 0 0 0 0 0 0 0 0 0 0 19
-3.2393 1.3204 0.8233 H 0 0 0 0 0 0 0 0 0 0 20
-5.5778 1.4738 -0.0853 H 0 0 0 0 0 0 0 0 0 0 21
-5.3929 -0.0159 0.8676 H 0 0 0 0 0 0 0 0 0 0 22
-5.3781 -0.0897 -0.9090 H 0 0 0 0 0 0 0 0 0 0 23
4.5233 0.3919 -1.0331 H 0 0 0 0 0 0 0 0 0 0 24
2 1 0 0 0 0
6 1 0 0 0 0
13 1 0 0 0 0
3 2 0 0 0 0
14 2 0 0 0 0
4 3 0 0 0 0
7 3 0 0 0 0
5 4 0 0 0 0
15 4 0 0 0 0
6 5 0 0 0 0
16 5 0 0 0 0
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8 6 0 0 0 0
11 7 0 0 0 0
12 7 0 0 0 0
9 8 0 0 0 0
17 8 0 0 0 0
18 8 0 0 0 0
10 9 0 0 0 0
19 9 0 0 0 0
20 9 0 0 0 0
21 10 0 0 0 0
22 10 0 0 0 0
23 10 0 0 0 0
12 24 0 0 0 0
M END
$$$$
4-sulfamoylbenzoicacid-anion.sdf
COSMOTHERM 3D 0

19 19 0 0 0 0 0 0 0 0 0 V2000
-0.0481 -0.0551 1.2165 C 0 0 0 0 0 0 0 0 0 0 1
1.3476 -0.0233 1.2076 C 0 0 0 0 0 0 0 0 0 0 2
2.0623 0.0002 -0.0011 C 0 0 0 0 0 0 0 0 0 0 3
1.3532 -0.0029 -1.2129 C 0 0 0 0 0 0 0 0 0 0 4
-0.0433 -0.0307 -1.2289 C 0 0 0 0 0 0 0 0 0 0 5
-0.7253 -0.0552 -0.0080 C 0 0 0 0 0 0 0 0 0 0 6
3.5989 0.0249 0.0035 C 0 0 0 0 0 0 0 0 0 0 7
-2.5391 -0.0849 -0.0073 S 0 0 0 0 0 0 0 0 0 0 8
-2.9886 -0.7789 1.2362 O 0 0 0 0 0 0 0 0 0 0 9
-2.9977 -0.5703 -1.3423 O 0 0 0 0 0 0 0 0 0 0 10
-3.1272 1.5023 0.1238 N 0 0 0 0 0 0 0 0 0 0 11
4.1654 0.0557 1.1374 O 0 0 0 0 0 0 0 0 0 0 12
4.1733 0.0117 -1.1270 O 0 0 0 0 0 0 0 0 0 0 13
-2.8241 1.9378 1.0011 H 0 0 0 0 0 0 0 0 0 0 14
-2.8282 2.0721 -0.6747 H 0 0 0 0 0 0 0 0 0 0 15
-0.5986 -0.0876 2.1575 H 0 0 0 0 0 0 0 0 0 0 16
1.9036 -0.0251 2.1459 H 0 0 0 0 0 0 0 0 0 0 17
1.9135 0.0087 -2.1486 H 0 0 0 0 0 0 0 0 0 0 18
-0.5916 -0.0411 -2.1714 H 0 0 0 0 0 0 0 0 0 0 19
2 1 0 0 0 0
6 1 0 0 0 0
16 1 0 0 0 0
3 2 0 0 0 0
17 2 0 0 0 0
4 3 0 0 0 0
7 3 0 0 0 0
5 4 0 0 0 0
18 4 0 0 0 0
6 5 0 0 0 0
8 6 0 0 0 0
12 7 0 0 0 0
13 7 0 0 0 0
9 8 0 0 0 0
10 8 0 0 0 0
11 8 0 0 0 0
14 11 0 0 0 0
15 11 0 0 0 0
5 19 0 0 0 0
M END
$$$$
4-sulfamoylbenzoicacid.sdf
COSMOTHERM 3D 0

20 20 0 0 0 0 0 0 0 0 0 V2000
-0.0765 -0.0461 1.2276 C 0 0 0 0 0 0 0 0 0 0 1
1.3166 -0.0166 1.2336 C 0 0 0 0 0 0 0 0 0 0 2
2.0303 0.0073 0.0234 C 0 0 0 0 0 0 0 0 0 0 3
1.3407 0.0074 -1.2007 C 0 0 0 0 0 0 0 0 0 0 4
-0.0546 -0.0163 -1.2189 C 0 0 0 0 0 0 0 0 0 0 5
-0.7415 -0.0423 -0.0030 C 0 0 0 0 0 0 0 0 0 0 6
3.5225 0.0229 0.0850 C 0 0 0 0 0 0 0 0 0 0 7
-2.5619 -0.0865 -0.0186 S 0 0 0 0 0 0 0 0 0 0 8
-3.0022 -0.8491 1.1851 O 0 0 0 0 0 0 0 0 0 0 9
-2.9957 -0.5079 -1.3814 O 0 0 0 0 0 0 0 0 0 0 10
-3.1552 1.4840 0.1899 N 0 0 0 0 0 0 0 0 0 0 11
4.1691 0.0531 1.1250 O 0 0 0 0 0 0 0 0 0 0 12
4.0998 -0.0035 -1.1393 O 0 0 0 0 0 0 0 0 0 0 13
-2.8745 1.8760 1.0945 H 0 0 0 0 0 0 0 0 0 0 14
-2.8638 2.1000 -0.5761 H 0 0 0 0 0 0 0 0 0 0 15
-0.6319 -0.0809 2.1651 H 0 0 0 0 0 0 0 0 0 0 16
1.8601 -0.0215 2.1785 H 0 0 0 0 0 0 0 0 0 0 17
1.8903 0.0210 -2.1408 H 0 0 0 0 0 0 0 0 0 0 18
-0.5966 -0.0235 -2.1643 H 0 0 0 0 0 0 0 0 0 0 19
5.0733 0.0090 -1.0139 H 0 0 0 0 0 0 0 0 0 0 20
2 1 0 0 0 0
6 1 0 0 0 0
16 1 0 0 0 0
3 2 0 0 0 0
17 2 0 0 0 0
4 3 0 0 0 0
7 3 0 0 0 0
5 4 0 0 0 0
18 4 0 0 0 0
6 5 0 0 0 0
19 5 0 0 0 0
8 6 0 0 0 0
12 7 0 0 0 0
13 7 0 0 0 0
9 8 0 0 0 0
10 8 0 0 0 0
11 8 0 0 0 0
14 11 0 0 0 0
15 11 0 0 0 0
13 20 0 0 0 0
M END
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4-trifluoromethylbenzoicacid-anion.sdf
COSMOTHERM      3D      0

17 17 0 0 0 0 0 0 0 0 0 V2000
  0.2651 1.2178 -0.0294 C 0 0 0 0 0 0 0 0 0 0 1
 -1.1306 1.2087 -0.0163 C 0 0 0 0 0 0 0 0 0 0 2
 -1.8443 0.0002 -0.0123 C 0 0 0 0 0 0 0 0 0 0 3
 -1.1288 -1.2076 -0.0292 C 0 0 0 0 0 0 0 0 0 0 4
  0.2667 -1.2144 -0.0443 C 0 0 0 0 0 0 0 0 0 0 5
  0.9647 0.0024 -0.0470 C 0 0 0 0 0 0 0 0 0 0 6
 -3.3801 -0.0007 0.0105 C 0 0 0 0 0 0 0 0 0 0 7
  2.4672 0.0010 -0.0013 C 0 0 0 0 0 0 0 0 0 0 8
  2.9450 -0.0595 1.2888 F 0 0 0 0 0 0 0 0 0 0 9
  3.0147 1.1232 -0.5539 F 0 0 0 0 0 0 0 0 0 0 10
  3.0157 -1.0668 -0.6547 F 0 0 0 0 0 0 0 0 0 0 11
 -3.9530 1.1310 0.0062 O 0 0 0 0 0 0 0 0 0 0 12
 -3.9513 -1.1331 0.0336 O 0 0 0 0 0 0 0 0 0 0 13
  0.8061 2.1649 -0.0321 H 0 0 0 0 0 0 0 0 0 0 14
 -1.6881 2.1462 -0.0074 H 0 0 0 0 0 0 0 0 0 0 15
 -1.6851 -2.1458 -0.0292 H 0 0 0 0 0 0 0 0 0 0 16
  0.8089 -2.1609 -0.0588 H 0 0 0 0 0 0 0 0 0 0 17
  2 1 0 0 0 0
  6 1 0 0 0 0
14 1 0 0 0 0
  3 2 0 0 0 0
15 2 0 0 0 0
  4 3 0 0 0 0
  7 3 0 0 0 0
  5 4 0 0 0 0
16 4 0 0 0 0
  6 5 0 0 0 0
  8 6 0 0 0 0
12 7 0 0 0 0
13 7 0 0 0 0
  9 8 0 0 0 0
10 8 0 0 0 0
11 8 0 0 0 0
  5 17 0 0 0 0
M END
$$$$
4-trifluoromethylbenzoicacid.sdf
COSMOTHERM      3D      0

18 18 0 0 0 0 0 0 0 0 0 V2000
  0.2943 1.2296 -0.0284 C 0 0 0 0 0 0 0 0 0 0 1
 -1.0989 1.2345 -0.0147 C 0 0 0 0 0 0 0 0 0 0 2
 -1.8109 0.0244 -0.0116 C 0 0 0 0 0 0 0 0 0 0 3
 -1.1147 -1.1960 -0.0271 C 0 0 0 0 0 0 0 0 0 0 4
  0.2793 -1.2053 -0.0420 C 0 0 0 0 0 0 0 0 0 0 5
  0.9810 0.0077 -0.0434 C 0 0 0 0 0 0 0 0 0 0 6
 -3.3026 0.0808 0.0076 C 0 0 0 0 0 0 0 0 0 0 7
  2.4885 -0.0054 -0.0009 C 0 0 0 0 0 0 0 0 0 0 8
  2.9576 -0.0682 1.2879 F 0 0 0 0 0 0 0 0 0 0 9
  3.0375 1.1115 -0.5564 F 0 0 0 0 0 0 0 0 0 0 10
  3.0206 -1.0775 -0.6551 F 0 0 0 0 0 0 0 0 0 0 11
 -3.9541 1.1187 0.0063 O 0 0 0 0 0 0 0 0 0 0 12
 -3.8768 -1.1453 0.0288 O 0 0 0 0 0 0 0 0 0 0 13
  0.8411 2.1724 -0.0315 H 0 0 0 0 0 0 0 0 0 0 14
 -1.6441 2.1784 -0.0052 H 0 0 0 0 0 0 0 0 0 0 15
 -1.6604 -2.1385 -0.0288 H 0 0 0 0 0 0 0 0 0 0 16
  0.8144 -2.1548 -0.0561 H 0 0 0 0 0 0 0 0 0 0 17
 -4.8504 -1.0215 0.0396 H 0 0 0 0 0 0 0 0 0 0 18
  2 1 0 0 0 0
  6 1 0 0 0 0
14 1 0 0 0 0
  3 2 0 0 0 0
15 2 0 0 0 0
  4 3 0 0 0 0
  7 3 0 0 0 0
  5 4 0 0 0 0
16 4 0 0 0 0
  6 5 0 0 0 0
17 5 0 0 0 0
  8 6 0 0 0 0
12 7 0 0 0 0
13 7 0 0 0 0
  9 8 0 0 0 0
10 8 0 0 0 0
11 8 0 0 0 0
13 18 0 0 0 0
M END
$$$$
5-fluorouracil0-anion.sdf
COSMOTHERM      3D      0

11 11 0 0 0 0 0 0 0 0 0 V2000
 -1.4982 0.0296 0.0002 C 0 0 0 0 0 0 0 0 0 0 1
 -0.6920 1.0886 0.0007 N 0 0 0 0 0 0 0 0 0 0 2
  0.6744 0.8749 0.0001 C 0 0 0 0 0 0 0 0 0 0 3
  1.0716 -0.5146 -0.0002 C 0 0 0 0 0 0 0 0 0 0 4
  0.1502 -1.5256 0.0004 C 0 0 0 0 0 0 0 0 0 0 5
 -1.1916 -1.2750 0.0004 N 0 0 0 0 0 0 0 0 0 0 6
  1.4969 1.8325 0.0000 O 0 0 0 0 0 0 0 0 0 0 7
 -2.8349 0.3365 -0.0009 O 0 0 0 0 0 0 0 0 0 0 8
  2.4153 -0.8074 -0.0005 F 0 0 0 0 0 0 0 0 0 0 9
  0.4649 -2.5726 0.0006 H 0 0 0 0 0 0 0 0 0 0 10
 -3.3179 -0.5147 0.0011 H 0 0 0 0 0 0 0 0 0 0 11
  2 1 0 0 0 0
  6 1 0 0 0 0
  8 1 0 0 0 0
  3 2 0 0 0 0
  4 3 0 0 0 0
  7 3 0 0 0 0
  5 4 0 0 0 0
  9 4 0 0 0 0
```

```
6 5 0 0 0 0
10 5 0 0 0 0
8 11 0 0 0 0
M END
$$$$
5-fluorouracil0.sdf
COSMOTHERM 3D 0
12 12 0 0 0 0 0 0 0 0 0 V2000
-1.6641 0.0462 0.0000 C 0 0 0 0 0 0 0 0 0 0 1
-0.6838 1.0337 -0.0002 N 0 0 0 0 0 0 0 0 0 0 2
0.7109 0.8728 0.0000 C 0 0 0 0 0 0 0 0 0 0 3
1.1050 -0.5246 0.0000 C 0 0 0 0 0 0 0 0 0 0 4
0.1938 -1.5277 0.0001 C 0 0 0 0 0 0 0 0 0 0 5
-1.1483 -1.2402 -0.0001 N 0 0 0 0 0 0 0 0 0 0 6
1.4769 1.8416 0.0001 O 0 0 0 0 0 0 0 0 0 0 7
-2.8710 0.2920 0.0001 O 0 0 0 0 0 0 0 0 0 0 8
2.4325 -0.7908 0.0000 F 0 0 0 0 0 0 0 0 0 0 9
-1.0263 1.9962 -0.0002 H 0 0 0 0 0 0 0 0 0 0 10
-1.8239 -2.0023 0.0003 H 0 0 0 0 0 0 0 0 0 0 11
0.4707 -2.5802 0.0002 H 0 0 0 0 0 0 0 0 0 0 12
2 1 0 0 0 0
6 1 0 0 0 0
8 1 0 0 0 0
3 2 0 0 0 0
10 2 0 0 0 0
4 3 0 0 0 0
7 3 0 0 0 0
5 4 0 0 0 0
9 4 0 0 0 0
6 5 0 0 0 0
11 6 0 0 0 0
5 12 0 0 0 0
M END
$$$$
5-fluorouracil1-anion.sdf
COSMOTHERM 3D 0
11 11 0 0 0 0 0 0 0 0 0 V2000
-0.1043 -1.6198 0.0000 C 0 0 0 0 0 0 0 0 0 0 1
-1.1096 -0.7060 0.0001 N 0 0 0 0 0 0 0 0 0 0 2
-0.8816 0.6455 -0.0001 C 0 0 0 0 0 0 0 0 0 0 3
0.5132 1.0782 0.0000 C 0 0 0 0 0 0 0 0 0 0 4
1.5313 0.1853 -0.0001 C 0 0 0 0 0 0 0 0 0 0 5
1.2246 -1.1505 -0.0004 N 0 0 0 0 0 0 0 0 0 0 6
-1.8244 1.4831 -0.0002 O 0 0 0 0 0 0 0 0 0 0 7
-0.2884 -2.8635 0.0003 O 0 0 0 0 0 0 0 0 0 0 8
0.7835 2.4215 0.0002 F 0 0 0 0 0 0 0 0 0 0 9
1.9714 -1.8421 -0.0004 H 0 0 0 0 0 0 0 0 0 0 10
2.5842 0.4632 0.0000 H 0 0 0 0 0 0 0 0 0 0 11
2 1 0 0 0 0
6 1 0 0 0 0
8 1 0 0 0 0
3 2 0 0 0 0
4 3 0 0 0 0
7 3 0 0 0 0
5 4 0 0 0 0
9 4 0 0 0 0
6 5 0 0 0 0
10 6 0 0 0 0
5 11 0 0 0 0
M END
$$$$
5-fluorouracil1.sdf
COSMOTHERM 3D 0
12 12 0 0 0 0 0 0 0 0 0 V2000
-0.1142 -1.6391 0.0000 C 0 0 0 0 0 0 0 0 0 0 1
-1.1024 -0.6803 0.0003 N 0 0 0 0 0 0 0 0 0 0 2
-0.7927 0.5992 0.0001 C 0 0 0 0 0 0 0 0 0 0 3
0.5550 1.0585 0.0001 C 0 0 0 0 0 0 0 0 0 0 4
1.5576 0.1364 -0.0001 C 0 0 0 0 0 0 0 0 0 0 5
1.2186 -1.1785 0.0004 N 0 0 0 0 0 0 0 0 0 0 6
-1.8191 1.4678 0.0000 O 0 0 0 0 0 0 0 0 0 0 7
-0.3420 -2.8580 -0.0005 O 0 0 0 0 0 0 0 0 0 0 8
0.8082 2.3956 -0.0002 F 0 0 0 0 0 0 0 0 0 0 9
1.9543 -1.8850 -0.0001 H 0 0 0 0 0 0 0 0 0 0 10
2.6152 0.3938 -0.0003 H 0 0 0 0 0 0 0 0 0 0 11
-1.4829 2.3885 -0.0011 H 0 0 0 0 0 0 0 0 0 0 12
2 1 0 0 0 0
6 1 0 0 0 0
8 1 0 0 0 0
3 2 0 0 0 0
4 3 0 0 0 0
7 3 0 0 0 0
5 4 0 0 0 0
9 4 0 0 0 0
6 5 0 0 0 0
11 5 0 0 0 0
10 6 0 0 0 0
7 12 0 0 0 0
M END
$$$$
5-fluorouracil2-anion.sdf
COSMOTHERM 3D 0
11 11 0 0 0 0 0 0 0 0 0 V2000
-1.6487 -0.0175 0.0000 C 0 0 0 0 0 0 0 0 0 0 1
-0.6826 1.0118 -0.0004 N 0 0 0 0 0 0 0 0 0 0 2
0.7089 0.8650 0.0000 C 0 0 0 0 0 0 0 0 0 0 3
1.0793 -0.5178 0.0000 C 0 0 0 0 0 0 0 0 0 0 4
0.1329 -1.5144 0.0001 C 0 0 0 0 0 0 0 0 0 0 5
-1.2065 -1.3076 0.0001 N 0 0 0 0 0 0 0 0 0 0 6
1.4743 1.8547 0.0002 O 0 0 0 0 0 0 0 0 0 0 7
-2.8626 0.3027 0.0001 O 0 0 0 0 0 0 0 0 0 0 8
```

```
2.4199 -0.8186 0.0000 F 0 0 0 0 0 0 0 0 0 0 9
-1.0351 1.9705 0.0001 H 0 0 0 0 0 0 0 0 0 0 10
0.4662 -2.5577 0.0001 H 0 0 0 0 0 0 0 0 0 0 11
2 1 0 0 0 0
6 1 0 0 0 0
8 1 0 0 0 0
3 2 0 0 0 0
10 2 0 0 0 0
4 3 0 0 0 0
7 3 0 0 0 0
5 4 0 0 0 0
9 4 0 0 0 0
6 5 0 0 0 0
5 11 0 0 0 0
M END
$$$$
5-fluorouracil2.sdf
COSMOTHERM 3D 0
12 12 0 0 0 0 0 0 0 0 0 V2000
-0.0324 1.5451 -0.0001 C 0 0 0 0 0 0 0 0 0 0 1
1.0154 0.6759 -0.0001 N 0 0 0 0 0 0 0 0 0 0 2
0.8684 -0.7261 0.0000 C 0 0 0 0 0 0 0 0 0 0 3
-0.5271 -1.1002 -0.0001 C 0 0 0 0 0 0 0 0 0 0 4
-1.5286 -0.1716 0.0000 C 0 0 0 0 0 0 0 0 0 0 5
-1.2920 1.1788 0.0001 N 0 0 0 0 0 0 0 0 0 0 6
1.8481 -1.4808 0.0002 O 0 0 0 0 0 0 0 0 0 0 7
0.3292 2.8338 -0.0001 O 0 0 0 0 0 0 0 0 0 0 8
-0.8008 -2.4293 -0.0001 F 0 0 0 0 0 0 0 0 0 0 9
1.9704 1.0426 -0.0003 H 0 0 0 0 0 0 0 0 0 0 10
-2.5740 -0.4864 0.0002 H 0 0 0 0 0 0 0 0 0 0 11
-0.4860 3.3784 0.0015 H 0 0 0 0 0 0 0 0 0 0 12
2 1 0 0 0 0
6 1 0 0 0 0
8 1 0 0 0 0
3 2 0 0 0 0
10 2 0 0 0 0
4 3 0 0 0 0
7 3 0 0 0 0
5 4 0 0 0 0
9 4 0 0 0 0
6 5 0 0 0 0
11 5 0 0 0 0
8 12 0 0 0 0
M END
$$$$
5-fluorouracil3-anion.sdf
COSMOTHERM 3D 0
11 11 0 0 0 0 0 0 0 0 0 V2000
-1.6263 0.0552 0.0000 C 0 0 0 0 0 0 0 0 0 0 1
-0.6875 1.0861 0.0000 N 0 0 0 0 0 0 0 0 0 0 2
0.5976 0.7819 0.0001 C 0 0 0 0 0 0 0 0 0 0 3
1.0358 -0.5504 -0.0004 C 0 0 0 0 0 0 0 0 0 0 4
0.0759 -1.5455 0.0004 C 0 0 0 0 0 0 0 0 0 0 5
-1.2385 -1.2813 0.0005 N 0 0 0 0 0 0 0 0 0 0 6
1.4715 1.8299 0.0004 O 0 0 0 0 0 0 0 0 0 0 7
-2.8569 0.3468 -0.0005 O 0 0 0 0 0 0 0 0 0 0 8
2.3871 -0.8343 -0.0004 F 0 0 0 0 0 0 0 0 0 0 9
0.3842 -2.5967 0.0005 H 0 0 0 0 0 0 0 0 0 0 10
2.3872 1.4846 0.0002 H 0 0 0 0 0 0 0 0 0 0 11
2 1 0 0 0 0
6 1 0 0 0 0
8 1 0 0 0 0
3 2 0 0 0 0
4 3 0 0 0 0
7 3 0 0 0 0
5 4 0 0 0 0
9 4 0 0 0 0
6 5 0 0 0 0
10 5 0 0 0 0
7 11 0 0 0 0
M END
$$$$
5-fluorouracil3.sdf
COSMOTHERM 3D 0
12 12 0 0 0 0 0 0 0 0 0 V2000
-1.5186 0.0377 -0.0002 C 0 0 0 0 0 0 0 0 0 0 1
-0.6733 1.0780 0.0003 N 0 0 0 0 0 0 0 0 0 0 2
0.6248 0.7852 0.0001 C 0 0 0 0 0 0 0 0 0 0 3
1.0560 -0.5544 -0.0005 C 0 0 0 0 0 0 0 0 0 0 4
0.1054 -1.5537 0.0007 C 0 0 0 0 0 0 0 0 0 0 5
-1.2136 -1.2670 0.0010 N 0 0 0 0 0 0 0 0 0 0 6
1.4718 1.8298 0.0007 O 0 0 0 0 0 0 0 0 0 0 7
-2.8251 0.3802 -0.0010 O 0 0 0 0 0 0 0 0 0 0 8
2.3910 -0.8275 -0.0009 F 0 0 0 0 0 0 0 0 0 0 9
0.3991 -2.6055 0.0015 H 0 0 0 0 0 0 0 0 0 0 10
-3.3491 -0.4472 0.0005 H 0 0 0 0 0 0 0 0 0 0 11
2.3979 1.5109 -0.0002 H 0 0 0 0 0 0 0 0 0 0 12
2 1 0 0 0 0
6 1 0 0 0 0
8 1 0 0 0 0
3 2 0 0 0 0
4 3 0 0 0 0
7 3 0 0 0 0
5 4 0 0 0 0
9 4 0 0 0 0
6 5 0 0 0 0
10 5 0 0 0 0
11 8 0 0 0 0
7 12 0 0 0 0
M END
$$$$
5-iodo-2-hydroxybenzoicacid-anion0.sdf
```



```

9 13 0 0 0 0
M END
$$$$
5-nitrouracil-anion1.sdf
COSMOTHERM 3D 0

13 13 0 0 0 0 0 0 0 0 V2000
0.1753 -1.3717 -0.0004 C 0 0 0 0 0 0 0 0 0 0 1
-0.6070 -0.2001 -0.0005 C 0 0 0 0 0 0 0 0 0 0 2
0.0531 1.0972 -0.0001 C 0 0 0 0 0 0 0 0 0 0 3
1.4492 0.9519 0.0003 N 0 0 0 0 0 0 0 0 0 0 4
2.1942 -0.2315 0.0001 C 0 0 0 0 0 0 0 0 0 0 5
1.4982 -1.4298 -0.0003 N 0 0 0 0 0 0 0 0 0 0 6
-0.4409 2.2327 -0.0002 O 0 0 0 0 0 0 0 0 0 0 7
3.4349 -0.1800 0.0003 O 0 0 0 0 0 0 0 0 0 0 8
-2.0237 -0.3279 0.0000 N 0 0 0 0 0 0 0 0 0 0 9
-0.3546 -2.3277 -0.0006 H 0 0 0 0 0 0 0 0 0 0 10
1.9797 1.8252 0.0008 H 0 0 0 0 0 0 0 0 0 0 11
-2.5277 -1.4842 0.0005 O 0 0 0 0 0 0 0 0 0 0 12
-2.7404 0.6988 0.0001 O 0 0 0 0 0 0 0 0 0 0 13
2 1 0 0 0 0
6 1 0 0 0 0
10 1 0 0 0 0
3 2 0 0 0 0
9 2 0 0 0 0
4 3 0 0 0 0
7 3 0 0 0 0
5 4 0 0 0 0
11 4 0 0 0 0
6 5 0 0 0 0
8 5 0 0 0 0
12 9 0 0 0 0
9 13 0 0 0 0
M END
$$$$
5-nitrouracil.sdf
COSMOTHERM 3D 0

14 14 0 0 0 0 0 0 0 0 V2000
0.1145 -1.3626 -0.0001 C 0 0 0 0 0 0 0 0 0 0 1
-0.6205 -0.2010 -0.0002 C 0 0 0 0 0 0 0 0 0 0 2
0.0513 1.1042 -0.0002 C 0 0 0 0 0 0 0 0 0 0 3
1.4579 0.9722 -0.0002 N 0 0 0 0 0 0 0 0 0 0 4
2.2273 -0.1744 0.0000 C 0 0 0 0 0 0 0 0 0 0 5
1.4577 -1.3500 0.0000 N 0 0 0 0 0 0 0 0 0 0 6
-0.4501 2.2234 -0.0002 O 0 0 0 0 0 0 0 0 0 0 7
3.4511 -0.1917 0.0003 O 0 0 0 0 0 0 0 0 0 0 8
-2.0634 -0.3258 0.0000 N 0 0 0 0 0 0 0 0 0 0 9
-0.3668 -2.3389 -0.0002 H 0 0 0 0 0 0 0 0 0 0 10
1.9768 1.8529 0.0001 H 0 0 0 0 0 0 0 0 0 0 11
1.9740 -2.2304 0.0002 H 0 0 0 0 0 0 0 0 0 0 12
-2.5520 -1.4745 -0.0002 O 0 0 0 0 0 0 0 0 0 0 13
-2.7516 0.7058 0.0005 O 0 0 0 0 0 0 0 0 0 0 14
2 1 0 0 0 0
6 1 0 0 0 0
10 1 0 0 0 0
3 2 0 0 0 0
9 2 0 0 0 0
4 3 0 0 0 0
7 3 0 0 0 0
5 4 0 0 0 0
11 4 0 0 0 0
6 5 0 0 0 0
8 5 0 0 0 0
12 6 0 0 0 0
13 9 0 0 0 0
9 14 0 0 0 0
M END
$$$$
5-nitrouracil2-anion.sdf
COSMOTHERM 3D 0

13 13 0 0 0 0 0 0 0 0 V2000
-0.2417 -1.4325 -0.0038 C 0 0 0 0 0 0 0 0 0 0 1
0.5633 -0.2680 0.0006 C 0 0 0 0 0 0 0 0 0 0 2
-0.1321 0.9893 -0.0017 C 0 0 0 0 0 0 0 0 0 0 3
-1.4459 1.0454 -0.0018 N 0 0 0 0 0 0 0 0 0 0 4
-2.1793 -0.1361 0.0005 C 0 0 0 0 0 0 0 0 0 0 5
-1.5544 -1.4042 -0.0042 N 0 0 0 0 0 0 0 0 0 0 6
0.5358 2.1501 -0.0035 O 0 0 0 0 0 0 0 0 0 0 7
-3.4264 -0.0886 0.0063 O 0 0 0 0 0 0 0 0 0 0 8
1.9630 -0.3653 0.0016 N 0 0 0 0 0 0 0 0 0 0 9
0.2498 -2.4097 -0.0067 H 0 0 0 0 0 0 0 0 0 0 10
2.5286 -1.4778 0.0008 O 0 0 0 0 0 0 0 0 0 0 11
2.6527 0.7193 0.0041 O 0 0 0 0 0 0 0 0 0 0 12
1.5153 1.8869 -0.0026 H 0 0 0 0 0 0 0 0 0 0 13
2 1 0 0 0 0
6 1 0 0 0 0
10 1 0 0 0 0
3 2 0 0 0 0
9 2 0 0 0 0
4 3 0 0 0 0
7 3 0 0 0 0
5 4 0 0 0 0
6 5 0 0 0 0
8 5 0 0 0 0
11 9 0 0 0 0
12 9 0 0 0 0
7 13 0 0 0 0
M END
$$$$
aceticacid-anion.sdf
COSMOTHERM 3D 0

7 6 0 0 0 0 0 0 0 0 V2000
```

1.4421	-0.0806	-0.0002	C	0	0	0	0	0	0	0	0	1
-0.0963	-0.0003	-0.0011	C	0	0	0	0	0	0	0	0	2
-0.7505	-1.0903	0.0003	O	0	0	0	0	0	0	0	0	3
-0.6054	1.1662	0.0003	O	0	0	0	0	0	0	0	0	4
1.8011	-1.1172	-0.0340	H	0	0	0	0	0	0	0	0	5
1.8457	0.4703	-0.8631	H	0	0	0	0	0	0	0	0	6
1.8376	0.4064	0.9044	H	0	0	0	0	0	0	0	0	7
2	1	0	0	0	0							
5	1	0	0	0	0							
6	1	0	0	0	0							
3	2	0	0	0	0							
4	2	0	0	0	0							
1	7	0	0	0	0							
M	END											
\$\$\$\$												
aceticacid.sdf												
COSMOtherm		3D								0		
8	7	0	0	0	0	0	0	0	0	V2000		
1.4608	0.0493	-0.0001	C	0	0	0	0	0	0	0	0	1
-0.0345	-0.0960	-0.0011	C	0	0	0	0	0	0	0	0	2
-0.6519	-1.1529	0.0002	O	0	0	0	0	0	0	0	0	3
-0.6624	1.1098	-0.0001	O	0	0	0	0	0	0	0	0	4
1.9331	-0.9368	-0.0341	H	0	0	0	0	0	0	0	0	5
1.7812	0.6484	-0.8639	H	0	0	0	0	0	0	0	0	6
1.7813	0.5833	0.9059	H	0	0	0	0	0	0	0	0	7
-1.6307	0.9458	0.0044	H	0	0	0	0	0	0	0	0	8
2	1	0	0	0	0							
5	1	0	0	0	0							
6	1	0	0	0	0							
7	1	0	0	0	0							
3	2	0	0	0	0							
4	2	0	0	0	0							
4	8	0	0	0	0							
M	END											
\$\$\$\$												
acrylicacid0-anion.sdf												
COSMOtherm		3D								0		
8	7	0	0	0	0	0	0	0	0	V2000		
2.0014	-0.0221	-0.0049	C	0	0	0	0	0	0	0	0	1
0.8399	0.6448	0.0067	C	0	0	0	0	0	0	0	0	2
-0.5250	-0.0220	0.0014	C	0	0	0	0	0	0	0	0	3
-1.5247	0.7691	-0.0044	O	0	0	0	0	0	0	0	0	4
-0.5800	-1.2906	0.0022	O	0	0	0	0	0	0	0	0	5
2.9643	0.4941	-0.0031	H	0	0	0	0	0	0	0	0	6
2.0101	-1.1152	-0.0167	H	0	0	0	0	0	0	0	0	7
0.8306	1.7397	0.0177	H	0	0	0	0	0	0	0	0	8
2	1	0	0	0	0							
6	1	0	0	0	0							
7	1	0	0	0	0							
3	2	0	0	0	0							
4	3	0	0	0	0							
5												

[illegible]


```
3 2 0 0 0 0
6 2 0 0 0 0
7 2 0 0 0 0
4 3 0 0 0 0
5 3 0 0 0 0
4 8 0 0 0 0
M END
$$$$
carbonicacid0-anion.sdf
COSMOTHERM 3D 0

5 4 0 0 0 0 0 0 0 0 0 V2000
-0.1133 -0.0487 0.0000 C 0 0 0 0 0 0 0 0 0 0 1
-0.0620 -1.3081 0.0000 O 0 0 0 0 0 0 0 0 0 0 2
1.1382 0.6301 0.0000 O 0 0 0 0 0 0 0 0 0 0 3
-1.1060 0.7187 0.0000 O 0 0 0 0 0 0 0 0 0 0 4
1.8234 -0.0665 -0.0005 H 0 0 0 0 0 0 0 0 0 0 5
2 1 0 0 0 0
3 1 0 0 0 0
4 1 0 0 0 0
3 5 0 0 0 0
M END
$$$$
carbonicacid0.sdf
COSMOTHERM 3D 0

6 5 0 0 0 0 0 0 0 0 0 V2000
-0.0002 -0.0991 0.0000 C 0 0 0 0 0 0 0 0 0 0 1
-0.0019 -1.3196 0.0000 O 0 0 0 0 0 0 0 0 0 0 2
1.0909 0.6885 0.0001 O 0 0 0 0 0 0 0 0 0 0 3
-1.0888 0.6915 -0.0001 O 0 0 0 0 0 0 0 0 0 0 4
1.8797 0.1090 -0.0012 H 0 0 0 0 0 0 0 0 0 0 5
-1.8794 0.1144 0.0013 H 0 0 0 0 0 0 0 0 0 0 6
2 1 0 0 0 0
3 1 0 0 0 0
4 1 0 0 0 0
5 3 0 0 0 0
4 6 0 0 0 0
M END
$$$$
carbonicacid1.sdf
COSMOTHERM 3D 0

6 5 0 0 0 0 0 0 0 0 0 V2000
0.0683 -0.0825 0.0000 C 0 0 0 0 0 0 0 0 0 0 1
0.8932 -0.9774 0.0000 O 0 0 0 0 0 0 0 0 0 0 2
0.3372 1.2425 0.0001 O 0 0 0 0 0 0 0 0 0 0 3
-1.2538 -0.3218 0.0001 O 0 0 0 0 0 0 0 0 0 0 4
1.3096 1.3606 -0.0007 H 0 0 0 0 0 0 0 0 0 0 5
-1.7525 0.5215 -0.0011 H 0 0 0 0 0 0 0 0 0 0 6
2 1 0 0 0 0
3 1 0 0 0 0
4 1 0 0 0 0
5 3 0 0 0 0
4 6 0 0 0 0
M END
$$$$
chloroaceticacid0-anion.sdf
COSMOTHERM 3D 0

7 6 0 0 0 0 0 0 0 0 0 V2000
-0.0332 -1.7617 -0.0041 Cl 0 0 0 0 0 0 0 0 0 0 1
0.8419 -0.1342 0.0132 C 0 0 0 0 0 0 0 0 0 0 2
-0.0664 1.1152 0.0009 C 0 0 0 0 0 0 0 0 0 0 3
-1.3180 1.0040 0.0044 O 0 0 0 0 0 0 0 0 0 0 4
0.6236 2.1807 -0.0089 O 0 0 0 0 0 0 0 0 0 0 5
1.4907 -0.1378 -0.8689 H 0 0 0 0 0 0 0 0 0 0 6
1.4592 -0.1408 0.9179 H 0 0 0 0 0 0 0 0 0 0 7
2 1 0 0 0 0
3 2 0 0 0 0
6 2 0 0 0 0
4 3 0 0 0 0
5 3 0 0 0 0
2 7 0 0 0 0
M END
$$$$
chloroaceticacid0.sdf
COSMOTHERM 3D 0

8 7 0 0 0 0 0 0 0 0 0 V2000
-0.0428 -1.7452 -0.0080 Cl 0 0 0 0 0 0 0 0 0 0 1
0.8763 -0.1782 0.0242 C 0 0 0 0 0 0 0 0 0 0 2
0.0480 1.0899 0.0016 C 0 0 0 0 0 0 0 0 0 0 3
-1.2808 0.9110 0.0097 O 0 0 0 0 0 0 0 0 0 0 4
0.5988 2.1806 -0.0167 O 0 0 0 0 0 0 0 0 0 0 5
1.5418 -0.1724 -0.8458 H 0 0 0 0 0 0 0 0 0 0 6
1.4841 -0.1768 0.9359 H 0 0 0 0 0 0 0 0 0 0 7
-1.7089 1.7958 -0.0027 H 0 0 0 0 0 0 0 0 0 0 8
2 1 0 0 0 0
3 2 0 0 0 0
6 2 0 0 0 0
7 2 0 0 0 0
4 3 0 0 0 0
5 3 0 0 0 0
4 8 0 0 0 0
M END
$$$$
chloroaceticacid1-anion.sdf
COSMOTHERM 3D 0

7 6 0 0 0 0 0 0 0 0 0 V2000
1.7617 0.0332 0.0049 Cl 0 0 0 0 0 0 0 0 0 0 1
0.1342 -0.8419 -0.0156 C 0 0 0 0 0 0 0 0 0 0 2
-1.1152 0.0664 -0.0010 C 0 0 0 0 0 0 0 0 0 0 3
-2.1807 -0.6236 0.0105 O 0 0 0 0 0 0 0 0 0 0 4
```


-1.0040	1.3180	-0.0052	O	0	0	0	0	0	0	0	0	5
0.1375	-1.4935	0.8645	H	0	0	0	0	0	0	0	0	6
0.1412	-1.4564	-0.9222	H	0	0	0	0	0	0	0	0	7
2	1	0	0	0	0							
3	2	0	0	0	0							
6	2	0	0	0	0							
4	3	0	0	0	0							
5	3	0	0	0	0							
2	7	0	0	0	0							
M_END												
\$\$\$\$												
chloroaceticacid1.sdf												
COSMOtherm				3D				0				
8	7	0	0	0	0	0	0	0	V2000			
1.7597	0.0337	0.0067	C1	0	0	0	0	0	0	0	0	1
0.1842	-0.8458	-0.0204	C	0	0	0	0	0	0	0	0	2
-1.0068	0.0967	-0.0033	C	0	0	0	0	0	0	0	0	3
-2.1422	-0.6366	0.0134	O	0	0	0	0	0	0	0	0	4
-0.9756	1.3124	-0.0069	O	0	0	0	0	0	0	0	0	5
0.1501	-1.5049	0.8541	H	0	0	0	0	0	0	0	0	6
0.1563	-1.4583	-0.9287	H	0	0	0	0	0	0	0	0	7
-2.9087	-0.0222	0.0157	H	0	0	0	0	0	0	0	0	8
2	1	0	0	0	0							
3	2	0	0	0	0							
6	2	0	0	0	0							
7	2	0	0	0	0							
4	3	0	0	0	0							
5	3	0	0	0	0							
4	8	0	0	0	0							
M_END												
\$\$\$\$												
cis-5-formyluracil-anion0.sdf												
COSMOtherm				3D				0				
13	13	0	0	0	0	0	0	0	V2000			
0.0850	-1.5082	0.0083	C	0	0	0	0	0	0	0	0	1
-0.8309	-0.4735	0.0046	C	0	0	0	0	0	0	0	0	2
-0.3039	0.9149	0.0044	C	0	0	0	0	0	0	0	0	3
1.0621	1.0961	-0.0021	N	0	0	0	0	0	0	0	0	4
1.9319	0.0679	-0.0034	C	0	0	0	0	0	0	0	0	5
1.4029	-1.2639	0.0055	N	0	0	0	0	0	0	0	0	6
-1.0681	1.9089	0.0111	O	0	0	0	0	0	0	0	0	7
3.1778	0.1769	-0.0109	O	0	0	0	0	0	0	0	0	8
-2.2285	-0.8618	0.0009	C	0	0	0	0	0	0	0	0	9
-0.2205	-2.5569	0.0118	H	0	0	0	0	0	0	0	0	10
2.0742	-2.0311	0.0060	H	0	0	0	0	0	0	0	0	11
-3.2245	-0.1286	-0.0164	O	0	0	0	0	0	0	0	0	12
-2.3697	-1.9728	0.0136	H	0	0	0	0	0	0	0	0	13
2	1	0	0	0	0							
6	1	0	0	0	0							
10	1	0	0	0	0							
3	2	0	0	0	0							
9	2	0	0	0	0							
4	3	0	0	0	0							
7	3	0	0	0	0							
5	4	0	0	0	0							
6												

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1
2
3      -1.2761  -1.4096   0.0020 N   0  0  0  0  0  0  0  0  0  0  0  0  6
4      1.9182   1.0687   0.0078 O   0  0  0  0  0  0  0  0  0  0  0  0  7
5      0.1927  -3.1862  -0.0082 O   0  0  0  0  0  0  0  0  0  0  0  0  8
6     -0.8756   2.2589   0.0034 C   0  0  0  0  0  0  0  0  0  0  0  0  9
7     -2.5527   0.2200   0.0091 H   0  0  0  0  0  0  0  0  0  0  0  0 10
8      1.9688  -1.4009  -0.0013 H   0  0  0  0  0  0  0  0  0  0  0  0 11
9     -2.0573  -2.0655   0.0007 H   0  0  0  0  0  0  0  0  0  0  0  0 12
10    -0.1210   3.2302  -0.0153 O   0  0  0  0  0  0  0  0  0  0  0  0 13
11    -1.9821   2.4079   0.0186 H   0  0  0  0  0  0  0  0  0  0  0  0 14
12
13    2  1  0  0  0  0
14    6  1  0  0  0  0
15   10  1  0  0  0  0
16    3  2  0  0  0  0
17    9  2  0  0  0  0
18    4  3  0  0  0  0
19    7  3  0  0  0  0
20    5  4  0  0  0  0
21   11  4  0  0  0  0
22    6  5  0  0  0  0
23    8  5  0  0  0  0
24   12  6  0  0  0  0
25   13  9  0  0  0  0
26    9 14  0  0  0  0
27 M  END
28 $$$$
29 cis-5-formyluracil2-anion.sdf
30 COSMOTHERM      3D      0
31
32   13 13  0  0  0  0  0  0  0  0  0  0  0  0 0 V2000
33   -1.5697  -0.2689   0.0010 C   0  0  0  0  0  0  0  0  0  0  0  0  1
34   -0.6003   0.7615   0.0008 C   0  0  0  0  0  0  0  0  0  0  0  0  2
35    0.7620   0.3063   0.0008 C   0  0  0  0  0  0  0  0  0  0  0  0  3
36    1.0980  -0.9662   0.0007 N   0  0  0  0  0  0  0  0  0  0  0  0  4
37    0.0784  -1.9169  -0.0003 C   0  0  0  0  0  0  0  0  0  0  0  0  5
38   -1.2847  -1.5566   0.0011 N   0  0  0  0  0  0  0  0  0  0  0  0  6
39    1.7540   1.2161   0.0010 O   0  0  0  0  0  0  0  0  0  0  0  0  7
40    0.3755  -3.1331  -0.0021 O   0  0  0  0  0  0  0  0  0  0  0  0  8
41   -0.9264   2.1462  -0.0008 C   0  0  0  0  0  0  0  0  0  0  0  0  9
42   -2.6326   0.0048   0.0014 H   0  0  0  0  0  0  0  0  0  0  0  0 10
43   -0.0615   3.0674  -0.0016 O   0  0  0  0  0  0  0  0  0  0  0  0 11
44   -2.0016   2.4161  -0.0015 H   0  0  0  0  0  0  0  0  0  0  0  0 12
45    1.2870   2.1234  -0.0006 H   0  0  0  0  0  0  0  0  0  0  0  0 13
46
47    2  1  0  0  0  0
48    6  1  0  0  0  0
49   10  1  0  0  0  0
50    3  2  0  0  0  0
51    9  2  0  0  0  0
52    4  3  0  0  0  0
53    7  3  0  0  0  0
54    5  4  0  0  0  0
55    6  5  0  0  0  0
56    8  5  0  0  0  0
57   11  9  0  0  0  0
58   12  9  0  0  0  0
59    7 13  0  0  0  0
60 M  END
$$$
cyanoaceticacid0-anion.sdf
COSMOTHERM      3D      0
8  7  0  0  0  0  0  0  0  0  0  0  0  0 0 V2000
1.5333  -0.2852  -0.0038 C   0  0  0  0  0  0  0  0  0  0  0  0  1
0.2303  -0.9179  -0.0502 C   0  0  0  0  0  0  0  0  0  0  0  0  2
-0.9912   0.0851  -0.0028 C   0  0  0  0  0  0  0  0  0  0  0  0  3
-0.7398   1.3183  -0.0254 O   0  0  0  0  0  0  0  0  0  0  0  0  4
-2.1144  -0.4860   0.0450 O   0  0  0  0  0  0  0  0  0  0  0  0  5
2.5768   0.2336   0.0397 N   0  0  0  0  0  0  0  0  0  0  0  0  6
0.1413  -1.6236   0.7893 H   0  0  0  0  0  0  0  0  0  0  0  0  7
0.1517  -1.5105  -0.9747 H   0  0  0  0  0  0  0  0  0  0  0  0  8
2  1  0  0  0  0
6  1  0  0  0  0
3  2  0  0  0  0
7  2  0  0  0  0
4  3  0  0  0  0
5  3  0  0  0  0
2  8  0  0  0  0
M  END
$$$
cyanoaceticacid0.sdf
COSMOTHERM      3D      0
9  8  0  0  0  0  0  0  0  0  0  0  0  0 0 V2000
1.5649  -0.2644  -0.0017 C   0  0  0  0  0  0  0  0  0  0  0  0  1
0.2567  -0.8959  -0.0431 C   0  0  0  0  0  0  0  0  0  0  0  0  2
-0.8906   0.1119  -0.0066 C   0  0  0  0  0  0  0  0  0  0  0  0  3
-0.7710   1.3226  -0.0197 O   0  0  0  0  0  0  0  0  0  0  0  0  4
-2.0666  -0.5426   0.0362 O   0  0  0  0  0  0  0  0  0  0  0  0  5
2.6204   0.2221   0.0332 N   0  0  0  0  0  0  0  0  0  0  0  0  6
0.1569  -1.5940   0.8023 H   0  0  0  0  0  0  0  0  0  0  0  0  7
0.1698  -1.5003  -0.9600 H   0  0  0  0  0  0  0  0  0  0  0  0  8
-2.7918   0.1203   0.0472 H   0  0  0  0  0  0  0  0  0  0  0  0  9
2  1  0  0  0  0
6  1  0  0  0  0
3  2  0  0  0  0
7  2  0  0  0  0
8  2  0  0  0  0
4  3  0  0  0  0
5  3  0  0  0  0
5  9  0  0  0  0
M  END
$$$
cyanoaceticacid1-anion.sdf
COSMOTHERM      3D      0
8  7  0  0  0  0  0  0  0  0  0  0  0  0 0 V2000
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1.5200 -0.1306 -0.0167 C 0 0 0 0 0 0 0 0 0 0 0 0 1
0.3263 -0.9477 -0.0627 C 0 0 0 0 0 0 0 0 0 0 0 0 2
-0.9792 -0.0384 0.0034 C 0 0 0 0 0 0 0 0 0 0 0 0 3
-1.4561 0.3117 -1.1080 O 0 0 0 0 0 0 0 0 0 0 0 0 4
-1.3919 0.2372 1.1606 O 0 0 0 0 0 0 0 0 0 0 0 0 5
2.4613 0.5588 0.0199 N 0 0 0 0 0 0 0 0 0 0 0 0 6
0.3393 -1.6409 0.7904 H 0 0 0 0 0 0 0 0 0 0 0 0 7
0.3312 -1.5296 -0.9950 H 0 0 0 0 0 0 0 0 0 0 0 0 8
2 1 0 0 0 0 0
6 1 0 0 0 0
3 2 0 0 0 0
7 2 0 0 0 0
4 3 0 0 0 0
5 3 0 0 0 0
2 8 0 0 0 0
M END
$$$$
cyanoaceticacid1.sdf
COSMOTHERM 3D 0
9 8 0 0 0 0 0 0 0 0 0 V2000
1.5357 -0.2679 0.0081 C 0 0 0 0 0 0 0 0 0 0 0 0 1
0.2500 -0.9214 0.1954 C 0 0 0 0 0 0 0 0 0 0 0 0 2
-0.9787 -0.0310 0.0078 C 0 0 0 0 0 0 0 0 0 0 0 0 3
-2.0920 -0.4873 -0.1735 O 0 0 0 0 0 0 0 0 0 0 0 0 4
-0.6923 1.2792 0.1021 O 0 0 0 0 0 0 0 0 0 0 0 0 5
2.5717 0.2366 -0.1521 N 0 0 0 0 0 0 0 0 0 0 0 0 6
0.2014 -1.3323 1.2176 H 0 0 0 0 0 0 0 0 0 0 0 0 7
0.1664 -1.7739 -0.4932 H 0 0 0 0 0 0 0 0 0 0 0 0 8
-1.5262 1.7900 0.0034 H 0 0 0 0 0 0 0 0 0 0 0 0 9
2 1 0 0 0 0
6 1 0 0 0 0
3 2 0 0 0 0
7 2 0 0 0 0
8 2 0 0 0 0
4 3 0 0 0 0
5 3 0 0 0 0
5 9 0 0 0 0
M END
$$$$
dichloroaceticacid0-anion.sdf
COSMOTHERM 3D 0
7 6 0 0 0 0 0 0 0 0 0 V2000
-1.0342 0.0138 1.4985 Cl 0 0 0 0 0 0 0 0 0 0 0 0 1
-0.1317 -0.5202 -0.0003 C 0 0 0 0 0 0 0 0 0 0 0 0 2
1.3310 0.0351 0.0013 C 0 0 0 0 0 0 0 0 0 0 0 0 3
1.4849 1.2800 0.0043 O 0 0 0 0 0 0 0 0 0 0 0 0 4
2.2015 -0.8797 -0.0006 O 0 0 0 0 0 0 0 0 0 0 0 0 5
-1.0310 0.0157 -1.5005 Cl 0 0 0 0 0 0 0 0 0 0 0 0 6
-0.1681 -1.6104 -0.0010 H 0 0 0 0 0 0 0 0 0 0 0 0 7
2 1 0 0 0 0
3 2 0 0 0 0
6 2 0 0 0 0
4 3 0 0 0 0
5 3 0 0 0 0
2 7 0 0 0 0
M END
$$$$
dichloroaceticacid0.sdf
COSMOTHERM 3D 0
8 7 0 0 0 0 0 0 0 0 0 V2000
1.4996 1.0305 -0.0156 Cl 0 0 0 0 0 0 0 0 0 0 0 0 1
0.0008 0.1748 0.5137 C 0 0 0 0 0 0 0 0 0 0 0 0 2
-0.0066 -1.2357 -0.0945 C 0 0 0 0 0 0 0 0 0 0 0 0 3
-0.0155 -1.4781 -1.2841 O 0 0 0 0 0 0 0 0 0 0 0 0 4
-0.0008 -2.1457 0.8929 O 0 0 0 0 0 0 0 0 0 0 0 0 5
-1.4903 1.0465 -0.0096 Cl 0 0 0 0 0 0 0 0 0 0 0 0 6
0.0032 0.1556 1.6039 H 0 0 0 0 0 0 0 0 0 0 0 0 7
-0.0039 -3.0456 0.4959 H 0 0 0 0 0 0 0 0 0 0 0 0 8
2 1 0 0 0 0
3 2 0 0 0 0
6 2 0 0 0 0
7 2 0 0 0 0
4 3 0 0 0 0
5 3 0 0 0 0
5 8 0 0 0 0
M END
$$$$
dimethadione0-anion.sdf
COSMOTHERM 3D 0
15 15 0 0 0 0 0 0 0 0 0 V2000
0.7500 -0.5547 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 1
0.4961 0.9706 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 2
-0.6162 -1.0791 0.0000 O 0 0 0 0 0 0 0 0 0 0 0 0 3
-1.4856 0.0182 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 4
-0.8385 1.2206 0.0002 N 0 0 0 0 0 0 0 0 0 0 0 0 5
1.4632 -1.0082 -1.2721 C 0 0 0 0 0 0 0 0 0 0 0 0 6
1.4633 -1.0081 1.2721 C 0 0 0 0 0 0 0 0 0 0 0 0 7
1.4126 1.8145 -0.0001 O 0 0 0 0 0 0 0 0 0 0 0 0 8
-2.7021 -0.1934 -0.0001 O 0 0 0 0 0 0 0 0 0 0 0 0 9
0.8953 -0.7152 -2.1664 H 0 0 0 0 0 0 0 0 0 0 0 0 10
2.4565 -0.5411 -1.3225 H 0 0 0 0 0 0 0 0 0 0 0 0 11
1.5892 -2.1002 -1.2731 H 0 0 0 0 0 0 0 0 0 0 0 0 12
0.8952 -0.7155 2.1664 H 0 0 0 0 0 0 0 0 0 0 0 0 13
2.4564 -0.5407 1.3227 H 0 0 0 0 0 0 0 0 0 0 0 0 14
1.5898 -2.1001 1.2730 H 0 0 0 0 0 0 0 0 0 0 0 0 15
2 1 0 0 0 0
3 1 0 0 0 0
6 1 0 0 0 0
7 1 0 0 0 0
5 2 0 0 0 0
8 2 0 0 0 0
```

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4    3    0    0    0    0
5    4    0    0    0    0
9    4    0    0    0    0
10   6    0    0    0    0
11   6    0    0    0    0
12   6    0    0    0    0
13   7    0    0    0    0
14   7    0    0    0    0
17   5    0    0    0    0
M      END
$$$$
dimethadione0.sdf
COSMOtherm          3D                      0

16 16 0 0 0 0 0 0 0 0 V2000
-0.7691      0.5618      0.0000 C      0 0 0 0 0 0 0 0 0 0 0 0 1
-0.5691     -0.9626      0.0001 C      0 0 0 0 0 0 0 0 0 0 0 2
0.6262      1.0735      0.0004 O      0 0 0 0 0 0 0 0 0 0 0 3
1.5080      0.0409      0.0001 C      0 0 0 0 0 0 0 0 0 0 0 4
0.7949     -1.1558      0.0002 N      0 0 0 0 0 0 0 0 0 0 0 5
-1.4585      1.0319      1.2759 C      0 0 0 0 0 0 0 0 0 0 0 6
-1.4575      1.0316     -1.2765 C      0 0 0 0 0 0 0 0 0 0 0 7
-1.4365     -1.8228      0.0000 O      0 0 0 0 0 0 0 0 0 0 0 8
2.7154      0.1782      0.0000 O      0 0 0 0 0 0 0 0 0 0 0 9
1.2553     -2.0654     -0.0003 H      0 0 0 0 0 0 0 0 0 0 0 10
-0.9021      0.7155      2.1683 H      0 0 0 0 0 0 0 0 0 0 0 11
-2.4687      0.6037      1.3203 H      0 0 0 0 0 0 0 0 0 0 0 12
-1.5401      2.1266      1.2711 H      0 0 0 0 0 0 0 0 0 0 0 13
-0.9020      0.7124     -2.1685 H      0 0 0 0 0 0 0 0 0 0 0 14
-2.4688      0.6059     -1.3202 H      0 0 0 0 0 0 0 0 0 0 0 15
-1.5362      2.1265     -1.2733 H      0 0 0 0 0 0 0 0 0 0 0 16

2    1    0    0    0    0
3    1    0    0    0    0
6    1    0    0    0    0
7    1    0    0    0    0
5    2    0    0    0    0
8    2    0    0    0    0
4    3    0    0    0    0
5    4    0    0    0    0
9    4    0    0    0    0
10   5    0    0    0    0
11   6    0    0    0    0
12   6    0    0    0    0
13   6    0    0    0    0
14   7    0    0    0    0
15   7    0    0    0    0
17   6    0    0    0    0
M      END
$$$$
dimethadionel-anion.sdf
COSMOtherm          3D                      0

15 15 0 0 0 0 0 0 0 0 V2000
0.7500     -0.5547      0.0000 C      0 0 0 0 0 0 0 0 0 0 0 1
0.4961      0.9706      0.0000 C      0 0 0 0 0 0 0 0 0 0 0 2
-0.6162     -1.0791      0.0000 O      0 0 0 0 0 0 0 0 0 0 0 3
-1.4856      0.0182      0.0000 C      0 0 0 0 0 0 0 0 0 0 0 4
-0.8385      1.2206      0.0002 N      0 0 0 0 0 0 0 0 0 0 0 5
1.4632     -1.0082     -1.2721 C      0 0 0 0 0 0 0 0 0 0 0 6
1.4633     -1.0081      1.2721 C      0 0 0 0 0 0 0 0 0 0 0 7
1.4126      1.8145     -0.0001 O      0 0 0 0 0 0 0 0 0 0 0 8
-2.7021     -0.1934     -0.0001 O      0 0 0 0 0 0 0 0 0 0 0 9
0.8953     -0.7152     -2.1664 H      0 0 0 0 0 0 0 0 0 0 0 10
2.4565     -0.5411     -1.3225 H      0 0 0 0 0 0 0 0 0 0 0 11
1.5892     -2.1002     -1.2731 H      0 0 0 0 0 0 0 0 0 0 0 12
0.8952     -0.7155      2.1664 H      0 0 0 0 0 0 0 0 0 0 0 13
2.4564     -0.5407      1.3227 H      0 0 0 0 0 0 0 0 0 0 0 14
1.5898     -2.1001      1.2730 H      0 0 0 0 0 0 0 0 0 0 0 15

2    1    0    0    0    0
3    1    0    0    0    0
6    1    0    0    0    0
7    1    0    0    0    0
5    2    0    0    0    0
8    2    0    0    0    0
4    3    0    0    0    0
5    4    0    0    0    0
9    4    0    0    0    0
10   6    0    0    0    0
11   6    0    0    0    0
12   6    0    0    0    0
13   7    0    0    0    0
14   7    0    0    0    0
17   5    0    0    0    0
M      END
$$$$
dimethadionel1.sdf
COSMOtherm          3D                      0

16 16 0 0 0 0 0 0 0 0 V2000
0.7876      0.5560      0.0000 C      0 0 0 0 0 0 0 0 0 0 0 1
0.5436     -0.9727      0.0000 C      0 0 0 0 0 0 0 0 0 0 0 2
-0.6223      1.0597     -0.0008 O      0 0 0 0 0 0 0 0 0 0 0 3
-1.3848     -0.0375     -0.0002 C      0 0 0 0 0 0 0 0 0 0 0 4
-0.8236     -1.2250      0.0002 N      0 0 0 0 0 0 0 0 0 0 0 5
1.4661      1.0290      1.2772 C      0 0 0 0 0 0 0 0 0 0 0 6
1.4678      1.0294     -1.2761 C      0 0 0 0 0 0 0 0 0 0 0 7
1.4327     -1.8181     -0.0003 O      0 0 0 0 0 0 0 0 0 0 0 8
-2.6904      0.1266      0.0000 O      0 0 0 0 0 0 0 0 0 0 0 9
0.8982      0.7253      2.1669 H      0 0 0 0 0 0 0 0 0 0 0 10
2.4663      0.5782      1.3315 H      0 0 0 0 0 0 0 0 0 0 0 11
1.5726      2.1218      1.2706 H      0 0 0 0 0 0 0 0 0 0 0 12
0.9015      0.7252     -2.1666 H      0 0 0 0 0 0 0 0 0 0 0 13
2.4685      0.5795     -1.3287 H      0 0 0 0 0 0 0 0 0 0 0 14
1.5734      2.1222     -1.2693 H      0 0 0 0 0 0 0 0 0 0 0 15
-2.9162      1.0817     -0.0023 H      0 0 0 0 0 0 0 0 0 0 0 16

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[illegible]

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4 1 0 0 0 0
5 1 0 0 0 0
6 1 0 0 0 0
3 2 0 0 0 0
7 2 0 0 0 0
2 8 0 0 0 0
M END
$$$$
ethanol.sdf
COSMOTHERM 3D 0
9 8 0 0 0 0 0 0 0 0 0 V2000
1.2720 0.0000 0.2530 C 0 0 0 0 0 0 0 0 0 0 1
0.0012 0.0000 -0.5761 C 0 0 0 0 0 0 0 0 0 0 2
-1.1321 0.0000 0.3241 O 0 0 0 0 0 0 0 0 0 0 3
2.1521 0.0008 -0.4063 H 0 0 0 0 0 0 0 0 0 0 4
1.3239 0.8929 0.8933 H 0 0 0 0 0 0 0 0 0 0 5
1.3246 -0.8937 0.8922 H 0 0 0 0 0 0 0 0 0 0 6
-0.0318 -0.8924 -1.2259 H 0 0 0 0 0 0 0 0 0 0 7
-0.0318 0.8925 -1.2258 H 0 0 0 0 0 0 0 0 0 0 8
-1.9393 -0.0004 -0.2211 H 0 0 0 0 0 0 0 0 0 0 9
2 1 0 0 0 0
4 1 0 0 0 0
5 1 0 0 0 0
6 1 0 0 0 0
3 2 0 0 0 0
7 2 0 0 0 0
8 2 0 0 0 0
3 9 0 0 0 0
M END
$$$$
fluoroaceticacid0-anion.sdf
COSMOTHERM 3D 0
7 6 0 0 0 0 0 0 0 0 0 V2000
-0.0701 -1.8291 -0.0065 F 0 0 0 0 0 0 0 0 0 0 1
0.7532 -0.6667 0.0096 C 0 0 0 0 0 0 0 0 0 0 2
-0.0496 0.6469 0.0005 C 0 0 0 0 0 0 0 0 0 0 3
-1.3090 0.5981 0.0030 O 0 0 0 0 0 0 0 0 0 0 4
0.6892 1.6789 -0.0055 O 0 0 0 0 0 0 0 0 0 0 5
1.4027 -0.7141 -0.8765 H 0 0 0 0 0 0 0 0 0 0 6
1.3718 -0.7184 0.9175 H 0 0 0 0 0 0 0 0 0 0 7
2 1 0 0 0 0
3 2 0 0 0 0
6 2 0 0 0 0
4 3 0 0 0 0
5 3 0 0 0 0
2 7 0 0 0 0
M END
$$$$
fluoroaceticacid0.sdf
COSMOTHERM 3D 0
8 7 0 0 0 0 0 0 0 0 0 V2000
-0.0925 -1.8060 -0.0073 F 0 0 0 0 0 0 0 0 0 0 1
0.7798 -0.7071 0.0102 C 0 0 0 0 0 0 0 0 0 0 2
0.0619 0.6286 0.0006 C 0 0 0 0 0 0 0 0 0 0 3
-1.2773 0.5276 0.0039 O 0 0 0 0 0 0 0 0 0 0 4
0.6813 1.6813 -0.0060 O 0 0 0 0 0 0 0 0 0 0 5
1.4296 -0.7595 -0.8750 H 0 0 0 0 0 0 0 0 0 0 6
1.3968 -0.7632 0.9186 H 0 0 0 0 0 0 0 0 0 0 7
-1.6534 1.4359 -0.0018 H 0 0 0 0 0 0 0 0 0 0 8
2 1 0 0 0 0
3 2 0 0 0 0
6 2 0 0 0 0
7 2 0 0 0 0
4 3 0 0 0 0
5 3 0 0 0 0
4 8 0 0 0 0
M END
$$$$
fluoroaceticacid1-anion.sdf
COSMOTHERM 3D 0
7 6 0 0 0 0 0 0 0 0 0 V2000
1.8290 0.0701 0.0005 F 0 0 0 0 0 0 0 0 0 0 1
0.6666 -0.7533 -0.0008 C 0 0 0 0 0 0 0 0 0 0 2
-0.6469 0.0496 -0.0001 C 0 0 0 0 0 0 0 0 0 0 3
-1.6789 -0.6890 0.0004 O 0 0 0 0 0 0 0 0 0 0 4
-0.5980 1.3090 -0.0002 O 0 0 0 0 0 0 0 0 0 0 5
0.7160 -1.3887 0.8956 H 0 0 0 0 0 0 0 0 0 0 6
0.7162 -1.3862 -0.8988 H 0 0 0 0 0 0 0 0 0 0 7
2 1 0 0 0 0
3 2 0 0 0 0
6 2 0 0 0 0
4 3 0 0 0 0
5 3 0 0 0 0
2 7 0 0 0 0
M END
$$$$
fluoroaceticacid1.sdf
COSMOTHERM 3D 0
8 7 0 0 0 0 0 0 0 0 0 V2000
1.8340 0.0683 0.0074 F 0 0 0 0 0 0 0 0 0 0 1
0.7052 -0.7562 -0.0105 C 0 0 0 0 0 0 0 0 0 0 2
-0.5548 0.0914 -0.0017 C 0 0 0 0 0 0 0 0 0 0 3
-1.6436 -0.7060 0.0061 O 0 0 0 0 0 0 0 0 0 0 4
-0.5847 1.3082 -0.0032 O 0 0 0 0 0 0 0 0 0 0 5
0.7247 -1.4072 0.8754 H 0 0 0 0 0 0 0 0 0 0 6
0.7308 -1.3750 -0.9193 H 0 0 0 0 0 0 0 0 0 0 7
-2.4473 -0.1412 0.0045 H 0 0 0 0 0 0 0 0 0 0 8
2 1 0 0 0 0
3 2 0 0 0 0
6 2 0 0 0 0
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7 2 0 0 0 0
4 3 0 0 0 0
5 3 0 0 0 0
4 8 0 0 0 0
M END
$$$$
formicacid-anion.sdf
COSMOTHERM 3D 0

4 3 0 0 0 0 0 0 0 0 0 V2000
-0.3690 0.0000 0.0000 C 0 0 0 0 0 0 0 0 0 0 1
0.1857 1.1375 0.0000 O 0 0 0 0 0 0 0 0 0 0 2
0.1857 -1.1375 0.0000 O 0 0 0 0 0 0 0 0 0 0 3
-1.4974 0.0000 0.0000 H 0 0 0 0 0 0 0 0 0 0 4
2 1 0 0 0 0
3 1 0 0 0 0
1 4 0 0 0 0
M END
$$$$
formicacid.sdf
COSMOTHERM 3D 0

5 4 0 0 0 0 0 0 0 0 0 V2000
-0.4154 -0.0935 0.0000 C 0 0 0 0 0 0 0 0 0 0 1
0.1224 1.1398 0.0000 O 0 0 0 0 0 0 0 0 0 0 2
0.2155 -1.1348 0.0000 O 0 0 0 0 0 0 0 0 0 0 3
-1.5169 -0.0240 -0.0001 H 0 0 0 0 0 0 0 0 0 0 4
1.1032 1.0584 -0.0003 H 0 0 0 0 0 0 0 0 0 0 5
2 1 0 0 0 0
3 1 0 0 0 0
4 1 0 0 0 0
2 5 0 0 0 0
M END
$$$$
fumaricacid-anion.sdf
COSMOTHERM 3D 0

11 10 0 0 0 0 0 0 0 0 0 V2000
0.4898 0.3983 -0.0002 C 0 0 0 0 0 0 0 0 0 0 1
-0.5575 -0.4432 -0.0051 C 0 0 0 0 0 0 0 0 0 0 2
-2.0068 0.0182 -0.0010 C 0 0 0 0 0 0 0 0 0 0 3
1.8859 -0.0842 -0.0009 C 0 0 0 0 0 0 0 0 0 0 4
2.2540 -1.2553 -0.0160 O 0 0 0 0 0 0 0 0 0 0 5
2.7666 0.9554 0.0178 O 0 0 0 0 0 0 0 0 0 0 6
-2.8702 -0.9152 0.0204 O 0 0 0 0 0 0 0 0 0 0 7
-2.2364 1.2646 -0.0175 O 0 0 0 0 0 0 0 0 0 0 8
0.3271 1.4779 0.0057 H 0 0 0 0 0 0 0 0 0 0 9
-0.3870 -1.5238 -0.0101 H 0 0 0 0 0 0 0 0 0 0 10
3.6743 0.5809 0.0156 H 0 0 0 0 0 0 0 0 0 0 11
2 1 0 0 0 0
4 1 0 0 0 0
9 1 0 0 0 0
3 2 0 0 0 0
10 2 0 0 0 0
7 3 0 0 0 0
8 3 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
6 11 0 0 0 0
M END
$$$$
fumaricacid.sdf
COSMOTHERM 3D 0

12 11 0 0 0 0 0 0 0 0 0 V2000
0.5222 0.4207 -0.0018 C 0 0 0 0 0 0 0 0 0 0 1
-0.5222 -0.4208 -0.0017 C 0 0 0 0 0 0 0 0 0 0 2
-1.9185 0.0858 -0.0009 C 0 0 0 0 0 0 0 0 0 0 3
1.9185 -0.0858 -0.0009 C 0 0 0 0 0 0 0 0 0 0 4
2.2500 -1.2642 -0.0096 O 0 0 0 0 0 0 0 0 0 0 5
2.8032 0.9402 0.0110 O 0 0 0 0 0 0 0 0 0 0 6
-2.8033 -0.9402 0.0109 O 0 0 0 0 0 0 0 0 0 0 7
-2.2499 1.2642 -0.0096 O 0 0 0 0 0 0 0 0 0 0 8
0.3752 1.5021 -0.0011 H 0 0 0 0 0 0 0 0 0 0 9
-0.3752 -1.5022 -0.0009 H 0 0 0 0 0 0 0 0 0 0 10
3.7109 0.5642 0.0105 H 0 0 0 0 0 0 0 0 0 0 11
-3.7109 -0.5641 0.0105 H 0 0 0 0 0 0 0 0 0 0 12
2 1 0 0 0 0
4 1 0 0 0 0
9 1 0 0 0 0
3 2 0 0 0 0
10 2 0 0 0 0
7 3 0 0 0 0
8 3 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
11 6 0 0 0 0
7 12 0 0 0 0
M END
$$$$
hypobromousacid-anion.sdf
COSMOTHERM 3D 0

2 0 0 0 0 0 0 0 0 0 0 V2000
-1.5538 0.0000 0.0000 O 0 0 0 0 0 0 0 0 0 0 1
0.3111 0.0000 0.0000 Br 0 0 0 0 0 0 0 0 0 0 2
M END
$$$$
hypobromousacid.sdf
COSMOTHERM 3D 0

3 1 0 0 0 0 0 0 0 0 0 V2000
-1.5419 0.0632 0.0000 O 0 0 0 0 0 0 0 0 0 0 1
0.3313 -0.0015 0.0000 Br 0 0 0 0 0 0 0 0 0 0 2
-1.7912 -0.8853 0.0000 H 0 0 0 0 0 0 0 0 0 0 3
```

```
1 3 0 0 0 0
M END
$$$$
hypochlorousacid-anion.sdf
COSMOtherm 3D 0

2 1 0 0 0 0 0 0 0 0 0 V2000
-1.2070 0.0000 0.0000 O 0 0 0 0 0 0 0 0 0 0 1
0.5447 0.0000 0.0000 Cl 0 0 0 0 0 0 0 0 0 0 2
1 2 0 0 0 0
M END
$$$$
hypochlorousacid.sdf
COSMOtherm 3D 0

3 2 0 0 0 0 0 0 0 0 0 V2000
-1.1727 0.0638 0.0000 O 0 0 0 0 0 0 0 0 0 0 1
0.5697 -0.0036 0.0000 Cl 0 0 0 0 0 0 0 0 0 0 2
-1.4219 -0.8856 0.0000 H 0 0 0 0 0 0 0 0 0 0 3
2 1 0 0 0 0
1 3 0 0 0 0
M END
$$$$
hypoiodousacid-anion.sdf
COSMOtherm 3D 0

2 0 0 0 0 0 0 0 0 0 0 V2000
-1.8041 0.0000 0.0000 O 0 0 0 0 0 0 0 0 0 0 1
0.2274 0.0000 0.0000 I 0 0 0 0 0 0 0 0 0 0 2
M END
$$$$
hypoiodousacid.sdf
COSMOtherm 3D 0

3 1 0 0 0 0 0 0 0 0 0 V2000
-1.8114 0.0626 0.0000 O 0 0 0 0 0 0 0 0 0 0 1
0.2448 -0.0009 0.0000 I 0 0 0 0 0 0 0 0 0 0 2
-2.0735 -0.8813 0.0000 H 0 0 0 0 0 0 0 0 0 0 3
1 3 0 0 0 0
M END
$$$$
hypophosphorousacid-anion.sdf
COSMOtherm 3D 0

5 4 0 0 0 0 0 0 0 0 0 V2000
1.3430 -0.4208 0.0000 O 0 0 0 0 0 0 0 0 0 0 1
0.0000 0.3520 0.0000 P 0 0 0 0 0 0 0 0 0 0 2
-1.3430 -0.4208 0.0000 O 0 0 0 0 0 0 0 0 0 0 3
0.0000 1.2710 1.1157 H 0 0 0 0 0 0 0 0 0 0 4
0.0001 1.2711 -1.1157 H 0 0 0 0 0 0 0 0 0 0 5
2 1 0 0 0 0
3 2 0 0 0 0
4 2 0 0 0 0
2 5 0 0 0 0
M END
$$$$
hypophosphorousacid.sdf
COSMOtherm 3D 0

6 5 0 0 0 0 0 0 0 0 0 V2000
-0.0222 1.1316 1.2714 H 0 0 0 0 0 0 0 0 0 0 1
0.0815 -0.0004 0.4132 P 0 0 0 0 0 0 0 0 0 0 2
-0.0175 -1.1343 1.2692 H 0 0 0 0 0 0 0 0 0 0 3
1.2913 0.0010 -0.5059 O 0 0 0 0 0 0 0 0 0 0 4
-1.3133 -0.0016 -0.4605 O 0 0 0 0 0 0 0 0 0 0 5
-2.1151 0.0223 0.1008 H 0 0 0 0 0 0 0 0 0 0 6
2 1 0 0 0 0
3 2 0 0 0 0
4 2 0 0 0 0
5 2 0 0 0 0
5 6 0 0 0 0
M END
$$$$
iodoaceticacid0-anion.sdf
COSMOtherm 3D 0

7 5 0 0 0 0 0 0 0 0 0 V2000
-0.0077 -1.0024 -0.0018 I 0 0 0 0 0 0 0 0 0 0 1
0.8993 1.0299 0.0231 C 0 0 0 0 0 0 0 0 0 0 2
-0.0767 2.2226 0.0013 C 0 0 0 0 0 0 0 0 0 0 3
-1.3214 2.0633 0.0082 O 0 0 0 0 0 0 0 0 0 0 4
0.5725 3.3153 -0.0171 O 0 0 0 0 0 0 0 0 0 0 5
1.5525 1.0389 -0.8544 H 0 0 0 0 0 0 0 0 0 0 6
1.5048 1.0362 0.9346 H 0 0 0 0 0 0 0 0 0 0 7
3 2 0 0 0 0
6 2 0 0 0 0
4 3 0 0 0 0
5 3 0 0 0 0
2 7 0 0 0 0
M END
$$$$
iodoaceticacid0.sdf
COSMOtherm 3D 0

8 6 0 0 0 0 0 0 0 0 0 V2000
-0.0101 -1.0009 -0.0031 I 0 0 0 0 0 0 0 0 0 0 1
0.9342 0.9722 0.0364 C 0 0 0 0 0 0 0 0 0 0 2
0.0422 2.1901 0.0025 C 0 0 0 0 0 0 0 0 0 0 3
-1.2783 1.9541 0.0153 O 0 0 0 0 0 0 0 0 0 0 4
0.5379 3.3079 -0.0279 O 0 0 0 0 0 0 0 0 0 0 5
1.6045 0.9980 -0.8279 H 0 0 0 0 0 0 0 0 0 0 6
1.5313 0.9952 0.9536 H 0 0 0 0 0 0 0 0 0 0 7
-1.7452 2.8190 -0.0032 H 0 0 0 0 0 0 0 0 0 0 8
3 2 0 0 0 0
6 2 0 0 0 0
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7 2 0 0 0 0
4 3 0 0 0 0
5 3 0 0 0 0
4 8 0 0 0 0
M END
$$$$
iodoaceticacid1-anion.sdf
COSMOtherm 3D 0

7 5 0 0 0 0 0 0 0 0 0 V2000
1.0024 0.0077 0.0018 I 0 0 0 0 0 0 0 0 0 0 1
-1.0299 -0.8993 -0.0224 C 0 0 0 0 0 0 0 0 0 0 2
-2.2227 0.0768 -0.0012 C 0 0 0 0 0 0 0 0 0 0 3
-3.3153 -0.5725 0.0165 O 0 0 0 0 0 0 0 0 0 0 4
-2.0634 1.3214 -0.0080 O 0 0 0 0 0 0 0 0 0 0 5
-1.0388 -1.5517 0.8558 H 0 0 0 0 0 0 0 0 0 0 6
-1.0363 -1.5057 -0.9333 H 0 0 0 0 0 0 0 0 0 0 7
3 2 0 0 0 0
6 2 0 0 0 0
4 3 0 0 0 0
5 3 0 0 0 0
2 7 0 0 0 0
M END
$$$$
iodoaceticacid1.sdf
COSMOtherm 3D 0

8 6 0 0 0 0 0 0 0 0 0 V2000
1.0043 0.0083 0.0030 I 0 0 0 0 0 0 0 0 0 0 1
-0.9625 -0.9064 -0.0359 C 0 0 0 0 0 0 0 0 0 0 2
-2.0981 0.0956 -0.0056 C 0 0 0 0 0 0 0 0 0 0 3
-3.2728 -0.5780 0.0258 O 0 0 0 0 0 0 0 0 0 0 4
-2.0150 1.3097 -0.0132 O 0 0 0 0 0 0 0 0 0 0 5
-1.0172 -1.5732 0.8302 H 0 0 0 0 0 0 0 0 0 0 6
-1.0109 -1.5042 -0.9518 H 0 0 0 0 0 0 0 0 0 0 7
-4.0036 0.0787 0.0338 H 0 0 0 0 0 0 0 0 0 0 8
3 2 0 0 0 0
6 2 0 0 0 0
7 2 0 0 0 0
4 3 0 0 0 0
5 3 0 0 0 0
4 8 0 0 0 0
M END
$$$$
maleicacid3-anion.sdf
COSMOtherm 3D 0

11 11 0 0 0 0 0 0 0 0 0 V2000
0.6754 -1.1413 -0.0155 C 0 0 0 0 0 0 0 0 0 0 1
-0.6754 -1.1413 -0.0156 C 0 0 0 0 0 0 0 0 0 0 2
1.6558 -0.0014 0.0011 C 0 0 0 0 0 0 0 0 0 0 3
-1.6558 -0.0011 0.0010 C 0 0 0 0 0 0 0 0 0 0 4
1.2076 1.2286 -0.0084 O 0 0 0 0 0 0 0 0 0 0 5
2.8710 -0.2770 0.0211 O 0 0 0 0 0 0 0 0 0 0 6
-2.8711 -0.2770 0.0212 O 0 0 0 0 0 0 0 0 0 0 7
-1.2075 1.2285 -0.0083 O 0 0 0 0 0 0 0 0 0 0 8
1.1731 -2.1144 -0.0247 H 0 0 0 0 0 0 0 0 0 0 9
-1.1732 -2.1144 -0.0250 H 0 0 0 0 0 0 0 0 0 0 10
0.0010 1.2511 -0.0129 H 0 0 0 0 0 0 0 0 0 0 11
2 1 0 0 0 0
3 1 0 0 0 0
9 1 0 0 0 0
4 2 0 0 0 0
10 2 0 0 0 0
5 3 0 0 0 0
6 3 0 0 0 0
7 4 0 0 0 0
8 4 0 0 0 0
5 11 0 0 0 0
8 11 0 0 0 0
M END
$$$$
maleicacid3.sdf
COSMOtherm 3D 0

12 11 0 0 0 0 0 0 0 0 0 V2000
0.6669 -1.1230 -0.0048 C 0 0 0 0 0 0 0 0 0 0 1
-0.6827 -1.1277 -0.0089 C 0 0 0 0 0 0 0 0 0 0 2
1.5784 0.0394 -0.0008 C 0 0 0 0 0 0 0 0 0 0 3
-1.6979 -0.0244 0.0001 C 0 0 0 0 0 0 0 0 0 0 4
1.2471 1.2338 -0.0077 O 0 0 0 0 0 0 0 0 0 0 5
2.8603 -0.3417 0.0104 O 0 0 0 0 0 0 0 0 0 0 6
-2.8929 -0.3162 0.0079 O 0 0 0 0 0 0 0 0 0 0 7
-1.3114 1.2538 0.0012 O 0 0 0 0 0 0 0 0 0 0 8
1.1744 -2.0888 -0.0074 H 0 0 0 0 0 0 0 0 0 0 9
-1.1660 -2.1063 -0.0131 H 0 0 0 0 0 0 0 0 0 0 10
3.4323 0.4579 0.0127 H 0 0 0 0 0 0 0 0 0 0 11
-0.2913 1.3341 -0.0068 H 0 0 0 0 0 0 0 0 0 0 12
2 1 0 0 0 0
3 1 0 0 0 0
9 1 0 0 0 0
4 2 0 0 0 0
10 2 0 0 0 0
5 3 0 0 0 0
6 3 0 0 0 0
7 4 0 0 0 0
8 4 0 0 0 0
11 6 0 0 0 0
8 12 0 0 0 0
M END
$$$$
mandelicacid-anion0.sdf
COSMOtherm 3D 0

18 18 0 0 0 0 0 0 0 0 0 V2000
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14 1 0 0 0 0
3 2 0 0 0 0
15 2 0 0 0 0
4 3 0 0 0 0
16 3 0 0 0 0
5 4 0 0 0 0
7 4 0 0 0 0
6 5 0 0 0 0
17 5 0 0 0 0
18 6 0 0 0 0
8 7 0 0 0 0
9 7 0 0 0 0
12 8 0 0 0 0
10 9 0 0 0 0
11 9 0 0 0 0
13 10 0 0 0 0
7 19 0 0 0 0
M END
$$$$
mandelicacid1.sdf
COSMOtherm 3D 0
19 19 0 0 0 0 0 0 0 0 0 V2000
0.1979 0.4805 -3.0994 C 0 0 0 0 0 0 0 0 0 0 1
0.4300 -0.8489 -2.7293 C 0 0 0 0 0 0 0 0 0 0 2
0.2618 -1.2454 -1.3977 C 0 0 0 0 0 0 0 0 0 0 3
-0.1413 -0.3175 -0.4264 C 0 0 0 0 0 0 0 0 0 0 4
-0.3696 1.0173 -0.8035 C 0 0 0 0 0 0 0 0 0 0 5
-0.2046 1.4125 -2.1344 C 0 0 0 0 0 0 0 0 0 0 6
-0.3661 -0.7714 1.0123 C 0 0 0 0 0 0 0 0 0 0 7
-1.7475 -0.7717 1.3922 O 0 0 0 0 0 0 0 0 0 0 8
0.5261 0.0462 1.9577 C 0 0 0 0 0 0 0 0 0 0 9
-0.1464 1.0468 2.5666 O 0 0 0 0 0 0 0 0 0 0 10
1.7173 -0.1690 2.1168 O 0 0 0 0 0 0 0 0 0 0 11
-2.0823 0.1439 1.3418 H 0 0 0 0 0 0 0 0 0 0 12
0.4844 1.5543 3.1235 H 0 0 0 0 0 0 0 0 0 0 13
0.3304 0.7910 -4.1372 H 0 0 0 0 0 0 0 0 0 0 14
0.7417 -1.5799 -3.4775 H 0 0 0 0 0 0 0 0 0 0 15
0.4393 -2.2844 -1.1112 H 0 0 0 0 0 0 0 0 0 0 16
-0.6767 1.7566 -0.0594 H 0 0 0 0 0 0 0 0 0 0 17
-0.3835 2.4512 -2.4174 H 0 0 0 0 0 0 0 0 0 0 18
-0.0339 -1.8133 1.1094 H 0 0 0 0 0 0 0 0 0 0 19
2 1 0 0 0 0
6 1 0 0 0 0
14 1 0 0 0 0
3 2 0 0 0 0
15 2 0 0 0 0
4 3 0 0 0 0
16 3 0 0 0 0
5 4 0 0 0 0
7 4 0 0 0 0
6 5 0 0 0 0
17 5 0 0 0 0
18 6 0 0 0 0
8 7 0 0 0 0
9 7 0 0 0 0
12 8 0 0 0 0
10 9 0 0 0 0
11 9 0 0 0 0
13 10 0 0 0 0
7 19 0 0 0 0
M END
$$$$
methanol-anion.sdf
COSMOtherm 3D 0
5 4 0 0 0 0 0 0 0 0 0 V2000
-0.6612 0.0000 0.0000 C 0 0 0 0 0 0 0 0 0 0 1
0.7119 0.0000 0.0000 O 0 0 0 0 0 0 0 0 0 0 2
-1.1400 0.3315 0.9691 H 0 0 0 0 0 0 0 0 0 0 3
-1.1400 0.6732 -0.7717 H 0 0 0 0 0 0 0 0 0 0 4
-1.1402 -1.0049 -0.1973 H 0 0 0 0 0 0 0 0 0 0 5
2 1 0 0 0 0
3 1 0 0 0 0
4 1 0 0 0 0
1 5 0 0 0 0
M END
$$$$
methanol.sdf
COSMOtherm 3D 0
6 5 0 0 0 0 0 0 0 0 0 V2000
-0.7382 0.0127 0.0000 C 0 0 0 0 0 0 0 0 0 0 1
0.7000 -0.0651 0.0000 O 0 0 0 0 0 0 0 0 0 0 2
-1.1138 -1.0183 0.0001 H 0 0 0 0 0 0 0 0 0 0 3
-1.1211 0.5268 -0.8972 H 0 0 0 0 0 0 0 0 0 0 4
-1.1211 0.5269 0.8971 H 0 0 0 0 0 0 0 0 0 0 5
1.0413 0.8466 0.0000 H 0 0 0 0 0 0 0 0 0 0 6
2 1 0 0 0 0
3 1 0 0 0 0
4 1 0 0 0 0
5 1 0 0 0 0
2 6 0 0 0 0
M END
$$$$
methylthiouracil0-anion.sdf
COSMOtherm 3D 0
14 14 0 0 0 0 0 0 0 0 0 V2000
-0.8379 -0.0328 0.0001 C 0 0 0 0 0 0 0 0 0 0 1
-0.3249 1.1936 -0.0003 N 0 0 0 0 0 0 0 0 0 0 2
1.0644 1.2997 0.0000 C 0 0 0 0 0 0 0 0 0 0 3
1.8112 0.0645 0.0000 C 0 0 0 0 0 0 0 0 0 0 4
1.1467 -1.1460 0.0000 C 0 0 0 0 0 0 0 0 0 0 5
-0.2236 -1.2205 0.0003 N 0 0 0 0 0 0 0 0 0 0 6
```

URL: <http://mc.manuscriptcentral.com/tandf/tmph>


```
1
2
3      1.6019      2.4178     -0.0049 O   0   0   0   0   0   0   0   0   0   0   7
4     -2.6840     -0.0342     -0.0014 S   0   0   0   0   0   0   0   0   0   0   8
5      2.8888      0.0182      0.0172 H   0   0   0   0   0   0   0   0   0   0   9
6      1.7758     -2.5269     -0.0107 C   0   0   0   0   0   0   0   0   0   0  10
7      2.5746      2.3251     -0.0033 H   0   0   0   0   0   0   0   0   0   0  11
8      1.7933     -2.9264     -1.0375 H   0   0   0   0   0   0   0   0   0   0  12
9      2.8138     -2.4442      0.3363 H   0   0   0   0   0   0   0   0   0   0  13
10     1.2378     -3.2528      0.6138 H   0   0   0   0   0   0   0   0   0   0  14
11
12      2   1   0   0   0   0
13      6   1   0   0   0   0
14      8   1   0   0   0   0
15      3   2   0   0   0   0
16      4   3   0   0   0   0
17      7   3   0   0   0   0
18      5   4   0   0   0   0
19      9   4   0   0   0   0
20      6   5   0   0   0   0
21     10   5   0   0   0   0
22     11   7   0   0   0   0
23     12  10   0   0   0   0
24     13  10   0   0   0   0
25     10  14   0   0   0   0
26
27 M   END
28 $$$
29 methylthiouracil3.sdf
30 COSMOTHERM      3D      0
31
32 15 15   0   0   0   0   0   0   0   0   0   0 V2000
33     -0.8636     -0.0436      0.0005 C   0   0   0   0   0   0   0   0   0   0   1
34     -0.3057      1.1771     -0.0026 N   0   0   0   0   0   0   0   0   0   0   2
35      1.0314      1.1961     -0.0001 C   0   0   0   0   0   0   0   0   0   0   3
36      1.8044      0.0236      0.0062 C   0   0   0   0   0   0   0   0   0   0   4
37      1.1140     -1.1875      0.0057 C   0   0   0   0   0   0   0   0   0   0   5
38     -0.2445     -1.2274      0.0044 N   0   0   0   0   0   0   0   0   0   0   6
39      1.5698      2.4358     -0.0025 O   0   0   0   0   0   0   0   0   0   0   7
40     -2.6540     -0.0140     -0.0008 S   0   0   0   0   0   0   0   0   0   0   8
41      2.8939      0.0587      0.0107 H   0   0   0   0   0   0   0   0   0   0   9
42      1.8253     -2.5078     -0.0059 C   0   0   0   0   0   0   0   0   0   0  10
43     -2.8002     -1.3659      0.0039 H   0   0   0   0   0   0   0   0   0   0  11
44      2.5455      2.3727     -0.0015 H   0   0   0   0   0   0   0   0   0   0  12
45      1.6687     -3.0081     -0.9744 H   0   0   0   0   0   0   0   0   0   0  13
46      2.9032     -2.3871      0.1542 H   0   0   0   0   0   0   0   0   0   0  14
47      1.4135     -3.1685      0.7702 H   0   0   0   0   0   0   0   0   0   0  15
48
49      2   1   0   0   0   0
50      6   1   0   0   0   0
51      8   1   0   0   0   0
52      3   2   0   0   0   0
53      4   3   0   0   0   0
54      7   3   0   0   0   0
55      5   4   0   0   0   0
56      9   4   0   0   0   0
57      6   5   0   0   0   0
58     10   5   0   0   0   0
59     12   7   0   0   0   0
60     11   8   0   0   0   0
61     13  10   0   0   0   0
62     14  10   0   0   0   0
63     10  15   0   0   0   0
64
65 M   END
66 $$$
67 n-pentanoicacid-anion.sdf
68 COSMOTHERM      3D      0
69
70 16 15   0   0   0   0   0   0   0   0   0   0 V2000
71      3.4621      0.3252      0.0088 C   0   0   0   0   0   0   0   0   0   0   1
72      2.2171     -0.5690     -0.0087 C   0   0   0   0   0   0   0   0   0   0   2
73      0.9015      0.2218      0.0055 C   0   0   0   0   0   0   0   0   0   0   3
74     -0.3385     -0.6732     -0.0111 C   0   0   0   0   0   0   0   0   0   0   4
75     -1.7095      0.0430     -0.0004 C   0   0   0   0   0   0   0   0   0   0   5
76     -1.7358      1.3116     -0.0065 O   0   0   0   0   0   0   0   0   0   0   6
77     -2.7340     -0.7150      0.0118 O   0   0   0   0   0   0   0   0   0   0   7
78      4.3881     -0.2692     -0.0039 H   0   0   0   0   0   0   0   0   0   0   8
79      3.4825      0.9937     -0.8666 H   0   0   0   0   0   0   0   0   0   0   9
80      3.4833      0.9575      0.9105 H   0   0   0   0   0   0   0   0   0   0  10
81      2.2415     -1.2493      0.8608 H   0   0   0   0   0   0   0   0   0   0  11
82      2.2421     -1.2158     -0.9032 H   0   0   0   0   0   0   0   0   0   0  12
83      0.8724      0.9023     -0.8623 H   0   0   0   0   0   0   0   0   0   0  13
84      0.8725      0.8696      0.8982 H   0   0   0   0   0   0   0   0   0   0  14
85     -0.3237     -1.3597      0.8537 H   0   0   0   0   0   0   0   0   0   0  15
86     -0.3223     -1.3268     -0.9012 H   0   0   0   0   0   0   0   0   0   0  16
87
88      2   1   0   0   0   0
89      8   1   0   0   0   0
90      9   1   0   0   0   0
91     10   1   0   0   0   0
92      3   2   0   0   0   0
93     11   2   0   0   0   0
94     12   2   0   0   0   0
95      4   3   0   0   0   0
96     13   3   0   0   0   0
97     14   3   0   0   0   0
98      5   4   0   0   0   0
99     15   4   0   0   0   0
100      6   5   0   0   0   0
101      7   5   0   0   0   0
102      4  16   0   0   0   0
103
104 M   END
105 $$$
106 n-pentanoicacid.sdf
107 COSMOTHERM      3D      0
108
109 17 16   0   0   0   0   0   0   0   0   0   0 V2000
110      3.4908      0.3137      0.0067 C   0   0   0   0   0   0   0   0   0   0   1
111      2.2388     -0.5694     -0.0064 C   0   0   0   0   0   0   0   0   0   0   2
112      0.9359      0.2407      0.0041 C   0   0   0   0   0   0   0   0   0   0   3
113     -0.3026     -0.6552     -0.0086 C   0   0   0   0   0   0   0   0   0   0   4
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nitrousacid-anion.sdf
COSMOTHERM 3D 0

3 2 0 0 0 0 0 0 0 0 0 V2000
0.0000 -0.4717 0.0000 N 0 0 0 0 0 0 0 0 0 0 1
-1.0785 0.2065 0.0000 O 0 0 0 0 0 0 0 0 0 0 2
1.0785 0.2065 0.0000 O 0 0 0 0 0 0 0 0 0 0 3
2 1 0 0 0 0
1 3 0 0 0 0
M END
$$$$
nitrousacid.sdf
COSMOTHERM 3D 0

4 3 0 0 0 0 0 0 0 0 0 V2000
0.1449 -0.5058 0.0000 N 0 0 0 0 0 0 0 0 0 0 1
-1.1286 0.1212 0.0000 O 0 0 0 0 0 0 0 0 0 0 2
1.0626 0.2522 0.0000 O 0 0 0 0 0 0 0 0 0 0 3
-0.9674 1.1007 -0.0002 H 0 0 0 0 0 0 0 0 0 0 4
2 1 0 0 0 0
3 1 0 0 0 0
2 4 0 0 0 0
M END
$$$$
oxalicacid0.sdf
COSMOTHERM 3D 0

8 7 0 0 0 0 0 0 0 0 0 V2000
0.7669 0.1136 -0.0002 C 0 0 0 0 0 0 0 0 0 0 1
-0.7668 -0.1136 -0.0002 C 0 0 0 0 0 0 0 0 0 0 2
1.2892 1.2109 0.0000 O 0 0 0 0 0 0 0 0 0 0 3
-1.4058 1.0623 0.0001 O 0 0 0 0 0 0 0 0 0 0 4
-1.2892 -1.2109 0.0000 O 0 0 0 0 0 0 0 0 0 0 5
1.4058 -1.0623 0.0001 O 0 0 0 0 0 0 0 0 0 0 6
-2.3737 0.8904 0.0011 H 0 0 0 0 0 0 0 0 0 0 7
2.3737 -0.8904 0.0011 H 0 0 0 0 0 0 0 0 0 0 8
2 1 0 0 0 0
3 1 0 0 0 0
6 1 0 0 0 0
4 2 0 0 0 0
5 2 0 0 0 0
7 4 0 0 0 0
6 8 0 0 0 0
M END
$$$$
oxalicacid2-anion.sdf
COSMOTHERM 3D 0

7 6 0 0 0 0 0 0 0 0 0 V2000
0.7547 -0.1253 -0.0002 C 0 0 0 0 0 0 0 0 0 0 1
-0.8215 -0.0393 -0.0001 C 0 0 0 0 0 0 0 0 0 0 2
1.4226 -1.1457 -0.0008 O 0 0 0 0 0 0 0 0 0 0 3
-1.6059 -1.6301 0.0584 C 0 0 0 0 0 0 0 0 0 0 4
-1.2374 1.1645 -0.0009 O 0 0 0 0 0 0 0 0 0 0 5
1.3037 1.1049 0.0010 O 0 0 0 0 0 0 0 0 0 0 6
0.4819 1.6887 0.0006 H 0 0 0 0 0 0 0 0 0 0 7
2 1 0 0 0 0
3 1 0 0 0 0
6 1 0 0 0 0
4 2 0 0 0 0
5 2 0 0 0 0
6 7 0 0 0 0
M END
$$$$
pamoicacid-anion0.sdf
COSMOTHERM 3D 0

44 48 0 0 0 0 0 0 0 0 0 V2000
4.6749 -2.6323 -0.4341 C 0 0 0 0 0 0 0 0 0 0 1
3.5586 -3.0106 -1.2204 C 0 0 0 0 0 0 0 0 0 0 2
2.4672 -2.1726 -1.3604 C 0 0 0 0 0 0 0 0 0 0 3
2.4154 -0.8927 -0.7262 C 0 0 0 0 0 0 0 0 0 0 4
3.5749 -0.5060 0.0422 C 0 0 0 0 0 0 0 0 0 0 5
4.6783 -1.3958 0.1780 C 0 0 0 0 0 0 0 0 0 0 6
1.2980 0.0024 -0.8287 C 0 0 0 0 0 0 0 0 0 0 7
1.4098 1.3004 -0.3011 C 0 0 0 0 0 0 0 0 0 0 8
2.5759 1.6820 0.4523 C 0 0 0 0 0 0 0 0 0 0 9
3.6077 0.7746 0.6346 C 0 0 0 0 0 0 0 0 0 0 10
0.0154 -0.4033 -1.5507 C 0 0 0 0 0 0 0 0 0 0 11
-1.2595 -0.4812 -0.7149 C 0 0 0 0 0 0 0 0 0 0 12
-1.6059 -1.6301 0.0584 C 0 0 0 0 0 0 0 0 0 0 13
-2.8867 -1.6866 0.7305 C 0 0 0 0 0 0 0 0 0 0 14
-3.7755 -0.5931 0.6126 C 0 0 0 0 0 0 0 0 0 0 15
-3.4381 0.5319 -0.1184 C 0 0 0 0 0 0 0 0 0 0 16
-2.1594 0.5983 -0.7887 C 0 0 0 0 0 0 0 0 0 0 17
-1.1131 -3.8581 0.9598 C 0 0 0 0 0 0 0 0 0 0 18
-2.3728 -3.9075 1.6092 C 0 0 0 0 0 0 0 0 0 0 19
-3.2371 -2.8370 1.4931 C 0 0 0 0 0 0 0 0 0 0 20
-0.7419 -2.7569 0.2102 C 0 0 0 0 0 0 0 0 0 0 21
-1.8336 1.7072 -1.4623 O 0 0 0 0 0 0 0 0 0 0 22
0.4525 2.2421 -0.4266 O 0 0 0 0 0 0 0 0 0 0 23
-4.3972 1.6784 -0.2007 C 0 0 0 0 0 0 0 0 0 0 24
2.7313 3.0573 0.9995 C 0 0 0 0 0 0 0 0 0 0 25
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2.3147 4.0937 0.4974 O 0 0 0 0 0 0 0 0 0 0 30
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5.5254 -3.3074 -0.3286 H 0 0 0 0 0 0 0 0 0 0 32
3.5592 -3.9768 -1.7287 H 0 0 0 0 0 0 0 0 0 0 33
1.6460 -2.5029 -1.9955 H 0 0 0 0 0 0 0 0 0 0 34
5.5352 -1.0714 0.7730 H 0 0 0 0 0 0 0 0 0 0 35
4.4817 1.0647 1.2184 H 0 0 0 0 0 0 0 0 0 0 36

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31 44 0 0 0 0
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pamoicacid0.sdf
COSMOTHERM 3D 0
45 48 0 0 0 0 0 0 0 0 0 0 V2000
4.9793 -2.1643 1.0661 C 0 0 0 0 0 0 0 0 0 0 1
3.8258 -2.6199 1.7539 C 0 0 0 0 0 0 0 0 0 0 2
2.6350 -1.9208 1.6940 C 0 0 0 0 0 0 0 0 0 0 3
2.5168 -0.7071 0.9500 C 0 0 0 0 0 0 0 0 0 0 4
3.7019 -0.2486 0.2571 C 0 0 0 0 0 0 0 0 0 0 5
4.9132 -0.9961 0.3378 C 0 0 0 0 0 0 0 0 0 0 6
1.3010 0.0428 0.8528 C 0 0 0 0 0 0 0 0 0 0 7
1.3076 1.2508 0.1477 C 0 0 0 0 0 0 0 0 0 0 8
2.4848 1.7029 -0.5472 C 0 0 0 0 0 0 0 0 0 0 9
3.6509 0.9501 -0.4810 C 0 0 0 0 0 0 0 0 0 0 10
0.0251 -0.3805 1.5683 C 0 0 0 0 0 0 0 0 0 0 11
-1.2329 -0.5024 0.7199 C 0 0 0 0 0 0 0 0 0 0 12
-1.3295 -1.4270 -0.3635 C 0 0 0 0 0 0 0 0 0 0 13
-2.5461 -1.5111 -1.1396 C 0 0 0 0 0 0 0 0 0 0 14
-3.6404 -0.6959 -0.7908 C 0 0 0 0 0 0 0 0 0 0 15
-3.5678 0.1783 0.2879 C 0 0 0 0 0 0 0 0 0 0 16
-2.3516 0.2656 1.0558 C 0 0 0 0 0 0 0 0 0 0 17
-0.3832 -3.1831 -1.7852 C 0 0 0 0 0 0 0 0 0 0 18
-1.5769 -3.2501 -2.5499 C 0 0 0 0 0 0 0 0 0 0 19
-2.6356 -2.4281 -2.2279 C 0 0 0 0 0 0 0 0 0 0 20
-0.2617 -2.3006 -0.7288 C 0 0 0 0 0 0 0 0 0 0 21
-2.2806 1.1039 2.1213 O 0 0 0 0 0 0 0 0 0 0 22
0.1738 1.9923 0.1290 O 0 0 0 0 0 0 0 0 0 0 23
-4.7171 1.0140 0.6657 C 0 0 0 0 0 0 0 0 0 0 24
2.4355 2.9685 -1.2949 C 0 0 0 0 0 0 0 0 0 0 25
-3.1679 1.5727 2.1711 H 0 0 0 0 0 0 0 0 0 0 26
0.3728 2.7986 -0.4358 H 0 0 0 0 0 0 0 0 0 0 27
-4.7017 1.8266 1.6078 O 0 0 0 0 0 0 0 0 0 0 28
-5.8196 0.8363 -0.0864 O 0 0 0 0 0 0 0 0 0 0 29
1.4260 3.6920 -1.3615 O 0 0 0 0 0 0 0 0 0 0 30
3.5800 3.3031 -1.9196 O 0 0 0 0 0 0 0 0 0 0 31
5.9102 -2.7300 1.1251 H 0 0 0 0 0 0 0 0 0 0 32
3.8759 -3.5422 2.3357 H 0 0 0 0 0 0 0 0 0 0 33
1.7796 -2.3090 2.2461 H 0 0 0 0 0 0 0 0 0 0 34
5.7891 -0.6225 -0.1974 H 0 0 0 0 0 0 0 0 0 0 35
4.5434 1.2889 -1.0075 H 0 0 0 0 0 0 0 0 0 0 36
-0.1819 0.3490 2.3636 H 0 0 0 0 0 0 0 0 0 0 37
0.1895 -1.3397 2.0768 H 0 0 0 0 0 0 0 0 0 0 38
-4.5595 -0.7588 -1.3738 H 0 0 0 0 0 0 0 0 0 0 39
0.4514 -3.8414 -2.0348 H 0 0 0 0 0 0 0 0 0 0 40
-1.6531 -3.9518 -3.3818 H 0 0 0 0 0 0 0 0 0 0 41
-3.5669 -2.4694 -2.7973 H 0 0 0 0 0 0 0 0 0 0 42
0.6684 -2.2764 -0.1638 H 0 0 0 0 0 0 0 0 0 0 43
-6.5154 1.4436 0.2464 H 0 0 0 0 0 0 0 0 0 0 44
3.4360 4.1572 -2.3817 H 0 0 0 0 0 0 0 0 0 0 45
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32 1 0 0 0 0
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URL: <http://mc.manuscriptcentral.com/tandf/tmph>

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30 25 0 0 0 0
31 25 0 0 0 0
44 29 0 0 0 0
31 45 0 0 0 0
M END
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pamoicacid3.sdf
COSMOtherm 3D 0
45 48 0 0 0 0 0 0 0 0 0 V2000
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3.6428 -1.3041 -2.9453 C 0 0 0 0 0 0 0 0 0 0 2
2.5259 -1.3882 -2.1349 C 0 0 0 0 0 0 0 0 0 0 3
2.4801 -0.7485 -0.8597 C 0 0 0 0 0 0 0 0 0 0 4
3.6631 -0.0292 -0.4456 C 0 0 0 0 0 0 0 0 0 0 5
4.7938 0.0474 -1.3101 C 0 0 0 0 0 0 0 0 0 0 6
1.3447 -0.7984 0.0134 C 0 0 0 0 0 0 0 0 0 0 7
1.4573 -0.2551 1.2942 C 0 0 0 0 0 0 0 0 0 0 8
2.6286 0.4632 1.7120 C 0 0 0 0 0 0 0 0 0 0 9
3.6953 0.5685 0.8290 C 0 0 0 0 0 0 0 0 0 0 10
0.0459 -1.5009 -0.3706 C 0 0 0 0 0 0 0 0 0 0 11
-1.2319 -0.6638 -0.4358 C 0 0 0 0 0 0 0 0 0 0 12
-1.5100 0.1661 -1.5715 C 0 0 0 0 0 0 0 0 0 0 13
-2.8118 0.7674 -1.7167 C 0 0 0 0 0 0 0 0 0 0 14
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5.6570 -0.5124 -3.1970 H 0 0 0 0 0 0 0 0 0 0 32
3.6424 -1.8139 -3.9104 H 0 0 0 0 0 0 0 0 0 0 33
1.6788 -1.9780 -2.4837 H 0 0 0 0 0 0 0 0 0 0 34
5.6704 0.6027 -0.9696 H 0 0 0 0 0 0 0 0 0 0 35
4.5824 1.1200 1.1438 H 0 0 0 0 0 0 0 0 0 0 36
-0.1207 -2.3334 0.3308 H 0 0 0 0 0 0 0 0 0 0 37
0.1712 -1.9785 -1.3496 H 0 0 0 0 0 0 0 0 0 0 38
-4.7779 0.9855 -0.8298 H 0 0 0 0 0 0 0 0 0 0 39
-0.1166 1.3685 -4.4700 H 0 0 0 0 0 0 0 0 0 0 40
-2.3824 2.3999 -4.7037 H 0 0 0 0 0 0 0 0 0 0 41
-4.0970 2.0148 -2.9392 H 0 0 0 0 0 0 0 0 0 0 42
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-4.9820 -0.3580 3.2743 H 0 0 0 0 0 0 0 0 0 0 44
1.8790 1.3566 4.7284 H 0 0 0 0 0 0 0 0 0 0 45
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43	21	0	0	0	0
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30	25	0	0	0	0
31	25	0	0	0	0
44	29	0	0	0	0
31	45	0	0	0	0
M	END				
\$\$\$\$					
pamoicacid4.sdf					
COSMOtherm	3D				0
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0	0	0	0	0	V2000
4.5647	-2.6153	1.0755	C	0	0
3.3965	-2.8289	1.8524	C	0	0
2.3293	-1.9545	1.7930	C	0	0
2.3577	-0.7970	0.9579	C	0	0
3.5543	-0.5871	0.1715	C	0	0
4.6350	-1.5144	0.2509	C	0	0
1.2810	0.1398	0.8757	C	0	0
1.4323	1.2737	0.0724	C	0	0
2.6115	1.4707	-0.7286	C	0	0
3.6448	0.5433	-0.6629	C	0	0
0.0000	0.0001	1.6867	C	0	0
-1.2812	-0.1399	0.8759	C	0	0
-2.3578	0.7970	0.9579	C	0	0
-3.5545	0.5868	0.1717	C	0	0
-3.6449	-0.5436	-0.6626	C	0	0
-2.6116	-1.4709	-0.7283	C	0	0
-1.4324	-1.2738	0.0726	C	0	0
-3.3967	2.8290	1.8521	C	0	0
-4.5649	2.6153	1.0753	C	0	0
-4.6352	1.5143	0.2508	C	0	0
-2.3295	1.9546	1.7929	C	0	0
-0.4343	-2.1927	0.0647	O	0	0
0.4342	2.1925	0.0642	O	0	0
-2.7068	-2.6613	-1.5847	C	0	0
-2.7071	2.6615	-1.5844	C	0	0
-0.7174	-2.9110	-0.5767	H	0	0
0.7178	2.9114	-0.5764	H	0	0
-1.8249	-3.5360	-1.6534	O	0	0
-3.8360	-2.7470	-2.3135	O	0	0
1.8255	3.5364	-1.6527	O	0	0
3.8364	2.7472	-2.3132	O	0	0
5.3961	-3.3195	1.1341	H	0	0
3.3387	-3.7018	2.5058	H	0	0
1.4484	-2.1665	2.3967	H	0	0
5.5237	-1.3281	-0.3566	H	0	0
4.5435	0.6916	-1.2626	H	0	0
-0.0816	0.8721	2.3478	H	0	0
0.0817	-0.8717	2.3481	H	0	0
-4.5436	-0.6919	-1.2624	H	0	0
-3.3389	3.7020	2.5054	H	0	0
-5.3963	3.3196	1.1336	H	0	0
-5.5239	1.3279	-0.3566	H	0	0
-1.4486	2.1667	2.3965	H	0	0
-3.7937	-3.5728	-2.8425	H	0	0
3.7943	3.5734	-2.8417	H	0	0
2	1	0	0	0	
6	1	0	0	0	
32	1	0	0	0	
3	2	0	0	0	
33	2	0	0	0	
4	3	0	0	0	
34	3	0	0	0	
5	4	0	0	0	
7	4	0	0	0	
6	5	0	0	0	
10	5	0	0	0	
35	6	0	0	0	
8	7	0	0	0	
11	7	0	0	0	
9	8	0	0	0	
23	8	0	0	0	
10	9	0	0	0	
25	9	0	0	0	
36	10	0	0	0	
12	11	0	0	0	
37	11	0	0	0	
38	11	0	0	0	
13	12	0	0	0	
17	12	0	0	0	
14	13	0	0	0	
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29 24 0 0 0 0
30 25 0 0 0 0
31 25 0 0 0 0
44 29 0 0 0 0
31 45 0 0 0 0
M END
$$$$
pentachlorophenol-anion.sdf
COSMOTHERM 3D 0

12 12 0 0 0 0 0 0 0 0 0 V2000
0.4489 1.2096 0.0000 C 0 0 0 0 0 0 0 0 0 0 1
-0.9459 1.2075 0.0001 C 0 0 0 0 0 0 0 0 0 0 2
-1.7440 0.0000 -0.0002 C 0 0 0 0 0 0 0 0 0 0 3
-0.9459 -1.2075 0.0001 C 0 0 0 0 0 0 0 0 0 0 4
0.4489 -1.2096 0.0000 C 0 0 0 0 0 0 0 0 0 0 5
1.1690 0.0000 0.0000 C 0 0 0 0 0 0 0 0 0 0 6
-3.0121 0.0000 -0.0005 O 0 0 0 0 0 0 0 0 0 0 7
-1.8479 2.7192 0.0002 Cl 0 0 0 0 0 0 0 0 0 0 8
1.3301 2.7349 0.0000 Cl 0 0 0 0 0 0 0 0 0 0 9
2.9266 0.0000 -0.0001 Cl 0 0 0 0 0 0 0 0 0 0 10
1.3301 -2.7349 0.0001 Cl 0 0 0 0 0 0 0 0 0 0 11
-1.8480 -2.7192 0.0001 Cl 0 0 0 0 0 0 0 0 0 0 12
2 1 0 0 0 0
6 1 0 0 0 0
9 1 0 0 0 0
3 2 0 0 0 0
8 2 0 0 0 0
4 3 0 0 0 0
7 3 0 0 0 0
5 4 0 0 0 0
6 5 0 0 0 0
11 5 0 0 0 0
10 6 0 0 0 0
4 12 0 0 0 0
M END
$$$$
pentachlorophenol.sdf
COSMOTHERM 3D 0

13 13 0 0 0 0 0 0 0 0 0 V2000
0.4687 1.2149 0.0000 C 0 0 0 0 0 0 0 0 0 0 1
-0.9327 1.2089 0.0001 C 0 0 0 0 0 0 0 0 0 0 2
-1.6437 -0.0048 -0.0001 C 0 0 0 0 0 0 0 0 0 0 3
-0.9185 -1.2102 0.0000 C 0 0 0 0 0 0 0 0 0 0 4
0.4815 -1.2146 0.0000 C 0 0 0 0 0 0 0 0 0 0 5
1.1828 0.0030 -0.0001 C 0 0 0 0 0 0 0 0 0 0 6
-2.9929 0.0373 -0.0006 O 0 0 0 0 0 0 0 0 0 0 7
-1.8495 2.6950 0.0001 Cl 0 0 0 0 0 0 0 0 0 0 8
1.3262 2.7343 0.0001 Cl 0 0 0 0 0 0 0 0 0 0 9
2.9293 0.0096 -0.0002 Cl 0 0 0 0 0 0 0 0 0 0 10
1.3435 -2.7310 0.0001 Cl 0 0 0 0 0 0 0 0 0 0 11
-1.8424 -2.6987 0.0001 Cl 0 0 0 0 0 0 0 0 0 0 12
-3.3420 -0.8815 0.0018 H 0 0 0 0 0 0 0 0 0 0 13
2 1 0 0 0 0
6 1 0 0 0 0
9 1 0 0 0 0
3 2 0 0 0 0
8 2 0 0 0 0
4 3 0 0 0 0
7 3 0 0 0 0
5 4 0 0 0 0
12 4 0 0 0 0
6 5 0 0 0 0
11 5 0 0 0 0
10 6 0 0 0 0
7 13 0 0 0 0
M END
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phenol-anion.sdf
COSMOTHERM 3D 0

12 12 0 0 0 0 0 0 0 0 0 V2000
1.2060 -1.1540 -0.0002 C 0 0 0 0 0 0 0 0 0 0 1
1.2142 0.2421 0.0004 C 0 0 0 0 0 0 0 0 0 0 2
0.0000 1.0174 0.0000 C 0 0 0 0 0 0 0 0 0 0 3
-1.2142 0.2421 0.0004 C 0 0 0 0 0 0 0 0 0 0 4
-1.2060 -1.1540 -0.0001 C 0 0 0 0 0 0 0 0 0 0 5
0.0000 -1.8763 0.0000 C 0 0 0 0 0 0 0 0 0 0 6
0.0000 2.3153 -0.0003 O 0 0 0 0 0 0 0 0 0 0 7
2.1585 -1.6937 -0.0002 H 0 0 0 0 0 0 0 0 0 0 8
2.1640 0.7866 0.0003 H 0 0 0 0 0 0 0 0 0 0 9
-2.1640 0.7866 0.0002 H 0 0 0 0 0 0 0 0 0 0 10
-2.1585 -1.6937 -0.0009 H 0 0 0 0 0 0 0 0 0 0 11
0.0000 -2.9678 -0.0006 H 0 0 0 0 0 0 0 0 0 0 12
2 1 0 0 0 0
6 1 0 0 0 0
8 1 0 0 0 0
3 2 0 0 0 0
9 2 0 0 0 0
4 3 0 0 0 0
7 3 0 0 0 0
5 4 0 0 0 0
10 4 0 0 0 0
6 5 0 0 0 0
11 5 0 0 0 0
6 12 0 0 0 0
M END
$$$$
phenol.sdf
COSMOTHERM 3D 0

13 13 0 0 0 0 0 0 0 0 0 V2000
-1.8845 -0.0020 0.0001 C 0 0 0 0 0 0 0 0 0 0 1
-1.1762 1.2074 0.0000 C 0 0 0 0 0 0 0 0 0 0 2
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[illegible]

URL: <http://mc.manuscriptcentral.com/tandf/tmph>

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11 7 0 0 0 0
12 7 0 0 0 0
11 10 0 0 0 0
14 10 0 0 0 0
21 10 0 0 0 0
22 11 0 0 0 0
13 12 0 0 0 0
23 12 0 0 0 0
14 13 0 0 0 0
24 13 0 0 0 0
25 14 0 0 0 0
16 15 0 0 0 0
26 15 0 0 0 0
17 16 0 0 0 0
27 16 0 0 0 0
18 17 0 0 0 0
28 17 0 0 0 0
19 18 0 0 0 0
29 18 0 0 0 0
19 30 0 0 0 0
M END
$$$$
phenytoin1.sdf
COSMOTHERM 3D 0
31 33 0 0 0 0 0 0 0 0 0 V2000
-0.9493 2.5609 0.2123 N 0 0 0 0 0 0 0 0 0 0 1
0.4403 2.6153 0.1747 C 0 0 0 0 0 0 0 0 0 0 2
-1.3416 1.2418 0.1526 C 0 0 0 0 0 0 0 0 0 0 3
0.0063 0.4464 0.0267 C 0 0 0 0 0 0 0 0 0 0 4
1.0556 1.4897 0.0839 N 0 0 0 0 0 0 0 0 0 0 5
0.1106 -0.3056 -1.3141 C 0 0 0 0 0 0 0 0 0 0 6
0.1018 -0.5253 1.2155 C 0 0 0 0 0 0 0 0 0 0 7
0.9824 3.8356 0.2346 O 0 0 0 0 0 0 0 0 0 0 8
-2.4903 0.8227 0.2096 O 0 0 0 0 0 0 0 0 0 0 9
1.0265 -1.1504 3.3759 C 0 0 0 0 0 0 0 0 0 0 10
0.9715 -0.2730 2.2857 C 0 0 0 0 0 0 0 0 0 0 11
-0.7147 -1.6682 1.2535 C 0 0 0 0 0 0 0 0 0 0 12
-0.6652 -2.5380 2.3467 C 0 0 0 0 0 0 0 0 0 0 13
0.2081 -2.2838 3.4119 C 0 0 0 0 0 0 0 0 0 0 14
-1.0068 -0.6452 -2.0894 C 0 0 0 0 0 0 0 0 0 0 15
-0.8490 -1.3572 -3.2866 C 0 0 0 0 0 0 0 0 0 0 16
0.4234 -1.7363 -3.7217 C 0 0 0 0 0 0 0 0 0 0 17
1.5435 -1.3993 -2.9503 C 0 0 0 0 0 0 0 0 0 0 18
1.3888 -0.6891 -1.7577 C 0 0 0 0 0 0 0 0 0 0 19
-1.5742 3.3585 0.3193 H 0 0 0 0 0 0 0 0 0 0 20
1.7134 -0.9439 4.1990 H 0 0 0 0 0 0 0 0 0 0 21
1.6117 0.6087 2.2571 H 0 0 0 0 0 0 0 0 0 0 22
-1.3920 -1.8818 0.4257 H 0 0 0 0 0 0 0 0 0 0 23
-1.3069 -3.4211 2.3630 H 0 0 0 0 0 0 0 0 0 0 24
0.2510 -2.9670 4.2621 H 0 0 0 0 0 0 0 0 0 0 25
-2.0079 -0.3626 -1.7638 H 0 0 0 0 0 0 0 0 0 0 26
-1.7297 -1.6107 -3.8799 H 0 0 0 0 0 0 0 0 0 0 27
0.5442 -2.2893 -4.6550 H 0 0 0 0 0 0 0 0 0 0 28
2.5432 -1.6878 -3.2807 H 0 0 0 0 0 0 0 0 0 0 29
2.2641 -0.4202 -1.1657 H 0 0 0 0 0 0 0 0 0 0 30
1.9576 3.7430 0.2000 H 0 0 0 0 0 0 0 0 0 0 31
2 1 0 0 0 0
3 1 0 0 0 0
20 1 0 0 0 0
5 2 0 0 0 0
8 2 0 0 0 0
4 3 0 0 0 0
9 3 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
7 4 0 0 0 0
15 6 0 0 0 0
19 6 0 0 0 0
11 7 0 0 0 0
12 7 0 0 0 0
11 10 0 0 0 0
14 10 0 0 0 0
21 10 0 0 0 0
22 11 0 0 0 0
13 12 0 0 0 0
23 12 0 0 0 0
14 13 0 0 0 0
24 13 0 0 0 0
25 14 0 0 0 0
16 15 0 0 0 0
26 15 0 0 0 0
17 16 0 0 0 0
27 16 0 0 0 0
18 17 0 0 0 0
28 17 0 0 0 0
19 18 0 0 0 0
29 18 0 0 0 0
30 19 0 0 0 0
8 31 0 0 0 0
M END
$$$$
phenytoin2-anion.sdf
COSMOTHERM 3D 0
30 32 0 0 0 0 0 0 0 0 0 V2000
-0.8564 2.6146 0.0241 N 0 0 0 0 0 0 0 0 0 0 1
0.6245 2.6262 -0.0658 C 0 0 0 0 0 0 0 0 0 0 2
-1.1518 1.3646 0.0493 C 0 0 0 0 0 0 0 0 0 0 3
0.0697 0.4371 -0.0072 C 0 0 0 0 0 0 0 0 0 0 4
1.1676 1.4067 -0.0679 N 0 0 0 0 0 0 0 0 0 0 5
0.0851 -0.4164 1.2776 C 0 0 0 0 0 0 0 0 0 0 6
0.1040 -0.4283 -1.2780 C 0 0 0 0 0 0 0 0 0 0 7
1.2209 3.7363 -0.1256 O 0 0 0 0 0 0 0 0 0 0 8
-2.3929 0.8569 0.1348 O 0 0 0 0 0 0 0 0 0 0 9
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2
3      1.2144   -2.1791   -2.5622  C    0    0    0    0    0    0    0    0    0    10
4      1.0841   -1.4308   -1.3898  C    0    0    0    0    0    0    0    0    0    11
5     -0.7474   -0.2013   -2.3697  C    0    0    0    0    0    0    0    0    0    12
6     -0.6207   -0.9524   -3.5459  C    0    0    0    0    0    0    0    0    0    13
7      0.3594   -1.9440   -3.6474  C    0    0    0    0    0    0    0    0    0    14
8      0.8828   -0.0452   2.3684  C    0    0    0    0    0    0    0    0    0    15
9      0.8605   -0.7889   3.5554  C    0    0    0    0    0    0    0    0    0    16
10     0.0400   -1.9171   3.6655  C    0    0    0    0    0    0    0    0    0    17
11     -0.7575   -2.2970   2.5780  C    0    0    0    0    0    0    0    0    0    18
12     -0.7333   -1.5533   1.3942  C    0    0    0    0    0    0    0    0    0    19
13      1.9848   -2.9502   -2.6296  H    0    0    0    0    0    0    0    0    0    20
14      1.7535   -1.6235   -0.5491  H    0    0    0    0    0    0    0    0    0    21
15     -1.5227    0.5646   -2.3133  H    0    0    0    0    0    0    0    0    0    22
16     -1.2968   -0.7618   -4.3819  H    0    0    0    0    0    0    0    0    0    23
17      0.4561   -2.5320   -4.5621  H    0    0    0    0    0    0    0    0    0    24
18      1.5247    0.8311    2.2695  H    0    0    0    0    0    0    0    0    0    25
19      1.4880   -0.4849    4.3961  H    0    0    0    0    0    0    0    0    0    26
20      0.0222   -2.4980    4.5896  H    0    0    0    0    0    0    0    0    0    27
21     -1.4001   -3.1769    2.6513  H    0    0    0    0    0    0    0    0    0    28
22     -1.3583   -1.8600    0.5537  H    0    0    0    0    0    0    0    0    0    29
23     -3.0292    1.6024    0.1732  H    0    0    0    0    0    0    0    0    0    30
24
25      2  1  0  0  0  0
26      3  1  0  0  0  0
27      5  2  0  0  0  0
28      8  2  0  0  0  0
29      4  3  0  0  0  0
30      9  3  0  0  0  0
31      5  4  0  0  0  0
32      6  4  0  0  0  0
33      7  4  0  0  0  0
34     15  6  0  0  0  0
35     19  6  0  0  0  0
36     11  7  0  0  0  0
37     12  7  0  0  0  0
38     11 10  0  0  0  0
39     14 10  0  0  0  0
40     20 10  0  0  0  0
41     21 11  0  0  0  0
42     13 12  0  0  0  0
43     22 12  0  0  0  0
44     14 13  0  0  0  0
45     23 13  0  0  0  0
46     24 14  0  0  0  0
47     16 15  0  0  0  0
48     25 15  0  0  0  0
49     17 16  0  0  0  0
50     26 16  0  0  0  0
51     18 17  0  0  0  0
52     27 17  0  0  0  0
53     19 18  0  0  0  0
54     28 18  0  0  0  0
55     29 19  0  0  0  0
56      9 30  0  0  0  0
57
58 M      END
59 $$$$
60 phenytoin2.sdf
    COSMOTHERM      3D      0
    31 33  0  0  0  0  0  0  0  0  0  0 V2000
    -0.8514    2.6179   -0.1383  N    0    0    0    0    0    0    0    0    0    1
    0.5741    2.6842   -0.2704  C    0    0    0    0    0    0    0    0    0    2
    -1.1420    1.3630   -0.0181  C    0    0    0    0    0    0    0    0    0    3
    0.0554    0.4007   -0.0152  C    0    0    0    0    0    0    0    0    0    4
    1.0997    1.4247   -0.1174  N    0    0    0    0    0    0    0    0    0    5
    0.0866   -0.3624    1.3232  C    0    0    0    0    0    0    0    0    0    6
    0.0933   -0.5249   -1.2432  C    0    0    0    0    0    0    0    0    0    7
    1.2042    3.7209   -0.4768  O    0    0    0    0    0    0    0    0    0    8
    -2.3602    0.8637    0.1207  O    0    0    0    0    0    0    0    0    0    9
    1.1169   -2.4073   -2.3940  C    0    0    0    0    0    0    0    0    0    10
    0.9932   -1.6030   -1.2577  C    0    0    0    0    0    0    0    0    0    11
    -0.6797   -0.2666   -2.3849  C    0    0    0    0    0    0    0    0    0    12
    -0.5615   -1.0781   -3.5188  C    0    0    0    0    0    0    0    0    0    13
    0.3363   -2.1500   -3.5269  C    0    0    0    0    0    0    0    0    0    14
    0.8912    0.0748    2.3840  C    0    0    0    0    0    0    0    0    0    15
    0.8788   -0.6061    3.6078  C    0    0    0    0    0    0    0    0    0    16
    0.0539   -1.7210    3.7861  C    0    0    0    0    0    0    0    0    0    17
    -0.7583   -2.1557    2.7311  C    0    0    0    0    0    0    0    0    0    18
    -0.7427   -1.4813    1.5074  C    0    0    0    0    0    0    0    0    0    19
    1.8222   -3.2404   -2.3916  H    0    0    0    0    0    0    0    0    0    20
    1.6008   -1.8180   -0.3769  H    0    0    0    0    0    0    0    0    0    21
    -1.3846    0.5665   -2.4025  H    0    0    0    0    0    0    0    0    0    22
    -1.1760   -0.8698   -4.3964  H    0    0    0    0    0    0    0    0    0    23
    0.4271   -2.7829   -4.4114  H    0    0    0    0    0    0    0    0    0    24
    1.5360    0.9440    2.2522  H    0    0    0    0    0    0    0    0    0    25
    1.5170   -0.2603    4.4229  H    0    0    0    0    0    0    0    0    0    26
    0.0444   -2.2510    4.7401  H    0    0    0    0    0    0    0    0    0    27
    -1.4057   -3.0249    2.8595  H    0    0    0    0    0    0    0    0    0    28
    -1.3746   -1.8329    0.6908  H    0    0    0    0    0    0    0    0    0    29
    2.0609    1.2066   -0.3677  H    0    0    0    0    0    0    0    0    0    30
    -3.0145    1.5964    0.1225  H    0    0    0    0    0    0    0    0    0    31
    2  1  0  0  0  0
    3  1  0  0  0  0
    5  2  0  0  0  0
    8  2  0  0  0  0
    4  3  0  0  0  0
    9  3  0  0  0  0
    5  4  0  0  0  0
    6  4  0  0  0  0
    7  4  0  0  0  0
    30  5  0  0  0  0
    15  6  0  0  0  0
    19  6  0  0  0  0
    11  7  0  0  0  0
    12  7  0  0  0  0
    11 10  0  0  0  0
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14 10 0 0 0 0
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21 11 0 0 0 0
13 12 0 0 0 0
22 12 0 0 0 0
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16 15 0 0 0 0
25 15 0 0 0 0
17 16 0 0 0 0
26 16 0 0 0 0
18 17 0 0 0 0
27 17 0 0 0 0
19 18 0 0 0 0
28 18 0 0 0 0
29 19 0 0 0 0
9 31 0 0 0 0
M END
$$$$
phenytoin3-anion.sdf
COSMOtherm 3D 0
30 32 0 0 0 0 0 0 0 0 0 V2000
-2.6042 -1.0045 0.2574 N 0 0 0 0 0 0 0 0 0 0 1
-2.6092 0.3681 0.1980 C 0 0 0 0 0 0 0 0 0 0 2
-1.2892 -1.3272 0.1711 C 0 0 0 0 0 0 0 0 0 0 3
-0.4557 0.0196 0.0280 C 0 0 0 0 0 0 0 0 0 0 4
-1.5046 1.0549 0.0858 N 0 0 0 0 0 0 0 0 0 0 5
0.2905 0.1169 -1.3129 C 0 0 0 0 0 0 0 0 0 0 6
0.5216 0.1120 1.2049 C 0 0 0 0 0 0 0 0 0 0 7
-3.8296 0.9653 0.2651 O 0 0 0 0 0 0 0 0 0 0 8
-0.7974 -2.4726 0.2182 O 0 0 0 0 0 0 0 0 0 0 9
1.1330 0.9969 3.3922 C 0 0 0 0 0 0 0 0 0 0 10
0.2596 0.9519 2.2983 C 0 0 0 0 0 0 0 0 0 0 11
1.6810 -0.6841 1.2312 C 0 0 0 0 0 0 0 0 0 0 12
2.5518 -0.6427 2.3248 C 0 0 0 0 0 0 0 0 0 0 13
2.2824 0.1992 3.4118 C 0 0 0 0 0 0 0 0 0 0 14
0.6872 1.3879 -1.7686 C 0 0 0 0 0 0 0 0 0 0 15
1.3784 1.5343 -2.9740 C 0 0 0 0 0 0 0 0 0 0 16
1.6882 0.4095 -3.7509 C 0 0 0 0 0 0 0 0 0 0 17
1.2985 -0.8572 -3.3067 C 0 0 0 0 0 0 0 0 0 0 18
0.6061 -1.0032 -2.0960 C 0 0 0 0 0 0 0 0 0 0 19
0.9133 1.6608 4.2313 H 0 0 0 0 0 0 0 0 0 0 20
-0.6349 1.5752 2.2772 H 0 0 0 0 0 0 0 0 0 0 21
1.9033 -1.3408 0.3893 H 0 0 0 0 0 0 0 0 0 0 22
3.4470 -1.2685 2.3269 H 0 0 0 0 0 0 0 0 0 0 23
2.9645 0.2347 4.2635 H 0 0 0 0 0 0 0 0 0 0 24
0.4368 2.2670 -1.1731 H 0 0 0 0 0 0 0 0 0 0 25
1.6755 2.5300 -3.3103 H 0 0 0 0 0 0 0 0 0 0 26
2.2262 0.5223 -4.6942 H 0 0 0 0 0 0 0 0 0 0 27
1.5302 -1.7417 -3.9041 H 0 0 0 0 0 0 0 0 0 0 28
0.3119 -1.9962 -1.7538 H 0 0 0 0 0 0 0 0 0 0 29
-3.6803 1.9317 0.2116 H 0 0 0 0 0 0 0 0 0 0 30
2 1 0 0 0 0
3 1 0 0 0 0
5 2 0 0 0 0
8 2 0 0 0 0
4 3 0 0 0 0
9 3 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
7 4 0 0 0 0
15 6 0 0 0 0
19 6 0 0 0 0
11 7 0 0 0 0
12 7 0 0 0 0
11 10 0 0 0 0
14 10 0 0 0 0
20 10 0 0 0 0
21 11 0 0 0 0
13 12 0 0 0 0
22 12 0 0 0 0
14 13 0 0 0 0
23 13 0 0 0 0
24 14 0 0 0 0
16 15 0 0 0 0
25 15 0 0 0 0
17 16 0 0 0 0
26 16 0 0 0 0
18 17 0 0 0 0
27 17 0 0 0 0
19 18 0 0 0 0
28 18 0 0 0 0
29 19 0 0 0 0
8 30 0 0 0 0
M END
$$$$
phenytoin3.sdf
COSMOtherm 3D 0
31 33 0 0 0 0 0 0 0 0 0 V2000
-2.6104 -0.8648 0.0648 N 0 0 0 0 0 0 0 0 0 0 1
-2.5659 0.5437 -0.0128 C 0 0 0 0 0 0 0 0 0 0 2
-1.3489 -1.1784 0.0667 C 0 0 0 0 0 0 0 0 0 0 3
-0.4241 0.0474 -0.0024 C 0 0 0 0 0 0 0 0 0 0 4
-1.4178 1.1457 -0.0369 N 0 0 0 0 0 0 0 0 0 0 5
0.4153 0.1064 -1.2881 C 0 0 0 0 0 0 0 0 0 0 6
0.4468 0.0817 1.2672 C 0 0 0 0 0 0 0 0 0 0 7
-3.7615 1.1500 -0.0558 O 0 0 0 0 0 0 0 0 0 0 8
-0.8643 -2.4081 0.1482 O 0 0 0 0 0 0 0 0 0 0 9
0.8835 0.8813 3.5204 C 0 0 0 0 0 0 0 0 0 0 10
0.1040 0.8936 2.3568 C 0 0 0 0 0 0 0 0 0 0 11
1.5788 -0.7456 1.3584 C 0 0 0 0 0 0 0 0 0 0 12
2.3533 -0.7595 2.5216 C 0 0 0 0 0 0 0 0 0 0 13
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[illegible]

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3 1 0 0 0 0
4 1 0 0 0 0
5 1 0 0 0 0
6 2 0 0 0 0
4 7 0 0 0 0
M END
$$$$
phosphoricacid1.sdf
COSMOTHERM 3D 0

8 7 0 0 0 0 0 0 0 0 0 V2000
0.0495 -0.0253 0.0995 P 0 0 0 0 0 0 0 0 0 0 1
1.0212 0.3502 -1.1462 O 0 0 0 0 0 0 0 0 0 0 2
-0.9031 1.2865 0.1683 O 0 0 0 0 0 0 0 0 0 0 3
-0.8234 -1.2493 -0.5369 O 0 0 0 0 0 0 0 0 0 0 4
0.6715 -0.2989 1.4417 O 0 0 0 0 0 0 0 0 0 0 5
1.6434 -0.3715 -1.3691 H 0 0 0 0 0 0 0 0 0 0 6
-1.3335 1.4975 -0.6848 H 0 0 0 0 0 0 0 0 0 0 7
-1.2959 -1.7516 0.1575 H 0 0 0 0 0 0 0 0 0 0 8
2 1 0 0 0 0
3 1 0 0 0 0
4 1 0 0 0 0
5 1 0 0 0 0
6 2 0 0 0 0
7 3 0 0 0 0
4 8 0 0 0 0
M END
$$$$
phosphoricacid2-anion.sdf
COSMOTHERM 3D 0

7 6 0 0 0 0 0 0 0 0 0 V2000
-0.0017 0.0077 -0.1316 P 0 0 0 0 0 0 0 0 0 0 1
1.3034 0.2022 0.9059 O 0 0 0 0 0 0 0 0 0 0 2
-1.2937 -0.1923 0.9203 O 0 0 0 0 0 0 0 0 0 0 3
-0.2150 1.3721 -0.7821 O 0 0 0 0 0 0 0 0 0 0 4
0.1907 -1.2832 -0.9367 O 0 0 0 0 0 0 0 0 0 0 5
1.6539 -0.6720 1.1634 H 0 0 0 0 0 0 0 0 0 0 6
-1.3681 -1.1313 1.1763 H 0 0 0 0 0 0 0 0 0 0 7
2 1 0 0 0 0
3 1 0 0 0 0
4 1 0 0 0 0
5 1 0 0 0 0
6 2 0 0 0 0
3 7 0 0 0 0
M END
$$$$
phosphoricacid2.sdf
COSMOTHERM 3D 0

8 7 0 0 0 0 0 0 0 0 0 V2000
-0.0004 -0.1182 0.0013 P 0 0 0 0 0 0 0 0 0 0 1
1.2113 0.5964 -0.8134 O 0 0 0 0 0 0 0 0 0 0 2
0.0963 0.6231 1.4447 O 0 0 0 0 0 0 0 0 0 0 3
-1.3022 0.6060 -0.6496 O 0 0 0 0 0 0 0 0 0 0 4
-0.0049 -1.6257 0.0160 O 0 0 0 0 0 0 0 0 0 0 5
1.4109 0.1311 -1.6507 H 0 0 0 0 0 0 0 0 0 0 6
0.7265 0.1747 2.0441 H 0 0 0 0 0 0 0 0 0 0 7
-2.1338 0.1563 -0.3973 H 0 0 0 0 0 0 0 0 0 0 8
2 1 0 0 0 0
3 1 0 0 0 0
4 1 0 0 0 0
5 1 0 0 0 0
6 2 0 0 0 0
7 3 0 0 0 0
4 8 0 0 0 0
M END
$$$$
phthalicacid0-anion.sdf
COSMOTHERM 3D 0

17 17 0 0 0 0 0 0 0 0 0 V2000
-1.5099 -2.3763 0.0036 C 0 0 0 0 0 0 0 0 0 0 1
-0.1860 -2.8314 -0.0130 C 0 0 0 0 0 0 0 0 0 0 2
0.8644 -1.9098 -0.0122 C 0 0 0 0 0 0 0 0 0 0 3
0.6169 -0.5293 0.0084 C 0 0 0 0 0 0 0 0 0 0 4
-0.7172 -0.0802 0.0127 C 0 0 0 0 0 0 0 0 0 0 5
-1.7749 -1.0034 0.0173 C 0 0 0 0 0 0 0 0 0 0 6
1.7695 0.4714 0.0662 C 0 0 0 0 0 0 0 0 0 0 7
-1.0747 1.3812 0.0306 C 0 0 0 0 0 0 0 0 0 0 8
2.9452 0.0296 -0.0938 O 0 0 0 0 0 0 0 0 0 0 9
1.4378 1.6782 0.2877 O 0 0 0 0 0 0 0 0 0 0 10
-1.5274 1.9691 1.0061 O 0 0 0 0 0 0 0 0 0 0 11
-1.0574 1.9287 -1.2132 O 0 0 0 0 0 0 0 0 0 0 12
-2.3377 -3.0875 0.0052 H 0 0 0 0 0 0 0 0 0 0 13
0.0249 -3.9025 -0.0232 H 0 0 0 0 0 0 0 0 0 0 14
1.9033 -2.2436 -0.0169 H 0 0 0 0 0 0 0 0 0 0 15
-2.8073 -0.6481 0.0239 H 0 0 0 0 0 0 0 0 0 0 16
-1.3522 2.8621 -1.1321 H 0 0 0 0 0 0 0 0 0 0 17
2 1 0 0 0 0
6 1 0 0 0 0
13 1 0 0 0 0
3 2 0 0 0 0
14 2 0 0 0 0
4 3 0 0 0 0
15 3 0 0 0 0
5 4 0 0 0 0
7 4 0 0 0 0
6 5 0 0 0 0
8 5 0 0 0 0
16 6 0 0 0 0
9 7 0 0 0 0
10 7 0 0 0 0
11 8 0 0 0 0
12 8 0 0 0 0
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12 17 0 0 0 0
M END
$$$$
phthalicacid0.sdf
COSMOTHERM 3D 0

18 18 0 0 0 0 0 0 0 0 0 V2000
-2.8234 -0.0134 -0.0085 C 0 0 0 0 0 0 0 0 0 0 0 1
-2.4705 -1.3660 -0.0093 C 0 0 0 0 0 0 0 0 0 0 0 2
-1.1227 -1.7387 -0.0002 C 0 0 0 0 0 0 0 0 0 0 0 3
-0.1174 -0.7639 -0.0014 C 0 0 0 0 0 0 0 0 0 0 0 4
-0.4706 0.6041 0.0186 C 0 0 0 0 0 0 0 0 0 0 0 5
-1.8280 0.9656 0.0083 C 0 0 0 0 0 0 0 0 0 0 0 6
1.3031 -1.2488 -0.0528 C 0 0 0 0 0 0 0 0 0 0 0 7
0.5841 1.6467 0.1662 C 0 0 0 0 0 0 0 0 0 0 0 8
1.8004 -1.9909 0.7817 O 0 0 0 0 0 0 0 0 0 0 0 9
1.9377 -0.8588 -1.1804 O 0 0 0 0 0 0 0 0 0 0 0 10
1.6910 1.4423 0.6505 O 0 0 0 0 0 0 0 0 0 0 0 11
0.1822 2.8661 -0.2639 O 0 0 0 0 0 0 0 0 0 0 0 12
-3.8736 0.2810 -0.0122 H 0 0 0 0 0 0 0 0 0 0 0 13
-3.2433 -2.1358 -0.0176 H 0 0 0 0 0 0 0 0 0 0 0 14
-0.8470 -2.7939 -0.0151 H 0 0 0 0 0 0 0 0 0 0 0 15
-2.0992 2.0203 0.0390 H 0 0 0 0 0 0 0 0 0 0 0 16
2.8521 -1.2184 -1.1584 H 0 0 0 0 0 0 0 0 0 0 0 17
0.9064 3.5035 -0.0814 H 0 0 0 0 0 0 0 0 0 0 0 18

2 1 0 0 0 0
6 1 0 0 0 0
13 1 0 0 0 0
3 2 0 0 0 0
14 2 0 0 0 0
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16 6 0 0 0 0
9 7 0 0 0 0
10 7 0 0 0 0
11 8 0 0 0 0
12 8 0 0 0 0
17 10 0 0 0 0
12 18 0 0 0 0
M END
$$$$
phthalicacid1-anion.sdf
COSMOTHERM 3D 0

17 17 0 0 0 0 0 0 0 0 0 V2000
0.1883 -2.8314 -0.0124 C 0 0 0 0 0 0 0 0 0 0 0 1
1.5117 -2.3750 0.0025 C 0 0 0 0 0 0 0 0 0 0 0 2
1.7755 -1.0018 0.0167 C 0 0 0 0 0 0 0 0 0 0 0 3
0.7169 -0.0797 0.0124 C 0 0 0 0 0 0 0 0 0 0 0 4
-0.6167 -0.5300 0.0081 C 0 0 0 0 0 0 0 0 0 0 0 5
-0.8630 -1.9109 -0.0097 C 0 0 0 0 0 0 0 0 0 0 0 6
1.0729 1.3821 0.0317 C 0 0 0 0 0 0 0 0 0 0 0 7
-1.7698 0.4703 0.0645 C 0 0 0 0 0 0 0 0 0 0 0 8
1.5206 1.9703 1.0095 O 0 0 0 0 0 0 0 0 0 0 0 9
1.0618 1.9296 -1.2121 O 0 0 0 0 0 0 0 0 0 0 0 10
-2.9456 0.0270 -0.0941 O 0 0 0 0 0 0 0 0 0 0 0 11
-1.4387 1.6774 0.2831 O 0 0 0 0 0 0 0 0 0 0 0 12
-0.0215 -3.9027 -0.0231 H 0 0 0 0 0 0 0 0 0 0 0 13
2.3402 -3.0854 0.0033 H 0 0 0 0 0 0 0 0 0 0 0 14
2.8075 -0.6456 0.0230 H 0 0 0 0 0 0 0 0 0 0 0 15
-1.9017 -2.2455 -0.0142 H 0 0 0 0 0 0 0 0 0 0 0 16
1.3565 2.8629 -1.1291 H 0 0 0 0 0 0 0 0 0 0 0 17

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10 17 0 0 0 0
M END
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phthalicacid1.sdf
COSMOTHERM 3D 0

18 18 0 0 0 0 0 0 0 0 0 V2000
-0.5046 -2.7893 -0.0106 C 0 0 0 0 0 0 0 0 0 0 0 1
0.8897 -2.6876 0.0108 C 0 0 0 0 0 0 0 0 0 0 0 2
1.4978 -1.4299 0.0173 C 0 0 0 0 0 0 0 0 0 0 0 3
0.7216 -0.2623 -0.0042 C 0 0 0 0 0 0 0 0 0 0 0 4
-0.6885 -0.3641 0.0112 C 0 0 0 0 0 0 0 0 0 0 0 5
-1.2870 -1.6328 -0.0113 C 0 0 0 0 0 0 0 0 0 0 0 6
1.4591 1.0375 -0.1053 C 0 0 0 0 0 0 0 0 0 0 0 7
-1.6011 0.8149 0.1176 C 0 0 0 0 0 0 0 0 0 0 0 8
2.4264 1.3339 0.5817 O 0 0 0 0 0 0 0 0 0 0 0 9
0.9840 1.8201 -1.1015 O 0 0 0 0 0 0 0 0 0 0 0 10
-2.6991 0.8870 -0.4188 O 0 0 0 0 0 0 0 0 0 0 0 11
-1.1079 1.7786 0.9299 O 0 0 0 0 0 0 0 0 0 0 0 12
-0.9847 -3.7687 -0.0198 H 0 0 0 0 0 0 0 0 0 0 0 13
1.5070 -3.5868 0.0182 H 0 0 0 0 0 0 0 0 0 0 0 14
2.5851 -1.3455 0.0069 H 0 0 0 0 0 0 0 0 0 0 0 15
-2.3752 -1.7037 0.0028 H 0 0 0 0 0 0 0 0 0 0 0 16
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16 6 0 0 0 0
9 7 0 0 0 0
10 7 0 0 0 0
11 8 0 0 0 0
12 8 0 0 0 0
17 10 0 0 0 0
12 18 0 0 0 0
M END
$$$$
phthalimide0-anion.sdf
COSMOtherm 3D 0
15 16 0 0 0 0 0 0 0 0 0 V2000
-2.6044 0.7013 -0.0001 C 0 0 0 0 0 0 0 0 0 0 1
-2.6044 -0.7013 0.0001 C 0 0 0 0 0 0 0 0 0 0 2
-1.3970 -1.4253 0.0002 C 0 0 0 0 0 0 0 0 0 0 3
-0.2118 -0.6990 0.0000 C 0 0 0 0 0 0 0 0 0 0 4
-0.2118 0.6990 0.0000 C 0 0 0 0 0 0 0 0 0 0 5
-1.3970 1.4252 -0.0002 C 0 0 0 0 0 0 0 0 0 0 6
1.2447 1.1146 0.0000 C 0 0 0 0 0 0 0 0 0 0 7
1.2447 -1.1146 0.0000 C 0 0 0 0 0 0 0 0 0 0 8
2.0502 0.0000 0.0000 N 0 0 0 0 0 0 0 0 0 0 9
1.6432 -2.2963 -0.0001 O 0 0 0 0 0 0 0 0 0 0 10
1.6431 2.2963 0.0001 O 0 0 0 0 0 0 0 0 0 0 11
-3.5555 1.2371 -0.0002 H 0 0 0 0 0 0 0 0 0 0 12
-3.5555 -1.2371 0.0002 H 0 0 0 0 0 0 0 0 0 0 13
-1.3971 -2.5172 0.0004 H 0 0 0 0 0 0 0 0 0 0 14
-1.3971 2.5171 -0.0003 H 0 0 0 0 0 0 0 0 0 0 15
2 1 0 0 0 0
6 1 0 0 0 0
12 1 0 0 0 0
3 2 0 0 0 0
13 2 0 0 0 0
4 3 0 0 0 0
14 3 0 0 0 0
5 4 0 0 0 0
8 4 0 0 0 0
6 5 0 0 0 0
7 5 0 0 0 0
9 7 0 0 0 0
11 7 0 0 0 0
9 8 0 0 0 0
10 8 0 0 0 0
6 15 0 0 0 0
M END
$$$$
phthalimide0.sdf
COSMOtherm 3D 0
16 17 0 0 0 0 0 0 0 0 0 V2000
-2.6101 0.7013 0.0000 C 0 0 0 0 0 0 0 0 0 0 1
-2.6101 -0.7013 0.0000 C 0 0 0 0 0 0 0 0 0 0 2
-1.4073 -1.4274 0.0000 C 0 0 0 0 0 0 0 0 0 0 3
-0.2219 -0.7018 0.0000 C 0 0 0 0 0 0 0 0 0 0 4
-0.2219 0.7018 0.0000 C 0 0 0 0 0 0 0 0 0 0 5
-1.4073 1.4274 0.0001 C 0 0 0 0 0 0 0 0 0 0 6
1.1975 1.1682 0.0000 C 0 0 0 0 0 0 0 0 0 0 7
1.1975 -1.1682 0.0001 C 0 0 0 0 0 0 0 0 0 0 8
1.9708 0.0000 0.0005 N 0 0 0 0 0 0 0 0 0 0 9
1.6396 -2.3108 -0.0002 O 0 0 0 0 0 0 0 0 0 0 10
1.6396 2.3108 -0.0003 O 0 0 0 0 0 0 0 0 0 0 11
2.9900 0.0000 -0.0003 H 0 0 0 0 0 0 0 0 0 0 12
-3.5605 1.2369 0.0000 H 0 0 0 0 0 0 0 0 0 0 13
-3.5604 -1.2369 -0.0001 H 0 0 0 0 0 0 0 0 0 0 14
-1.4068 -2.5181 0.0001 H 0 0 0 0 0 0 0 0 0 0 15
-1.4069 2.5181 0.0001 H 0 0 0 0 0 0 0 0 0 0 16
2 1 0 0 0 0
6 1 0 0 0 0
13 1 0 0 0 0
3 2 0 0 0 0
14 2 0 0 0 0
4 3 0 0 0 0
15 3 0 0 0 0
5 4 0 0 0 0
8 4 0 0 0 0
6 5 0 0 0 0
7 5 0 0 0 0
9 7 0 0 0 0
11 7 0 0 0 0
9 8 0 0 0 0
10 8 0 0 0 0
12 9 0 0 0 0
6 16 0 0 0 0
M END
$$$$
phthalimide1-anion.sdf
COSMOtherm 3D 0
15 16 0 0 0 0 0 0 0 0 0 V2000
-2.6044 0.7013 -0.0001 C 0 0 0 0 0 0 0 0 0 0 1
-2.6044 -0.7013 0.0001 C 0 0 0 0 0 0 0 0 0 0 2
-1.3970 -1.4253 0.0002 C 0 0 0 0 0 0 0 0 0 0 3
-0.2118 -0.6990 0.0000 C 0 0 0 0 0 0 0 0 0 0 4
-0.2118 0.6990 0.0000 C 0 0 0 0 0 0 0 0 0 0 5
-1.3970 1.4252 -0.0002 C 0 0 0 0 0 0 0 0 0 0 6
```

URL: <http://mc.manuscriptcentral.com/tandf/tmph>

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15 15 0 0 0 0 0 0 0 0 0 V2000
1.8791 -0.0117 1.5268 C 0 0 0 0 0 0 0 0 0 1
2.6213 -0.0034 0.3387 C 0 0 0 0 0 0 0 0 0 2
1.9603 0.0060 -0.8882 C 0 0 0 0 0 0 0 0 0 3
0.5533 0.0059 -0.9557 C 0 0 0 0 0 0 0 0 0 4
-0.2183 -0.0018 0.2336 C 0 0 0 0 0 0 0 0 0 5
0.4861 -0.0100 1.4534 C 0 0 0 0 0 0 0 0 0 6
-0.0555 0.0164 -2.1866 O 0 0 0 0 0 0 0 0 0 7
-1.7536 -0.0017 0.2902 C 0 0 0 0 0 0 0 0 0 8
-2.2730 0.0347 1.4519 O 0 0 0 0 0 0 0 0 0 9
-2.3987 -0.0388 -0.7997 O 0 0 0 0 0 0 0 0 0 10
2.3821 -0.0191 2.4953 H 0 0 0 0 0 0 0 0 0 11
3.7128 -0.0034 0.3633 H 0 0 0 0 0 0 0 0 0 12
2.5332 0.0137 -1.8202 H 0 0 0 0 0 0 0 0 0 13
-0.1188 -0.0140 2.3616 H 0 0 0 0 0 0 0 0 0 14
0.6488 0.0261 -2.8644 H 0 0 0 0 0 0 0 0 0 15
2 1 0 0 0 0
6 1 0 0 0 0
11 1 0 0 0 0
3 2 0 0 0 0
12 2 0 0 0 0
4 3 0 0 0 0
13 3 0 0 0 0
5 4 0 0 0 0
7 4 0 0 0 0
6 5 0 0 0 0
8 5 0 0 0 0
14 6 0 0 0 0
9 8 0 0 0 0
10 8 0 0 0 0
7 15 0 0 0 0
M END
$$$$
salicylicacid-anion2.sdf
COSMOtherm 3D 0
15 15 0 0 0 0 0 0 0 0 0 V2000
1.9626 -1.4503 -0.0138 C 0 0 0 0 0 0 0 0 0 1
2.6334 -0.2225 -0.0041 C 0 0 0 0 0 0 0 0 0 2
1.9050 0.9727 0.0087 C 0 0 0 0 0 0 0 0 0 3
0.5036 0.9394 0.0087 C 0 0 0 0 0 0 0 0 0 4
-0.1889 -0.2866 -0.0016 C 0 0 0 0 0 0 0 0 0 5
0.5617 -1.4715 -0.0113 C 0 0 0 0 0 0 0 0 0 6
-0.2521 2.0934 0.0224 O 0 0 0 0 0 0 0 0 0 7
-1.7161 -0.3256 -0.0035 C 0 0 0 0 0 0 0 0 0 8
-2.2847 -0.3944 1.1267 O 0 0 0 0 0 0 0 0 0 9
-2.2835 -0.3015 -1.1362 O 0 0 0 0 0 0 0 0 0 10
2.5241 -2.3861 -0.0237 H 0 0 0 0 0 0 0 0 0 11
3.7243 -0.1873 -0.0051 H 0 0 0 0 0 0 0 0 0 12
2.4221 1.9362 0.0180 H 0 0 0 0 0 0 0 0 0 13
0.0359 -2.4297 -0.0180 H 0 0 0 0 0 0 0 0 0 14
0.3463 2.8644 0.0254 H 0 0 0 0 0 0 0 0 0 15
2 1 0 0 0 0
6 1 0 0 0 0
11 1 0 0 0 0
3 2 0 0 0 0
12 2 0 0 0 0
4 3 0 0 0 0
13 3 0 0 0 0
5 4 0 0 0 0
7 4 0 0 0 0
6 5 0 0 0 0
8 5 0 0 0 0
14 6 0 0 0 0
9 8 0 0 0 0
10 8 0 0 0 0
7 15 0 0 0 0
M END
$$$$
salicylicacid0.sdf
COSMOtherm 3D 0
16 16 0 0 0 0 0 0 0 0 0 V2000
1.9437 -1.4792 -0.0009 C 0 0 0 0 0 0 0 0 0 1
2.6327 -0.2522 0.0005 C 0 0 0 0 0 0 0 0 0 2
1.9427 0.9560 0.0010 C 0 0 0 0 0 0 0 0 0 3
0.5371 0.9648 0.0003 C 0 0 0 0 0 0 0 0 0 4
-0.1718 -0.2708 -0.0006 C 0 0 0 0 0 0 0 0 0 5
0.5549 -1.4820 -0.0012 C 0 0 0 0 0 0 0 0 0 6
-0.0979 2.1606 0.0003 O 0 0 0 0 0 0 0 0 0 7
-1.6370 -0.2430 -0.0003 C 0 0 0 0 0 0 0 0 0 8
-2.3052 0.8076 -0.0017 O 0 0 0 0 0 0 0 0 0 9
-2.2310 -1.4522 0.0023 O 0 0 0 0 0 0 0 0 0 10
2.4950 -2.4198 -0.0015 H 0 0 0 0 0 0 0 0 0 11
3.7241 -0.2427 0.0010 H 0 0 0 0 0 0 0 0 0 12
2.4727 1.9094 0.0020 H 0 0 0 0 0 0 0 0 0 13
0.0072 -2.4245 -0.0022 H 0 0 0 0 0 0 0 0 0 14
-1.0821 1.9529 -0.0002 H 0 0 0 0 0 0 0 0 0 15
-3.2027 -1.3130 0.0010 H 0 0 0 0 0 0 0 0 0 16
2 1 0 0 0 0
6 1 0 0 0 0
11 1 0 0 0 0
3 2 0 0 0 0
12 2 0 0 0 0
4 3 0 0 0 0
13 3 0 0 0 0
5 4 0 0 0 0
7 4 0 0 0 0
6 5 0 0 0 0
8 5 0 0 0 0
14 6 0 0 0 0
15 7 0 0 0 0
9 8 0 0 0 0
10 8 0 0 0 0
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10 16 0 0 0 0
M END
$$$$
salicylicacid1.sdf
COSMOtherm 3D 0

16 16 0 0 0 0 0 0 0 0 0 V2000
1.9715 -1.4610 -0.0320 C 0 0 0 0 0 0 0 0 0 0 0 1
2.6400 -0.2246 -0.0025 C 0 0 0 0 0 0 0 0 0 0 0 2
1.9244 0.9673 0.0219 C 0 0 0 0 0 0 0 0 0 0 0 3
0.5178 0.9589 0.0163 C 0 0 0 0 0 0 0 0 0 0 0 4
-0.1720 -0.2862 -0.0092 C 0 0 0 0 0 0 0 0 0 0 0 5
0.5836 -1.4800 -0.0308 C 0 0 0 0 0 0 0 0 0 0 0 6
-0.0920 2.1735 0.0418 O 0 0 0 0 0 0 0 0 0 0 0 7
-1.6436 -0.4208 0.0039 C 0 0 0 0 0 0 0 0 0 0 0 8
-2.2655 -1.4717 0.0889 O 0 0 0 0 0 0 0 0 0 0 0 9
-2.2911 0.7850 -0.0999 O 0 0 0 0 0 0 0 0 0 0 0 10
2.5351 -2.3940 -0.0536 H 0 0 0 0 0 0 0 0 0 0 0 11
3.7310 -0.1927 -0.0003 H 0 0 0 0 0 0 0 0 0 0 0 12
2.4359 1.9307 0.0437 H 0 0 0 0 0 0 0 0 0 0 0 13
0.0408 -2.4259 -0.0498 H 0 0 0 0 0 0 0 0 0 0 0 14
-1.0702 2.0368 0.0097 H 0 0 0 0 0 0 0 0 0 0 0 15
-3.2603 0.6394 -0.0506 H 0 0 0 0 0 0 0 0 0 0 0 16

2 1 0 0 0 0
6 1 0 0 0 0
11 1 0 0 0 0
3 2 0 0 0 0
12 2 0 0 0 0
4 3 0 0 0 0
13 3 0 0 0 0
5 4 0 0 0 0
7 4 0 0 0 0
6 5 0 0 0 0
8 5 0 0 0 0
14 6 0 0 0 0
15 7 0 0 0 0
9 8 0 0 0 0
10 8 0 0 0 0
10 16 0 0 0 0
M END
$$$$
salicylicacid2.sdf
COSMOtherm 3D 0

16 16 0 0 0 0 0 0 0 0 0 V2000
1.9317 -1.4943 -0.0426 C 0 0 0 0 0 0 0 0 0 0 0 1
2.6385 -0.2825 -0.0182 C 0 0 0 0 0 0 0 0 0 0 0 2
1.9533 0.9281 0.0169 C 0 0 0 0 0 0 0 0 0 0 0 3
0.5467 0.9625 0.0248 C 0 0 0 0 0 0 0 0 0 0 0 4
-0.1830 -0.2553 -0.0031 C 0 0 0 0 0 0 0 0 0 0 0 5
0.5426 -1.4666 -0.0311 C 0 0 0 0 0 0 0 0 0 0 0 6
-0.1079 2.1566 0.0694 O 0 0 0 0 0 0 0 0 0 0 0 7
-1.6636 -0.3820 0.0043 C 0 0 0 0 0 0 0 0 0 0 0 8
-2.2529 -1.4555 0.1264 O 0 0 0 0 0 0 0 0 0 0 0 9
-2.3413 0.7817 -0.1506 O 0 0 0 0 0 0 0 0 0 0 0 10
2.4632 -2.4459 -0.0703 H 0 0 0 0 0 0 0 0 0 0 0 11
3.7298 -0.2802 -0.0257 H 0 0 0 0 0 0 0 0 0 0 0 12
2.5024 1.8728 0.0404 H 0 0 0 0 0 0 0 0 0 0 0 13
-0.0288 -2.3952 -0.0481 H 0 0 0 0 0 0 0 0 0 0 0 14
0.5561 2.8732 0.1006 H 0 0 0 0 0 0 0 0 0 0 0 15
-3.2967 0.5540 -0.1305 H 0 0 0 0 0 0 0 0 0 0 0 16

2 1 0 0 0 0
6 1 0 0 0 0
11 1 0 0 0 0
3 2 0 0 0 0
12 2 0 0 0 0
4 3 0 0 0 0
13 3 0 0 0 0
5 4 0 0 0 0
7 4 0 0 0 0
6 5 0 0 0 0
8 5 0 0 0 0
14 6 0 0 0 0
15 7 0 0 0 0
9 8 0 0 0 0
10 8 0 0 0 0
10 16 0 0 0 0
M END
$$$$
succinimide0-anion.sdf
COSMOtherm 3D 0

11 11 0 0 0 0 0 0 0 0 0 V2000
-0.7642 -1.3025 0.0003 C 0 0 0 0 0 0 0 0 0 0 0 1
-1.1140 0.1968 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 2
0.7642 -1.3025 -0.0003 C 0 0 0 0 0 0 0 0 0 0 0 3
1.1140 0.1968 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 4
0.0000 0.9894 0.0000 N 0 0 0 0 0 0 0 0 0 0 0 5
2.2894 0.6213 0.0001 O 0 0 0 0 0 0 0 0 0 0 0 6
-2.2894 0.6213 -0.0001 O 0 0 0 0 0 0 0 0 0 0 0 7
-1.2087 -1.7807 -0.8848 H 0 0 0 0 0 0 0 0 0 0 0 8
-1.2079 -1.7800 0.8861 H 0 0 0 0 0 0 0 0 0 0 0 9
1.2079 -1.7800 -0.8861 H 0 0 0 0 0 0 0 0 0 0 0 10
1.2087 -1.7806 0.8848 H 0 0 0 0 0 0 0 0 0 0 0 11

2 1 0 0 0 0
3 1 0 0 0 0
8 1 0 0 0 0
9 1 0 0 0 0
5 2 0 0 0 0
7 2 0 0 0 0
4 3 0 0 0 0
10 3 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
3 11 0 0 0 0
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M END
$$$$
succinimide0.sdf
COSMOTHERM 3D 0

12 12 0 0 0 0 0 0 0 0 V2000
-0.7686 -1.3091 0.0000 C 0 0 0 0 0 0 0 0 0 0 1
-1.1700 0.1577 0.0000 C 0 0 0 0 0 0 0 0 0 0 2
0.7686 -1.3091 -0.0001 C 0 0 0 0 0 0 0 0 0 0 3
1.1700 0.1577 0.0000 C 0 0 0 0 0 0 0 0 0 0 4
0.0000 0.9110 -0.0005 N 0 0 0 0 0 0 0 0 0 0 5
2.3005 0.6308 0.0003 O 0 0 0 0 0 0 0 0 0 0 6
-2.3005 0.6307 0.0003 O 0 0 0 0 0 0 0 0 0 0 7
-1.2031 -1.7935 -0.8850 H 0 0 0 0 0 0 0 0 0 0 8
-1.2029 -1.7935 0.8851 H 0 0 0 0 0 0 0 0 0 0 9
1.2029 -1.7935 -0.8852 H 0 0 0 0 0 0 0 0 0 0 10
1.2030 -1.7936 0.8849 H 0 0 0 0 0 0 0 0 0 0 11
0.0000 1.9318 -0.0010 H 0 0 0 0 0 0 0 0 0 0 12

2 1 0 0 0 0
3 1 0 0 0 0
8 1 0 0 0 0
9 1 0 0 0 0
5 2 0 0 0 0
7 2 0 0 0 0
4 3 0 0 0 0
10 3 0 0 0 0
11 3 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
5 12 0 0 0 0

M END
$$$$
succinimide1-anion.sdf
COSMOTHERM 3D 0

11 11 0 0 0 0 0 0 0 0 V2000
-0.7642 -1.3025 0.0003 C 0 0 0 0 0 0 0 0 0 0 1
-1.1140 0.1968 0.0000 C 0 0 0 0 0 0 0 0 0 0 2
0.7642 -1.3025 -0.0003 C 0 0 0 0 0 0 0 0 0 0 3
1.1140 0.1968 0.0000 C 0 0 0 0 0 0 0 0 0 0 4
0.0000 0.9894 0.0000 N 0 0 0 0 0 0 0 0 0 0 5
2.2894 0.6213 0.0001 O 0 0 0 0 0 0 0 0 0 0 6
-2.2894 0.6213 -0.0001 O 0 0 0 0 0 0 0 0 0 0 7
-1.2087 -1.7807 -0.8848 H 0 0 0 0 0 0 0 0 0 0 8
-1.2079 -1.7800 0.8861 H 0 0 0 0 0 0 0 0 0 0 9
1.2079 -1.7800 -0.8861 H 0 0 0 0 0 0 0 0 0 0 10
1.2087 -1.7806 0.8848 H 0 0 0 0 0 0 0 0 0 0 11

2 1 0 0 0 0
3 1 0 0 0 0
8 1 0 0 0 0
9 1 0 0 0 0
5 2 0 0 0 0
7 2 0 0 0 0
4 3 0 0 0 0
10 3 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
3 11 0 0 0 0

M END
$$$$
succinimide1.sdf
COSMOTHERM 3D 0

12 12 0 0 0 0 0 0 0 0 V2000
-0.8108 -1.3030 0.0008 C 0 0 0 0 0 0 0 0 0 0 1
-1.1547 0.1908 0.0000 C 0 0 0 0 0 0 0 0 0 0 2
0.7226 -1.3195 -0.0007 C 0 0 0 0 0 0 0 0 0 0 3
1.0279 0.1510 -0.0001 C 0 0 0 0 0 0 0 0 0 0 4
0.0185 0.9790 0.0000 N 0 0 0 0 0 0 0 0 0 0 5
2.2943 0.5414 0.0002 O 0 0 0 0 0 0 0 0 0 0 6
-2.2849 0.6685 -0.0003 O 0 0 0 0 0 0 0 0 0 0 7
-1.2528 -1.7802 -0.8842 H 0 0 0 0 0 0 0 0 0 0 8
-1.2506 -1.7784 0.8879 H 0 0 0 0 0 0 0 0 0 0 9
1.1627 -1.7975 -0.8874 H 0 0 0 0 0 0 0 0 0 0 10
1.1647 -1.7988 0.8843 H 0 0 0 0 0 0 0 0 0 0 11
2.3328 1.5235 0.0013 H 0 0 0 0 0 0 0 0 0 0 12

2 1 0 0 0 0
3 1 0 0 0 0
8 1 0 0 0 0
9 1 0 0 0 0
5 2 0 0 0 0
7 2 0 0 0 0
4 3 0 0 0 0
10 3 0 0 0 0
11 3 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
6 12 0 0 0 0

M END
$$$$
sulfurousacid-anion.sdf
COSMOTHERM 3D 0

5 4 0 0 0 0 0 0 0 0 V2000
-0.3954 0.0003 0.1433 S 0 0 0 0 0 0 0 0 0 0 1
0.1242 -0.0091 -1.5871 O 0 0 0 0 0 0 0 0 0 0 2
0.2999 -1.2545 0.7067 O 0 0 0 0 0 0 0 0 0 0 3
0.2988 1.2627 0.6908 O 0 0 0 0 0 0 0 0 0 0 4
1.1052 0.0044 -1.5476 H 0 0 0 0 0 0 0 0 0 0 5

2 1 0 0 0 0
3 1 0 0 0 0
4 1 0 0 0 0
2 5 0 0 0 0

M END
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10 1 0 0 0 0
3 2 0 0 0 0
9 2 0 0 0 0
4 3 0 0 0 0
7 3 0 0 0 0
5 4 0 0 0 0
11 4 0 0 0 0
6 5 0 0 0 0
8 5 0 0 0 0
12 9 0 0 0 0
13 9 0 0 0 0
9 14 0 0 0 0
M END
$$$$
thymine.sdf
COSMOTHERM 3D 0
15 15 0 0 0 0 0 0 0 0 0 V2000
-0.2358 -1.5308 0.0005 C 0 0 0 0 0 0 0 0 0 1
-1.1931 -0.5610 0.0012 C 0 0 0 0 0 0 0 0 0 2
-0.7573 0.8299 0.0002 C 0 0 0 0 0 0 0 0 0 3
0.6382 1.0148 0.0015 N 0 0 0 0 0 0 0 0 0 4
1.6228 0.0390 0.0000 C 0 0 0 0 0 0 0 0 0 5
1.1098 -1.2457 -0.0010 N 0 0 0 0 0 0 0 0 0 6
-1.5071 1.8174 -0.0011 O 0 0 0 0 0 0 0 0 0 7
2.8316 0.2902 -0.0004 O 0 0 0 0 0 0 0 0 0 8
-2.6630 -0.8607 -0.0002 C 0 0 0 0 0 0 0 0 0 9
-0.4772 -2.5931 0.0004 H 0 0 0 0 0 0 0 0 0 10
0.9694 1.9810 0.0019 H 0 0 0 0 0 0 0 0 0 11
1.7880 -2.0053 -0.0018 H 0 0 0 0 0 0 0 0 0 12
-3.1480 -0.4549 -0.9011 H 0 0 0 0 0 0 0 0 0 13
-3.1600 -0.4000 0.8667 H 0 0 0 0 0 0 0 0 0 14
-2.8404 -1.9432 0.0313 H 0 0 0 0 0 0 0 0 0 15
2 1 0 0 0 0
6 1 0 0 0 0
10 1 0 0 0 0
3 2 0 0 0 0
9 2 0 0 0 0
4 3 0 0 0 0
7 3 0 0 0 0
5 4 0 0 0 0
11 4 0 0 0 0
6 5 0 0 0 0
8 5 0 0 0 0
12 6 0 0 0 0
13 9 0 0 0 0
14 9 0 0 0 0
9 15 0 0 0 0
M END
$$$$
trans-5-formyluracil-anion0.sdf
COSMOTHERM 3D 0
13 13 0 0 0 0 0 0 0 0 0 V2000
-0.2798 -1.3087 -0.0001 C 0 0 0 0 0 0 0 0 0 1
-0.9153 -0.0847 0.0001 C 0 0 0 0 0 0 0 0 0 2
-0.0774 1.1359 0.0000 C 0 0 0 0 0 0 0 0 0 3
1.2907 0.9994 0.0000 N 0 0 0 0 0 0 0 0 0 4
1.8897 -0.2079 0.0000 C 0 0 0 0 0 0 0 0 0 5
1.0596 -1.3779 -0.0001 N 0 0 0 0 0 0 0 0 0 6
-0.6008 2.2805 0.0000 O 0 0 0 0 0 0 0 0 0 7
3.1253 -0.3988 0.0001 O 0 0 0 0 0 0 0 0 0 8
-2.3637 -0.0062 -0.0003 C 0 0 0 0 0 0 0 0 0 9
-0.8290 -2.2518 -0.0001 H 0 0 0 0 0 0 0 0 0 10
1.5337 -2.2806 -0.0003 H 0 0 0 0 0 0 0 0 0 11
-3.1410 -0.9756 0.0003 O 0 0 0 0 0 0 0 0 0 12
-2.7665 1.0298 -0.0012 H 0 0 0 0 0 0 0 0 0 13
2 1 0 0 0 0
6 1 0 0 0 0
10 1 0 0 0 0
3 2 0 0 0 0
9 2 0 0 0 0
4 3 0 0 0 0
7 3 0 0 0 0
5 4 0 0 0 0
6 5 0 0 0 0
8 5 0 0 0 0
11 6 0 0 0 0
12 9 0 0 0 0
9 13 0 0 0 0
M END
$$$$
trans-5-formyluracil-anion1.sdf
COSMOTHERM 3D 0
13 13 0 0 0 0 0 0 0 0 0 V2000
-0.2325 -1.3051 0.0000 C 0 0 0 0 0 0 0 0 0 1
-0.9240 -0.0791 -0.0003 C 0 0 0 0 0 0 0 0 0 2
-0.1404 1.1418 0.0000 C 0 0 0 0 0 0 0 0 0 3
1.2390 0.9038 0.0006 N 0 0 0 0 0 0 0 0 0 4
1.8773 -0.3441 0.0000 C 0 0 0 0 0 0 0 0 0 5
1.0863 -1.4787 0.0000 N 0 0 0 0 0 0 0 0 0 6
-0.5688 2.3129 -0.0001 O 0 0 0 0 0 0 0 0 0 7
3.1211 -0.3936 -0.0002 O 0 0 0 0 0 0 0 0 0 8
-2.3648 -0.0173 -0.0003 C 0 0 0 0 0 0 0 0 0 9
-0.8348 -2.2210 0.0001 H 0 0 0 0 0 0 0 0 0 10
1.8441 1.7270 0.0003 H 0 0 0 0 0 0 0 0 0 11
-3.1365 -0.9955 0.0003 O 0 0 0 0 0 0 0 0 0 12
-2.7856 1.0133 -0.0008 H 0 0 0 0 0 0 0 0 0 13
2 1 0 0 0 0
6 1 0 0 0 0
10 1 0 0 0 0
3 2 0 0 0 0
9 2 0 0 0 0
4 3 0 0 0 0
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7 3 0 0 0 0
5 4 0 0 0 0
11 4 0 0 0 0
6 5 0 0 0 0
8 5 0 0 0 0
12 9 0 0 0 0
9 13 0 0 0 0
M END
$$$$
trans-5-formyluracil.sdf
COSMOTHERM 3D 0

14 14 0 0 0 0 0 0 0 0 0 V2000
-0.2914 -1.2943 -0.0001 C 0 0 0 0 0 0 0 0 0 0 1
-0.9385 -0.0802 -0.0001 C 0 0 0 0 0 0 0 0 0 0 2
-0.1445 1.1475 0.0000 C 0 0 0 0 0 0 0 0 0 0 3
1.2468 0.9277 0.0006 N 0 0 0 0 0 0 0 0 0 0 4
1.9141 -0.2832 0.0000 C 0 0 0 0 0 0 0 0 0 0 5
1.0539 -1.3916 -0.0001 N 0 0 0 0 0 0 0 0 0 0 6
-0.5863 2.2999 -0.0002 O 0 0 0 0 0 0 0 0 0 0 7
3.1347 -0.3996 -0.0002 O 0 0 0 0 0 0 0 0 0 0 8
-2.3993 -0.0103 -0.0003 C 0 0 0 0 0 0 0 0 0 0 9
-0.8435 -2.2347 -0.0004 H 0 0 0 0 0 0 0 0 0 0 10
1.8389 1.7607 0.0008 H 0 0 0 0 0 0 0 0 0 0 11
1.5034 -2.3076 -0.0004 H 0 0 0 0 0 0 0 0 0 0 12
-3.1466 -0.9923 0.0004 O 0 0 0 0 0 0 0 0 0 0 13
-2.8163 1.0190 -0.0012 H 0 0 0 0 0 0 0 0 0 0 14
2 1 0 0 0 0
6 1 0 0 0 0
10 1 0 0 0 0
3 2 0 0 0 0
9 2 0 0 0 0
4 3 0 0 0 0
7 3 0 0 0 0
5 4 0 0 0 0
11 4 0 0 0 0
6 5 0 0 0 0
8 5 0 0 0 0
12 6 0 0 0 0
13 9 0 0 0 0
9 14 0 0 0 0
M END
$$$$
trans-5-formyluracil2-anion.sdf
COSMOTHERM 3D 0

13 13 0 0 0 0 0 0 0 0 0 V2000
-1.5697 -0.2689 0.0010 C 0 0 0 0 0 0 0 0 0 0 1
-0.6003 0.7615 0.0008 C 0 0 0 0 0 0 0 0 0 0 2
0.7620 0.3063 0.0008 C 0 0 0 0 0 0 0 0 0 0 3
1.0980 -0.9662 0.0007 N 0 0 0 0 0 0 0 0 0 0 4
0.0784 -1.9169 -0.0003 C 0 0 0 0 0 0 0 0 0 0 5
-1.2847 -1.5566 0.0011 N 0 0 0 0 0 0 0 0 0 0 6
1.7540 1.2161 0.0010 O 0 0 0 0 0 0 0 0 0 0 7
0.3755 -3.1331 -0.0021 O 0 0 0 0 0 0 0 0 0 0 8
-0.9264 2.1462 -0.0008 C 0 0 0 0 0 0 0 0 0 0 9
-2.6326 0.0048 0.0014 H 0 0 0 0 0 0 0 0 0 0 10
-0.0615 3.0674 -0.0016 O 0 0 0 0 0 0 0 0 0 0 11
-2.0016 2.4161 -0.0015 H 0 0 0 0 0 0 0 0 0 0 12
1.2870 2.1234 -0.0006 H 0 0 0 0 0 0 0 0 0 0 13
2 1 0 0 0 0
6 1 0 0 0 0
10 1 0 0 0 0
3 2 0 0 0 0
9 2 0 0 0 0
4 3 0 0 0 0
7 3 0 0 0 0
5 4 0 0 0 0
6 5 0 0 0 0
8 5 0 0 0 0
11 9 0 0 0 0
12 9 0 0 0 0
7 13 0 0 0 0
M END
$$$$
trichloroaceticacid-anion.sdf
COSMOTHERM 3D 0

7 6 0 0 0 0 0 0 0 0 0 V2000
0.5429 -0.9834 1.4795 Cl 0 0 0 0 0 0 0 0 0 0 1
0.1183 0.0008 0.0002 C 0 0 0 0 0 0 0 0 0 0 2
-1.4656 0.3101 0.0022 C 0 0 0 0 0 0 0 0 0 0 3
-1.7804 1.5177 0.0029 O 0 0 0 0 0 0 0 0 0 0 4
-2.1651 -0.7259 0.0022 O 0 0 0 0 0 0 0 0 0 0 5
0.5400 -0.9721 -1.4876 Cl 0 0 0 0 0 0 0 0 0 0 6
1.1542 1.4928 0.0050 Cl 0 0 0 0 0 0 0 0 0 0 7
2 1 0 0 0 0
3 2 0 0 0 0
6 2 0 0 0 0
4 3 0 0 0 0
5 3 0 0 0 0
2 7 0 0 0 0
M END
$$$$
trichloroaceticacid.sdf
COSMOTHERM 3D 0

8 7 0 0 0 0 0 0 0 0 0 V2000
0.4436 -1.0530 1.4593 Cl 0 0 0 0 0 0 0 0 0 0 1
0.1685 -0.0162 0.0008 C 0 0 0 0 0 0 0 0 0 0 2
-1.3106 0.4953 0.0139 C 0 0 0 0 0 0 0 0 0 0 3
-1.6056 1.6688 0.0200 O 0 0 0 0 0 0 0 0 0 0 4
-2.1550 -0.5380 0.0139 O 0 0 0 0 0 0 0 0 0 0 5
0.4295 -0.9851 -1.5075 Cl 0 0 0 0 0 0 0 0 0 0 6
1.2984 1.3710 0.0274 Cl 0 0 0 0 0 0 0 0 0 0 7
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-3.0760 -0.1950 0.0170 H 0 0 0 0 0 0 0 0 0 0 8
2 1 0 0 0 0
3 2 0 0 0 0
6 2 0 0 0 0
7 2 0 0 0 0
4 3 0 0 0 0
5 3 0 0 0 0
5 8 0 0 0 0
M END
$$$$
uracil-anion1.sdf
COSMOtherm 3D 0

11 11 0 0 0 0 0 0 0 0 0 V2000
-1.7175 -0.0934 0.0000 C 0 0 0 0 0 0 0 0 0 0 1
-1.1520 1.1701 -0.0001 C 0 0 0 0 0 0 0 0 0 0 2
0.2744 1.2861 0.0000 C 0 0 0 0 0 0 0 0 0 0 3
0.9235 0.0429 0.0002 N 0 0 0 0 0 0 0 0 0 0 4
0.3106 -1.2236 0.0000 C 0 0 0 0 0 0 0 0 0 0 5
-1.0540 -1.2735 0.0001 N 0 0 0 0 0 0 0 0 0 0 6
0.9526 2.3436 0.0000 O 0 0 0 0 0 0 0 0 0 0 7
1.0423 -2.2442 -0.0001 O 0 0 0 0 0 0 0 0 0 0 8
-1.7627 2.0714 -0.0003 H 0 0 0 0 0 0 0 0 0 0 9
-2.8100 -0.1813 0.0001 H 0 0 0 0 0 0 0 0 0 0 10
1.9446 0.0575 -0.0001 H 0 0 0 0 0 0 0 0 0 0 11
2 1 0 0 0 0
6 1 0 0 0 0
10 1 0 0 0 0
3 2 0 0 0 0
9 2 0 0 0 0
4 3 0 0 0 0
7 3 0 0 0 0
5 4 0 0 0 0
6 5 0 0 0 0
8 5 0 0 0 0
4 11 0 0 0 0
M END
$$$$
uracil.sdf
COSMOtherm 3D 0

12 12 0 0 0 0 0 0 0 0 0 V2000
-1.7458 -0.0178 0.0001 C 0 0 0 0 0 0 0 0 0 0 1
-1.1435 1.2015 0.0002 C 0 0 0 0 0 0 0 0 0 0 2
0.3006 1.2898 0.0000 C 0 0 0 0 0 0 0 0 0 0 3
0.9514 0.0380 0.0001 N 0 0 0 0 0 0 0 0 0 0 4
0.3676 -1.2192 0.0000 C 0 0 0 0 0 0 0 0 0 0 5
-1.0204 -1.1808 -0.0002 N 0 0 0 0 0 0 0 0 0 0 6
0.9722 2.3320 -0.0001 O 0 0 0 0 0 0 0 0 0 0 7
1.0127 -2.2697 0.0000 O 0 0 0 0 0 0 0 0 0 0 8
-1.7286 2.1172 0.0001 H 0 0 0 0 0 0 0 0 0 0 9
-2.8272 -0.1450 0.0001 H 0 0 0 0 0 0 0 0 0 0 10
1.9727 0.0527 0.0003 H 0 0 0 0 0 0 0 0 0 0 11
-1.4980 -2.0805 -0.0002 H 0 0 0 0 0 0 0 0 0 0 12
2 1 0 0 0 0
6 1 0 0 0 0
10 1 0 0 0 0
3 2 0 0 0 0
9 2 0 0 0 0
4 3 0 0 0 0
7 3 0 0 0 0
5 4 0 0 0 0
11 4 0 0 0 0
6 5 0 0 0 0
8 5 0 0 0 0
6 12 0 0 0 0
M END
$$$$
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S4 b) Mono-solvated Acids & Anions

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2,2,2-trichloroethanol-anion.sdf
COSMOtherm 3D 0

11 9 0 0 0 0 0 0 0 0 0 V2000
-3.6769 0.3261 -0.1977 O 0 0 0 0 0 0 0 0 0 0 1
-2.8189 -0.2320 -0.4323 H 0 0 0 0 0 0 0 0 0 0 2
-3.3556 1.0180 0.4044 H 0 0 0 0 0 0 0 0 0 0 3
0.4442 0.0021 -0.1189 C 0 0 0 0 0 0 0 0 0 0 4
-0.5978 -0.3217 -1.2362 C 0 0 0 0 0 0 0 0 0 0 5
1.8215 1.0060 -0.8113 Cl 0 0 0 0 0 0 0 0 0 0 6
-0.3203 0.9475 1.2462 Cl 0 0 0 0 0 0 0 0 0 0 7
1.1489 -1.5258 0.5881 Cl 0 0 0 0 0 0 0 0 0 0 8
-1.6380 -1.0768 -0.8202 O 0 0 0 0 0 0 0 0 0 0 9
0.0305 -0.7975 -2.0288 H 0 0 0 0 0 0 0 0 0 0 10
-0.8733 0.6927 -1.6205 H 0 0 0 0 0 0 0 0 0 0 11
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
7 4 0 0 0 0
8 4 0 0 0 0
9 5 0 0 0 0
10 5 0 0 0 0
5 11 0 0 0 0
M END
$$$$
2,2,2-trichloroethanol.sdf
COSMOtherm 3D 0
```

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12 10 0 0 0 0 0 0 0 0 0 V2000
-3.7463 -0.1444 -0.2754 O 0 0 0 0 0 0 0 0 0 0 1
-4.1383 -0.8906 -0.7645 H 0 0 0 0 0 0 0 0 0 0 2
-3.6522 0.5606 -0.9411 H 0 0 0 0 0 0 0 0 0 0 3
0.4943 -0.1048 -0.0131 C 0 0 0 0 0 0 0 0 0 0 4
-0.4905 -1.2470 0.3210 C 0 0 0 0 0 0 0 0 0 0 5
1.8410 -0.7910 -1.0234 Cl 0 0 0 0 0 0 0 0 0 0 6
-0.3344 1.2146 -0.9466 Cl 0 0 0 0 0 0 0 0 0 0 7
1.1920 0.6075 1.5014 Cl 0 0 0 0 0 0 0 0 0 0 8
-1.5531 -0.8387 1.1413 O 0 0 0 0 0 0 0 0 0 0 9
0.0952 -2.0150 0.8479 H 0 0 0 0 0 0 0 0 0 0 10
-0.8304 -1.6628 -0.6415 H 0 0 0 0 0 0 0 0 0 0 11
-2.3191 -0.5464 0.5673 H 0 0 0 0 0 0 0 0 0 0 12
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
7 4 0 0 0 0
8 4 0 0 0 0
9 5 0 0 0 0
10 5 0 0 0 0
11 5 0 0 0 0
9 12 0 0 0 0
M END
$$$$
2,2-dimethylpropanoicacid-anion.sdf
COSMOTHERM 3D 0
19 17 0 0 0 0 0 0 0 0 0 V2000
-3.5942 -0.1554 0.0014 O 0 0 0 0 0 0 0 0 0 0 1
-2.6125 -0.4207 -0.0002 H 0 0 0 0 0 0 0 0 0 0 2
-3.5437 0.8166 -0.0025 H 0 0 0 0 0 0 0 0 0 0 3
2.0250 1.2678 -0.0139 C 0 0 0 0 0 0 0 0 0 0 4
1.2526 -0.0598 0.0001 C 0 0 0 0 0 0 0 0 0 0 5
1.6186 -0.8592 1.2686 C 0 0 0 0 0 0 0 0 0 0 6
1.6210 -0.8871 -1.2495 C 0 0 0 0 0 0 0 0 0 0 7
-0.2917 0.1845 -0.0023 C 0 0 0 0 0 0 0 0 0 0 8
-0.7329 1.3673 -0.0019 O 0 0 0 0 0 0 0 0 0 0 9
-1.0278 -0.8674 -0.0029 O 0 0 0 0 0 0 0 0 0 0 10
3.1096 1.0743 -0.0116 H 0 0 0 0 0 0 0 0 0 0 11
1.7828 1.8602 -0.9079 H 0 0 0 0 0 0 0 0 0 0 12
1.7820 1.8793 0.8668 H 0 0 0 0 0 0 0 0 0 0 13
2.6995 -1.0724 1.2881 H 0 0 0 0 0 0 0 0 0 0 14
1.0747 -1.8133 1.2968 H 0 0 0 0 0 0 0 0 0 0 15
1.3701 -0.2936 2.1806 H 0 0 0 0 0 0 0 0 0 0 16
2.7019 -1.1007 -1.2621 H 0 0 0 0 0 0 0 0 0 0 17
1.0767 -1.8413 -1.2577 H 0 0 0 0 0 0 0 0 0 0 18
1.3744 -0.3418 -2.1743 H 0 0 0 0 0 0 0 0 0 0 19
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
11 4 0 0 0 0
12 4 0 0 0 0
13 4 0 0 0 0
6 5 0 0 0 0
7 5 0 0 0 0
8 5 0 0 0 0
14 6 0 0 0 0
15 6 0 0 0 0
16 6 0 0 0 0
17 7 0 0 0 0
18 7 0 0 0 0
9 8 0 0 0 0
10 8 0 0 0 0
7 19 0 0 0 0
M END
$$$$
2,2-dimethylpropanoicacid.sdf
COSMOTHERM 3D 0
20 18 0 0 0 0 0 0 0 0 0 V2000
-3.6236 -0.0263 0.1980 O 0 0 0 0 0 0 0 0 0 0 1
-3.8516 -0.5483 -0.5932 H 0 0 0 0 0 0 0 0 0 0 2
-3.9862 0.8606 0.0180 H 0 0 0 0 0 0 0 0 0 0 3
2.1551 0.0265 -1.1735 C 0 0 0 0 0 0 0 0 0 0 4
1.2852 -0.0005 0.0924 C 0 0 0 0 0 0 0 0 0 0 5
1.5802 1.2441 0.9616 C 0 0 0 0 0 0 0 0 0 0 6
1.5755 -1.2846 0.9045 C 0 0 0 0 0 0 0 0 0 0 7
-0.1994 0.0071 -0.3029 C 0 0 0 0 0 0 0 0 0 0 8
-0.6120 0.0134 -1.4605 O 0 0 0 0 0 0 0 0 0 0 9
-1.0254 0.0018 0.7585 O 0 0 0 0 0 0 0 0 0 0 10
3.2170 0.0139 -0.8876 H 0 0 0 0 0 0 0 0 0 0 11
1.9592 -0.8459 -1.8121 H 0 0 0 0 0 0 0 0 0 0 12
1.9690 0.9321 -1.7678 H 0 0 0 0 0 0 0 0 0 0 13
2.6458 1.2522 1.2353 H 0 0 0 0 0 0 0 0 0 0 14
0.9859 1.2371 1.8847 H 0 0 0 0 0 0 0 0 0 0 15
1.3631 2.1732 0.4134 H 0 0 0 0 0 0 0 0 0 0 16
2.6409 -1.3089 1.1783 H 0 0 0 0 0 0 0 0 0 0 17
0.9802 -1.3171 1.8264 H 0 0 0 0 0 0 0 0 0 0 18
1.3556 -2.1871 0.3145 H 0 0 0 0 0 0 0 0 0 0 19
-1.9947 0.0035 0.4452 H 0 0 0 0 0 0 0 0 0 0 20
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
11 4 0 0 0 0
12 4 0 0 0 0
13 4 0 0 0 0
6 5 0 0 0 0
7 5 0 0 0 0
8 5 0 0 0 0
14 6 0 0 0 0
15 6 0 0 0 0
16 6 0 0 0 0
17 7 0 0 0 0
18 7 0 0 0 0
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19 7 0 0 0 0
9 8 0 0 0 0
10 8 0 0 0 0
10 20 0 0 0 0
M END
$$$$
2,3,4,6-tetrachlorophenol-anion.sdf
COSMOtherm 3D 0

15 14 0 0 0 0 0 0 0 0 0 V2000
-4.8073 -0.8001 -0.5123 O 0 0 0 0 0 0 0 0 0 0 1
-3.8395 -0.7857 -0.2498 H 0 0 0 0 0 0 0 0 0 0 2
-5.0111 0.1257 -0.7273 H 0 0 0 0 0 0 0 0 0 0 3
0.0775 1.7612 0.0246 C 0 0 0 0 0 0 0 0 0 0 4
-1.0981 1.0271 0.0961 C 0 0 0 0 0 0 0 0 0 0 5
-1.1580 -0.4079 0.1235 C 0 0 0 0 0 0 0 0 0 0 6
0.1500 -1.0213 0.0657 C 0 0 0 0 0 0 0 0 0 0 7
1.3470 -0.2995 -0.0054 C 0 0 0 0 0 0 0 0 0 0 8
1.3082 1.1038 -0.0274 C 0 0 0 0 0 0 0 0 0 0 9
-2.2361 -1.0951 0.1965 O 0 0 0 0 0 0 0 0 0 0 10
0.1729 -2.7818 0.0919 Cl 0 0 0 0 0 0 0 0 0 0 11
2.8951 -1.1370 -0.0702 Cl 0 0 0 0 0 0 0 0 0 0 12
2.7840 2.0707 -0.1141 Cl 0 0 0 0 0 0 0 0 0 0 13
-2.6354 1.9082 0.1686 Cl 0 0 0 0 0 0 0 0 0 0 14
0.0450 2.8500 0.0099 H 0 0 0 0 0 0 0 0 0 0 15

2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
9 4 0 0 0 0
6 5 0 0 0 0
14 5 0 0 0 0
7 6 0 0 0 0
10 6 0 0 0 0
8 7 0 0 0 0
11 7 0 0 0 0
9 8 0 0 0 0
12 8 0 0 0 0
13 9 0 0 0 0
4 15 0 0 0 0
M END
$$$$
2,3,4,6-tetrachlorophenol.sdf
COSMOtherm 3D 0

16 15 0 0 0 0 0 0 0 0 0 V2000
-4.3041 0.0409 -1.5728 O 0 0 0 0 0 0 0 0 0 0 1
-4.3084 -0.6487 -2.2610 H 0 0 0 0 0 0 0 0 0 0 2
-4.4164 0.8761 -2.0621 H 0 0 0 0 0 0 0 0 0 0 3
-0.3255 -0.0089 -0.7504 C 0 0 0 0 0 0 0 0 0 0 4
1.0752 -0.0010 -0.6249 C 0 0 0 0 0 0 0 0 0 0 5
1.6486 0.0046 0.6537 C 0 0 0 0 0 0 0 0 0 0 6
0.8363 0.0029 1.7873 C 0 0 0 0 0 0 0 0 0 0 7
-0.5448 -0.0042 1.6447 C 0 0 0 0 0 0 0 0 0 0 8
-1.1743 -0.0094 0.3800 C 0 0 0 0 0 0 0 0 0 0 9
3.3929 0.0144 0.8707 Cl 0 0 0 0 0 0 0 0 0 0 10
-2.5139 -0.0207 0.3449 O 0 0 0 0 0 0 0 0 0 0 11
-1.0668 -0.0193 -2.3383 Cl 0 0 0 0 0 0 0 0 0 0 12
2.0851 0.0001 -2.0520 Cl 0 0 0 0 0 0 0 0 0 0 13
1.2841 0.0075 2.7795 H 0 0 0 0 0 0 0 0 0 0 14
-1.5521 -0.0057 3.0867 Cl 0 0 0 0 0 0 0 0 0 0 15
-2.9541 0.0083 -0.5662 H 0 0 0 0 0 0 0 0 0 0 16

2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
9 4 0 0 0 0
12 4 0 0 0 0
6 5 0 0 0 0
13 5 0 0 0 0
7 6 0 0 0 0
10 6 0 0 0 0
8 7 0 0 0 0
14 7 0 0 0 0
9 8 0 0 0 0
15 8 0 0 0 0
11 9 0 0 0 0
11 16 0 0 0 0
M END
$$$$
2,3,4-trichlorophenol-anion.sdf
COSMOtherm 3D 0

15 14 0 0 0 0 0 0 0 0 0 V2000
-4.8410 -0.0444 1.4948 O 0 0 0 0 0 0 0 0 0 0 1
-4.0333 -0.0101 0.8812 H 0 0 0 0 0 0 0 0 0 0 2
-4.8468 0.8208 1.9384 H 0 0 0 0 0 0 0 0 0 0 3
-1.2265 -0.0064 1.5919 C 0 0 0 0 0 0 0 0 0 0 4
0.0934 -0.0051 2.0259 C 0 0 0 0 0 0 0 0 0 0 5
1.1482 -0.0018 1.1080 C 0 0 0 0 0 0 0 0 0 0 6
0.8642 0.0002 -0.2677 C 0 0 0 0 0 0 0 0 0 0 7
-0.4674 -0.0007 -0.7025 C 0 0 0 0 0 0 0 0 0 0 8
-1.5872 -0.0027 0.2069 C 0 0 0 0 0 0 0 0 0 0 9
2.8142 0.0005 1.7076 Cl 0 0 0 0 0 0 0 0 0 0 10
-2.8103 -0.0029 -0.2105 O 0 0 0 0 0 0 0 0 0 0 11
-2.0358 -0.0132 2.3247 H 0 0 0 0 0 0 0 0 0 0 12
0.3179 -0.0072 3.0934 H 0 0 0 0 0 0 0 0 0 0 13
2.1847 0.0031 -1.4378 Cl 0 0 0 0 0 0 0 0 0 0 14
-0.8465 0.0010 -2.4261 Cl 0 0 0 0 0 0 0 0 0 0 15

2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
9 4 0 0 0 0
12 4 0 0 0 0
6 5 0 0 0 0
13 5 0 0 0 0
7 6 0 0 0 0
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10 6 0 0 0 0
8 7 0 0 0 0
14 7 0 0 0 0
9 8 0 0 0 0
11 9 0 0 0 0
8 15 0 0 0 0
M END
$$$$
2,3,4-trichlorophenol.sdf
COSMOtherm 3D 0
16 15 0 0 0 0 0 0 0 0 0 V2000
-4.6384 0.0030 1.5542 O 0 0 0 0 0 0 0 0 0 0 0 1
-5.1834 -0.8050 1.5313 H 0 0 0 0 0 0 0 0 0 0 0 2
-5.2725 0.7341 1.4365 H 0 0 0 0 0 0 0 0 0 0 0 3
0.0609 0.0011 2.0153 C 0 0 0 0 0 0 0 0 0 0 0 4
-1.2513 0.0012 1.5516 C 0 0 0 0 0 0 0 0 0 0 0 5
-1.5308 0.0008 0.1736 C 0 0 0 0 0 0 0 0 0 0 0 6
-0.4445 0.0002 -0.7301 C 0 0 0 0 0 0 0 0 0 0 0 7
0.8812 0.0002 -0.2660 C 0 0 0 0 0 0 0 0 0 0 0 8
1.1281 0.0003 1.1163 C 0 0 0 0 0 0 0 0 0 0 0 9
-2.7831 0.0004 -0.3272 O 0 0 0 0 0 0 0 0 0 0 0 10
-0.7968 -0.0004 -2.4490 Cl 0 0 0 0 0 0 0 0 0 0 0 11
2.2110 -0.0004 -1.4062 Cl 0 0 0 0 0 0 0 0 0 0 0 12
2.7745 -0.0001 1.7451 Cl 0 0 0 0 0 0 0 0 0 0 0 13
0.2606 0.0014 3.0864 H 0 0 0 0 0 0 0 0 0 0 0 14
-2.0787 0.0022 2.2620 H 0 0 0 0 0 0 0 0 0 0 0 15
-3.4737 -0.0003 0.4166 H 0 0 0 0 0 0 0 0 0 0 0 16
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
9 4 0 0 0 0
14 4 0 0 0 0
6 5 0 0 0 0
15 5 0 0 0 0
7 6 0 0 0 0
10 6 0 0 0 0
8 7 0 0 0 0
11 7 0 0 0 0
9 8 0 0 0 0
12 8 0 0 0 0
13 9 0 0 0 0
10 16 0 0 0 0
M END
$$$$
2,3-dichlorophenol-anion.sdf
COSMOtherm 3D 0
15 14 0 0 0 0 0 0 0 0 0 V2000
-4.6680 -0.0414 -0.1072 O 0 0 0 0 0 0 0 0 0 0 0 1
-3.6763 -0.0126 -0.3310 H 0 0 0 0 0 0 0 0 0 0 0 2
-4.8342 0.7907 0.3677 H 0 0 0 0 0 0 0 0 0 0 0 3
-1.4122 -0.0080 1.4709 C 0 0 0 0 0 0 0 0 0 0 0 4
-0.3781 -0.0058 2.4015 C 0 0 0 0 0 0 0 0 0 0 0 5
0.9666 -0.0016 2.0031 C 0 0 0 0 0 0 0 0 0 0 0 6
1.2403 0.0003 0.6316 C 0 0 0 0 0 0 0 0 0 0 0 7
0.2182 -0.0018 -0.3207 C 0 0 0 0 0 0 0 0 0 0 0 8
-1.1753 -0.0029 0.0579 C 0 0 0 0 0 0 0 0 0 0 0 9
1.7802 0.0010 2.7268 H 0 0 0 0 0 0 0 0 0 0 0 10
-2.1232 -0.0011 -0.8236 O 0 0 0 0 0 0 0 0 0 0 0 11
-2.4530 -0.0158 1.8022 H 0 0 0 0 0 0 0 0 0 0 0 12
-0.6131 -0.0087 3.4684 H 0 0 0 0 0 0 0 0 0 0 0 13
2.9467 0.0043 0.1273 Cl 0 0 0 0 0 0 0 0 0 0 0 14
0.5797 0.0001 -2.0511 Cl 0 0 0 0 0 0 0 0 0 0 0 15
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
9 4 0 0 0 0
12 4 0 0 0 0
6 5 0 0 0 0
13 5 0 0 0 0
7 6 0 0 0 0
10 6 0 0 0 0
8 7 0 0 0 0
14 7 0 0 0 0
9 8 0 0 0 0
11 9 0 0 0 0
8 15 0 0 0 0
M END
$$$$
2,3-dichlorophenol.sdf
COSMOtherm 3D 0
16 15 0 0 0 0 0 0 0 0 0 V2000
-4.5363 -0.0092 0.0042 O 0 0 0 0 0 0 0 0 0 0 0 1
-5.0499 -0.7579 -0.3510 H 0 0 0 0 0 0 0 0 0 0 0 2
-5.0335 0.7842 -0.2674 H 0 0 0 0 0 0 0 0 0 0 0 3
-0.4281 0.0016 2.3772 C 0 0 0 0 0 0 0 0 0 0 0 4
-1.4377 0.0035 1.4156 C 0 0 0 0 0 0 0 0 0 0 0 5
-1.1194 0.0029 0.0450 C 0 0 0 0 0 0 0 0 0 0 0 6
0.2436 0.0013 -0.3342 C 0 0 0 0 0 0 0 0 0 0 0 7
1.2428 -0.0004 0.6482 C 0 0 0 0 0 0 0 0 0 0 0 8
0.9196 -0.0001 2.0071 C 0 0 0 0 0 0 0 0 0 0 0 9
-2.0542 0.0045 -0.9311 O 0 0 0 0 0 0 0 0 0 0 0 10
0.6373 0.0010 -2.0468 Cl 0 0 0 0 0 0 0 0 0 0 0 11
2.9465 -0.0028 0.1869 Cl 0 0 0 0 0 0 0 0 0 0 0 12
-2.9885 0.0017 -0.5396 H 0 0 0 0 0 0 0 0 0 0 0 13
-0.6923 0.0020 3.4355 H 0 0 0 0 0 0 0 0 0 0 0 14
-2.4877 0.0043 1.7114 H 0 0 0 0 0 0 0 0 0 0 0 15
1.7119 -0.0014 2.7543 H 0 0 0 0 0 0 0 0 0 0 0 16
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
9 4 0 0 0 0
14 4 0 0 0 0
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6 5 0 0 0 0
15 5 0 0 0 0
7 6 0 0 0 0
10 6 0 0 0 0
8 7 0 0 0 0
11 7 0 0 0 0
9 8 0 0 0 0
12 8 0 0 0 0
13 10 0 0 0 0
9 16 0 0 0 0
M END
$$$$
2,4,5-trichlorophenol-anion.sdf
COSMOtherm 3D 0

15 14 0 0 0 0 0 0 0 0 0 V2000
-3.3026 3.2156 0.0065 O 0 0 0 0 0 0 0 0 0 0 1
-2.3210 2.9607 -0.0019 H 0 0 0 0 0 0 0 0 0 0 2
-3.6270 2.9590 -0.8734 H 0 0 0 0 0 0 0 0 0 0 3
-1.1848 0.3035 0.0213 C 0 0 0 0 0 0 0 0 0 0 4
-0.7324 -1.0105 0.0109 C 0 0 0 0 0 0 0 0 0 0 5
0.6382 -1.3052 -0.0039 C 0 0 0 0 0 0 0 0 0 0 6
1.5515 -0.2443 -0.0072 C 0 0 0 0 0 0 0 0 0 0 7
1.0962 1.0679 0.0052 C 0 0 0 0 0 0 0 0 0 0 8
-0.2950 1.4294 0.0161 C 0 0 0 0 0 0 0 0 0 0 9
1.2486 -2.9643 -0.0205 Cl 0 0 0 0 0 0 0 0 0 0 10
-0.7084 2.6525 0.0225 O 0 0 0 0 0 0 0 0 0 0 11
-2.2566 0.5052 0.0360 H 0 0 0 0 0 0 0 0 0 0 12
-1.9335 -2.3176 0.0162 Cl 0 0 0 0 0 0 0 0 0 0 13
2.6210 -0.4536 -0.0178 H 0 0 0 0 0 0 0 0 0 0 14
2.2900 2.3823 0.0012 Cl 0 0 0 0 0 0 0 0 0 0 15
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
9 4 0 0 0 0
12 4 0 0 0 0
6 5 0 0 0 0
13 5 0 0 0 0
7 6 0 0 0 0
10 6 0 0 0 0
8 7 0 0 0 0
14 7 0 0 0 0
9 8 0 0 0 0
11 9 0 0 0 0
8 15 0 0 0 0
M END
$$$$
2,4,5-trichlorophenol.sdf
COSMOtherm 3D 0

16 15 0 0 0 0 0 0 0 0 0 V2000
-3.3246 -0.0105 -2.8674 O 0 0 0 0 0 0 0 0 0 0 1
-3.6428 -0.7450 -3.4235 H 0 0 0 0 0 0 0 0 0 0 2
-3.6762 0.7942 -3.2906 H 0 0 0 0 0 0 0 0 0 0 3
-0.7075 0.0009 1.0244 C 0 0 0 0 0 0 0 0 0 0 4
-1.1784 0.0023 -0.2881 C 0 0 0 0 0 0 0 0 0 0 5
-0.2869 0.0031 -1.3759 C 0 0 0 0 0 0 0 0 0 0 6
1.0952 0.0008 -1.0902 C 0 0 0 0 0 0 0 0 0 0 7
1.5690 0.0002 0.2179 C 0 0 0 0 0 0 0 0 0 0 8
0.6689 -0.0006 1.2868 C 0 0 0 0 0 0 0 0 0 0 9
-0.6945 0.0079 -2.6602 O 0 0 0 0 0 0 0 0 0 0 10
2.2476 -0.0015 -2.4242 Cl 0 0 0 0 0 0 0 0 0 0 11
1.3010 -0.0014 2.9295 Cl 0 0 0 0 0 0 0 0 0 0 12
-1.8823 0.0003 2.3359 Cl 0 0 0 0 0 0 0 0 0 0 13
-2.2517 0.0037 -0.4784 H 0 0 0 0 0 0 0 0 0 0 14
2.6410 -0.0017 0.4098 H 0 0 0 0 0 0 0 0 0 0 15
-1.7084 0.0034 -2.7257 H 0 0 0 0 0 0 0 0 0 0 16
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
9 4 0 0 0 0
13 4 0 0 0 0
6 5 0 0 0 0
14 5 0 0 0 0
7 6 0 0 0 0
10 6 0 0 0 0
8 7 0 0 0 0
11 7 0 0 0 0
9 8 0 0 0 0
15 8 0 0 0 0
12 9 0 0 0 0
10 16 0 0 0 0
M END
$$$$
2,4,6-trichlorophenol-anion.sdf
COSMOtherm 3D 0

15 14 0 0 0 0 0 0 0 0 0 V2000
-4.1763 0.2917 -1.0099 O 0 0 0 0 0 0 0 0 0 0 1
-3.3671 0.0083 -0.4825 H 0 0 0 0 0 0 0 0 0 0 2
-4.0925 1.2588 -1.0677 H 0 0 0 0 0 0 0 0 0 0 3
1.5516 -0.9830 -0.0559 C 0 0 0 0 0 0 0 0 0 0 4
0.2050 -1.3038 0.0865 C 0 0 0 0 0 0 0 0 0 0 5
-0.8635 -0.3487 0.2208 C 0 0 0 0 0 0 0 0 0 0 6
-0.3774 1.0059 0.1844 C 0 0 0 0 0 0 0 0 0 0 7
0.9581 1.3718 0.0392 C 0 0 0 0 0 0 0 0 0 0 8
1.9158 0.3643 -0.0825 C 0 0 0 0 0 0 0 0 0 0 9
-2.0975 -0.6792 0.3633 O 0 0 0 0 0 0 0 0 0 0 10
-1.5829 2.3001 0.3567 Cl 0 0 0 0 0 0 0 0 0 0 11
-0.2520 -3.0196 0.1181 Cl 0 0 0 0 0 0 0 0 0 0 12
3.6292 0.8036 -0.2684 Cl 0 0 0 0 0 0 0 0 0 0 13
2.2997 -1.7692 -0.1494 H 0 0 0 0 0 0 0 0 0 0 14
1.2434 2.4231 0.0234 H 0 0 0 0 0 0 0 0 0 0 15
2 1 0 0 0 0
3 1 0 0 0 0
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5 4 0 0 0 0
9 4 0 0 0 0
14 4 0 0 0 0
6 5 0 0 0 0
12 5 0 0 0 0
7 6 0 0 0 0
10 6 0 0 0 0
8 7 0 0 0 0
11 7 0 0 0 0
9 8 0 0 0 0
13 9 0 0 0 0
8 15 0 0 0 0
M END
$$$$
2,4,6-trichlorophenol.sdf
COSMOTHERM 3D 0
16 15 0 0 0 0 0 0 0 0 0 V2000
-4.3902 0.0737 -0.3079 O 0 0 0 0 0 0 0 0 0 0 1
-4.6586 -0.6530 -0.8987 H 0 0 0 0 0 0 0 0 0 0 2
-4.6285 0.8842 -0.7935 H 0 0 0 0 0 0 0 0 0 0 3
0.2953 -0.0061 1.3121 C 0 0 0 0 0 0 0 0 0 0 4
1.6356 0.0051 0.9359 C 0 0 0 0 0 0 0 0 0 0 5
1.9443 0.0076 -0.4242 C 0 0 0 0 0 0 0 0 0 0 6
0.9460 -0.0018 -1.3950 C 0 0 0 0 0 0 0 0 0 0 7
-0.3870 -0.0142 -0.9828 C 0 0 0 0 0 0 0 0 0 0 8
-0.7665 -0.0147 0.3775 C 0 0 0 0 0 0 0 0 0 0 9
3.6404 0.0226 -0.9263 Cl 0 0 0 0 0 0 0 0 0 0 10
-2.0248 -0.0301 0.8453 O 0 0 0 0 0 0 0 0 0 0 11
-0.1036 -0.0091 3.0287 Cl 0 0 0 0 0 0 0 0 0 0 12
2.4177 0.0121 1.6930 H 0 0 0 0 0 0 0 0 0 0 13
1.1893 -0.0013 -2.4560 H 0 0 0 0 0 0 0 0 0 0 14
-1.6443 -0.0321 -2.2198 Cl 0 0 0 0 0 0 0 0 0 0 15
-2.7638 0.0080 0.1571 H 0 0 0 0 0 0 0 0 0 0 16
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
9 4 0 0 0 0
12 4 0 0 0 0
6 5 0 0 0 0
13 5 0 0 0 0
7 6 0 0 0 0
10 6 0 0 0 0
8 7 0 0 0 0
14 7 0 0 0 0
9 8 0 0 0 0
15 8 0 0 0 0
11 9 0 0 0 0
11 16 0 0 0 0
M END
$$$$
2,4-dichlorophenol-anion.sdf
COSMOTHERM 3D 0
15 14 0 0 0 0 0 0 0 0 0 V2000
-2.2785 -3.9859 0.0307 O 0 0 0 0 0 0 0 0 0 0 1
-1.4803 -3.3532 0.0077 H 0 0 0 0 0 0 0 0 0 0 2
-2.6902 -3.8923 -0.8452 H 0 0 0 0 0 0 0 0 0 0 3
-1.4855 -0.4651 0.0203 C 0 0 0 0 0 0 0 0 0 0 4
-1.5916 0.9246 0.0139 C 0 0 0 0 0 0 0 0 0 0 5
-0.4303 1.7013 0.0015 C 0 0 0 0 0 0 0 0 0 0 6
0.8314 1.1021 -0.0046 C 0 0 0 0 0 0 0 0 0 0 7
0.9100 -0.2884 0.0025 C 0 0 0 0 0 0 0 0 0 0 8
-0.2313 -1.1609 0.0107 C 0 0 0 0 0 0 0 0 0 0 9
-0.5486 3.4811 -0.0069 Cl 0 0 0 0 0 0 0 0 0 0 10
-0.1316 -2.4531 0.0124 O 0 0 0 0 0 0 0 0 0 0 11
-2.3934 -1.0725 0.0321 H 0 0 0 0 0 0 0 0 0 0 12
-2.5738 1.4000 0.0196 H 0 0 0 0 0 0 0 0 0 0 13
1.7391 1.7056 -0.0122 H 0 0 0 0 0 0 0 0 0 0 14
2.5233 -1.0415 -0.0049 Cl 0 0 0 0 0 0 0 0 0 0 15
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
9 4 0 0 0 0
12 4 0 0 0 0
6 5 0 0 0 0
13 5 0 0 0 0
7 6 0 0 0 0
10 6 0 0 0 0
8 7 0 0 0 0
14 7 0 0 0 0
9 8 0 0 0 0
11 9 0 0 0 0
8 15 0 0 0 0
M END
$$$$
2,4-dichlorophenol.sdf
COSMOTHERM 3D 0
16 15 0 0 0 0 0 0 0 0 0 V2000
-2.3387 -0.0153 -3.7655 O 0 0 0 0 0 0 0 0 0 0 1
-2.5232 -0.8833 -4.1690 H 0 0 0 0 0 0 0 0 0 0 2
-2.3443 0.6116 -4.5121 H 0 0 0 0 0 0 0 0 0 0 3
-1.5842 0.0164 0.9106 C 0 0 0 0 0 0 0 0 0 0 4
-1.4621 0.0238 -0.4796 C 0 0 0 0 0 0 0 0 0 0 5
-0.2014 0.0159 -1.1060 C 0 0 0 0 0 0 0 0 0 0 6
0.9384 0.0025 -0.2747 C 0 0 0 0 0 0 0 0 0 0 7
0.8387 -0.0043 1.1161 C 0 0 0 0 0 0 0 0 0 0 8
-0.4307 0.0020 1.6947 C 0 0 0 0 0 0 0 0 0 0 9
-0.0369 0.0198 -2.4478 O 0 0 0 0 0 0 0 0 0 0 10
2.5412 -0.0063 -1.0174 Cl 0 0 0 0 0 0 0 0 0 0 11
-0.5694 -0.0085 3.4639 Cl 0 0 0 0 0 0 0 0 0 0 12
-2.5714 0.0216 1.3720 H 0 0 0 0 0 0 0 0 0 0 13
-2.3595 0.0357 -1.1003 H 0 0 0 0 0 0 0 0 0 0 14
1.7384 -0.0150 1.7295 H 0 0 0 0 0 0 0 0 0 0 15
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-0.9304 0.0073 -2.9243 H 0 0 0 0 0 0 0 0 0 0 16
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
9 4 0 0 0 0
13 4 0 0 0 0
16 5 0 0 0 0
14 5 0 0 0 0
7 6 0 0 0 0
10 6 0 0 0 0
8 7 0 0 0 0
11 7 0 0 0 0
9 8 0 0 0 0
15 8 0 0 0 0
12 9 0 0 0 0
10 16 0 0 0 0
M END
$$$$
2,4-dihydroxybenzoicacid-anion.sdf
COSMOtherm 3D 0
19 19 0 0 0 0 0 0 0 0 V2000
-4.9400 -0.6471 -0.0063 O 0 0 0 0 0 0 0 0 0 0 1
-3.9395 -0.7527 0.0010 H 0 0 0 0 0 0 0 0 0 0 2
-5.0702 0.3131 -0.0900 H 0 0 0 0 0 0 0 0 0 0 3
1.9604 -1.5251 0.0001 C 0 0 0 0 0 0 0 0 0 0 4
0.5756 -1.3987 0.0031 C 0 0 0 0 0 0 0 0 0 0 5
-0.0590 -0.1444 0.0036 C 0 0 0 0 0 0 0 0 0 0 6
0.7571 1.0242 0.0014 C 0 0 0 0 0 0 0 0 0 0 7
2.1579 0.9085 -0.0017 C 0 0 0 0 0 0 0 0 0 0 8
2.7489 -0.3578 -0.0026 C 0 0 0 0 0 0 0 0 0 0 9
-1.5512 -0.0188 0.0048 C 0 0 0 0 0 0 0 0 0 0 10
-2.2693 -1.0631 0.0078 O 0 0 0 0 0 0 0 0 0 0 11
-2.0351 1.1823 0.0016 O 0 0 0 0 0 0 0 0 0 0 12
0.1946 2.2532 0.0023 O 0 0 0 0 0 0 0 0 0 0 13
4.1115 -0.5242 -0.0060 O 0 0 0 0 0 0 0 0 0 0 14
-0.8391 2.0247 0.0012 H 0 0 0 0 0 0 0 0 0 0 15
4.5463 0.3501 -0.0085 H 0 0 0 0 0 0 0 0 0 0 16
2.4438 -2.5026 -0.0005 H 0 0 0 0 0 0 0 0 0 0 17
-0.0529 -2.2911 0.0047 H 0 0 0 0 0 0 0 0 0 0 18
2.7706 1.8132 -0.0034 H 0 0 0 0 0 0 0 0 0 0 19
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
9 4 0 0 0 0
17 4 0 0 0 0
6 5 0 0 0 0
18 5 0 0 0 0
7 6 0 0 0 0
10 6 0 0 0 0
8 7 0 0 0 0
13 7 0 0 0 0
9 8 0 0 0 0
14 9 0 0 0 0
11 10 0 0 0 0
12 10 0 0 0 0
15 12 0 0 0 0
15 13 0 0 0 0
16 14 0 0 0 0
8 19 0 0 0 0
M END
$$$$
2,4-dihydroxybenzoicacid.sdf
COSMOtherm 3D 0
20 19 0 0 0 0 0 0 0 0 V2000
-4.8399 -0.0160 0.7259 O 0 0 0 0 0 0 0 0 0 0 1
-5.1871 -0.6872 0.1104 H 0 0 0 0 0 0 0 0 0 0 2
-5.2197 0.8263 0.4151 H 0 0 0 0 0 0 0 0 0 0 3
1.9124 -0.0010 1.5503 C 0 0 0 0 0 0 0 0 0 0 4
0.5385 -0.0001 1.3809 C 0 0 0 0 0 0 0 0 0 0 5
-0.0500 0.0010 0.0969 C 0 0 0 0 0 0 0 0 0 0 6
0.8076 0.0005 -1.0432 C 0 0 0 0 0 0 0 0 0 0 7
2.1992 0.0003 -0.8775 C 0 0 0 0 0 0 0 0 0 0 8
2.7438 -0.0011 0.4093 C 0 0 0 0 0 0 0 0 0 0 9
-1.5007 0.0029 -0.1017 C 0 0 0 0 0 0 0 0 0 0 10
-2.2387 0.0038 1.0081 O 0 0 0 0 0 0 0 0 0 0 11
-2.0206 0.0029 -1.2442 O 0 0 0 0 0 0 0 0 0 0 12
0.3105 0.0006 -2.3017 O 0 0 0 0 0 0 0 0 0 0 13
4.0910 -0.0021 0.6278 O 0 0 0 0 0 0 0 0 0 0 14
-3.2394 0.0023 0.7826 H 0 0 0 0 0 0 0 0 0 0 15
-0.6975 0.0024 -2.1854 H 0 0 0 0 0 0 0 0 0 0 16
4.5657 -0.0011 -0.2261 H 0 0 0 0 0 0 0 0 0 0 17
2.3620 -0.0018 2.5432 H 0 0 0 0 0 0 0 0 0 0 18
-0.1126 0.0001 2.2551 H 0 0 0 0 0 0 0 0 0 0 19
2.8421 0.0003 -1.7599 H 0 0 0 0 0 0 0 0 0 0 20
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
9 4 0 0 0 0
18 4 0 0 0 0
6 5 0 0 0 0
19 5 0 0 0 0
7 6 0 0 0 0
10 6 0 0 0 0
8 7 0 0 0 0
13 7 0 0 0 0
9 8 0 0 0 0
14 9 0 0 0 0
11 10 0 0 0 0
12 10 0 0 0 0
15 11 0 0 0 0
16 13 0 0 0 0
17 14 0 0 0 0
8 20 0 0 0 0
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[illegible]

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13 11 0 0 0 0 0 0 0 0 0 V2000
-3.6800 0.7084 -0.2821 O 0 0 0 0 0 0 0 0 0 1
-2.6740 0.6378 -0.2909 H 0 0 0 0 0 0 0 0 0 2
-3.9651 -0.1442 0.0890 H 0 0 0 0 0 0 0 0 0 3
1.4551 -1.4915 -0.9427 C 0 0 0 0 0 0 0 0 0 4
1.0243 -0.6153 0.2247 C 0 0 0 0 0 0 0 0 0 5
-0.5079 -0.3844 0.2359 C 0 0 0 0 0 0 0 0 0 6
-1.1502 -1.2937 0.8288 O 0 0 0 0 0 0 0 0 0 7
-0.9867 0.6208 -0.3730 O 0 0 0 0 0 0 0 0 0 8
1.9757 0.9906 0.1621 Cl 0 0 0 0 0 0 0 0 0 9
2.5354 -1.6853 -0.9169 H 0 0 0 0 0 0 0 0 0 10
0.9294 -2.4557 -0.8736 H 0 0 0 0 0 0 0 0 0 11
1.1983 -1.0225 -1.9025 H 0 0 0 0 0 0 0 0 0 12
1.3256 -1.0505 1.1827 H 0 0 0 0 0 0 0 0 0 13
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
10 4 0 0 0 0
11 4 0 0 0 0
12 4 0 0 0 0
6 5 0 0 0 0
9 5 0 0 0 0
7 6 0 0 0 0
8 6 0 0 0 0
5 13 0 0 0 0
M END
$$$
2-chloropropanoicacid.sdf
COSMOtherm 3D 0
14 12 0 0 0 0 0 0 0 0 0 V2000
-3.7186 0.4046 -0.0182 O 0 0 0 0 0 0 0 0 0 1
-4.0492 -0.4400 -0.3758 H 0 0 0 0 0 0 0 0 0 2
-3.8832 1.0546 -0.7260 H 0 0 0 0 0 0 0 0 0 3
1.8130 -1.6321 0.2712 C 0 0 0 0 0 0 0 0 0 4
1.0307 -0.3737 0.5662 C 0 0 0 0 0 0 0 0 0 5
-0.4060 -0.4026 0.0361 C 0 0 0 0 0 0 0 0 0 6
-1.2277 0.3390 0.7812 O 0 0 0 0 0 0 0 0 0 7
-0.7430 -1.0394 -0.9546 O 0 0 0 0 0 0 0 0 0 8
1.8293 1.0929 -0.2536 Cl 0 0 0 0 0 0 0 0 0 9
2.8435 -1.5389 0.6350 H 0 0 0 0 0 0 0 0 0 10
1.3371 -2.4749 0.7961 H 0 0 0 0 0 0 0 0 0 11
1.8195 -1.8530 -0.8034 H 0 0 0 0 0 0 0 0 0 12
1.0314 -0.1165 1.6297 H 0 0 0 0 0 0 0 0 0 13
-2.1812 0.3215 0.3961 H 0 0 0 0 0 0 0 0 0 14
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
10 4 0 0 0 0
11 4 0 0 0 0
12 4 0 0 0 0
6 5 0 0 0 0
9 5 0 0 0 0
13 5 0 0 0 0
7 6 0 0 0 0
8 6 0 0 0 0
7 14 0 0 0 0
M END
$$$
2-hydroxypropanoicacid-anion.sdf
COSMOtherm 3D 0
14 12 0 0 0 0 0 0 0 0 0 V2000
-3.5184 -0.1169 -0.0702 O 0 0 0 0 0 0 0 0 0 1
-2.5399 -0.3212 0.0635 H 0 0 0 0 0 0 0 0 0 2
-3.5201 0.7802 -0.4452 H 0 0 0 0 0 0 0 0 0 3
1.8879 -1.3884 -0.4831 C 0 0 0 0 0 0 0 0 0 4
1.4007 -0.2219 0.3765 C 0 0 0 0 0 0 0 0 0 5
-0.0880 0.1199 0.1052 C 0 0 0 0 0 0 0 0 0 6
-0.3200 1.2894 -0.3249 O 0 0 0 0 0 0 0 0 0 7
-0.9463 -0.7888 0.3346 O 0 0 0 0 0 0 0 0 0 8
2.1952 0.9544 0.1371 O 0 0 0 0 0 0 0 0 0 9
2.9461 -1.5990 -0.2723 H 0 0 0 0 0 0 0 0 0 10
1.3036 -2.2939 -0.2700 H 0 0 0 0 0 0 0 0 0 11
1.7867 -1.1473 -1.5521 H 0 0 0 0 0 0 0 0 0 12
1.4839 -0.4976 1.4438 H 0 0 0 0 0 0 0 0 0 13
1.5029 1.5985 -0.1660 H 0 0 0 0 0 0 0 0 0 14
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
10 4 0 0 0 0
11 4 0 0 0 0
12 4 0 0 0 0
6 5 0 0 0 0
9 5 0 0 0 0
13 5 0 0 0 0
7 6 0 0 0 0
8 6 0 0 0 0
9 14 0 0 0 0
M END
$$$
2-hydroxypropanoicacid.sdf
COSMOtherm 3D 0
15 13 0 0 0 0 0 0 0 0 0 V2000
-3.4289 -0.0743 0.1351 O 0 0 0 0 0 0 0 0 0 1
-3.6127 -0.9739 -0.1922 H 0 0 0 0 0 0 0 0 0 2
-3.8090 0.5189 -0.5388 H 0 0 0 0 0 0 0 0 0 3
1.8198 -0.5247 1.4109 C 0 0 0 0 0 0 0 0 0 4
1.4079 0.3722 0.2378 C 0 0 0 0 0 0 0 0 0 5
-0.0319 0.0936 -0.1954 C 0 0 0 0 0 0 0 0 0 6
-0.2855 -0.3875 -1.3002 O 0 0 0 0 0 0 0 0 0 7
-0.9371 0.4060 0.7249 O 0 0 0 0 0 0 0 0 0 8
2.2745 0.1814 -0.8864 O 0 0 0 0 0 0 0 0 0 9
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2
3      2.8660   -0.3178   1.6729 H   0   0   0   0   0   0   0   0   0   0   10
4      1.1943   -0.3293   2.2923 H   0   0   0   0   0   0   0   0   0   0   11
5      1.7288   -1.5855   1.1361 H   0   0   0   0   0   0   0   0   0   0   12
6      1.4639   1.4292   0.5493 H   0   0   0   0   0   0   0   0   0   0   13
7     -1.8903   0.1855   0.4019 H   0   0   0   0   0   0   0   0   0   0   14
8      1.7064   -0.2204  -1.5815 H   0   0   0   0   0   0   0   0   0   0   15
9
10     2   1   0   0   0   0
11     3   1   0   0   0   0
12     5   4   0   0   0   0
13    10   4   0   0   0   0
14    11   4   0   0   0   0
15    12   4   0   0   0   0
16     6   5   0   0   0   0
17     9   5   0   0   0   0
18    13   5   0   0   0   0
19     7   6   0   0   0   0
20     8   6   0   0   0   0
21    14   8   0   0   0   0
22     9  15   0   0   0   0
23
24 M  END
25 $$$
26 3,3-dimethylsuccinimide-anion.sdf
27 COSMOtherm      3D      0
28
29 20 19 0 0 0 0 0 0 0 0 0 V2000
30 -3.4991 1.0516 -0.0097 O 0 0 0 0 0 0 0 0 0 0 0 1
31 -2.5708 0.6385 -0.0005 H 0 0 0 0 0 0 0 0 0 0 0 2
32 -3.3296 2.0096 -0.0090 H 0 0 0 0 0 0 0 0 0 0 0 3
33 1.4611 0.0243 -0.0038 C 0 0 0 0 0 0 0 0 0 0 0 4
34 0.9693 -1.4348 -0.0052 C 0 0 0 0 0 0 0 0 0 0 0 5
35 0.1186 0.8084 0.0078 C 0 0 0 0 0 0 0 0 0 0 0 6
36 -0.9725 -0.0207 0.0111 N 0 0 0 0 0 0 0 0 0 0 0 7
37 -0.5591 -1.3252 0.0035 C 0 0 0 0 0 0 0 0 0 0 0 8
38 2.2541 0.3897 -1.2712 C 0 0 0 0 0 0 0 0 0 0 0 9
39 2.2717 0.3815 1.2549 C 0 0 0 0 0 0 0 0 0 0 0 10
40 -1.3222 -2.3116 0.0029 O 0 0 0 0 0 0 0 0 0 0 0 11
41 0.0568 2.0514 0.0128 O 0 0 0 0 0 0 0 0 0 0 0 12
42 1.2985 -2.0060 0.8761 H 0 0 0 0 0 0 0 0 0 0 0 13
43 1.2885 -2.0009 -0.8936 H 0 0 0 0 0 0 0 0 0 0 0 14
44 1.6933 0.1321 -2.1826 H 0 0 0 0 0 0 0 0 0 0 0 15
45 2.4691 1.4680 -1.2936 H 0 0 0 0 0 0 0 0 0 0 0 16
46 3.2104 -0.1543 -1.2928 H 0 0 0 0 0 0 0 0 0 0 0 17
47 1.7235 0.1180 2.1723 H 0 0 0 0 0 0 0 0 0 0 0 18
48 2.4870 1.4597 1.2812 H 0 0 0 0 0 0 0 0 0 0 0 19
49 3.2281 -0.1626 1.2598 H 0 0 0 0 0 0 0 0 0 0 0 20
50
51 2   1   0   0   0   0
52 3   1   0   0   0   0
53 5   4   0   0   0   0
54 6   4   0   0   0   0
55 9   4   0   0   0   0
56 10  4   0   0   0   0
57 8   5   0   0   0   0
58 13  5   0   0   0   0
59 14  5   0   0   0   0
60 7   6   0   0   0   0
61 12  6   0   0   0   0
62 8   7   0   0   0   0
63 11  8   0   0   0   0
64 15  9   0   0   0   0
65 16  9   0   0   0   0
66 17  9   0   0   0   0
67 18 10   0   0   0   0
68 19 10   0   0   0   0
69 10 20   0   0   0   0
70
71 M  END
72 $$$
73 3,3-dimethylsuccinimide.sdf
74 COSMOtherm      3D      0
75
76 21 20 0 0 0 0 0 0 0 0 0 V2000
77 -3.5316 -0.0012 1.0718 O 0 0 0 0 0 0 0 0 0 0 0 1
78 -4.0472 -0.7741 0.7785 H 0 0 0 0 0 0 0 0 0 0 0 2
79 -4.0571 0.7640 0.7759 H 0 0 0 0 0 0 0 0 0 0 0 3
80 1.5002 -0.0006 -0.0190 C 0 0 0 0 0 0 0 0 0 0 0 4
81 0.9240 0.0000 -1.4561 C 0 0 0 0 0 0 0 0 0 0 0 5
82 0.2383 0.0012 0.8659 C 0 0 0 0 0 0 0 0 0 0 0 6
83 -0.8833 0.0010 0.0494 N 0 0 0 0 0 0 0 0 0 0 0 7
84 -0.5874 0.0007 -1.3062 C 0 0 0 0 0 0 0 0 0 0 0 8
85 2.3257 1.2644 0.2852 C 0 0 0 0 0 0 0 0 0 0 0 9
86 2.3218 -1.2681 0.2854 C 0 0 0 0 0 0 0 0 0 0 0 10
87 -1.4281 0.0010 -2.2012 O 0 0 0 0 0 0 0 0 0 0 0 11
88 0.2016 0.0025 2.0924 O 0 0 0 0 0 0 0 0 0 0 0 12
89 -1.8617 0.0022 0.4195 H 0 0 0 0 0 0 0 0 0 0 0 13
90 1.2216 -0.8840 -2.0382 H 0 0 0 0 0 0 0 0 0 0 0 14
91 1.2222 0.8842 -2.0376 H 0 0 0 0 0 0 0 0 0 0 0 15
92 1.7513 2.1788 0.0760 H 0 0 0 0 0 0 0 0 0 0 0 16
93 2.6326 1.2802 1.3403 H 0 0 0 0 0 0 0 0 0 0 0 17
94 3.2299 1.2747 -0.3398 H 0 0 0 0 0 0 0 0 0 0 0 18
95 1.7445 -2.1808 0.0762 H 0 0 0 0 0 0 0 0 0 0 0 19
96 2.6286 -1.2848 1.3404 H 0 0 0 0 0 0 0 0 0 0 0 20
97 3.2260 -1.2813 -0.3396 H 0 0 0 0 0 0 0 0 0 0 0 21
98
99 2   1   0   0   0   0
100 3   1   0   0   0   0
101 5   4   0   0   0   0
102 6   4   0   0   0   0
103 9   4   0   0   0   0
104 10  4   0   0   0   0
105 8   5   0   0   0   0
106 14  5   0   0   0   0
107 15  5   0   0   0   0
108 7   6   0   0   0   0
109 12  6   0   0   0   0
110 8   7   0   0   0   0
111 13  7   0   0   0   0
112 11  8   0   0   0   0
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16 9 0 0 0 0
17 9 0 0 0 0
18 9 0 0 0 0
19 10 0 0 0 0
20 10 0 0 0 0
10 21 0 0 0 0
M END
$$$$
3,3-methylphenylglutarimide-anion.sdf
COSMOtherm 3D 0

30 30 0 0 0 0 0 0 0 0 0 V2000
-3.8285 -2.0707 0.6172 O 0 0 0 0 0 0 0 0 0 0 0 1
-3.1343 -1.3309 0.5215 H 0 0 0 0 0 0 0 0 0 0 0 2
-4.0012 -2.3250 -0.3062 H 0 0 0 0 0 0 0 0 0 0 0 3
-1.3713 0.6418 1.2145 C 0 0 0 0 0 0 0 0 0 0 0 4
-1.9606 -0.1046 0.2361 N 0 0 0 0 0 0 0 0 0 0 0 5
-1.6459 0.0725 -1.0800 C 0 0 0 0 0 0 0 0 0 0 0 6
-0.5932 1.0985 -1.4980 C 0 0 0 0 0 0 0 0 0 0 0 7
0.4641 1.3972 -0.4216 C 0 0 0 0 0 0 0 0 0 0 0 8
-0.3406 1.7135 0.8598 C 0 0 0 0 0 0 0 0 0 0 0 9
-2.2354 -0.5853 -1.9694 O 0 0 0 0 0 0 0 0 0 0 0 10
-1.6856 0.4807 2.4167 O 0 0 0 0 0 0 0 0 0 0 0 11
1.2913 2.6308 -0.8443 C 0 0 0 0 0 0 0 0 0 0 0 12
1.4182 0.2129 -0.1762 C 0 0 0 0 0 0 0 0 0 0 0 13
-1.1337 2.0373 -1.7119 H 0 0 0 0 0 0 0 0 0 0 0 14
-0.1498 0.7766 -2.4500 H 0 0 0 0 0 0 0 0 0 0 0 15
-0.8920 2.6580 0.7032 H 0 0 0 0 0 0 0 0 0 0 0 16
0.3062 1.8672 1.7334 H 0 0 0 0 0 0 0 0 0 0 0 17
3.2587 -1.8943 0.2999 C 0 0 0 0 0 0 0 0 0 0 0 18
2.3277 -1.9873 -0.7379 C 0 0 0 0 0 0 0 0 0 0 0 19
1.4201 -0.9450 -0.9723 C 0 0 0 0 0 0 0 0 0 0 0 20
2.3640 0.2884 0.8651 C 0 0 0 0 0 0 0 0 0 0 0 21
3.2726 -0.7467 1.1025 C 0 0 0 0 0 0 0 0 0 0 0 22
0.6296 3.4931 -1.0181 H 0 0 0 0 0 0 0 0 0 0 0 23
2.0187 2.9090 -0.0686 H 0 0 0 0 0 0 0 0 0 0 0 24
1.8449 2.4282 -1.7738 H 0 0 0 0 0 0 0 0 0 0 0 25
3.9667 -2.7048 0.4828 H 0 0 0 0 0 0 0 0 0 0 0 26
2.3025 -2.8750 -1.3734 H 0 0 0 0 0 0 0 0 0 0 0 27
0.7084 -1.0528 -1.7912 H 0 0 0 0 0 0 0 0 0 0 0 28
2.3991 1.1735 1.5037 H 0 0 0 0 0 0 0 0 0 0 0 29
3.9941 -0.6559 1.9171 H 0 0 0 0 0 0 0 0 0 0 0 30
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
9 4 0 0 0 0
11 4 0 0 0 0
6 5 0 0 0 0
7 6 0 0 0 0
10 6 0 0 0 0
8 7 0 0 0 0
14 7 0 0 0 0
15 7 0 0 0 0
9 8 0 0 0 0
12 8 0 0 0 0
13 8 0 0 0 0
16 9 0 0 0 0
17 9 0 0 0 0
23 12 0 0 0 0
24 12 0 0 0 0
25 12 0 0 0 0
20 13 0 0 0 0
21 13 0 0 0 0
19 18 0 0 0 0
22 18 0 0 0 0
26 18 0 0 0 0
20 19 0 0 0 0
27 19 0 0 0 0
28 20 0 0 0 0
22 21 0 0 0 0
29 21 0 0 0 0
22 30 0 0 0 0
M END
$$$$
3,3-methylphenylglutarimide.sdf
COSMOtherm 3D 0

31 31 0 0 0 0 0 0 0 0 0 V2000
-3.8756 0.4543 2.1072 O 0 0 0 0 0 0 0 0 0 0 0 1
-4.3923 -0.3620 2.2338 H 0 0 0 0 0 0 0 0 0 0 0 2
-4.5445 1.1265 1.8830 H 0 0 0 0 0 0 0 0 0 0 0 3
-1.3621 1.2514 -0.5332 C 0 0 0 0 0 0 0 0 0 0 0 4
-1.8959 0.1070 0.0480 N 0 0 0 0 0 0 0 0 0 0 0 5
-1.5485 -1.2053 -0.2497 C 0 0 0 0 0 0 0 0 0 0 0 6
-0.4996 -1.4025 -1.3226 C 0 0 0 0 0 0 0 0 0 0 0 7
0.5102 -0.2439 -1.4475 C 0 0 0 0 0 0 0 0 0 0 0 8
-0.3372 1.0406 -1.6260 C 0 0 0 0 0 0 0 0 0 0 0 9
-2.1063 -2.1385 0.3314 O 0 0 0 0 0 0 0 0 0 0 10
-1.7478 2.3649 -0.1716 O 0 0 0 0 0 0 0 0 0 0 11
1.3730 -0.4663 -2.7089 C 0 0 0 0 0 0 0 0 0 0 0 12
1.4324 -0.1182 -0.2200 C 0 0 0 0 0 0 0 0 0 0 0 13
-2.6239 0.2444 0.7855 H 0 0 0 0 0 0 0 0 0 0 0 14
-1.0435 -1.4893 -2.2794 H 0 0 0 0 0 0 0 0 0 0 0 15
-0.0171 -2.3738 -1.1546 H 0 0 0 0 0 0 0 0 0 0 0 16
-0.8934 0.9691 -2.5773 H 0 0 0 0 0 0 0 0 0 0 0 17
0.2764 1.9474 -1.6873 H 0 0 0 0 0 0 0 0 0 0 0 18
3.2126 0.1488 1.9704 C 0 0 0 0 0 0 0 0 0 0 0 19
2.3793 -0.9674 1.8677 C 0 0 0 0 0 0 0 0 0 0 0 20
1.5012 -1.0989 0.7836 C 0 0 0 0 0 0 0 0 0 0 0 21
2.2831 0.9982 -0.1022 C 0 0 0 0 0 0 0 0 0 0 0 22
3.1614 1.1328 0.9759 C 0 0 0 0 0 0 0 0 0 0 0 23
0.7359 -0.5515 -3.6020 H 0 0 0 0 0 0 0 0 0 0 0 24
2.0695 0.3700 -2.8620 H 0 0 0 0 0 0 0 0 0 0 0 25
1.9633 -1.3892 -2.6137 H 0 0 0 0 0 0 0 0 0 0 0 26
3.8963 0.2526 2.8149 H 0 0 0 0 0 0 0 0 0 0 0 27
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URL: <http://mc.manuscriptcentral.com/tandf/tmph>

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14 9 0 0 0 0
13 16 0 0 0 0
M END
$$$$
3,5-dichlorophenol-anion.sdf
COSMOtherm 3D 0

15 14 0 0 0 0 0 0 0 0 0 V2000
-4.3366 -0.0302 1.4849 O 0 0 0 0 0 0 0 0 0 0 1
-3.3357 -0.0071 1.6682 H 0 0 0 0 0 0 0 0 0 0 2
-4.5354 0.8434 1.1072 H 0 0 0 0 0 0 0 0 0 0 3
1.4997 0.0013 0.4850 C 0 0 0 0 0 0 0 0 0 0 4
0.5447 -0.0046 1.4896 C 0 0 0 0 0 0 0 0 0 0 5
-0.8530 -0.0102 1.1575 C 0 0 0 0 0 0 0 0 0 0 6
-1.1785 -0.0096 -0.2425 C 0 0 0 0 0 0 0 0 0 0 7
-0.1677 -0.0031 -1.1915 C 0 0 0 0 0 0 0 0 0 0 8
1.1973 0.0033 -0.8820 C 0 0 0 0 0 0 0 0 0 0 9
-1.7645 -0.0159 2.0830 O 0 0 0 0 0 0 0 0 0 0 10
-0.6203 -0.0025 -2.9225 Cl 0 0 0 0 0 0 0 0 0 0 11
3.2279 0.0078 0.9470 Cl 0 0 0 0 0 0 0 0 0 0 12
0.8341 -0.0058 2.5407 H 0 0 0 0 0 0 0 0 0 0 13
-2.2271 -0.0179 -0.5405 H 0 0 0 0 0 0 0 0 0 0 14
1.9681 0.0086 -1.6487 H 0 0 0 0 0 0 0 0 0 0 15

2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
9 4 0 0 0 0
12 4 0 0 0 0
6 5 0 0 0 0
13 5 0 0 0 0
7 6 0 0 0 0
10 6 0 0 0 0
8 7 0 0 0 0
14 7 0 0 0 0
9 8 0 0 0 0
11 8 0 0 0 0
9 15 0 0 0 0
M END
$$$$
3,5-dichlorophenol.sdf
COSMOtherm 3D 0

16 15 0 0 0 0 0 0 0 0 0 V2000
-4.1729 -0.0063 -1.3906 O 0 0 0 0 0 0 0 0 0 0 1
-4.6544 -0.7825 -1.7316 H 0 0 0 0 0 0 0 0 0 0 2
-4.6653 0.7612 -1.7358 H 0 0 0 0 0 0 0 0 0 0 3
-1.6378 0.0056 -2.1905 O 0 0 0 0 0 0 0 0 0 0 4
-0.7605 0.0033 -1.1578 C 0 0 0 0 0 0 0 0 0 0 5
0.6118 0.0020 -1.4741 C 0 0 0 0 0 0 0 0 0 0 6
1.5366 -0.0003 -0.4360 C 0 0 0 0 0 0 0 0 0 0 7
3.2642 -0.0023 -0.8361 Cl 0 0 0 0 0 0 0 0 0 0 8
1.1694 -0.0009 0.9127 C 0 0 0 0 0 0 0 0 0 0 9
-0.2002 0.0008 1.1838 C 0 0 0 0 0 0 0 0 0 0 10
-0.7209 0.0004 2.8793 Cl 0 0 0 0 0 0 0 0 0 0 11
-1.1748 0.0029 0.1887 C 0 0 0 0 0 0 0 0 0 0 12
-2.5948 0.0015 -1.8622 H 0 0 0 0 0 0 0 0 0 0 13
0.9270 0.0022 -2.5166 H 0 0 0 0 0 0 0 0 0 0 14
1.9110 -0.0026 1.7083 H 0 0 0 0 0 0 0 0 0 0 15
-2.2347 0.0044 0.4402 H 0 0 0 0 0 0 0 0 0 0 16

2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
13 4 0 0 0 0
6 5 0 0 0 0
12 5 0 0 0 0
7 6 0 0 0 0
14 6 0 0 0 0
8 7 0 0 0 0
9 7 0 0 0 0
10 9 0 0 0 0
15 9 0 0 0 0
11 10 0 0 0 0
12 10 0 0 0 0
12 16 0 0 0 0
M END
$$$$
3-chlorophenol-anion.sdf
COSMOtherm 3D 0

15 14 0 0 0 0 0 0 0 0 0 V2000
-4.5282 0.0705 0.2863 O 0 0 0 0 0 0 0 0 0 0 1
-3.5501 0.0160 0.5805 H 0 0 0 0 0 0 0 0 0 0 2
-4.5941 0.9195 -0.1828 H 0 0 0 0 0 0 0 0 0 0 3
-0.1073 -0.0238 -1.9379 C 0 0 0 0 0 0 0 0 0 0 4
-1.2073 -0.0566 -1.0833 C 0 0 0 0 0 0 0 0 0 0 5
-1.0518 -0.0617 0.3420 C 0 0 0 0 0 0 0 0 0 0 6
0.2993 -0.0292 0.8291 C 0 0 0 0 0 0 0 0 0 0 7
1.3635 0.0017 -0.0620 C 0 0 0 0 0 0 0 0 0 0 8
1.2110 0.0072 -1.4510 C 0 0 0 0 0 0 0 0 0 0 9
-2.0611 -0.0928 1.1684 O 0 0 0 0 0 0 0 0 0 0 10
3.0318 0.0415 0.6059 Cl 0 0 0 0 0 0 0 0 0 0 11
-0.2681 -0.0214 -3.0192 H 0 0 0 0 0 0 0 0 0 0 12
-2.2201 -0.0841 -1.4924 H 0 0 0 0 0 0 0 0 0 0 13
0.4688 -0.0314 1.9069 H 0 0 0 0 0 0 0 0 0 0 14
2.0699 0.0326 -2.1197 H 0 0 0 0 0 0 0 0 0 0 15

2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
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12 4 0 0 0 0
6 5 0 0 0 0
13 5 0 0 0 0
7 6 0 0 0 0
10 6 0 0 0 0
8 7 0 0 0 0
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14 7 0 0 0 0
9 8 0 0 0 0
11 8 0 0 0 0
9 15 0 0 0 0
M END
$$$$
3-chlorophenol.sdf
COSMOTHERM 3D 0
16 15 0 0 0 0 0 0 0 0 0 V2000
-4.4971 0.2757 0.0146 O 0 0 0 0 0 0 0 0 0 0 0 1
-4.7624 -0.3314 0.7292 H 0 0 0 0 0 0 0 0 0 0 0 2
-4.8122 -0.1492 -0.8039 H 0 0 0 0 0 0 0 0 0 0 0 3
0.3313 0.8307 -0.0023 C 0 0 0 0 0 0 0 0 0 0 0 4
1.3969 -0.0651 0.0001 C 0 0 0 0 0 0 0 0 0 0 0 5
1.2198 -1.4501 0.0002 C 0 0 0 0 0 0 0 0 0 0 0 6
-0.0936 -1.9357 -0.0024 C 0 0 0 0 0 0 0 0 0 0 0 7
-1.1899 -1.0702 -0.0055 C 0 0 0 0 0 0 0 0 0 0 0 8
-0.9815 0.3219 -0.0043 C 0 0 0 0 0 0 0 0 0 0 0 9
2.0732 -2.1266 0.0026 H 0 0 0 0 0 0 0 0 0 0 0 10
-1.9983 1.2257 -0.0053 O 0 0 0 0 0 0 0 0 0 0 0 11
0.4945 1.9082 -0.0022 H 0 0 0 0 0 0 0 0 0 0 0 12
3.0516 0.5891 0.0031 Cl 0 0 0 0 0 0 0 0 0 0 0 13
-0.2628 -3.0139 -0.0029 H 0 0 0 0 0 0 0 0 0 0 0 14
-2.2058 -1.4686 -0.0089 H 0 0 0 0 0 0 0 0 0 0 0 15
-2.8954 0.7691 0.0011 H 0 0 0 0 0 0 0 0 0 0 0 16
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
9 4 0 0 0 0
12 4 0 0 0 0
6 5 0 0 0 0
13 5 0 0 0 0
7 6 0 0 0 0
10 6 0 0 0 0
8 7 0 0 0 0
14 7 0 0 0 0
9 8 0 0 0 0
15 8 0 0 0 0
11 9 0 0 0 0
11 16 0 0 0 0
M END
$$$$
3-chloropropanoicacid-anion.sdf
COSMOTHERM 3D 0
13 11 0 0 0 0 0 0 0 0 0 V2000
-4.3547 -0.0171 0.0841 O 0 0 0 0 0 0 0 0 0 0 0 1
-3.4274 -0.0009 -0.3196 H 0 0 0 0 0 0 0 0 0 0 0 2
-4.1707 -0.0275 1.0396 H 0 0 0 0 0 0 0 0 0 0 0 3
1.4415 0.0227 0.5583 C 0 0 0 0 0 0 0 0 0 0 0 4
0.4515 -0.0111 -0.5875 C 0 0 0 0 0 0 0 0 0 0 0 5
-1.0149 0.0064 -0.0937 C 0 0 0 0 0 0 0 0 0 0 0 6
-1.2368 0.0030 1.1479 O 0 0 0 0 0 0 0 0 0 0 0 7
-1.9029 0.0204 -1.0140 O 0 0 0 0 0 0 0 0 0 0 0 8
0.5952 -0.9158 -1.1976 H 0 0 0 0 0 0 0 0 0 0 0 9
1.3719 0.9392 1.1504 H 0 0 0 0 0 0 0 0 0 0 0 10
1.3607 -0.8498 1.2120 H 0 0 0 0 0 0 0 0 0 0 0 11
3.1890 -0.0087 -0.0746 Cl 0 0 0 0 0 0 0 0 0 0 0 12
0.6004 0.8496 -1.2565 H 0 0 0 0 0 0 0 0 0 0 0 13
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
10 4 0 0 0 0
11 4 0 0 0 0
12 4 0 0 0 0
6 5 0 0 0 0
9 5 0 0 0 0
7 6 0 0 0 0
8 6 0 0 0 0
5 13 0 0 0 0
M END
$$$$
3-chloropropanoicacid.sdf
COSMOTHERM 3D 0
14 12 0 0 0 0 0 0 0 0 0 V2000
-4.3705 0.0076 0.1087 O 0 0 0 0 0 0 0 0 0 0 0 1
-4.6486 -0.8101 -0.3434 H 0 0 0 0 0 0 0 0 0 0 0 2
-4.5989 0.7232 -0.5128 H 0 0 0 0 0 0 0 0 0 0 0 3
1.5247 -0.0213 -0.5790 C 0 0 0 0 0 0 0 0 0 0 0 4
0.4766 0.0017 0.5191 C 0 0 0 0 0 0 0 0 0 0 0 5
-0.9306 0.0010 -0.0516 C 0 0 0 0 0 0 0 0 0 0 0 6
-1.8624 -0.0028 0.9110 O 0 0 0 0 0 0 0 0 0 0 0 7
-1.1869 0.0059 -1.2526 O 0 0 0 0 0 0 0 0 0 0 0 8
0.5883 0.8955 1.1514 H 0 0 0 0 0 0 0 0 0 0 0 9
3.2112 0.0053 0.1550 Cl 0 0 0 0 0 0 0 0 0 0 0 10
1.4786 -0.9327 -1.1815 H 0 0 0 0 0 0 0 0 0 0 0 11
1.4693 0.8575 -1.2273 H 0 0 0 0 0 0 0 0 0 0 0 12
0.5804 -0.8690 1.1836 H 0 0 0 0 0 0 0 0 0 0 0 13
-2.8008 0.0000 0.5021 H 0 0 0 0 0 0 0 0 0 0 0 14
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
10 4 0 0 0 0
11 4 0 0 0 0
12 4 0 0 0 0
6 5 0 0 0 0
9 5 0 0 0 0
13 5 0 0 0 0
7 6 0 0 0 0
8 6 0 0 0 0
7 14 0 0 0 0
M END
$$$$
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3-hydroxy-2-naphtoicacid-anion.sdf											
COSMOtherm				3D				0			
24	25	0	0	0	0	0	0	0	0	0	V2000
-5.3919	-1.4569	0.0296	O	0	0	0	0	0	0	0	0
-4.3943	-1.3496	0.0075	H	0	0	0	0	0	0	0	0
-5.7210	-0.5419	0.0062	H	0	0	0	0	0	0	0	0
4.3276	-0.2922	0.0081	C	0	0	0	0	0	0	0	0
3.8190	-1.6185	0.0020	C	0	0	0	0	0	0	0	0
2.4541	-1.8341	-0.0032	C	0	0	0	0	0	0	0	0
1.5421	-0.7406	-0.0025	C	0	0	0	0	0	0	0	0
2.0570	0.6071	0.0037	C	0	0	0	0	0	0	0	0
3.4710	0.7922	0.0089	C	0	0	0	0	0	0	0	0
0.1372	-0.9272	-0.0076	C	0	0	0	0	0	0	0	0
-0.7470	0.1399	-0.0067	C	0	0	0	0	0	0	0	0
-0.2234	1.4840	-0.0005	C	0	0	0	0	0	0	0	0
1.1501	1.6951	0.0044	C	0	0	0	0	0	0	0	0
-2.2398	-0.0934	-0.0118	C	0	0	0	0	0	0	0	0
-2.6805	-1.2785	-0.0201	O	0	0	0	0	0	0	0	0
-2.9892	0.9564	-0.0078	O	0	0	0	0	0	0	0	0
-1.0738	2.5384	0.0005	O	0	0	0	0	0	0	0	0
-2.0157	2.0781	-0.0021	H	0	0	0	0	0	0	0	0
5.4076	-0.1306	0.0121	H	0	0	0	0	0	0	0	0
4.5097	-2.4634	0.0013	H	0	0	0	0	0	0	0	0
2.0536	-2.8507	-0.0080	H	0	0	0	0	0	0	0	0
3.8694	1.8097	0.0137	H	0	0	0	0	0	0	0	0
-0.2717	-1.9401	-0.0123	H	0	0	0	0	0	0	0	0
1.5300	2.7192	0.0092	H	0	0	0	0	0	0	0	0
2	1	0	0	0	0						
3	1	0	0	0	0						
5	4	0	0	0	0						
9	4	0	0	0	0						
19	4	0	0	0	0						
6	5	0	0	0	0						
20	5	0	0	0	0						
7	6	0	0	0	0						
21	6	0	0	0	0						
8	7	0	0	0	0						
10	7	0	0	0	0						
9	8	0	0	0	0						
13	8	0	0	0	0						
22	9	0	0	0	0						
11	10	0	0	0	0						
23	10	0	0	0	0						
12	11	0	0	0	0						
14	11	0	0	0	0						
13	12	0	0	0	0						
17	12	0	0	0	0						
15	14	0	0	0	0						
16	14	0	0	0	0						
18	16	0	0	0	0						
18	17	0	0	0	0						
13	24	0	0	0	0						
M END											
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3-hydroxy-2-naphtoicacid.sdf											
COSMOtherm				3D				0			
25	25	0	0	0	0	0	0	0	0	0	V

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3 16 14 0 0 0 0
4 18 15 0 0 0 0
5 19 17 0 0 0 0
6 13 25 0 0 0 0
7 M END
8 $$$
9 3-hydroxybenzoicacid-anion.sdf
10 COSMOTHERM 3D 0
11
12 18 17 0 0 0 0 0 0 0 0 0 V2000
13 -4.6337 -0.8075 0.0085 O 0 0 0 0 0 0 0 0 0 0 1
14 -3.6218 -0.8227 0.0028 H 0 0 0 0 0 0 0 0 0 0 2
15 -4.8357 0.1438 0.0361 H 0 0 0 0 0 0 0 0 0 0 3
16 2.1057 1.6867 0.0047 C 0 0 0 0 0 0 0 0 0 0 4
17 0.7087 1.6100 0.0014 C 0 0 0 0 0 0 0 0 0 0 5
18 0.0742 0.3574 -0.0021 C 0 0 0 0 0 0 0 0 0 0 6
19 0.8530 -0.8098 -0.0027 C 0 0 0 0 0 0 0 0 0 0 7
20 2.2508 -0.7255 0.0006 C 0 0 0 0 0 0 0 0 0 0 8
21 2.8847 0.5260 0.0042 C 0 0 0 0 0 0 0 0 0 0 9
22 -1.4506 0.2643 -0.0052 C 0 0 0 0 0 0 0 0 0 0 10
23 3.0560 -1.8432 0.0004 O 0 0 0 0 0 0 0 0 0 0 11
24 -1.9531 -0.9144 -0.0053 O 0 0 0 0 0 0 0 0 0 0 12
25 -2.1113 1.3403 -0.0071 O 0 0 0 0 0 0 0 0 0 0 13
26 2.5998 2.6606 0.0080 H 0 0 0 0 0 0 0 0 0 0 14
27 0.0962 2.5119 0.0021 H 0 0 0 0 0 0 0 0 0 0 15
28 0.3540 -1.7815 -0.0054 H 0 0 0 0 0 0 0 0 0 0 16
29 3.9750 0.5774 0.0068 H 0 0 0 0 0 0 0 0 0 0 17
30 2.4950 -2.6420 -0.0032 H 0 0 0 0 0 0 0 0 0 0 18
31
32 2 1 0 0 0 0
33 3 1 0 0 0 0
34 5 4 0 0 0 0
35 9 4 0 0 0 0
36 14 4 0 0 0 0
37 6 5 0 0 0 0
38 15 5 0 0 0 0
39 7 6 0 0 0 0
40 10 6 0 0 0 0
41 8 7 0 0 0 0
42 16 7 0 0 0 0
43 9 8 0 0 0 0
44 11 8 0 0 0 0
45 17 9 0 0 0 0
46 12 10 0 0 0 0
47 13 10 0 0 0 0
48 11 18 0 0 0 0
49 M END
50 $$$
51 3-hydroxybenzoicacid.sdf
52 COSMOTHERM 3D 0
53
54 19 18 0 0 0 0 0 0 0 0 0 V2000
55 2.1269 -3.3585 0.0059 O 0 0 0 0 0 0 0 0 0 0 1
56 2.6851 -3.0513 0.7431 H 0 0 0 0 0 0 0 0 0 0 2
57 2.6421 -3.1605 -0.7971 H 0 0 0 0 0 0 0 0 0 0 3
58 -2.4915 0.3502 0.0016 C 0 0 0 0 0 0 0 0 0 0 4
59 -1.5191 1.3533 0.0011 C 0 0 0 0 0 0 0 0 0 0 5
60 -0.1611 0.9926 -0.0012 C 0 0 0 0 0 0 0 0 0 0 6
61 0.2165 -0.3615 -0.0030 C 0 0 0 0 0 0 0 0 0 0 7
62 -0.7672 -1.3631 -0.0013 C 0 0 0 0 0 0 0 0 0 0 8
63 -2.1267 -0.9979 0.0005 C 0 0 0 0 0 0 0 0 0 0 9
64 0.8580 2.0773 -0.0006 C 0 0 0 0 0 0 0 0 0 0 10
65 -0.4665 -2.6909 -0.0008 O 0 0 0 0 0 0 0 0 0 0 11
66 2.1349 1.6139 0.0002 O 0 0 0 0 0 0 0 0 0 0 12
67 0.5999 3.2774 0.0000 O 0 0 0 0 0 0 0 0 0 0 13
68 -3.5492 0.6183 0.0030 H 0 0 0 0 0 0 0 0 0 0 14
69 -1.7975 2.4067 0.0025 H 0 0 0 0 0 0 0 0 0 0 15
70 1.2713 -0.6352 -0.0058 H 0 0 0 0 0 0 0 0 0 0 16
71 -2.8852 -1.7827 0.0013 H 0 0 0 0 0 0 0 0 0 0 17
72 0.5281 -2.8420 0.0020 H 0 0 0 0 0 0 0 0 0 0 18
73 2.7319 2.3926 0.0016 H 0 0 0 0 0 0 0 0 0 0 19
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75 2 1 0 0 0 0
76 3 1 0 0 0 0
77 5 4 0 0 0 0
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79 14 4 0 0 0 0
80 6 5 0 0 0 0
81 15 5 0 0 0 0
82 7 6 0 0 0 0
83 10 6 0 0 0 0
84 8 7 0 0 0 0
85 16 7 0 0 0 0
86 9 8 0 0 0 0
87 11 8 0 0 0 0
88 17 9 0 0 0 0
89 12 10 0 0 0 0
90 13 10 0 0 0 0
91 18 11 0 0 0 0
92 12 19 0 0 0 0
93 M END
94 $$$
95 4-(1,1-dimethylethyl)-benzoicacid-anion.sdf
96 COSMOTHERM 3D 0
97
98 29 28 0 0 0 0 0 0 0 0 0 V2000
99 -5.8865 -0.4862 -0.0059 O 0 0 0 0 0 0 0 0 0 0 1
100 -4.8840 -0.6315 -0.0039 H 0 0 0 0 0 0 0 0 0 0 2
101 -5.9617 0.4839 0.0082 H 0 0 0 0 0 0 0 0 0 0 3
102 1.0772 1.2472 -0.0020 C 0 0 0 0 0 0 0 0 0 0 4
103 -0.3211 1.3020 -0.0009 C 0 0 0 0 0 0 0 0 0 0 5
104 -1.0915 0.1311 0.0014 C 0 0 0 0 0 0 0 0 0 0 6
105 -0.4165 -1.1014 0.0029 C 0 0 0 0 0 0 0 0 0 0 7
106 0.9780 -1.1540 0.0022 C 0 0 0 0 0 0 0 0 0 0 8
107 1.7615 0.0189 -0.0003 C 0 0 0 0 0 0 0 0 0 0 9
108 -2.6127 0.2028 0.0022 C 0 0 0 0 0 0 0 0 0 0 10
109 3.2967 -0.0808 -0.0008 C 0 0 0 0 0 0 0 0 0 0 11
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3.7601	-0.8461	1.2623	C	0	0	0	0	0	0	0	0	0	12
3.9738	1.3027	-0.0041	C	0	0	0	0	0	0	0	0	0	13
3.7588	-0.8516	-1.2610	C	0	0	0	0	0	0	0	0	0	14
-3.1553	1.3446	0.0039	O	0	0	0	0	0	0	0	0	0	15
-3.2421	-0.9145	0.0006	O	0	0	0	0	0	0	0	0	0	16
1.6350	2.1842	-0.0041	H	0	0	0	0	0	0	0	0	0	17
-0.8336	2.2658	-0.0021	H	0	0	0	0	0	0	0	0	0	18
-1.0022	-2.0224	0.0047	H	0	0	0	0	0	0	0	0	0	19
1.4653	-2.1316	0.0034	H	0	0	0	0	0	0	0	0	0	20
4.8578	-0.9294	1.2710	H	0	0	0	0	0	0	0	0	0	21
3.3440	-1.8630	1.2963	H	0	0	0	0	0	0	0	0	0	22
3.4495	-0.3191	2.1772	H	0	0	0	0	0	0	0	0	0	23
5.0660	1.1733	-0.0044	H	0	0	0	0	0	0	0	0	0	24
3.7067	1.8876	-0.8970	H	0	0	0	0	0	0	0	0	0	25
3.7076	1.8914	0.8866	H	0	0	0	0	0	0	0	0	0	26
4.8566	-0.9342	-1.2709	H	0	0	0	0	0	0	0	0	0	27
3.4466	-0.3289	-2.1778	H	0	0	0	0	0	0	0	0	0	28
3.3434	-1.8689	-1.2898	H	0	0	0	0	0	0	0	0	0	29
2	1	0	0	0	0	0	0	0	0	0	0	0	0
3	1	0	0	0	0	0	0	0	0	0	0	0	0
5	4	0	0	0	0	0	0	0	0	0	0	0	0
9	4	0	0	0	0	0	0	0	0	0	0	0	0
17	4	0	0	0	0	0	0	0	0	0	0	0	0
6	5	0	0	0	0	0	0	0	0	0	0	0	0
18	5	0	0	0	0	0	0	0	0	0	0	0	0
7	6	0	0	0	0	0	0	0	0	0	0	0	0
10	6	0	0	0	0	0	0	0	0	0	0	0	0
8	7	0	0	0	0	0	0	0	0	0	0	0	0
19	7	0	0	0	0	0	0	0	0	0	0	0	0
9	8	0	0	0	0	0	0	0	0	0	0	0	0
20	8	0	0	0	0	0	0	0	0	0	0	0	0
11	9	0	0	0	0	0	0	0	0	0	0	0	0
15	10	0	0	0	0	0	0	0	0	0	0	0	0
16	10	0	0	0	0	0	0	0	0	0	0	0	0
12	11	0	0	0	0	0	0	0	0	0	0	0	0
13	11	0	0	0	0	0	0	0	0	0	0	0	0
14	11	0	0	0	0	0	0	0	0	0	0	0	0
21	12	0	0	0	0	0	0	0	0	0	0	0	0
22	12	0	0	0	0	0	0	0	0	0	0	0	0
23	12	0	0	0	0	0	0	0	0	0	0	0	0
24	13	0	0	0	0	0	0	0	0	0	0	0	0
25	13	0	0	0	0	0	0	0	0	0	0	0	0
26	13	0	0	0	0	0	0	0	0	0	0	0	0
27	14	0	0	0	0	0	0	0	0	0	0	0	0
28	14	0	0	0	0	0	0	0	0	0	0	0	0
14	29	0	0	0	0	0	0	0	0	0	0	0	0
M END													
\$\$\$\$													
4-(1,1-dimethylethyl)-benzoicacid.sdf													
COSMOtherm 3D 0													
30	29	0	0	0	0	0	0	0	0	0	0	0	0
-5.8363	-0.0006	0.6861	O	0	0	0	0	0	0	0	0	0	1
-6.2225	-0.6468	0.0669	H	0	0	0	0	0	0	0	0	0	2
-6.2058	0.8575	0.4077	H	0	0	0	0	0	0	0	0	0	3
1.1347	-0.0121	-1.2643	C	0	0	0	0	0	0	0	0	0	4
-0.2582	-0.0129	-1.3611	C	0	0	0	0	0	0	0	0	0	5
-1.0552	-0.0067	-0.2066	C	0	0	0	0	0	0	0	0	0	6
-0.4225	0.0008	1.0500	C	0	0	0	0	0	0	0	0	0	7
0.9680	0.0041	1.1366	C	0	0	0	0	0	0	0	0	0	8
1.7817	-0.0023	-0.0154	C	0	0	0	0	0	0	0	0	0	9
-2.5392	-0.0020	-0.3519	C	0	0	0	0	0	0	0	0	0	10
3.3122	0.0031	0.1273	C	0	0	0	0	0	0	0	0	0	11
3.7460	1.2764	0.8939	C	0	0	0	0	0	0	0	0	0	12
4.0282	-0.0115	-1.2362	C	0	0	0	0	0	0	0	0	0	13
3.7535	-1.2484	0.9245	C	0	0	0	0	0	0	0	0	0	14
-3.1148	0.0234	-1.4419	O	0	0	0	0	0	0	0	0	0	15
-3.1961	-0.0288	0.8207	O	0	0	0	0	0	0	0	0	0	16
1.7187	-0.0181	-2.1843	H	0	0	0	0	0	0	0	0	0	17
-0.7403	-0.0180	-2.3399	H	0	0	0	0	0	0	0	0	0	18
-1.0232	0.0062	1.9597	H	0	0	0	0	0	0	0	0	0	19
1.4279	0.0121	2.1263	H	0	0	0	0	0	0	0	0	0	20
4.8407	1.2898	1.0073	H	0	0	0	0	0	0	0	0	0	21
3.3018	1.3178	1.8983	H	0	0	0	0	0	0	0	0	0	22
3.4470	2.1846	0.3491	H	0	0	0	0	0	0	0	0	0	23
5.1157	-0.0052	-1.0743	H	0	0	0	0	0	0	0	0	0	24
3.7827	-0.9122	-1.8185	H	0	0	0	0	0	0	0	0	0	25
3.7757	0.8716	-1.8416	H	0	0	0	0	0	0	0	0	0	26
4.8485	-1.2533	1.0366	H	0	0	0	0	0	0	0	0	0	27
3.4586	-2.1714	0.4029	H	0	0	0	0	0	0	0	0	0	28
3.3112	-1.2674	1.9304	H	0	0	0	0	0	0	0	0	0	29
-4.2033	-0.0154	0.6577	H	0	0	0	0	0	0	0	0	0	30
2	1	0	0	0	0	0	0	0	0	0	0	0	0
3	1	0	0	0	0	0	0	0	0	0	0	0	0
5	4	0	0	0	0	0	0	0	0	0	0	0	0
9	4	0	0	0	0	0	0	0	0	0	0	0	0
17	4	0	0	0	0	0	0	0	0	0	0	0	0
6	5	0	0	0	0	0	0	0	0	0	0	0	0
18	5	0	0	0	0	0	0	0	0	0	0	0	0
7	6	0	0	0	0	0	0	0	0	0	0	0	0
10	6	0	0	0	0	0	0	0	0	0	0	0	0
8	7	0	0	0	0	0	0	0	0	0	0	0	0
19	7	0	0	0	0	0	0	0	0	0	0	0	0
9	8	0	0	0	0	0	0	0	0	0	0	0	0
20	8	0	0	0	0	0	0	0	0	0	0	0	0
11	9	0	0	0	0	0	0	0	0	0	0	0	0
15	10	0	0	0	0	0	0	0	0	0	0	0	0
16	10	0	0	0	0	0	0	0	0	0	0	0	0
12	11	0	0	0	0	0	0	0	0	0	0	0	0
13	11	0	0	0	0	0	0	0	0	0	0	0	0
14	11	0	0	0	0	0	0	0	0	0	0	0	0
21	12	0	0	0	0	0	0	0	0	0	0	0	0
22	12	0	0	0	0	0	0	0	0	0	0	0	0
23	12	0	0	0	0	0	0	0	0	0	0	0	0
24	13	0	0	0	0	0	0	0	0	0	0	0	0

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25 13 0 0 0 0
26 13 0 0 0 0
27 14 0 0 0 0
28 14 0 0 0 0
29 14 0 0 0 0
16 30 0 0 0 0
M END
$$$$
4-(1-methylethyl)-benzoicacid-anion.sdf
COSMOtherm 3D 0

26 25 0 0 0 0 0 0 0 0 0 V2000
-5.6228 0.0118 0.2988 O 0 0 0 0 0 0 0 0 0 0 0 1
-4.6272 -0.0014 0.4867 H 0 0 0 0 0 0 0 0 0 0 0 2
-5.6586 0.0589 -0.6723 H 0 0 0 0 0 0 0 0 0 0 0 3
1.1906 0.0204 1.3603 C 0 0 0 0 0 0 0 0 0 0 0 4
-0.2009 0.0147 1.2200 C 0 0 0 0 0 0 0 0 0 0 0 5
-0.7930 -0.0033 -0.0523 C 0 0 0 0 0 0 0 0 0 0 0 6
0.0489 -0.0170 -1.1775 C 0 0 0 0 0 0 0 0 0 0 0 7
1.4377 -0.0132 -1.0351 C 0 0 0 0 0 0 0 0 0 0 0 8
2.0367 0.0063 0.2384 C 0 0 0 0 0 0 0 0 0 0 0 9
-2.3071 -0.0076 -0.2212 C 0 0 0 0 0 0 0 0 0 0 0 10
3.5494 0.0105 0.4047 C 0 0 0 0 0 0 0 0 0 0 0 11
4.1885 -1.2721 -0.1624 C 0 0 0 0 0 0 0 0 0 0 0 12
4.1898 1.2654 -0.2197 C 0 0 0 0 0 0 0 0 0 0 0 13
-3.0058 -0.0174 0.8545 O 0 0 0 0 0 0 0 0 0 0 0 14
-2.7756 -0.0010 -1.3947 O 0 0 0 0 0 0 0 0 0 0 0 15
1.6324 0.0357 2.3604 H 0 0 0 0 0 0 0 0 0 0 0 16
-0.8455 0.0249 2.1006 H 0 0 0 0 0 0 0 0 0 0 0 17
-0.4066 -0.0305 -2.1694 H 0 0 0 0 0 0 0 0 0 0 0 18
2.0641 -0.0252 -1.9306 H 0 0 0 0 0 0 0 0 0 0 0 19
3.7518 0.0348 1.4883 H 0 0 0 0 0 0 0 0 0 0 0 20
5.2736 -1.2738 0.0215 H 0 0 0 0 0 0 0 0 0 0 0 21
3.7608 -2.1719 0.3038 H 0 0 0 0 0 0 0 0 0 0 0 22
4.0320 -1.3457 -1.2498 H 0 0 0 0 0 0 0 0 0 0 0 23
5.2742 1.2763 -0.0323 H 0 0 0 0 0 0 0 0 0 0 0 24
3.7602 2.1860 0.2021 H 0 0 0 0 0 0 0 0 0 0 0 25
4.0375 1.2878 -1.3099 H 0 0 0 0 0 0 0 0 0 0 0 26
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
9 4 0 0 0 0
16 4 0 0 0 0
6 5 0 0 0 0
17 5 0 0 0 0
7 6 0 0 0 0
10 6 0 0 0 0
8 7 0 0 0 0
18 7 0 0 0 0
9 8 0 0 0 0
19 8 0 0 0 0
11 9 0 0 0 0
14 10 0 0 0 0
15 10 0 0 0 0
12 11 0 0 0 0
13 11 0 0 0 0
20 11 0 0 0 0
21 12 0 0 0 0
22 12 0 0 0 0
23 12 0 0 0 0
24 13 0 0 0 0
25 13 0 0 0 0
13 26 0 0 0 0
M END
$$$$
4-(1-methylethyl)-benzoicacid.sdf
COSMOtherm 3D 0

27 26 0 0 0 0 0 0 0 0 0 V2000
-5.4969 -0.0215 0.8029 O 0 0 0 0 0 0 0 0 0 0 0 1
-5.8656 -0.3928 -0.0199 H 0 0 0 0 0 0 0 0 0 0 0 2
-5.8766 0.8750 0.8584 H 0 0 0 0 0 0 0 0 0 0 0 3
1.3747 0.0012 -1.4007 C 0 0 0 0 0 0 0 0 0 0 0 4
-0.0197 0.0007 -1.4371 C 0 0 0 0 0 0 0 0 0 0 0 5
-0.7609 -0.0021 -0.2437 C 0 0 0 0 0 0 0 0 0 0 0 6
-0.0739 -0.0045 0.9845 C 0 0 0 0 0 0 0 0 0 0 0 7
1.3202 -0.0039 1.0109 C 0 0 0 0 0 0 0 0 0 0 0 8
2.0720 -0.0009 -0.1797 C 0 0 0 0 0 0 0 0 0 0 0 9
-2.2503 -0.0025 -0.3201 C 0 0 0 0 0 0 0 0 0 0 0 10
3.5921 0.0009 -0.1563 C 0 0 0 0 0 0 0 0 0 0 0 11
4.1474 1.2746 0.5107 C 0 0 0 0 0 0 0 0 0 0 0 12
4.1524 -1.2654 0.5201 C 0 0 0 0 0 0 0 0 0 0 0 13
-2.8764 0.0026 -1.3824 O 0 0 0 0 0 0 0 0 0 0 0 14
-2.8530 -0.0113 0.8816 O 0 0 0 0 0 0 0 0 0 0 0 15
1.9372 0.0038 -2.3376 H 0 0 0 0 0 0 0 0 0 0 0 16
-0.5482 0.0031 -2.3916 H 0 0 0 0 0 0 0 0 0 0 0 17
-0.6361 -0.0064 1.9186 H 0 0 0 0 0 0 0 0 0 0 0 18
1.8301 -0.0053 1.9768 H 0 0 0 0 0 0 0 0 0 0 0 19
3.9282 -0.0023 -1.2063 H 0 0 0 0 0 0 0 0 0 0 0 20
5.2466 1.2816 0.4612 H 0 0 0 0 0 0 0 0 0 0 0 21
3.7759 2.1821 0.0126 H 0 0 0 0 0 0 0 0 0 0 0 22
3.8585 1.3258 1.5717 H 0 0 0 0 0 0 0 0 0 0 0 23
5.2515 -1.2688 0.4696 H 0 0 0 0 0 0 0 0 0 0 0 24
3.7838 -2.1780 0.0292 H 0 0 0 0 0 0 0 0 0 0 0 25
3.8647 -1.3097 1.5817 H 0 0 0 0 0 0 0 0 0 0 0 26
-3.8665 -0.0043 0.7601 H 0 0 0 0 0 0 0 0 0 0 0 27
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
9 4 0 0 0 0
16 4 0 0 0 0
6 5 0 0 0 0
17 5 0 0 0 0
7 6 0 0 0 0
10 6 0 0 0 0
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18 7 0 0 0 0
  9 8 0 0 0 0
19 8 0 0 0 0
11 9 0 0 0 0
14 10 0 0 0 0
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12 11 0 0 0 0
13 11 0 0 0 0
20 11 0 0 0 0
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22 12 0 0 0 0
23 12 0 0 0 0
24 13 0 0 0 0
25 13 0 0 0 0
26 13 0 0 0 0
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M END
$$$$
4-aminobenzoicacid-anion.sdf
COSMOtherm 3D 0

19 18 0 0 0 0 0 0 0 0 V2000
-4.8386 -0.0115 -0.4115 O 0 0 0 0 0 0 0 0 0 0 1
-3.8354 -0.0055 -0.5688 H 0 0 0 0 0 0 0 0 0 0 2
-4.9036 -0.0010 0.5593 H 0 0 0 0 0 0 0 0 0 0 3
1.9931 0.0069 -1.2635 C 0 0 0 0 0 0 0 0 0 0 4
0.6041 0.0072 -1.1574 C 0 0 0 0 0 0 0 0 0 0 5
-0.0381 0.0049 0.0947 C 0 0 0 0 0 0 0 0 0 0 6
0.7732 0.0052 1.2443 C 0 0 0 0 0 0 0 0 0 0 7
2.1631 0.0052 1.1565 C 0 0 0 0 0 0 0 0 0 0 8
2.8028 0.0043 -0.1044 C 0 0 0 0 0 0 0 0 0 0 9
-1.5475 0.0033 0.2119 C 0 0 0 0 0 0 0 0 0 0 10
4.1868 -0.0629 -0.2010 N 0 0 0 0 0 0 0 0 0 0 11
-2.2156 0.0048 -0.8868 O 0 0 0 0 0 0 0 0 0 0 12
-2.0623 -0.0002 1.3687 O 0 0 0 0 0 0 0 0 0 0 13
4.7106 0.2555 0.6113 H 0 0 0 0 0 0 0 0 0 0 14
4.5934 0.2580 -1.0767 H 0 0 0 0 0 0 0 0 0 0 15
2.4685 0.0088 -2.2478 H 0 0 0 0 0 0 0 0 0 0 16
-0.0092 0.0115 -2.0603 H 0 0 0 0 0 0 0 0 0 0 17
0.2890 0.0081 2.2227 H 0 0 0 0 0 0 0 0 0 0 18
2.7706 0.0062 2.0650 H 0 0 0 0 0 0 0 0 0 0 19
  2 1 0 0 0 0
  3 1 0 0 0 0
  5 4 0 0 0 0
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18 7 0 0 0 0
  9 8 0 0 0 0
11 9 0 0 0 0
12 10 0 0 0 0
13 10 0 0 0 0
14 11 0 0 0 0
15 11 0 0 0 0
  8 19 0 0 0 0
M END
$$$$
4-aminobenzoicacid.sdf
COSMOtherm 3D 0

20 19 0 0 0 0 0 0 0 0 V2000
-4.8277 -0.0075 0.5422 O 0 0 0 0 0 0 0 0 0 0 1
-5.1612 -0.5247 -0.2137 H 0 0 0 0 0 0 0 0 0 0 2
-5.1878 0.8876 0.4030 H 0 0 0 0 0 0 0 0 0 0 3
2.2290 0.0060 -1.1351 C 0 0 0 0 0 0 0 0 0 0 4
0.8500 0.0024 -1.2730 C 0 0 0 0 0 0 0 0 0 0 5
-0.0014 -0.0038 -0.1474 C 0 0 0 0 0 0 0 0 0 0 6
0.5916 -0.0070 1.1340 C 0 0 0 0 0 0 0 0 0 0 7
1.9702 -0.0034 1.2878 C 0 0 0 0 0 0 0 0 0 0 8
2.8248 0.0032 0.1540 C 0 0 0 0 0 0 0 0 0 0 9
-1.4626 -0.0057 -0.3472 C 0 0 0 0 0 0 0 0 0 0 10
4.1802 0.0067 0.2986 N 0 0 0 0 0 0 0 0 0 0 11
-2.0107 -0.0018 -1.4567 O 0 0 0 0 0 0 0 0 0 0 12
-2.1739 -0.0137 0.8036 O 0 0 0 0 0 0 0 0 0 0 13
4.6107 0.0074 1.2162 H 0 0 0 0 0 0 0 0 0 0 14
4.7944 0.0117 -0.5076 H 0 0 0 0 0 0 0 0 0 0 15
2.8694 0.0109 -2.0197 H 0 0 0 0 0 0 0 0 0 0 16
0.4053 0.0047 -2.2695 H 0 0 0 0 0 0 0 0 0 0 17
-0.0434 -0.0120 2.0204 H 0 0 0 0 0 0 0 0 0 0 18
2.4103 -0.0057 2.2873 H 0 0 0 0 0 0 0 0 0 0 19
-3.1666 -0.0083 0.5908 H 0 0 0 0 0 0 0 0 0 0 20
  2 1 0 0 0 0
  3 1 0 0 0 0
  5 4 0 0 0 0
  9 4 0 0 0 0
16 4 0 0 0 0
  6 5 0 0 0 0
17 5 0 0 0 0
  7 6 0 0 0 0
10 6 0 0 0 0
  8 7 0 0 0 0
18 7 0 0 0 0
  9 8 0 0 0 0
19 8 0 0 0 0
11 9 0 0 0 0
12 10 0 0 0 0
13 10 0 0 0 0
14 11 0 0 0 0
15 11 0 0 0 0
13 20 0 0 0 0
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1
2
3 M END
4 $$$$
5 4-bromobenzoicacid-anion.sdf
6 COSMOTHERM 3D 0
7
8 17 16 0 0 0 0 0 0 0 0 V2000
9 -6.2493 -0.0142 -0.5404 O 0 0 0 0 0 0 0 0 0 0 1
10 -5.2433 -0.0061 -0.6393 H 0 0 0 0 0 0 0 0 0 0 2
11 -6.3782 -0.0721 0.4220 H 0 0 0 0 0 0 0 0 0 0 3
12 0.6193 0.0067 -1.1810 C 0 0 0 0 0 0 0 0 0 0 4
13 -0.7769 0.0084 -1.1026 C 0 0 0 0 0 0 0 0 0 0 5
14 -1.4339 0.0048 0.1379 C 0 0 0 0 0 0 0 0 0 0 6
15 -0.6619 -0.0008 1.3102 C 0 0 0 0 0 0 0 0 0 0 7
16 0.7349 -0.0035 1.2572 C 0 0 0 0 0 0 0 0 0 0 8
17 1.3553 0.0005 0.0060 C 0 0 0 0 0 0 0 0 0 0 9
18 -2.9577 0.0071 0.2210 C 0 0 0 0 0 0 0 0 0 0 10
19 3.2848 -0.0027 -0.0851 Br 0 0 0 0 0 0 0 0 0 0 11
20 -3.5893 0.0032 -0.8930 O 0 0 0 0 0 0 0 0 0 0 12
21 -3.4863 0.0113 1.3673 O 0 0 0 0 0 0 0 0 0 0 13
22 1.1213 0.0096 -2.1487 H 0 0 0 0 0 0 0 0 0 0 14
23 -1.3719 0.0125 -2.0169 H 0 0 0 0 0 0 0 0 0 0 15
24 -1.1705 -0.0036 2.2754 H 0 0 0 0 0 0 0 0 0 0 16
25 1.3255 -0.0080 2.1735 H 0 0 0 0 0 0 0 0 0 0 17
26
27 2 1 0 0 0 0 0
28 3 1 0 0 0 0 0
29 5 4 0 0 0 0 0
30 9 4 0 0 0 0 0
31 14 4 0 0 0 0 0
32 6 5 0 0 0 0 0
33 15 5 0 0 0 0 0
34 7 6 0 0 0 0 0
35 10 6 0 0 0 0 0
36 8 7 0 0 0 0 0
37 16 7 0 0 0 0 0
38 9 8 0 0 0 0 0
39 11 9 0 0 0 0 0
40 12 10 0 0 0 0 0
41 13 10 0 0 0 0 0
42 8 17 0 0 0 0 0
43 M END
44 $$$$
45 4-bromobenzoicacid.sdf
46 COSMOTHERM 3D 0
47
48 18 17 0 0 0 0 0 0 0 0 V2000
49 -6.1691 -0.0241 0.6974 O 0 0 0 0 0 0 0 0 0 0 1
50 -6.5382 -0.6800 0.0775 H 0 0 0 0 0 0 0 0 0 0 2
51 -6.5623 0.8244 0.4215 H 0 0 0 0 0 0 0 0 0 0 3
52 0.7814 -0.0072 -1.2761 C 0 0 0 0 0 0 0 0 0 0 4
53 -0.6110 -0.0053 -1.3611 C 0 0 0 0 0 0 0 0 0 0 5
54 -1.4012 0.0028 -0.1998 C 0 0 0 0 0 0 0 0 0 0 6
55 -0.7771 0.0093 1.0593 C 0 0 0 0 0 0 0 0 0 0 7
56 0.6154 0.0086 1.1609 C 0 0 0 0 0 0 0 0 0 0 8
57 1.3754 0.0000 -0.0112 C 0 0 0 0 0 0 0 0 0 0 9
58 -2.8892 0.0061 -0.3455 C 0 0 0 0 0 0 0 0 0 0 10
59 3.2959 -0.0016 0.1195 Br 0 0 0 0 0 0 0 0 0 0 11
60 -3.4582 0.0191 -1.4376 O 0 0 0 0 0 0 0 0 0 0 12
-3.5410 -0.0070 0.8266 O 0 0 0 0 0 0 0 0 0 0 13
1.3899 -0.0145 -2.1797 H 0 0 0 0 0 0 0 0 0 0 14
-1.0957 -0.0100 -2.3380 H 0 0 0 0 0 0 0 0 0 0 15
-1.3795 0.0159 1.9672 H 0 0 0 0 0 0 0 0 0 0 16
1.0966 0.0148 2.1386 H 0 0 0 0 0 0 0 0 0 0 17
-4.5520 -0.0034 0.6700 H 0 0 0 0 0 0 0 0 0 0 18
2 1 0 0 0 0 0
3 1 0 0 0 0 0
5 4 0 0 0 0 0
9 4 0 0 0 0 0
14 4 0 0 0 0 0
6 5 0 0 0 0 0
15 5 0 0 0 0 0
7 6 0 0 0 0 0
10 6 0 0 0 0 0
8 7 0 0 0 0 0
16 7 0 0 0 0 0
9 8 0 0 0 0 0
17 8 0 0 0 0 0
11 9 0 0 0 0 0
12 10 0 0 0 0 0
13 10 0 0 0 0 0
13 18 0 0 0 0 0
M END
$$$$
4-butylbenzoicacid-anion.sdf
COSMOTHERM 3D 0
29 28 0 0 0 0 0 0 0 0 V2000
-6.1262 -0.6464 -0.5764 O 0 0 0 0 0 0 0 0 0 0 1
-5.1342 -0.7448 -0.3962 H 0 0 0 0 0 0 0 0 0 0 2
-6.2235 0.3100 -0.7258 H 0 0 0 0 0 0 0 0 0 0 3
0.6272 -1.0442 0.7500 C 0 0 0 0 0 0 0 0 0 0 4
-0.7450 -1.0409 0.4852 C 0 0 0 0 0 0 0 0 0 0 5
-1.4108 0.1511 0.1538 C 0 0 0 0 0 0 0 0 0 0 6
-0.6618 1.3379 0.0953 C 0 0 0 0 0 0 0 0 0 0 7
0.7103 1.3327 0.3587 C 0 0 0 0 0 0 0 0 0 0 8
1.3813 0.1420 0.6915 C 0 0 0 0 0 0 0 0 0 0 9
-2.9078 0.1681 -0.1292 C 0 0 0 0 0 0 0 0 0 0 10
2.8721 0.1314 0.9417 C 0 0 0 0 0 0 0 0 0 0 11
3.6984 -0.1219 -0.3366 C 0 0 0 0 0 0 0 0 0 0 12
5.2111 -0.1291 -0.0807 C 0 0 0 0 0 0 0 0 0 0 13
6.0339 -0.3842 -1.3480 C 0 0 0 0 0 0 0 0 0 0 14
-3.5165 -0.9596 -0.0749 O 0 0 0 0 0 0 0 0 0 0 15
-3.4516 1.2770 -0.3967 O 0 0 0 0 0 0 0 0 0 0 16
1.1236 -1.9821 1.0139 H 0 0 0 0 0 0 0 0 0 0 17
-1.3207 -1.9665 0.5384 H 0 0 0 0 0 0 0 0 0 0 18
-1.1747 2.2681 -0.1557 H 0 0 0 0 0 0 0 0 0 0 19
```

1	2.726	2.2694	0.3132	H	0	0	0	0	0	0	0	0	0	20
3	3.1152	-0.6477	1.6824	H	0	0	0	0	0	0	0	0	0	21
3	3.1782	1.0964	1.3779	H	0	0	0	0	0	0	0	0	0	22
3	3.4547	0.6525	-1.0840	H	0	0	0	0	0	0	0	0	0	23
3	3.3948	-1.0869	-0.7781	H	0	0	0	0	0	0	0	0	0	24
5	5.4460	-0.8995	0.6737	H	0	0	0	0	0	0	0	0	0	25
5	5.5069	0.8370	0.3636	H	0	0	0	0	0	0	0	0	0	26
7	7.1129	-0.3845	-1.1330	H	0	0	0	0	0	0	0	0	0	27
5	5.8436	0.3903	-2.1072	H	0	0	0	0	0	0	0	0	0	28
5	5.7820	-1.3584	-1.7958	H	0	0	0	0	0	0	0	0	0	29
2	1	0	0	0	0									
3	1	0	0	0	0									
5	4	0	0	0	0									
9	4	0	0	0	0									
17	4	0	0	0	0									
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27	14	0	0	0	0									
28	14	0	0	0	0									
14	29	0	0	0	0									
M END														
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4-butylbenzoicacid.sdf														
COSMOTHERM 3D 0														
30	29	0	0	0	0	0	0	0	0	V2000				
-6.0620	0.4963	0.8843	O	0	0	0	0	0	0	0	0	0	0	1
-6.5843	-0.2201	0.4799	H	0	0	0	0	0	0	0	0	0	0	2
-6.3339	1.2994	0.4043	H	0	0	0	0	0	0	0	0	0	0	3
0.7586	-0.2980	-1.3843	C	0	0	0	0	0	0	0	0	0	0	4
-0.6088	-0.0271	-1.4052	C	0	0	0	0	0	0	0	0	0	0	5
-1.3737	-0.1365	-0.2308	C	0	0	0	0	0	0	0	0	0	0	6
-0.7383	-0.5236	0.963												

URL: <http://mc.manuscriptcentral.com/tandf/tmph>

[illegible]

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4-chlorophenol.sdf
COSMOtherm 3D 0

16 15 0 0 0 0 0 0 0 0 0 V2000
1.0105 4.3857 -0.0118 O 0 0 0 0 0 0 0 0 0 0 0 1
1.6704 4.3586 -0.7281 H 0 0 0 0 0 0 0 0 0 0 0 2
1.5332 4.4803 0.8052 H 0 0 0 0 0 0 0 0 0 0 0 3
-1.6023 0.2789 -0.0011 C 0 0 0 0 0 0 0 0 0 0 0 4
-1.2902 -1.0816 -0.0020 C 0 0 0 0 0 0 0 0 0 0 0 5
0.0498 -1.4757 0.0007 C 0 0 0 0 0 0 0 0 0 0 0 6
1.0792 -0.5344 0.0056 C 0 0 0 0 0 0 0 0 0 0 0 7
0.7626 0.8275 0.0069 C 0 0 0 0 0 0 0 0 0 0 0 8
-0.5808 1.2457 0.0025 C 0 0 0 0 0 0 0 0 0 0 0 9
0.4505 -3.2096 -0.0021 Cl 0 0 0 0 0 0 0 0 0 0 0 10
-0.9482 2.5577 0.0016 O 0 0 0 0 0 0 0 0 0 0 0 11
-2.6445 0.6015 -0.0036 H 0 0 0 0 0 0 0 0 0 0 0 12
-2.0873 -1.8254 -0.0052 H 0 0 0 0 0 0 0 0 0 0 0 13
2.1223 -0.8512 0.0082 H 0 0 0 0 0 0 0 0 0 0 0 14
1.5661 1.5660 0.0119 H 0 0 0 0 0 0 0 0 0 0 0 15
-0.1456 3.1633 -0.0028 H 0 0 0 0 0 0 0 0 0 0 0 16
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
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12 4 0 0 0 0
6 5 0 0 0 0
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7 6 0 0 0 0
10 6 0 0 0 0
8 7 0 0 0 0
14 7 0 0 0 0
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15 8 0 0 0 0
11 9 0 0 0 0
11 16 0 0 0 0
M END
\$\$\$
4-cyanobenzoicacid-anion.sdf
COSMOtherm 3D 0

18 17 0 0 0 0 0 0 0 0 0 V2000
-5.2051 -0.4934 -0.0142 O 0 0 0 0 0 0 0 0 0 0 0 1
-4.2020 -0.6096 -0.0011 H 0 0 0 0 0 0 0 0 0 0 0 2
-5.3163 0.4712 -0.0751 H 0 0 0 0 0 0 0 0 0 0 0 3
1.6501 -1.2344 0.0021 C 0 0 0 0 0 0 0 0 0 0 0 4
0.2605 -1.1364 0.0052 C 0 0 0 0 0 0 0 0 0 0 0 5
-0.3737 0.1167 0.0044 C 0 0 0 0 0 0 0 0 0 0 0 6
0.4118 1.2811 0.0005 C 0 0 0 0 0 0 0 0 0 0 0 7
1.8024 1.2067 -0.0026 C 0 0 0 0 0 0 0 0 0 0 0 8
2.4277 -0.0576 -0.0017 C 0 0 0 0 0 0 0 0 0 0 0 9
-1.9009 0.2229 0.0076 C 0 0 0 0 0 0 0 0 0 0 0 10
3.8525 -0.1460 -0.0047 C 0 0 0 0 0 0 0 0 0 0 0 11
5.0184 -0.2175 -0.0067 N 0 0 0 0 0 0 0 0 0 0 0 12
-2.5439 -0.8824 0.0092 O 0 0 0 0 0 0 0 0 0 0 0 13
-2.4070 1.3776 0.0073 O 0 0 0 0 0 0 0 0 0 0 0 14
2.1387 -2.2092 0.0025 H 0 0 0 0 0 0 0 0 0 0 0 15
-0.3530 -2.0378 0.0079 H 0 0 0 0 0 0 0 0 0 0 0 16
-0.0880 2.2503 -0.0001 H 0 0 0 0 0 0 0 0 0 0 0 17
2.4076 2.1137 -0.0054 H 0 0 0 0 0 0 0 0 0 0 0 18
2 1 0 0 0 0
3 1 0 0 0 0
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10 6 0 0 0 0
8 7 0 0 0 0
17 7 0 0 0 0
9 8 0 0 0 0
11 9 0 0 0 0
13 10 0 0 0 0
14 10 0 0 0 0
12 11 0 0 0 0
8 18 0 0 0 0
M END
\$\$\$
4-cyanobenzoicacid.sdf
COSMOtherm 3D 0

19 18 0 0 0 0 0 0 0 0 0 V2000
-5.1214 0.0027 0.6330 O 0 0 0 0 0 0 0 0 0 0 0 1
-5.4905 -0.6689 0.0302 H 0 0 0 0 0 0 0 0 0 0 0 2
-5.4953 0.8474 0.3211 H 0 0 0 0 0 0 0 0 0 0 0 3
1.8509 -0.0038 -1.2035 C 0 0 0 0 0 0 0 0 0 0 0 4
0.4644 -0.0069 -1.3164 C 0 0 0 0 0 0 0 0 0 0 0 5
-0.3443 -0.0072 -0.1680 C 0 0 0 0 0 0 0 0 0 0 0 6
0.2494 -0.0045 1.1055 C 0 0 0 0 0 0 0 0 0 0 0 7
1.6359 -0.0007 1.2343 C 0 0 0 0 0 0 0 0 0 0 0 8
2.4403 0.0000 0.0772 C 0 0 0 0 0 0 0 0 0 0 0 9
-1.8346 -0.0045 -0.3449 C 0 0 0 0 0 0 0 0 0 0 0 10
3.8637 0.0053 0.2023 C 0 0 0 0 0 0 0 0 0 0 0 11
5.0266 0.0105 0.3036 N 0 0 0 0 0 0 0 0 0 0 0 12
-2.3737 0.0116 -1.4508 O 0 0 0 0 0 0 0 0 0 0 0 13
-2.5065 -0.0170 0.8113 O 0 0 0 0 0 0 0 0 0 0 0 14
2.4785 -0.0034 -2.0944 H 0 0 0 0 0 0 0 0 0 0 0 15
-0.0056 -0.0079 -2.2999 H 0 0 0 0 0 0 0 0 0 0 0 16
-0.3753 -0.0040 1.9977 H 0 0 0 0 0 0 0 0 0 0 0 17
2.0986 0.0027 2.2210 H 0 0 0 0 0 0 0 0 0 0 0 18
-3.5177 -0.0015 0.6378 H 0 0 0 0 0 0 0 0 0 0 0 19
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0


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9 4 0 0 0 0
16 4 0 0 0 0
6 5 0 0 0 0
17 5 0 0 0 0
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10 6 0 0 0 0
8 7 0 0 0 0
18 7 0 0 0 0
9 8 0 0 0 0
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11 9 0 0 0 0
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15 10 0 0 0 0
12 11 0 0 0 0
13 11 0 0 0 0
20 12 0 0 0 0
21 12 0 0 0 0
22 12 0 0 0 0
23 13 0 0 0 0
24 13 0 0 0 0
25 13 0 0 0 0
15 26 0 0 0 0
M END
$$$$
4-ethylbenzoicacid-anion.sdf
COSMOtherm 3D 0
23 22 0 0 0 0 0 0 0 0 0 V2000
-5.2314 -0.4470 0.2623 O 0 0 0 0 0 0 0 0 0 0 0 0 1
-4.2366 -0.6051 0.1597 H 0 0 0 0 0 0 0 0 0 0 0 0 2
-5.2850 0.5203 0.3499 H 0 0 0 0 0 0 0 0 0 0 0 0 3
1.7332 1.1979 -0.2249 C 0 0 0 0 0 0 0 0 0 0 0 0 4
0.3418 1.2723 -0.1242 C 0 0 0 0 0 0 0 0 0 0 0 0 5
-0.4424 0.1071 -0.1069 C 0 0 0 0 0 0 0 0 0 0 0 0 6
0.2078 -1.1350 -0.1939 C 0 0 0 0 0 0 0 0 0 0 0 0 7
1.6000 -1.2078 -0.2928 C 0 0 0 0 0 0 0 0 0 0 0 0 8
2.3889 -0.0434 -0.3110 C 0 0 0 0 0 0 0 0 0 0 0 0 9
-1.9595 0.1995 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 10
3.8979 -0.1233 -0.3785 C 0 0 0 0 0 0 0 0 0 0 0 0 11
4.5536 -0.1883 1.0149 C 0 0 0 0 0 0 0 0 0 0 0 0 12
-2.4818 1.3476 0.0811 O 0 0 0 0 0 0 0 0 0 0 0 0 13
-2.6062 -0.9077 0.0016 O 0 0 0 0 0 0 0 0 0 0 0 0 14
2.3233 2.1184 -0.2450 H 0 0 0 0 0 0 0 0 0 0 0 0 15
-0.1592 2.2402 -0.0630 H 0 0 0 0 0 0 0 0 0 0 0 0 16
-0.3946 -2.0450 -0.1869 H 0 0 0 0 0 0 0 0 0 0 0 0 17
2.0857 -2.1849 -0.3658 H 0 0 0 0 0 0 0 0 0 0 0 0 18
4.2860 0.7539 -0.9195 H 0 0 0 0 0 0 0 0 0 0 0 0 19
4.1916 -1.0130 -0.9575 H 0 0 0 0 0 0 0 0 0 0 0 0 20
5.6487 -0.2431 0.9272 H 0 0 0 0 0 0 0 0 0 0 0 0 21
4.2112 -1.0737 1.5711 H 0 0 0 0 0 0 0 0 0 0 0 0 22
4.3037 0.7024 1.6104 H 0 0 0 0 0 0 0 0 0 0 0 0 23
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
9 4 0 0 0 0
15 4 0 0 0 0
6 5 0 0 0 0
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7 6 0 0 0 0
10 6 0 0 0 0
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17 7 0 0 0 0
9 8 0 0 0 0
18 8 0 0 0 0
11 9 0 0 0 0
13 10 0 0 0 0
14 10 0 0 0 0
12 11 0 0 0 0
19 11 0 0 0 0
20 11 0 0 0 0
21 12 0 0 0 0
22 12 0 0 0 0
12 23 0 0 0 0
M END
$$$$
4-ethylbenzoicacid.sdf
COSMOtherm 3D 0
24 23 0 0 0 0 0 0 0 0 0 V2000
-5.1912 0.2092 0.6380 O 0 0 0 0 0 0 0 0 0 0 0 0 1
-5.6117 -0.5207 0.1474 H 0 0 0 0 0 0 0 0 0 0 0 0 2
-5.5033 1.0172 0.1909 H 0 0 0 0 0 0 0 0 0 0 0 0 3
1.7920 -0.2099 -1.2045 C 0 0 0 0 0 0 0 0 0 0 0 0 4
0.4073 -0.1021 -1.3228 C 0 0 0 0 0 0 0 0 0 0 0 0 5
-0.4064 -0.0974 -0.1764 C 0 0 0 0 0 0 0 0 0 0 0 0 6
0.1975 -0.2061 1.0892 C 0 0 0 0 0 0 0 0 0 0 0 0 7
1.5844 -0.3125 1.1984 C 0 0 0 0 0 0 0 0 0 0 0 0 8
2.4065 -0.3156 0.0568 C 0 0 0 0 0 0 0 0 0 0 0 0 9
-1.8837 0.0202 -0.3437 C 0 0 0 0 0 0 0 0 0 0 0 0 10
3.9105 -0.3891 0.1830 C 0 0 0 0 0 0 0 0 0 0 0 0 11
4.5599 1.0023 0.3201 C 0 0 0 0 0 0 0 0 0 0 0 0 12
-2.4359 0.1239 -1.4410 O 0 0 0 0 0 0 0 0 0 0 0 0 13
-2.5621 0.0052 0.8168 O 0 0 0 0 0 0 0 0 0 0 0 0 14
2.4099 -0.2183 -2.1056 H 0 0 0 0 0 0 0 0 0 0 0 0 15
-0.0600 -0.0245 -2.3055 H 0 0 0 0 0 0 0 0 0 0 0 0 16
-0.4218 -0.2101 1.9863 H 0 0 0 0 0 0 0 0 0 0 0 0 17
2.0395 -0.4014 2.1877 H 0 0 0 0 0 0 0 0 0 0 0 0 18
4.3260 -0.8976 -0.7006 H 0 0 0 0 0 0 0 0 0 0 0 0 19
4.1739 -0.9992 1.0608 H 0 0 0 0 0 0 0 0 0 0 0 0 20
5.6521 0.9109 0.4096 H 0 0 0 0 0 0 0 0 0 0 0 0 21
4.1866 1.5260 1.2125 H 0 0 0 0 0 0 0 0 0 0 0 0 22
4.3408 1.6286 -0.5572 H 0 0 0 0 0 0 0 0 0 0 0 0 23
-3.5632 0.0916 0.6380 H 0 0 0 0 0 0 0 0 0 0 0 0 24
2 1 0 0 0 0
3 1 0 0 0 0
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15 4 0 0 0 0
6 5 0 0 0 0
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7 6 0 0 0 0
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8 7 0 0 0 0
17 7 0 0 0 0
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14 10 0 0 0 0
12 11 0 0 0 0
19 11 0 0 0 0
20 11 0 0 0 0
21 12 0 0 0 0
22 12 0 0 0 0
23 12 0 0 0 0
14 24 0 0 0 0
M END
$$$$
4-fluorobenzoicacid-anion.sdf
COSMOtherm 3D 0

17 16 0 0 0 0 0 0 0 0 0 V2000
-4.9128 -0.4385 0.0394 O 0 0 0 0 0 0 0 0 0 0 1
-3.9098 -0.5722 0.0151 H 0 0 0 0 0 0 0 0 0 0 2
-5.0069 0.5297 0.0258 H 0 0 0 0 0 0 0 0 0 0 3
1.9284 -1.2710 -0.0047 C 0 0 0 0 0 0 0 0 0 0 4
0.5353 -1.1560 -0.0127 C 0 0 0 0 0 0 0 0 0 0 5
-0.0886 0.1028 -0.0093 C 0 0 0 0 0 0 0 0 0 0 6
0.7137 1.2560 0.0015 C 0 0 0 0 0 0 0 0 0 0 7
2.1083 1.1665 0.0104 C 0 0 0 0 0 0 0 0 0 0 8
2.6834 -0.1013 0.0067 C 0 0 0 0 0 0 0 0 0 0 9
-1.6079 0.2259 -0.0173 C 0 0 0 0 0 0 0 0 0 0 10
4.0507 -0.2020 0.0152 F 0 0 0 0 0 0 0 0 0 0 11
-2.2702 -0.8711 -0.0214 O 0 0 0 0 0 0 0 0 0 0 12
-2.1086 1.3851 -0.0193 O 0 0 0 0 0 0 0 0 0 0 13
2.4230 -2.2432 -0.0072 H 0 0 0 0 0 0 0 0 0 0 14
-0.0856 -2.0525 -0.0212 H 0 0 0 0 0 0 0 0 0 0 15
0.2279 2.2326 0.0037 H 0 0 0 0 0 0 0 0 0 0 16
2.7394 2.0560 0.0194 H 0 0 0 0 0 0 0 0 0 0 17
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
9 4 0 0 0 0
14 4 0 0 0 0
6 5 0 0 0 0
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10 6 0 0 0 0
8 7 0 0 0 0
16 7 0 0 0 0
9 8 0 0 0 0
11 9 0 0 0 0
12 10 0 0 0 0
13 10 0 0 0 0
8 17 0 0 0 0
M END
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4-fluorobenzoicacid.sdf
COSMOtherm 3D 0

18 17 0 0 0 0 0 0 0 0 0 V2000
-4.8584 -0.0236 0.5657 O 0 0 0 0 0 0 0 0 0 0 1
-5.2027 -0.6683 -0.0794 H 0 0 0 0 0 0 0 0 0 0 2
-5.2480 0.8281 0.2951 H 0 0 0 0 0 0 0 0 0 0 3
2.1663 0.0004 -1.1453 C 0 0 0 0 0 0 0 0 0 0 4
0.7790 0.0029 -1.2837 C 0 0 0 0 0 0 0 0 0 0 5
-0.0555 0.0030 -0.1522 C 0 0 0 0 0 0 0 0 0 0 6
0.5187 0.0009 1.1319 C 0 0 0 0 0 0 0 0 0 0 7
1.9054 -0.0018 1.2880 C 0 0 0 0 0 0 0 0 0 0 8
2.6977 -0.0019 0.1425 C 0 0 0 0 0 0 0 0 0 0 9
-1.5348 0.0053 -0.3554 C 0 0 0 0 0 0 0 0 0 0 10
4.0549 -0.0046 0.2877 F 0 0 0 0 0 0 0 0 0 0 11
-2.0633 0.0027 -1.4682 O 0 0 0 0 0 0 0 0 0 0 12
-2.2336 0.0090 0.7908 O 0 0 0 0 0 0 0 0 0 0 13
2.8265 0.0005 -2.0127 H 0 0 0 0 0 0 0 0 0 0 14
0.3300 0.0052 -2.2771 H 0 0 0 0 0 0 0 0 0 0 15
-0.1208 0.0012 2.0138 H 0 0 0 0 0 0 0 0 0 0 16
2.3674 -0.0037 2.2755 H 0 0 0 0 0 0 0 0 0 0 17
-3.2365 0.0080 0.5940 H 0 0 0 0 0 0 0 0 0 0 18
2 1 0 0 0 0
3 1 0 0 0 0
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14 4 0 0 0 0
6 5 0 0 0 0
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16 7 0 0 0 0
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11 9 0 0 0 0
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13 10 0 0 0 0
13 18 0 0 0 0
M END
$$$$
4-hydroxybenzoicacid-anion.sdf
COSMOtherm 3D 0
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URL: <http://mc.manuscriptcentral.com/tandf/tmph>

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4.1368 -1.0803 0.9099 H 0 0 0 0 0 0 0 0 0 0 0 20
4.2392 0.7060 0.9662 H 0 0 0 0 0 0 0 0 0 0 0 21
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
9 4 0 0 0 0
16 4 0 0 0 0
6 5 0 0 0 0
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8 7 0 0 0 0
18 7 0 0 0 0
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19 8 0 0 0 0
11 9 0 0 0 0
13 10 0 0 0 0
14 10 0 0 0 0
12 11 0 0 0 0
20 11 0 0 0 0
15 12 0 0 0 0
11 21 0 0 0 0
M END
$$$$
4-hydroxymethylbenzoicacid.sdf
COSMOtherm 3D 0
22 21 0 0 0 0 0 0 0 0 0 V2000
-5.2315 0.2116 0.6140 O 0 0 0 0 0 0 0 0 0 0 0 1
-5.6667 -0.5638 0.2128 H 0 0 0 0 0 0 0 0 0 0 0 2
-5.5481 0.9703 0.0891 H 0 0 0 0 0 0 0 0 0 0 0 3
1.7589 -0.2420 -1.1766 C 0 0 0 0 0 0 0 0 0 0 0 4
0.3755 -0.1350 -1.3082 C 0 0 0 0 0 0 0 0 0 0 0 5
-0.4436 -0.0960 -0.1664 C 0 0 0 0 0 0 0 0 0 0 0 6
0.1458 -0.1669 1.1075 C 0 0 0 0 0 0 0 0 0 0 0 7
1.5324 -0.2722 1.2312 C 0 0 0 0 0 0 0 0 0 0 0 8
2.3546 -0.3115 0.0941 C 0 0 0 0 0 0 0 0 0 0 0 9
-1.9229 0.0161 -0.3494 C 0 0 0 0 0 0 0 0 0 0 0 10
3.8532 -0.3921 0.2315 C 0 0 0 0 0 0 0 0 0 0 0 11
4.3848 0.9563 0.1870 O 0 0 0 0 0 0 0 0 0 0 0 12
-2.4611 0.1094 -1.4537 O 0 0 0 0 0 0 0 0 0 0 0 13
-2.6100 0.0070 0.8036 O 0 0 0 0 0 0 0 0 0 0 0 14
5.3553 0.8795 0.2432 H 0 0 0 0 0 0 0 0 0 0 0 15
2.3868 -0.2778 -2.0695 H 0 0 0 0 0 0 0 0 0 0 0 16
-0.0861 -0.0848 -2.2952 H 0 0 0 0 0 0 0 0 0 0 0 17
-0.4821 -0.1411 1.9978 H 0 0 0 0 0 0 0 0 0 0 0 18
1.9835 -0.3285 2.2242 H 0 0 0 0 0 0 0 0 0 0 0 19
4.2757 -0.9913 -0.5926 H 0 0 0 0 0 0 0 0 0 0 0 20
4.1198 -0.8742 1.1869 H 0 0 0 0 0 0 0 0 0 0 0 21
-3.6112 0.0892 0.6175 H 0 0 0 0 0 0 0 0 0 0 0 22
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
9 4 0 0 0 0
16 4 0 0 0 0
6 5 0 0 0 0
17 5 0 0 0 0
7 6 0 0 0 0
10 6 0 0 0 0
8 7 0 0 0 0
18 7 0 0 0 0
9 8 0 0 0 0
19 8 0 0 0 0
11 9 0 0 0 0
13 10 0 0 0 0
14 10 0 0 0 0
12 11 0 0 0 0
20 11 0 0 0 0
21 11 0 0 0 0
15 12 0 0 0 0
14 22 0 0 0 0
M END
$$$$
4-iodobenzoicacid-anion.sdf
COSMOtherm 3D 0
17 15 0 0 0 0 0 0 0 0 0 V2000
-6.9293 -0.5578 -0.0118 O 0 0 0 0 0 0 0 0 0 0 0 1
-5.9231 -0.6601 0.0040 H 0 0 0 0 0 0 0 0 0 0 0 2
-7.0525 0.4056 -0.0668 H 0 0 0 0 0 0 0 0 0 0 0 3
-0.0581 -1.1612 0.0026 C 0 0 0 0 0 0 0 0 0 0 0 4
-1.4554 -1.0928 0.0041 C 0 0 0 0 0 0 0 0 0 0 0 5
-2.1211 0.1427 0.0035 C 0 0 0 0 0 0 0 0 0 0 0 6
-1.3572 1.3200 0.0015 C 0 0 0 0 0 0 0 0 0 0 0 7
0.0407 1.2764 0.0001 C 0 0 0 0 0 0 0 0 0 0 0 8
0.6728 0.0300 0.0007 C 0 0 0 0 0 0 0 0 0 0 0 9
-3.6461 0.2150 0.0055 C 0 0 0 0 0 0 0 0 0 0 0 10
2.8149 -0.0567 -0.0014 I 0 0 0 0 0 0 0 0 0 0 0 11
-4.2691 -0.9036 0.0081 O 0 0 0 0 0 0 0 0 0 0 0 12
-4.1827 1.3575 0.0043 O 0 0 0 0 0 0 0 0 0 0 0 13
0.4441 -2.1288 0.0031 H 0 0 0 0 0 0 0 0 0 0 0 14
-2.0435 -2.0116 0.0057 H 0 0 0 0 0 0 0 0 0 0 0 15
-1.8718 2.2821 0.0013 H 0 0 0 0 0 0 0 0 0 0 0 16
0.6187 2.2006 -0.0013 H 0 0 0 0 0 0 0 0 0 0 0 17
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
9 4 0 0 0 0
14 4 0 0 0 0
6 5 0 0 0 0
15 5 0 0 0 0
7 6 0 0 0 0
10 6 0 0 0 0
8 7 0 0 0 0
16 7 0 0 0 0
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9 8 0 0 0 0
12 10 0 0 0 0
13 10 0 0 0 0
8 17 0 0 0 0
M END
$$$$
4-iodobenzoicacid.sdf
COSMOTHERM 3D 0

18 16 0 0 0 0 0 0 0 0 0 V2000
-6.8490 -0.0028 0.7379 O 0 0 0 0 0 0 0 0 0 0 0 1
-7.2459 -0.6559 0.1328 H 0 0 0 0 0 0 0 0 0 0 0 2
-7.2347 0.8507 0.4674 H 0 0 0 0 0 0 0 0 0 0 0 3
0.0854 -0.0066 -1.3053 C 0 0 0 0 0 0 0 0 0 0 0 4
-1.3083 -0.0077 -1.3791 C 0 0 0 0 0 0 0 0 0 0 0 5
-2.0887 -0.0051 -0.2115 C 0 0 0 0 0 0 0 0 0 0 0 6
-1.4538 -0.0017 1.0419 C 0 0 0 0 0 0 0 0 0 0 0 7
-0.0599 0.0003 1.1316 C 0 0 0 0 0 0 0 0 0 0 0 8
0.6936 -0.0022 -0.0460 C 0 0 0 0 0 0 0 0 0 0 0 9
-3.5783 -0.0018 -0.3442 C 0 0 0 0 0 0 0 0 0 0 0 10
2.8277 0.0016 0.0815 I 0 0 0 0 0 0 0 0 0 0 0 11
-4.1566 0.0153 -1.4315 O 0 0 0 0 0 0 0 0 0 0 0 12
-4.2197 -0.0175 0.8332 O 0 0 0 0 0 0 0 0 0 0 0 13
0.6804 -0.0092 -2.2181 H 0 0 0 0 0 0 0 0 0 0 0 14
-1.8007 -0.0101 -2.3523 H 0 0 0 0 0 0 0 0 0 0 0 15
-2.0482 0.0009 1.9553 H 0 0 0 0 0 0 0 0 0 0 0 16
0.4231 0.0044 2.1083 H 0 0 0 0 0 0 0 0 0 0 0 17
-5.2322 -0.0065 0.6862 H 0 0 0 0 0 0 0 0 0 0 0 18
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
9 4 0 0 0 0
14 4 0 0 0 0
6 5 0 0 0 0
15 5 0 0 0 0
7 6 0 0 0 0
10 6 0 0 0 0
8 7 0 0 0 0
16 7 0 0 0 0
9 8 0 0 0 0
17 8 0 0 0 0
12 10 0 0 0 0
13 10 0 0 0 0
13 18 0 0 0 0
M END
$$$$
4-methoxybenzoicacid-anion.sdf
COSMOTHERM 3D 0

21 20 0 0 0 0 0 0 0 0 0 V2000
-5.2950 0.0169 0.2474 O 0 0 0 0 0 0 0 0 0 0 0 1
-4.3024 -0.0005 0.4529 H 0 0 0 0 0 0 0 0 0 0 0 2
-5.3121 0.0449 -0.7250 H 0 0 0 0 0 0 0 0 0 0 0 3
1.4933 0.0002 1.4062 C 0 0 0 0 0 0 0 0 0 0 0 4
0.1116 -0.0032 1.2402 C 0 0 0 0 0 0 0 0 0 0 0 5
-0.4688 -0.0045 -0.0427 C 0 0 0 0 0 0 0 0 0 0 0 6
0.3868 -0.0034 -1.1536 C 0 0 0 0 0 0 0 0 0 0 0 7
1.7782 -0.0002 -1.0097 C 0 0 0 0 0 0 0 0 0 0 0 8
2.3377 0.0014 0.2791 C 0 0 0 0 0 0 0 0 0 0 0 9
-1.9769 -0.0075 -0.2282 C 0 0 0 0 0 0 0 0 0 0 0 10
3.6835 0.0043 0.5390 O 0 0 0 0 0 0 0 0 0 0 0 11
4.5853 0.0067 -0.5855 C 0 0 0 0 0 0 0 0 0 0 0 12
-2.6885 -0.0120 0.8401 O 0 0 0 0 0 0 0 0 0 0 0 13
-2.4351 -0.0052 -1.4068 O 0 0 0 0 0 0 0 0 0 0 0 14
1.9410 0.0019 2.4019 H 0 0 0 0 0 0 0 0 0 0 0 15
-0.5425 -0.0040 2.1134 H 0 0 0 0 0 0 0 0 0 0 0 16
-0.0540 -0.0041 -2.1519 H 0 0 0 0 0 0 0 0 0 0 0 17
2.4108 0.0008 -1.8966 H 0 0 0 0 0 0 0 0 0 0 0 18
5.5915 0.0093 -0.1542 H 0 0 0 0 0 0 0 0 0 0 0 19
4.4505 -0.8939 -1.2035 H 0 0 0 0 0 0 0 0 0 0 0 20
4.4458 0.9064 -1.2037 H 0 0 0 0 0 0 0 0 0 0 0 21
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
9 4 0 0 0 0
15 4 0 0 0 0
6 5 0 0 0 0
16 5 0 0 0 0
7 6 0 0 0 0
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11 9 0 0 0 0
13 10 0 0 0 0
14 10 0 0 0 0
12 11 0 0 0 0
19 12 0 0 0 0
20 12 0 0 0 0
12 21 0 0 0 0
M END
$$$$
4-methoxybenzoicacid.sdf
COSMOTHERM 3D 0

22 21 0 0 0 0 0 0 0 0 0 V2000
-5.1836 -0.0015 0.8186 O 0 0 0 0 0 0 0 0 0 0 0 1
-5.5860 -0.6814 0.2478 H 0 0 0 0 0 0 0 0 0 0 0 2
-5.5631 0.8393 0.5036 H 0 0 0 0 0 0 0 0 0 0 0 3
1.7072 -0.0077 -1.3933 C 0 0 0 0 0 0 0 0 0 0 0 4
0.3207 -0.0069 -1.4318 C 0 0 0 0 0 0 0 0 0 0 0 5
-0.4358 -0.0021 -0.2416 C 0 0 0 0 0 0 0 0 0 0 0 6
0.2425 0.0032 0.9888 C 0 0 0 0 0 0 0 0 0 0 0 7
1.6371 0.0033 1.0436 C 0 0 0 0 0 0 0 0 0 0 0 8
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2.3775 -0.0024 -0.1525 C 0 0 0 0 0 0 0 0 0 0 0 9
-1.9181 -0.0003 -0.3306 C 0 0 0 0 0 0 0 0 0 0 0 10
3.7391 -0.0042 -0.2143 O 0 0 0 0 0 0 0 0 0 0 0 11
4.4760 0.0124 1.0279 C 0 0 0 0 0 0 0 0 0 0 0 12
-2.5370 0.0218 -1.3985 O 0 0 0 0 0 0 0 0 0 0 0 13
-2.5346 -0.0273 0.8662 O 0 0 0 0 0 0 0 0 0 0 0 14
2.2951 -0.0125 -2.3123 H 0 0 0 0 0 0 0 0 0 0 0 15
-0.1985 -0.0102 -2.3911 H 0 0 0 0 0 0 0 0 0 0 0 16
-0.3252 0.0074 1.9193 H 0 0 0 0 0 0 0 0 0 0 0 17
2.1347 0.0080 2.0122 H 0 0 0 0 0 0 0 0 0 0 0 18
5.5317 0.0148 0.7392 H 0 0 0 0 0 0 0 0 0 0 0 19
4.2476 0.9185 1.6081 H 0 0 0 0 0 0 0 0 0 0 0 20
4.2569 -0.8834 1.6272 H 0 0 0 0 0 0 0 0 0 0 0 21
-3.5448 -0.0171 0.7358 H 0 0 0 0 0 0 0 0 0 0 0 22
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
9 4 0 0 0 0
15 4 0 0 0 0
6 5 0 0 0 0
16 5 0 0 0 0
7 6 0 0 0 0
10 6 0 0 0 0
8 7 0 0 0 0
17 7 0 0 0 0
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11 9 0 0 0 0
13 10 0 0 0 0
14 10 0 0 0 0
12 11 0 0 0 0
19 12 0 0 0 0
20 12 0 0 0 0
21 12 0 0 0 0
14 22 0 0 0 0
M END
$$$$
4-methylaminobenzoicacid-anion.sdf
COSMOTHERM 3D 0
22 21 0 0 0 0 0 0 0 0 0 V2000
-5.2730 -0.2012 0.0272 O 0 0 0 0 0 0 0 0 0 0 0 1
-4.2862 -0.4420 0.0178 H 0 0 0 0 0 0 0 0 0 0 0 2
-5.2481 0.7716 0.0300 H 0 0 0 0 0 0 0 0 0 0 0 3
1.4991 -1.4168 -0.0013 C 0 0 0 0 0 0 0 0 0 0 0 4
0.1197 -1.2515 0.0078 C 0 0 0 0 0 0 0 0 0 0 0 5
-0.4699 0.0295 -0.0098 C 0 0 0 0 0 0 0 0 0 0 0 6
0.3912 1.1395 -0.0336 C 0 0 0 0 0 0 0 0 0 0 0 7
1.7787 0.9967 -0.0420 C 0 0 0 0 0 0 0 0 0 0 0 8
2.3659 -0.2926 -0.0317 C 0 0 0 0 0 0 0 0 0 0 0 9
-1.9707 0.2124 -0.0006 C 0 0 0 0 0 0 0 0 0 0 0 10
3.7299 -0.4766 -0.0816 N 0 0 0 0 0 0 0 0 0 0 0 11
4.6838 0.6053 0.1117 C 0 0 0 0 0 0 0 0 0 0 0 12
-2.6878 -0.8558 0.0069 O 0 0 0 0 0 0 0 0 0 0 0 13
-2.4363 1.3908 -0.0012 O 0 0 0 0 0 0 0 0 0 0 0 14
4.0606 -1.4096 0.1466 H 0 0 0 0 0 0 0 0 0 0 0 15
1.9322 -2.4205 0.0129 H 0 0 0 0 0 0 0 0 0 0 0 16
-0.5317 -2.1271 0.0319 H 0 0 0 0 0 0 0 0 0 0 0 17
-0.0498 2.1382 -0.0414 H 0 0 0 0 0 0 0 0 0 0 0 18
2.4105 1.8853 -0.0569 H 0 0 0 0 0 0 0 0 0 0 0 19
5.6956 0.1862 0.0730 H 0 0 0 0 0 0 0 0 0 0 0 20
4.5967 1.3560 -0.6887 H 0 0 0 0 0 0 0 0 0 0 0 21
4.5538 1.1202 1.0810 H 0 0 0 0 0 0 0 0 0 0 0 22
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
9 4 0 0 0 0
16 4 0 0 0 0
6 5 0 0 0 0
17 5 0 0 0 0
7 6 0 0 0 0
10 6 0 0 0 0
8 7 0 0 0 0
18 7 0 0 0 0
9 8 0 0 0 0
19 8 0 0 0 0
11 9 0 0 0 0
13 10 0 0 0 0
14 10 0 0 0 0
12 11 0 0 0 0
15 11 0 0 0 0
20 12 0 0 0 0
21 12 0 0 0 0
12 22 0 0 0 0
M END
$$$$
4-methylaminobenzoicacid.sdf
COSMOTHERM 3D 0
23 22 0 0 0 0 0 0 0 0 0 V2000
-5.1921 -0.0057 0.8235 O 0 0 0 0 0 0 0 0 0 0 0 1
-5.5839 -0.5868 0.1459 H 0 0 0 0 0 0 0 0 0 0 0 2
-5.5661 0.8747 0.6353 H 0 0 0 0 0 0 0 0 0 0 0 3
1.7063 -0.0047 -1.4106 C 0 0 0 0 0 0 0 0 0 0 0 4
0.3236 -0.0049 -1.4378 C 0 0 0 0 0 0 0 0 0 0 0 5
-0.4352 -0.0038 -0.2444 C 0 0 0 0 0 0 0 0 0 0 0 6
0.2602 -0.0010 0.9820 C 0 0 0 0 0 0 0 0 0 0 0 7
1.6491 0.0011 1.0280 C 0 0 0 0 0 0 0 0 0 0 0 8
2.4098 -0.0010 -0.1723 C 0 0 0 0 0 0 0 0 0 0 0 9
-1.9067 -0.0022 -0.3247 C 0 0 0 0 0 0 0 0 0 0 0 10
3.7724 -0.0009 -0.1627 N 0 0 0 0 0 0 0 0 0 0 0 11
4.5916 0.0110 1.0382 C 0 0 0 0 0 0 0 0 0 0 0 12
-2.5430 0.0185 -1.3864 O 0 0 0 0 0 0 0 0 0 0 0 13
-2.5240 -0.0278 0.8795 O 0 0 0 0 0 0 0 0 0 0 0 14
4.2493 0.0047 -1.0585 H 0 0 0 0 0 0 0 0 0 0 0 15
```

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2.2741 -0.0067 -2.3441 H 0 0 0 0 0 0 0 0 0 0 0 16
-0.2001 -0.0066 -2.3954 H 0 0 0 0 0 0 0 0 0 0 0 17
-0.3012 0.0010 1.9170 H 0 0 0 0 0 0 0 0 0 0 0 18
2.1541 0.0056 1.9939 H 0 0 0 0 0 0 0 0 0 0 0 19
5.6445 -0.0012 0.7368 H 0 0 0 0 0 0 0 0 0 0 0 20
4.4147 0.9145 1.6446 H 0 0 0 0 0 0 0 0 0 0 0 21
4.4016 -0.8724 1.6691 H 0 0 0 0 0 0 0 0 0 0 0 22
-3.5298 -0.0129 0.7445 H 0 0 0 0 0 0 0 0 0 0 0 23
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
9 4 0 0 0 0
16 4 0 0 0 0
6 5 0 0 0 0
17 5 0 0 0 0
7 6 0 0 0 0
10 6 0 0 0 0
8 7 0 0 0 0
18 7 0 0 0 0
9 8 0 0 0 0
19 8 0 0 0 0
11 9 0 0 0 0
13 10 0 0 0 0
14 10 0 0 0 0
12 11 0 0 0 0
15 11 0 0 0 0
20 12 0 0 0 0
21 12 0 0 0 0
22 12 0 0 0 0
14 23 0 0 0 0
M END
$$$$
4-methylbenzoicacid-anion.sdf
COSMOTHERM 3D 0
20 19 0 0 0 0 0 0 0 0 0 V2000
-4.8384 -0.0034 -0.4293 O 0 0 0 0 0 0 0 0 0 0 0 1
-3.8348 0.0002 -0.5695 H 0 0 0 0 0 0 0 0 0 0 0 2
-4.9240 -0.0094 0.5398 H 0 0 0 0 0 0 0 0 0 0 0 3
2.0063 -0.0082 -1.2579 C 0 0 0 0 0 0 0 0 0 0 0 4
0.6124 -0.0019 -1.1570 C 0 0 0 0 0 0 0 0 0 0 0 5
-0.0181 0.0003 0.0979 C 0 0 0 0 0 0 0 0 0 0 0 6
0.7892 -0.0064 1.2474 C 0 0 0 0 0 0 0 0 0 0 0 7
2.1822 -0.0131 1.1453 C 0 0 0 0 0 0 0 0 0 0 0 8
2.8181 -0.0102 -0.1094 C 0 0 0 0 0 0 0 0 0 0 0 9
4.3228 0.0167 -0.2178 C 0 0 0 0 0 0 0 0 0 0 0 10
-1.5366 0.0050 0.2201 C 0 0 0 0 0 0 0 0 0 0 0 11
-2.2018 0.0035 -0.8763 O 0 0 0 0 0 0 0 0 0 0 0 12
-2.0409 0.0105 1.3789 O 0 0 0 0 0 0 0 0 0 0 0 13
2.4759 -0.0140 -2.2452 H 0 0 0 0 0 0 0 0 0 0 0 14
-0.0063 -0.0023 -2.0561 H 0 0 0 0 0 0 0 0 0 0 0 15
0.3049 -0.0102 2.2256 H 0 0 0 0 0 0 0 0 0 0 0 16
2.7898 -0.0229 2.0541 H 0 0 0 0 0 0 0 0 0 0 0 17
4.6974 1.0536 -0.2087 H 0 0 0 0 0 0 0 0 0 0 0 18
4.6670 -0.4457 -1.1533 H 0 0 0 0 0 0 0 0 0 0 0 19
4.7956 -0.5065 0.6251 H 0 0 0 0 0 0 0 0 0 0 0 20
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
9 4 0 0 0 0
14 4 0 0 0 0
6 5 0 0 0 0
15 5 0 0 0 0
7 6 0 0 0 0
11 6 0 0 0 0
8 7 0 0 0 0
16 7 0 0 0 0
9 8 0 0 0 0
17 8 0 0 0 0
10 9 0 0 0 0
18 10 0 0 0 0
19 10 0 0 0 0
12 11 0 0 0 0
13 11 0 0 0 0
10 20 0 0 0 0
M END
$$$$
4-methylbenzoicacid.sdf
COSMOTHERM 3D 0
21 20 0 0 0 0 0 0 0 0 0 V2000
-4.7971 -0.0001 0.5584 O 0 0 0 0 0 0 0 0 0 0 0 1
-5.1508 -0.5968 -0.1265 H 0 0 0 0 0 0 0 0 0 0 0 2
-5.1632 0.8752 0.3345 H 0 0 0 0 0 0 0 0 0 0 0 3
2.2418 -0.0039 -1.1225 C 0 0 0 0 0 0 0 0 0 0 0 4
0.8563 -0.0021 -1.2745 C 0 0 0 0 0 0 0 0 0 0 0 5
0.0160 -0.0045 -0.1475 C 0 0 0 0 0 0 0 0 0 0 0 6
0.5959 -0.0117 1.1337 C 0 0 0 0 0 0 0 0 0 0 0 7
1.9835 -0.0135 1.2771 C 0 0 0 0 0 0 0 0 0 0 0 8
2.8320 -0.0059 0.1550 C 0 0 0 0 0 0 0 0 0 0 0 9
4.3299 0.0253 0.3160 C 0 0 0 0 0 0 0 0 0 0 0 10
-1.4611 -0.0036 -0.3509 C 0 0 0 0 0 0 0 0 0 0 0 11
-1.9938 0.0018 -1.4629 O 0 0 0 0 0 0 0 0 0 0 0 12
-2.1638 -0.0096 0.7953 O 0 0 0 0 0 0 0 0 0 0 0 13
2.8801 -0.0064 -2.0089 H 0 0 0 0 0 0 0 0 0 0 0 14
0.4095 -0.0019 -2.2697 H 0 0 0 0 0 0 0 0 0 0 0 15
-0.0425 -0.0190 2.0172 H 0 0 0 0 0 0 0 0 0 0 0 16
2.4192 -0.0234 2.2788 H 0 0 0 0 0 0 0 0 0 0 0 17
4.6910 1.0655 0.3694 H 0 0 0 0 0 0 0 0 0 0 0 18
4.8352 -0.4524 -0.5344 H 0 0 0 0 0 0 0 0 0 0 0 19
4.6452 -0.4767 1.2411 H 0 0 0 0 0 0 0 0 0 0 0 20
-3.1638 -0.0022 0.5934 H 0 0 0 0 0 0 0 0 0 0 0 21
2 1 0 0 0 0
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5 4 0 0 0 0
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  9  4  0  0  0  0
 14  4  0  0  0  0
   6  5  0  0  0  0
 15  5  0  0  0  0
   7  6  0  0  0  0
 11  6  0  0  0  0
   8  7  0  0  0  0
 16  7  0  0  0  0
   9  8  0  0  0  0
 17  8  0  0  0  0
 10  9  0  0  0  0
 18 10  0  0  0  0
 19 10  0  0  0  0
 20 10  0  0  0  0
 12 11  0  0  0  0
 13 11  0  0  0  0
 13 21  0  0  0  0
M  END
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4-nitrobenzoicacid-anion.sdf
COSMOtherm      3D      0

19 18  0  0  0  0  0  0  0  0  0  0 V2000
-5.6415 -0.5179  0.0209 O  0  0  0  0  0  0  0  0  0  0  1
-4.6376 -0.6212  0.0045 H  0  0  0  0  0  0  0  0  0  0  2
-5.7662  0.4459  0.0639 H  0  0  0  0  0  0  0  0  0  0  3
 1.3619  1.2328  0.0008 C  0  0  0  0  0  0  0  0  0  0  4
-0.0295  1.3012 -0.0031 C  0  0  0  0  0  0  0  0  0  0  5
-0.8095  0.1322 -0.0052 C  0  0  0  0  0  0  0  0  0  0  6
-0.1703 -1.1193 -0.0037 C  0  0  0  0  0  0  0  0  0  0  7
 1.2201 -1.2111 -0.0008 C  0  0  0  0  0  0  0  0  0  0  8
 1.9675 -0.0283  0.0014 C  0  0  0  0  0  0  0  0  0  0  9
-2.3382  0.2317 -0.0098 C  0  0  0  0  0  0  0  0  0  0 10
 3.4386 -0.1138  0.0040 N  0  0  0  0  0  0  0  0  0  0 11
 3.9644 -1.2394 -0.0060 O  0  0  0  0  0  0  0  0  0  0 12
 4.0914  0.9432  0.0158 O  0  0  0  0  0  0  0  0  0  0 13
-2.8476  1.3843 -0.0143 O  0  0  0  0  0  0  0  0  0  0 14
-2.9741 -0.8772 -0.0085 O  0  0  0  0  0  0  0  0  0  0 15
 1.9724  2.1344  0.0024 H  0  0  0  0  0  0  0  0  0  0 16
-0.5329  2.2682 -0.0045 H  0  0  0  0  0  0  0  0  0  0 17
-0.7794 -2.0232 -0.0049 H  0  0  0  0  0  0  0  0  0  0 18
 1.7232 -2.1767  0.0002 H  0  0  0  0  0  0  0  0  0  0 19
 2  1  0  0  0  0
 3  1  0  0  0  0
 5  4  0  0  0  0
 9  4  0  0  0  0
16  4  0  0  0  0
 6  5  0  0  0  0
17  5  0  0  0  0
 7  6  0  0  0  0
10  6  0  0  0  0
 8  7  0  0  0  0
18  7  0  0  0  0
 9  8  0  0  0  0
11  9  0  0  0  0
14 10  0  0  0  0
15 10  0  0  0  0
12 11  0  0  0  0
13 11  0  0  0  0
 8 19  0  0  0  0
M  END
$$$$
4-nitrobenzoicacid.sdf
COSMOtherm      3D      0

20 19  0  0  0  0  0  0  0  0  0  0 V2000
-5.5407 -0.0020  0.6619 O  0  0  0  0  0  0  0  0  0  0  1
-5.9135 -0.7433  0.1502 H  0  0  0  0  0  0  0  0  0  0  2
-5.9294  0.7980  0.2629 H  0  0  0  0  0  0  0  0  0  0  3
 1.4079  0.0006 -1.2406 C  0  0  0  0  0  0  0  0  0  0  4
 0.0196 -0.0005 -1.3452 C  0  0  0  0  0  0  0  0  0  0  5
-0.7809 -0.0009 -0.1902 C  0  0  0  0  0  0  0  0  0  0  6
-0.1792 -0.0011  1.0800 C  0  0  0  0  0  0  0  0  0  0  7
 1.2088 -0.0015  1.1995 C  0  0  0  0  0  0  0  0  0  0  8
 1.9787 -0.0001  0.0349 C  0  0  0  0  0  0  0  0  0  0  9
-2.2749 -0.0010 -0.3541 C  0  0  0  0  0  0  0  0  0  0 10
 3.4541  0.0006  0.1569 N  0  0  0  0  0  0  0  0  0  0 11
 3.9459 -0.0139  1.2956 O  0  0  0  0  0  0  0  0  0  0 12
 4.1284  0.0154 -0.8831 O  0  0  0  0  0  0  0  0  0  0 13
-2.8217 -0.0128 -1.4563 O  0  0  0  0  0  0  0  0  0  0 14
-2.9330  0.0123  0.8087 O  0  0  0  0  0  0  0  0  0  0 15
 2.0395  0.0013 -2.1268 H  0  0  0  0  0  0  0  0  0  0 16
-0.4560 -0.0013 -2.3257 H  0  0  0  0  0  0  0  0  0  0 17
-0.7974 -0.0016  1.9763 H  0  0  0  0  0  0  0  0  0  0 18
 1.6891 -0.0021  2.1762 H  0  0  0  0  0  0  0  0  0  0 19
-3.9486  0.0102  0.6539 H  0  0  0  0  0  0  0  0  0  0 20
 2  1  0  0  0  0
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14 10  0  0  0  0
15 10  0  0  0  0
12 11  0  0  0  0
13 11  0  0  0  0
15 20  0  0  0  0
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3 M END
4 $$$$
5 4-phenylbenzoicacid-anion.sdf
6 COSMOtherm 3D 0
7
8 27 27 0 0 0 0 0 0 0 0 V2000
9 -6.5743 -0.5328 0.1106 O 0 0 0 0 0 0 0 0 0 0 1
10 -5.5690 -0.6498 0.1330 H 0 0 0 0 0 0 0 0 0 0 2
11 -6.6786 0.4219 -0.0456 H 0 0 0 0 0 0 0 0 0 0 3
12 0.2947 -1.1218 0.2705 C 0 0 0 0 0 0 0 0 0 0 4
13 -1.1000 -1.0705 0.2601 C 0 0 0 0 0 0 0 0 0 0 5
14 -1.7763 0.1270 -0.0248 C 0 0 0 0 0 0 0 0 0 0 6
15 -1.0126 1.2724 -0.3025 C 0 0 0 0 0 0 0 0 0 0 7
16 0.3817 1.2247 -0.2965 C 0 0 0 0 0 0 0 0 0 0 8
17 1.0659 0.0256 -0.0083 C 0 0 0 0 0 0 0 0 0 0 9
18 2.5498 -0.0258 0.0026 C 0 0 0 0 0 0 0 0 0 0 10
19 -3.2989 0.1926 -0.0367 C 0 0 0 0 0 0 0 0 0 0 11
20 4.7068 1.0302 0.4516 C 0 0 0 0 0 0 0 0 0 0 12
21 3.3101 1.0782 0.4404 C 0 0 0 0 0 0 0 0 0 0 13
22 3.2396 -1.1794 -0.4235 C 0 0 0 0 0 0 0 0 0 0 14
23 4.6364 -1.2270 -0.4124 C 0 0 0 0 0 0 0 0 0 0 15
24 5.3774 -0.1225 0.0250 C 0 0 0 0 0 0 0 0 0 0 16
25 -3.9215 -0.9059 0.1851 O 0 0 0 0 0 0 0 0 0 0 17
26 -3.8434 1.3098 -0.2616 O 0 0 0 0 0 0 0 0 0 0 18
27 0.7935 -2.0604 0.5197 H 0 0 0 0 0 0 0 0 0 0 19
28 -1.6848 -1.9640 0.4840 H 0 0 0 0 0 0 0 0 0 0 20
29 -1.5319 2.2042 -0.5326 H 0 0 0 0 0 0 0 0 0 0 21
30 0.9488 2.1253 -0.5402 H 0 0 0 0 0 0 0 0 0 0 22
31 5.2737 1.8947 0.8027 H 0 0 0 0 0 0 0 0 0 0 23
32 2.8024 1.9764 0.7968 H 0 0 0 0 0 0 0 0 0 0 24
33 2.6774 -2.0410 -0.7885 H 0 0 0 0 0 0 0 0 0 0 25
34 5.1484 -2.1284 -0.7551 H 0 0 0 0 0 0 0 0 0 0 26
35 6.4681 -0.1598 0.0338 H 0 0 0 0 0 0 0 0 0 0 27
36
37 2 1 0 0 0 0
38 3 1 0 0 0 0
39 5 4 0 0 0 0
40 9 4 0 0 0 0
41 19 4 0 0 0 0
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60 25 14 0 0 0 0
16 15 0 0 0 0
26 15 0 0 0 0
16 27 0 0 0 0
M END
$$$$
4-phenylbenzoicacid.sdf
COSMOtherm 3D 0
28 28 0 0 0 0 0 0 0 0 V2000
-6.5044 0.1720 0.7282 O 0 0 0 0 0 0 0 0 0 0 1
-6.8950 -0.5998 0.2785 H 0 0 0 0 0 0 0 0 0 0 2
-6.8750 0.9425 0.2595 H 0 0 0 0 0 0 0 0 0 0 3
0.4280 -0.2856 -1.2613 C 0 0 0 0 0 0 0 0 0 0 4
-0.9619 -0.3002 -1.3367 C 0 0 0 0 0 0 0 0 0 0 5
-1.7418 -0.0461 -0.1956 C 0 0 0 0 0 0 0 0 0 0 6
-1.0959 0.2227 1.0242 C 0 0 0 0 0 0 0 0 0 0 7
0.2956 0.2381 1.0963 C 0 0 0 0 0 0 0 0 0 0 8
1.0870 -0.0157 -0.0431 C 0 0 0 0 0 0 0 0 0 0 9
2.5686 0.0034 0.0356 C 0 0 0 0 0 0 0 0 0 0 10
-3.2284 -0.0708 -0.3186 C 0 0 0 0 0 0 0 0 0 0 11
4.6331 -0.4140 1.2702 C 0 0 0 0 0 0 0 0 0 0 12
3.2379 -0.4333 1.1970 C 0 0 0 0 0 0 0 0 0 0 13
3.3441 0.4617 -1.0490 C 0 0 0 0 0 0 0 0 0 0 14
4.7391 0.4835 -0.9735 C 0 0 0 0 0 0 0 0 0 0 15
5.3903 0.0451 0.1858 C 0 0 0 0 0 0 0 0 0 0 16
-3.8156 -0.2927 -1.3794 O 0 0 0 0 0 0 0 0 0 0 17
-3.8687 0.1710 0.8372 O 0 0 0 0 0 0 0 0 0 0 18
1.0121 -0.5087 -2.1554 H 0 0 0 0 0 0 0 0 0 0 19
-1.4595 -0.5176 -2.2827 H 0 0 0 0 0 0 0 0 0 0 20
-1.6870 0.4300 1.9161 H 0 0 0 0 0 0 0 0 0 0 21
0.7757 0.4721 2.0475 H 0 0 0 0 0 0 0 0 0 0 22
5.1314 -0.7657 2.1755 H 0 0 0 0 0 0 0 0 0 0 23
2.6627 -0.8143 2.0427 H 0 0 0 0 0 0 0 0 0 0 24
2.8509 0.8270 -1.9515 H 0 0 0 0 0 0 0 0 0 0 25
5.3197 0.8513 -1.8216 H 0 0 0 0 0 0 0 0 0 0 26
6.4800 0.0614 0.2437 H 0 0 0 0 0 0 0 0 0 0 27
-4.8789 0.1482 0.6895 H 0 0 0 0 0 0 0 0 0 0 28
2 1 0 0 0 0
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20 5 0 0 0 0
7 6 0 0 0 0
11 6 0 0 0 0
8 7 0 0 0 0
21 7 0 0 0 0
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URL: <http://mc.manuscriptcentral.com/tandf/tmph>

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-4.6243 -0.0037 0.6635 H 0 0 0 0 0 0 0 0 0 0 23
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6 5 0 0 0 0
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8 7 0 0 0 0
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22 8 0 0 0 0
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15 10 0 0 0 0
16 10 0 0 0 0
12 11 0 0 0 0
13 11 0 0 0 0
14 11 0 0 0 0
17 14 0 0 0 0
18 14 0 0 0 0
16 23 0 0 0 0
M END
$$$$
4-trifluoromethylbenzoicacid-anion.sdf
COSMOtherm 3D 0
20 19 0 0 0 0 0 0 0 0 0 V2000
-6.0797 0.1181 -0.5241 O 0 0 0 0 0 0 0 0 0 0 1
-5.0772 0.0488 -0.6318 H 0 0 0 0 0 0 0 0 0 0 2
-6.1950 0.1881 0.4394 H 0 0 0 0 0 0 0 0 0 0 3
0.7776 -0.0617 -1.1867 C 0 0 0 0 0 0 0 0 0 0 4
-0.6162 -0.0650 -1.1082 C 0 0 0 0 0 0 0 0 0 0 5
-1.2661 -0.0501 0.1353 C 0 0 0 0 0 0 0 0 0 0 6
-0.4918 -0.0410 1.3063 C 0 0 0 0 0 0 0 0 0 0 7
0.9017 -0.0385 1.2425 C 0 0 0 0 0 0 0 0 0 0 8
1.5367 -0.0507 -0.0082 C 0 0 0 0 0 0 0 0 0 0 9
-2.7936 -0.0374 0.2241 C 0 0 0 0 0 0 0 0 0 0 10
3.0371 0.0168 -0.0790 C 0 0 0 0 0 0 0 0 0 0 11
3.4994 1.3112 -0.0054 F 0 0 0 0 0 0 0 0 0 0 12
3.5364 -0.4979 -1.2398 F 0 0 0 0 0 0 0 0 0 0 13
3.6437 -0.6567 0.9438 F 0 0 0 0 0 0 0 0 0 0 14
-3.4255 -0.0532 -0.8883 O 0 0 0 0 0 0 0 0 0 0 15
-3.3152 -0.0062 1.3715 O 0 0 0 0 0 0 0 0 0 0 16
1.2703 -0.0725 -2.1594 H 0 0 0 0 0 0 0 0 0 0 17
-1.2173 -0.0769 -2.0180 H 0 0 0 0 0 0 0 0 0 0 18
-1.0000 -0.0334 2.2712 H 0 0 0 0 0 0 0 0 0 0 19
1.4908 -0.0321 2.1605 H 0 0 0 0 0 0 0 0 0 0 20
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
9 4 0 0 0 0
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6 5 0 0 0 0
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8 7 0 0 0 0
19 7 0 0 0 0
9 8 0 0 0 0
11 9 0 0 0 0
15 10 0 0 0 0
16 10 0 0 0 0
12 11 0 0 0 0
13 11 0 0 0 0
14 11 0 0 0 0
8 20 0 0 0 0
M END
$$$$
4-trifluoromethylbenzoicacid.sdf
COSMOtherm 3D 0
21 20 0 0 0 0 0 0 0 0 0 V2000
-5.9974 -0.0471 0.6916 O 0 0 0 0 0 0 0 0 0 0 1
-6.3554 -0.6547 0.0185 H 0 0 0 0 0 0 0 0 0 0 2
-6.4122 0.8128 0.4942 H 0 0 0 0 0 0 0 0 0 0 3
0.9466 -0.0139 -1.2686 C 0 0 0 0 0 0 0 0 0 0 4
-0.4439 0.0034 -1.3630 C 0 0 0 0 0 0 0 0 0 0 5
-1.2347 0.0122 -0.2033 C 0 0 0 0 0 0 0 0 0 0 6
-0.6179 0.0078 1.0585 C 0 0 0 0 0 0 0 0 0 0 7
0.7727 -0.0098 1.1594 C 0 0 0 0 0 0 0 0 0 0 8
1.5526 -0.0276 -0.0050 C 0 0 0 0 0 0 0 0 0 0 9
-2.7271 0.0163 -0.3528 C 0 0 0 0 0 0 0 0 0 0 10
3.0555 -0.0101 0.1095 C 0 0 0 0 0 0 0 0 0 0 11
3.5457 1.2688 0.2102 F 0 0 0 0 0 0 0 0 0 0 12
3.6705 -0.5734 -0.9690 F 0 0 0 0 0 0 0 0 0 0 13
3.5009 -0.6780 1.2135 F 0 0 0 0 0 0 0 0 0 0 14
-3.2895 0.0095 -1.4472 O 0 0 0 0 0 0 0 0 0 0 15
-3.3776 0.0238 0.8171 O 0 0 0 0 0 0 0 0 0 0 16
1.5531 -0.0258 -2.1741 H 0 0 0 0 0 0 0 0 0 0 17
-0.9280 0.0067 -2.3397 H 0 0 0 0 0 0 0 0 0 0 18
-1.2257 0.0140 1.9622 H 0 0 0 0 0 0 0 0 0 0 19
1.2454 -0.0189 2.1416 H 0 0 0 0 0 0 0 0 0 0 20
-4.3908 0.0115 0.6638 H 0 0 0 0 0 0 0 0 0 0 21
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
9 4 0 0 0 0
17 4 0 0 0 0
6 5 0 0 0 0
18 5 0 0 0 0
7 6 0 0 0 0
10 6 0 0 0 0
8 7 0 0 0 0
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19 7 0 0 0 0
9 8 0 0 0 0
20 8 0 0 0 0
11 9 0 0 0 0
15 10 0 0 0 0
16 10 0 0 0 0
12 11 0 0 0 0
13 11 0 0 0 0
14 11 0 0 0 0
16 21 0 0 0 0
M END
$$$$
5-fluorouracil-anion.sdf
COSMOtherm 3D 0
14 13 0 0 0 0 0 0 0 0 V2000
-3.7914 -0.0069 1.1967 O 0 0 0 0 0 0 0 0 0 1
-2.8562 -0.0079 0.8114 H 0 0 0 0 0 0 0 0 0 2
-3.8603 0.8454 1.6602 H 0 0 0 0 0 0 0 0 0 3
-0.8644 -0.0147 -1.0683 C 0 0 0 0 0 0 0 0 0 4
0.5086 0.0094 -1.3888 N 0 0 0 0 0 0 0 0 0 5
1.5883 0.0140 -0.4990 C 0 0 0 0 0 0 0 0 0 6
1.1375 -0.0099 0.8625 C 0 0 0 0 0 0 0 0 0 7
-0.1977 -0.0327 1.1750 C 0 0 0 0 0 0 0 0 0 8
-1.1971 -0.0363 0.2569 N 0 0 0 0 0 0 0 0 0 9
2.7708 0.0376 -0.9005 O 0 0 0 0 0 0 0 0 0 10
-1.7027 -0.0159 -1.9974 O 0 0 0 0 0 0 0 0 0 11
2.0927 -0.0084 1.8472 F 0 0 0 0 0 0 0 0 0 12
0.7423 0.0263 -2.3830 H 0 0 0 0 0 0 0 0 0 13
-0.5009 -0.0510 2.2264 H 0 0 0 0 0 0 0 0 0 14
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
9 4 0 0 0 0
11 4 0 0 0 0
6 5 0 0 0 0
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7 6 0 0 0 0
10 6 0 0 0 0
8 7 0 0 0 0
12 7 0 0 0 0
9 8 0 0 0 0
8 14 0 0 0 0
M END
$$$$
5-fluorouracil.sdf
COSMOtherm 3D 0
15 14 0 0 0 0 0 0 0 0 V2000
-1.2340 0.0219 3.7206 O 0 0 0 0 0 0 0 0 0 1
-0.8340 0.6890 4.3072 H 0 0 0 0 0 0 0 0 0 2
-1.1409 -0.8176 4.2069 H 0 0 0 0 0 0 0 0 0 3
1.1142 -0.0050 0.8419 C 0 0 0 0 0 0 0 0 0 4
1.4045 -0.0013 -0.5219 N 0 0 0 0 0 0 0 0 0 5
0.5056 0.0030 -1.5989 C 0 0 0 0 0 0 0 0 0 6
-0.8758 -0.0010 -1.1588 C 0 0 0 0 0 0 0 0 0 7
-1.2090 -0.0079 0.1562 C 0 0 0 0 0 0 0 0 0 8
-0.2397 -0.0075 1.1251 N 0 0 0 0 0 0 0 0 0 9
0.8947 0.0095 -2.7726 O 0 0 0 0 0 0 0 0 0 10
1.9914 -0.0058 1.7094 O 0 0 0 0 0 0 0 0 0 11
-1.8316 -0.0002 -2.1210 F 0 0 0 0 0 0 0 0 0 12
2.3973 0.0022 -0.7627 H 0 0 0 0 0 0 0 0 0 13
-0.5272 -0.0134 2.1334 H 0 0 0 0 0 0 0 0 0 14
-2.2433 -0.0115 0.4971 H 0 0 0 0 0 0 0 0 0 15
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
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6 5 0 0 0 0
13 5 0 0 0 0
7 6 0 0 0 0
10 6 0 0 0 0
8 7 0 0 0 0
12 7 0 0 0 0
9 8 0 0 0 0
14 9 0 0 0 0
8 15 0 0 0 0
M END
$$$$
5-iodo-2-hydroxybenzoicacid-anion.sdf
COSMOtherm 3D 0
18 17 0 0 0 0 0 0 0 0 V2000
-5.3732 -2.8086 -0.0218 O 0 0 0 0 0 0 0 0 0 1
-4.4985 -2.3172 -0.0058 H 0 0 0 0 0 0 0 0 0 2
-6.0372 -2.0980 -0.0292 H 0 0 0 0 0 0 0 0 0 3
0.7179 0.5374 -0.0010 C 0 0 0 0 0 0 0 0 0 4
-0.4627 -0.1969 0.0064 C 0 0 0 0 0 0 0 0 0 5
-1.7019 0.4646 0.0059 C 0 0 0 0 0 0 0 0 0 6
-1.7333 1.8869 -0.0014 C 0 0 0 0 0 0 0 0 0 7
-0.5233 2.6072 -0.0092 C 0 0 0 0 0 0 0 0 0 8
0.6996 1.9392 -0.0089 C 0 0 0 0 0 0 0 0 0 9
-2.9892 -0.3207 0.0117 C 0 0 0 0 0 0 0 0 0 10
-4.0798 0.3698 0.0094 O 0 0 0 0 0 0 0 0 0 11
-2.9465 -1.5835 0.0167 O 0 0 0 0 0 0 0 0 0 12
-2.9075 2.5520 -0.0010 O 0 0 0 0 0 0 0 0 0 13
2.6046 -0.4874 -0.0003 I 0 0 0 0 0 0 0 0 0 14
-3.6118 1.7662 0.0031 H 0 0 0 0 0 0 0 0 0 15
-0.4624 -1.2870 0.0122 H 0 0 0 0 0 0 0 0 0 16
-0.5538 3.6982 -0.0151 H 0 0 0 0 0 0 0 0 0 17
1.6265 2.5128 -0.0150 H 0 0 0 0 0 0 0 0 0 18
2 1 0 0 0 0
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12 10  0  0  0  0
15 11  0  0  0  0
15 13  0  0  0  0
  9 18  0  0  0  0
M  END
$$$$
5-iodo-2-hydroxybenzoicacid.sdf
COSMOtherm      3D      0

19 17  0  0  0  0  0  0  0  0  0  0 V2000
-5.1021 -0.0135  2.8996 O  0  0  0  0  0  0  0  0  0  0  1
-5.6507 -0.8081  2.7647 H  0  0  0  0  0  0  0  0  0  0  2
-5.7034  0.7365  2.7364 H  0  0  0  0  0  0  0  0  0  0  3
  0.7187 -0.0011 -0.5470 C  0  0  0  0  0  0  0  0  0  0  4
-0.4667  0.0039  0.1734 C  0  0  0  0  0  0  0  0  0  0  5
-1.7013  0.0036 -0.5080 C  0  0  0  0  0  0  0  0  0  0  6
-1.7171 -0.0018 -1.9302 C  0  0  0  0  0  0  0  0  0  0  7
-0.4997 -0.0073 -2.6339 C  0  0  0  0  0  0  0  0  0  0  8
  0.7118 -0.0070 -1.9508 C  0  0  0  0  0  0  0  0  0  0  9
-2.9839  0.0084  0.2238 C  0  0  0  0  0  0  0  0  0  0 10
-2.8886  0.0108  1.5470 O  0  0  0  0  0  0  0  0  0  0 11
-4.0818  0.0099 -0.3746 O  0  0  0  0  0  0  0  0  0  0 12
-2.8701 -0.0021 -2.6345 O  0  0  0  0  0  0  0  0  0  0 13
  2.5899  0.0001  0.4931 I  0  0  0  0  0  0  0  0  0  0 14
-3.8208  0.0078  1.9903 H  0  0  0  0  0  0  0  0  0  0 15
-3.6073  0.0033 -1.9405 H  0  0  0  0  0  0  0  0  0  0 16
-0.4686  0.0083  1.2621 H  0  0  0  0  0  0  0  0  0  0 17
-0.5186 -0.0117 -3.7244 H  0  0  0  0  0  0  0  0  0  0 18
  1.6448 -0.0113 -2.5141 H  0  0  0  0  0  0  0  0  0  0 19

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  3  1  0  0  0  0
  5  4  0  0  0  0
  9  4  0  0  0  0
  6  5  0  0  0  0
17  5  0  0  0  0
  7  6  0  0  0  0
10  6  0  0  0  0
  8  7  0  0  0  0
13  7  0  0  0  0
  9  8  0  0  0  0
18  8  0  0  0  0
11 10  0  0  0  0
12 10  0  0  0  0
15 11  0  0  0  0
16 13  0  0  0  0
  9 19  0  0  0  0
M  END
$$$$
5-nitrouracil-anion.sdf
COSMOtherm      3D      0

16 15  0  0  0  0  0  0  0  0  0  0 V2000
-3.7511 -0.1078 -2.0922 O  0  0  0  0  0  0  0  0  0  0  1
-2.9974 -0.0414 -1.4342 H  0  0  0  0  0  0  0  0  0  0  2
-3.9499  0.8161 -2.3221 H  0  0  0  0  0  0  0  0  0  0  3
-0.3357  0.0270 -0.9117 C  0  0  0  0  0  0  0  0  0  0  4
  0.8822  0.0047 -0.2132 C  0  0  0  0  0  0  0  0  0  0  5
  0.8708 -0.0123  1.2434 C  0  0  0  0  0  0  0  0  0  0  6
-0.4431 -0.0018  1.7386 N  0  0  0  0  0  0  0  0  0  0  7
-1.6402  0.0194  1.0183 C  0  0  0  0  0  0  0  0  0  0  8
-1.5436  0.0315 -0.3659 N  0  0  0  0  0  0  0  0  0  0  9
  1.8200 -0.0332  2.0364 O  0  0  0  0  0  0  0  0  0  0 10
-2.7273  0.0260  1.6124 O  0  0  0  0  0  0  0  0  0  0 11
  2.0948  0.0037 -0.9617 N  0  0  0  0  0  0  0  0  0  0 12
-0.2947  0.0368 -2.0035 H  0  0  0  0  0  0  0  0  0  0 13
-0.5268 -0.0119  2.7569 H  0  0  0  0  0  0  0  0  0  0 14
  2.0286  0.0234 -2.2196 O  0  0  0  0  0  0  0  0  0  0 15
  3.1919 -0.0171 -0.3610 O  0  0  0  0  0  0  0  0  0  0 16

  2  1  0  0  0  0
  3  1  0  0  0  0
  5  4  0  0  0  0
  9  4  0  0  0  0
13  4  0  0  0  0
  6  5  0  0  0  0
12  5  0  0  0  0
  7  6  0  0  0  0
10  6  0  0  0  0
  8  7  0  0  0  0
14  7  0  0  0  0
  9  8  0  0  0  0
11  8  0  0  0  0
15 12  0  0  0  0
12 16  0  0  0  0
M  END
$$$$
5-nitrouracil.sdf
COSMOtherm      3D      0

17 16  0  0  0  0  0  0  0  0  0  0 V2000
-2.1028 -3.5784  0.0025 O  0  0  0  0  0  0  0  0  0  0  1
-1.9729 -4.2456  0.7011 H  0  0  0  0  0  0  0  0  0  0  2
-2.1392 -4.0909 -0.8260 H  0  0  0  0  0  0  0  0  0  0  3
-0.9333 -0.2794  0.0012 C  0  0  0  0  0  0  0  0  0  0  4
-0.2068  0.8915  0.0017 C  0  0  0  0  0  0  0  0  0  0  5
  1.2588  0.8513  0.0034 C  0  0  0  0  0  0  0  0  0  0  6
```

```
1
2
3      1.7454 -0.4734 0.0026 N 0 0 0 0 0 0 0 0 0 0 0 7
4      1.0389 -1.6627 -0.0004 C 0 0 0 0 0 0 0 0 0 0 0 8
5     -0.3519 -1.4871 0.0000 N 0 0 0 0 0 0 0 0 0 0 0 9
6      2.0529 1.7877 0.0077 O 0 0 0 0 0 0 0 0 0 0 0 10
7      1.5625 -2.7712 -0.0031 O 0 0 0 0 0 0 0 0 0 0 0 11
8     -0.9426 2.1350 -0.0010 N 0 0 0 0 0 0 0 0 0 0 0 12
9     -2.0222 -0.2597 0.0008 H 0 0 0 0 0 0 0 0 0 0 0 13
10      2.7635 -0.5629 0.0041 H 0 0 0 0 0 0 0 0 0 0 0 14
11     -0.9569 -2.3559 -0.0023 H 0 0 0 0 0 0 0 0 0 0 0 15
12     -2.1912 2.0799 0.0207 O 0 0 0 0 0 0 0 0 0 0 0 16
13     -0.3125 3.2043 -0.0258 O 0 0 0 0 0 0 0 0 0 0 0 17
14
15      2 1 0 0 0 0
16      3 1 0 0 0 0
17      5 4 0 0 0 0
18      9 4 0 0 0 0
19     13 4 0 0 0 0
20      6 5 0 0 0 0
21     12 5 0 0 0 0
22      7 6 0 0 0 0
23     10 6 0 0 0 0
24      8 7 0 0 0 0
25     14 7 0 0 0 0
26      9 8 0 0 0 0
27     11 8 0 0 0 0
28     15 9 0 0 0 0
29     16 12 0 0 0 0
30     12 17 0 0 0 0
31
32 M END
33 $$$
34 aceticacid-anion.sdf
35 COSMOTHERM 3D 0
36
37      10 8 0 0 0 0 0 0 0 0 0 V2000
38     -2.6444 -0.0635 -0.0058 O 0 0 0 0 0 0 0 0 0 0 0 1
39     -1.6798 -0.3817 0.0017 H 0 0 0 0 0 0 0 0 0 0 0 2
40     -2.5492 0.9048 -0.0039 H 0 0 0 0 0 0 0 0 0 0 0 3
41      2.1955 -0.3112 -0.0073 C 0 0 0 0 0 0 0 0 0 0 0 4
42      0.7003 0.0343 0.0054 C 0 0 0 0 0 0 0 0 0 0 0 5
43     -0.1274 -0.9468 0.0074 O 0 0 0 0 0 0 0 0 0 0 0 6
44      0.3779 1.2565 0.0033 O 0 0 0 0 0 0 0 0 0 0 0 7
45      2.3728 -1.3892 0.0936 H 0 0 0 0 0 0 0 0 0 0 0 8
46      2.6397 0.0363 -0.9527 H 0 0 0 0 0 0 0 0 0 0 0 9
47      2.7089 0.2225 0.8058 H 0 0 0 0 0 0 0 0 0 0 0 10
48
49      2 1 0 0 0 0
50      3 1 0 0 0 0
51      5 4 0 0 0 0
52      8 4 0 0 0 0
53      9 4 0 0 0 0
54      6 5 0 0 0 0
55      7 5 0 0 0 0
56      4 10 0 0 0 0
57
58 M END
59 $$$
60 aceticacid.sdf
COSMOTHERM 3D 0

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```
11 9 0 0 0 0 0 0 0 0 0 V2000
-2.6632 -0.0231 0.0932 O 0 0 0 0 0 0 0 0 0 0 0 1
-2.8339 -0.5955 -0.6771 H 0 0 0 0 0 0 0 0 0 0 0 2
-2.9948 0.8534 -0.1753 H 0 0 0 0 0 0 0 0 0 0 0 3
2.2026 -0.0055 0.4247 C 0 0 0 0 0 0 0 0 0 0 0 4
0.7914 0.0037 -0.1040 C 0 0 0 0 0 0 0 0 0 0 0 5
0.4952 0.0091 -1.2971 O 0 0 0 0 0 0 0 0 0 0 0 6
-0.1272 0.0009 0.8789 O 0 0 0 0 0 0 0 0 0 0 0 7
2.9163 0.0324 -0.4042 H 0 0 0 0 0 0 0 0 0 0 0 8
2.3613 0.8523 1.0931 H 0 0 0 0 0 0 0 0 0 0 0 9
2.3721 -0.9165 1.0166 H 0 0 0 0 0 0 0 0 0 0 0 10
-1.0668 0.0031 0.4835 H 0 0 0 0 0 0 0 0 0 0 0 11
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
8 4 0 0 0 0
9 4 0 0 0 0
10 4 0 0 0 0
6 5 0 0 0 0
7 5 0 0 0 0
7 11 0 0 0 0
M END
$$$
acrylicacid-anion.sdf
COSMOTHERM 3D 0

```

```
11 9 0 0 0 0 0 0 0 0 0 V2000
-3.0979 0.0891 -0.0036 O 0 0 0 0 0 0 0 0 0 0 0 1
-2.1603 -0.2967 -0.0023 H 0 0 0 0 0 0 0 0 0 0 0 2
-2.9385 1.0483 0.0325 H 0 0 0 0 0 0 0 0 0 0 0 3
2.7509 0.2383 0.0003 C 0 0 0 0 0 0 0 0 0 0 0 4
1.6817 -0.5680 -0.0029 C 0 0 0 0 0 0 0 0 0 0 0 5
0.2534 -0.0659 0.0002 C 0 0 0 0 0 0 0 0 0 0 0 6
-0.6462 -0.9855 0.0038 O 0 0 0 0 0 0 0 0 0 0 0 7
0.0309 1.1766 -0.0002 O 0 0 0 0 0 0 0 0 0 0 0 8
3.7696 -0.1553 0.0000 H 0 0 0 0 0 0 0 0 0 0 0 9
2.6250 1.3241 0.0036 H 0 0 0 0 0 0 0 0 0 0 0 10
1.8040 -1.6556 -0.0048 H 0 0 0 0 0 0 0 0 0 0 0 11
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
9 4 0 0 0 0
10 4 0 0 0 0
6 5 0 0 0 0
7 6 0 0 0 0
8 6 0 0 0 0
5 11 0 0 0 0
M END
$$$
```



```
1
2
3      -3.4957    0.5498    0.1903 C    0    0    0    0    0    0    0    0    0    9
4      0.2475    0.2296   -0.1203 C    0    0    0    0    0    0    0    0    0    10
5      0.4198   -1.1739   -0.0612 C    0    0    0    0    0    0    0    0    0    11
6     -0.7518   -2.0202    0.0659 C    0    0    0    0    0    0    0    0    0    12
7     -2.0222   -1.4329    0.1473 C    0    0    0    0    0    0    0    0    0    13
8      1.6997   -1.8098   -0.1587 C    0    0    0    0    0    0    0    0    0    14
9      1.8169   -3.1805   -0.1199 C    0    0    0    0    0    0    0    0    0    15
10     0.6649   -4.0084    0.0156 C    0    0    0    0    0    0    0    0    0    16
11    -0.5839   -3.4409    0.1059 C    0    0    0    0    0    0    0    0    0    17
12     1.4459    1.1228   -0.3038 C    0    0    0    0    0    0    0    0    0    18
13     1.6481    1.7697   -1.3289 O    0    0    0    0    0    0    0    0    0    19
14     2.2564    1.1426    0.7607 O    0    0    0    0    0    0    0    0    0    20
15    -4.6518    2.3548    0.2201 H    0    0    0    0    0    0    0    0    0    21
16    -2.6579    3.8450   -0.0208 H    0    0    0    0    0    0    0    0    0    22
17    -0.3971    2.9015   -0.1962 H    0    0    0    0    0    0    0    0    0    23
18    -4.3596   -0.1095    0.3003 H    0    0    0    0    0    0    0    0    0    24
19    -2.9001   -2.0758    0.2510 H    0    0    0    0    0    0    0    0    0    25
20     2.5964   -1.1976   -0.2607 H    0    0    0    0    0    0    0    0    0    26
21     2.8032   -3.6418   -0.1961 H    0    0    0    0    0    0    0    0    0    27
22     0.7809   -5.0931    0.0456 H    0    0    0    0    0    0    0    0    0    28
23    -1.4742   -4.0657    0.2046 H    0    0    0    0    0    0    0    0    0    29
24     3.0615    1.7588    0.5926 H    0    0    0    0    0    0    0    0    0    30
25
26      2 1 0 0 0 0
27      3 1 0 0 0 0
28      5 4 0 0 0 0
29      9 4 0 0 0 0
30     21 4 0 0 0 0
31      6 5 0 0 0 0
32     22 5 0 0 0 0
33      7 6 0 0 0 0
34     23 6 0 0 0 0
35      8 7 0 0 0 0
36     10 7 0 0 0 0
37      9 8 0 0 0 0
38     13 8 0 0 0 0
39     24 9 0 0 0 0
40     11 10 0 0 0 0
41     18 10 0 0 0 0
42     12 11 0 0 0 0
43     14 11 0 0 0 0
44     13 12 0 0 0 0
45     17 12 0 0 0 0
46     25 13 0 0 0 0
47     15 14 0 0 0 0
48     26 14 0 0 0 0
49     16 15 0 0 0 0
50     27 15 0 0 0 0
51     17 16 0 0 0 0
52     28 16 0 0 0 0
53     29 17 0 0 0 0
54     19 18 0 0 0 0
55     20 18 0 0 0 0
56     20 30 0 0 0 0
57
58 M END
59 $$$
60 benzoicacid-anion.sdf
   COSMOTHERM      3D      0
17 16 0 0 0 0 0 0 0 0 0 0 V2000
-4.3945 -0.3391 0.0040 O 0 0 0 0 0 0 0 0 0 0 1
-3.3979 -0.5181 0.0029 H 0 0 0 0 0 0 0 0 0 0 2
-4.4394 0.6325 0.0276 H 0 0 0 0 0 0 0 0 0 0 3
2.4269 -1.3406 0.0020 C 0 0 0 0 0 0 0 0 0 0 4
1.0343 -1.2087 0.0002 C 0 0 0 0 0 0 0 0 0 0 5
0.4357 0.0624 -0.0013 C 0 0 0 0 0 0 0 0 0 0 6
1.2605 1.1998 -0.0010 C 0 0 0 0 0 0 0 0 0 0 7
2.6531 1.0720 0.0009 C 0 0 0 0 0 0 0 0 0 0 8
3.2403 -0.1999 0.0025 C 0 0 0 0 0 0 0 0 0 0 9
-1.0830 0.2161 -0.0028 C 0 0 0 0 0 0 0 0 0 0 10
-1.7684 -0.8670 -0.0060 O 0 0 0 0 0 0 0 0 0 0 11
-1.5618 1.3847 -0.0006 O 0 0 0 0 0 0 0 0 0 0 12
2.8806 -2.3341 0.0032 H 0 0 0 0 0 0 0 0 0 0 13
0.3922 -2.0909 -0.0005 H 0 0 0 0 0 0 0 0 0 0 14
0.7902 2.1845 -0.0022 H 0 0 0 0 0 0 0 0 0 0 15
3.2827 1.9642 0.0009 H 0 0 0 0 0 0 0 0 0 0 16
4.3274 -0.3020 0.0040 H 0 0 0 0 0 0 0 0 0 0 17
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
9 4 0 0 0 0
13 4 0 0 0 0
6 5 0 0 0 0
14 5 0 0 0 0
7 6 0 0 0 0
10 6 0 0 0 0
8 7 0 0 0 0
15 7 0 0 0 0
9 8 0 0 0 0
16 8 0 0 0 0
11 10 0 0 0 0
12 10 0 0 0 0
9 17 0 0 0 0
M END
$$$
benzoicacid.sdf
COSMOTHERM      3D      0
18 17 0 0 0 0 0 0 0 0 0 0 V2000
-4.3632 0.0074 0.4523 O 0 0 0 0 0 0 0 0 0 0 1
-4.7151 -0.6120 -0.2134 H 0 0 0 0 0 0 0 0 0 0 2
-4.7170 0.8776 0.1908 H 0 0 0 0 0 0 0 0 0 0 3
2.3790 0.0004 1.4007 C 0 0 0 0 0 0 0 0 0 0 4
0.9959 -0.0067 1.2045 C 0 0 0 0 0 0 0 0 0 0 5
0.4698 -0.0047 -0.0996 C 0 0 0 0 0 0 0 0 0 0 6
1.3438 0.0046 -1.2005 C 0 0 0 0 0 0 0 0 0 0 7
```



```
1
2
3      -4.6437    0.7622   -0.8494 H    0 0 0 0 0 0 0 0 0 0 0 3
4      1.8363    0.0052   -0.0963 Br   0 0 0 0 0 0 0 0 0 0 0 4
5      0.1822   -0.0221    0.9630 C    0 0 0 0 0 0 0 0 0 0 0 5
6     -1.0784   -0.0094    0.1094 C    0 0 0 0 0 0 0 0 0 0 0 6
7     -2.1470    0.0093    0.9126 O    0 0 0 0 0 0 0 0 0 0 0 7
8     -1.1183   -0.0191   -1.1115 O    0 0 0 0 0 0 0 0 0 0 0 8
9      0.2079    0.8556    1.6167 H    0 0 0 0 0 0 0 0 0 0 0 9
10     0.2128   -0.9291    1.5757 H    0 0 0 0 0 0 0 0 0 0 0 10
11     -3.0196    0.0091    0.3662 H    0 0 0 0 0 0 0 0 0 0 0 11
12
13     2 1 0 0 0 0
14     3 1 0 0 0 0
15     6 5 0 0 0 0
16     9 5 0 0 0 0
17    10 5 0 0 0 0
18     7 6 0 0 0 0
19     8 6 0 0 0 0
20     7 11 0 0 0 0
21
22 M END
23 $$$
24 carbonicacid-anion.sdf
25 COSMOTHERM      3D      0
26
27     8 6 0 0 0 0 0 0 0 0 0 0 V2000
28     -2.7019   -0.0378   -0.0070 O    0 0 0 0 0 0 0 0 0 0 0 1
29     -1.7426   -0.3446   -0.0030 H    0 0 0 0 0 0 0 0 0 0 0 2
30     -2.6325    0.9275    0.0888 H    0 0 0 0 0 0 0 0 0 0 0 3
31     0.6704    0.0340    0.0005 C    0 0 0 0 0 0 0 0 0 0 0 4
32     0.4603    1.2701   -0.0015 O    0 0 0 0 0 0 0 0 0 0 0 5
33     2.0126   -0.3983   -0.0014 O    0 0 0 0 0 0 0 0 0 0 0 6
34     -0.1600   -0.9222    0.0044 O    0 0 0 0 0 0 0 0 0 0 0 7
35     2.5600    0.4114   -0.0037 H    0 0 0 0 0 0 0 0 0 0 0 8
36
37     2 1 0 0 0 0
38     3 1 0 0 0 0
39     5 4 0 0 0 0
40     6 4 0 0 0 0
41     7 4 0 0 0 0
42     6 8 0 0 0 0
43
44 M END
45 $$$
46 carbonicacid.sdf
47 COSMOTHERM      3D      0
48
49     9 7 0 0 0 0 0 0 0 0 0 0 V2000
50     -2.6404    0.0053    0.0548 O    0 0 0 0 0 0 0 0 0 0 0 1
51     -2.9165   -0.7935   -0.4317 H    0 0 0 0 0 0 0 0 0 0 0 2
52     -2.8856    0.7493   -0.5258 H    0 0 0 0 0 0 0 0 0 0 0 3
53     0.7465   -0.0005   -0.0871 C    0 0 0 0 0 0 0 0 0 0 0 4
54     0.5495   -0.0026   -1.2964 O    0 0 0 0 0 0 0 0 0 0 0 5
55     1.9764    0.0032    0.4837 O    0 0 0 0 0 0 0 0 0 0 0 6
56     -0.1760   -0.0023    0.8699 O    0 0 0 0 0 0 0 0 0 0 0 7
57     2.6347   -0.0041   -0.2401 H    0 0 0 0 0 0 0 0 0 0 0 8
58     -1.1165   -0.0014    0.4566 H    0 0 0 0 0 0 0 0 0 0 0 9
59
60     2 1 0 0 0 0
61     3 1 0 0 0 0
62     5 4 0 0 0 0
63     6 4 0 0 0 0
64     7 4 0 0 0 0
65     8 6 0 0 0 0
66     7 9 0 0 0 0
67
68 M END
69 $$$
70 chloroaceticacid-anion.sdf
71 COSMOTHERM      3D      0
72
73    10 8 0 0 0 0 0 0 0 0 0 0 V2000
74     -3.4582   -0.8948    0.0042 O    0 0 0 0 0 0 0 0 0 0 0 1
75     -2.4577   -0.7761   -0.0009 H    0 0 0 0 0 0 0 0 0 0 0 2
76     -3.7929    0.0185    0.0173 H    0 0 0 0 0 0 0 0 0 0 0 3
77     2.2625   -0.5579    0.0009 Cl    0 0 0 0 0 0 0 0 0 0 0 4
78     1.1148    0.8849    0.0045 C    0 0 0 0 0 0 0 0 0 0 0 5
79     -0.3882    0.5466   -0.0025 C    0 0 0 0 0 0 0 0 0 0 0 6
80     -0.7688   -0.6618   -0.0077 O    0 0 0 0 0 0 0 0 0 0 0 7
81     -1.1100    1.5812   -0.0021 O    0 0 0 0 0 0 0 0 0 0 0 8
82     1.3678    1.4704   -0.8854 H    0 0 0 0 0 0 0 0 0 0 0 9
83     1.3614    1.4607    0.9026 H    0 0 0 0 0 0 0 0 0 0 0 10
84
85     2 1 0 0 0 0
86     3 1 0 0 0 0
87     5 4 0 0 0 0
88     6 5 0 0 0 0
89     9 5 0 0 0 0
90     7 6 0 0 0 0
91     8 6 0 0 0 0
92     5 10 0 0 0 0
93
94 M END
95 $$$
96 chloroaceticacid_270.sdf
97 COSMOTHERM      3D      0
98
99    11 9 0 0 0 0 0 0 0 0 0 0 V2000
100     -3.7212   -0.0019   -0.1683 O    0 0 0 0 0 0 0 0 0 0 0 1
101     -3.9278   -0.7977   -0.6924 H    0 0 0 0 0 0 0 0 0 0 0 2
102     -3.9107    0.7459   -0.7646 H    0 0 0 0 0 0 0 0 0 0 0 3
103     2.4612   -0.0025   -0.1807 Cl    0 0 0 0 0 0 0 0 0 0 0 4
104     0.9862    0.0007    0.8665 C    0 0 0 0 0 0 0 0 0 0 0 5
105     -0.3086    0.0027    0.0629 C    0 0 0 0 0 0 0 0 0 0 0 6
106     -1.3462    0.0038    0.9048 O    0 0 0 0 0 0 0 0 0 0 0 7
107     -0.3898    0.0039   -1.1559 O    0 0 0 0 0 0 0 0 0 0 0 8
108     1.0317    0.8929    1.5007 H    0 0 0 0 0 0 0 0 0 0 0 9
109     1.0285   -0.8909    1.5017 H    0 0 0 0 0 0 0 0 0 0 0 10
110     -2.2388    0.0037    0.3914 H    0 0 0 0 0 0 0 0 0 0 0 11
111
112     2 1 0 0 0 0
113     3 1 0 0 0 0
114     5 4 0 0 0 0
115     6 5 0 0 0 0
116     9 5 0 0 0 0
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```
10 5 0 0 0 0
7 6 0 0 0 0
8 6 0 0 0 0
7 11 0 0 0 0
M END
$$$$
cis-5-formyluracil-anion.sdf
COSMOtherm 3D 0

16 15 0 0 0 0 0 0 0 0 0 V2000
-3.8198 -0.0183 1.7575 O 0 0 0 0 0 0 0 0 0 0 1
-2.9687 -0.0185 1.2203 H 0 0 0 0 0 0 0 0 0 0 2
-3.9854 0.9224 1.9407 H 0 0 0 0 0 0 0 0 0 0 3
-0.2625 -0.0273 1.0768 C 0 0 0 0 0 0 0 0 0 0 4
1.0450 -0.0074 0.5631 C 0 0 0 0 0 0 0 0 0 0 5
1.2015 0.0108 -0.8837 C 0 0 0 0 0 0 0 0 0 0 6
-0.0281 0.0077 -1.5602 N 0 0 0 0 0 0 0 0 0 0 7
-1.3106 -0.0125 -0.9992 C 0 0 0 0 0 0 0 0 0 0 8
-1.3976 -0.0307 0.3811 N 0 0 0 0 0 0 0 0 0 0 9
2.2590 0.0280 -1.5338 O 0 0 0 0 0 0 0 0 0 0 10
-2.3091 -0.0144 -1.7382 O 0 0 0 0 0 0 0 0 0 0 11
2.1385 -0.0105 1.5057 C 0 0 0 0 0 0 0 0 0 0 12
-0.3801 -0.0425 2.1676 H 0 0 0 0 0 0 0 0 0 0 13
0.0194 0.0196 -2.5807 H 0 0 0 0 0 0 0 0 0 0 14
3.3548 0.0064 1.2638 O 0 0 0 0 0 0 0 0 0 0 15
1.7937 -0.0298 2.5700 H 0 0 0 0 0 0 0 0 0 0 16
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
9 4 0 0 0 0
13 4 0 0 0 0
6 5 0 0 0 0
12 5 0 0 0 0
7 6 0 0 0 0
10 6 0 0 0 0
8 7 0 0 0 0
14 7 0 0 0 0
9 8 0 0 0 0
11 8 0 0 0 0
15 12 0 0 0 0
12 16 0 0 0 0
M END
$$$$
cis-5-formyluracil.sdf
COSMOtherm 3D 0

17 16 0 0 0 0 0 0 0 0 0 V2000
-1.7705 0.0238 -3.6982 O 0 0 0 0 0 0 0 0 0 0 1
-1.7186 -0.7922 -4.2288 H 0 0 0 0 0 0 0 0 0 0 2
-1.5137 0.7339 -4.3144 H 0 0 0 0 0 0 0 0 0 0 3
-1.1032 -0.0121 -0.2167 C 0 0 0 0 0 0 0 0 0 0 4
-0.5690 -0.0035 1.0563 C 0 0 0 0 0 0 0 0 0 0 5
0.8888 0.0038 1.2025 C 0 0 0 0 0 0 0 0 0 0 6
1.5754 0.0011 -0.0302 N 0 0 0 0 0 0 0 0 0 0 7
1.0438 -0.0062 -1.3077 C 0 0 0 0 0 0 0 0 0 0 8
-0.3542 -0.0135 -1.3353 N 0 0 0 0 0 0 0 0 0 0 9
1.5304 0.0116 2.2539 O 0 0 0 0 0 0 0 0 0 0 10
1.7254 -0.0065 -2.3297 O 0 0 0 0 0 0 0 0 0 0 11
-1.5063 -0.0033 2.1739 C 0 0 0 0 0 0 0 0 0 0 12
-2.1841 -0.0185 -0.3724 H 0 0 0 0 0 0 0 0 0 0 13
2.5959 0.0067 0.0253 H 0 0 0 0 0 0 0 0 0 0 14
-0.8204 -0.0197 -2.2805 H 0 0 0 0 0 0 0 0 0 0 15
-1.2274 0.0043 3.3733 O 0 0 0 0 0 0 0 0 0 0 16
-2.5747 -0.0112 1.8481 H 0 0 0 0 0 0 0 0 0 0 17
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
9 4 0 0 0 0
13 4 0 0 0 0
6 5 0 0 0 0
12 5 0 0 0 0
7 6 0 0 0 0
10 6 0 0 0 0
8 7 0 0 0 0
14 7 0 0 0 0
9 8 0 0 0 0
11 8 0 0 0 0
15 9 0 0 0 0
16 12 0 0 0 0
12 17 0 0 0 0
M END
$$$$
cyanoaceticacid-anion.sdf
COSMOtherm 3D 0

11 9 0 0 0 0 0 0 0 0 0 V2000
-3.2330 -1.0223 -0.0108 O 0 0 0 0 0 0 0 0 0 0 1
-2.2427 -0.8419 0.0086 H 0 0 0 0 0 0 0 0 0 0 2
-3.6260 -0.1329 -0.0346 H 0 0 0 0 0 0 0 0 0 0 3
2.1766 -0.2380 -0.0030 C 0 0 0 0 0 0 0 0 0 0 4
1.3058 0.9211 0.0276 C 0 0 0 0 0 0 0 0 0 0 5
-0.2313 0.5919 0.0079 C 0 0 0 0 0 0 0 0 0 0 6
-0.5611 -0.6338 0.0391 O 0 0 0 0 0 0 0 0 0 0 7
-0.9841 1.5934 -0.0301 O 0 0 0 0 0 0 0 0 0 0 8
2.8725 -1.1729 -0.0314 N 0 0 0 0 0 0 0 0 0 0 9
1.5356 1.5688 -0.8315 H 0 0 0 0 0 0 0 0 0 0 10
1.5195 1.5079 0.9342 H 0 0 0 0 0 0 0 0 0 0 11
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
9 4 0 0 0 0
6 5 0 0 0 0
10 5 0 0 0 0
7 6 0 0 0 0
8 6 0 0 0 0
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5 11 0 0 0 0
M END
$$$$
cyanoaceticacid.sdf
COSMOTHERM 3D 0

12 10 0 0 0 0 0 0 0 0 V2000
-3.5386 -0.0110 -0.2633 O 0 0 0 0 0 0 0 0 0 0 1
-3.7068 -0.7890 -0.8264 H 0 0 0 0 0 0 0 0 0 0 2
-3.7173 0.7557 -0.8385 H 0 0 0 0 0 0 0 0 0 0 3
2.3388 -0.0045 0.1020 C 0 0 0 0 0 0 0 0 0 0 4
1.1412 0.0122 0.9245 C 0 0 0 0 0 0 0 0 0 0 5
-0.1527 0.0087 0.0985 C 0 0 0 0 0 0 0 0 0 0 6
-0.1860 0.0185 -1.1233 O 0 0 0 0 0 0 0 0 0 0 7
-1.2126 -0.0042 0.9024 O 0 0 0 0 0 0 0 0 0 0 8
3.3055 -0.0184 -0.5452 N 0 0 0 0 0 0 0 0 0 0 9
1.1517 0.9044 1.5704 H 0 0 0 0 0 0 0 0 0 0 10
1.1448 -0.8609 1.5955 H 0 0 0 0 0 0 0 0 0 0 11
-2.0870 -0.0027 0.3572 H 0 0 0 0 0 0 0 0 0 0 12
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
9 4 0 0 0 0
6 5 0 0 0 0
10 5 0 0 0 0
11 5 0 0 0 0
7 6 0 0 0 0
8 6 0 0 0 0
8 12 0 0 0 0
M END
$$$$
dichloroaceticacid-anion.sdf
COSMOTHERM 3D 0

10 8 0 0 0 0 0 0 0 0 V2000
-3.9580 -0.6585 0.0135 O 0 0 0 0 0 0 0 0 0 0 1
-2.9549 -0.6254 -0.0082 H 0 0 0 0 0 0 0 0 0 0 2
-4.2200 0.2776 0.0449 H 0 0 0 0 0 0 0 0 0 0 3
1.4953 -0.2293 1.5204 Cl 0 0 0 0 0 0 0 0 0 0 4
0.8396 0.5387 -0.0016 C 0 0 0 0 0 0 0 0 0 0 5
-0.7177 0.4697 -0.0317 C 0 0 0 0 0 0 0 0 0 0 6
-1.2446 -0.6792 -0.0291 O 0 0 0 0 0 0 0 0 0 0 7
-1.2746 1.5949 -0.0554 O 0 0 0 0 0 0 0 0 0 0 8
1.5561 -0.2630 -1.4780 Cl 0 0 0 0 0 0 0 0 0 0 9
1.2061 1.5659 -0.0056 H 0 0 0 0 0 0 0 0 0 0 10
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 5 0 0 0 0
9 5 0 0 0 0
7 6 0 0 0 0
8 6 0 0 0 0
5 10 0 0 0 0
M END
$$$$
dichloroaceticacid.sdf
COSMOTHERM 3D 0

11 9 0 0 0 0 0 0 0 0 V2000
-4.0484 0.0000 0.0828 O 0 0 0 0 0 0 0 0 0 0 1
-4.3079 -0.7642 -0.4646 H 0 0 0 0 0 0 0 0 0 0 2
-4.3146 0.7830 -0.4340 H 0 0 0 0 0 0 0 0 0 0 3
1.6062 -1.4969 -0.0065 Cl 0 0 0 0 0 0 0 0 0 0 4
0.7350 -0.0003 0.5151 C 0 0 0 0 0 0 0 0 0 0 5
-0.6766 0.0033 -0.1024 C 0 0 0 0 0 0 0 0 0 0 6
-0.8819 0.0099 -1.3054 O 0 0 0 0 0 0 0 0 0 0 7
-1.5908 -0.0031 0.8577 O 0 0 0 0 0 0 0 0 0 0 8
1.6144 1.4924 -0.0019 Cl 0 0 0 0 0 0 0 0 0 0 9
0.7133 -0.0025 1.6052 H 0 0 0 0 0 0 0 0 0 0 10
-2.5532 -0.0009 0.4621 H 0 0 0 0 0 0 0 0 0 0 11
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 5 0 0 0 0
9 5 0 0 0 0
10 5 0 0 0 0
7 6 0 0 0 0
8 6 0 0 0 0
8 11 0 0 0 0
M END
$$$$
dimethadione-anion.sdf
COSMOTHERM 3D 0

18 17 0 0 0 0 0 0 0 0 V2000
-3.6149 -0.0411 0.8752 O 0 0 0 0 0 0 0 0 0 0 1
-2.6496 -0.0235 0.5847 H 0 0 0 0 0 0 0 0 0 0 2
-3.8216 0.8876 1.0767 H 0 0 0 0 0 0 0 0 0 0 3
1.4169 0.0067 0.0588 C 0 0 0 0 0 0 0 0 0 0 4
0.1237 -0.0128 0.9049 C 0 0 0 0 0 0 0 0 0 0 5
0.8799 0.0107 -1.3046 O 0 0 0 0 0 0 0 0 0 0 6
-0.5119 -0.0048 -1.2133 C 0 0 0 0 0 0 0 0 0 0 7
-0.9583 -0.0184 0.0805 N 0 0 0 0 0 0 0 0 0 0 8
2.2188 1.2865 0.2859 C 0 0 0 0 0 0 0 0 0 0 9
2.2452 -1.2593 0.2678 C 0 0 0 0 0 0 0 0 0 0 10
0.1164 -0.0212 2.1470 O 0 0 0 0 0 0 0 0 0 0 11
-1.1797 -0.0048 -2.2483 O 0 0 0 0 0 0 0 0 0 0 12
1.6069 2.1755 0.0778 H 0 0 0 0 0 0 0 0 0 0 13
2.5523 1.3301 1.3319 H 0 0 0 0 0 0 0 0 0 0 14
3.1044 1.3031 -0.3648 H 0 0 0 0 0 0 0 0 0 0 15
1.6519 -2.1577 0.0467 H 0 0 0 0 0 0 0 0 0 0 16
2.5796 -1.3109 1.3131 H 0 0 0 0 0 0 0 0 0 0 17
3.1309 -1.2483 -0.3829 H 0 0 0 0 0 0 0 0 0 0 18
2 1 0 0 0 0
3 1 0 0 0 0
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5 4 0 0 0 0
6 4 0 0 0 0
9 4 0 0 0 0
10 4 0 0 0 0
8 5 0 0 0 0
11 5 0 0 0 0
7 6 0 0 0 0
8 7 0 0 0 0
12 7 0 0 0 0
13 9 0 0 0 0
14 9 0 0 0 0
15 9 0 0 0 0
16 10 0 0 0 0
17 10 0 0 0 0
10 18 0 0 0 0
M END
$$$$
dimethadione.sdf
COSMOTHERM 3D 0
19 18 0 0 0 0 0 0 0 0 0 V2000
-3.5434 -0.0016 0.9055 O 0 0 0 0 0 0 0 0 0 0 1
-4.0496 -0.7842 0.6219 H 0 0 0 0 0 0 0 0 0 0 2
-4.0675 0.7562 0.5888 H 0 0 0 0 0 0 0 0 0 0 3
1.4375 -0.0013 0.0582 C 0 0 0 0 0 0 0 0 0 0 4
0.1800 0.0025 0.9440 C 0 0 0 0 0 0 0 0 0 0 5
0.8664 -0.0007 -1.3106 O 0 0 0 0 0 0 0 0 0 0 6
-0.4937 0.0012 -1.2479 C 0 0 0 0 0 0 0 0 0 0 7
-0.8927 0.0042 0.0833 N 0 0 0 0 0 0 0 0 0 0 8
2.2479 -1.2792 0.2469 C 0 0 0 0 0 0 0 0 0 0 9
2.2543 1.2730 0.2453 C 0 0 0 0 0 0 0 0 0 0 10
0.1462 0.0035 2.1676 O 0 0 0 0 0 0 0 0 0 0 11
-1.2091 0.0009 -2.2327 O 0 0 0 0 0 0 0 0 0 0 12
-1.9041 0.0038 0.3707 H 0 0 0 0 0 0 0 0 0 0 13
1.6337 -2.1698 0.0576 H 0 0 0 0 0 0 0 0 0 0 14
2.6227 -1.3226 1.2782 H 0 0 0 0 0 0 0 0 0 0 15
3.1053 -1.2806 -0.4390 H 0 0 0 0 0 0 0 0 0 0 16
1.6446 2.1664 0.0551 H 0 0 0 0 0 0 0 0 0 0 17
2.6292 1.3157 1.2766 H 0 0 0 0 0 0 0 0 0 0 18
3.1118 1.2692 -0.4405 H 0 0 0 0 0 0 0 0 0 0 19
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
9 4 0 0 0 0
10 4 0 0 0 0
8 5 0 0 0 0
11 5 0 0 0 0
7 6 0 0 0 0
8 7 0 0 0 0
12 7 0 0 0 0
13 8 0 0 0 0
14 9 0 0 0 0
15 9 0 0 0 0
16 9 0 0 0 0
17 10 0 0 0 0
18 10 0 0 0 0
10 19 0 0 0 0
M END
$$$$
ethanol-anion.sdf
COSMOTHERM 3D 0
11 10 0 0 0 0 0 0 0 0 V2000
-2.1626 -0.0818 -0.4034 O 0 0 0 0 0 0 0 0 0 0 1
-1.1989 0.1183 0.1648 H 0 0 0 0 0 0 0 0 0 0 2
-1.9491 0.0950 -1.3348 H 0 0 0 0 0 0 0 0 0 0 3
1.6899 0.1740 -0.7831 C 0 0 0 0 0 0 0 0 0 0 4
0.9362 -0.4516 0.4030 C 0 0 0 0 0 0 0 0 0 0 5
-0.1076 0.3459 0.8870 O 0 0 0 0 0 0 0 0 0 0 6
2.5249 -0.4645 -1.1207 H 0 0 0 0 0 0 0 0 0 0 7
1.0093 0.3245 -1.6364 H 0 0 0 0 0 0 0 0 0 0 8
2.1017 1.1564 -0.5007 H 0 0 0 0 0 0 0 0 0 0 9
1.6830 -0.6579 1.2051 H 0 0 0 0 0 0 0 0 0 0 10
0.5714 -1.4571 0.0763 H 0 0 0 0 0 0 0 0 0 0 11
2 1 0 0 0 0
3 1 0 0 0 0
6 2 0 0 0 0
5 4 0 0 0 0
7 4 0 0 0 0
8 4 0 0 0 0
9 4 0 0 0 0
6 5 0 0 0 0
10 5 0 0 0 0
5 11 0 0 0 0
M END
$$$$
ethanol.sdf
COSMOTHERM 3D 0
12 10 0 0 0 0 0 0 0 0 V2000
-2.6448 0.0041 -0.0905 O 0 0 0 0 0 0 0 0 0 0 1
-2.9169 -0.7967 -0.5739 H 0 0 0 0 0 0 0 0 0 0 2
-2.8884 0.7371 -0.6843 H 0 0 0 0 0 0 0 0 0 0 3
2.3421 0.0006 -0.0340 C 0 0 0 0 0 0 0 0 0 0 4
0.8934 -0.0036 -0.4914 C 0 0 0 0 0 0 0 0 0 0 5
0.0379 0.0024 0.6676 O 0 0 0 0 0 0 0 0 0 0 6
3.0160 -0.0027 -0.9034 H 0 0 0 0 0 0 0 0 0 0 7
2.5609 0.8964 0.5660 H 0 0 0 0 0 0 0 0 0 0 8
2.5634 -0.8887 0.5748 H 0 0 0 0 0 0 0 0 0 0 9
0.6966 -0.8985 -1.1105 H 0 0 0 0 0 0 0 0 0 0 10
0.6949 0.8838 -1.1208 H 0 0 0 0 0 0 0 0 0 0 11
-0.9025 0.0010 0.3529 H 0 0 0 0 0 0 0 0 0 0 12
2 1 0 0 0 0
3 1 0 0 0 0
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5 4 0 0 0 0
7 4 0 0 0 0
8 4 0 0 0 0
9 4 0 0 0 0
6 5 0 0 0 0
10 5 0 0 0 0
11 5 0 0 0 0
6 12 0 0 0 0
M END
$$$$
fluoroaceticacid-anion.sdf
COSMOTHERM 3D 0
10 8 0 0 0 0 0 0 0 0 0 V2000
-3.1347 0.0075 0.5646 O 0 0 0 0 0 0 0 0 0 0 1
-2.1261 0.0009 0.5713 H 0 0 0 0 0 0 0 0 0 0 2
-3.3585 -0.0334 -0.3810 H 0 0 0 0 0 0 0 0 0 0 3
2.2604 0.0002 0.8647 F 0 0 0 0 0 0 0 0 0 0 4
1.6800 0.0069 -0.4326 C 0 0 0 0 0 0 0 0 0 0 5
0.1439 -0.0024 -0.4135 C 0 0 0 0 0 0 0 0 0 0 6
-0.4463 -0.0087 0.7113 O 0 0 0 0 0 0 0 0 0 0 7
-0.3841 -0.0021 -1.5590 O 0 0 0 0 0 0 0 0 0 0 8
2.0475 -0.8835 -0.9633 H 0 0 0 0 0 0 0 0 0 0 9
2.0359 0.9105 -0.9488 H 0 0 0 0 0 0 0 0 0 0 10
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 5 0 0 0 0
9 5 0 0 0 0
7 6 0 0 0 0
8 6 0 0 0 0
5 10 0 0 0 0
M END
$$$$
fluoroaceticacid.sdf
COSMOTHERM 3D 0
11 9 0 0 0 0 0 0 0 0 V2000
-3.2375 0.0056 -0.0564 O 0 0 0 0 0 0 0 0 0 0 1
-3.4816 -0.7893 -0.5652 H 0 0 0 0 0 0 0 0 0 0 2
-3.4394 0.7530 -0.6491 H 0 0 0 0 0 0 0 0 0 0 3
2.5721 -0.0097 -0.2316 F 0 0 0 0 0 0 0 0 0 0 4
1.5311 0.0178 0.7069 C 0 0 0 0 0 0 0 0 0 0 5
0.1826 0.0007 0.0010 C 0 0 0 0 0 0 0 0 0 0 6
-0.8084 -0.0113 0.8952 O 0 0 0 0 0 0 0 0 0 0 7
0.0453 0.0016 -1.2141 O 0 0 0 0 0 0 0 0 0 0 8
1.6243 0.9333 1.3090 H 0 0 0 0 0 0 0 0 0 0 9
1.6238 -0.8605 1.3618 H 0 0 0 0 0 0 0 0 0 0 10
-1.7275 -0.0073 0.4314 H 0 0 0 0 0 0 0 0 0 0 11
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 5 0 0 0 0
9 5 0 0 0 0
10 5 0 0 0 0
7 6 0 0 0 0
8 6 0 0 0 0
7 11 0 0 0 0
M END
$$$$
formicacid-anion.sdf
COSMOTHERM 3D 0
7 5 0 0 0 0 0 0 0 0 V2000
-2.1773 0.2336 0.0005 O 0 0 0 0 0 0 0 0 0 0 1
-1.2740 -0.2195 0.0038 H 0 0 0 0 0 0 0 0 0 0 2
-1.9545 1.1801 -0.0311 H 0 0 0 0 0 0 0 0 0 0 3
1.1851 -0.2583 -0.0046 C 0 0 0 0 0 0 0 0 0 0 4
1.1672 0.9993 0.0032 O 0 0 0 0 0 0 0 0 0 0 5
0.1857 -1.0517 0.0027 O 0 0 0 0 0 0 0 0 0 0 6
2.1905 -0.7601 -0.0192 H 0 0 0 0 0 0 0 0 0 0 7
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
4 7 0 0 0 0
M END
$$$$
formicacid.sdf
COSMOTHERM 3D 0
8 6 0 0 0 0 0 0 0 0 V2000
-2.1614 0.0015 -0.2298 O 0 0 0 0 0 0 0 0 0 0 1
-2.3313 -0.7855 -0.7790 H 0 0 0 0 0 0 0 0 0 0 2
-2.3101 0.7578 -0.8264 H 0 0 0 0 0 0 0 0 0 0 3
1.2470 -0.0012 0.2592 C 0 0 0 0 0 0 0 0 0 0 4
0.1513 0.0014 1.0169 O 0 0 0 0 0 0 0 0 0 0 5
1.2745 -0.0002 -0.9643 O 0 0 0 0 0 0 0 0 0 0 6
2.1568 -0.0040 0.8882 H 0 0 0 0 0 0 0 0 0 0 7
-0.6996 0.0022 0.4417 H 0 0 0 0 0 0 0 0 0 0 8
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
7 4 0 0 0 0
5 8 0 0 0 0
M END
$$$$
fumaricacid-anion.sdf
COSMOTHERM 3D 0
14 12 0 0 0 0 0 0 0 0 V2000
-4.6310 0.0519 0.0034 O 0 0 0 0 0 0 0 0 0 0 1
-3.6951 -0.3253 0.0029 H 0 0 0 0 0 0 0 0 0 0 2
-4.4754 1.0125 0.0103 H 0 0 0 0 0 0 0 0 0 0 3
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1.1952 0.3899 0.0013 C 0 0 0 0 0 0 0 0 0 0 0 0 4
0.1660 -0.4728 -0.0042 C 0 0 0 0 0 0 0 0 0 0 0 0 5
-1.2829 -0.0263 -0.0027 C 0 0 0 0 0 0 0 0 0 0 0 0 6
2.6022 -0.0622 0.0012 C 0 0 0 0 0 0 0 0 0 0 0 0 7
2.9944 -1.2250 -0.0019 O 0 0 0 0 0 0 0 0 0 0 0 0 8
3.4573 0.9976 0.0044 O 0 0 0 0 0 0 0 0 0 0 0 0 9
-2.1378 -0.9819 0.0030 O 0 0 0 0 0 0 0 0 0 0 0 0 10
-1.5419 1.2074 -0.0064 O 0 0 0 0 0 0 0 0 0 0 0 0 11
1.0098 1.4659 0.0053 H 0 0 0 0 0 0 0 0 0 0 0 0 12
0.3524 -1.5503 -0.0084 H 0 0 0 0 0 0 0 0 0 0 0 0 13
4.3743 0.6462 0.0033 H 0 0 0 0 0 0 0 0 0 0 0 0 14
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
7 4 0 0 0 0
12 4 0 0 0 0
6 5 0 0 0 0
13 5 0 0 0 0
10 6 0 0 0 0
11 6 0 0 0 0
8 7 0 0 0 0
9 7 0 0 0 0
9 14 0 0 0 0
M END
$$$$
fumaricacid.sdf
COSMOTHERM 3D 0
15 13 0 0 0 0 0 0 0 0 0 V2000
-4.6194 0.0106 0.1322 O 0 0 0 0 0 0 0 0 0 0 0 0 1
-4.9049 -0.8119 -0.3067 H 0 0 0 0 0 0 0 0 0 0 0 0 2
-4.8611 0.7205 -0.4910 H 0 0 0 0 0 0 0 0 0 0 0 0 3
1.2480 0.0004 -0.4144 C 0 0 0 0 0 0 0 0 0 0 0 0 4
0.1906 -0.0038 0.4109 C 0 0 0 0 0 0 0 0 0 0 0 0 5
-1.2042 -0.0035 -0.1175 C 0 0 0 0 0 0 0 0 0 0 0 0 6
2.6378 0.0007 0.1049 C 0 0 0 0 0 0 0 0 0 0 0 0 7
2.9621 -0.0066 1.2859 O 0 0 0 0 0 0 0 0 0 0 0 0 8
3.5336 0.0095 -0.9135 O 0 0 0 0 0 0 0 0 0 0 0 0 9
-2.1054 0.0087 0.8736 O 0 0 0 0 0 0 0 0 0 0 0 0 10
-1.4890 -0.0125 -1.3135 O 0 0 0 0 0 0 0 0 0 0 0 0 11
1.1126 0.0032 -1.4974 H 0 0 0 0 0 0 0 0 0 0 0 0 12
0.3222 -0.0058 1.4946 H 0 0 0 0 0 0 0 0 0 0 0 0 13
4.4370 0.0059 -0.5277 H 0 0 0 0 0 0 0 0 0 0 0 0 14
-3.0592 0.0084 0.4927 H 0 0 0 0 0 0 0 0 0 0 0 0 15
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
7 4 0 0 0 0
12 4 0 0 0 0
6 5 0 0 0 0
13 5 0 0 0 0
10 6 0 0 0 0
11 6 0 0 0 0
8 7 0 0 0 0
9 7 0 0 0 0
14 9 0 0 0 0
10 15 0 0 0 0
M END
$$$$
hypobromousacid-anion.sdf
COSMOTHERM 3D 0
5 2 0 0 0 0 0 0 0 0 0 V2000
-2.8958 -0.0595 0.3746 O 0 0 0 0 0 0 0 0 0 0 0 0 1
-1.9839 -0.0209 -0.1272 H 0 0 0 0 0 0 0 0 0 0 0 0 2
-3.1596 0.8710 0.4733 H 0 0 0 0 0 0 0 0 0 0 0 0 3
-0.7130 0.0041 -0.9832 O 0 0 0 0 0 0 0 0 0 0 0 0 4
0.7874 0.0004 0.1175 Br 0 0 0 0 0 0 0 0 0 0 0 0 5
2 1 0 0 0 0
3 1 0 0 0 0
M END
$$$$
hypobromousacid.sdf
COSMOTHERM 3D 0
6 3 0 0 0 0 0 0 0 0 0 V2000
-2.7993 -0.0165 0.4151 O 0 0 0 0 0 0 0 0 0 0 0 0 1
-3.4604 -0.6421 0.0660 H 0 0 0 0 0 0 0 0 0 0 0 0 2
-3.2525 0.8467 0.4140 H 0 0 0 0 0 0 0 0 0 0 0 0 3
-0.6180 0.0104 -1.0964 O 0 0 0 0 0 0 0 0 0 0 0 0 4
0.7871 -0.0014 0.1367 Br 0 0 0 0 0 0 0 0 0 0 0 0 5
-1.4453 0.0050 -0.5059 H 0 0 0 0 0 0 0 0 0 0 0 0 6
2 1 0 0 0 0
3 1 0 0 0 0
4 6 0 0 0 0
M END
$$$$
hypochlorousacid-anion.sdf
COSMOTHERM 3D 0
5 3 0 0 0 0 0 0 0 0 0 V2000
-2.3659 0.2896 0.0592 O 0 0 0 0 0 0 0 0 0 0 0 0 1
-1.4202 -0.1415 0.0162 H 0 0 0 0 0 0 0 0 0 0 0 0 2
-2.4965 0.6832 -0.8200 H 0 0 0 0 0 0 0 0 0 0 0 0 3
-0.0842 -0.9022 -0.0176 O 0 0 0 0 0 0 0 0 0 0 0 0 4
1.2171 0.2611 0.0041 Cl 0 0 0 0 0 0 0 0 0 0 0 0 5
2 1 0 0 0 0
3 1 0 0 0 0
4 5 0 0 0 0
M END
$$$$
hypochlorousacid.sdf
COSMOTHERM 3D 0
6 4 0 0 0 0 0 0 0 0 0 V2000
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```

-2.2723 -0.0113 0.3352 O 0 0 0 0 0 0 0 0 0 0 0 1
-2.8788 -0.6891 -0.0155 H 0 0 0 0 0 0 0 0 0 0 0 2
-2.7569 0.8289 0.2402 H 0 0 0 0 0 0 0 0 0 0 0 3
0.0126 0.0079 -0.9742 O 0 0 0 0 0 0 0 0 0 0 0 4
1.2047 -0.0025 0.2950 Cl 0 0 0 0 0 0 0 0 0 0 0 5
-0.8701 0.0027 -0.4595 H 0 0 0 0 0 0 0 0 0 0 0 6
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
4 6 0 0 0 0
M END
$$$$
hypoiodousacid-anion.sdf
COSMOTHERM 3D 0
5 2 0 0 0 0 0 0 0 0 0 V2000
-3.2394 -0.0573 -0.4281 O 0 0 0 0 0 0 0 0 0 0 0 1
-2.3436 -0.0217 0.1086 H 0 0 0 0 0 0 0 0 0 0 0 2
-3.5621 0.8599 -0.4295 H 0 0 0 0 0 0 0 0 0 0 0 3
-1.1204 -0.0008 1.0103 O 0 0 0 0 0 0 0 0 0 0 0 4
0.5966 0.0007 -0.0709 I 0 0 0 0 0 0 0 0 0 0 0 5
2 1 0 0 0 0
3 1 0 0 0 0
M END
$$$$
hypoiodousacid.sdf
COSMOTHERM 3D 0
6 3 0 0 0 0 0 0 0 0 0 V2000
-3.1660 0.0074 0.4760 O 0 0 0 0 0 0 0 0 0 0 0 1
-3.6826 -0.8135 0.3740 H 0 0 0 0 0 0 0 0 0 0 0 2
-3.7857 0.7190 0.2298 H 0 0 0 0 0 0 0 0 0 0 0 3
-1.0344 -0.0044 -1.1480 O 0 0 0 0 0 0 0 0 0 0 0 4
0.6034 0.0004 0.0840 I 0 0 0 0 0 0 0 0 0 0 0 5
-1.8226 0.0014 -0.5153 H 0 0 0 0 0 0 0 0 0 0 0 6
2 1 0 0 0 0
3 1 0 0 0 0
4 6 0 0 0 0
M END
$$$$
hypophosphorousacid-anion.sdf
COSMOTHERM 3D 0
8 6 0 0 0 0 0 0 0 0 0 V2000
-2.8099 -0.1697 0.3622 O 0 0 0 0 0 0 0 0 0 0 0 1
-1.9056 0.0768 -0.0066 H 0 0 0 0 0 0 0 0 0 0 0 2
-3.0263 0.5547 0.9736 H 0 0 0 0 0 0 0 0 0 0 0 3
-0.4335 0.4850 -0.6914 O 0 0 0 0 0 0 0 0 0 0 0 4
0.9001 -0.2271 -0.3075 P 0 0 0 0 0 0 0 0 0 0 0 5
1.6589 0.1955 0.9711 O 0 0 0 0 0 0 0 0 0 0 0 6
0.6487 -1.6457 -0.2622 H 0 0 0 0 0 0 0 0 0 0 0 7
1.7764 -0.1164 -1.4447 H 0 0 0 0 0 0 0 0 0 0 0 8
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 5 0 0 0 0
7 5 0 0 0 0
5 8 0 0 0 0
M END
$$$$
hypophosphorousacid.sdf
COSMOTHERM 3D 0
9 7 0 0 0 0 0 0 0 0 0 V2000
-0.4413 2.5662 -0.1387 O 0 0 0 0 0 0 0 0 0 0 0 1
0.1073 3.2172 -0.6141 H 0 0 0 0 0 0 0 0 0 0 0 2
-0.7671 3.0413 0.6479 H 0 0 0 0 0 0 0 0 0 0 0 3
0.2747 -0.6548 -1.6453 H 0 0 0 0 0 0 0 0 0 0 0 4
0.2783 -0.9412 -0.2484 P 0 0 0 0 0 0 0 0 0 0 0 5
1.3654 -1.8317 -0.0404 H 0 0 0 0 0 0 0 0 0 0 0 6
-1.0692 -1.4545 0.2526 O 0 0 0 0 0 0 0 0 0 0 0 7
0.8868 0.3942 0.4562 O 0 0 0 0 0 0 0 0 0 0 0 8
0.3675 1.2478 0.2356 H 0 0 0 0 0 0 0 0 0 0 0 9
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 5 0 0 0 0
7 5 0 0 0 0
8 5 0 0 0 0
8 9 0 0 0 0
M END
$$$$
iodoaceticacid-anion.sdf
COSMOTHERM 3D 0
10 7 0 0 0 0 0 0 0 0 0 V2000
-4.5085 -1.2652 0.0007 O 0 0 0 0 0 0 0 0 0 0 0 1
-3.5440 -0.9744 -0.0006 H 0 0 0 0 0 0 0 0 0 0 0 2
-4.9996 -0.4258 0.0231 H 0 0 0 0 0 0 0 0 0 0 0 3
1.3945 -0.1694 0.0000 I 0 0 0 0 0 0 0 0 0 0 0 4
-0.2970 1.2682 0.0029 C 0 0 0 0 0 0 0 0 0 0 0 5
-1.7130 0.6738 -0.0011 C 0 0 0 0 0 0 0 0 0 0 0 6
-1.8960 -0.5784 -0.0025 O 0 0 0 0 0 0 0 0 0 0 0 7
-2.5925 1.5809 -0.0019 O 0 0 0 0 0 0 0 0 0 0 0 8
-0.1307 1.8801 -0.8888 H 0 0 0 0 0 0 0 0 0 0 0 9
-0.1332 1.8735 0.8994 H 0 0 0 0 0 0 0 0 0 0 0 10
2 1 0 0 0 0
3 1 0 0 0 0
6 5 0 0 0 0
9 5 0 0 0 0
7 6 0 0 0 0
8 6 0 0 0 0
5 10 0 0 0 0
M END
$$$$

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9 8 0 0 0 0
10 8 0 0 0 0
5 12 0 0 0 0
M END
$$$$
nitroaceticacid.sdf
COSMOtherm 3D 0
13 11 0 0 0 0 0 0 0 0 0 V2000
-3.9122 0.0075 -0.2555 O 0 0 0 0 0 0 0 0 0 0 1
-4.1002 -0.7614 -0.8251 H 0 0 0 0 0 0 0 0 0 0 2
-4.0823 0.7858 -0.8180 H 0 0 0 0 0 0 0 0 0 0 3
-0.5400 0.0132 0.1148 C 0 0 0 0 0 0 0 0 0 0 4
0.7319 -0.0331 0.9693 C 0 0 0 0 0 0 0 0 0 0 5
-1.6069 -0.0517 0.9007 O 0 0 0 0 0 0 0 0 0 0 6
-0.5406 0.1019 -1.1033 O 0 0 0 0 0 0 0 0 0 0 7
1.9430 -0.0168 0.0788 N 0 0 0 0 0 0 0 0 0 0 8
2.4459 1.0793 -0.1856 O 0 0 0 0 0 0 0 0 0 0 9
2.3431 -1.1009 -0.3581 O 0 0 0 0 0 0 0 0 0 0 10
0.7853 0.8444 1.6225 H 0 0 0 0 0 0 0 0 0 0 11
0.7650 -0.9559 1.5581 H 0 0 0 0 0 0 0 0 0 0 12
-2.4860 -0.0174 0.3500 H 0 0 0 0 0 0 0 0 0 0 13
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
7 4 0 0 0 0
8 5 0 0 0 0
11 5 0 0 0 0
12 5 0 0 0 0
9 8 0 0 0 0
10 8 0 0 0 0
6 13 0 0 0 0
M END
$$$$
nitromethane-anion.sdf
COSMOtherm 3D 0
9 7 0 0 0 0 0 0 0 0 V2000
-2.5945 0.0071 -0.0427 O 0 0 0 0 0 0 0 0 0 0 1
-1.6366 -0.0137 -0.3581 H 0 0 0 0 0 0 0 0 0 0 2
-2.4955 0.0465 0.9244 H 0 0 0 0 0 0 0 0 0 0 3
2.1000 0.0136 -0.2417 C 0 0 0 0 0 0 0 0 0 0 4
0.7960 -0.0021 0.0082 N 0 0 0 0 0 0 0 0 0 0 5
-0.0694 -0.0112 -0.9931 O 0 0 0 0 0 0 0 0 0 0 6
0.3232 -0.0088 1.2167 O 0 0 0 0 0 0 0 0 0 0 7
2.7781 0.0204 0.6053 H 0 0 0 0 0 0 0 0 0 0 8
2.4233 0.0177 -1.2771 H 0 0 0 0 0 0 0 0 0 0 9
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
8 4 0 0 0 0
6 5 0 0 0 0
7 5 0 0 0 0
4 9 0 0 0 0
M END
$$$$
nitromethane.sdf
COSMOtherm 3D 0
10 8 0 0 0 0 0 0 0 0 V2000
-2.9359 0.0843 -0.0271 O 0 0 0 0 0 0 0 0 0 0 1
-3.2711 -0.8260 0.0452 H 0 0 0 0 0 0 0 0 0 0 2
-1.9759 -0.0253 -0.2029 H 0 0 0 0 0 0 0 0 0 0 3
2.2019 0.0384 -0.4329 C 0 0 0 0 0 0 0 0 0 0 4
0.7796 -0.0116 0.0367 N 0 0 0 0 0 0 0 0 0 0 5
0.5725 -0.0133 1.2512 O 0 0 0 0 0 0 0 0 0 0 6
-0.1175 -0.0458 -0.8230 O 0 0 0 0 0 0 0 0 0 0 7
2.2081 0.0087 -1.5236 H 0 0 0 0 0 0 0 0 0 0 8
2.6322 0.9679 -0.0444 H 0 0 0 0 0 0 0 0 0 0 9
2.7149 -0.8230 0.0078 H 0 0 0 0 0 0 0 0 0 0 10
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
8 4 0 0 0 0
9 4 0 0 0 0
6 5 0 0 0 0
7 5 0 0 0 0
4 10 0 0 0 0
M END
$$$$
nitrousacid-anion.sdf
COSMOtherm 3D 0
6 4 0 0 0 0 0 0 0 0 V2000
-1.0327 0.0013 -0.2995 O 0 0 0 0 0 0 0 0 0 0 1
-0.2103 -0.0023 -1.2866 N 0 0 0 0 0 0 0 0 0 0 2
1.0139 0.0012 -0.9815 O 0 0 0 0 0 0 0 0 0 0 3
1.1094 -0.0023 2.0527 H 0 0 0 0 0 0 0 0 0 0 4
0.1471 -0.0005 2.1983 O 0 0 0 0 0 0 0 0 0 0 5
-0.2245 0.0030 1.2667 H 0 0 0 0 0 0 0 0 0 0 6
2 1 0 0 0 0
3 2 0 0 0 0
5 4 0 0 0 0
5 6 0 0 0 0
M END
$$$$
nitrousacid.sdf
COSMOtherm 3D 0
7 5 0 0 0 0 0 0 0 0 V2000
-2.4332 -0.0005 -0.1442 O 0 0 0 0 0 0 0 0 0 0 1
0.0440 -0.0006 0.7156 O 0 0 0 0 0 0 0 0 0 0 2
0.8652 0.0001 -0.4228 N 0 0 0 0 0 0 0 0 0 0 3
2.0263 0.0004 -0.1356 O 0 0 0 0 0 0 0 0 0 0 4
```

URL: <http://mc.manuscriptcentral.com/tandf/tmph>


```
M END
$$$$
pentachlorophenol.sdf
COSMOTHERM 3D 0

16 15 0 0 0 0 0 0 0 0 V2000
-4.7676 0.0374 1.0985 O 0 0 0 0 0 0 0 0 0 0 1
-5.1921 -0.6217 0.5197 H 0 0 0 0 0 0 0 0 0 0 2
-5.1490 0.8901 0.8199 H 0 0 0 0 0 0 0 0 0 0 3
1.3527 0.0005 0.7238 C 0 0 0 0 0 0 0 0 0 0 4
0.1526 -0.0062 1.4435 C 0 0 0 0 0 0 0 0 0 0 5
-1.1010 -0.0095 0.7881 C 0 0 0 0 0 0 0 0 0 0 6
-1.1000 -0.0086 -0.6230 C 0 0 0 0 0 0 0 0 0 0 7
0.0996 -0.0018 -1.3507 C 0 0 0 0 0 0 0 0 0 0 8
1.3334 0.0029 -0.6817 C 0 0 0 0 0 0 0 0 0 0 9
-2.1954 -0.0177 1.5574 O 0 0 0 0 0 0 0 0 0 0 10
0.1538 -0.0092 3.1918 Cl 0 0 0 0 0 0 0 0 0 0 11
2.8778 0.0058 1.5753 Cl 0 0 0 0 0 0 0 0 0 0 12
2.8295 0.0117 -1.5858 Cl 0 0 0 0 0 0 0 0 0 0 13
0.0538 0.0001 -3.0971 Cl 0 0 0 0 0 0 0 0 0 0 14
-2.6405 -0.0172 -1.4535 Cl 0 0 0 0 0 0 0 0 0 0 15
-3.0955 0.0015 1.0903 H 0 0 0 0 0 0 0 0 0 0 16

2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
9 4 0 0 0 0
12 4 0 0 0 0
6 5 0 0 0 0
11 5 0 0 0 0
7 6 0 0 0 0
10 6 0 0 0 0
8 7 0 0 0 0
15 7 0 0 0 0
9 8 0 0 0 0
14 8 0 0 0 0
13 9 0 0 0 0
10 16 0 0 0 0

M END
$$$$
phenol--anion.sdf
COSMOTHERM 3D 0

15 14 0 0 0 0 0 0 0 0 V2000
-3.5738 0.0043 -0.4792 O 0 0 0 0 0 0 0 0 0 0 1
-2.7002 -0.0038 0.0655 H 0 0 0 0 0 0 0 0 0 0 2
-3.5120 0.8038 -1.0289 H 0 0 0 0 0 0 0 0 0 0 3
2.2149 0.0402 0.7436 C 0 0 0 0 0 0 0 0 0 0 4
0.9349 0.0182 1.3011 C 0 0 0 0 0 0 0 0 0 0 5
-0.2430 -0.0250 0.4872 C 0 0 0 0 0 0 0 0 0 0 6
-0.0221 -0.0452 -0.9284 C 0 0 0 0 0 0 0 0 0 0 7
1.2642 -0.0223 -1.4718 C 0 0 0 0 0 0 0 0 0 0 8
2.4009 0.0205 -0.6486 C 0 0 0 0 0 0 0 0 0 0 9
-1.4423 -0.0460 1.0182 O 0 0 0 0 0 0 0 0 0 0 10
3.0851 0.0733 1.4059 H 0 0 0 0 0 0 0 0 0 0 11
0.8055 0.0343 2.3873 H 0 0 0 0 0 0 0 0 0 0 12
-0.8946 -0.0837 -1.5866 H 0 0 0 0 0 0 0 0 0 0 13
1.3835 -0.0393 -2.5593 H 0 0 0 0 0 0 0 0 0 0 14
3.4036 0.0387 -1.0794 H 0 0 0 0 0 0 0 0 0 0 15

2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
9 4 0 0 0 0
11 4 0 0 0 0
6 5 0 0 0 0
12 5 0 0 0 0
7 6 0 0 0 0
10 6 0 0 0 0
8 7 0 0 0 0
13 7 0 0 0 0
9 8 0 0 0 0
14 8 0 0 0 0
9 15 0 0 0 0

M END
$$$$
phenol.sdf
COSMOTHERM 3D 0

16 15 0 0 0 0 0 0 0 0 V2000
-3.5672 -0.0001 -0.4511 O 0 0 0 0 0 0 0 0 0 0 1
-3.7241 -0.7853 -1.0059 H 0 0 0 0 0 0 0 0 0 0 2
-3.6989 0.7573 -1.0495 H 0 0 0 0 0 0 0 0 0 0 3
2.2597 -0.0013 0.7048 C 0 0 0 0 0 0 0 0 0 0 4
0.9926 -0.0006 1.2935 C 0 0 0 0 0 0 0 0 0 0 5
-0.1586 0.0009 0.4853 C 0 0 0 0 0 0 0 0 0 0 6
-0.0223 0.0012 -0.9150 C 0 0 0 0 0 0 0 0 0 0 7
1.2526 0.0003 -1.4911 C 0 0 0 0 0 0 0 0 0 0 8
2.4008 -0.0009 -0.6899 C 0 0 0 0 0 0 0 0 0 0 9
-1.3742 0.0022 1.1101 O 0 0 0 0 0 0 0 0 0 0 10
3.1451 -0.0024 1.3439 H 0 0 0 0 0 0 0 0 0 0 11
0.8786 -0.0010 2.3793 H 0 0 0 0 0 0 0 0 0 0 12
-0.9125 0.0020 -1.5471 H 0 0 0 0 0 0 0 0 0 0 13
1.3447 0.0006 -2.5793 H 0 0 0 0 0 0 0 0 0 0 14
3.3924 -0.0014 -1.1451 H 0 0 0 0 0 0 0 0 0 0 15
-2.1240 0.0007 0.4429 H 0 0 0 0 0 0 0 0 0 0 16

2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
9 4 0 0 0 0
11 4 0 0 0 0
6 5 0 0 0 0
12 5 0 0 0 0
7 6 0 0 0 0
10 6 0 0 0 0
8 7 0 0 0 0
13 7 0 0 0 0
```

9 8 0 0 0 0
14 8 0 0 0 0
15 9 0 0 0 0
10 16 0 0 0 0

M END

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phenytoin-anion.sdf
COSMOtherm 3D

0

33 34 0 0 0 0 0 0 0 0 0 V2000
-4.8650 -1.2640 0.8897 O 0 0 0 0 0 0 0 0 0 0 1
-3.9569 -0.8562 0.7072 H 0 0 0 0 0 0 0 0 0 0 2
-5.1347 -0.8783 1.7408 H 0 0 0 0 0 0 0 0 0 0 3
-2.3916 -0.1564 0.3786 N 0 0 0 0 0 0 0 0 0 0 4
-2.1674 1.1978 0.1775 C 0 0 0 0 0 0 0 0 0 0 5
-1.2079 -0.8091 0.3120 C 0 0 0 0 0 0 0 0 0 0 6
-0.0363 0.2205 0.0373 C 0 0 0 0 0 0 0 0 0 0 7
-0.8051 1.4635 0.1115 N 0 0 0 0 0 0 0 0 0 0 8
0.5664 0.0549 -1.3657 C 0 0 0 0 0 0 0 0 0 0 9
1.0103 0.0912 1.1444 C 0 0 0 0 0 0 0 0 0 0 10
-3.0453 2.0760 0.0879 O 0 0 0 0 0 0 0 0 0 0 11
-1.0159 -2.0286 0.4425 O 0 0 0 0 0 0 0 0 0 0 12
1.9639 0.8054 3.2680 C 0 0 0 0 0 0 0 0 0 0 13
1.0295 0.9693 2.2379 C 0 0 0 0 0 0 0 0 0 0 14
1.9403 -0.9620 1.1065 C 0 0 0 0 0 0 0 0 0 0 15
2.8697 -1.1297 2.1370 C 0 0 0 0 0 0 0 0 0 0 16
2.8868 -0.2449 3.2228 C 0 0 0 0 0 0 0 0 0 0 17
-0.0151 -0.7689 -2.3416 C 0 0 0 0 0 0 0 0 0 0 18
0.5187 -0.8276 -3.6355 C 0 0 0 0 0 0 0 0 0 0 19
1.6379 -0.0609 -3.9736 C 0 0 0 0 0 0 0 0 0 0 20
2.2252 0.7649 -3.0068 C 0 0 0 0 0 0 0 0 0 0 21
1.6962 0.8169 -1.7143 C 0 0 0 0 0 0 0 0 0 0 22
-0.4867 2.3107 -0.3543 H 0 0 0 0 0 0 0 0 0 0 23
1.9693 1.5028 4.1083 H 0 0 0 0 0 0 0 0 0 0 24
0.3093 1.7879 2.2766 H 0 0 0 0 0 0 0 0 0 0 25
1.9370 -1.6531 0.2626 H 0 0 0 0 0 0 0 0 0 0 26
3.5860 -1.9526 2.0902 H 0 0 0 0 0 0 0 0 0 0 27
3.6170 -0.3719 4.0244 H 0 0 0 0 0 0 0 0 0 0 28
-0.8839 -1.3806 -2.0951 H 0 0 0 0 0 0 0 0 0 0 29
0.0558 -1.4784 -4.3800 H 0 0 0 0 0 0 0 0 0 0 30
2.0533 -0.1081 -4.9819 H 0 0 0 0 0 0 0 0 0 0 31
3.1009 1.3666 -3.2579 H 0 0 0 0 0 0 0 0 0 0 32
2.1688 1.4567 -0.9656 H 0 0 0 0 0 0 0 0 0 0 33

2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
8 5 0 0 0 0
11 5 0 0 0 0
7 6 0 0 0 0
12 6 0 0 0 0
8 7 0 0 0 0
9 7 0 0 0 0
10 7 0 0 0 0
23 8 0 0 0 0
18 9 0 0 0 0
22 9 0 0 0 0
14 10 0 0 0 0
15 10 0 0 0 0
14 13 0 0 0 0
17 13 0 0 0 0
24 13 0 0 0 0
25 14 0 0 0 0
16 15 0 0 0 0
26 15 0 0 0 0
17 16 0 0 0 0
27 16 0 0 0 0
28 17 0 0 0 0
19 18 0 0 0 0
29 18 0 0 0 0
20 19 0 0 0 0
30 19 0 0 0 0
21 20 0 0 0 0
31 20 0 0 0 0
22 21 0 0 0 0
32 21 0 0 0 0
22 33 0 0 0 0

M END

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phenytoin.sdf
COSMOtherm 3D

0

34 35 0 0 0 0 0 0 0 0 0 V2000
-4.9128 -0.4614 -1.2180 O 0 0 0 0 0 0 0 0 0 0 1
-5.0153 -1.2380 -1.7978 H 0 0 0 0 0 0 0 0 0 0 2
-5.1697 0.2938 -1.7777 H 0 0 0 0 0 0 0 0 0 0 3
-2.3532 -0.1929 -0.1021 N 0 0 0 0 0 0 0 0 0 0 4
-2.1391 -0.0434 1.2838 C 0 0 0 0 0 0 0 0 0 0 5
-1.1890 -0.1637 -0.8212 C 0 0 0 0 0 0 0 0 0 0 6
-0.0217 -0.0078 0.2136 C 0 0 0 0 0 0 0 0 0 0 7
-0.7860 -0.0135 1.4686 N 0 0 0 0 0 0 0 0 0 0 8
0.7178 1.3301 0.0565 C 0 0 0 0 0 0 0 0 0 0 9
0.9014 -1.2253 0.0734 C 0 0 0 0 0 0 0 0 0 0 10
-3.0216 0.0342 2.1374 O 0 0 0 0 0 0 0 0 0 0 11
-1.0721 -0.2559 -2.0366 O 0 0 0 0 0 0 0 0 0 0 12
1.6667 -3.4134 0.8039 C 0 0 0 0 0 0 0 0 0 0 13
0.8400 -2.2962 0.9748 C 0 0 0 0 0 0 0 0 0 0 14
1.7930 -1.2932 -1.0104 C 0 0 0 0 0 0 0 0 0 0 15
2.6114 -2.4119 -1.1839 C 0 0 0 0 0 0 0 0 0 0 16
2.5529 -3.4760 -0.2753 C 0 0 0 0 0 0 0 0 0 0 17
0.1607 2.4059 -0.6516 C 0 0 0 0 0 0 0 0 0 0 18
0.8205 3.6394 -0.7015 C 0 0 0 0 0 0 0 0 0 0 19
2.0395 3.8142 -0.0389 C 0 0 0 0 0 0 0 0 0 0 20
2.5982 2.7469 0.6741 C 0 0 0 0 0 0 0 0 0 0 21
1.9437 1.5126 0.7177 C 0 0 0 0 0 0 0 0 0 0 22

[illegible]

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-1.1071 -0.0316 -2.3094 O 0 0 0 0 0 0 0 0 0 0 0 14
4.0814 0.0459 -1.2174 H 0 0 0 0 0 0 0 0 0 0 0 15
4.0668 0.0472 1.2569 H 0 0 0 0 0 0 0 0 0 0 0 16
1.9016 0.0136 2.5243 H 0 0 0 0 0 0 0 0 0 0 0 17
1.9314 0.0094 -2.5102 H 0 0 0 0 0 0 0 0 0 0 0 18
2 1 0 0 0 0 0
3 1 0 0 0 0 0
5 4 0 0 0 0 0
9 4 0 0 0 0 0
15 4 0 0 0 0 0
6 5 0 0 0 0 0
16 5 0 0 0 0 0
7 6 0 0 0 0 0
17 6 0 0 0 0 0
8 7 0 0 0 0 0
11 7 0 0 0 0 0
9 8 0 0 0 0 0
10 8 0 0 0 0 0
12 10 0 0 0 0 0
14 10 0 0 0 0 0
12 11 0 0 0 0 0
13 11 0 0 0 0 0
9 18 0 0 0 0 0
M END
$$$$
phthalimide.sdf
COSMOtherm 3D 0
19 19 0 0 0 0 0 0 0 0 0 V2000
-4.2758 -0.0009 0.0432 O 0 0 0 0 0 0 0 0 0 0 0 1
-4.6637 -0.7828 -0.3898 H 0 0 0 0 0 0 0 0 0 0 0 2
-4.6682 0.7555 -0.4295 H 0 0 0 0 0 0 0 0 0 0 0 3
3.1453 -0.0010 0.6834 C 0 0 0 0 0 0 0 0 0 0 0 4
3.1353 -0.0010 -0.7193 C 0 0 0 0 0 0 0 0 0 0 0 5
1.9270 -0.0004 -1.4364 C 0 0 0 0 0 0 0 0 0 0 0 6
0.7469 0.0002 -0.7020 C 0 0 0 0 0 0 0 0 0 0 0 7
0.7568 0.0001 0.7006 C 0 0 0 0 0 0 0 0 0 0 0 8
1.9474 -0.0003 1.4179 C 0 0 0 0 0 0 0 0 0 0 0 9
-0.6632 0.0010 1.1718 C 0 0 0 0 0 0 0 0 0 0 0 10
-0.6794 0.0008 -1.1526 C 0 0 0 0 0 0 0 0 0 0 0 11
-1.4487 0.0015 0.0150 N 0 0 0 0 0 0 0 0 0 0 0 12
-1.1242 0.0008 -2.2962 O 0 0 0 0 0 0 0 0 0 0 0 13
-1.0907 0.0012 2.3220 O 0 0 0 0 0 0 0 0 0 0 0 14
-2.4936 0.0012 0.0171 H 0 0 0 0 0 0 0 0 0 0 0 15
4.0996 -0.0015 1.2122 H 0 0 0 0 0 0 0 0 0 0 0 16
4.0818 -0.0015 -1.2617 H 0 0 0 0 0 0 0 0 0 0 0 17
1.9184 -0.0003 -2.5272 H 0 0 0 0 0 0 0 0 0 0 0 18
1.9548 -0.0004 2.5087 H 0 0 0 0 0 0 0 0 0 0 0 19
2 1 0 0 0 0 0
3 1 0 0 0 0 0
5 4 0 0 0 0 0
9 4 0 0 0 0 0
16 4 0 0 0 0 0
6 5 0 0 0 0 0
17 5 0 0 0 0 0
7 6 0 0 0 0 0
18 6 0 0 0 0 0
8 7 0 0 0 0 0
11 7 0 0 0 0 0
9 8 0 0 0 0 0
10 8 0 0 0 0 0
12 10 0 0 0 0 0
14 10 0 0 0 0 0
12 11 0 0 0 0 0
13 11 0 0 0 0 0
15 12 0 0 0 0 0
9 19 0 0 0 0 0
M END
$$$$
salicylicacid-anion.sdf
COSMOtherm 3D 0
18 18 0 0 0 0 0 0 0 0 0 V2000
-4.5414 -0.4262 0.0222 O 0 0 0 0 0 0 0 0 0 0 0 1
-3.5514 -0.5993 0.0083 H 0 0 0 0 0 0 0 0 0 0 0 2
-4.6069 0.5402 -0.0662 H 0 0 0 0 0 0 0 0 0 0 0 3
2.2980 -1.7028 0.0008 C 0 0 0 0 0 0 0 0 0 0 0 4
3.1516 -0.5862 0.0066 C 0 0 0 0 0 0 0 0 0 0 0 5
2.6317 0.7072 0.0075 C 0 0 0 0 0 0 0 0 0 0 0 6
1.2378 0.9084 0.0025 C 0 0 0 0 0 0 0 0 0 0 0 7
0.3625 -0.2147 -0.0040 C 0 0 0 0 0 0 0 0 0 0 0 8
0.9173 -1.5059 -0.0046 C 0 0 0 0 0 0 0 0 0 0 0 9
0.7456 2.1693 0.0032 O 0 0 0 0 0 0 0 0 0 0 0 10
-1.1282 -0.0074 -0.0091 C 0 0 0 0 0 0 0 0 0 0 0 11
-1.8968 -1.0132 -0.0102 O 0 0 0 0 0 0 0 0 0 0 0 12
-1.5444 1.2159 -0.0120 O 0 0 0 0 0 0 0 0 0 0 0 13
2.7119 -2.7123 0.0001 H 0 0 0 0 0 0 0 0 0 0 0 14
4.2346 -0.7276 0.0106 H 0 0 0 0 0 0 0 0 0 0 0 15
3.2894 1.5787 0.0122 H 0 0 0 0 0 0 0 0 0 0 0 16
0.2330 -2.3563 -0.0093 H 0 0 0 0 0 0 0 0 0 0 0 17
-0.2935 2.0056 -0.0033 H 0 0 0 0 0 0 0 0 0 0 0 18
2 1 0 0 0 0 0
3 1 0 0 0 0 0
5 4 0 0 0 0 0
9 4 0 0 0 0 0
14 4 0 0 0 0 0
6 5 0 0 0 0 0
15 5 0 0 0 0 0
7 6 0 0 0 0 0
16 6 0 0 0 0 0
8 7 0 0 0 0 0
10 7 0 0 0 0 0
9 8 0 0 0 0 0
11 8 0 0 0 0 0
17 9 0 0 0 0 0
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12 11 0 0 0 0
13 11 0 0 0 0
10 18 0 0 0 0
13 18 0 0 0 0
M END
$$$$
salicylicacid.sdf
COSMOTHERM 3D 0
19 18 0 0 0 0 0 0 0 0 0 V2000
-4.4471 -0.0150 0.4652 O 0 0 0 0 0 0 0 0 0 0 1
-4.7314 -0.5387 -0.3066 H 0 0 0 0 0 0 0 0 0 0 2
-4.8093 0.8765 0.3073 H 0 0 0 0 0 0 0 0 0 0 3
2.2205 0.0040 1.7646 C 0 0 0 0 0 0 0 0 0 0 4
3.1266 0.0043 0.6887 C 0 0 0 0 0 0 0 0 0 0 5
2.6732 0.0010 -0.6274 C 0 0 0 0 0 0 0 0 0 0 6
1.2932 -0.0015 -0.8973 C 0 0 0 0 0 0 0 0 0 0 7
0.3658 -0.0030 0.1836 C 0 0 0 0 0 0 0 0 0 0 8
0.8545 -0.0003 1.5070 C 0 0 0 0 0 0 0 0 0 0 9
0.8866 -0.0025 -2.1892 O 0 0 0 0 0 0 0 0 0 0 10
-1.0772 -0.0017 -0.1154 C 0 0 0 0 0 0 0 0 0 0 11
-1.5136 0.0122 -1.2887 O 0 0 0 0 0 0 0 0 0 0 12
-1.8841 -0.0192 0.9416 O 0 0 0 0 0 0 0 0 0 0 13
2.5858 0.0076 2.7919 H 0 0 0 0 0 0 0 0 0 0 14
4.2009 0.0081 0.8829 H 0 0 0 0 0 0 0 0 0 0 15
3.3715 0.0020 -1.4656 H 0 0 0 0 0 0 0 0 0 0 16
0.1384 -0.0001 2.3290 H 0 0 0 0 0 0 0 0 0 0 17
-0.1246 0.0071 -2.1500 H 0 0 0 0 0 0 0 0 0 0 18
-2.8706 -0.0081 0.6513 H 0 0 0 0 0 0 0 0 0 0 19
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
9 4 0 0 0 0
14 4 0 0 0 0
6 5 0 0 0 0
15 5 0 0 0 0
7 6 0 0 0 0
16 6 0 0 0 0
8 7 0 0 0 0
10 7 0 0 0 0
9 8 0 0 0 0
11 8 0 0 0 0
17 9 0 0 0 0
18 10 0 0 0 0
12 11 0 0 0 0
13 11 0 0 0 0
13 19 0 0 0 0
M END
$$$$
succinimide-anion.sdf
COSMOTHERM 3D 0
14 13 0 0 0 0 0 0 0 0 0 V2000
-3.1345 -0.3613 -0.0460 O 0 0 0 0 0 0 0 0 0 0 1
-2.1233 -0.2684 -0.0163 H 0 0 0 0 0 0 0 0 0 0 2
-3.4574 0.3853 0.4872 H 0 0 0 0 0 0 0 0 0 0 3
1.7388 1.0098 -0.0105 C 0 0 0 0 0 0 0 0 0 0 4
0.2069 1.1367 0.0024 C 0 0 0 0 0 0 0 0 0 0 5
1.9693 -0.5017 -0.0128 C 0 0 0 0 0 0 0 0 0 0 6
0.5450 -1.0799 0.0067 C 0 0 0 0 0 0 0 0 0 0 7
-0.4031 -0.0906 0.0139 N 0 0 0 0 0 0 0 0 0 0 8
0.2983 -2.3012 0.0140 O 0 0 0 0 0 0 0 0 0 0 9
-0.3939 2.2281 0.0052 O 0 0 0 0 0 0 0 0 0 0 10
2.1519 1.5190 0.8723 H 0 0 0 0 0 0 0 0 0 0 11
2.1383 1.5208 -0.8984 H 0 0 0 0 0 0 0 0 0 0 12
2.5222 -0.8677 0.8644 H 0 0 0 0 0 0 0 0 0 0 13
2.4960 -0.8676 -0.9061 H 0 0 0 0 0 0 0 0 0 0 14
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
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11 4 0 0 0 0
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8 5 0 0 0 0
10 5 0 0 0 0
7 6 0 0 0 0
13 6 0 0 0 0
8 7 0 0 0 0
9 7 0 0 0 0
6 14 0 0 0 0
M END
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succinimide.sdf
COSMOTHERM 3D 0
15 14 0 0 0 0 0 0 0 0 0 V2000
-3.1705 -0.0001 0.1081 O 0 0 0 0 0 0 0 0 0 0 1
-3.5705 -0.7714 -0.3329 H 0 0 0 0 0 0 0 0 0 0 2
-3.5728 0.7670 -0.3381 H 0 0 0 0 0 0 0 0 0 0 3
1.9147 -0.0003 0.7222 C 0 0 0 0 0 0 0 0 0 0 4
0.4556 0.0001 1.1569 C 0 0 0 0 0 0 0 0 0 0 5
1.8742 -0.0003 -0.8131 C 0 0 0 0 0 0 0 0 0 0 6
0.3941 0.0001 -1.1697 C 0 0 0 0 0 0 0 0 0 0 7
-0.3332 0.0000 0.0137 N 0 0 0 0 0 0 0 0 0 0 8
-0.1023 0.0004 -2.2923 O 0 0 0 0 0 0 0 0 0 0 9
0.0199 0.0004 2.3046 O 0 0 0 0 0 0 0 0 0 0 10
2.4094 -0.8855 1.1449 H 0 0 0 0 0 0 0 0 0 0 11
2.4099 0.8846 1.1449 H 0 0 0 0 0 0 0 0 0 0 12
2.3459 -0.8855 -1.2613 H 0 0 0 0 0 0 0 0 0 0 13
2.3463 0.8846 -1.2612 H 0 0 0 0 0 0 0 0 0 0 14
-1.3784 0.0005 0.0375 H 0 0 0 0 0 0 0 0 0 0 15
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
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11 4 0 0 0 0
12 4 0 0 0 0
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10 5 0 0 0 0
7 6 0 0 0 0
13 6 0 0 0 0
14 6 0 0 0 0
8 7 0 0 0 0
9 7 0 0 0 0
8 15 0 0 0 0
M END
$$$$
sulfurousacid-anion.sdf
COSMOTHERM 3D 0
8 6 0 0 0 0 0 0 0 0 0 V2000
-2.4129 -0.0777 0.4723 O 0 0 0 0 0 0 0 0 0 0 1
-0.1362 1.4151 -0.3776 O 0 0 0 0 0 0 0 0 0 0 2
0.8751 -0.0444 -0.3264 S 0 0 0 0 0 0 0 0 0 0 3
1.3459 -0.1055 1.1345 O 0 0 0 0 0 0 0 0 0 0 4
-0.1831 -1.1680 -0.5690 O 0 0 0 0 0 0 0 0 0 0 5
-1.0105 1.1348 0.0115 H 0 0 0 0 0 0 0 0 0 0 6
-3.1084 -0.0451 -0.2086 H 0 0 0 0 0 0 0 0 0 0 7
-1.7150 -0.6921 0.0993 H 0 0 0 0 0 0 0 0 0 0 8
7 1 0 0 0 0
3 2 0 0 0 0
6 2 0 0 0 0
4 3 0 0 0 0
5 3 0 0 0 0
1 8 0 0 0 0
M END
$$$$
sulfurousacid.sdf
COSMOTHERM 3D 0
9 7 0 0 0 0 0 0 0 0 0 V2000
-2.2515 -0.0001 0.3788 O 0 0 0 0 0 0 0 0 0 0 1
-2.5222 0.0116 1.3157 H 0 0 0 0 0 0 0 0 0 0 2
-3.0823 -0.0061 -0.1323 H 0 0 0 0 0 0 0 0 0 0 3
0.9256 0.0012 -0.2169 S 0 0 0 0 0 0 0 0 0 0 4
-0.0693 -1.2979 -0.6307 O 0 0 0 0 0 0 0 0 0 0 5
-0.0817 1.2839 -0.6496 O 0 0 0 0 0 0 0 0 0 0 6
1.0223 0.0125 1.2879 O 0 0 0 0 0 0 0 0 0 0 7
-0.9597 -1.1324 -0.1988 H 0 0 0 0 0 0 0 0 0 0 8
-0.9720 1.1131 -0.2171 H 0 0 0 0 0 0 0 0 0 0 9
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
7 4 0 0 0 0
8 5 0 0 0 0
6 9 0 0 0 0
M END
$$$$
tert-butanol-anion.sdf
COSMOTHERM 3D 0
17 16 0 0 0 0 0 0 0 0 0 V2000
-2.6693 -0.0044 0.0878 O 0 0 0 0 0 0 0 0 0 0 1
-1.4218 -0.0208 0.5344 H 0 0 0 0 0 0 0 0 0 0 2
-2.5795 0.0638 -0.8775 H 0 0 0 0 0 0 0 0 0 0 3
0.6201 0.0000 -0.0066 C 0 0 0 0 0 0 0 0 0 0 4
0.4773 1.2893 -0.8457 C 0 0 0 0 0 0 0 0 0 0 5
0.4914 -1.2346 -0.9264 C 0 0 0 0 0 0 0 0 0 0 6
1.9936 -0.0132 0.6840 C 0 0 0 0 0 0 0 0 0 0 7
1.2402 1.3548 -1.6384 H 0 0 0 0 0 0 0 0 0 0 8
0.6123 -2.1563 -0.3362 H 0 0 0 0 0 0 0 0 0 0 9
2.0925 0.8587 1.3490 H 0 0 0 0 0 0 0 0 0 0 10
1.2468 -1.2354 -1.7290 H 0 0 0 0 0 0 0 0 0 0 11
-0.5155 1.3254 -1.3198 H 0 0 0 0 0 0 0 0 0 0 12
0.5769 2.1727 -0.1960 H 0 0 0 0 0 0 0 0 0 0 13
2.1033 -0.9240 1.2927 H 0 0 0 0 0 0 0 0 0 0 14
-0.5061 -1.2560 -1.3911 H 0 0 0 0 0 0 0 0 0 0 15
2.8168 0.0154 -0.0477 H 0 0 0 0 0 0 0 0 0 0 16
-0.3770 -0.0393 1.0087 O 0 0 0 0 0 0 0 0 0 0 17
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
7 4 0 0 0 0
8 5 0 0 0 0
12 5 0 0 0 0
13 5 0 0 0 0
9 6 0 0 0 0
11 6 0 0 0 0
15 6 0 0 0 0
10 7 0 0 0 0
14 7 0 0 0 0
16 7 0 0 0 0
2 17 0 0 0 0
4 17 0 0 0 0
M END
$$$$
tert-butanol.sdf
COSMOTHERM 3D 0
18 16 0 0 0 0 0 0 0 0 0 V2000
-2.9378 0.0008 0.0920 O 0 0 0 0 0 0 0 0 0 0 1
-3.2268 -0.7770 -0.4184 H 0 0 0 0 0 0 0 0 0 0 2
-3.2135 0.7599 -0.4527 H 0 0 0 0 0 0 0 0 0 0 3
0.7440 0.0005 -0.0308 C 0 0 0 0 0 0 0 0 0 0 4
0.5994 1.2815 -0.8674 C 0 0 0 0 0 0 0 0 0 0 5
0.5960 -1.2458 -0.9177 C 0 0 0 0 0 0 0 0 0 0 6
2.0843 -0.0160 0.7078 C 0 0 0 0 0 0 0 0 0 0 7
1.3747 1.3361 -1.6468 H 0 0 0 0 0 0 0 0 0 0 8
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2
3      0.6815   -2.1592   -0.3109 H   0   0   0   0   0   0   0   0   0   0   9
4      2.1727    0.8631    1.3633 H   0   0   0   0   0   0   0   0   0   0  10
5      1.3726   -1.2730   -1.6973 H   0   0   0   0   0   0   0   0   0   0  11
6     -0.3820    1.3111   -1.3652 H   0   0   0   0   0   0   0   0   0   0  12
7      0.6903    2.1700   -0.2254 H   0   0   0   0   0   0   0   0   0   0  13
8      2.1712   -0.9218    1.3260 H   0   0   0   0   0   0   0   0   0   0  14
9     -0.3846   -1.2518   -1.4180 H   0   0   0   0   0   0   0   0   0   0  15
10     2.9214   -0.0015   -0.0049 H   0   0   0   0   0   0   0   0   0   0  16
11    -0.2728   -0.0188    1.0092 O   0   0   0   0   0   0   0   0   0   0  17
12    -1.1638   -0.0107    0.5760 H   0   0   0   0   0   0   0   0   0   0  18
13
14  2   1   0   0   0   0   0
15  3   1   0   0   0   0   0
16  5   4   0   0   0   0   0
17  6   4   0   0   0   0   0
18  7   4   0   0   0   0   0
19 17   4   0   0   0   0   0
20  8   5   0   0   0   0   0
21 12   5   0   0   0   0   0
22 13   5   0   0   0   0   0
23  9   6   0   0   0   0   0
24 11   6   0   0   0   0   0
25 15   6   0   0   0   0   0
26 10   7   0   0   0   0   0
27 14   7   0   0   0   0   0
28 16   7   0   0   0   0   0
29 17  18   0   0   0   0   0
30 M  END
31 $$$$
32 thymine-anion.sdf
33 COSMOTHERM      3D      0
34
35 17 16   0   0   0   0   0   0   0   0   0   0 V2000
36   -3.7378   -0.0331   -1.2111 O   0   0   0   0   0   0   0   0   0   0   1
37   -2.7966   -0.0211   -0.8297 H   0   0   0   0   0   0   0   0   0   0   2
38   -3.9778    0.9064   -1.2859 H   0   0   0   0   0   0   0   0   0   0   3
39   -0.1453   -0.0164   -1.2008 C   0   0   0   0   0   0   0   0   0   0   4
40    1.2114   -0.0046   -0.9356 C   0   0   0   0   0   0   0   0   0   0   5
41    1.6108    0.0075    0.4488 C   0   0   0   0   0   0   0   0   0   0   6
42    0.5393    0.0056    1.3502 N   0   0   0   0   0   0   0   0   0   0   7
43   -0.8289   -0.0083    1.0333 C   0   0   0   0   0   0   0   0   0   0   8
44   -1.1548   -0.0192   -0.2910 N   0   0   0   0   0   0   0   0   0   0   9
45    2.7886    0.0188    0.8810 O   0   0   0   0   0   0   0   0   0   0  10
46   -1.6703   -0.0102    1.9637 O   0   0   0   0   0   0   0   0   0   0  11
47    2.2619   -0.0025   -2.0100 C   0   0   0   0   0   0   0   0   0   0  12
48   -0.4755   -0.0249   -2.2461 H   0   0   0   0   0   0   0   0   0   0  13
49    0.7771    0.0134    2.3432 H   0   0   0   0   0   0   0   0   0   0  14
50    2.9337   -0.8714   -1.9219 H   0   0   0   0   0   0   0   0   0   0  15
51    2.8988    0.8952   -1.9547 H   0   0   0   0   0   0   0   0   0   0  16
52    1.7983   -0.0295   -3.0059 H   0   0   0   0   0   0   0   0   0   0  17
53
54  2   1   0   0   0   0   0
55  3   1   0   0   0   0   0
56  5   4   0   0   0   0   0
57  9   4   0   0   0   0   0
58 13   4   0   0   0   0   0
59  6   5   0   0   0   0   0
60 12   5   0   0   0   0   0
61  7   6   0   0   0   0   0
62 10   6   0   0   0   0   0
63  8   7   0   0   0   0   0
64 14   7   0   0   0   0   0
65  9   8   0   0   0   0   0
66 11   8   0   0   0   0   0
67 15  12   0   0   0   0   0
68 16  12   0   0   0   0   0
69 12  17   0   0   0   0   0
70 M  END
71 $$$$
72 thymine.sdf
73 COSMOTHERM      3D      0
74
75 18 17   0   0   0   0   0   0   0   0   0   0 V2000
76   -3.7154   -0.0052    1.2303 O   0   0   0   0   0   0   0   0   0   0   1
77   -4.2437   -0.7725    0.9453 H   0   0   0   0   0   0   0   0   0   0   2
78   -4.2467    0.7668    0.9637 H   0   0   0   0   0   0   0   0   0   0   3
79   -0.1090    0.0032    1.2297 C   0   0   0   0   0   0   0   0   0   0   4
80    1.2269    0.0013    0.9517 C   0   0   0   0   0   0   0   0   0   0   5
81    1.6299   -0.0013   -0.4472 C   0   0   0   0   0   0   0   0   0   0   6
82    0.5667   -0.0016   -1.3677 N   0   0   0   0   0   0   0   0   0   0   7
83   -0.7943    0.0018   -1.0914 C   0   0   0   0   0   0   0   0   0   0   8
84   -1.0804    0.0035    0.2592 N   0   0   0   0   0   0   0   0   0   0   9
85    2.8011   -0.0039   -0.8593 O   0   0   0   0   0   0   0   0   0   0  10
86   -1.6594    0.0029   -1.9749 O   0   0   0   0   0   0   0   0   0   0  11
87    2.2866    0.0008    2.0136 C   0   0   0   0   0   0   0   0   0   0  12
88   -0.4865    0.0045    2.2526 H   0   0   0   0   0   0   0   0   0   0  13
89    0.8202   -0.0028   -2.3569 H   0   0   0   0   0   0   0   0   0   0  14
90   -2.0869    0.0033    0.5385 H   0   0   0   0   0   0   0   0   0   0  15
91    2.9358    0.8853    1.9255 H   0   0   0   0   0   0   0   0   0   0  16
92    2.9362   -0.8832    1.9240 H   0   0   0   0   0   0   0   0   0   0  17
93    1.8360   -0.0001    3.0144 H   0   0   0   0   0   0   0   0   0   0  18
94
95  2   1   0   0   0   0   0
96  3   1   0   0   0   0   0
97  5   4   0   0   0   0   0
98  9   4   0   0   0   0   0
99 13   4   0   0   0   0   0
100  6   5   0   0   0   0   0
101 12   5   0   0   0   0   0
102  7   6   0   0   0   0   0
103 10   6   0   0   0   0   0
104  8   7   0   0   0   0   0
105 14   7   0   0   0   0   0
106  9   8   0   0   0   0   0
107 11   8   0   0   0   0   0
108 15   9   0   0   0   0   0
109 16  12   0   0   0   0   0
110 17  12   0   0   0   0   0
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12 18 0 0 0 0
M END
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trans-5-formyluracil-anion.sdf
COSMOtherm 3D 0

16 15 0 0 0 0 0 0 0 0 0 V2000
-3.5639 -0.0749 -1.9373 O 0 0 0 0 0 0 0 0 0 0 0 1
-2.7607 -0.0286 -1.3330 H 0 0 0 0 0 0 0 0 0 0 0 2
-3.7862 0.8555 -2.1130 H 0 0 0 0 0 0 0 0 0 0 0 3
-0.0736 0.0085 -0.9682 C 0 0 0 0 0 0 0 0 0 0 0 4
1.1791 0.0012 -0.3353 C 0 0 0 0 0 0 0 0 0 0 0 5
1.2089 -0.0051 1.1162 C 0 0 0 0 0 0 0 0 0 0 0 6
-0.0683 0.0000 1.6896 N 0 0 0 0 0 0 0 0 0 0 0 7
-1.2956 0.0078 1.0157 C 0 0 0 0 0 0 0 0 0 0 0 8
-1.2627 0.0123 -0.3690 N 0 0 0 0 0 0 0 0 0 0 0 9
2.2176 -0.0140 1.8467 O 0 0 0 0 0 0 0 0 0 0 0 10
-2.3557 0.0106 1.6624 O 0 0 0 0 0 0 0 0 0 0 0 11
2.4122 -0.0005 -1.0870 C 0 0 0 0 0 0 0 0 0 0 0 12
-0.0906 0.0125 -2.0636 H 0 0 0 0 0 0 0 0 0 0 0 13
-0.1107 -0.0041 2.7104 H 0 0 0 0 0 0 0 0 0 0 0 14
2.5065 0.0065 -2.3280 O 0 0 0 0 0 0 0 0 0 0 0 15
3.3349 -0.0087 -0.4649 H 0 0 0 0 0 0 0 0 0 0 0 16

2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
9 4 0 0 0 0
13 4 0 0 0 0
6 5 0 0 0 0
12 5 0 0 0 0
7 6 0 0 0 0
10 6 0 0 0 0
8 7 0 0 0 0
14 7 0 0 0 0
9 8 0 0 0 0
11 8 0 0 0 0
15 12 0 0 0 0
12 16 0 0 0 0
M END
$$$$
trans-5-formyluracil.sdf
COSMOtherm 3D 0

17 16 0 0 0 0 0 0 0 0 0 V2000
-1.9653 3.4283 0.0117 O 0 0 0 0 0 0 0 0 0 0 0 1
-2.0287 3.8719 -0.8538 H 0 0 0 0 0 0 0 0 0 0 0 2
-1.7122 4.1363 0.6318 H 0 0 0 0 0 0 0 0 0 0 0 3
-0.9856 0.0203 0.0056 C 0 0 0 0 0 0 0 0 0 0 0 4
-0.3280 -1.1912 0.0001 C 0 0 0 0 0 0 0 0 0 0 0 5
1.1326 -1.2003 -0.0014 C 0 0 0 0 0 0 0 0 0 0 0 6
1.7080 0.0836 -0.0045 N 0 0 0 0 0 0 0 0 0 0 0 7
1.0560 1.3056 -0.0007 C 0 0 0 0 0 0 0 0 0 0 0 8
-0.3402 1.2019 0.0046 N 0 0 0 0 0 0 0 0 0 0 0 9
1.8569 -2.2014 -0.0006 O 0 0 0 0 0 0 0 0 0 0 0 10
1.6372 2.3874 -0.0011 O 0 0 0 0 0 0 0 0 0 0 0 11
-1.0698 -2.4489 0.0020 C 0 0 0 0 0 0 0 0 0 0 0 12
-2.0759 0.0662 0.0105 H 0 0 0 0 0 0 0 0 0 0 0 13
2.7292 0.1248 -0.0065 H 0 0 0 0 0 0 0 0 0 0 0 14
-0.8890 2.1010 0.0089 H 0 0 0 0 0 0 0 0 0 0 0 15
-2.3020 -2.5384 -0.0016 O 0 0 0 0 0 0 0 0 0 0 0 16
-0.4376 -3.3624 0.0072 H 0 0 0 0 0 0 0 0 0 0 0 17

2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
9 4 0 0 0 0
13 4 0 0 0 0
6 5 0 0 0 0
12 5 0 0 0 0
7 6 0 0 0 0
10 6 0 0 0 0
8 7 0 0 0 0
14 7 0 0 0 0
9 8 0 0 0 0
11 8 0 0 0 0
15 9 0 0 0 0
16 12 0 0 0 0
12 17 0 0 0 0
M END
$$$$
trichloroaceticacid-anion.sdf
COSMOtherm 3D 0

10 8 0 0 0 0 0 0 0 0 0 V2000
-4.3883 -0.0641 0.0317 O 0 0 0 0 0 0 0 0 0 0 0 1
-3.4013 -0.2175 -0.0096 H 0 0 0 0 0 0 0 0 0 0 0 2
-4.4923 0.8734 -0.2056 H 0 0 0 0 0 0 0 0 0 0 0 3
0.9349 -1.0183 1.4816 Cl 0 0 0 0 0 0 0 0 0 0 0 4
0.6035 -0.0050 0.0010 C 0 0 0 0 0 0 0 0 0 0 0 5
-0.9517 0.3955 -0.0296 C 0 0 0 0 0 0 0 0 0 0 0 6
-1.2130 1.6101 -0.0268 O 0 0 0 0 0 0 0 0 0 0 0 7
-1.7100 -0.6097 -0.0540 O 0 0 0 0 0 0 0 0 0 0 0 8
1.0007 -0.9865 -1.4847 Cl 0 0 0 0 0 0 0 0 0 0 0 9
1.7063 1.4313 0.0410 Cl 0 0 0 0 0 0 0 0 0 0 0 10

2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 5 0 0 0 0
9 5 0 0 0 0
7 6 0 0 0 0
8 6 0 0 0 0
5 10 0 0 0 0
M END
$$$$
trichloroaceticacid.sdf
COSMOtherm 3D 0
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-2.8748 -0.3169 2.2388 H 0 0 0 0 0 0 0 0 0 0 0 3
2.3407 0.2110 2.8389 O 0 0 0 0 0 0 0 0 0 0 0 4
1.4219 0.2831 2.3795 H 0 0 0 0 0 0 0 0 0 0 0 5
2.8888 -0.2823 2.2058 H 0 0 0 0 0 0 0 0 0 0 0 6
-0.0009 0.0994 -0.6836 C 0 0 0 0 0 0 0 0 0 0 0 7
-0.0018 1.0625 0.5386 C 0 0 0 0 0 0 0 0 0 0 0 8
-0.0048 1.0717 -2.2372 Cl 0 0 0 0 0 0 0 0 0 0 0 9
1.4761 -0.9691 -0.6763 Cl 0 0 0 0 0 0 0 0 0 0 0 10
-1.4736 -0.9753 -0.6726 Cl 0 0 0 0 0 0 0 0 0 0 0 11
0.0009 0.4229 1.7418 O 0 0 0 0 0 0 0 0 0 0 0 12
-0.8979 1.7026 0.3713 H 0 0 0 0 0 0 0 0 0 0 0 13
0.8910 1.7067 0.3692 H 0 0 0 0 0 0 0 0 0 0 0 14
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
8 7 0 0 0 0
9 7 0 0 0 0
10 7 0 0 0 0
11 7 0 0 0 0
12 8 0 0 0 0
13 8 0 0 0 0
8 14 0 0 0 0
M END
$$$$
2,2,2-trichloroethanol.sdf
COSMOtherm 3D 0
15 12 0 0 0 0 0 0 0 0 0 0 V2000
1.2372 -4.1821 -0.0446 O 0 0 0 0 0 0 0 0 0 0 0 1
1.9033 -3.8530 0.5855 H 0 0 0 0 0 0 0 0 0 0 0 2
1.6490 -4.0684 -0.9201 H 0 0 0 0 0 0 0 0 0 0 0 3
-1.2727 -3.1606 0.2053 O 0 0 0 0 0 0 0 0 0 0 0 4
-1.6546 -3.6927 0.9258 H 0 0 0 0 0 0 0 0 0 0 0 5
-0.3330 -3.4876 0.1130 H 0 0 0 0 0 0 0 0 0 0 0 6
0.0521 0.9057 0.1037 C 0 0 0 0 0 0 0 0 0 0 0 7
-0.6703 0.0999 1.2061 C 0 0 0 0 0 0 0 0 0 0 0 8
1.4362 1.8056 0.8668 Cl 0 0 0 0 0 0 0 0 0 0 0 9
0.6983 -0.1951 -1.1861 Cl 0 0 0 0 0 0 0 0 0 0 0 10
-1.0786 2.0994 -0.6640 Cl 0 0 0 0 0 0 0 0 0 0 0 11
-1.7863 -0.6014 0.7308 O 0 0 0 0 0 0 0 0 0 0 0 12
-0.9919 0.8333 1.9615 H 0 0 0 0 0 0 0 0 0 0 0 13
0.0866 -0.5611 1.6603 H 0 0 0 0 0 0 0 0 0 0 0 14
-1.5155 -1.5444 0.5009 H 0 0 0 0 0 0 0 0 0 0 0 15
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
8 7 0 0 0 0
9 7 0 0 0 0
10 7 0 0 0 0
11 7 0 0 0 0
12 8 0 0 0 0
13 8 0 0 0 0
14 8 0 0 0 0
12 15 0 0 0 0
M END
$$$$
2,2-dimethylpropanoicacid-anion.sdf
COSMOtherm 3D 0
22 19 0 0 0 0 0 0 0 0 0 0 V2000
-4.6509 0.4669 0.7999 O 0 0 0 0 0 0 0 0 0 0 0 1
-3.9291 0.1017 0.2070 H 0 0 0 0 0 0 0 0 0 0 0 2
-4.3280 1.3454 1.0640 H 0 0 0 0 0 0 0 0 0 0 0 3
-2.7486 -0.6201 -0.7992 O 0 0 0 0 0 0 0 0 0 0 0 4
-1.8205 -0.6194 -0.3402 H 0 0 0 0 0 0 0 0 0 0 0 5
-2.5958 -0.0802 -1.5955 H 0 0 0 0 0 0 0 0 0 0 0 6
2.8253 0.8076 -0.7289 C 0 0 0 0 0 0 0 0 0 0 0 7
1.8862 0.0497 0.2209 C 0 0 0 0 0 0 0 0 0 0 0 8
1.8408 0.7671 1.5877 C 0 0 0 0 0 0 0 0 0 0 0 9
2.3990 -1.3925 0.4169 C 0 0 0 0 0 0 0 0 0 0 0 10
0.4345 -0.0095 -0.3515 C 0 0 0 0 0 0 0 0 0 0 0 11
0.1704 0.5557 -1.4475 O 0 0 0 0 0 0 0 0 0 0 0 12
-0.4235 -0.6532 0.3588 O 0 0 0 0 0 0 0 0 0 0 0 13
3.8429 0.8408 -0.3078 H 0 0 0 0 0 0 0 0 0 0 0 14
2.8759 0.3192 -1.7128 H 0 0 0 0 0 0 0 0 0 0 0 15
2.4839 1.8408 -0.8868 H 0 0 0 0 0 0 0 0 0 0 0 16
2.8478 0.8025 2.0336 H 0 0 0 0 0 0 0 0 0 0 0 17
1.1713 0.2406 2.2821 H 0 0 0 0 0 0 0 0 0 0 0 18
1.4814 1.8028 1.4814 H 0 0 0 0 0 0 0 0 0 0 0 19
3.4127 -1.3813 0.8484 H 0 0 0 0 0 0 0 0 0 0 0 20
1.7385 -1.9520 1.0936 H 0 0 0 0 0 0 0 0 0 0 0 21
2.4455 -1.9316 -0.5423 H 0 0 0 0 0 0 0 0 0 0 0 22
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
8 7 0 0 0 0
14 7 0 0 0 0
15 7 0 0 0 0
16 7 0 0 0 0
9 8 0 0 0 0
10 8 0 0 0 0
11 8 0 0 0 0
17 9 0 0 0 0
18 9 0 0 0 0
19 9 0 0 0 0
20 10 0 0 0 0
21 10 0 0 0 0
12 11 0 0 0 0
13 11 0 0 0 0
10 22 0 0 0 0
M END
$$$$
```

```
2,2-dimethylpropanoicacid.sdf
COSMOtherm      3D      0

23 20 0 0 0 0 0 0 0 0 0 V2000
-1.2902 3.2387 0.0671 O 0 0 0 0 0 0 0 0 0 0 1
-1.3329 2.2469 -0.0082 H 0 0 0 0 0 0 0 0 0 0 2
-1.7079 3.5781 -0.7446 H 0 0 0 0 0 0 0 0 0 0 3
1.3522 2.9043 0.0398 O 0 0 0 0 0 0 0 0 0 0 4
0.4000 3.2285 -0.0085 H 0 0 0 0 0 0 0 0 0 0 5
1.7902 3.2433 -0.7618 H 0 0 0 0 0 0 0 0 0 0 6
-1.5118 -2.2240 0.0610 C 0 0 0 0 0 0 0 0 0 0 7
-0.0593 -1.7286 0.0012 C 0 0 0 0 0 0 0 0 0 0 8
0.6145 -2.2276 -1.2994 C 0 0 0 0 0 0 0 0 0 0 9
0.7261 -2.2477 1.2275 C 0 0 0 0 0 0 0 0 0 0 10
-0.0297 -0.1941 0.0008 C 0 0 0 0 0 0 0 0 0 0 11
-1.0556 0.5003 -0.0176 O 0 0 0 0 0 0 0 0 0 0 12
1.2004 0.3130 0.0157 O 0 0 0 0 0 0 0 0 0 0 13
-1.5220 -3.3238 0.0576 H 0 0 0 0 0 0 0 0 0 0 14
-2.0158 -1.8787 0.9748 H 0 0 0 0 0 0 0 0 0 0 15
-2.0925 -1.8716 -0.8027 H 0 0 0 0 0 0 0 0 0 0 16
0.5868 -3.3269 -1.3222 H 0 0 0 0 0 0 0 0 0 0 17
1.6629 -1.9058 -1.3549 H 0 0 0 0 0 0 0 0 0 0 18
0.0869 -1.8550 -2.1902 H 0 0 0 0 0 0 0 0 0 0 19
0.6996 -3.3473 1.2356 H 0 0 0 0 0 0 0 0 0 0 20
1.7752 -1.9264 1.1959 H 0 0 0 0 0 0 0 0 0 0 21
0.2798 -1.8896 2.1673 H 0 0 0 0 0 0 0 0 0 0 22
1.2066 1.3519 0.0016 H 0 0 0 0 0 0 0 0 0 0 23

2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
8 7 0 0 0 0
14 7 0 0 0 0
15 7 0 0 0 0
16 7 0 0 0 0
9 8 0 0 0 0
10 8 0 0 0 0
11 8 0 0 0 0
17 9 0 0 0 0
18 9 0 0 0 0
19 9 0 0 0 0
20 10 0 0 0 0
21 10 0 0 0 0
22 10 0 0 0 0
12 11 0 0 0 0
13 11 0 0 0 0
13 23 0 0 0 0
M END
$$$$
```

```
2,3,4,6-tetrachlorophenol-anion.sdf
COSMOtherm      3D      0

18 16 0 0 0 0 0 0 0 0 0 V2000
-1.1870 2.6366 4.3085 O 0 0 0 0 0 0 0 0 0 0 1
-0.8420 1.6995 4.2754 H 0 0 0 0 0 0 0 0 0 0 2
-1.8494 2.6234 5.0204 H 0 0 0 0 0 0 0 0 0 0 3
-0.2269 0.0697 4.2771 O 0 0 0 0 0 0 0 0 0 0 4
-0.3004 -0.3688 3.3644 H 0 0 0 0 0 0 0 0 0 0 5
0.7283 0.0921 4.4622 H 0 0 0 0 0 0 0 0 0 0 6
1.8215 0.0147 -0.5909 C 0 0 0 0 0 0 0 0 0 0 7
1.2912 -0.4193 0.6163 C 0 0 0 0 0 0 0 0 0 0 8
-0.1015 -0.6839 0.8395 C 0 0 0 0 0 0 0 0 0 0 9
-0.9136 -0.4439 -0.3292 C 0 0 0 0 0 0 0 0 0 0 10
-0.3994 -0.0085 -1.5566 C 0 0 0 0 0 0 0 0 0 0 11
0.9793 0.2248 -1.6845 C 0 0 0 0 0 0 0 0 0 0 12
-0.5933 -1.0984 1.9506 O 0 0 0 0 0 0 0 0 0 0 13
-2.6386 -0.7374 -0.1409 Cl 0 0 0 0 0 0 0 0 0 0 14
-1.4671 0.2541 -2.9316 Cl 0 0 0 0 0 0 0 0 0 0 15
1.6873 0.7744 -3.2064 Cl 0 0 0 0 0 0 0 0 0 0 16
2.3993 -0.6913 1.9735 Cl 0 0 0 0 0 0 0 0 0 0 17
2.8920 0.1901 -0.6904 H 0 0 0 0 0 0 0 0 0 0 18

2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
8 7 0 0 0 0
12 7 0 0 0 0
9 8 0 0 0 0
17 8 0 0 0 0
10 9 0 0 0 0
13 9 0 0 0 0
11 10 0 0 0 0
14 10 0 0 0 0
12 11 0 0 0 0
15 11 0 0 0 0
16 12 0 0 0 0
7 18 0 0 0 0
M END
$$$$
```

```
2,3,4,6-tetrachlorophenol.sdf
COSMOtherm      3D      0

19 17 0 0 0 0 0 0 0 0 0 V2000
-1.2725 -5.3102 -1.1426 O 0 0 0 0 0 0 0 0 0 0 1
-0.8371 -6.1063 -1.4985 H 0 0 0 0 0 0 0 0 0 0 2
-1.4682 -4.7706 -1.9299 H 0 0 0 0 0 0 0 0 0 0 3
0.2782 -4.0988 0.7202 O 0 0 0 0 0 0 0 0 0 0 4
-0.3062 -4.5280 0.0286 H 0 0 0 0 0 0 0 0 0 0 5
-0.2093 -4.1816 1.5587 H 0 0 0 0 0 0 0 0 0 0 6
-0.4825 -0.2025 0.1592 C 0 0 0 0 0 0 0 0 0 0 7
-0.8924 1.1385 0.0448 C 0 0 0 0 0 0 0 0 0 0 8
0.0742 2.1422 -0.1027 C 0 0 0 0 0 0 0 0 0 0 9
1.4288 1.8112 -0.1352 C 0 0 0 0 0 0 0 0 0 0 10
1.8152 0.4828 -0.0199 C 0 0 0 0 0 0 0 0 0 0 11
0.8837 -0.5709 0.1315 C 0 0 0 0 0 0 0 0 0 0 12
```

[illegible]

```
13 19 0 0 0 0
M END
$$$$
2,3-dichlorophenol-anion.sdf
COSMOTHERM 3D 0

18 16 0 0 0 0 0 0 0 0 0 V2000
-1.0148 0.6403 5.1994 O 0 0 0 0 0 0 0 0 0 0 0 1
-0.2368 0.2272 4.7212 H 0 0 0 0 0 0 0 0 0 0 0 2
-1.2014 1.4549 4.7020 H 0 0 0 0 0 0 0 0 0 0 0 3
1.1119 -0.5278 3.9650 O 0 0 0 0 0 0 0 0 0 0 0 4
1.1246 -0.3490 2.9457 H 0 0 0 0 0 0 0 0 0 0 0 5
1.0303 -1.4935 4.0554 H 0 0 0 0 0 0 0 0 0 0 0 6
-1.1023 -0.2051 1.1423 C 0 0 0 0 0 0 0 0 0 0 0 7
-2.2006 -0.2379 0.2884 C 0 0 0 0 0 0 0 0 0 0 0 8
-2.0498 -0.1546 -1.1027 C 0 0 0 0 0 0 0 0 0 0 0 9
-0.7538 -0.0321 -1.6125 C 0 0 0 0 0 0 0 0 0 0 0 10
0.3634 0.0034 -0.7743 C 0 0 0 0 0 0 0 0 0 0 0 11
0.2390 -0.0827 0.6595 C 0 0 0 0 0 0 0 0 0 0 0 12
-2.9058 -0.1791 -1.7751 H 0 0 0 0 0 0 0 0 0 0 0 13
1.2787 -0.0463 1.4350 O 0 0 0 0 0 0 0 0 0 0 0 14
-1.2442 -0.2642 2.2236 H 0 0 0 0 0 0 0 0 0 0 0 15
-3.2053 -0.3314 0.7065 H 0 0 0 0 0 0 0 0 0 0 0 16
-0.5636 0.0779 -3.3772 Cl 0 0 0 0 0 0 0 0 0 0 0 17
1.9962 0.1589 -1.4318 Cl 0 0 0 0 0 0 0 0 0 0 0 18

2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
8 7 0 0 0 0
12 7 0 0 0 0
15 7 0 0 0 0
9 8 0 0 0 0
16 8 0 0 0 0
10 9 0 0 0 0
13 9 0 0 0 0
11 10 0 0 0 0
17 10 0 0 0 0
12 11 0 0 0 0
14 12 0 0 0 0
11 18 0 0 0 0
M END
$$$$
2,3-dichlorophenol.sdf
COSMOTHERM 3D 0

19 17 0 0 0 0 0 0 0 0 0 V2000
-5.6465 -0.4216 1.0804 O 0 0 0 0 0 0 0 0 0 0 0 1
-5.7636 -1.3895 1.0754 H 0 0 0 0 0 0 0 0 0 0 0 2
-6.5449 -0.0689 0.9449 H 0 0 0 0 0 0 0 0 0 0 0 3
-3.8703 0.4728 -0.7449 O 0 0 0 0 0 0 0 0 0 0 0 4
-4.5572 0.1198 -0.1036 H 0 0 0 0 0 0 0 0 0 0 0 5
-4.2300 0.3049 -1.6342 H 0 0 0 0 0 0 0 0 0 0 0 6
0.3573 2.4523 -0.0119 C 0 0 0 0 0 0 0 0 0 0 0 7
-0.7238 1.5965 -0.2173 C 0 0 0 0 0 0 0 0 0 0 0 8
-0.5360 0.2017 -0.2613 C 0 0 0 0 0 0 0 0 0 0 0 9
0.7740 -0.3076 -0.0933 C 0 0 0 0 0 0 0 0 0 0 0 10
1.8469 0.5698 0.1114 C 0 0 0 0 0 0 0 0 0 0 0 11
1.6519 1.9519 0.1542 C 0 0 0 0 0 0 0 0 0 0 0 12
-1.5432 -0.6733 -0.4572 O 0 0 0 0 0 0 0 0 0 0 0 13
1.0078 -2.0491 -0.1493 Cl 0 0 0 0 0 0 0 0 0 0 0 14
3.4833 -0.0569 0.3205 Cl 0 0 0 0 0 0 0 0 0 0 0 15
-2.4398 -0.1916 -0.5676 H 0 0 0 0 0 0 0 0 0 0 0 16
0.1925 3.5303 0.0196 H 0 0 0 0 0 0 0 0 0 0 0 17
-1.7316 1.9934 -0.3468 H 0 0 0 0 0 0 0 0 0 0 0 18
2.4998 2.6165 0.3141 H 0 0 0 0 0 0 0 0 0 0 0 19

2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
8 7 0 0 0 0
12 7 0 0 0 0
17 7 0 0 0 0
9 8 0 0 0 0
18 8 0 0 0 0
10 9 0 0 0 0
13 9 0 0 0 0
11 10 0 0 0 0
14 10 0 0 0 0
12 11 0 0 0 0
15 11 0 0 0 0
16 13 0 0 0 0
12 19 0 0 0 0
M END
$$$$
2,4,5-trichlorophenol-anion.sdf
COSMOTHERM 3D 0

18 16 0 0 0 0 0 0 0 0 0 V2000
2.4166 -4.5640 1.0951 O 0 0 0 0 0 0 0 0 0 0 0 1
1.6990 -4.3802 0.4229 H 0 0 0 0 0 0 0 0 0 0 0 2
2.1216 -5.3726 1.5479 H 0 0 0 0 0 0 0 0 0 0 0 3
0.4649 -4.1138 -0.7541 O 0 0 0 0 0 0 0 0 0 0 0 4
-0.1446 -3.3026 -0.5815 H 0 0 0 0 0 0 0 0 0 0 0 5
0.8346 -3.9791 -1.6438 H 0 0 0 0 0 0 0 0 0 0 0 6
0.5846 -0.5454 -0.2584 C 0 0 0 0 0 0 0 0 0 0 0 7
0.9947 0.7782 -0.1430 C 0 0 0 0 0 0 0 0 0 0 0 8
0.0662 1.8081 0.0613 C 0 0 0 0 0 0 0 0 0 0 0 9
-1.2918 1.4794 0.1477 C 0 0 0 0 0 0 0 0 0 0 0 10
-1.6980 0.1560 0.0323 C 0 0 0 0 0 0 0 0 0 0 0 11
-0.7916 -0.9374 -0.1784 C 0 0 0 0 0 0 0 0 0 0 0 12
0.5509 3.5012 0.2107 Cl 0 0 0 0 0 0 0 0 0 0 0 13
-1.1838 -2.1662 -0.2843 O 0 0 0 0 0 0 0 0 0 0 0 14
1.3291 -1.3263 -0.4160 H 0 0 0 0 0 0 0 0 0 0 0 15
2.7278 1.1378 -0.2592 Cl 0 0 0 0 0 0 0 0 0 0 0 16
```

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-2.0284 2.2669 0.3060 H 0 0 0 0 0 0 0 0 0 0 0 0 17
-3.4295 -0.2156 0.1480 Cl 0 0 0 0 0 0 0 0 0 0 0 0 18
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
8 7 0 0 0 0
12 7 0 0 0 0
15 7 0 0 0 0
9 8 0 0 0 0
16 8 0 0 0 0
10 9 0 0 0 0
13 9 0 0 0 0
11 10 0 0 0 0
17 10 0 0 0 0
12 11 0 0 0 0
14 12 0 0 0 0
11 18 0 0 0 0
M END
$$$$
2,4,5-trichlorophenol.sdf
COSMOTHERM 3D 0
19 17 0 0 0 0 0 0 0 0 0 V2000
-5.5912 1.5439 1.0458 O 0 0 0 0 0 0 0 0 0 0 0 1
-6.3673 0.9933 0.8354 H 0 0 0 0 0 0 0 0 0 0 0 2
-5.9467 2.4484 1.1204 H 0 0 0 0 0 0 0 0 0 0 0 3
-3.5750 1.3576 -0.7269 O 0 0 0 0 0 0 0 0 0 0 0 4
-4.3614 1.4274 -0.1055 H 0 0 0 0 0 0 0 0 0 0 0 5
-3.9411 1.4173 -1.6274 H 0 0 0 0 0 0 0 0 0 0 0 6
1.0313 0.9829 -0.0952 C 0 0 0 0 0 0 0 0 0 0 0 7
-0.3344 0.7612 -0.2666 C 0 0 0 0 0 0 0 0 0 0 0 8
-0.8664 -0.5417 -0.2397 C 0 0 0 0 0 0 0 0 0 0 0 9
0.0356 -1.6097 -0.0383 C 0 0 0 0 0 0 0 0 0 0 0 10
1.3988 -1.3923 0.1328 C 0 0 0 0 0 0 0 0 0 0 0 11
1.9081 -0.0915 0.1042 C 0 0 0 0 0 0 0 0 0 0 0 12
-2.1759 -0.8027 -0.3989 O 0 0 0 0 0 0 0 0 0 0 0 13
-0.5839 -3.2598 0.0003 Cl 0 0 0 0 0 0 0 0 0 0 0 14
3.6384 0.1492 0.3238 Cl 0 0 0 0 0 0 0 0 0 0 0 15
1.6223 2.6416 -0.1390 Cl 0 0 0 0 0 0 0 0 0 0 0 16
-1.0067 1.6053 -0.4206 H 0 0 0 0 0 0 0 0 0 0 0 17
2.0708 -2.2354 0.2873 H 0 0 0 0 0 0 0 0 0 0 0 18
-2.7188 0.0600 -0.5303 H 0 0 0 0 0 0 0 0 0 0 0 19
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
8 7 0 0 0 0
12 7 0 0 0 0
16 7 0 0 0 0
9 8 0 0 0 0
17 8 0 0 0 0
10 9 0 0 0 0
13 9 0 0 0 0
11 10 0 0 0 0
14 10 0 0 0 0
12 11 0 0 0 0
18 11 0 0 0 0
15 12 0 0 0 0
13 19 0 0 0 0
M END
$$$$
2,4,6-trichlorophenol-anion.sdf
COSMOTHERM 3D 0
18 16 0 0 0 0 0 0 0 0 0 V2000
-2.5580 4.2129 0.2005 O 0 0 0 0 0 0 0 0 0 0 0 1
-1.5946 4.0610 -0.0204 H 0 0 0 0 0 0 0 0 0 0 0 2
-2.5373 4.7624 1.0025 H 0 0 0 0 0 0 0 0 0 0 0 3
0.0776 3.8686 -0.4506 O 0 0 0 0 0 0 0 0 0 0 0 4
0.4405 2.9703 -0.1339 H 0 0 0 0 0 0 0 0 0 0 0 5
0.1425 3.8297 -1.4209 H 0 0 0 0 0 0 0 0 0 0 0 6
-0.1322 -1.8143 1.0344 C 0 0 0 0 0 0 0 0 0 0 0 7
0.3008 -0.5162 1.2873 C 0 0 0 0 0 0 0 0 0 0 0 8
0.6168 0.4588 0.2786 C 0 0 0 0 0 0 0 0 0 0 0 9
0.4291 -0.0603 -1.0493 C 0 0 0 0 0 0 0 0 0 0 0 10
-0.0050 -1.3492 -1.3476 C 0 0 0 0 0 0 0 0 0 0 0 11
-0.2847 -2.2187 -0.2928 C 0 0 0 0 0 0 0 0 0 0 0 12
1.0287 1.6480 0.5488 O 0 0 0 0 0 0 0 0 0 0 0 13
0.8065 1.0254 -2.4045 Cl 0 0 0 0 0 0 0 0 0 0 0 14
0.4897 -0.0081 2.9768 Cl 0 0 0 0 0 0 0 0 0 0 0 15
-0.8402 -3.8706 -0.6455 Cl 0 0 0 0 0 0 0 0 0 0 0 16
-0.3505 -2.4940 1.8573 H 0 0 0 0 0 0 0 0 0 0 0 17
-0.1187 -1.6674 -2.3833 H 0 0 0 0 0 0 0 0 0 0 0 18
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
8 7 0 0 0 0
12 7 0 0 0 0
17 7 0 0 0 0
9 8 0 0 0 0
15 8 0 0 0 0
10 9 0 0 0 0
13 9 0 0 0 0
11 10 0 0 0 0
14 10 0 0 0 0
12 11 0 0 0 0
16 12 0 0 0 0
11 18 0 0 0 0
M END
$$$$
2,4,6-trichlorophenol.sdf
COSMOTHERM 3D 0
```



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6 4 0 0 0 0
8 7 0 0 0 0
12 7 0 0 0 0
16 7 0 0 0 0
9 8 0 0 0 0
17 8 0 0 0 0
10 9 0 0 0 0
13 9 0 0 0 0
11 10 0 0 0 0
14 10 0 0 0 0
12 11 0 0 0 0
18 11 0 0 0 0
15 12 0 0 0 0
13 19 0 0 0 0
M END
$$$$
2,4-dihydroxybenzoicacid-anion.sdf
COSMOtherm 3D 0
22 21 0 0 0 0 0 0 0 0 0 V2000
0.9480 5.2316 -0.0160 O 0 0 0 0 0 0 0 0 0 0 1
1.5959 5.1705 -0.7412 H 0 0 0 0 0 0 0 0 0 0 2
1.4874 5.2881 0.7938 H 0 0 0 0 0 0 0 0 0 0 3
-0.1190 -5.5108 -0.0178 O 0 0 0 0 0 0 0 0 0 0 4
-0.3823 -4.5397 -0.0105 H 0 0 0 0 0 0 0 0 0 0 5
0.8527 -5.4815 0.0126 H 0 0 0 0 0 0 0 0 0 0 6
-1.8457 1.2280 0.0032 C 0 0 0 0 0 0 0 0 0 0 7
-1.5704 -0.1342 0.0053 C 0 0 0 0 0 0 0 0 0 0 8
-0.2539 -0.6305 0.0046 C 0 0 0 0 0 0 0 0 0 0 9
0.8164 0.3109 0.0035 C 0 0 0 0 0 0 0 0 0 0 10
0.5497 1.6901 0.0026 C 0 0 0 0 0 0 0 0 0 0 11
-0.7747 2.1491 0.0014 C 0 0 0 0 0 0 0 0 0 0 12
0.0333 -2.0978 0.0048 C 0 0 0 0 0 0 0 0 0 0 13
-0.9254 -2.9286 0.0010 O 0 0 0 0 0 0 0 0 0 0 14
1.2805 -2.4495 0.0082 O 0 0 0 0 0 0 0 0 0 0 15
2.1013 -0.1130 0.0043 O 0 0 0 0 0 0 0 0 0 0 16
-1.0878 3.4749 -0.0028 O 0 0 0 0 0 0 0 0 0 0 17
1.9892 -1.1639 0.0063 H 0 0 0 0 0 0 0 0 0 0 18
-0.2613 4.0462 -0.0073 H 0 0 0 0 0 0 0 0 0 0 19
-2.8709 1.6004 0.0034 H 0 0 0 0 0 0 0 0 0 0 20
-2.3891 -0.8562 0.0068 H 0 0 0 0 0 0 0 0 0 0 21
1.3849 2.3931 0.0033 H 0 0 0 0 0 0 0 0 0 0 22
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
8 7 0 0 0 0
12 7 0 0 0 0
20 7 0 0 0 0
9 8 0 0 0 0
21 8 0 0 0 0
10 9 0 0 0 0
13 9 0 0 0 0
11 10 0 0 0 0
16 10 0 0 0 0
12 11 0 0 0 0
17 12 0 0 0 0
14 13 0 0 0 0
15 13 0 0 0 0
18 15 0 0 0 0
18 16 0 0 0 0
19 17 0 0 0 0
11 22 0 0 0 0
M END
$$$$
2,4-dihydroxybenzoicacid.sdf
COSMOtherm 3D 0
23 21 0 0 0 0 0 0 0 0 0 V2000
-0.9255 0.0060 -5.1222 O 0 0 0 0 0 0 0 0 0 0 1
-0.9328 -0.7807 -5.6979 H 0 0 0 0 0 0 0 0 0 0 2
-0.9017 0.7623 -5.7370 H 0 0 0 0 0 0 0 0 0 0 3
0.2824 -0.0101 5.4344 O 0 0 0 0 0 0 0 0 0 0 4
-0.3330 -0.7139 5.7107 H 0 0 0 0 0 0 0 0 0 0 5
-0.1209 0.8146 5.7626 H 0 0 0 0 0 0 0 0 0 0 6
1.8425 -0.0015 -1.1945 C 0 0 0 0 0 0 0 0 0 0 7
1.5306 -0.0001 0.1533 C 0 0 0 0 0 0 0 0 0 0 8
0.1911 0.0011 0.6057 C 0 0 0 0 0 0 0 0 0 0 9
-0.8497 0.0003 -0.3706 C 0 0 0 0 0 0 0 0 0 0 10
-0.5407 -0.0007 -1.7363 C 0 0 0 0 0 0 0 0 0 0 11
0.7987 -0.0022 -2.1519 C 0 0 0 0 0 0 0 0 0 0 12
-0.1598 0.0017 2.0247 C 0 0 0 0 0 0 0 0 0 0 13
0.8651 0.0062 2.8794 O 0 0 0 0 0 0 0 0 0 0 14
-1.3513 -0.0016 2.4227 O 0 0 0 0 0 0 0 0 0 0 15
-2.1555 0.0005 -0.0081 O 0 0 0 0 0 0 0 0 0 0 16
1.1545 -0.0050 -3.4584 O 0 0 0 0 0 0 0 0 0 0 17
0.5290 0.0039 3.8476 H 0 0 0 0 0 0 0 0 0 0 18
-2.1458 -0.0001 1.0063 H 0 0 0 0 0 0 0 0 0 0 19
0.3450 -0.0006 -4.0640 H 0 0 0 0 0 0 0 0 0 0 20
2.8780 -0.0026 -1.5348 H 0 0 0 0 0 0 0 0 0 0 21
2.3314 0.0001 0.8930 H 0 0 0 0 0 0 0 0 0 0 22
-1.3510 -0.0015 -2.4666 H 0 0 0 0 0 0 0 0 0 0 23
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
8 7 0 0 0 0
12 7 0 0 0 0
21 7 0 0 0 0
9 8 0 0 0 0
22 8 0 0 0 0
10 9 0 0 0 0
13 9 0 0 0 0
11 10 0 0 0 0
16 10 0 0 0 0
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12 11 0 0 0 0
17 12 0 0 0 0
14 13 0 0 0 0
15 13 0 0 0 0
18 14 0 0 0 0
19 16 0 0 0 0
20 17 0 0 0 0
11 23 0 0 0 0
M END
$$$$
2,5-dichlorophenol-anion.sdf
COSMOtherm 3D 0

18 16 0 0 0 0 0 0 0 0 0 V2000
-4.3079 1.7869 -1.0748 O 0 0 0 0 0 0 0 0 0 0 1
-3.6450 2.0233 -0.3631 H 0 0 0 0 0 0 0 0 0 0 2
-4.7360 2.6317 -1.2957 H 0 0 0 0 0 0 0 0 0 0 3
-2.5226 2.4667 0.8660 O 0 0 0 0 0 0 0 0 0 0 4
-1.5509 2.1674 0.6879 H 0 0 0 0 0 0 0 0 0 0 5
-2.7609 2.0866 1.7293 H 0 0 0 0 0 0 0 0 0 0 6
-0.5210 -0.4742 0.2466 C 0 0 0 0 0 0 0 0 0 0 7
-0.0457 -1.7628 0.0441 C 0 0 0 0 0 0 0 0 0 0 8
1.2935 -2.0519 -0.2251 C 0 0 0 0 0 0 0 0 0 0 9
2.1798 -0.9661 -0.2873 C 0 0 0 0 0 0 0 0 0 0 10
1.7260 0.3321 -0.0877 C 0 0 0 0 0 0 0 0 0 0 11
0.3566 0.6603 0.1926 C 0 0 0 0 0 0 0 0 0 0 12
1.6425 -3.0712 -0.3805 H 0 0 0 0 0 0 0 0 0 0 13
-0.0522 1.8760 0.3793 O 0 0 0 0 0 0 0 0 0 0 14
-1.5768 -0.2958 0.4529 H 0 0 0 0 0 0 0 0 0 0 15
-1.2076 -3.1224 0.1314 Cl 0 0 0 0 0 0 0 0 0 0 16
3.2358 -1.1444 -0.4956 H 0 0 0 0 0 0 0 0 0 0 17
2.8903 1.6753 -0.1783 Cl 0 0 0 0 0 0 0 0 0 0 18

2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
8 7 0 0 0 0
12 7 0 0 0 0
15 7 0 0 0 0
9 8 0 0 0 0
16 8 0 0 0 0
10 9 0 0 0 0
13 9 0 0 0 0
11 10 0 0 0 0
17 10 0 0 0 0
12 11 0 0 0 0
14 12 0 0 0 0
11 18 0 0 0 0
M END
$$$$
2,5-dichlorophenol.sdf
COSMOtherm 3D 0

19 17 0 0 0 0 0 0 0 0 0 V2000
-5.0823 1.1694 0.9141 O 0 0 0 0 0 0 0 0 0 0 1
-5.8208 0.5750 0.6890 H 0 0 0 0 0 0 0 0 0 0 2
-5.4934 2.0486 1.0013 H 0 0 0 0 0 0 0 0 0 0 3
-3.0461 1.1240 -0.8480 O 0 0 0 0 0 0 0 0 0 0 4
-3.8375 1.1402 -0.2307 H 0 0 0 0 0 0 0 0 0 0 5
-3.4126 1.1165 -1.7503 H 0 0 0 0 0 0 0 0 0 0 6
1.5659 1.1285 0.0426 C 0 0 0 0 0 0 0 0 0 0 7
0.2321 0.8179 -0.2079 C 0 0 0 0 0 0 0 0 0 0 8
-0.1837 -0.5294 -0.2080 C 0 0 0 0 0 0 0 0 0 0 9
0.7909 -1.5191 0.0476 C 0 0 0 0 0 0 0 0 0 0 10
2.1201 -1.1864 0.2954 C 0 0 0 0 0 0 0 0 0 0 11
2.5283 0.1517 0.2959 C 0 0 0 0 0 0 0 0 0 0 12
-1.4582 -0.8994 -0.4398 O 0 0 0 0 0 0 0 0 0 0 13
0.3018 -3.2178 0.0521 Cl 0 0 0 0 0 0 0 0 0 0 14
2.0531 2.8364 0.0356 Cl 0 0 0 0 0 0 0 0 0 0 15
-0.5005 1.6008 -0.4040 H 0 0 0 0 0 0 0 0 0 0 16
2.8471 -1.9752 0.4896 H 0 0 0 0 0 0 0 0 0 0 17
3.5669 0.4145 0.4889 H 0 0 0 0 0 0 0 0 0 0 18
-2.0611 -0.0864 -0.6021 H 0 0 0 0 0 0 0 0 0 0 19

2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
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8 7 0 0 0 0
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16 8 0 0 0 0
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13 9 0 0 0 0
11 10 0 0 0 0
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12 11 0 0 0 0
17 11 0 0 0 0
18 12 0 0 0 0
13 19 0 0 0 0
M END
$$$$
2,6-dichlorophenol-anion.sdf
COSMOtherm 3D 0

18 16 0 0 0 0 0 0 0 0 0 V2000
-4.1808 -1.4341 1.7405 O 0 0 0 0 0 0 0 0 0 0 1
-3.8355 -0.6528 1.2193 H 0 0 0 0 0 0 0 0 0 0 2
-5.0620 -1.1527 2.0402 H 0 0 0 0 0 0 0 0 0 0 3
-3.2348 0.7098 0.3319 O 0 0 0 0 0 0 0 0 0 0 4
-2.2154 0.7117 0.3436 H 0 0 0 0 0 0 0 0 0 0 5
-3.4712 0.6069 -0.6059 H 0 0 0 0 0 0 0 0 0 0 6
2.7324 -0.5524 0.0655 C 0 0 0 0 0 0 0 0 0 0 7
1.6121 -0.0206 0.6950 C 0 0 0 0 0 0 0 0 0 0 8
0.3673 0.2830 0.0402 C 0 0 0 0 0 0 0 0 0 0 9
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0.4138 -0.0247 -1.3635 C 0 0 0 0 0 0 0 0 0 0 0 10
1.5185 -0.5578 -2.0215 C 0 0 0 0 0 0 0 0 0 0 0 11
2.6915 -0.8293 -1.3071 C 0 0 0 0 0 0 0 0 0 0 0 12
-0.6482 0.7776 0.6603 O 0 0 0 0 0 0 0 0 0 0 0 13
-1.0494 0.3270 -2.3211 Cl 0 0 0 0 0 0 0 0 0 0 0 14
1.6941 0.3178 2.4422 Cl 0 0 0 0 0 0 0 0 0 0 0 15
3.6343 -0.7524 0.6461 H 0 0 0 0 0 0 0 0 0 0 0 16
1.4628 -0.7582 -3.0925 H 0 0 0 0 0 0 0 0 0 0 0 17
3.5622 -1.2467 -1.8130 H 0 0 0 0 0 0 0 0 0 0 0 18
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
8 7 0 0 0 0
12 7 0 0 0 0
16 7 0 0 0 0
9 8 0 0 0 0
15 8 0 0 0 0
10 9 0 0 0 0
13 9 0 0 0 0
11 10 0 0 0 0
14 10 0 0 0 0
12 11 0 0 0 0
17 11 0 0 0 0
12 18 0 0 0 0
M END
$$$$
2,6-dichlorophenol.sdf
COSMOtherm 3D 0
19 17 0 0 0 0 0 0 0 0 0 V2000
-4.6682 -1.1539 -1.1131 O 0 0 0 0 0 0 0 0 0 0 0 1
-4.8261 -2.0801 -1.3719 H 0 0 0 0 0 0 0 0 0 0 0 2
-4.3614 -0.7237 -1.9317 H 0 0 0 0 0 0 0 0 0 0 0 3
-2.9315 -1.0402 0.9702 O 0 0 0 0 0 0 0 0 0 0 0 4
-3.5640 -1.0498 0.1941 H 0 0 0 0 0 0 0 0 0 0 0 5
-3.2695 -0.3522 1.5700 H 0 0 0 0 0 0 0 0 0 0 0 6
2.8428 0.4641 -0.3286 C 0 0 0 0 0 0 0 0 0 0 0 7
1.8370 -0.4642 -0.0778 C 0 0 0 0 0 0 0 0 0 0 0 8
0.4834 -0.0961 0.1162 C 0 0 0 0 0 0 0 0 0 0 0 9
0.2102 1.2884 0.0381 C 0 0 0 0 0 0 0 0 0 0 0 10
1.2033 2.2362 -0.2113 C 0 0 0 0 0 0 0 0 0 0 0 11
2.5243 1.8240 -0.3953 C 0 0 0 0 0 0 0 0 0 0 0 12
-0.4122 -1.0688 0.3482 O 0 0 0 0 0 0 0 0 0 0 0 13
-1.4551 1.8465 0.2563 Cl 0 0 0 0 0 0 0 0 0 0 0 14
2.2514 -2.1813 0.0076 Cl 0 0 0 0 0 0 0 0 0 0 0 15
3.8682 0.1228 -0.4688 H 0 0 0 0 0 0 0 0 0 0 0 16
0.9351 3.2920 -0.2613 H 0 0 0 0 0 0 0 0 0 0 0 17
3.3045 2.5596 -0.5906 H 0 0 0 0 0 0 0 0 0 0 0 18
-1.3725 -0.7909 0.5522 H 0 0 0 0 0 0 0 0 0 0 0 19
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
8 7 0 0 0 0
12 7 0 0 0 0
16 7 0 0 0 0
9 8 0 0 0 0
15 8 0 0 0 0
10 9 0 0 0 0
13 9 0 0 0 0
11 10 0 0 0 0
14 10 0 0 0 0
12 11 0 0 0 0
17 11 0 0 0 0
18 12 0 0 0 0
13 19 0 0 0 0
M END
$$$$
2-acetylbutanedioicacid-anion.sdf
COSMOtherm 3D 0
24 22 0 0 0 0 0 0 0 0 0 V2000
-0.9899 0.6208 5.5458 O 0 0 0 0 0 0 0 0 0 0 0 1
-0.2207 0.5123 4.9184 H 0 0 0 0 0 0 0 0 0 0 0 2
-1.5183 1.3389 5.1576 H 0 0 0 0 0 0 0 0 0 0 0 3
1.1702 0.2478 3.8993 O 0 0 0 0 0 0 0 0 0 0 0 4
0.9359 -0.2671 3.0618 H 0 0 0 0 0 0 0 0 0 0 0 5
1.5272 1.0937 3.5761 H 0 0 0 0 0 0 0 0 0 0 0 6
0.6737 -0.6589 0.6346 C 0 0 0 0 0 0 0 0 0 0 0 7
0.3551 -1.4718 -0.6277 C 0 0 0 0 0 0 0 0 0 0 0 8
-0.2706 -0.6914 -1.8148 C 0 0 0 0 0 0 0 0 0 0 0 9
-1.5244 0.1109 -1.4242 C 0 0 0 0 0 0 0 0 0 0 0 10
-1.6856 1.2652 -1.8095 O 0 0 0 0 0 0 0 0 0 0 0 11
-2.5550 -0.6027 -0.5859 C 0 0 0 0 0 0 0 0 0 0 0 12
0.7022 0.1974 -2.6067 C 0 0 0 0 0 0 0 0 0 0 0 13
1.5057 0.9794 -1.9051 O 0 0 0 0 0 0 0 0 0 0 0 14
0.7221 0.1797 -3.8393 O 0 0 0 0 0 0 0 0 0 0 0 15
0.5309 -1.2194 1.7531 O 0 0 0 0 0 0 0 0 0 0 0 16
1.0907 0.5509 0.4890 O 0 0 0 0 0 0 0 0 0 0 0 17
-0.3032 -2.3025 -0.3452 H 0 0 0 0 0 0 0 0 0 0 0 18
1.2980 -1.9298 -0.9681 H 0 0 0 0 0 0 0 0 0 0 0 19
-0.6344 -1.4479 -2.5299 H 0 0 0 0 0 0 0 0 0 0 0 20
-3.4890 -0.0296 -0.5745 H 0 0 0 0 0 0 0 0 0 0 0 21
-2.7351 -1.6208 -0.9609 H 0 0 0 0 0 0 0 0 0 0 0 22
-2.1895 -0.7049 0.4489 H 0 0 0 0 0 0 0 0 0 0 0 23
1.3274 0.8344 -0.8323 H 0 0 0 0 0 0 0 0 0 0 0 24
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
8 7 0 0 0 0
16 7 0 0 0 0
17 7 0 0 0 0
9 8 0 0 0 0
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18 8 0 0 0 0
19 8 0 0 0 0
10 9 0 0 0 0
13 9 0 0 0 0
20 9 0 0 0 0
11 10 0 0 0 0
12 10 0 0 0 0
21 12 0 0 0 0
22 12 0 0 0 0
23 12 0 0 0 0
14 13 0 0 0 0
15 13 0 0 0 0
14 24 0 0 0 0
17 24 0 0 0 0
M END
$$$$
2-acetylbutanedioicacid.sdf
COSMOTHERM 3D 0
25 22 0 0 0 0 0 0 0 0 0 V2000
-0.5714 3.0738 -2.0986 O 0 0 0 0 0 0 0 0 0 0 1
-0.4355 2.2051 -1.6384 H 0 0 0 0 0 0 0 0 0 0 2
0.0875 3.0895 -2.8158 H 0 0 0 0 0 0 0 0 0 0 3
0.0982 4.2162 0.2057 O 0 0 0 0 0 0 0 0 0 0 4
-0.1095 3.9631 -0.7485 H 0 0 0 0 0 0 0 0 0 0 5
0.9230 4.7342 0.1746 H 0 0 0 0 0 0 0 0 0 0 6
0.1382 0.9189 0.7781 C 0 0 0 0 0 0 0 0 0 0 7
0.2772 -0.3543 1.5908 C 0 0 0 0 0 0 0 0 0 0 8
0.1197 -1.6151 0.7333 C 0 0 0 0 0 0 0 0 0 0 9
-1.2710 -1.8039 0.1162 C 0 0 0 0 0 0 0 0 0 0 10
-1.4089 -2.3967 -0.9639 O 0 0 0 0 0 0 0 0 0 0 11
-2.4678 -1.3505 0.8925 C 0 0 0 0 0 0 0 0 0 0 12
1.3099 -1.7705 -0.2395 C 0 0 0 0 0 0 0 0 0 0 13
1.0862 -2.4419 -1.3729 O 0 0 0 0 0 0 0 0 0 0 14
2.4222 -1.3423 0.0347 O 0 0 0 0 0 0 0 0 0 0 15
0.4233 2.0097 1.4676 O 0 0 0 0 0 0 0 0 0 0 16
-0.2221 0.8985 -0.4078 O 0 0 0 0 0 0 0 0 0 0 17
-0.4618 -0.3302 2.4048 H 0 0 0 0 0 0 0 0 0 0 18
1.2610 -0.3554 2.0771 H 0 0 0 0 0 0 0 0 0 0 19
0.2112 -2.4819 1.4184 H 0 0 0 0 0 0 0 0 0 0 20
-3.3819 -1.7256 0.4198 H 0 0 0 0 0 0 0 0 0 0 21
-2.4079 -1.6998 1.9341 H 0 0 0 0 0 0 0 0 0 0 22
-2.5051 -0.2508 0.9253 H 0 0 0 0 0 0 0 0 0 0 23
0.0767 -2.6027 -1.4289 H 0 0 0 0 0 0 0 0 0 0 24
0.3000 2.8929 0.9092 H 0 0 0 0 0 0 0 0 0 0 25
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
8 7 0 0 0 0
16 7 0 0 0 0
17 7 0 0 0 0
9 8 0 0 0 0
18 8 0 0 0 0
19 8 0 0 0 0
10 9 0 0 0 0
13 9 0 0 0 0
20 9 0 0 0 0
11 10 0 0 0 0
12 10 0 0 0 0
21 12 0 0 0 0
22 12 0 0 0 0
23 12 0 0 0 0
14 13 0 0 0 0
15 13 0 0 0 0
24 14 0 0 0 0
16 25 0 0 0 0
M END
$$$$
2-chlorophenol-anion.sdf
COSMOTHERM 3D 0
18 16 0 0 0 0 0 0 0 0 0 V2000
3.0533 1.4364 0.5681 O 0 0 0 0 0 0 0 0 0 0 1
2.3141 0.8205 0.2741 H 0 0 0 0 0 0 0 0 0 0 2
2.6296 2.3107 0.6046 H 0 0 0 0 0 0 0 0 0 0 3
2.8373 -2.5587 -0.2786 O 0 0 0 0 0 0 0 0 0 0 4
2.2128 -1.7632 -0.2337 H 0 0 0 0 0 0 0 0 0 0 5
2.7416 -2.9910 0.5872 H 0 0 0 0 0 0 0 0 0 0 6
-0.6690 -1.7928 0.0528 C 0 0 0 0 0 0 0 0 0 0 7
-2.0497 -1.9299 0.1884 C 0 0 0 0 0 0 0 0 0 0 8
-2.8860 -0.8037 0.2081 C 0 0 0 0 0 0 0 0 0 0 9
-2.3078 0.4658 0.0821 C 0 0 0 0 0 0 0 0 0 0 10
-0.9265 0.5924 -0.0540 C 0 0 0 0 0 0 0 0 0 0 11
-0.0269 -0.5205 -0.0757 C 0 0 0 0 0 0 0 0 0 0 12
-3.9670 -0.9036 0.3144 H 0 0 0 0 0 0 0 0 0 0 13
1.2692 -0.4027 -0.2092 O 0 0 0 0 0 0 0 0 0 0 14
-0.0268 -2.6768 0.0351 H 0 0 0 0 0 0 0 0 0 0 15
-2.4799 -2.9303 0.2827 H 0 0 0 0 0 0 0 0 0 0 16
-2.9313 1.3616 0.0878 H 0 0 0 0 0 0 0 0 0 0 17
-0.2415 2.2321 -0.2278 Cl 0 0 0 0 0 0 0 0 0 0 18
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
8 7 0 0 0 0
12 7 0 0 0 0
15 7 0 0 0 0
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14 12 0 0 0 0
11 18 0 0 0 0
M END
$$$$
2-chlorophenol.sdf
COSMOtherm 3D 0

19 17 0 0 0 0 0 0 0 0 0 V2000
-5.0646 -0.4542 0.7725 O 0 0 0 0 0 0 0 0 0 0 1
-5.2985 -1.3542 0.4809 H 0 0 0 0 0 0 0 0 0 0 2
-5.9043 0.0390 0.7336 H 0 0 0 0 0 0 0 0 0 0 3
-3.1040 0.6966 -0.6908 O 0 0 0 0 0 0 0 0 0 0 4
-3.8561 0.2595 -0.1910 H 0 0 0 0 0 0 0 0 0 0 5
-3.3859 0.7158 -1.6227 H 0 0 0 0 0 0 0 0 0 0 6
1.2476 2.4063 0.1228 C 0 0 0 0 0 0 0 0 0 0 7
0.1202 1.6164 -0.1133 C 0 0 0 0 0 0 0 0 0 0 8
0.2170 0.2108 -0.1609 C 0 0 0 0 0 0 0 0 0 0 9
1.4919 -0.3597 0.0377 C 0 0 0 0 0 0 0 0 0 0 10
2.6207 0.4236 0.2739 C 0 0 0 0 0 0 0 0 0 0 11
2.5023 1.8173 0.3169 C 0 0 0 0 0 0 0 0 0 0 12
-0.8422 -0.5990 -0.3879 O 0 0 0 0 0 0 0 0 0 0 13
1.6549 -2.1250 -0.0150 Cl 0 0 0 0 0 0 0 0 0 0 14
-1.7001 -0.0608 -0.5105 H 0 0 0 0 0 0 0 0 0 0 15
1.1408 3.4921 0.1539 H 0 0 0 0 0 0 0 0 0 0 16
-0.8582 2.0768 -0.2638 H 0 0 0 0 0 0 0 0 0 0 17
3.5874 -0.0588 0.4221 H 0 0 0 0 0 0 0 0 0 0 18
3.3852 2.4303 0.5009 H 0 0 0 0 0 0 0 0 0 0 19

2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
8 7 0 0 0 0
12 7 0 0 0 0
16 7 0 0 0 0
9 8 0 0 0 0
17 8 0 0 0 0
10 9 0 0 0 0
13 9 0 0 0 0
11 10 0 0 0 0
14 10 0 0 0 0
12 11 0 0 0 0
18 11 0 0 0 0
15 13 0 0 0 0
12 19 0 0 0 0
M END
$$$$
2-chloropropanoicacid-anion.sdf
COSMOtherm 3D 0

16 13 0 0 0 0 0 0 0 0 0 V2000
-4.6596 0.2006 -1.1768 O 0 0 0 0 0 0 0 0 0 0 1
-4.0192 -0.0452 -0.4497 H 0 0 0 0 0 0 0 0 0 0 2
-4.3932 1.0965 -1.4448 H 0 0 0 0 0 0 0 0 0 0 3
-2.9520 -0.5851 0.7936 O 0 0 0 0 0 0 0 0 0 0 4
-1.9791 -0.5265 0.4853 H 0 0 0 0 0 0 0 0 0 0 5
-2.9855 0.0021 1.5690 H 0 0 0 0 0 0 0 0 0 0 6
2.6233 -0.6403 1.1760 C 0 0 0 0 0 0 0 0 0 0 7
1.7955 0.3359 0.3502 C 0 0 0 0 0 0 0 0 0 0 8
0.2861 0.2289 0.6776 C 0 0 0 0 0 0 0 0 0 0 9
-0.0525 0.8646 1.7100 O 0 0 0 0 0 0 0 0 0 0 10
-0.4569 -0.4993 -0.0543 O 0 0 0 0 0 0 0 0 0 0 11
2.1500 0.0553 -1.4589 Cl 0 0 0 0 0 0 0 0 0 0 12
3.6951 -0.5269 0.9673 H 0 0 0 0 0 0 0 0 0 0 13
2.4541 -0.4323 2.2430 H 0 0 0 0 0 0 0 0 0 0 14
2.3275 -1.6786 0.9707 H 0 0 0 0 0 0 0 0 0 0 15
2.1195 1.3687 0.5152 H 0 0 0 0 0 0 0 0 0 0 16

2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
8 7 0 0 0 0
13 7 0 0 0 0
14 7 0 0 0 0
15 7 0 0 0 0
9 8 0 0 0 0
12 8 0 0 0 0
10 9 0 0 0 0
11 9 0 0 0 0
8 16 0 0 0 0
M END
$$$$
2-chloropropanoicacid.sdf
COSMOtherm 3D 0

17 14 0 0 0 0 0 0 0 0 0 V2000
-0.7472 -4.6021 0.1642 O 0 0 0 0 0 0 0 0 0 0 1
-1.0291 -4.9398 -0.7059 H 0 0 0 0 0 0 0 0 0 0 2
-1.5582 -4.2296 0.5561 H 0 0 0 0 0 0 0 0 0 0 3
1.3053 -2.8705 -0.0901 O 0 0 0 0 0 0 0 0 0 0 4
0.5260 -3.4910 0.0332 H 0 0 0 0 0 0 0 0 0 0 5
1.8029 -2.9013 0.7473 H 0 0 0 0 0 0 0 0 0 0 6
-1.8500 2.0694 -0.3704 C 0 0 0 0 0 0 0 0 0 0 7
-0.4330 1.5900 -0.5865 C 0 0 0 0 0 0 0 0 0 0 8
-0.1757 0.1690 -0.0687 C 0 0 0 0 0 0 0 0 0 0 9
0.7095 -0.4833 -0.8200 O 0 0 0 0 0 0 0 0 0 0 10
-0.7328 -0.2905 0.9224 O 0 0 0 0 0 0 0 0 0 0 11
0.7654 2.6744 0.3369 Cl 0 0 0 0 0 0 0 0 0 0 12
-1.9636 3.1067 -0.7095 H 0 0 0 0 0 0 0 0 0 0 13
-2.5309 1.4375 -0.9624 H 0 0 0 0 0 0 0 0 0 0 14
-2.1377 1.9932 0.6863 H 0 0 0 0 0 0 0 0 0 0 15
-0.1143 1.6731 -1.6299 H 0 0 0 0 0 0 0 0 0 0 16
0.8937 -1.4407 -0.4463 H 0 0 0 0 0 0 0 0 0 0 17

2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
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6 4 0 0 0 0
8 7 0 0 0 0
13 7 0 0 0 0
14 7 0 0 0 0
15 7 0 0 0 0
9 8 0 0 0 0
12 8 0 0 0 0
16 8 0 0 0 0
10 9 0 0 0 0
11 9 0 0 0 0
10 17 0 0 0 0
M END
$$$$
2-hydroxypropanoicacid-anion.sdf
COSMOTHERM 3D 0
17 14 0 0 0 0 0 0 0 0 0 V2000
-4.6815 -0.7525 0.3319 O 0 0 0 0 0 0 0 0 0 0 1
-3.9195 -0.1632 0.0618 H 0 0 0 0 0 0 0 0 0 0 2
-4.5741 -0.8634 1.2919 H 0 0 0 0 0 0 0 0 0 0 3
-2.6256 0.8269 -0.5174 O 0 0 0 0 0 0 0 0 0 0 4
-1.7209 0.4115 -0.2889 H 0 0 0 0 0 0 0 0 0 0 5
-2.6217 1.6967 -0.0813 H 0 0 0 0 0 0 0 0 0 0 6
2.2965 -1.6074 -0.6287 C 0 0 0 0 0 0 0 0 0 0 7
2.0237 -0.4967 0.3859 C 0 0 0 0 0 0 0 0 0 0 8
0.7190 0.2775 0.0646 C 0 0 0 0 0 0 0 0 0 0 9
0.8439 1.5184 -0.1518 O 0 0 0 0 0 0 0 0 0 0 10
-0.3635 -0.3921 0.0492 O 0 0 0 0 0 0 0 0 0 0 11
3.1178 0.4373 0.4264 O 0 0 0 0 0 0 0 0 0 0 12
3.2312 -2.1296 -0.3778 H 0 0 0 0 0 0 0 0 0 0 13
1.4778 -2.3401 -0.6264 H 0 0 0 0 0 0 0 0 0 0 14
2.3920 -1.1890 -1.6419 H 0 0 0 0 0 0 0 0 0 0 15
1.8991 -0.9438 1.3893 H 0 0 0 0 0 0 0 0 0 0 16
2.6596 1.2883 0.2010 H 0 0 0 0 0 0 0 0 0 0 17
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
8 7 0 0 0 0
13 7 0 0 0 0
14 7 0 0 0 0
15 7 0 0 0 0
9 8 0 0 0 0
12 8 0 0 0 0
16 8 0 0 0 0
10 9 0 0 0 0
11 9 0 0 0 0
12 17 0 0 0 0
M END
$$$$
2-hydroxypropanoicacid.sdf
COSMOTHERM 3D 0
18 15 0 0 0 0 0 0 0 0 0 V2000
-0.7805 0.9213 -3.9008 O 0 0 0 0 0 0 0 0 0 0 1
-1.5951 0.4925 -4.2194 H 0 0 0 0 0 0 0 0 0 0 2
-0.3737 1.2964 -4.7029 H 0 0 0 0 0 0 0 0 0 0 3
0.9074 -0.7137 -2.6025 O 0 0 0 0 0 0 0 0 0 0 4
0.2492 -0.1374 -3.0996 H 0 0 0 0 0 0 0 0 0 0 5
0.6820 -1.6334 -2.8304 H 0 0 0 0 0 0 0 0 0 0 6
0.8324 1.2947 2.3916 C 0 0 0 0 0 0 0 0 0 0 7
0.2196 -0.0826 2.1237 C 0 0 0 0 0 0 0 0 0 0 8
0.0032 -0.3331 0.6290 C 0 0 0 0 0 0 0 0 0 0 9
-1.1283 -0.5365 0.1796 O 0 0 0 0 0 0 0 0 0 0 10
1.1144 -0.3085 -0.0878 O 0 0 0 0 0 0 0 0 0 0 11
-1.0355 -0.2224 2.8010 O 0 0 0 0 0 0 0 0 0 0 12
0.9408 1.4391 3.4749 H 0 0 0 0 0 0 0 0 0 0 13
1.8253 1.3756 1.9286 H 0 0 0 0 0 0 0 0 0 0 14
0.1861 2.0901 1.9934 H 0 0 0 0 0 0 0 0 0 0 15
0.9105 -0.8647 2.4862 H 0 0 0 0 0 0 0 0 0 0 16
0.9307 -0.4854 -1.1046 H 0 0 0 0 0 0 0 0 0 0 17
-1.6873 -0.4008 2.0850 H 0 0 0 0 0 0 0 0 0 0 18
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
8 7 0 0 0 0
13 7 0 0 0 0
14 7 0 0 0 0
15 7 0 0 0 0
9 8 0 0 0 0
12 8 0 0 0 0
16 8 0 0 0 0
10 9 0 0 0 0
11 9 0 0 0 0
17 11 0 0 0 0
12 18 0 0 0 0
M END
$$$$
3,3-dimethylsuccinimide-anion.sdf
COSMOTHERM 3D 0
23 21 0 0 0 0 0 0 0 0 0 V2000
-3.9266 0.6553 -0.0049 O 0 0 0 0 0 0 0 0 0 0 1
-3.6720 -0.3029 -0.0079 H 0 0 0 0 0 0 0 0 0 0 2
-3.0355 1.0974 0.0055 H 0 0 0 0 0 0 0 0 0 0 3
-2.7020 -1.8646 -0.0602 O 0 0 0 0 0 0 0 0 0 0 4
-1.8271 -1.3357 -0.0143 H 0 0 0 0 0 0 0 0 0 0 5
-2.7548 -2.3387 0.7882 H 0 0 0 0 0 0 0 0 0 0 6
1.9131 0.2577 -0.0032 C 0 0 0 0 0 0 0 0 0 0 7
1.0530 1.5353 0.0168 C 0 0 0 0 0 0 0 0 0 0 8
0.8268 -0.8526 0.0063 C 0 0 0 0 0 0 0 0 0 0 9
-0.4481 -0.3369 0.0079 N 0 0 0 0 0 0 0 0 0 0 10
-0.3863 1.0246 0.0115 C 0 0 0 0 0 0 0 0 0 0 11
2.8050 0.1141 1.2426 C 0 0 0 0 0 0 0 0 0 0 12
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1
2
3 1.7690 0.1033 -0.0903 C 0 0 0 0 0 0 0 0 0 0 16
4 -0.1520 -0.1445 -2.9973 H 0 0 0 0 0 0 0 0 0 0 17
5 0.8739 -1.3983 -2.3068 H 0 0 0 0 0 0 0 0 0 0 18
6 -0.4517 2.0795 -1.8955 H 0 0 0 0 0 0 0 0 0 0 19
7 0.3649 2.4635 -0.3778 H 0 0 0 0 0 0 0 0 0 0 20
8 3.2377 -0.7070 2.1989 C 0 0 0 0 0 0 0 0 0 0 21
9 2.6018 -1.6548 1.3928 C 0 0 0 0 0 0 0 0 0 0 22
10 1.8781 -1.2527 0.2616 C 0 0 0 0 0 0 0 0 0 0 23
11 2.4176 1.0439 0.7342 C 0 0 0 0 0 0 0 0 0 0 24
12 3.1420 0.6492 1.8622 C 0 0 0 0 0 0 0 0 0 0 25
13 1.5159 1.5583 -3.2387 H 0 0 0 0 0 0 0 0 0 0 26
14 2.5642 2.0482 -1.8850 H 0 0 0 0 0 0 0 0 0 0 27
15 2.7791 0.4499 -2.6382 H 0 0 0 0 0 0 0 0 0 0 28
16 3.8024 -1.0191 3.0793 H 0 0 0 0 0 0 0 0 0 0 29
17 2.6657 -2.7167 1.6403 H 0 0 0 0 0 0 0 0 0 0 30
18 1.3962 -2.0207 -0.3442 H 0 0 0 0 0 0 0 0 0 0 31
19 2.3632 2.1075 0.4930 H 0 0 0 0 0 0 0 0 0 0 32
20 3.6341 1.4036 2.4797 H 0 0 0 0 0 0 0 0 0 0 33
21 2 1 0 0 0 0
22 3 1 0 0 0 0
23 5 4 0 0 0 0
24 6 4 0 0 0 0
25 8 7 0 0 0 0
26 12 7 0 0 0 0
27 14 7 0 0 0 0
28 9 8 0 0 0 0
29 10 9 0 0 0 0
30 13 9 0 0 0 0
31 11 10 0 0 0 0
32 17 10 0 0 0 0
33 18 10 0 0 0 0
34 12 11 0 0 0 0
35 15 11 0 0 0 0
36 16 11 0 0 0 0
37 19 12 0 0 0 0
38 20 12 0 0 0 0
39 26 15 0 0 0 0
40 27 15 0 0 0 0
41 28 15 0 0 0 0
42 23 16 0 0 0 0
43 24 16 0 0 0 0
44 22 21 0 0 0 0
45 25 21 0 0 0 0
46 29 21 0 0 0 0
47 23 22 0 0 0 0
48 30 22 0 0 0 0
49 31 23 0 0 0 0
50 25 24 0 0 0 0
51 32 24 0 0 0 0
52 25 33 0 0 0 0
53 M END
54 \$\$\$\$
55 3,3-methylphenylglutarimide.sdf
56 COSMOtherm 3D 0
57
58 34 33 0 0 0 0 0 0 0 0 0 0 V2000
59 -5.8549 -0.9267 0.7630 O 0 0 0 0 0 0 0 0 0 0 1
60 -6.6389 -1.3850 0.4094 H 0 0 0 0 0 0 0 0 0 0 2
-6.1151 0.0120 0.7853 H 0 0 0 0 0 0 0 0 0 0 3
-3.5970 -1.3928 -0.7205 O 0 0 0 0 0 0 0 0 0 0 4
-3.8418 -1.2735 -1.6552 H 0 0 0 0 0 0 0 0 0 0 5
-4.4331 -1.2038 -0.2087 H 0 0 0 0 0 0 0 0 0 0 6
-0.9813 0.4810 1.1277 C 0 0 0 0 0 0 0 0 0 0 7
-1.4009 0.3131 -0.1865 N 0 0 0 0 0 0 0 0 0 0 8
-0.8196 0.8867 -1.3098 C 0 0 0 0 0 0 0 0 0 0 9
0.3800 1.7798 -1.0768 C 0 0 0 0 0 0 0 0 0 0 10
1.2029 1.4293 0.1799 C 0 0 0 0 0 0 0 0 0 0 11
0.1944 1.4064 1.3540 C 0 0 0 0 0 0 0 0 0 0 12
-1.2973 0.6791 -2.4280 O 0 0 0 0 0 0 0 0 0 0 13
-1.5764 -0.0901 2.0440 O 0 0 0 0 0 0 0 0 0 0 14
2.2476 2.5408 0.4205 C 0 0 0 0 0 0 0 0 0 0 15
1.9260 0.0731 0.0600 C 0 0 0 0 0 0 0 0 0 0 16
-2.2333 -0.3083 -0.3506 H 0 0 0 0 0 0 0 0 0 0 17
-0.0119 2.8047 -0.9558 H 0 0 0 0 0 0 0 0 0 0 18
0.9827 1.7886 -1.9936 H 0 0 0 0 0 0 0 0 0 0 19
-0.2181 2.4221 1.4871 H 0 0 0 0 0 0 0 0 0 0 20
0.6593 1.1283 2.3072 H 0 0 0 0 0 0 0 0 0 0 21
3.3354 -2.3826 -0.0965 C 0 0 0 0 0 0 0 0 0 0 22
2.7230 -1.8446 -1.2309 C 0 0 0 0 0 0 0 0 0 0 23
2.0275 -0.6302 -1.1520 C 0 0 0 0 0 0 0 0 0 0 24
2.5546 -0.4814 1.1921 C 0 0 0 0 0 0 0 0 0 0 25
3.2493 -1.6915 1.1183 C 0 0 0 0 0 0 0 0 0 0 26
1.7537 3.5191 0.5179 H 0 0 0 0 0 0 0 0 0 0 27
2.8199 2.3501 1.3389 H 0 0 0 0 0 0 0 0 0 0 28
2.9565 2.5916 -0.4190 H 0 0 0 0 0 0 0 0 0 0 29
3.8757 -3.3291 -0.1560 H 0 0 0 0 0 0 0 0 0 0 30
2.7820 -2.3682 -2.1870 H 0 0 0 0 0 0 0 0 0 0 31
1.5680 -0.2404 -2.0605 H 0 0 0 0 0 0 0 0 0 0 32
2.5096 0.0373 2.1517 H 0 0 0 0 0 0 0 0 0 0 33
3.7250 -2.0958 2.0139 H 0 0 0 0 0 0 0 0 0 0 34
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
8 7 0 0 0 0
12 7 0 0 0 0
14 7 0 0 0 0
9 8 0 0 0 0
17 8 0 0 0 0
10 9 0 0 0 0
13 9 0 0 0 0
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18 10 0 0 0 0
19 10 0 0 0 0
12 11 0 0 0 0

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15 11 0 0 0 0
16 11 0 0 0 0
20 12 0 0 0 0
21 12 0 0 0 0
27 15 0 0 0 0
28 15 0 0 0 0
29 15 0 0 0 0
24 16 0 0 0 0
25 16 0 0 0 0
23 22 0 0 0 0
26 22 0 0 0 0
30 22 0 0 0 0
24 23 0 0 0 0
31 23 0 0 0 0
32 24 0 0 0 0
26 25 0 0 0 0
33 25 0 0 0 0
26 34 0 0 0 0
M END
$$$$
3,4-dichlorophenol-anion.sdf
COSMOTHERM 3D 0

18 16 0 0 0 0 0 0 0 0 0 V2000
-2.5391 3.5846 0.0374 O 0 0 0 0 0 0 0 0 0 0 1
-1.6007 3.2062 0.0433 H 0 0 0 0 0 0 0 0 0 0 2
-2.8513 3.4412 -0.8722 H 0 0 0 0 0 0 0 0 0 0 3
1.8945 4.4879 -0.0815 O 0 0 0 0 0 0 0 0 0 0 4
1.1854 3.7675 -0.0307 H 0 0 0 0 0 0 0 0 0 0 5
2.3429 4.3290 -0.9296 H 0 0 0 0 0 0 0 0 0 0 6
1.8132 -0.4924 0.0458 C 0 0 0 0 0 0 0 0 0 0 7
1.5538 0.8745 0.0744 C 0 0 0 0 0 0 0 0 0 0 8
0.2195 1.3820 0.0674 C 0 0 0 0 0 0 0 0 0 0 9
-0.8288 0.4121 0.0352 C 0 0 0 0 0 0 0 0 0 0 10
-0.5506 -0.9513 0.0076 C 0 0 0 0 0 0 0 0 0 0 11
0.7687 -1.4248 0.0122 C 0 0 0 0 0 0 0 0 0 0 12
-0.0403 2.6685 0.0911 O 0 0 0 0 0 0 0 0 0 0 13
-1.9159 -2.0867 -0.0331 Cl 0 0 0 0 0 0 0 0 0 0 14
1.1475 -3.1542 -0.0248 Cl 0 0 0 0 0 0 0 0 0 0 15
2.8435 -0.8518 0.0504 H 0 0 0 0 0 0 0 0 0 0 16
2.3848 1.5819 0.1038 H 0 0 0 0 0 0 0 0 0 0 17
-1.8646 0.7538 0.0331 H 0 0 0 0 0 0 0 0 0 0 18
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
8 7 0 0 0 0
12 7 0 0 0 0
16 7 0 0 0 0
9 8 0 0 0 0
17 8 0 0 0 0
10 9 0 0 0 0
13 9 0 0 0 0
11 10 0 0 0 0
12 11 0 0 0 0
14 11 0 0 0 0
15 12 0 0 0 0
10 18 0 0 0 0
M END
$$$$
3,4-dichlorophenol.sdf
COSMOTHERM 3D 0

19 17 0 0 0 0 0 0 0 0 0 V2000
-5.5639 0.7603 1.1710 O 0 0 0 0 0 0 0 0 0 0 1
-6.1476 -0.0099 1.2991 H 0 0 0 0 0 0 0 0 0 0 2
-6.1766 1.5024 1.0167 H 0 0 0 0 0 0 0 0 0 0 3
-3.7667 0.4429 -0.8199 O 0 0 0 0 0 0 0 0 0 0 4
-4.4739 0.5480 -0.1176 H 0 0 0 0 0 0 0 0 0 0 5
-4.2461 0.3399 -1.6615 H 0 0 0 0 0 0 0 0 0 0 6
0.8743 0.4669 -0.1176 C 0 0 0 0 0 0 0 0 0 0 7
1.8329 -0.5264 0.1210 C 0 0 0 0 0 0 0 0 0 0 8
1.4250 -1.8644 0.1741 C 0 0 0 0 0 0 0 0 0 0 9
0.0875 -2.2085 -0.0064 C 0 0 0 0 0 0 0 0 0 0 10
-0.8754 -1.2097 -0.2455 C 0 0 0 0 0 0 0 0 0 0 11
-0.4697 0.1373 -0.3014 C 0 0 0 0 0 0 0 0 0 0 12
3.5378 -0.1360 0.3565 Cl 0 0 0 0 0 0 0 0 0 0 13
2.1674 -2.6409 0.3597 H 0 0 0 0 0 0 0 0 0 0 14
-0.2220 -3.2536 0.0375 H 0 0 0 0 0 0 0 0 0 0 15
-2.1650 -1.5903 -0.4173 O 0 0 0 0 0 0 0 0 0 0 16
-1.2008 0.9229 -0.4879 H 0 0 0 0 0 0 0 0 0 0 17
1.3321 2.1701 -0.1957 Cl 0 0 0 0 0 0 0 0 0 0 18
-2.7740 -0.7862 -0.5710 H 0 0 0 0 0 0 0 0 0 0 19
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
8 7 0 0 0 0
12 7 0 0 0 0
18 7 0 0 0 0
9 8 0 0 0 0
13 8 0 0 0 0
10 9 0 0 0 0
14 9 0 0 0 0
11 10 0 0 0 0
15 10 0 0 0 0
12 11 0 0 0 0
16 11 0 0 0 0
17 12 0 0 0 0
16 19 0 0 0 0
M END
$$$$
3,5-dichlorophenol-anion.sdf
COSMOTHERM 3D 0
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18 16 0 0 0 0 0 0 0 0 0 V2000
-3.7523 -0.0685 2.2669 O 0 0 0 0 0 0 0 0 0 0 1
-3.1928 -0.0387 1.4264 H 0 0 0 0 0 0 0 0 0 0 2
-3.6881 0.8300 2.6336 H 0 0 0 0 0 0 0 0 0 0 3
-3.7497 0.0186 -2.2761 O 0 0 0 0 0 0 0 0 0 0 4
-3.1900 0.0122 -1.4346 H 0 0 0 0 0 0 0 0 0 0 5
-3.5936 0.8960 -2.6654 H 0 0 0 0 0 0 0 0 0 0 6
1.0923 0.0049 1.1842 C 0 0 0 0 0 0 0 0 0 0 7
-0.2940 -0.0129 1.2198 C 0 0 0 0 0 0 0 0 0 0 8
-1.0394 -0.0268 -0.0018 C 0 0 0 0 0 0 0 0 0 0 9
-0.2897 -0.0251 -1.2212 C 0 0 0 0 0 0 0 0 0 0 10
1.0962 -0.0088 -1.1810 C 0 0 0 0 0 0 0 0 0 0 11
1.8413 0.0076 0.0029 C 0 0 0 0 0 0 0 0 0 0 12
-2.3482 -0.0410 -0.0040 O 0 0 0 0 0 0 0 0 0 0 13
1.9959 -0.0083 -2.7242 Cl 0 0 0 0 0 0 0 0 0 0 14
1.9862 0.0228 2.7302 Cl 0 0 0 0 0 0 0 0 0 0 15
-0.8313 -0.0178 2.1683 H 0 0 0 0 0 0 0 0 0 0 16
-0.8237 -0.0411 -2.1713 H 0 0 0 0 0 0 0 0 0 0 17
2.9286 0.0217 0.0047 H 0 0 0 0 0 0 0 0 0 0 18
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
8 7 0 0 0 0
12 7 0 0 0 0
15 7 0 0 0 0
9 8 0 0 0 0
16 8 0 0 0 0
10 9 0 0 0 0
13 9 0 0 0 0
11 10 0 0 0 0
17 10 0 0 0 0
12 11 0 0 0 0
14 11 0 0 0 0
12 18 0 0 0 0
M END
$$$$
3,5-dichlorophenol.sdf
COSMOTHERM 3D 0
19 17 0 0 0 0 0 0 0 0 0 V2000
-5.5772 -0.7630 1.0927 O 0 0 0 0 0 0 0 0 0 0 1
-5.8509 -1.6984 1.0961 H 0 0 0 0 0 0 0 0 0 0 2
-6.4098 -0.2682 0.9840 H 0 0 0 0 0 0 0 0 0 0 3
-3.7406 -0.1736 -0.7947 O 0 0 0 0 0 0 0 0 0 0 4
-4.4539 -0.4098 -0.1285 H 0 0 0 0 0 0 0 0 0 0 5
-4.1425 -0.3133 -1.6707 H 0 0 0 0 0 0 0 0 0 0 6
-1.5602 -1.5950 -0.5431 O 0 0 0 0 0 0 0 0 0 0 7
-0.4623 -0.8366 -0.3239 C 0 0 0 0 0 0 0 0 0 0 8
0.7700 -1.5014 -0.1669 C 0 0 0 0 0 0 0 0 0 0 9
1.9146 -0.7450 0.0581 C 0 0 0 0 0 0 0 0 0 0 10
3.4644 -1.5860 0.2551 Cl 0 0 0 0 0 0 0 0 0 0 11
1.9049 0.6503 0.1371 C 0 0 0 0 0 0 0 0 0 0 12
0.6650 1.2712 -0.0236 C 0 0 0 0 0 0 0 0 0 0 13
0.5959 3.0420 0.0670 Cl 0 0 0 0 0 0 0 0 0 0 14
-0.5161 0.5705 -0.2513 C 0 0 0 0 0 0 0 0 0 0 15
-2.4013 -1.0216 -0.6391 H 0 0 0 0 0 0 0 0 0 0 16
0.8093 -2.5885 -0.2236 H 0 0 0 0 0 0 0 0 0 0 17
2.8139 1.2209 0.3140 H 0 0 0 0 0 0 0 0 0 0 18
-1.4653 1.0915 -0.3727 H 0 0 0 0 0 0 0 0 0 0 19
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
8 7 0 0 0 0
16 7 0 0 0 0
9 8 0 0 0 0
15 8 0 0 0 0
10 9 0 0 0 0
17 9 0 0 0 0
11 10 0 0 0 0
12 10 0 0 0 0
13 12 0 0 0 0
18 12 0 0 0 0
14 13 0 0 0 0
15 13 0 0 0 0
15 19 0 0 0 0
M END
$$$$
3-chlorophenol-anion.sdf
COSMOTHERM 3D 0
18 16 0 0 0 0 0 0 0 0 0 V2000
-3.0378 0.0518 2.1427 O 0 0 0 0 0 0 0 0 0 0 1
-2.0289 0.0329 2.0461 H 0 0 0 0 0 0 0 0 0 0 2
-3.2933 0.9412 1.8442 H 0 0 0 0 0 0 0 0 0 0 3
0.9537 -0.0544 4.2751 O 0 0 0 0 0 0 0 0 0 0 4
0.4785 -0.0552 3.3798 H 0 0 0 0 0 0 0 0 0 0 5
1.4702 -0.8783 4.2766 H 0 0 0 0 0 0 0 0 0 0 6
2.2879 0.0935 -0.5240 C 0 0 0 0 0 0 0 0 0 0 7
1.6525 0.0664 0.7163 C 0 0 0 0 0 0 0 0 0 0 8
0.2298 0.0002 0.8203 C 0 0 0 0 0 0 0 0 0 0 9
-0.5029 -0.0372 -0.4080 C 0 0 0 0 0 0 0 0 0 0 10
0.1732 -0.0067 -1.6213 C 0 0 0 0 0 0 0 0 0 0 11
1.5641 0.0572 -1.7274 C 0 0 0 0 0 0 0 0 0 0 12
-0.3873 -0.0265 1.9814 O 0 0 0 0 0 0 0 0 0 0 13
-0.7928 -0.0534 -3.1322 Cl 0 0 0 0 0 0 0 0 0 0 14
3.3786 0.1447 -0.5668 H 0 0 0 0 0 0 0 0 0 0 15
2.2389 0.1006 1.6369 H 0 0 0 0 0 0 0 0 0 0 16
-1.5919 -0.0900 -0.3739 H 0 0 0 0 0 0 0 0 0 0 17
2.0613 0.0796 -2.6960 H 0 0 0 0 0 0 0 0 0 0 18
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
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8 7 0 0 0 0
12 7 0 0 0 0
15 7 0 0 0 0
9 8 0 0 0 0
16 8 0 0 0 0
10 9 0 0 0 0
13 9 0 0 0 0
11 10 0 0 0 0
17 10 0 0 0 0
12 11 0 0 0 0
14 11 0 0 0 0
12 18 0 0 0 0
M END
$$$$
3-chlorophenol.sdf
COSMOTHERM 3D 0

19 17 0 0 0 0 0 0 0 0 0 V2000
-0.7238 1.1120 -5.0254 O 0 0 0 0 0 0 0 0 0 0 1
-1.5795 0.7700 -5.3422 H 0 0 0 0 0 0 0 0 0 0 2
-0.2884 1.4532 -5.8279 H 0 0 0 0 0 0 0 0 0 0 3
0.8399 -0.6880 -3.7461 O 0 0 0 0 0 0 0 0 0 0 4
0.2306 -0.0590 -4.2338 H 0 0 0 0 0 0 0 0 0 0 5
0.5041 -1.5824 -3.9323 H 0 0 0 0 0 0 0 0 0 0 6
0.8682 0.0681 1.0114 C 0 0 0 0 0 0 0 0 0 0 7
-0.1197 0.0384 1.9914 C 0 0 0 0 0 0 0 0 0 0 8
-1.4557 -0.2529 1.7094 C 0 0 0 0 0 0 0 0 0 0 9
-1.7918 -0.5245 0.3774 C 0 0 0 0 0 0 0 0 0 0 10
-0.8303 -0.5051 -0.6354 C 0 0 0 0 0 0 0 0 0 0 11
0.5103 -0.2064 -0.3233 C 0 0 0 0 0 0 0 0 0 0 12
-2.2072 -0.2678 2.4975 H 0 0 0 0 0 0 0 0 0 0 13
1.4985 -0.1669 -1.2537 O 0 0 0 0 0 0 0 0 0 0 14
1.9049 0.2981 1.2566 H 0 0 0 0 0 0 0 0 0 0 15
0.3465 0.3877 3.6735 Cl 0 0 0 0 0 0 0 0 0 0 16
-2.8286 -0.7560 0.1272 H 0 0 0 0 0 0 0 0 0 0 17
-1.1122 -0.7210 -1.6668 H 0 0 0 0 0 0 0 0 0 0 18
1.1491 -0.3813 -2.1829 H 0 0 0 0 0 0 0 0 0 0 19

2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
8 7 0 0 0 0
12 7 0 0 0 0
15 7 0 0 0 0
9 8 0 0 0 0
16 8 0 0 0 0
10 9 0 0 0 0
13 9 0 0 0 0
11 10 0 0 0 0
17 10 0 0 0 0
12 11 0 0 0 0
18 11 0 0 0 0
14 12 0 0 0 0
14 19 0 0 0 0
M END
$$$$
3-chloropropanoicacid-anion.sdf
COSMOTHERM 3D 0

16 13 0 0 0 0 0 0 0 0 0 V2000
-5.3061 0.9499 -0.6704 O 0 0 0 0 0 0 0 0 0 0 1
-4.6227 0.3279 -0.2832 H 0 0 0 0 0 0 0 0 0 0 2
-4.9468 1.1936 -1.5405 H 0 0 0 0 0 0 0 0 0 0 3
-3.5091 -0.7365 0.4820 O 0 0 0 0 0 0 0 0 0 0 4
-2.5958 -0.2874 0.6147 H 0 0 0 0 0 0 0 0 0 0 5
-3.3055 -1.4922 -0.0975 H 0 0 0 0 0 0 0 0 0 0 6
2.2085 -0.4155 -0.3406 C 0 0 0 0 0 0 0 0 0 0 7
1.1573 0.4044 0.3789 C 0 0 0 0 0 0 0 0 0 0 8
-0.2579 -0.1987 0.2279 C 0 0 0 0 0 0 0 0 0 0 9
-0.4121 -1.2250 -0.4868 O 0 0 0 0 0 0 0 0 0 0 10
-1.1849 0.4185 0.8612 O 0 0 0 0 0 0 0 0 0 0 11
1.1328 1.4330 -0.0124 H 0 0 0 0 0 0 0 0 0 0 12
2.3045 -1.4272 0.0633 H 0 0 0 0 0 0 0 0 0 0 13
2.0432 -0.4607 -1.4203 H 0 0 0 0 0 0 0 0 0 0 14
3.8905 0.3454 -0.1393 Cl 0 0 0 0 0 0 0 0 0 0 15
1.3878 0.4789 1.4521 H 0 0 0 0 0 0 0 0 0 0 16

2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
8 7 0 0 0 0
13 7 0 0 0 0
14 7 0 0 0 0
15 7 0 0 0 0
9 8 0 0 0 0
12 8 0 0 0 0
10 9 0 0 0 0
11 9 0 0 0 0
8 16 0 0 0 0
M END
$$$$
3-chloropropanoicacid.sdf
COSMOTHERM 3D 0

17 14 0 0 0 0 0 0 0 0 0 V2000
-1.2779 -0.5624 -4.7637 O 0 0 0 0 0 0 0 0 0 0 1
-1.0874 -1.0765 -5.5696 H 0 0 0 0 0 0 0 0 0 0 2
-1.8706 0.1499 -5.0650 H 0 0 0 0 0 0 0 0 0 0 3
0.9917 0.2836 -3.5747 O 0 0 0 0 0 0 0 0 0 0 4
1.0911 1.2367 -3.7469 H 0 0 0 0 0 0 0 0 0 0 5
0.1356 0.0145 -4.0251 H 0 0 0 0 0 0 0 0 0 0 6
-0.5467 0.2883 2.1256 C 0 0 0 0 0 0 0 0 0 0 7
0.5348 -0.2391 1.2001 C 0 0 0 0 0 0 0 0 0 0 8
0.2877 0.1738 -0.2421 C 0 0 0 0 0 0 0 0 0 0 9
1.1991 -0.3363 -1.0741 O 0 0 0 0 0 0 0 0 0 0 10
```

URL: <http://mc.manuscriptcentral.com/tandf/tmph>


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1
2
3      1.8267    0.0008   -3.5273 H    0    0    0    0    0    0    0    0    0    0    17
4     -0.6087    0.0031   -2.9455 H    0    0    0    0    0    0    0    0    0    0    18
5      0.4149   -0.0019    1.2485 H    0    0    0    0    0    0    0    0    0    0    19
6      3.5438   -0.0026   -1.7213 H    0    0    0    0    0    0    0    0    0    0    20
7      2.6930   -0.0023    1.7494 H    0    0    0    0    0    0    0    0    0    0    21
8     -2.9765   -0.0032    0.9765 H    0    0    0    0    0    0    0    0    0    0    22
9
10     2  1  0  0  0  0
11     3  1  0  0  0  0
12     5  4  0  0  0  0
13     6  4  0  0  0  0
14     8  7  0  0  0  0
15    12  7  0  0  0  0
16    17  7  0  0  0  0
17     9  8  0  0  0  0
18    18  8  0  0  0  0
19    10  9  0  0  0  0
20    13  9  0  0  0  0
21    11 10  0  0  0  0
22    19 10  0  0  0  0
23    12 11  0  0  0  0
24    14 11  0  0  0  0
25    20 12  0  0  0  0
26    15 13  0  0  0  0
27    16 13  0  0  0  0
28    21 14  0  0  0  0
29    15 22  0  0  0  0
30
31 M  END
32 $$$$
33 4-(1,1-dimethylethyl)-benzoicacid-anion.sdf
34 COSMOtherm      3D      0
35
36 32 30  0  0  0  0  0  0  0  0  0  0 V2000
37   -6.7350    0.8454    1.4462 O    0  0  0  0  0  0  0  0  0  0  0  1
38   -6.1553    0.3456    0.7990 H    0  0  0  0  0  0  0  0  0  0  0  2
39   -6.3518    1.7386    1.4761 H    0  0  0  0  0  0  0  0  0  0  0  3
40   -5.2147   -0.6131   -0.2678 O    0  0  0  0  0  0  0  0  0  0  0  4
41   -4.2149   -0.5742   -0.0290 H    0  0  0  0  0  0  0  0  0  0  0  5
42   -5.2429   -0.2656   -1.1770 H    0  0  0  0  0  0  0  0  0  0  0  6
43    1.7939    0.3143   -1.2154 C    0  0  0  0  0  0  0  0  0  0  0  7
44    0.4114    0.2519   -1.4216 C    0  0  0  0  0  0  0  0  0  0  0  8
45   -0.4595   -0.1002   -0.3815 C    0  0  0  0  0  0  0  0  0  0  0  9
46    0.0973   -0.3877    0.8764 C    0  0  0  0  0  0  0  0  0  0  0 10
47    1.4759   -0.3218    1.0800 C    0  0  0  0  0  0  0  0  0  0  0 11
48    2.3604    0.0304    0.0396 C    0  0  0  0  0  0  0  0  0  0  0 12
49   -1.9608   -0.1633   -0.6171 C    0  0  0  0  0  0  0  0  0  0  0 13
50    3.8748    0.0903    0.3046 C    0  0  0  0  0  0  0  0  0  0  0 14
51    4.1580    1.1239    1.4213 C    0  0  0  0  0  0  0  0  0  0  0 15
52    4.6735    0.4981   -0.9471 C    0  0  0  0  0  0  0  0  0  0  0 16
53    4.3682   -1.3032    0.7641 C    0  0  0  0  0  0  0  0  0  0  0 17
54   -2.4047    0.1534   -1.7559 O    0  0  0  0  0  0  0  0  0  0  0 18
55   -2.6820   -0.5425    0.3765 O    0  0  0  0  0  0  0  0  0  0  0 19
56    2.4335    0.5912   -2.0536 H    0  0  0  0  0  0  0  0  0  0  0 20
57   -0.0089    0.4785   -2.4031 H    0  0  0  0  0  0  0  0  0  0  0 21
58   -0.5679   -0.6641    1.6961 H    0  0  0  0  0  0  0  0  0  0  0 22
59    1.8697   -0.5501    2.0728 H    0  0  0  0  0  0  0  0  0  0  0 23
60    5.2387    1.1711    1.6257 H    0  0  0  0  0  0  0  0  0  0  0 24
61    3.6489    0.8592    2.3592 H    0  0  0  0  0  0  0  0  0  0  0 25
62    3.8213    2.1279    1.1219 H    0  0  0  0  0  0  0  0  0  0  0 26
63    5.7459    0.5255   -0.7031 H    0  0  0  0  0  0  0  0  0  0  0 27
64    4.5375   -0.2177   -1.7716 H    0  0  0  0  0  0  0  0  0  0  0 28
65    4.3880    1.4977   -1.3072 H    0  0  0  0  0  0  0  0  0  0  0 29
66    5.4500   -1.2717    0.9659 H    0  0  0  0  0  0  0  0  0  0  0 30
67    4.1861   -2.0604   -0.0135 H    0  0  0  0  0  0  0  0  0  0  0 31
68    3.8628   -1.6310    1.6838 H    0  0  0  0  0  0  0  0  0  0  0 32
69
70     2  1  0  0  0  0
71     3  1  0  0  0  0
72     5  4  0  0  0  0
73     6  4  0  0  0  0
74     8  7  0  0  0  0
75    12  7  0  0  0  0
76    20  7  0  0  0  0
77     9  8  0  0  0  0
78    21  8  0  0  0  0
79    10  9  0  0  0  0
80    13  9  0  0  0  0
81    11 10  0  0  0  0
82    22 10  0  0  0  0
83    12 11  0  0  0  0
84    23 11  0  0  0  0
85    14 12  0  0  0  0
86    18 13  0  0  0  0
87    19 13  0  0  0  0
88    15 14  0  0  0  0
89    16 14  0  0  0  0
90    17 14  0  0  0  0
91    24 15  0  0  0  0
92    25 15  0  0  0  0
93    26 15  0  0  0  0
94    27 16  0  0  0  0
95    28 16  0  0  0  0
96    29 16  0  0  0  0
97    30 17  0  0  0  0
98    31 17  0  0  0  0
99    17 32  0  0  0  0
100
101 M  END
102 $$$$
103 4-(1,1-dimethylethyl)-benzoicacid.sdf
104 COSMOtherm      3D      0
105
106 33 31  0  0  0  0  0  0  0  0  0  0 V2000
107   -0.8276    6.4010    1.0394 O    0  0  0  0  0  0  0  0  0  0  0  1
108   -1.7158    6.3418    0.6434 H    0  0  0  0  0  0  0  0  0  0  0  2
109   -0.6669    7.3580    1.1296 H    0  0  0  0  0  0  0  0  0  0  0  3
110    1.1202    5.1466   -0.3488 O    0  0  0  0  0  0  0  0  0  0  0  4
111    0.3734    5.6260    0.1195 H    0  0  0  0  0  0  0  0  0  0  0  5
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17 7 0 0 0 0
9 8 0 0 0 0
18 8 0 0 0 0
10 9 0 0 0 0
13 9 0 0 0 0
11 10 0 0 0 0
19 10 0 0 0 0
12 11 0 0 0 0
14 12 0 0 0 0
15 13 0 0 0 0
16 13 0 0 0 0
11 20 0 0 0 0
M END
$$$$
4-bromobenzoicacid.sdf
COSMOTHERM 3D 0

21 19 0 0 0 0 0 0 0 0 0 V2000
-0.1834 -1.5466 -6.8430 O 0 0 0 0 0 0 0 0 0 0 1
-0.0994 -1.4206 -7.8056 H 0 0 0 0 0 0 0 0 0 0 2
-0.9512 -2.1385 -6.7448 H 0 0 0 0 0 0 0 0 0 0 3
-0.5763 0.7906 -5.5368 O 0 0 0 0 0 0 0 0 0 0 4
-0.4182 -0.0686 -6.0326 H 0 0 0 0 0 0 0 0 0 0 5
0.1542 1.3797 -5.7981 H 0 0 0 0 0 0 0 0 0 0 6
1.2775 -0.0491 1.3465 C 0 0 0 0 0 0 0 0 0 0 7
1.3797 0.0857 -0.0382 C 0 0 0 0 0 0 0 0 0 0 8
0.2326 0.2598 -0.8296 C 0 0 0 0 0 0 0 0 0 0 9
-1.0296 0.3002 -0.2139 C 0 0 0 0 0 0 0 0 0 0 10
-1.1488 0.1687 1.1712 C 0 0 0 0 0 0 0 0 0 0 11
0.0096 -0.0055 1.9321 C 0 0 0 0 0 0 0 0 0 0 12
0.3959 0.3972 -2.3112 C 0 0 0 0 0 0 0 0 0 0 13
-0.1449 -0.1913 3.8422 Br 0 0 0 0 0 0 0 0 0 0 14
1.4973 0.3848 -2.8647 O 0 0 0 0 0 0 0 0 0 0 15
-0.7617 0.5287 -2.9685 O 0 0 0 0 0 0 0 0 0 0 16
2.1705 -0.1846 1.9558 H 0 0 0 0 0 0 0 0 0 0 17
2.3594 0.0562 -0.5163 H 0 0 0 0 0 0 0 0 0 0 18
-1.9266 0.4344 -0.8178 H 0 0 0 0 0 0 0 0 0 0 19
-2.1294 0.1998 1.6455 H 0 0 0 0 0 0 0 0 0 0 20
-0.5952 0.6202 -3.9881 H 0 0 0 0 0 0 0 0 0 0 21

2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
8 7 0 0 0 0
12 7 0 0 0 0
17 7 0 0 0 0
9 8 0 0 0 0
18 8 0 0 0 0
10 9 0 0 0 0
13 9 0 0 0 0
11 10 0 0 0 0
19 10 0 0 0 0
12 11 0 0 0 0
20 11 0 0 0 0
14 12 0 0 0 0
15 13 0 0 0 0
16 13 0 0 0 0
16 21 0 0 0 0
M END
$$$$
4-butylbenzoicacid-anion.sdf
COSMOTHERM 3D 0

32 30 0 0 0 0 0 0 0 0 0 V2000
-7.0625 0.5921 1.3293 O 0 0 0 0 0 0 0 0 0 0 1
-6.4388 0.0256 0.7863 H 0 0 0 0 0 0 0 0 0 0 2
-6.7395 1.5003 1.2015 H 0 0 0 0 0 0 0 0 0 0 3
-5.4093 -1.0348 -0.0851 O 0 0 0 0 0 0 0 0 0 0 4
-4.4198 -0.8384 0.1188 H 0 0 0 0 0 0 0 0 0 0 5
-5.4802 -0.8748 -1.0430 H 0 0 0 0 0 0 0 0 0 0 6
1.1585 0.3852 1.1316 C 0 0 0 0 0 0 0 0 0 0 7
-0.1927 0.0822 0.9459 C 0 0 0 0 0 0 0 0 0 0 8
-0.7605 0.0913 -0.3389 C 0 0 0 0 0 0 0 0 0 0 9
0.0636 0.4102 -1.4306 C 0 0 0 0 0 0 0 0 0 0 10
1.4155 0.7076 -1.2434 C 0 0 0 0 0 0 0 0 0 0 11
1.9884 0.7021 0.0411 C 0 0 0 0 0 0 0 0 0 0 12
-2.2327 -0.2269 -0.5541 C 0 0 0 0 0 0 0 0 0 0 13
3.4592 0.9880 0.2391 C 0 0 0 0 0 0 0 0 0 0 14
4.3320 -0.2847 0.1874 C 0 0 0 0 0 0 0 0 0 0 15
5.8253 0.0029 0.3866 C 0 0 0 0 0 0 0 0 0 0 16
6.6909 -1.2619 0.3471 C 0 0 0 0 0 0 0 0 0 0 17
-2.9045 -0.5649 0.4879 O 0 0 0 0 0 0 0 0 0 0 18
-2.7012 -0.1439 -1.7233 O 0 0 0 0 0 0 0 0 0 0 19
1.5788 0.3822 2.1410 H 0 0 0 0 0 0 0 0 0 0 20
-0.8274 -0.1600 1.7998 H 0 0 0 0 0 0 0 0 0 0 21
-0.3748 0.4246 -2.4300 H 0 0 0 0 0 0 0 0 0 0 22
2.0386 0.9564 -2.1066 H 0 0 0 0 0 0 0 0 0 0 23
3.6108 1.4839 1.2119 H 0 0 0 0 0 0 0 0 0 0 24
3.8058 1.6896 -0.5370 H 0 0 0 0 0 0 0 0 0 0 25
4.1796 -0.7883 -0.7829 H 0 0 0 0 0 0 0 0 0 0 26
3.9863 -0.9909 0.9619 H 0 0 0 0 0 0 0 0 0 0 27
5.9682 0.5182 1.3519 H 0 0 0 0 0 0 0 0 0 0 28
6.1647 0.7077 -0.3917 H 0 0 0 0 0 0 0 0 0 0 29
7.7554 -1.0243 0.4921 H 0 0 0 0 0 0 0 0 0 0 30
6.5920 -1.7806 -0.6192 H 0 0 0 0 0 0 0 0 0 0 31
6.3949 -1.9694 1.1373 H 0 0 0 0 0 0 0 0 0 0 32

2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
8 7 0 0 0 0
12 7 0 0 0 0
20 7 0 0 0 0
9 8 0 0 0 0
21 8 0 0 0 0
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10 9 0 0 0 0
13 9 0 0 0 0
11 10 0 0 0 0
22 10 0 0 0 0
12 11 0 0 0 0
23 11 0 0 0 0
14 12 0 0 0 0
18 13 0 0 0 0
19 13 0 0 0 0
15 14 0 0 0 0
24 14 0 0 0 0
25 14 0 0 0 0
16 15 0 0 0 0
26 15 0 0 0 0
27 15 0 0 0 0
17 16 0 0 0 0
28 16 0 0 0 0
29 16 0 0 0 0
30 17 0 0 0 0
31 17 0 0 0 0
17 32 0 0 0 0
M END
$$$$
4-butylbenzoicacid.sdf
COSMOTHERM 3D 0

33 31 0 0 0 0 0 0 0 0 0 V2000
-1.7363 -6.4760 0.7640 O 0 0 0 0 0 0 0 0 0 1
-1.7376 -7.3981 1.0820 H 0 0 0 0 0 0 0 0 0 2
-2.1564 -6.5196 -0.1139 H 0 0 0 0 0 0 0 0 0 3
0.7551 -5.4234 0.7432 O 0 0 0 0 0 0 0 0 0 4
1.2654 -5.8776 0.0491 H 0 0 0 0 0 0 0 0 0 5
-0.1636 -5.8241 0.7065 H 0 0 0 0 0 0 0 0 0 6
-0.3475 1.3593 -1.3953 C 0 0 0 0 0 0 0 0 0 7
-0.4591 -0.0294 -1.3312 C 0 0 0 0 0 0 0 0 0 8
0.2916 -0.7614 -0.3943 C 0 0 0 0 0 0 0 0 0 9
1.1566 -0.0720 0.4744 C 0 0 0 0 0 0 0 0 0 10
1.2637 1.3173 0.4029 C 0 0 0 0 0 0 0 0 0 11
0.5154 2.0586 -0.5305 C 0 0 0 0 0 0 0 0 0 12
0.1515 -2.2476 -0.3614 C 0 0 0 0 0 0 0 0 0 13
0.6078 3.5655 -0.5751 C 0 0 0 0 0 0 0 0 0 14
-0.3809 4.2559 0.3908 C 0 0 0 0 0 0 0 0 0 15
-0.2881 5.7857 0.3474 C 0 0 0 0 0 0 0 0 0 16
-1.2670 6.4729 1.3062 C 0 0 0 0 0 0 0 0 0 17
-0.5828 -2.8731 -1.1312 O 0 0 0 0 0 0 0 0 0 18
0.8972 -2.8380 0.5825 O 0 0 0 0 0 0 0 0 0 19
-0.9340 1.9136 -2.1323 H 0 0 0 0 0 0 0 0 0 20
-1.1255 -0.5626 -2.0094 H 0 0 0 0 0 0 0 0 0 21
1.7486 -0.6277 1.2017 H 0 0 0 0 0 0 0 0 0 22
1.9454 1.8393 1.0791 H 0 0 0 0 0 0 0 0 0 23
0.4082 3.9158 -1.6005 H 0 0 0 0 0 0 0 0 0 24
1.6327 3.8790 -0.3191 H 0 0 0 0 0 0 0 0 0 25
-0.1860 3.9042 1.4179 H 0 0 0 0 0 0 0 0 0 26
-1.4086 3.9406 0.1422 H 0 0 0 0 0 0 0 0 0 27
-0.4778 6.1298 -0.6839 H 0 0 0 0 0 0 0 0 0 28
0.7437 6.0918 0.5904 H 0 0 0 0 0 0 0 0 0 29
-1.1761 7.5684 1.2547 H 0 0 0 0 0 0 0 0 0 30
-1.0800 6.1700 2.3481 H 0 0 0 0 0 0 0 0 0 31
-2.3089 6.2108 1.0647 H 0 0 0 0 0 0 0 0 0 32
0.7693 -3.8636 0.5601 H 0 0 0 0 0 0 0 0 0 33

2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
8 7 0 0 0 0
12 7 0 0 0 0
20 7 0 0 0 0
9 8 0 0 0 0
21 8 0 0 0 0
10 9 0 0 0 0
13 9 0 0 0 0
11 10 0 0 0 0
22 10 0 0 0 0
12 11 0 0 0 0
23 11 0 0 0 0
14 12 0 0 0 0
18 13 0 0 0 0
19 13 0 0 0 0
15 14 0 0 0 0
24 14 0 0 0 0
25 14 0 0 0 0
16 15 0 0 0 0
26 15 0 0 0 0
27 15 0 0 0 0
17 16 0 0 0 0
28 16 0 0 0 0
29 16 0 0 0 0
30 17 0 0 0 0
31 17 0 0 0 0
32 17 0 0 0 0
19 33 0 0 0 0
M END
$$$$
4-carbamoylbenzoicacid-anion.sdf
COSMOTHERM 3D 0

24 22 0 0 0 0 0 0 0 0 0 V2000
-1.1115 6.4131 -1.2776 O 0 0 0 0 0 0 0 0 0 1
-0.4983 5.8516 -0.7188 H 0 0 0 0 0 0 0 0 0 2
-1.9962 6.0449 -1.1124 H 0 0 0 0 0 0 0 0 0 3
0.6479 4.9381 0.1815 O 0 0 0 0 0 0 0 0 0 4
0.5895 3.9389 -0.0424 H 0 0 0 0 0 0 0 0 0 5
0.4495 4.9715 1.1343 H 0 0 0 0 0 0 0 0 0 6
0.2015 -1.7451 -1.1737 C 0 0 0 0 0 0 0 0 0 7
0.2975 -0.3704 -0.9589 C 0 0 0 0 0 0 0 0 0 8
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1
2
3      0.1570      0.1644      0.3324 C      0      0      0      0      0      0      0      0      0      9
4     -0.0815     -0.7112      1.4034 C      0      0      0      0      0      0      0      0      0      10
5     -0.1851     -2.0868      1.1928 C      0      0      0      0      0      0      0      0      0      11
6     -0.0486     -2.6188     -0.1020 C      0      0      0      0      0      0      0      0      0      12
7      0.2648      1.6666      0.5800 C      0      0      0      0      0      0      0      0      0      13
8     -0.1292     -4.0930     -0.3918 C      0      0      0      0      0      0      0      0      0      14
9      0.3980     -4.5835     -1.4091 O      0      0      0      0      0      0      0      0      0      15
10    -0.7990     -4.8554      0.5074 N      0      0      0      0      0      0      0      0      0      16
11      0.5283      2.3934     -0.4433 O      0      0      0      0      0      0      0      0      0      17
12      0.0924      2.0893      1.7552 O      0      0      0      0      0      0      0      0      0      18
13    -0.8812     -5.8556      0.3455 H      0      0      0      0      0      0      0      0      0      19
14   -1.3233     -4.4572      1.2795 H      0      0      0      0      0      0      0      0      0      20
15      0.3165     -2.1592     -2.1764 H      0      0      0      0      0      0      0      0      0      21
16      0.4846      0.3077     -1.7923 H      0      0      0      0      0      0      0      0      0      22
17    -0.1785     -0.2968      2.4077 H      0      0      0      0      0      0      0      0      0      23
18    -0.3457     -2.7417      2.0514 H      0      0      0      0      0      0      0      0      0      24
19
20      2      1      0      0      0      0
21      3      1      0      0      0      0
22      5      4      0      0      0      0
23      6      4      0      0      0      0
24      8      7      0      0      0      0
25     12      7      0      0      0      0
26     21      7      0      0      0      0
27      9      8      0      0      0      0
28     22      8      0      0      0      0
29     10      9      0      0      0      0
30     13      9      0      0      0      0
31     11     10      0      0      0      0
32     23     10      0      0      0      0
33     12     11      0      0      0      0
34     14     12      0      0      0      0
35     17     13      0      0      0      0
36     18     13      0      0      0      0
37     15     14      0      0      0      0
38     16     14      0      0      0      0
39     19     16      0      0      0      0
40     20     16      0      0      0      0
41     11     24      0      0      0      0
42
43 M      END
44 $$$$
45 4-carbamoylbenzoicacid.sdf
46 COSMOTHERM      3D      0
47
48     25     23      0      0      0      0      0      0      0      0      0      0 V2000
49     -0.8195     -1.3390     -6.2495 O      0      0      0      0      0      0      0      0      0      0      1
50     -0.5276     -1.3186     -7.1792 H      0      0      0      0      0      0      0      0      0      0      2
51     -1.7880     -1.4362     -6.3026 H      0      0      0      0      0      0      0      0      0      0      3
52     -0.1479      0.8839     -4.8699 O      0      0      0      0      0      0      0      0      0      0      4
53     -0.3744      0.0612     -5.3999 H      0      0      0      0      0      0      0      0      0      0      5
54      0.7726      1.1010     -5.1028 H      0      0      0      0      0      0      0      0      0      0      6
55      1.1567     -0.3674      2.0658 C      0      0      0      0      0      0      0      0      0      0      7
56      1.3548     -0.2678      0.6912 C      0      0      0      0      0      0      0      0      0      0      8
57      0.3088      0.1525     -0.1474 C      0      0      0      0      0      0      0      0      0      0      9
58     -0.9387      0.4715      0.4139 C      0      0      0      0      0      0      0      0      0      0      10
59     -1.1380      0.3644      1.7906 C      0      0      0      0      0      0      0      0      0      0      11
60     -0.0933     -0.0603      2.6294 C      0      0      0      0      0      0      0      0      0      0      12
61      0.5635      0.2591     -1.6209 C      0      0      0      0      0      0      0      0      0      0      13
62     -0.2396     -0.1683      4.1258 C      0      0      0      0      0      0      0      0      0      0      14
63      0.7544     -0.1163      4.8739 O      0      0      0      0      0      0      0      0      0      0      15
64     -1.4978     -0.3161      4.6046 N      0      0      0      0      0      0      0      0      0      0      16
65      1.6660      0.0363     -2.1247 O      0      0      0      0      0      0      0      0      0      0      17
66     -0.5134      0.6193     -2.3254 O      0      0      0      0      0      0      0      0      0      0      18
67     -1.6396     -0.3977      5.6081 H      0      0      0      0      0      0      0      0      0      0      19
68     -2.2994     -0.4694      4.0016 H      0      0      0      0      0      0      0      0      0      0      20
69      1.9683     -0.6868      2.7204 H      0      0      0      0      0      0      0      0      0      0      21
70      2.3226     -0.5131      0.2528 H      0      0      0      0      0      0      0      0      0      0      22
71     -1.7513      0.8103     -0.2278 H      0      0      0      0      0      0      0      0      0      0      23
72     -2.1090      0.6421      2.2030 H      0      0      0      0      0      0      0      0      0      0      24
73     -0.2854      0.6889     -3.3357 H      0      0      0      0      0      0      0      0      0      0      25
74
75      2      1      0      0      0      0
76      3      1      0      0      0      0
77      5      4      0      0      0      0
78      6      4      0      0      0      0
79      8      7      0      0      0      0
80     12      7      0      0      0      0
81     21      7      0      0      0      0
82      9      8      0      0      0      0
83     22      8      0      0      0      0
84     10      9      0      0      0      0
85     13      9      0      0      0      0
86     11     10      0      0      0      0
87     23     10      0      0      0      0
88     12     11      0      0      0      0
89     24     11      0      0      0      0
90     14     12      0      0      0      0
91     17     13      0      0      0      0
92     18     13      0      0      0      0
93     15     14      0      0      0      0
94     16     14      0      0      0      0
95     19     16      0      0      0      0
96     20     16      0      0      0      0
97     18     25      0      0      0      0
98
99 M      END
100 $$$$
101 4-chlorobenzoicacid-anion.sdf
102 COSMOTHERM      3D      0
103
104     20     18      0      0      0      0      0      0      0      0      0      0 V2000
105     -6.1498      0.9741      1.3241 O      0      0      0      0      0      0      0      0      0      0      1
106     -5.5888      0.4039      0.7207 H      0      0      0      0      0      0      0      0      0      0      2
107     -5.7084      1.8406      1.3187 H      0      0      0      0      0      0      0      0      0      0      3
108     -4.6808     -0.6624     -0.2759 O      0      0      0      0      0      0      0      0      0      0      4
109     -3.6841     -0.6296     -0.0335 H      0      0      0      0      0      0      0      0      0      0      5
110     -4.6994     -0.3617     -1.2019 H      0      0      0      0      0      0      0      0      0      0      6
111      1.9828     -0.3447      1.1982 C      0      0      0      0      0      0      0      0      0      0      7
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0.6103 -0.4306 0.9483 C 0 0 0 0 0 0 0 0 0 0 8
0.0825 -0.1159 -0.3141 C 0 0 0 0 0 0 0 0 0 0 9
0.9607 0.2894 -1.3315 C 0 0 0 0 0 0 0 0 0 0 10
2.3363 0.3811 -1.1047 C 0 0 0 0 0 0 0 0 0 0 11
2.8273 0.0613 0.1629 C 0 0 0 0 0 0 0 0 0 0 12
-1.4146 -0.2066 -0.5860 C 0 0 0 0 0 0 0 0 0 0 13
4.5731 0.1744 0.4665 Cl 0 0 0 0 0 0 0 0 0 0 14
-2.1460 -0.6090 0.3885 O 0 0 0 0 0 0 0 0 0 0 15
-1.8324 0.1133 -1.7320 O 0 0 0 0 0 0 0 0 0 0 16
2.3879 -0.5886 2.1805 H 0 0 0 0 0 0 0 0 0 0 17
-0.0679 -0.7460 1.7419 H 0 0 0 0 0 0 0 0 0 0 18
0.5525 0.5346 -2.3129 H 0 0 0 0 0 0 0 0 0 0 19
3.0141 0.6950 -1.8988 H 0 0 0 0 0 0 0 0 0 0 20
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
8 7 0 0 0 0
12 7 0 0 0 0
17 7 0 0 0 0
9 8 0 0 0 0
18 8 0 0 0 0
10 9 0 0 0 0
13 9 0 0 0 0
11 10 0 0 0 0
19 10 0 0 0 0
12 11 0 0 0 0
14 12 0 0 0 0
15 13 0 0 0 0
16 13 0 0 0 0
11 20 0 0 0 0
M END
$$$$
4-chlorobenzoicacid.sdf
COSMOtherm 3D 0
21 19 0 0 0 0 0 0 0 0 0 V2000
-0.7679 5.8890 1.0494 O 0 0 0 0 0 0 0 0 0 0 1
-1.6677 5.8792 0.6757 H 0 0 0 0 0 0 0 0 0 0 2
-0.5623 6.8353 1.1593 H 0 0 0 0 0 0 0 0 0 0 3
1.0859 4.5945 -0.4194 O 0 0 0 0 0 0 0 0 0 0 4
0.3718 5.0894 0.0839 H 0 0 0 0 0 0 0 0 0 0 5
1.0046 4.8872 -1.3447 H 0 0 0 0 0 0 0 0 0 0 6
-1.2253 -2.2093 -0.1836 C 0 0 0 0 0 0 0 0 0 0 7
-1.2393 -0.8208 -0.3145 C 0 0 0 0 0 0 0 0 0 0 8
-0.0573 -0.0742 -0.1773 C 0 0 0 0 0 0 0 0 0 0 9
1.1500 -0.7400 0.0957 C 0 0 0 0 0 0 0 0 0 0 10
1.1808 -2.1292 0.2288 C 0 0 0 0 0 0 0 0 0 0 11
-0.0105 -2.8448 0.0866 C 0 0 0 0 0 0 0 0 0 0 12
-0.1243 1.4133 -0.3299 C 0 0 0 0 0 0 0 0 0 0 13
0.0197 -4.6064 0.2531 Cl 0 0 0 0 0 0 0 0 0 0 14
-1.1736 2.0133 -0.5723 O 0 0 0 0 0 0 0 0 0 0 15
1.0578 2.0204 -0.1792 O 0 0 0 0 0 0 0 0 0 0 16
-2.1427 -2.7877 -0.2903 H 0 0 0 0 0 0 0 0 0 0 17
-2.1761 -0.3043 -0.5259 H 0 0 0 0 0 0 0 0 0 0 18
2.0727 -0.1709 0.2046 H 0 0 0 0 0 0 0 0 0 0 19
2.1167 -2.6461 0.4397 H 0 0 0 0 0 0 0 0 0 0 20
0.9640 3.0464 -0.2968 H 0 0 0 0 0 0 0 0 0 0 21
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
8 7 0 0 0 0
12 7 0 0 0 0
17 7 0 0 0 0
9 8 0 0 0 0
18 8 0 0 0 0
10 9 0 0 0 0
13 9 0 0 0 0
11 10 0 0 0 0
19 10 0 0 0 0
12 11 0 0 0 0
20 11 0 0 0 0
14 12 0 0 0 0
15 13 0 0 0 0
16 13 0 0 0 0
16 21 0 0 0 0
M END
$$$$
4-chlorophenol-anion.sdf
COSMOtherm 3D 0
18 16 0 0 0 0 0 0 0 0 0 V2000
-2.2519 -0.0568 3.6678 O 0 0 0 0 0 0 0 0 0 0 1
-1.4103 -0.0221 3.0998 H 0 0 0 0 0 0 0 0 0 0 2
-2.6309 0.8356 3.5925 H 0 0 0 0 0 0 0 0 0 0 3
2.2532 0.0215 3.6640 O 0 0 0 0 0 0 0 0 0 0 4
1.4104 0.0095 3.0968 H 0 0 0 0 0 0 0 0 0 0 5
2.7035 -0.8128 3.4475 H 0 0 0 0 0 0 0 0 0 0 6
-1.2155 -0.0173 -1.1923 C 0 0 0 0 0 0 0 0 0 0 7
-1.2132 -0.0105 0.2036 C 0 0 0 0 0 0 0 0 0 0 8
-0.0003 0.0138 0.9560 C 0 0 0 0 0 0 0 0 0 0 9
1.2123 0.0306 0.2027 C 0 0 0 0 0 0 0 0 0 0 10
1.2140 0.0254 -1.1933 C 0 0 0 0 0 0 0 0 0 0 11
-0.0009 0.0003 -1.8828 C 0 0 0 0 0 0 0 0 0 0 12
0.0001 0.0196 2.2742 O 0 0 0 0 0 0 0 0 0 0 13
-0.0015 -0.0085 -3.6702 Cl 0 0 0 0 0 0 0 0 0 0 14
-2.1604 -0.0357 -1.7386 H 0 0 0 0 0 0 0 0 0 0 15
-2.1625 -0.0264 0.7439 H 0 0 0 0 0 0 0 0 0 0 16
2.1623 0.0559 0.7415 H 0 0 0 0 0 0 0 0 0 0 17
2.1588 0.0398 -1.7400 H 0 0 0 0 0 0 0 0 0 0 18
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
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8 7 0 0 0 0
12 7 0 0 0 0
15 7 0 0 0 0
9 8 0 0 0 0
16 8 0 0 0 0
10 9 0 0 0 0
13 9 0 0 0 0
11 10 0 0 0 0
17 10 0 0 0 0
12 11 0 0 0 0
14 12 0 0 0 0
11 18 0 0 0 0
M END
$$$$
4-chlorophenol.sdf
COSMOTHERM 3D 0

19 17 0 0 0 0 0 0 0 0 0 V2000
-1.7217 4.7271 0.8187 O 0 0 0 0 0 0 0 0 0 0 1
-2.5087 4.1585 0.8985 H 0 0 0 0 0 0 0 0 0 0 2
-2.0749 5.5958 0.5533 H 0 0 0 0 0 0 0 0 0 0 3
0.2658 3.8327 -0.8041 O 0 0 0 0 0 0 0 0 0 0 4
-0.5035 4.1447 -0.2433 H 0 0 0 0 0 0 0 0 0 0 5
-0.0691 3.7923 -1.7173 H 0 0 0 0 0 0 0 0 0 0 6
1.7447 -0.5877 0.4549 C 0 0 0 0 0 0 0 0 0 0 7
1.1630 -1.8570 0.4527 C 0 0 0 0 0 0 0 0 0 0 8
-0.1501 -2.0072 -0.0020 C 0 0 0 0 0 0 0 0 0 0 9
-0.8861 -0.9111 -0.4525 C 0 0 0 0 0 0 0 0 0 0 10
-0.2999 0.3591 -0.4482 C 0 0 0 0 0 0 0 0 0 0 11
1.0216 0.5325 0.0075 C 0 0 0 0 0 0 0 0 0 0 12
-0.8942 -3.6236 -0.0052 C1 0 0 0 0 0 0 0 0 0 0 13
1.6418 1.7442 0.0387 O 0 0 0 0 0 0 0 0 0 0 14
2.7696 -0.4560 0.8068 H 0 0 0 0 0 0 0 0 0 0 15
1.7320 -2.7200 0.8018 H 0 0 0 0 0 0 0 0 0 0 16
-1.9092 -1.0373 -0.8072 H 0 0 0 0 0 0 0 0 0 0 17
-0.8749 1.2174 -0.8000 H 0 0 0 0 0 0 0 0 0 0 18
1.0402 2.4831 -0.3057 H 0 0 0 0 0 0 0 0 0 0 19

2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
8 7 0 0 0 0
12 7 0 0 0 0
15 7 0 0 0 0
9 8 0 0 0 0
16 8 0 0 0 0
10 9 0 0 0 0
13 9 0 0 0 0
11 10 0 0 0 0
17 10 0 0 0 0
12 11 0 0 0 0
18 11 0 0 0 0
14 12 0 0 0 0
14 19 0 0 0 0
M END
$$$$
4-cyanobenzoicacid-anion.sdf
COSMOTHERM 3D 0

21 19 0 0 0 0 0 0 0 0 0 V2000
-6.1765 0.5578 1.4240 O 0 0 0 0 0 0 0 0 0 0 1
-5.5352 0.1903 0.7488 H 0 0 0 0 0 0 0 0 0 0 2
-5.8608 1.4619 1.5924 H 0 0 0 0 0 0 0 0 0 0 3
-4.4793 -0.5604 -0.3852 O 0 0 0 0 0 0 0 0 0 0 4
-3.4937 -0.4754 -0.1249 H 0 0 0 0 0 0 0 0 0 0 5
-4.5277 -0.1442 -1.2639 H 0 0 0 0 0 0 0 0 0 0 6
2.1389 -0.1456 1.2824 C 0 0 0 0 0 0 0 0 0 0 7
0.7754 -0.1813 0.9993 C 0 0 0 0 0 0 0 0 0 0 8
0.3089 -0.0282 -0.3166 C 0 0 0 0 0 0 0 0 0 0 9
1.2360 0.1588 -1.3549 C 0 0 0 0 0 0 0 0 0 0 10
2.6040 0.1856 -1.0958 C 0 0 0 0 0 0 0 0 0 0 11
3.0606 0.0352 0.2303 C 0 0 0 0 0 0 0 0 0 0 12
-1.1876 -0.0612 -0.6264 C 0 0 0 0 0 0 0 0 0 0 13
4.4606 0.0645 0.5084 C 0 0 0 0 0 0 0 0 0 0 14
5.6061 0.0874 0.7360 N 0 0 0 0 0 0 0 0 0 0 15
-1.9559 -0.3961 0.3422 O 0 0 0 0 0 0 0 0 0 0 16
-1.5546 0.2351 -1.7943 O 0 0 0 0 0 0 0 0 0 0 17
2.4967 -0.2590 2.3060 H 0 0 0 0 0 0 0 0 0 0 18
0.0525 -0.3286 1.8019 H 0 0 0 0 0 0 0 0 0 0 19
0.8666 0.2814 -2.3734 H 0 0 0 0 0 0 0 0 0 0 20
3.3204 0.3233 -1.9061 H 0 0 0 0 0 0 0 0 0 0 21

2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
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15 14 0 0 0 0
11 21 0 0 0 0
M END
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4-cyanobenzoicacid.sdf
COSMOTHERM 3D 0
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12 11 0 0 0 0
21 11 0 0 0 0
14 12 0 0 0 0
16 13 0 0 0 0
17 13 0 0 0 0
15 14 0 0 0 0
22 14 0 0 0 0
23 14 0 0 0 0
24 15 0 0 0 0
25 15 0 0 0 0
15 26 0 0 0 0
M END
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4-ethylbenzoicacid.sdf
COSMOTHERM 3D 0

27 25 0 0 0 0 0 0 0 0 0 V2000
-0.6942 1.3292 5.7722 O 0 0 0 0 0 0 0 0 0 0 1
-1.6350 1.2130 5.5468 H 0 0 0 0 0 0 0 0 0 0 2
-0.5039 2.2594 5.5522 H 0 0 0 0 0 0 0 0 0 0 3
0.9874 -0.3650 4.4979 O 0 0 0 0 0 0 0 0 0 0 4
0.7736 -1.2598 4.8171 H 0 0 0 0 0 0 0 0 0 0 5
0.3364 0.2454 4.9560 H 0 0 0 0 0 0 0 0 0 0 6
-1.1548 -0.4374 -2.3732 C 0 0 0 0 0 0 0 0 0 0 7
-1.2083 -0.5174 -0.9822 C 0 0 0 0 0 0 0 0 0 0 8
-0.0476 -0.3253 -0.2129 C 0 0 0 0 0 0 0 0 0 0 9
1.1670 -0.0548 -0.8685 C 0 0 0 0 0 0 0 0 0 0 10
1.2126 0.0208 -2.2611 C 0 0 0 0 0 0 0 0 0 0 11
0.0553 -0.1671 -3.0386 C 0 0 0 0 0 0 0 0 0 0 12
-0.1417 -0.4264 1.2741 C 0 0 0 0 0 0 0 0 0 0 13
0.1031 -0.0433 -4.5439 C 0 0 0 0 0 0 0 0 0 0 14
-0.1269 1.4026 -5.0257 C 0 0 0 0 0 0 0 0 0 0 15
-1.1883 -0.7041 1.8658 O 0 0 0 0 0 0 0 0 0 0 16
1.0162 -0.1872 1.9062 O 0 0 0 0 0 0 0 0 0 0 17
-2.0652 -0.5939 -2.9568 H 0 0 0 0 0 0 0 0 0 0 18
-2.1505 -0.7332 -0.4762 H 0 0 0 0 0 0 0 0 0 0 19
2.0758 0.0901 -0.2843 H 0 0 0 0 0 0 0 0 0 0 20
2.1651 0.2236 -2.7565 H 0 0 0 0 0 0 0 0 0 0 21
-0.6614 -0.6990 -4.9884 H 0 0 0 0 0 0 0 0 0 0 22
1.0809 -0.3945 -4.9078 H 0 0 0 0 0 0 0 0 0 0 23
-0.0837 1.4554 -6.1234 H 0 0 0 0 0 0 0 0 0 0 24
0.6395 2.0802 -4.6212 H 0 0 0 0 0 0 0 0 0 0 25
-1.1113 1.7734 -4.7046 H 0 0 0 0 0 0 0 0 0 0 26
0.8998 -0.2819 2.9284 H 0 0 0 0 0 0 0 0 0 0 27

2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
8 7 0 0 0 0
12 7 0 0 0 0
18 7 0 0 0 0
9 8 0 0 0 0
19 8 0 0 0 0
10 9 0 0 0 0
13 9 0 0 0 0
11 10 0 0 0 0
20 10 0 0 0 0
12 11 0 0 0 0
21 11 0 0 0 0
14 12 0 0 0 0
16 13 0 0 0 0
17 13 0 0 0 0
15 14 0 0 0 0
22 14 0 0 0 0
23 14 0 0 0 0
24 15 0 0 0 0
25 15 0 0 0 0
26 15 0 0 0 0
17 27 0 0 0 0
M END
$$$$
4-fluorobenzoicacid-anion.sdf
COSMOTHERM 3D 0

20 18 0 0 0 0 0 0 0 0 0 V2000
-5.7199 0.9290 1.2087 O 0 0 0 0 0 0 0 0 0 0 1
-5.1346 0.3762 0.6120 H 0 0 0 0 0 0 0 0 0 0 2
-5.3306 1.8194 1.1743 H 0 0 0 0 0 0 0 0 0 0 3
-4.1845 -0.6668 -0.3684 O 0 0 0 0 0 0 0 0 0 0 4
-3.1979 -0.6385 -0.0846 H 0 0 0 0 0 0 0 0 0 0 5
-4.1633 -0.3503 -1.2891 H 0 0 0 0 0 0 0 0 0 0 6
2.4160 -0.2667 1.3373 C 0 0 0 0 0 0 0 0 0 0 7
1.0533 -0.3728 1.0440 C 0 0 0 0 0 0 0 0 0 0 8
0.5654 -0.0951 -0.2440 C 0 0 0 0 0 0 0 0 0 0 9
1.4728 0.2938 -1.2435 C 0 0 0 0 0 0 0 0 0 0 10
2.8398 0.4033 -0.9750 C 0 0 0 0 0 0 0 0 0 0 11
3.2790 0.1200 0.3156 C 0 0 0 0 0 0 0 0 0 0 12
-0.9195 -0.2080 -0.5628 C 0 0 0 0 0 0 0 0 0 0 13
4.6175 0.2254 0.5917 F 0 0 0 0 0 0 0 0 0 0 14
-1.6778 -0.6170 0.3893 O 0 0 0 0 0 0 0 0 0 0 15
-1.3071 0.1017 -1.7223 O 0 0 0 0 0 0 0 0 0 0 16
2.8050 -0.4772 2.3342 H 0 0 0 0 0 0 0 0 0 0 17
0.3504 -0.6748 1.8209 H 0 0 0 0 0 0 0 0 0 0 18
1.0925 0.5097 -2.2425 H 0 0 0 0 0 0 0 0 0 0 19
3.5526 0.7019 -1.7447 H 0 0 0 0 0 0 0 0 0 0 20

2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
8 7 0 0 0 0
12 7 0 0 0 0
17 7 0 0 0 0
9 8 0 0 0 0
18 8 0 0 0 0
10 9 0 0 0 0
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13 9 0 0 0 0
11 10 0 0 0 0
19 10 0 0 0 0
12 11 0 0 0 0
14 12 0 0 0 0
15 13 0 0 0 0
16 13 0 0 0 0
11 20 0 0 0 0
M END
$$$$
4-fluorobenzoicacid.sdf
COSMOtherm 3D 0

21 19 0 0 0 0 0 0 0 0 0 V2000
-0.8236 5.4240 0.9369 O 0 0 0 0 0 0 0 0 0 0 1
-1.7013 5.4108 0.5138 H 0 0 0 0 0 0 0 0 0 0 2
-0.6229 6.3714 1.0471 H 0 0 0 0 0 0 0 0 0 0 3
1.1105 4.1141 -0.4125 O 0 0 0 0 0 0 0 0 0 0 4
0.3682 4.6132 0.0429 H 0 0 0 0 0 0 0 0 0 0 5
1.0816 4.3956 -1.3443 H 0 0 0 0 0 0 0 0 0 0 6
-1.2278 -2.6809 -0.1127 C 0 0 0 0 0 0 0 0 0 0 7
-1.2355 -1.2941 -0.2592 C 0 0 0 0 0 0 0 0 0 0 8
-0.0478 -0.5519 -0.1361 C 0 0 0 0 0 0 0 0 0 0 9
1.1595 -1.2195 0.1382 C 0 0 0 0 0 0 0 0 0 0 10
1.1853 -2.6069 0.2877 C 0 0 0 0 0 0 0 0 0 0 11
-0.0123 -3.3058 0.1582 C 0 0 0 0 0 0 0 0 0 0 12
-0.1084 0.9324 -0.3058 C 0 0 0 0 0 0 0 0 0 0 13
0.0053 -4.6632 0.3025 F 0 0 0 0 0 0 0 0 0 0 14
-1.1519 1.5355 -0.5661 O 0 0 0 0 0 0 0 0 0 0 15
1.0745 1.5388 -0.1476 O 0 0 0 0 0 0 0 0 0 0 16
-2.1404 -3.2700 -0.2049 H 0 0 0 0 0 0 0 0 0 0 17
-2.1696 -0.7735 -0.4718 H 0 0 0 0 0 0 0 0 0 0 18
2.0838 -0.6511 0.2352 H 0 0 0 0 0 0 0 0 0 0 19
2.1124 -3.1399 0.4996 H 0 0 0 0 0 0 0 0 0 0 20
0.9838 2.5623 -0.2763 H 0 0 0 0 0 0 0 0 0 0 21

2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
8 7 0 0 0 0
12 7 0 0 0 0
17 7 0 0 0 0
9 8 0 0 0 0
18 8 0 0 0 0
10 9 0 0 0 0
13 9 0 0 0 0
11 10 0 0 0 0
19 10 0 0 0 0
12 11 0 0 0 0
20 11 0 0 0 0
14 12 0 0 0 0
15 13 0 0 0 0
16 13 0 0 0 0
16 21 0 0 0 0
M END
$$$$
4-hydroxybenzoicacid-anion.sdf
COSMOtherm 3D 0

21 19 0 0 0 0 0 0 0 0 0 V2000
-1.4572 0.0138 5.0810 O 0 0 0 0 0 0 0 0 0 0 1
-2.0471 -0.7603 5.0367 H 0 0 0 0 0 0 0 0 0 0 2
-2.0521 0.7828 5.0186 H 0 0 0 0 0 0 0 0 0 0 3
-0.9993 0.0337 -5.3129 O 0 0 0 0 0 0 0 0 0 0 4
-1.0115 0.0076 -4.2987 H 0 0 0 0 0 0 0 0 0 0 5
-0.0468 0.0459 -5.5120 H 0 0 0 0 0 0 0 0 0 0 6
1.6701 0.0045 1.3340 C 0 0 0 0 0 0 0 0 0 0 7
1.5270 -0.0001 -0.0523 C 0 0 0 0 0 0 0 0 0 0 8
0.2568 -0.0091 -0.6577 C 0 0 0 0 0 0 0 0 0 0 9
-0.8724 -0.0134 0.1790 C 0 0 0 0 0 0 0 0 0 0 10
-0.7476 -0.0084 1.5694 C 0 0 0 0 0 0 0 0 0 0 11
0.5300 0.0009 2.1594 C 0 0 0 0 0 0 0 0 0 0 12
0.1214 -0.0129 -2.1691 C 0 0 0 0 0 0 0 0 0 0 13
-1.0721 -0.0288 -2.6438 O 0 0 0 0 0 0 0 0 0 0 14
1.1775 -0.0003 -2.8658 O 0 0 0 0 0 0 0 0 0 0 15
0.7213 0.0065 3.5094 O 0 0 0 0 0 0 0 0 0 0 16
-0.1536 0.0057 4.0037 H 0 0 0 0 0 0 0 0 0 0 17
2.6594 0.0114 1.7965 H 0 0 0 0 0 0 0 0 0 0 18
2.4108 0.0032 -0.6930 H 0 0 0 0 0 0 0 0 0 0 19
-1.8634 -0.0208 -0.2778 H 0 0 0 0 0 0 0 0 0 0 20
-1.6377 -0.0114 2.2026 H 0 0 0 0 0 0 0 0 0 0 21

2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
8 7 0 0 0 0
12 7 0 0 0 0
18 7 0 0 0 0
9 8 0 0 0 0
19 8 0 0 0 0
10 9 0 0 0 0
13 9 0 0 0 0
11 10 0 0 0 0
20 10 0 0 0 0
12 11 0 0 0 0
16 12 0 0 0 0
14 13 0 0 0 0
15 13 0 0 0 0
17 16 0 0 0 0
11 21 0 0 0 0
M END
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4-hydroxybenzoicacid.sdf
COSMOtherm 3D 0
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22 20 0 0 0 0 0 0 0 0 0 V2000
-5.2431 0.0177 1.1698 O 0 0 0 0 0 0 0 0 0 0 1
-5.6925 -0.7349 0.7429 H 0 0 0 0 0 0 0 0 0 0 2
-5.6544 0.8063 0.7703 H 0 0 0 0 0 0 0 0 0 0 3
4.8819 0.0178 1.6446 O 0 0 0 0 0 0 0 0 0 0 4
5.4734 0.7895 1.7146 H 0 0 0 0 0 0 0 0 0 0 5
5.4718 -0.7536 1.7287 H 0 0 0 0 0 0 0 0 0 0 6
1.4126 -0.0003 -1.6839 C 0 0 0 0 0 0 0 0 0 0 7
0.0272 -0.0018 -1.5873 C 0 0 0 0 0 0 0 0 0 0 8
-0.6127 -0.0074 -0.3317 C 0 0 0 0 0 0 0 0 0 0 9
0.1831 -0.0116 0.8304 C 0 0 0 0 0 0 0 0 0 0 10
1.5726 -0.0094 0.7464 C 0 0 0 0 0 0 0 0 0 0 11
2.2023 -0.0034 -0.5155 C 0 0 0 0 0 0 0 0 0 0 12
-2.0943 -0.0047 -0.2800 C 0 0 0 0 0 0 0 0 0 0 13
-2.5958 -0.0273 0.9715 O 0 0 0 0 0 0 0 0 0 0 14
-2.8148 0.0167 -1.2826 O 0 0 0 0 0 0 0 0 0 0 15
3.5490 -0.0008 -0.6645 O 0 0 0 0 0 0 0 0 0 0 16
-3.6129 -0.0146 0.9349 H 0 0 0 0 0 0 0 0 0 0 17
4.0213 0.0057 0.2291 H 0 0 0 0 0 0 0 0 0 0 18
1.9062 0.0036 -2.6572 H 0 0 0 0 0 0 0 0 0 0 19
-0.5823 0.0016 -2.4922 H 0 0 0 0 0 0 0 0 0 0 20
-0.2938 -0.0159 1.8107 H 0 0 0 0 0 0 0 0 0 0 21
2.1795 -0.0114 1.6534 H 0 0 0 0 0 0 0 0 0 0 22

2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
8 7 0 0 0 0
12 7 0 0 0 0
19 7 0 0 0 0
9 8 0 0 0 0
20 8 0 0 0 0
10 9 0 0 0 0
13 9 0 0 0 0
11 10 0 0 0 0
21 10 0 0 0 0
12 11 0 0 0 0
16 12 0 0 0 0
14 13 0 0 0 0
15 13 0 0 0 0
17 14 0 0 0 0
18 16 0 0 0 0
11 22 0 0 0 0

M END
$$$$
4-hydroxymethylbenzoicacid-anion.sdf
COSMOTHERM 3D 0

24 22 0 0 0 0 0 0 0 0 0 V2000
-6.1330 0.7800 1.2803 O 0 0 0 0 0 0 0 0 0 0 1
-5.5373 0.2480 0.6749 H 0 0 0 0 0 0 0 0 0 0 2
-5.7408 1.6697 1.2872 H 0 0 0 0 0 0 0 0 0 0 3
-4.5624 -0.7614 -0.3156 O 0 0 0 0 0 0 0 0 0 0 4
-3.5716 -0.6768 -0.0571 H 0 0 0 0 0 0 0 0 0 0 5
-4.5815 -0.4655 -1.2431 H 0 0 0 0 0 0 0 0 0 0 6
2.0394 -0.0333 1.2774 C 0 0 0 0 0 0 0 0 0 0 7
0.6797 -0.2131 1.0104 C 0 0 0 0 0 0 0 0 0 0 8
0.1706 -0.0011 -0.2814 C 0 0 0 0 0 0 0 0 0 0 9
1.0548 0.3946 -1.2984 C 0 0 0 0 0 0 0 0 0 0 10
2.4142 0.5722 -1.0310 C 0 0 0 0 0 0 0 0 0 0 11
2.9242 0.3618 0.2607 C 0 0 0 0 0 0 0 0 0 0 12
-1.3125 -0.1835 -0.5827 C 0 0 0 0 0 0 0 0 0 0 13
4.3956 0.5213 0.5415 C 0 0 0 0 0 0 0 0 0 0 14
5.0483 -0.7553 0.3098 O 0 0 0 0 0 0 0 0 0 0 15
-2.0503 -0.5701 0.3943 O 0 0 0 0 0 0 0 0 0 0 16
-1.7186 0.0517 -1.7537 O 0 0 0 0 0 0 0 0 0 0 17
5.9973 -0.6253 0.4929 H 0 0 0 0 0 0 0 0 0 0 18
2.4207 -0.1954 2.2886 H 0 0 0 0 0 0 0 0 0 0 19
-0.0061 -0.5158 1.8028 H 0 0 0 0 0 0 0 0 0 0 20
0.6577 0.5651 -2.3002 H 0 0 0 0 0 0 0 0 0 0 21
3.0898 0.8842 -1.8313 H 0 0 0 0 0 0 0 0 0 0 22
4.5497 0.8370 1.5872 H 0 0 0 0 0 0 0 0 0 0 23
4.8273 1.2891 -0.1227 H 0 0 0 0 0 0 0 0 0 0 24

2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
8 7 0 0 0 0
12 7 0 0 0 0
19 7 0 0 0 0
9 8 0 0 0 0
20 8 0 0 0 0
10 9 0 0 0 0
13 9 0 0 0 0
11 10 0 0 0 0
21 10 0 0 0 0
12 11 0 0 0 0
22 11 0 0 0 0
14 12 0 0 0 0
16 13 0 0 0 0
17 13 0 0 0 0
15 14 0 0 0 0
23 14 0 0 0 0
18 15 0 0 0 0
14 24 0 0 0 0

M END
$$$$
4-hydroxymethylbenzoicacid.sdf
COSMOTHERM 3D 0

25 23 0 0 0 0 0 0 0 0 0 V2000
-0.8166 -5.7453 1.2385 O 0 0 0 0 0 0 0 0 0 0 1
-0.6279 -6.6922 1.3702 H 0 0 0 0 0 0 0 0 0 0 2
-1.7155 -5.7286 0.8633 H 0 0 0 0 0 0 0 0 0 0 3
1.0497 -4.5252 -0.2799 O 0 0 0 0 0 0 0 0 0 0 4
```

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1
2
3      0.9554   -4.8517   -1.1925 H   0   0   0   0   0   0   0   0   0   0   5
4      0.3331   -4.9894    0.2481 H   0   0   0   0   0   0   0   0   0   0   6
5     -1.1493    2.3179   -0.4656 C   0   0   0   0   0   0   0   0   0   0   7
6     -1.1919    0.9252   -0.5277 C   0   0   0   0   0   0   0   0   0   0   8
7     -0.0276    0.1702   -0.3044 C   0   0   0   0   0   0   0   0   0   0   9
8      1.1788    0.8335   -0.0193 C   0   0   0   0   0   0   0   0   0   0   10
9      1.2142    2.2277    0.0395 C   0   0   0   0   0   0   0   0   0   0   11
10     0.0535    2.9861   -0.1830 C   0   0   0   0   0   0   0   0   0   0   12
11     -0.1090   -1.3224   -0.3924 C   0   0   0   0   0   0   0   0   0   0   13
12     0.0899    4.4899   -0.0842 C   0   0   0   0   0   0   0   0   0   0   14
13     -0.1902    4.8598    1.2900 O   0   0   0   0   0   0   0   0   0   0   15
14     -1.1497   -1.9212   -0.6737 O   0   0   0   0   0   0   0   0   0   0   16
15      1.0509   -1.9401   -0.1375 O   0   0   0   0   0   0   0   0   0   0   17
16     -0.1799    5.8344    1.3288 H   0   0   0   0   0   0   0   0   0   0   18
17     -2.0584    2.8965   -0.6450 H   0   0   0   0   0   0   0   0   0   0   19
18     -2.1255    0.4079   -0.7531 H   0   0   0   0   0   0   0   0   0   0   20
19      2.0871    0.2558    0.1498 H   0   0   0   0   0   0   0   0   0   0   21
20      2.1566    2.7358    0.2549 H   0   0   0   0   0   0   0   0   0   0   22
21     -0.6658    4.9306   -0.7557 H   0   0   0   0   0   0   0   0   0   0   23
22      1.0836    4.8642   -0.3814 H   0   0   0   0   0   0   0   0   0   0   24
23      0.9449   -2.9687   -0.2193 H   0   0   0   0   0   0   0   0   0   0   25
24
25  2   1   0   0   0   0   0
26  3   1   0   0   0   0   0
27  5   4   0   0   0   0   0
28  6   4   0   0   0   0   0
29  8   7   0   0   0   0   0
30 12   7   0   0   0   0   0
31 19   7   0   0   0   0   0
32  9   8   0   0   0   0   0
33 20   8   0   0   0   0   0
34 10   9   0   0   0   0   0
35 13   9   0   0   0   0   0
36 11  10   0   0   0   0   0
37 21  10   0   0   0   0   0
38 12  11   0   0   0   0   0
39 22  11   0   0   0   0   0
40 14  12   0   0   0   0   0
41 16  13   0   0   0   0   0
42 17  13   0   0   0   0   0
43 15  14   0   0   0   0   0
44 23  14   0   0   0   0   0
45 24  14   0   0   0   0   0
46 18  15   0   0   0   0   0
47 17  25   0   0   0   0   0
48
49 M   END
50 $$$$
51 4-iodobenzoicacid-anion.sdf
52 COSMOTHERM      3D      0
53
54 20 17   0   0   0   0   0   0   0   0   0   0 V2000
55 -7.8130   0.6164   1.7876 O   0   0   0   0   0   0   0   0   0   0   1
56 -7.2635   0.2535   1.0327 H   0   0   0   0   0   0   0   0   0   0   2
57 -7.4343   1.4943   1.9649 H   0   0   0   0   0   0   0   0   0   0   3
58 -6.3675  -0.4873  -0.2341 O   0   0   0   0   0   0   0   0   0   0   4
59 -5.3561  -0.4419  -0.0685 H   0   0   0   0   0   0   0   0   0   0   5
60 -6.4914  -0.0316  -1.0852 H   0   0   0   0   0   0   0   0   0   0   6
61  0.3522  -0.2771   0.9984 C   0   0   0   0   0   0   0   0   0   0   7
62 -1.0295  -0.3071   0.7820 C   0   0   0   0   0   0   0   0   0   0   8
63 -1.5689  -0.0710  -0.4919 C   0   0   0   0   0   0   0   0   0   0   9
64 -0.6943   0.1954  -1.5566 C   0   0   0   0   0   0   0   0   0   0   10
65  0.6906   0.2252  -1.3648 C   0   0   0   0   0   0   0   0   0   0   11
66  1.1959  -0.0113  -0.0835 C   0   0   0   0   0   0   0   0   0   0   12
67 -3.0757  -0.0968  -0.7251 C   0   0   0   0   0   0   0   0   0   0   13
68  3.3161   0.0356   0.2302 I   0   0   0   0   0   0   0   0   0   0   14
69 -3.8000  -0.4212   0.2827 O   0   0   0   0   0   0   0   0   0   0   15
70 -3.5052   0.1969  -1.8734 O   0   0   0   0   0   0   0   0   0   0   16
71  0.7555  -0.4589   1.9944 H   0   0   0   0   0   0   0   0   0   0   17
72 -1.7042  -0.5157   1.6132 H   0   0   0   0   0   0   0   0   0   0   18
73 -1.1107   0.3812  -2.5477 H   0   0   0   0   0   0   0   0   0   0   19
74  1.3563   0.4307  -2.2030 H   0   0   0   0   0   0   0   0   0   0   20
75
76  2   1   0   0   0   0   0
77  3   1   0   0   0   0   0
78  5   4   0   0   0   0   0
79  6   4   0   0   0   0   0
80  8   7   0   0   0   0   0
81 12   7   0   0   0   0   0
82 17   7   0   0   0   0   0
83  9   8   0   0   0   0   0
84 18   8   0   0   0   0   0
85 10   9   0   0   0   0   0
86 13   9   0   0   0   0   0
87 11  10   0   0   0   0   0
88 19  10   0   0   0   0   0
89 12  11   0   0   0   0   0
90 15  13   0   0   0   0   0
91 16  13   0   0   0   0   0
92 11  20   0   0   0   0   0
93
94 M   END
95 $$$$
96 4-iodobenzoicacid.sdf
97 COSMOTHERM      3D      0
98
99 21 18   0   0   0   0   0   0   0   0   0   0 V2000
100 -0.0919  -1.5447  -7.5842 O   0   0   0   0   0   0   0   0   0   0   1
101 -0.0551  -1.4210  -8.5507 H   0   0   0   0   0   0   0   0   0   0   2
102 -0.7827  -2.2201  -7.4545 H   0   0   0   0   0   0   0   0   0   0   3
103 -0.6872   0.7389  -6.2671 O   0   0   0   0   0   0   0   0   0   0   4
104 -0.4465  -0.0963  -6.7708 H   0   0   0   0   0   0   0   0   0   0   5
105 -0.0496   1.4147  -6.5593 H   0   0   0   0   0   0   0   0   0   0   6
106  1.3120   0.0278   0.6022 C   0   0   0   0   0   0   0   0   0   0   7
107  1.3954   0.1436  -0.7863 C   0   0   0   0   0   0   0   0   0   0   8
108  0.2355   0.2696  -1.5678 C   0   0   0   0   0   0   0   0   0   0   9
109 -1.0204   0.2789  -0.9385 C   0   0   0   0   0   0   0   0   0   0   10
110 -1.1203   0.1662   0.4505 C   0   0   0   0   0   0   0   0   0   0   11
111  0.0501   0.0421   1.2046 C   0   0   0   0   0   0   0   0   0   0   12
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URL: <http://mc.manuscriptcentral.com/tandf/tmph>

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-1.2258 -4.8003 0.1018 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 18
-2.3889 -2.7718 -0.2014 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 19
-2.2969 -0.3072 -0.4082 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 20
1.9833 -0.4101 0.1042 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 21
1.9200 -2.8582 0.3092 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 22
0.4770 -6.2728 0.4321 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 23
1.5525 -5.1633 -0.4562 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 24
1.3680 -5.0075 1.3145 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 25
1.0188 2.8710 -0.3006 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 26
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
8 7 0 0 0 0
12 7 0 0 0 0
19 7 0 0 0 0
9 8 0 0 0 0
20 8 0 0 0 0
10 9 0 0 0 0
13 9 0 0 0 0
11 10 0 0 0 0
21 10 0 0 0 0
12 11 0 0 0 0
22 11 0 0 0 0
14 12 0 0 0 0
16 13 0 0 0 0
17 13 0 0 0 0
15 14 0 0 0 0
18 14 0 0 0 0
23 15 0 0 0 0
24 15 0 0 0 0
25 15 0 0 0 0
17 26 0 0 0 0
M END
$$$$
4-methylbenzoicacid-anion.sdf
COSMOtherm 3D 0
23 21 0 0 0 0 0 0 0 0 0 0 V2000
-5.6243 0.9671 1.1706 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1
-5.0403 0.3924 0.5929 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 2
-5.1729 1.8280 1.1919 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 3
-4.0990 -0.6815 -0.3581 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 4
-3.1134 -0.6594 -0.0652 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 5
-4.0620 -0.3720 -1.2809 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 6
2.5044 -0.2516 1.3302 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 7
1.1399 -0.3749 1.0541 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 8
0.6382 -0.0981 -0.2282 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 9
1.5425 0.3059 -1.2241 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 10
2.9063 0.4256 -0.9474 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 11
3.4142 0.1465 0.3344 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 12
4.8916 0.2469 0.6239 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 13
-0.8452 -0.2218 -0.5408 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 14
-1.5998 -0.6432 0.4103 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 15
-1.2437 0.0910 -1.6975 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 16
2.8722 -0.4654 2.3371 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 17
0.4442 -0.6844 1.8355 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 18
1.1579 0.5286 -2.2209 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 19
3.5916 0.7435 -1.7376 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 20
5.4006 -0.7046 0.3976 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 21
5.0790 0.4727 1.6828 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 22
5.3692 1.0244 0.0112 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 23
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
8 7 0 0 0 0
12 7 0 0 0 0
17 7 0 0 0 0
9 8 0 0 0 0
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10 9 0 0 0 0
14 9 0 0 0 0
11 10 0 0 0 0
19 10 0 0 0 0
12 11 0 0 0 0
20 11 0 0 0 0
13 12 0 0 0 0
21 13 0 0 0 0
22 13 0 0 0 0
15 14 0 0 0 0
16 14 0 0 0 0
13 23 0 0 0 0
M END
$$$$
4-methylbenzoicacid.sdf
COSMOtherm 3D 0
24 22 0 0 0 0 0 0 0 0 0 0 V2000
-0.8344 5.3473 0.9272 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1
-1.7070 5.3434 0.4937 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 2
-0.6323 6.2921 1.0536 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 3
1.1159 4.0434 -0.4119 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 4
0.3691 4.5380 0.0395 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 5
1.0946 4.3322 -1.3416 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 6
-1.2127 -2.7621 -0.1057 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 7
-1.2305 -1.3766 -0.2597 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 8
-0.0468 -0.6299 -0.1301 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 9
1.1534 -1.3034 0.1595 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 10
1.1631 -2.6903 0.3121 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 11
-0.0162 -3.4460 0.1793 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 12
0.0060 -4.9468 0.3128 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 13
-0.1053 0.8524 -0.3011 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 14
-1.1483 1.4620 -0.5515 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 15
1.0819 1.4592 -0.1581 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 16
```

[illegible]

	2.1347	-2.3754	0.2984	H	0	0	0	0	0	0	0	0	0	0	22
	0.9243	3.3204	-0.3484	H	0	0	0	0	0	0	0	0	0	0	23
2	1	0	0	0											
3	1	0	0	0	0										
5	4	0	0	0	0										
6	4	0	0	0	0										
8	7	0	0	0	0										
12	7	0	0	0	0										
19	7	0	0	0	0										
9	8	0	0	0	0										
20	8	0	0	0	0										
10	9	0	0	0	0										
13	9	0	0	0	0										
11	10	0	0	0	0										
21	10	0	0	0	0										
12	11	0	0	0	0										
22	11	0	0	0	0										
14	12	0	0	0	0										
17	13	0	0	0	0										
18	13	0	0	0	0										
15	14	0	0	0	0										
16	14	0	0	0	0										
18	23	0	0	0	0										
M END															
\$\$\$\$															
4-phenylbenzoicacid-anion.sdf															
COSMOTHERM 3D 0															
30	29	0	0	0	0	0	0	0	0	V2000					
-1.4495	7.2516	-1.2665	O	0	0	0	0	0	0	0	0	0	0	0	1
-0.7315	6.7438	-0.7859	H	0	0	0	0	0	0	0	0	0	0	0	2
-2.2756	6.8119	-1.0023	H	0	0	0	0	0	0	0	0	0	0	0	3
0.5742	5.9226	-0.0341	O	0	0	0	0	0	0	0	0	0	0	0	4
0.5323	4.9126	-0.2199	H	0	0	0	0	0	0	0	0	0	0	0	5
0.5043	5.9781	0.9357	H	0	0	0	0	0	0	0	0	0	0	0	6
0.1548	-0.8163	-1.0650	C	0	0	0	0	0	0	0	0	0	0	0	7
0.2600	0.5674	-0.9190	C	0	0	0	0	0	0	0	0	0	0	0	8
0.2584	1.1601	0.3542	C	0	0	0	0	0	0	0	0	0	0	0	9
0.1492	0.3249	1.4779	C	0	0	0	0	0	0	0	0	0	0	0	10
0.0445	-1.0587	1.3358	C	0	0	0	0	0	0	0	0	0	0	0	11
0.0445	-1.6596	0.0600	C	0	0	0	0	0	0	0	0	0	0	0	12
-0.0668	-3.1323	-0.0922	C	0	0	0	0	0	0	0	0	0	0	0	13
0.3733	2.6687	0.5247	C	0	0	0	0	0	0	0	0	0	0	0	14
-0.9528	-5.2823	0.6566	C	0	0	0	0	0	0	0	0	0	0	0	15
-0.8494	-3.8959	0.7981	C	0	0	0	0	0	0	0	0	0	0	0	16
0.6082	-3.8078	-1.1296	C	0	0	0	0	0	0	0	0	0	0	0	17
0.5052	-5.1945	-1.2707	C	0											

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24 14 0 0 0 0
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25 15 0 0 0 0
26 15 0 0 0 0
27 16 0 0 0 0
28 16 0 0 0 0
16 29 0 0 0 0
M END
$$$$
4-propylbenzoicacid.sdf
COSMOtherm 3D 0

30 28 0 0 0 0 0 0 0 0 0 V2000
-0.7980 6.3382 0.6286 O 0 0 0 0 0 0 0 0 0 0 1
-1.6332 6.3598 0.1273 H 0 0 0 0 0 0 0 0 0 0 2
-0.5578 7.2764 0.7384 H 0 0 0 0 0 0 0 0 0 0 3
1.1818 4.9056 -0.5206 O 0 0 0 0 0 0 0 0 0 0 4
0.4257 5.4453 -0.1414 H 0 0 0 0 0 0 0 0 0 0 5
1.2067 5.1215 -1.4698 H 0 0 0 0 0 0 0 0 0 0 6
-1.2883 -1.8234 0.1202 C 0 0 0 0 0 0 0 0 0 0 7
-1.2746 -0.4483 -0.1094 C 0 0 0 0 0 0 0 0 0 0 8
-0.0787 0.2811 0.0078 C 0 0 0 0 0 0 0 0 0 0 9
1.1011 -0.3977 0.3617 C 0 0 0 0 0 0 0 0 0 0 10
1.0792 -1.7743 0.5888 C 0 0 0 0 0 0 0 0 0 0 11
-0.1127 -2.5126 0.4720 C 0 0 0 0 0 0 0 0 0 0 12
-0.1024 1.7525 -0.2467 C 0 0 0 0 0 0 0 0 0 0 13
-0.1215 -4.0087 0.6751 C 0 0 0 0 0 0 0 0 0 0 14
0.1435 -4.7912 -0.6300 C 0 0 0 0 0 0 0 0 0 0 15
0.1434 -6.3081 -0.4160 C 0 0 0 0 0 0 0 0 0 0 16
-1.1228 2.3637 -0.5743 O 0 0 0 0 0 0 0 0 0 0 17
1.0884 2.3474 -0.0862 O 0 0 0 0 0 0 0 0 0 0 18
-2.2276 -2.3747 0.0315 H 0 0 0 0 0 0 0 0 0 0 19
-2.1925 0.0769 -0.3780 H 0 0 0 0 0 0 0 0 0 0 20
2.0342 0.1569 0.4615 H 0 0 0 0 0 0 0 0 0 0 21
2.0030 -2.2870 0.8678 H 0 0 0 0 0 0 0 0 0 0 22
-1.0961 -4.3198 1.0850 H 0 0 0 0 0 0 0 0 0 0 23
0.6451 -4.2840 1.4172 H 0 0 0 0 0 0 0 0 0 0 24
1.1120 -4.4721 -1.0489 H 0 0 0 0 0 0 0 0 0 0 25
-0.6229 -4.5178 -1.3737 H 0 0 0 0 0 0 0 0 0 0 26
0.3297 -6.8418 -1.3595 H 0 0 0 0 0 0 0 0 0 0 27
-0.8244 -6.6533 -0.0204 H 0 0 0 0 0 0 0 0 0 0 28
0.9242 -6.6078 0.3000 H 0 0 0 0 0 0 0 0 0 0 29
1.0198 3.3595 -0.2830 H 0 0 0 0 0 0 0 0 0 0 30

2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
8 7 0 0 0 0
12 7 0 0 0 0
19 7 0 0 0 0
9 8 0 0 0 0
20 8 0 0 0 0
10 9 0 0 0 0
13 9 0 0 0 0
11 10 0 0 0 0
21 10 0 0 0 0
12 11 0 0 0 0
22 11 0 0 0 0
14 12 0 0 0 0
17 13 0 0 0 0
18 13 0 0 0 0
15 14 0 0 0 0
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24 14 0 0 0 0
16 15 0 0 0 0
25 15 0 0 0 0
26 15 0 0 0 0
27 16 0 0 0 0
28 16 0 0 0 0
29 16 0 0 0 0
18 30 0 0 0 0
M END
$$$$
4-sulfamoylbenzoicacid-anion.sdf
COSMOtherm 3D 0

25 23 0 0 0 0 0 0 0 0 0 V2000
-7.0507 0.8445 1.6226 O 0 0 0 0 0 0 0 0 0 0 1
-6.5336 0.3535 0.9195 H 0 0 0 0 0 0 0 0 0 0 2
-6.6293 1.7197 1.6672 H 0 0 0 0 0 0 0 0 0 0 3
-5.6892 -0.5945 -0.2448 O 0 0 0 0 0 0 0 0 0 0 4
-4.6810 -0.5783 -0.0649 H 0 0 0 0 0 0 0 0 0 0 5
-5.7749 -0.2188 -1.1389 H 0 0 0 0 0 0 0 0 0 0 6
1.0089 -0.3279 1.0636 C 0 0 0 0 0 0 0 0 0 0 7
-0.3653 -0.4068 0.8288 C 0 0 0 0 0 0 0 0 0 0 8
-0.8977 -0.1049 -0.4348 C 0 0 0 0 0 0 0 0 0 0 9
-0.0310 0.2785 -1.4707 C 0 0 0 0 0 0 0 0 0 0 10
1.3462 0.3617 -1.2584 C 0 0 0 0 0 0 0 0 0 0 11
1.8469 0.0530 0.0109 C 0 0 0 0 0 0 0 0 0 0 12
-2.4037 -0.1801 -0.6875 C 0 0 0 0 0 0 0 0 0 0 13
3.6359 0.1488 0.2996 S 0 0 0 0 0 0 0 0 0 0 14
3.8591 0.3323 1.7641 O 0 0 0 0 0 0 0 0 0 0 15
4.2079 1.1246 -0.6745 O 0 0 0 0 0 0 0 0 0 0 16
4.3482 -1.3432 -0.0847 N 0 0 0 0 0 0 0 0 0 0 17
-3.1204 -0.5790 0.2962 O 0 0 0 0 0 0 0 0 0 0 18
-2.8285 0.1495 -1.8266 O 0 0 0 0 0 0 0 0 0 0 19
3.9785 -2.0923 0.5098 H 0 0 0 0 0 0 0 0 0 0 20
4.2067 -1.5747 -1.0736 H 0 0 0 0 0 0 0 0 0 0 21
1.4201 -0.5512 2.0482 H 0 0 0 0 0 0 0 0 0 0 22
-1.0422 -0.6988 1.6319 H 0 0 0 0 0 0 0 0 0 0 23
-0.4517 0.5188 -2.4475 H 0 0 0 0 0 0 0 0 0 0 24
2.0162 0.6686 -2.0618 H 0 0 0 0 0 0 0 0 0 0 25

2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
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6 4 0 0 0 0
8 7 0 0 0 0
12 7 0 0 0 0
22 7 0 0 0 0
9 8 0 0 0 0
23 8 0 0 0 0
10 9 0 0 0 0
13 9 0 0 0 0
11 10 0 0 0 0
24 10 0 0 0 0
12 11 0 0 0 0
14 12 0 0 0 0
18 13 0 0 0 0
19 13 0 0 0 0
15 14 0 0 0 0
16 14 0 0 0 0
17 14 0 0 0 0
20 17 0 0 0 0
21 17 0 0 0 0
11 25 0 0 0 0
M END
$$$$
4-sulfamoylbenzoicacid.sdf
COSMOTHERM 3D 0

26 24 0 0 0 0 0 0 0 0 0 V2000
-0.8280 6.7706 1.0794 O 0 0 0 0 0 0 0 0 0 0 1
-1.7122 6.7583 0.6701 H 0 0 0 0 0 0 0 0 0 0 2
-0.6466 7.7155 1.2350 H 0 0 0 0 0 0 0 0 0 0 3
1.1013 5.5688 -0.3622 O 0 0 0 0 0 0 0 0 0 0 4
0.3589 6.0329 0.1311 H 0 0 0 0 0 0 0 0 0 0 5
1.0486 5.8909 -1.2798 H 0 0 0 0 0 0 0 0 0 0 6
-1.2339 -1.2051 -0.2264 C 0 0 0 0 0 0 0 0 0 0 7
-1.2339 0.1827 -0.3606 C 0 0 0 0 0 0 0 0 0 0 8
-0.0428 0.9124 -0.2158 C 0 0 0 0 0 0 0 0 0 0 9
1.1587 0.2410 0.0655 C 0 0 0 0 0 0 0 0 0 0 10
1.1743 -1.1483 0.2006 C 0 0 0 0 0 0 0 0 0 0 11
-0.0243 -1.8509 0.0482 C 0 0 0 0 0 0 0 0 0 0 12
-0.0980 2.4072 -0.3610 C 0 0 0 0 0 0 0 0 0 0 13
-0.0132 -3.6627 0.2140 S 0 0 0 0 0 0 0 0 0 0 14
-1.3791 -4.0903 0.6344 O 0 0 0 0 0 0 0 0 0 0 15
1.1792 -4.0389 1.0266 O 0 0 0 0 0 0 0 0 0 0 16
0.2343 -4.3556 -1.3107 N 0 0 0 0 0 0 0 0 0 0 17
-1.1428 3.0082 -0.6142 O 0 0 0 0 0 0 0 0 0 0 18
1.0828 3.0021 -0.1883 O 0 0 0 0 0 0 0 0 0 0 19
-0.5237 -4.1198 -1.9593 H 0 0 0 0 0 0 0 0 0 0 20
1.1412 -4.0827 -1.7031 H 0 0 0 0 0 0 0 0 0 0 21
-2.1593 -1.7722 -0.3272 H 0 0 0 0 0 0 0 0 0 0 22
-2.1630 0.7123 -0.5721 H 0 0 0 0 0 0 0 0 0 0 23
2.0825 0.8055 0.1854 H 0 0 0 0 0 0 0 0 0 0 24
2.1028 -1.6722 0.4277 H 0 0 0 0 0 0 0 0 0 0 25
0.9978 4.0355 -0.2878 H 0 0 0 0 0 0 0 0 0 0 26
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
8 7 0 0 0 0
12 7 0 0 0 0
22 7 0 0 0 0
9 8 0 0 0 0
23 8 0 0 0 0
10 9 0 0 0 0
13 9 0 0 0 0
11 10 0 0 0 0
24 10 0 0 0 0
12 11 0 0 0 0
25 11 0 0 0 0
14 12 0 0 0 0
18 13 0 0 0 0
19 13 0 0 0 0
15 14 0 0 0 0
16 14 0 0 0 0
17 14 0 0 0 0
20 17 0 0 0 0
21 17 0 0 0 0
19 26 0 0 0 0
M END
$$$$
4-trifluoromethylbenzoicacid-anion.sdf
COSMOTHERM 3D 0

23 21 0 0 0 0 0 0 0 0 0 V2000
-6.8334 0.9642 1.4738 O 0 0 0 0 0 0 0 0 0 0 1
-6.3047 0.4017 0.8353 H 0 0 0 0 0 0 0 0 0 0 2
-6.3955 1.8322 1.4526 H 0 0 0 0 0 0 0 0 0 0 3
-5.4442 -0.6600 -0.2116 O 0 0 0 0 0 0 0 0 0 0 4
-4.4371 -0.6191 -0.0237 H 0 0 0 0 0 0 0 0 0 0 5
-5.5214 -0.3663 -1.1366 H 0 0 0 0 0 0 0 0 0 0 6
1.2562 -0.3695 1.0841 C 0 0 0 0 0 0 0 0 0 0 7
-0.1189 -0.4461 0.8578 C 0 0 0 0 0 0 0 0 0 0 8
-0.6602 -0.1156 -0.3940 C 0 0 0 0 0 0 0 0 0 0 9
0.2033 0.2976 -1.4209 C 0 0 0 0 0 0 0 0 0 0 10
1.5796 0.3778 -1.2080 C 0 0 0 0 0 0 0 0 0 0 11
2.1056 0.0486 0.0502 C 0 0 0 0 0 0 0 0 0 0 12
-2.1658 -0.1953 -0.6441 C 0 0 0 0 0 0 0 0 0 0 13
3.5934 0.0873 0.2685 C 0 0 0 0 0 0 0 0 0 0 14
4.2047 -1.0804 -0.1273 F 0 0 0 0 0 0 0 0 0 0 15
3.9308 0.2669 1.5790 F 0 0 0 0 0 0 0 0 0 0 16
4.2029 1.0881 -0.4351 F 0 0 0 0 0 0 0 0 0 0 17
-2.8810 -0.5989 0.3401 O 0 0 0 0 0 0 0 0 0 0 18
-2.5963 0.1348 -1.7813 O 0 0 0 0 0 0 0 0 0 0 19
1.6635 -0.6254 2.0626 H 0 0 0 0 0 0 0 0 0 0 20
-0.7901 -0.7647 1.6556 H 0 0 0 0 0 0 0 0 0 0 21
-0.2206 0.5567 -2.3916 H 0 0 0 0 0 0 0 0 0 0 22
2.2387 0.7035 -2.0136 H 0 0 0 0 0 0 0 0 0 0 23
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21 8 0 0 0 0
10 9 0 0 0 0
13 9 0 0 0 0
11 10 0 0 0 0
22 10 0 0 0 0
12 11 0 0 0 0
14 12 0 0 0 0
18 13 0 0 0 0
19 13 0 0 0 0
15 14 0 0 0 0
16 14 0 0 0 0
17 14 0 0 0 0
11 23 0 0 0 0
M END
$$$$
4-trifluoromethylbenzoicacid.sdf
COSMOTHERM 3D 0

24 22 0 0 0 0 0 0 0 0 0 V2000
-1.3701 -5.6476 0.0630 O 0 0 0 0 0 0 0 0 0 1
-1.7761 -5.9650 -0.7636 H 0 0 0 0 0 0 0 0 0 2
-1.4012 -4.6556 0.0098 H 0 0 0 0 0 0 0 0 0 3
1.2723 -5.3791 -0.0001 O 0 0 0 0 0 0 0 0 0 4
0.3076 -5.6735 0.0285 H 0 0 0 0 0 0 0 0 0 5
1.6799 -5.7143 0.8191 H 0 0 0 0 0 0 0 0 0 6
-1.2141 1.3132 -0.0410 C 0 0 0 0 0 0 0 0 0 7
-1.1907 -0.0799 -0.0357 C 0 0 0 0 0 0 0 0 0 8
0.0326 -0.7687 -0.0299 C 0 0 0 0 0 0 0 0 0 9
1.2375 -0.0470 -0.0342 C 0 0 0 0 0 0 0 0 0 10
1.2201 1.3474 -0.0384 C 0 0 0 0 0 0 0 0 0 11
-0.0062 2.0250 -0.0453 C 0 0 0 0 0 0 0 0 0 12
0.0178 -2.2668 -0.0141 C 0 0 0 0 0 0 0 0 0 13
-0.0289 3.5314 0.0075 C 0 0 0 0 0 0 0 0 0 14
-0.0739 3.9925 1.3003 F 0 0 0 0 0 0 0 0 0 15
-1.1149 4.0613 -0.6256 F 0 0 0 0 0 0 0 0 0 16
1.0753 4.0927 -0.5621 F 0 0 0 0 0 0 0 0 0 17
-1.0457 -2.9035 0.0270 O 0 0 0 0 0 0 0 0 0 18
1.2233 -2.8164 -0.0457 O 0 0 0 0 0 0 0 0 0 19
-2.1680 1.8409 -0.0484 H 0 0 0 0 0 0 0 0 0 20
-2.1233 -0.6439 -0.0352 H 0 0 0 0 0 0 0 0 0 21
2.1891 -0.5769 -0.0315 H 0 0 0 0 0 0 0 0 0 22
2.1587 1.9014 -0.0415 H 0 0 0 0 0 0 0 0 0 23
1.1954 -3.8654 -0.0076 H 0 0 0 0 0 0 0 0 0 24
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
8 7 0 0 0 0
12 7 0 0 0 0
20 7 0 0 0 0
9 8 0 0 0 0
21 8 0 0 0 0
10 9 0 0 0 0
13 9 0 0 0 0
11 10 0 0 0 0
22 10 0 0 0 0
12 11 0 0 0 0
23 11 0 0 0 0
14 12 0 0 0 0
18 13 0 0 0 0
19 13 0 0 0 0
15 14 0 0 0 0
16 14 0 0 0 0
17 14 0 0 0 0
19 24 0 0 0 0
M END
$$$$
5-fluorouracil-anion.sdf
COSMOTHERM 3D 0

17 15 0 0 0 0 0 0 0 0 0 V2000
-1.4634 -0.6132 -4.5588 O 0 0 0 0 0 0 0 0 0 1
-0.6911 -0.1839 -4.0891 H 0 0 0 0 0 0 0 0 0 2
-2.1660 0.0585 -4.5371 H 0 0 0 0 0 0 0 0 0 3
0.7082 0.4673 -3.3102 O 0 0 0 0 0 0 0 0 0 4
0.6448 0.3714 -2.2909 H 0 0 0 0 0 0 0 0 0 5
0.7809 1.4239 -3.4727 H 0 0 0 0 0 0 0 0 0 6
1.4978 -0.0378 0.1959 C 0 0 0 0 0 0 0 0 0 7
1.2133 -0.1724 1.5698 N 0 0 0 0 0 0 0 0 0 8
-0.0404 -0.1106 2.1881 C 0 0 0 0 0 0 0 0 0 9
-1.0823 0.1157 1.2279 C 0 0 0 0 0 0 0 0 0 10
-0.8089 0.2445 -0.1089 C 0 0 0 0 0 0 0 0 0 11
0.4380 0.1743 -0.6413 N 0 0 0 0 0 0 0 0 0 12
-0.1715 -0.2437 3.4225 O 0 0 0 0 0 0 0 0 0 13
2.6846 -0.1172 -0.1897 O 0 0 0 0 0 0 0 0 0 14
-2.3680 0.1985 1.6958 F 0 0 0 0 0 0 0 0 0 15
2.0131 -0.3309 2.1851 H 0 0 0 0 0 0 0 0 0 16
-1.6306 0.4142 -0.8112 H 0 0 0 0 0 0 0 0 0 17
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
8 7 0 0 0 0
12 7 0 0 0 0
14 7 0 0 0 0
9 8 0 0 0 0
16 8 0 0 0 0
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10 9 0 0 0 0
13 9 0 0 0 0
11 10 0 0 0 0
15 10 0 0 0 0
12 11 0 0 0 0
11 17 0 0 0 0
M END
$$$$
5-fluorouracil.sdf
COSMOTHERM 3D 0
18 16 0 0 0 0 0 0 0 0 0 V2000
-4.8889 0.9926 -0.1165 O 0 0 0 0 0 0 0 0 0 0 1
-5.4730 0.6068 0.5613 H 0 0 0 0 0 0 0 0 0 0 2
-5.4989 1.3242 -0.8005 H 0 0 0 0 0 0 0 0 0 0 3
-3.0587 -0.7593 -1.1039 O 0 0 0 0 0 0 0 0 0 0 4
-3.7602 -0.1531 -0.7265 H 0 0 0 0 0 0 0 0 0 0 5
-3.3850 -1.6627 -0.9459 H 0 0 0 0 0 0 0 0 0 0 6
-0.2060 -0.2433 1.1447 C 0 0 0 0 0 0 0 0 0 0 7
1.1430 0.0036 1.4009 N 0 0 0 0 0 0 0 0 0 0 8
2.1839 0.1665 0.4755 C 0 0 0 0 0 0 0 0 0 0 9
1.7203 0.0549 -0.8927 C 0 0 0 0 0 0 0 0 0 0 10
0.4182 -0.1834 -1.1912 C 0 0 0 0 0 0 0 0 0 0 11
-0.5157 -0.3262 -0.1998 N 0 0 0 0 0 0 0 0 0 0 12
3.3488 0.3795 0.8345 O 0 0 0 0 0 0 0 0 0 0 13
-1.0392 -0.3733 2.0454 O 0 0 0 0 0 0 0 0 0 0 14
2.6474 0.1973 -1.8728 F 0 0 0 0 0 0 0 0 0 0 15
1.4014 0.0704 2.3870 H 0 0 0 0 0 0 0 0 0 0 16
-1.5228 -0.5073 -0.4657 H 0 0 0 0 0 0 0 0 0 0 17
0.0614 -0.2708 -2.2165 H 0 0 0 0 0 0 0 0 0 0 18
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
8 7 0 0 0 0
12 7 0 0 0 0
14 7 0 0 0 0
9 8 0 0 0 0
16 8 0 0 0 0
10 9 0 0 0 0
13 9 0 0 0 0
11 10 0 0 0 0
15 10 0 0 0 0
12 11 0 0 0 0
17 12 0 0 0 0
11 18 0 0 0 0
M END
$$$$
5-iodo-2-hydroxybenzoicacid-anion.sdf
COSMOTHERM 3D 0
21 19 0 0 0 0 0 0 0 0 0 V2000
-3.3919 0.8547 6.0064 O 0 0 0 0 0 0 0 0 0 0 1
-2.5722 0.3248 5.7924 H 0 0 0 0 0 0 0 0 0 0 2
-3.0940 1.7801 5.9880 H 0 0 0 0 0 0 0 0 0 0 3
-1.2228 -0.6954 5.4098 O 0 0 0 0 0 0 0 0 0 0 4
-0.9401 -0.5891 4.4411 H 0 0 0 0 0 0 0 0 0 0 5
-0.4268 -0.4705 5.9222 H 0 0 0 0 0 0 0 0 0 0 6
0.5587 0.0548 -1.2005 C 0 0 0 0 0 0 0 0 0 0 7
0.1411 -0.1116 0.1150 C 0 0 0 0 0 0 0 0 0 0 8
1.0765 -0.0583 1.1608 C 0 0 0 0 0 0 0 0 0 0 9
2.4485 0.1660 0.8593 C 0 0 0 0 0 0 0 0 0 0 10
2.8461 0.3304 -0.4810 C 0 0 0 0 0 0 0 0 0 0 11
1.9081 0.2758 -1.5099 C 0 0 0 0 0 0 0 0 0 0 12
0.6363 -0.2357 2.5921 C 0 0 0 0 0 0 0 0 0 0 13
1.5570 -0.1684 3.4909 O 0 0 0 0 0 0 0 0 0 0 14
-0.5892 -0.4373 2.8409 O 0 0 0 0 0 0 0 0 0 0 15
3.3730 0.2247 1.8412 O 0 0 0 0 0 0 0 0 0 0 16
-0.8834 -0.0258 -2.7896 I 0 0 0 0 0 0 0 0 0 0 17
2.7980 0.0721 2.7059 H 0 0 0 0 0 0 0 0 0 0 18
-0.9050 -0.2846 0.3689 H 0 0 0 0 0 0 0 0 0 0 19
3.9001 0.5014 -0.7066 H 0 0 0 0 0 0 0 0 0 0 20
2.2337 0.4063 -2.5422 H 0 0 0 0 0 0 0 0 0 0 21
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
8 7 0 0 0 0
12 7 0 0 0 0
9 8 0 0 0 0
19 8 0 0 0 0
10 9 0 0 0 0
13 9 0 0 0 0
11 10 0 0 0 0
16 10 0 0 0 0
12 11 0 0 0 0
20 11 0 0 0 0
14 13 0 0 0 0
15 13 0 0 0 0
18 14 0 0 0 0
18 16 0 0 0 0
12 21 0 0 0 0
M END
$$$$
5-iodo-2-hydroxybenzoicacid.sdf
COSMOTHERM 3D 0
22 19 0 0 0 0 0 0 0 0 0 V2000
1.2575 -1.7159 -6.6209 O 0 0 0 0 0 0 0 0 0 0 1
1.1299 -1.0496 -7.3210 H 0 0 0 0 0 0 0 0 0 0 2
1.4577 -2.5394 -7.1029 H 0 0 0 0 0 0 0 0 0 0 3
-0.8158 -2.0121 -4.9498 O 0 0 0 0 0 0 0 0 0 0 4
-0.0658 -1.8808 -5.6075 H 0 0 0 0 0 0 0 0 0 0 5
-1.6199 -1.6910 -5.3963 H 0 0 0 0 0 0 0 0 0 0 6
0.0406 0.5465 1.2056 C 0 0 0 0 0 0 0 0 0 0 7
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-0.1337      0.0017    -0.0586 C   0   0   0   0   0   0   0   0   0   0   8
-0.1438      0.8431    -1.1896 C   0   0   0   0   0   0   0   0   0   0   9
  0.0230      2.2456    -1.0212 C   0   0   0   0   0   0   0   0   0   0  10
  0.2001      2.7696     0.2720 C   0   0   0   0   0   0   0   0   0   0  11
  0.2089      1.9296     1.3800 C   0   0   0   0   0   0   0   0   0   0  12
-0.3268      0.2987    -2.5526 C   0   0   0   0   0   0   0   0   0   0  13
-0.4632     -1.0132    -2.6349 O   0   0   0   0   0   0   0   0   0   0  14
-0.3473      1.0488    -3.5557 O   0   0   0   0   0   0   0   0   0   0  15
  0.0173      3.0968    -2.0706 O   0   0   0   0   0   0   0   0   0   0  16
  0.0521     -0.7354     2.9195 I   0   0   0   0   0   0   0   0   0   0  17
-0.6002     -1.3315    -3.6274 H   0   0   0   0   0   0   0   0   0   0  18
-0.1260      2.5101    -2.8849 H   0   0   0   0   0   0   0   0   0   0  19
-0.2662     -1.0696    -0.2026 H   0   0   0   0   0   0   0   0   0   0  20
  0.3294      3.8459     0.3942 H   0   0   0   0   0   0   0   0   0   0  21
  0.3468      2.3538     2.3744 H   0   0   0   0   0   0   0   0   0   0  22

  2   1   0   0   0   0
  3   1   0   0   0   0
  5   4   0   0   0   0
  6   4   0   0   0   0
  8   7   0   0   0   0
12   7   0   0   0   0
  9   8   0   0   0   0
20   8   0   0   0   0
10   9   0   0   0   0
13   9   0   0   0   0
11  10   0   0   0   0
16  10   0   0   0   0
12  11   0   0   0   0
21  11   0   0   0   0
14  13   0   0   0   0
15  13   0   0   0   0
18  14   0   0   0   0
19  16   0   0   0   0
12  22   0   0   0   0
M   END
$$$$
5-nitrouracil-anion.sdf
COSMOTHERM      3D      0

19 17   0   0   0   0   0   0   0   0   0   0 V2000
-2.0359    -4.5691    -0.8592 O   0   0   0   0   0   0   0   0   0   0   1
-1.2714    -4.2524    -0.3002 H   0   0   0   0   0   0   0   0   0   0   2
-2.8266    -4.2307    -0.4057 H   0   0   0   0   0   0   0   0   0   0   3
  0.1341    -3.7581     0.6005 O   0   0   0   0   0   0   0   0   0   0   4
  0.3312    -2.7702     0.4946 H   0   0   0   0   0   0   0   0   0   0   5
  0.0110    -3.8922     1.5568 H   0   0   0   0   0   0   0   0   0   0   6
-0.4546    -0.2290     0.2661 C   0   0   0   0   0   0   0   0   0   0   7
-0.3848     1.1579     0.0649 C   0   0   0   0   0   0   0   0   0   0   8
  0.9087     1.7804    -0.1871 C   0   0   0   0   0   0   0   0   0   0   9
  1.9389     0.8258    -0.1829 N   0   0   0   0   0   0   0   0   0   0  10
  1.8428    -0.5522     0.0224 C   0   0   0   0   0   0   0   0   0   0  11
  0.5738    -1.0662     0.2526 N   0   0   0   0   0   0   0   0   0   0  12
  1.1812     2.9694    -0.3889 O   0   0   0   0   0   0   0   0   0   0  13
  2.8566    -1.2627    -0.0041 O   0   0   0   0   0   0   0   0   0   0  14
-1.5931     1.9134     0.1143 N   0   0   0   0   0   0   0   0   0   0  15
-1.4382    -0.6668     0.4511 H   0   0   0   0   0   0   0   0   0   0  16
  2.8768     1.1943    -0.3521 H   0   0   0   0   0   0   0   0   0   0  17
-2.6734     1.3080     0.3444 O   0   0   0   0   0   0   0   0   0   0  18
-1.5572     3.1495    -0.0697 O   0   0   0   0   0   0   0   0   0   0  19

  2   1   0   0   0   0
  3   1   0   0   0   0
  5   4   0   0   0   0
  6   4   0   0   0   0
  8   7   0   0   0   0
12   7   0   0   0   0
16   7   0   0   0   0
  9   8   0   0   0   0
15   8   0   0   0   0
10   9   0   0   0   0
13   9   0   0   0   0
11  10   0   0   0   0
17  10   0   0   0   0
12  11   0   0   0   0
14  11   0   0   0   0
18  15   0   0   0   0
15  19   0   0   0   0
M   END
$$$$
5-nitrouracil.sdf
COSMOTHERM      3D      0

20 18   0   0   0   0   0   0   0   0   0   0 V2000
-5.3012     0.7287     0.9415 O   0   0   0   0   0   0   0   0   0   0   1
-5.9765     0.1510     0.5416 H   0   0   0   0   0   0   0   0   0   0   2
-5.7962     1.5191     1.2248 H   0   0   0   0   0   0   0   0   0   0   3
-3.2571     1.3376    -0.7167 O   0   0   0   0   0   0   0   0   0   0   4
-4.0418     1.1047    -0.1364 H   0   0   0   0   0   0   0   0   0   0   5
-3.5794     1.2756    -1.6333 H   0   0   0   0   0   0   0   0   0   0   6
  0.1180     0.7932    -0.2004 C   0   0   0   0   0   0   0   0   0   0   7
  1.3847     0.2858    -0.0027 C   0   0   0   0   0   0   0   0   0   0   8
  1.5891    -1.1610     0.1126 C   0   0   0   0   0   0   0   0   0   0   9
  0.3757    -1.8707    -0.0050 N   0   0   0   0   0   0   0   0   0   0  10
-0.9046    -1.3836    -0.2033 C   0   0   0   0   0   0   0   0   0   0  11
-0.9668     0.0129    -0.2949 N   0   0   0   0   0   0   0   0   0   0  12
  2.6365    -1.7779     0.2903 O   0   0   0   0   0   0   0   0   0   0  13
-1.8994    -2.0952    -0.2915 O   0   0   0   0   0   0   0   0   0   0  14
  2.4779     1.2262     0.0819 N   0   0   0   0   0   0   0   0   0   0  15
-0.0438     1.8669    -0.2886 H   0   0   0   0   0   0   0   0   0   0  16
  0.4574    -2.8868     0.0678 H   0   0   0   0   0   0   0   0   0   0  17
-1.9247     0.4640    -0.4626 H   0   0   0   0   0   0   0   0   0   0  18
  2.2134     2.4455    -0.0079 O   0   0   0   0   0   0   0   0   0   0  19
  3.6311     0.7944     0.2388 O   0   0   0   0   0   0   0   0   0   0  20

  2   1   0   0   0   0
  3   1   0   0   0   0
  5   4   0   0   0   0
```

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6 4 0 0 0 0
8 7 0 0 0 0
12 7 0 0 0 0
16 7 0 0 0 0
9 8 0 0 0 0
15 8 0 0 0 0
10 9 0 0 0 0
13 9 0 0 0 0
11 10 0 0 0 0
17 10 0 0 0 0
12 11 0 0 0 0
14 11 0 0 0 0
18 12 0 0 0 0
19 15 0 0 0 0
15 20 0 0 0 0
M END
$$$$
aceticacid-anion.sdf
COSMOTHERM 3D 0
13 10 0 0 0 0 0 0 0 0 V2000
-2.9319 -0.0699 1.2546 O 0 0 0 0 0 0 0 0 0 0 1
-1.9830 0.0027 0.9219 H 0 0 0 0 0 0 0 0 0 0 2
-3.4174 0.6151 0.7648 H 0 0 0 0 0 0 0 0 0 0 3
2.9232 -0.0055 1.1675 O 0 0 0 0 0 0 0 0 0 0 4
2.2943 -0.0129 0.3761 H 0 0 0 0 0 0 0 0 0 0 5
2.3184 0.0251 1.9288 H 0 0 0 0 0 0 0 0 0 0 6
-0.9589 -0.0026 -1.7905 C 0 0 0 0 0 0 0 0 0 0 7
0.0745 0.0095 -0.6630 C 0 0 0 0 0 0 0 0 0 0 8
1.3079 -0.0299 -0.9798 O 0 0 0 0 0 0 0 0 0 0 9
-0.3528 0.0610 0.5372 O 0 0 0 0 0 0 0 0 0 0 10
-0.4843 -0.0674 -2.7767 H 0 0 0 0 0 0 0 0 0 0 11
-1.6427 -0.8537 -1.6578 H 0 0 0 0 0 0 0 0 0 0 12
-1.5685 0.9120 -1.7425 H 0 0 0 0 0 0 0 0 0 0 13
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
8 7 0 0 0 0
11 7 0 0 0 0
12 7 0 0 0 0
9 8 0 0 0 0
10 8 0 0 0 0
7 13 0 0 0 0
M END
$$$$
aceticacid.sdf
COSMOTHERM 3D 0
14 11 0 0 0 0 0 0 0 0 V2000
-0.7176 0.5610 -3.3800 O 0 0 0 0 0 0 0 0 0 0 1
-1.3312 -0.0617 -3.8115 H 0 0 0 0 0 0 0 0 0 0 2
-0.2453 0.9858 -4.1196 H 0 0 0 0 0 0 0 0 0 0 3
1.0173 -0.5927 -1.6558 O 0 0 0 0 0 0 0 0 0 0 4
0.3555 -0.2092 -2.3053 H 0 0 0 0 0 0 0 0 0 0 5
0.8859 -1.5570 -1.6870 H 0 0 0 0 0 0 0 0 0 0 6
-0.1340 0.5762 2.8934 C 0 0 0 0 0 0 0 0 0 0 7
-0.1399 -0.0384 1.5155 C 0 0 0 0 0 0 0 0 0 0 8
-0.9761 -0.8528 1.1258 O 0 0 0 0 0 0 0 0 0 0 9
0.8732 0.3971 0.7516 O 0 0 0 0 0 0 0 0 0 0 10
-0.9576 0.1728 3.4910 H 0 0 0 0 0 0 0 0 0 0 11
0.8234 0.3708 3.3929 H 0 0 0 0 0 0 0 0 0 0 12
-0.2343 1.6683 2.8163 H 0 0 0 0 0 0 0 0 0 0 13
0.8439 -0.0417 -0.1813 H 0 0 0 0 0 0 0 0 0 0 14
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
8 7 0 0 0 0
11 7 0 0 0 0
12 7 0 0 0 0
13 7 0 0 0 0
9 8 0 0 0 0
10 8 0 0 0 0
10 14 0 0 0 0
M END
$$$$
acrylicacid-anion.sdf
COSMOTHERM 3D 0
14 11 0 0 0 0 0 0 0 0 V2000
-4.1451 0.6031 -0.5848 O 0 0 0 0 0 0 0 0 0 0 1
-3.3786 0.1853 -0.0923 H 0 0 0 0 0 0 0 0 0 0 2
-3.9176 1.5474 -0.6318 H 0 0 0 0 0 0 0 0 0 0 3
-2.1167 -0.6398 0.7314 O 0 0 0 0 0 0 0 0 0 0 4
-1.2421 -0.6298 0.1897 H 0 0 0 0 0 0 0 0 0 0 5
-1.8741 -0.1803 1.5550 H 0 0 0 0 0 0 0 0 0 0 6
3.5032 0.4413 -0.1521 C 0 0 0 0 0 0 0 0 0 0 7
2.3885 -0.0589 -0.7008 C 0 0 0 0 0 0 0 0 0 0 8
1.0561 -0.1057 0.0127 C 0 0 0 0 0 0 0 0 0 0 9
0.0985 -0.6435 -0.6618 O 0 0 0 0 0 0 0 0 0 0 10
0.9520 0.3616 1.1791 O 0 0 0 0 0 0 0 0 0 0 11
4.4525 0.4584 -0.6916 H 0 0 0 0 0 0 0 0 0 0 12
3.4866 0.8487 0.8620 H 0 0 0 0 0 0 0 0 0 0 13
2.4007 -0.4686 -1.7152 H 0 0 0 0 0 0 0 0 0 0 14
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
8 7 0 0 0 0
12 7 0 0 0 0
13 7 0 0 0 0
9 8 0 0 0 0
10 9 0 0 0 0
11 9 0 0 0 0
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8 14 0 0 0 0
M END
$$$$
acrylicacid.sdf
COSMOtherm 3D 0
15 12 0 0 0 0 0 0 0 0 0 V2000
-1.0253 3.6936 -0.4305 O 0 0 0 0 0 0 0 0 0 0 0 1
-1.6497 3.2243 -1.0135 H 0 0 0 0 0 0 0 0 0 0 0 2
-0.7204 4.4508 -0.9632 H 0 0 0 0 0 0 0 0 0 0 0 3
1.0595 2.2055 0.4402 O 0 0 0 0 0 0 0 0 0 0 0 4
1.0587 2.2943 1.4101 H 0 0 0 0 0 0 0 0 0 0 0 5
0.2733 2.7405 0.1216 H 0 0 0 0 0 0 0 0 0 0 0 6
-0.6712 -3.3932 -0.1364 C 0 0 0 0 0 0 0 0 0 0 0 7
0.2227 -2.4433 -0.4394 C 0 0 0 0 0 0 0 0 0 0 0 8
0.0998 -1.0525 0.0785 C 0 0 0 0 0 0 0 0 0 0 0 9
1.0972 -0.2666 -0.3588 O 0 0 0 0 0 0 0 0 0 0 0 10
-0.8030 -0.6603 0.8188 O 0 0 0 0 0 0 0 0 0 0 0 11
-0.5710 -4.4092 -0.5200 H 0 0 0 0 0 0 0 0 0 0 0 12
-1.5277 -3.1745 0.5052 H 0 0 0 0 0 0 0 0 0 0 0 13
1.0820 -2.6525 -1.0798 H 0 0 0 0 0 0 0 0 0 0 0 14
0.9979 0.6948 0.0086 H 0 0 0 0 0 0 0 0 0 0 0 15
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
8 7 0 0 0 0
12 7 0 0 0 0
13 7 0 0 0 0
9 8 0 0 0 0
14 8 0 0 0 0
10 9 0 0 0 0
11 9 0 0 0 0
10 15 0 0 0 0
M END
$$$$
anthracene-9-carboxylicacid-anion.sdf
COSMOtherm 3D 0
32 32 0 0 0 0 0 0 0 0 0 V2000
-6.2568 -0.0651 -0.7905 O 0 0 0 0 0 0 0 0 0 0 0 1
-5.5670 0.5928 -0.4867 H 0 0 0 0 0 0 0 0 0 0 0 2
-6.8732 0.4628 -1.3262 H 0 0 0 0 0 0 0 0 0 0 0 3
-4.3850 1.7484 0.0294 O 0 0 0 0 0 0 0 0 0 0 0 4
-3.4387 1.4328 -0.1925 H 0 0 0 0 0 0 0 0 0 0 0 5
-4.3829 1.8132 1.0010 H 0 0 0 0 0 0 0 0 0 0 0 6
3.4290 2.8049 -0.2605 C 0 0 0 0 0 0 0 0 0 0 0 7
2.1125 3.3130 -0.0558 C 0 0 0 0 0 0 0 0 0 0 0 8
1.0456 2.4541 0.0828 C 0 0 0 0 0 0 0 0 0 0 0 9
1.2236 1.0341 0.0247 C 0 0 0 0 0 0 0 0 0 0 0 10
2.5639 0.5198 -0.1861 C 0 0 0 0 0 0 0 0 0 0 0 11
3.6454 1.4478 -0.3240 C 0 0 0 0 0 0 0 0 0 0 0 12
0.1443 0.1315 0.1697 C 0 0 0 0 0 0 0 0 0 0 0 13
0.3623 -1.2645 0.1041 C 0 0 0 0 0 0 0 0 0 0 0 14
1.7047 -1.7703 -0.1126 C 0 0 0 0 0 0 0 0 0 0 0 15
2.7702 -0.8670 -0.2486 C 0 0 0 0 0 0 0 0 0 0 0 16
-0.7039 -2.2113 0.2382 C 0 0 0 0 0 0 0 0 0 0 0 17
-0.4677 -3.5657 0.1681 C 0 0 0 0 0 0 0 0 0 0 0 18
0.8530 -4.0606 -0.0420 C 0 0 0 0 0 0 0 0 0 0 0 19
1.9064 -3.1863 -0.1782 C 0 0 0 0 0 0 0 0 0 0 0 20
-1.2598 0.6654 0.4278 C 0 0 0 0 0 0 0 0 0 0 0 21
-1.6239 0.7844 1.6263 O 0 0 0 0 0 0 0 0 0 0 0 22
-1.9530 0.9496 -0.6077 O 0 0 0 0 0 0 0 0 0 0 0 23
4.2641 3.4998 -0.3669 H 0 0 0 0 0 0 0 0 0 0 0 24
1.9540 4.3921 -0.0091 H 0 0 0 0 0 0 0 0 0 0 0 25
0.0417 2.8545 0.2371 H 0 0 0 0 0 0 0 0 0 0 0 26
4.6521 1.0531 -0.4806 H 0 0 0 0 0 0 0 0 0 0 0 27
3.7810 -1.2516 -0.4080 H 0 0 0 0 0 0 0 0 0 0 0 28
-1.7190 -1.8439 0.3994 H 0 0 0 0 0 0 0 0 0 0 0 29
-1.2952 -4.2699 0.2724 H 0 0 0 0 0 0 0 0 0 0 0 30
1.0227 -5.1376 -0.0945 H 0 0 0 0 0 0 0 0 0 0 0 31
2.9203 -3.5601 -0.3404 H 0 0 0 0 0 0 0 0 0 0 0 32
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
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18 17 0 0 0 0
29 17 0 0 0 0
19 18 0 0 0 0
30 18 0 0 0 0
20 19 0 0 0 0
31 19 0 0 0 0
22 21 0 0 0 0
23 21 0 0 0 0
20 32 0 0 0 0
M END
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17 8 0 0 0 0
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11 10 0 0 0 0
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19 11 0 0 0 0
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15 13 0 0 0 0
12 20 0 0 0 0
M END
$$$$
benzoicacid.sdf
COSMOtherm 3D 0
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-0.8035 4.9122 0.9008 O 0 0 0 0 0 0 0 0 0 1
-1.7008 4.8667 0.5237 H 0 0 0 0 0 0 0 0 0 2
-0.6168 5.8665 0.9657 H 0 0 0 0 0 0 0 0 0 3
1.0878 3.5814 -0.4899 O 0 0 0 0 0 0 0 0 0 4
0.3600 4.0871 -0.0188 H 0 0 0 0 0 0 0 0 0 5
1.0141 3.8319 -1.4281 H 0 0 0 0 0 0 0 0 0 6
1.1799 -3.1259 0.4030 C 0 0 0 0 0 0 0 0 0 7
1.1617 -1.7409 0.2184 C 0 0 0 0 0 0 0 0 0 8
-0.0462 -1.0849 -0.0797 C 0 0 0 0 0 0 0 0 0 9
-1.2317 -1.8327 -0.1884 C 0 0 0 0 0 0 0 0 0 10
-1.2106 -3.2162 -0.0019 C 0 0 0 0 0 0 0 0 0 11
-0.0045 -3.8652 0.2936 C 0 0 0 0 0 0 0 0 0 12
-0.1101 0.3960 -0.2905 C 0 0 0 0 0 0 0 0 0 13
1.0684 1.0128 -0.1382 O 0 0 0 0 0 0 0 0 0 14
-1.1528 0.9888 -0.5772 O 0 0 0 0 0 0 0 0 0 15
2.1200 -3.6302 0.6327 H 0 0 0 0 0 0 0 0 0 16
2.0826 -1.1641 0.3034 H 0 0 0 0 0 0 0 0 0 17
-2.1645 -1.3167 -0.4197 H 0 0 0 0 0 0 0 0 0 18
-2.1345 -3.7907 -0.0869 H 0 0 0 0 0 0 0 0 0 19
0.0121 -4.9469 0.4384 H 0 0 0 0 0 0 0 0 0 20
0.9731 2.0302 -0.3011 H 0 0 0 0 0 0 0 0 0 21
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
8 7 0 0 0 0
12 7 0 0 0 0
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18 10 0 0 0 0
12 11 0 0 0 0
19 11 0 0 0 0
20 12 0 0 0 0
14 13 0 0 0 0
15 13 0 0 0 0
14 21 0 0 0 0
M END
$$$$
boricacid-anion.sdf
COSMOtherm 3D 0
12 9 0 0 0 0 0 0 0 0 0 V2000
-2.5583 -0.0768 -1.1409 O 0 0 0 0 0 0 0 0 0 1
-1.5314 -0.0077 -1.1310 H 0 0 0 0 0 0 0 0 0 2
-2.8703 0.8015 -1.4206 H 0 0 0 0 0 0 0 0 0 3
2.5620 -0.0725 -1.1420 O 0 0 0 0 0 0 0 0 0 4
1.5353 0.0008 -1.1275 H 0 0 0 0 0 0 0 0 0 5
2.8790 0.8210 -1.3611 H 0 0 0 0 0 0 0 0 0 6
-0.0010 0.0160 0.6218 B 0 0 0 0 0 0 0 0 0 7
-1.1796 0.0036 1.4016 O 0 0 0 0 0 0 0 0 0 8
0.0021 0.0410 -0.7271 O 0 0 0 0 0 0 0 0 0 9
1.1738 -0.0070 1.4069 O 0 0 0 0 0 0 0 0 0 10
-1.9436 0.0044 0.7800 H 0 0 0 0 0 0 0 0 0 11
1.9403 -0.0203 0.7889 H 0 0 0 0 0 0 0 0 0 12
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
8 7 0 0 0 0
9 7 0 0 0 0
10 7 0 0 0 0
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10 12 0 0 0 0
M END
$$$$
boricacid.sdf
COSMOtherm 3D 0
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-3.6721 -0.0008 0.6790 O 0 0 0 0 0 0 0 0 0 1
-4.2466 -0.7742 0.5306 H 0 0 0 0 0 0 0 0 0 2
-4.2511 0.7669 0.5192 H 0 0 0 0 0 0 0 0 0 3
-1.4581 -0.0069 -0.8563 O 0 0 0 0 0 0 0 0 0 4
-1.7226 -0.0043 -1.7932 H 0 0 0 0 0 0 0 0 0 5
-2.3095 -0.0042 -0.3241 H 0 0 0 0 0 0 0 0 0 6
1.5365 0.0051 0.0647 B 0 0 0 0 0 0 0 0 0 7
2.8635 0.0549 0.4618 O 0 0 0 0 0 0 0 0 0 8
0.9045 1.2210 -0.1230 O 0 0 0 0 0 0 0 0 0 9
0.9130 -1.2175 -0.1227 O 0 0 0 0 0 0 0 0 0 10
3.2394 -0.8360 0.5716 H 0 0 0 0 0 0 0 0 0 11
-0.0314 1.0614 -0.4071 H 0 0 0 0 0 0 0 0 0 12
-0.0253 -1.0695 -0.4074 H 0 0 0 0 0 0 0 0 0 13
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
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6 4 0 0 0 0
8 7 0 0 0 0
9 7 0 0 0 0
10 7 0 0 0 0
11 8 0 0 0 0
12 9 0 0 0 0
10 13 0 0 0 0
M END
$$$$
bromoaceticacid-anion.sdf
COSMOTHERM 3D 0
13 9 0 0 0 0 0 0 0 0 0 V2000
1.6525 -0.4721 4.9433 O 0 0 0 0 0 0 0 0 0 0 1
0.8962 -0.0792 4.4192 H 0 0 0 0 0 0 0 0 0 0 2
1.8136 -1.3363 4.5276 H 0 0 0 0 0 0 0 0 0 0 3
-0.3742 0.7087 3.5508 O 0 0 0 0 0 0 0 0 0 0 4
-0.3003 0.5506 2.5461 H 0 0 0 0 0 0 0 0 0 0 5
-1.2454 0.3458 3.7889 H 0 0 0 0 0 0 0 0 0 0 6
0.5840 0.0316 -2.1064 Br 0 0 0 0 0 0 0 0 0 0 7
-1.1373 -0.3308 -1.1480 C 0 0 0 0 0 0 0 0 0 0 8
-1.1396 -0.0759 0.3675 C 0 0 0 0 0 0 0 0 0 0 9
-2.2598 -0.3324 0.8868 O 0 0 0 0 0 0 0 0 0 0 10
-0.0952 0.3435 0.9516 O 0 0 0 0 0 0 0 0 0 0 11
-1.3616 -1.3815 -1.3563 H 0 0 0 0 0 0 0 0 0 0 12
-1.8763 0.3078 -1.6417 H 0 0 0 0 0 0 0 0 0 0 13
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
9 8 0 0 0 0
12 8 0 0 0 0
10 9 0 0 0 0
11 9 0 0 0 0
8 13 0 0 0 0
M END
$$$$
bromoaceticacid.sdf
COSMOTHERM 3D 0
14 10 0 0 0 0 0 0 0 0 0 V2000
-1.4283 -4.8120 0.5141 O 0 0 0 0 0 0 0 0 0 0 1
-1.6518 -5.6884 0.1504 H 0 0 0 0 0 0 0 0 0 0 2
-2.2207 -4.2707 0.3440 H 0 0 0 0 0 0 0 0 0 0 3
0.8735 -3.8164 -0.4469 O 0 0 0 0 0 0 0 0 0 0 4
0.8748 -3.8956 -1.4178 H 0 0 0 0 0 0 0 0 0 0 5
-0.0128 -4.1837 -0.1443 H 0 0 0 0 0 0 0 0 0 0 6
-0.2885 2.3278 0.0035 Br 0 0 0 0 0 0 0 0 0 0 7
0.9205 0.8587 0.4990 C 0 0 0 0 0 0 0 0 0 0 8
0.4940 -0.4897 -0.0688 C 0 0 0 0 0 0 0 0 0 0 9
1.3443 -1.4275 0.3496 O 0 0 0 0 0 0 0 0 0 0 10
-0.4693 -0.6842 -0.7967 O 0 0 0 0 0 0 0 0 0 0 11
0.9438 0.8222 1.5926 H 0 0 0 0 0 0 0 0 0 0 12
1.9140 1.1279 0.1256 H 0 0 0 0 0 0 0 0 0 0 13
1.0859 -2.3713 -0.0241 H 0 0 0 0 0 0 0 0 0 0 14
2 1 0 0 0 0
3 1 0 0 0 0
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6 4 0 0 0 0
9 8 0 0 0 0
12 8 0 0 0 0
13 8 0 0 0 0
10 9 0 0 0 0
11 9 0 0 0 0
10 14 0 0 0 0
M END
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carbonicacid-anion.sdf
COSMOTHERM 3D 0
11 8 0 0 0 0 0 0 0 0 0 V2000
-3.8027 0.4365 -0.5538 O 0 0 0 0 0 0 0 0 0 0 1
-3.0104 0.0842 -0.0546 H 0 0 0 0 0 0 0 0 0 0 2
-3.6415 1.3931 -0.6205 H 0 0 0 0 0 0 0 0 0 0 3
-1.6845 -0.6334 0.7910 O 0 0 0 0 0 0 0 0 0 0 4
-0.8159 -0.5602 0.2607 H 0 0 0 0 0 0 0 0 0 0 5
-1.5041 -0.1612 1.6224 H 0 0 0 0 0 0 0 0 0 0 6
1.4924 0.0360 -0.0193 C 0 0 0 0 0 0 0 0 0 0 7
1.5343 0.5082 1.1396 O 0 0 0 0 0 0 0 0 0 0 8
2.6680 0.0810 -0.7904 O 0 0 0 0 0 0 0 0 0 0 9
0.5189 -0.4987 -0.6335 O 0 0 0 0 0 0 0 0 0 0 10
3.3471 0.5059 -0.2302 H 0 0 0 0 0 0 0 0 0 0 11
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
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8 7 0 0 0 0
9 7 0 0 0 0
10 7 0 0 0 0
9 11 0 0 0 0
M END
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carbonicacid.sdf
COSMOTHERM 3D 0
12 9 0 0 0 0 0 0 0 0 0 V2000
-3.3851 0.0055 -0.3588 O 0 0 0 0 0 0 0 0 0 0 1
-3.5453 -0.7840 -0.9079 H 0 0 0 0 0 0 0 0 0 0 2
-3.5155 0.7584 -0.9644 H 0 0 0 0 0 0 0 0 0 0 3
3.3848 -0.0033 -0.3596 O 0 0 0 0 0 0 0 0 0 0 4
3.5763 0.8270 -0.8330 H 0 0 0 0 0 0 0 0 0 0 5
3.4780 -0.7001 -1.0349 H 0 0 0 0 0 0 0 0 0 0 6
0.0003 -0.0022 0.1594 C 0 0 0 0 0 0 0 0 0 0 7
0.0007 -0.0032 -1.0700 O 0 0 0 0 0 0 0 0 0 0 8
-1.0949 0.0025 0.9300 O 0 0 0 0 0 0 0 0 0 0 9
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1.0948 -0.0061 0.9310 O 0 0 0 0 0 0 0 0 0 0 10
-1.9290 0.0030 0.3436 H 0 0 0 0 0 0 0 0 0 0 11
1.9293 -0.0043 0.3452 H 0 0 0 0 0 0 0 0 0 0 12
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
8 7 0 0 0 0
9 7 0 0 0 0
10 7 0 0 0 0
11 9 0 0 0 0
10 12 0 0 0 0
M END
$$$$
chloroaceticacid--anion.sdf
COSMOTHERM 3D 0
13 10 0 0 0 0 0 0 0 0 0 V2000
-4.4049 0.4776 -1.2896 O 0 0 0 0 0 0 0 0 0 0 1
-3.7928 0.0802 -0.6055 H 0 0 0 0 0 0 0 0 0 0 2
-4.4878 1.4105 -1.0282 H 0 0 0 0 0 0 0 0 0 0 3
-2.7510 -0.7184 0.5229 O 0 0 0 0 0 0 0 0 0 0 4
-1.7644 -0.5671 0.3124 H 0 0 0 0 0 0 0 0 0 0 5
-2.8622 -0.3698 1.4249 H 0 0 0 0 0 0 0 0 0 0 6
2.6446 -0.0587 -1.0673 Cl 0 0 0 0 0 0 0 0 0 0 7
2.0078 0.3096 0.6211 C 0 0 0 0 0 0 0 0 0 0 8
0.5030 0.0707 0.8384 C 0 0 0 0 0 0 0 0 0 0 9
-0.2123 -0.3725 -0.1118 O 0 0 0 0 0 0 0 0 0 0 10
0.1318 0.3575 2.0081 O 0 0 0 0 0 0 0 0 0 0 11
2.2479 1.3608 0.8108 H 0 0 0 0 0 0 0 0 0 0 12
2.5851 -0.3221 1.3044 H 0 0 0 0 0 0 0 0 0 0 13
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
8 7 0 0 0 0
9 8 0 0 0 0
12 8 0 0 0 0
10 9 0 0 0 0
11 9 0 0 0 0
8 13 0 0 0 0
M END
$$$$
chloroaceticacid.sdf
COSMOTHERM 3D 0
14 11 0 0 0 0 0 0 0 0 0 V2000
-1.2601 -4.0991 0.5078 O 0 0 0 0 0 0 0 0 0 0 1
-1.3871 -5.0035 0.1677 H 0 0 0 0 0 0 0 0 0 0 2
-2.0950 -3.6422 0.2985 H 0 0 0 0 0 0 0 0 0 0 3
0.9617 -2.9277 -0.4464 O 0 0 0 0 0 0 0 0 0 0 4
0.9743 -3.0106 -1.4168 H 0 0 0 0 0 0 0 0 0 0 5
0.1057 -3.3617 -0.1460 H 0 0 0 0 0 0 0 0 0 0 6
-0.5304 3.0050 0.0056 Cl 0 0 0 0 0 0 0 0 0 0 7
0.6783 1.7448 0.4845 C 0 0 0 0 0 0 0 0 0 0 8
0.3419 0.3617 -0.0640 C 0 0 0 0 0 0 0 0 0 0 9
1.2671 -0.5079 0.3392 O 0 0 0 0 0 0 0 0 0 0 10
-0.6243 0.0949 -0.7645 O 0 0 0 0 0 0 0 0 0 0 11
0.7086 1.7152 1.5790 H 0 0 0 0 0 0 0 0 0 0 12
1.6559 2.0660 0.1087 H 0 0 0 0 0 0 0 0 0 0 13
1.0701 -1.4700 -0.0226 H 0 0 0 0 0 0 0 0 0 0 14
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
8 7 0 0 0 0
9 8 0 0 0 0
12 8 0 0 0 0
13 8 0 0 0 0
10 9 0 0 0 0
11 9 0 0 0 0
10 14 0 0 0 0
M END
$$$$
cis-5-formyluracil--anion.sdf
COSMOTHERM 3D 0
19 17 0 0 0 0 0 0 0 0 0 V2000
-4.4743 0.3799 -0.2295 O 0 0 0 0 0 0 0 0 0 0 1
-4.1993 -0.5648 -0.1156 H 0 0 0 0 0 0 0 0 0 0 2
-3.6083 0.8468 -0.1272 H 0 0 0 0 0 0 0 0 0 0 3
-3.1464 -2.0688 0.0983 O 0 0 0 0 0 0 0 0 0 0 4
-2.3030 -1.5080 0.1007 H 0 0 0 0 0 0 0 0 0 0 5
-3.2287 -2.4031 1.0088 H 0 0 0 0 0 0 0 0 0 0 6
0.3154 -1.1317 -0.0077 C 0 0 0 0 0 0 0 0 0 0 7
1.5804 -0.5279 -0.0203 C 0 0 0 0 0 0 0 0 0 0 8
1.6368 0.9256 0.0199 C 0 0 0 0 0 0 0 0 0 0 9
0.3611 1.5141 0.0558 N 0 0 0 0 0 0 0 0 0 0 10
-0.8715 0.8639 0.0519 C 0 0 0 0 0 0 0 0 0 0 11
-0.8675 -0.5152 0.0267 N 0 0 0 0 0 0 0 0 0 0 12
2.6441 1.6483 0.0246 O 0 0 0 0 0 0 0 0 0 0 13
-1.9195 1.5436 0.0734 O 0 0 0 0 0 0 0 0 0 0 14
2.7382 -1.3932 -0.0631 C 0 0 0 0 0 0 0 0 0 0 15
0.2724 -2.2274 -0.0307 H 0 0 0 0 0 0 0 0 0 0 16
0.3358 2.5357 0.0771 H 0 0 0 0 0 0 0 0 0 0 17
3.9324 -1.0638 -0.0767 O 0 0 0 0 0 0 0 0 0 0 18
2.4690 -2.4786 -0.0861 H 0 0 0 0 0 0 0 0 0 0 19
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
8 7 0 0 0 0
12 7 0 0 0 0
16 7 0 0 0 0
9 8 0 0 0 0
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15 8 0 0 0 0
10 9 0 0 0 0
13 9 0 0 0 0
11 10 0 0 0 0
17 10 0 0 0 0
12 11 0 0 0 0
14 11 0 0 0 0
18 15 0 0 0 0
15 19 0 0 0 0
M END
$$$$
cis-5-formyluracil.sdf
COSMOtherm 3D 0

20 18 0 0 0 0 0 0 0 0 0 V2000
-5.1383 -0.5699 1.0003 O 0 0 0 0 0 0 0 0 0 0 1
-5.6866 -1.3385 1.2422 H 0 0 0 0 0 0 0 0 0 0 2
-5.7765 0.0871 0.6679 H 0 0 0 0 0 0 0 0 0 0 3
-3.1929 -1.2320 -0.7683 O 0 0 0 0 0 0 0 0 0 0 4
-3.5394 -1.0854 -1.6662 H 0 0 0 0 0 0 0 0 0 0 5
-3.9354 -0.9718 -0.1478 H 0 0 0 0 0 0 0 0 0 0 6
0.2445 -0.9937 -0.2394 C 0 0 0 0 0 0 0 0 0 0 7
1.5579 -0.6287 -0.0158 C 0 0 0 0 0 0 0 0 0 0 8
1.8712 0.7943 0.1331 C 0 0 0 0 0 0 0 0 0 0 9
0.7404 1.6302 0.0210 N 0 0 0 0 0 0 0 0 0 0 10
-0.5770 1.2663 -0.2059 C 0 0 0 0 0 0 0 0 0 0 11
-0.7684 -0.1128 -0.3304 N 0 0 0 0 0 0 0 0 0 0 12
2.9785 1.2949 0.3364 O 0 0 0 0 0 0 0 0 0 0 13
-1.4990 2.0737 -0.2915 O 0 0 0 0 0 0 0 0 0 0 14
2.5455 -1.6987 0.0549 C 0 0 0 0 0 0 0 0 0 0 15
-0.0328 -2.0436 -0.3556 H 0 0 0 0 0 0 0 0 0 0 16
0.9128 2.6329 0.1176 H 0 0 0 0 0 0 0 0 0 0 17
-1.7578 -0.4643 -0.5058 H 0 0 0 0 0 0 0 0 0 0 18
3.7565 -1.5773 0.2451 O 0 0 0 0 0 0 0 0 0 0 19
2.1007 -2.7136 -0.0856 H 0 0 0 0 0 0 0 0 0 0 20
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
8 7 0 0 0 0
12 7 0 0 0 0
16 7 0 0 0 0
9 8 0 0 0 0
15 8 0 0 0 0
10 9 0 0 0 0
13 9 0 0 0 0
11 10 0 0 0 0
17 10 0 0 0 0
12 11 0 0 0 0
14 11 0 0 0 0
18 12 0 0 0 0
19 15 0 0 0 0
15 20 0 0 0 0
M END
$$$$
cyanoaceticacid-anion.sdf
COSMOtherm 3D 0

14 11 0 0 0 0 0 0 0 0 0 V2000
-4.2229 0.4596 -1.2793 O 0 0 0 0 0 0 0 0 0 0 1
-3.6001 0.0791 -0.5957 H 0 0 0 0 0 0 0 0 0 0 2
-4.3134 1.3952 -1.0303 H 0 0 0 0 0 0 0 0 0 0 3
-2.5394 -0.6940 0.5347 O 0 0 0 0 0 0 0 0 0 0 4
-1.5559 -0.5390 0.3193 H 0 0 0 0 0 0 0 0 0 0 5
-2.6489 -0.3449 1.4366 H 0 0 0 0 0 0 0 0 0 0 6
2.6399 0.0401 -0.8402 C 0 0 0 0 0 0 0 0 0 0 7
2.2580 0.2685 0.5403 C 0 0 0 0 0 0 0 0 0 0 8
0.7313 0.0665 0.8450 C 0 0 0 0 0 0 0 0 0 0 9
-0.0003 -0.3389 -0.1131 O 0 0 0 0 0 0 0 0 0 0 10
0.3854 0.3229 2.0213 O 0 0 0 0 0 0 0 0 0 0 11
2.9428 -0.1412 -1.9511 N 0 0 0 0 0 0 0 0 0 0 12
2.5405 1.2918 0.8290 H 0 0 0 0 0 0 0 0 0 0 13
2.8300 -0.4132 1.1884 H 0 0 0 0 0 0 0 0 0 0 14
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
8 7 0 0 0 0
12 7 0 0 0 0
9 8 0 0 0 0
13 8 0 0 0 0
10 9 0 0 0 0
11 9 0 0 0 0
8 14 0 0 0 0
M END
$$$$
cyanoaceticacid.sdf
COSMOtherm 3D 0

15 12 0 0 0 0 0 0 0 0 0 V2000
1.2978 3.8757 -0.5318 O 0 0 0 0 0 0 0 0 0 0 1
2.1053 3.7973 0.0081 H 0 0 0 0 0 0 0 0 0 0 2
1.1862 4.8349 -0.6639 H 0 0 0 0 0 0 0 0 0 0 3
-0.8984 2.7366 0.5031 O 0 0 0 0 0 0 0 0 0 0 4
-0.0545 3.1717 0.1690 H 0 0 0 0 0 0 0 0 0 0 5
-0.8766 2.8210 1.4731 H 0 0 0 0 0 0 0 0 0 0 6
0.2690 -2.9507 -0.1632 C 0 0 0 0 0 0 0 0 0 0 7
-0.7070 -1.9317 -0.5099 C 0 0 0 0 0 0 0 0 0 0 8
-0.3580 -0.5465 0.0575 C 0 0 0 0 0 0 0 0 0 0 9
0.6253 -0.3233 0.7514 O 0 0 0 0 0 0 0 0 0 0 10
-1.2673 0.3463 -0.3103 O 0 0 0 0 0 0 0 0 0 0 11
1.0442 -3.7751 0.1063 N 0 0 0 0 0 0 0 0 0 0 12
-1.6983 -2.2328 -0.1370 H 0 0 0 0 0 0 0 0 0 0 13
-0.7915 -1.8633 -1.6054 H 0 0 0 0 0 0 0 0 0 0 14
-1.0434 1.3003 0.0689 H 0 0 0 0 0 0 0 0 0 0 15
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2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
8 7 0 0 0 0
12 7 0 0 0 0
9 8 0 0 0 0
13 8 0 0 0 0
14 8 0 0 0 0
10 9 0 0 0 0
11 9 0 0 0 0
11 15 0 0 0 0
M END
$$$$
dichloroaceticacid-anion.sdf
COSMOtherm 3D 0

13 10 0 0 0 0 0 0 0 0 0 V2000
-4.9776 0.9794 -0.7027 O 0 0 0 0 0 0 0 0 0 0 1
-4.3324 0.2755 -0.4069 H 0 0 0 0 0 0 0 0 0 0 2
-4.6393 1.8012 -0.3078 H 0 0 0 0 0 0 0 0 0 0 3
-3.2579 -1.0172 0.0208 O 0 0 0 0 0 0 0 0 0 0 4
-2.2871 -0.7375 -0.0742 H 0 0 0 0 0 0 0 0 0 0 5
-3.3537 -1.2552 0.9600 H 0 0 0 0 0 0 0 0 0 0 6
2.3029 -0.9671 -0.9289 Cl 0 0 0 0 0 0 0 0 0 0 7
1.5303 -0.0610 0.4547 C 0 0 0 0 0 0 0 0 0 0 8
0.0404 -0.4805 0.6320 C 0 0 0 0 0 0 0 0 0 0 9
-0.7362 -0.2699 -0.3456 O 0 0 0 0 0 0 0 0 0 0 10
-0.2196 -0.9877 1.7493 O 0 0 0 0 0 0 0 0 0 0 11
1.6679 1.7409 0.1920 Cl 0 0 0 0 0 0 0 0 0 0 12
2.1277 -0.2868 1.3389 H 0 0 0 0 0 0 0 0 0 0 13
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
8 7 0 0 0 0
9 8 0 0 0 0
12 8 0 0 0 0
10 9 0 0 0 0
11 9 0 0 0 0
8 13 0 0 0 0
M END
$$$$
dichloroaceticacid.sdf
COSMOtherm 3D 0

14 12 0 0 0 0 0 0 0 0 0 V2000
-1.0981 -1.0396 3.4734 O 0 0 0 0 0 0 0 0 0 0 1
-0.8612 -1.9509 3.7236 H 0 0 0 0 0 0 0 0 0 0 2
-1.0971 -1.0285 2.4835 H 0 0 0 0 0 0 0 0 0 0 3
0.8806 0.7000 3.4195 O 0 0 0 0 0 0 0 0 0 0 4
0.1398 0.0383 3.6230 H 0 0 0 0 0 0 0 0 0 0 5
0.6568 1.5213 3.8946 H 0 0 0 0 0 0 0 0 0 0 6
1.3511 -0.7597 -1.8655 Cl 0 0 0 0 0 0 0 0 0 0 7
0.1916 0.4953 -1.2423 C 0 0 0 0 0 0 0 0 0 0 8
0.0408 0.2756 0.2755 C 0 0 0 0 0 0 0 0 0 0 9
-0.7605 -0.5319 0.7426 O 0 0 0 0 0 0 0 0 0 0 10
0.8826 1.0371 0.9333 O 0 0 0 0 0 0 0 0 0 0 11
-1.3958 0.3973 -2.0793 Cl 0 0 0 0 0 0 0 0 0 0 12
0.6277 1.4685 -1.4713 H 0 0 0 0 0 0 0 0 0 0 13
0.8493 0.8874 2.0040 H 0 0 0 0 0 0 0 0 0 0 14
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
8 7 0 0 0 0
9 8 0 0 0 0
12 8 0 0 0 0
13 8 0 0 0 0
10 9 0 0 0 0
11 9 0 0 0 0
4 14 0 0 0 0
11 14 0 0 0 0
M END
$$$$
dimethadione-anion.sdf
COSMOtherm 3D 0

21 19 0 0 0 0 0 0 0 0 0 V2000
-3.8925 0.7602 -0.1031 O 0 0 0 0 0 0 0 0 0 0 1
-3.6721 -0.2057 -0.0592 H 0 0 0 0 0 0 0 0 0 0 2
-2.9979 1.1757 -0.0337 H 0 0 0 0 0 0 0 0 0 0 3
-2.7941 -1.8188 0.0056 O 0 0 0 0 0 0 0 0 0 0 4
-1.8894 -1.3589 0.0373 H 0 0 0 0 0 0 0 0 0 0 5
-2.9039 -2.2214 0.8847 H 0 0 0 0 0 0 0 0 0 0 6
1.8554 0.2152 -0.0113 C 0 0 0 0 0 0 0 0 0 0 7
0.8307 -0.9400 -0.0123 C 0 0 0 0 0 0 0 0 0 0 8
0.9756 1.3907 0.0282 O 0 0 0 0 0 0 0 0 0 0 9
-0.3324 0.9365 0.0442 C 0 0 0 0 0 0 0 0 0 0 10
-0.4316 -0.4250 0.0222 N 0 0 0 0 0 0 0 0 0 0 11
2.7235 0.1995 1.2439 C 0 0 0 0 0 0 0 0 0 0 12
2.6720 0.2456 -1.3004 C 0 0 0 0 0 0 0 0 0 0 13
1.1430 -2.1396 -0.0395 O 0 0 0 0 0 0 0 0 0 0 14
-1.2503 1.7681 0.0763 O 0 0 0 0 0 0 0 0 0 0 15
2.1050 0.2250 2.1518 H 0 0 0 0 0 0 0 0 0 0 16
3.3271 -0.7185 1.2593 H 0 0 0 0 0 0 0 0 0 0 17
3.4011 1.0650 1.2502 H 0 0 0 0 0 0 0 0 0 0 18
2.0172 0.3104 -2.1804 H 0 0 0 0 0 0 0 0 0 0 19
3.2684 -0.6741 -1.3766 H 0 0 0 0 0 0 0 0 0 0 20
3.3546 1.1071 -1.3003 H 0 0 0 0 0 0 0 0 0 0 21
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
8 7 0 0 0 0
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9 7 0 0 0 0
12 7 0 0 0 0
13 7 0 0 0 0
11 8 0 0 0 0
14 8 0 0 0 0
10 9 0 0 0 0
11 10 0 0 0 0
15 10 0 0 0 0
16 12 0 0 0 0
17 12 0 0 0 0
18 12 0 0 0 0
19 13 0 0 0 0
20 13 0 0 0 0
13 21 0 0 0 0
M END
$$$$
dimethadione.sdf
COSMOTHERM 3D 0
22 20 0 0 0 0 0 0 0 0 0 V2000
-4.7085 0.0916 0.9286 O 0 0 0 0 0 0 0 0 0 0 1
-5.1609 -0.7480 0.7282 H 0 0 0 0 0 0 0 0 0 0 2
-5.4291 0.7436 1.0035 H 0 0 0 0 0 0 0 0 0 0 3
-2.8444 0.7939 -0.9198 O 0 0 0 0 0 0 0 0 0 0 4
-3.5563 0.5150 -0.2749 H 0 0 0 0 0 0 0 0 0 0 5
-3.1480 0.4870 -1.7920 H 0 0 0 0 0 0 0 0 0 0 6
1.9779 0.0909 0.2014 C 0 0 0 0 0 0 0 0 0 0 7
0.7269 0.9351 -0.0939 C 0 0 0 0 0 0 0 0 0 0 8
1.4579 -1.2938 0.1129 O 0 0 0 0 0 0 0 0 0 0 9
0.1287 -1.2724 -0.1885 C 0 0 0 0 0 0 0 0 0 0 10
-0.2978 0.0435 -0.3060 N 0 0 0 0 0 0 0 0 0 0 11
2.4908 0.3296 1.6172 C 0 0 0 0 0 0 0 0 0 0 12
3.0436 0.2819 -0.8722 C 0 0 0 0 0 0 0 0 0 0 13
0.6632 2.1575 -0.1315 O 0 0 0 0 0 0 0 0 0 0 14
-0.5400 -2.2811 -0.3227 O 0 0 0 0 0 0 0 0 0 0 15
-1.2985 0.3040 -0.5441 H 0 0 0 0 0 0 0 0 0 0 16
1.7051 0.1435 2.3616 H 0 0 0 0 0 0 0 0 0 0 17
2.8255 1.3713 1.7123 H 0 0 0 0 0 0 0 0 0 0 18
3.3427 -0.3325 1.8211 H 0 0 0 0 0 0 0 0 0 0 19
2.6472 0.0523 -1.8704 H 0 0 0 0 0 0 0 0 0 0 20
3.3868 1.3249 -0.8618 H 0 0 0 0 0 0 0 0 0 0 21
3.9011 -0.3725 -0.6669 H 0 0 0 0 0 0 0 0 0 0 22
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
8 7 0 0 0 0
9 7 0 0 0 0
12 7 0 0 0 0
13 7 0 0 0 0
11 8 0 0 0 0
14 8 0 0 0 0
10 9 0 0 0 0
11 10 0 0 0 0
15 10 0 0 0 0
16 11 0 0 0 0
17 12 0 0 0 0
18 12 0 0 0 0
19 12 0 0 0 0
20 13 0 0 0 0
21 13 0 0 0 0
13 22 0 0 0 0
M END
$$$$
ethanol-anion.sdf
COSMOTHERM 3D 0
14 13 0 0 0 0 0 0 0 0 0 V2000
-2.1617 -1.2703 -0.2007 O 0 0 0 0 0 0 0 0 0 0 1
-1.2549 -0.8172 0.1017 H 0 0 0 0 0 0 0 0 0 0 2
-2.2958 -0.9691 -1.1152 H 0 0 0 0 0 0 0 0 0 0 3
2.2509 -1.1336 -0.2266 O 0 0 0 0 0 0 0 0 0 0 4
1.3206 -0.7377 0.0853 H 0 0 0 0 0 0 0 0 0 0 5
2.3973 -0.7624 -1.1130 H 0 0 0 0 0 0 0 0 0 0 6
-0.1157 1.8634 -0.6841 C 0 0 0 0 0 0 0 0 0 0 7
-0.0111 1.1642 0.6804 C 0 0 0 0 0 0 0 0 0 0 8
0.0203 -0.2394 0.5970 O 0 0 0 0 0 0 0 0 0 0 9
-0.1319 2.9610 -0.5755 H 0 0 0 0 0 0 0 0 0 0 10
0.7409 1.5967 -1.3236 H 0 0 0 0 0 0 0 0 0 0 11
-1.0361 1.5576 -1.2064 H 0 0 0 0 0 0 0 0 0 0 12
-0.8678 1.5034 1.3059 H 0 0 0 0 0 0 0 0 0 0 13
0.9009 1.5461 1.1934 H 0 0 0 0 0 0 0 0 0 0 14
2 1 0 0 0 0
3 1 0 0 0 0
9 2 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
9 5 0 0 0 0
8 7 0 0 0 0
10 7 0 0 0 0
11 7 0 0 0 0
12 7 0 0 0 0
9 8 0 0 0 0
13 8 0 0 0 0
8 14 0 0 0 0
M END
$$$$
ethanol.sdf
COSMOTHERM 3D 0
15 12 0 0 0 0 0 0 0 0 0 V2000
-0.9476 3.2338 -0.1529 O 0 0 0 0 0 0 0 0 0 0 1
-0.6628 4.1626 -0.2295 H 0 0 0 0 0 0 0 0 0 0 2
-1.5882 3.2390 0.5813 H 0 0 0 0 0 0 0 0 0 0 3
1.1687 1.5360 0.1937 O 0 0 0 0 0 0 0 0 0 0 4
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1
2
3 7 10 0 0 0 0
4 M END
5 $$$
6 formicacid.sdf
7 COSMOTHERM 3D 0
8
9 11 8 0 0 0 0 0 0 0 0 0 V2000
10 -3.0716 -0.5713 -0.3489 O 0 0 0 0 0 0 0 0 0 0 1
11 -2.8136 -1.4068 -0.7796 H 0 0 0 0 0 0 0 0 0 0 2
12 -3.5079 -0.0583 -1.0539 H 0 0 0 0 0 0 0 0 0 0 3
13 -1.0579 0.8184 0.7750 O 0 0 0 0 0 0 0 0 0 0 4
14 -0.9560 0.4752 1.6806 H 0 0 0 0 0 0 0 0 0 0 5
15 -1.7907 0.2717 0.3577 H 0 0 0 0 0 0 0 0 0 0 6
16 2.0038 -0.1166 -0.3435 C 0 0 0 0 0 0 0 0 0 0 7
17 1.1317 0.8542 -0.5960 O 0 0 0 0 0 0 0 0 0 0 8
18 1.8644 -1.0157 0.4771 O 0 0 0 0 0 0 0 0 0 0 9
19 2.9030 -0.0155 -0.9810 H 0 0 0 0 0 0 0 0 0 0 10
20 0.2774 0.7644 -0.0071 H 0 0 0 0 0 0 0 0 0 0 11
21 2 1 0 0 0 0
22 3 1 0 0 0 0
23 5 4 0 0 0 0
24 6 4 0 0 0 0
25 8 7 0 0 0 0
26 9 7 0 0 0 0
27 10 7 0 0 0 0
28 8 11 0 0 0 0
29 M END
30 $$$
31 fumaricacid-anion.sdf
32 COSMOTHERM 3D 0
33
34 17 14 0 0 0 0 0 0 0 0 V2000
35 -5.3168 -0.0065 0.1831 O 0 0 0 0 0 0 0 0 0 0 1
36 -5.4836 -0.4035 -0.6915 H 0 0 0 0 0 0 0 0 0 0 2
37 -5.7024 0.8871 0.1244 H 0 0 0 0 0 0 0 0 0 0 3
38 5.3716 0.0431 0.0689 O 0 0 0 0 0 0 0 0 0 0 4
39 4.4268 0.0276 -0.2879 H 0 0 0 0 0 0 0 0 0 0 5
40 5.2428 0.0251 1.0331 H 0 0 0 0 0 0 0 0 0 0 6
41 -0.4858 -0.0124 0.3631 C 0 0 0 0 0 0 0 0 0 0 7
42 0.5643 -0.0167 -0.4735 C 0 0 0 0 0 0 0 0 0 0 8
43 2.0035 -0.0174 -0.0001 C 0 0 0 0 0 0 0 0 0 0 9
44 -1.8879 -0.0043 -0.1228 C 0 0 0 0 0 0 0 0 0 0 10
45 -2.2256 -0.0142 -1.3077 O 0 0 0 0 0 0 0 0 0 0 11
46 -2.7688 0.0145 0.8958 O 0 0 0 0 0 0 0 0 0 0 12
47 2.8765 0.0106 -0.9402 O 0 0 0 0 0 0 0 0 0 0 13
48 2.2430 -0.0429 1.2374 O 0 0 0 0 0 0 0 0 0 0 14
49 -0.3262 -0.0120 1.4435 H 0 0 0 0 0 0 0 0 0 0 15
50 0.4004 -0.0152 -1.5549 H 0 0 0 0 0 0 0 0 0 0 16
51 -3.7240 0.0231 0.5341 H 0 0 0 0 0 0 0 0 0 0 17
52 2 1 0 0 0 0
53 3 1 0 0 0 0
54 5 4 0 0 0 0
55 6 4 0 0 0 0
56 8 7 0 0 0 0
57 10 7 0 0 0 0
58 15 7 0 0 0 0
59 9 8 0 0 0 0
60 16 8 0 0 0 0
13 9 0 0 0 0
14 9 0 0 0 0
11 10 0 0 0 0
12 10 0 0 0 0
12 17 0 0 0 0
M END
$$$
fumaricacid.sdf
COSMOTHERM 3D 0
18 15 0 0 0 0 0 0 0 0 V2000
-5.3501 0.0220 0.1214 O 0 0 0 0 0 0 0 0 0 0 1
-5.6451 -0.7885 -0.3334 H 0 0 0 0 0 0 0 0 0 0 2
-5.5944 0.7478 -0.4820 H 0 0 0 0 0 0 0 0 0 0 3
5.3524 0.0227 -0.1246 O 0 0 0 0 0 0 0 0 0 0 4
5.6497 -0.7785 0.3445 H 0 0 0 0 0 0 0 0 0 0 5
5.5949 0.7595 0.4660 H 0 0 0 0 0 0 0 0 0 0 6
-0.5340 -0.0073 0.4072 C 0 0 0 0 0 0 0 0 0 0 7
0.5332 -0.0104 -0.4053 C 0 0 0 0 0 0 0 0 0 0 8
1.9234 -0.0075 0.1301 C 0 0 0 0 0 0 0 0 0 0 9
-1.9242 -0.0061 -0.1288 C 0 0 0 0 0 0 0 0 0 0 10
-2.2060 -0.0081 -1.3261 O 0 0 0 0 0 0 0 0 0 0 11
-2.8320 0.0010 0.8581 O 0 0 0 0 0 0 0 0 0 0 12
2.8303 -0.0003 -0.8578 O 0 0 0 0 0 0 0 0 0 0 13
2.2065 -0.0095 1.3270 O 0 0 0 0 0 0 0 0 0 0 14
-0.4104 -0.0057 1.4919 H 0 0 0 0 0 0 0 0 0 0 15
0.4093 -0.0126 -1.4903 H 0 0 0 0 0 0 0 0 0 0 16
-3.7831 0.0062 0.4736 H 0 0 0 0 0 0 0 0 0 0 17
3.7812 0.0025 -0.4745 H 0 0 0 0 0 0 0 0 0 0 18
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
8 7 0 0 0 0
10 7 0 0 0 0
15 7 0 0 0 0
9 8 0 0 0 0
16 8 0 0 0 0
13 9 0 0 0 0
14 9 0 0 0 0
11 10 0 0 0 0
12 10 0 0 0 0
17 12 0 0 0 0
13 18 0 0 0 0
M END
$$$
hypobromousacid-anion.sdf
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1
2
3      -0.4824   -1.0592   -0.5618 O   0   0   0   0   0   0   0   0   0   0   7
4      1.0952    0.0674    0.0992 I   0   0   0   0   0   0   0   0   0   0   8
5     -1.2478   -0.3927   -0.6600 H   0   0   0   0   0   0   0   0   0   0   9
6
7      2 1 0 0 0 0
8      3 1 0 0 0 0
9      5 4 0 0 0 0
10     6 4 0 0 0 0
11     7 9 0 0 0 0
12
13 M  END
14 $$$$
15 hypophosphorousacid-anion.sdf
16 COSMOTHERM      3D                                0
17
18 11 8 0 0 0 0 0 0 0 0 0 V2000
19   -1.2749   -2.0941    0.0517 O   0   0   0   0   0   0   0   0   0   0   1
20   -1.3437   -1.0900   -0.0448 H   0   0   0   0   0   0   0   0   0   0   2
21   -1.5930   -2.4510   -0.7961 H   0   0   0   0   0   0   0   0   0   0   3
22    1.5468   -1.8908    0.0906 O   0   0   0   0   0   0   0   0   0   0   4
23    1.5329   -0.9037   -0.0433 H   0   0   0   0   0   0   0   0   0   0   5
24    0.5819   -2.1144    0.0761 H   0   0   0   0   0   0   0   0   0   0   6
25    1.3089    0.8484   -0.2797 O   0   0   0   0   0   0   0   0   0   0   7
26   -0.0793    1.3995    0.1483 P   0   0   0   0   0   0   0   0   0   0   8
27   -1.3558    0.5642   -0.1704 O   0   0   0   0   0   0   0   0   0   0   9
28   -0.0573    1.6788    1.5591 H   0   0   0   0   0   0   0   0   0   0  10
29   -0.2533    2.7052   -0.4229 H   0   0   0   0   0   0   0   0   0   0  11
30
31     2 1 0 0 0 0
32     3 1 0 0 0 0
33     5 4 0 0 0 0
34     6 4 0 0 0 0
35     8 7 0 0 0 0
36     9 8 0 0 0 0
37    10 8 0 0 0 0
38     8 11 0 0 0 0
39
40 M  END
41 $$$$
42 hypophosphorousacid.sdf
43 COSMOTHERM      3D                                0
44
45 12 9 0 0 0 0 0 0 0 0 0 V2000
46   -3.6294    0.2901    0.6882 O   0   0   0   0   0   0   0   0   0   0   1
47   -4.4726   -0.1838    0.5682 H   0   0   0   0   0   0   0   0   0   0   2
48   -3.8380    1.2164    0.4687 H   0   0   0   0   0   0   0   0   0   0   3
49   -1.6148   -0.7541   -0.7512 O   0   0   0   0   0   0   0   0   0   0   4
50   -1.9324   -0.9284   -1.6554 H   0   0   0   0   0   0   0   0   0   0   5
51   -2.3952   -0.3548   -0.2584 H   0   0   0   0   0   0   0   0   0   0   6
52    1.9564   -1.1818   -0.9301 H   0   0   0   0   0   0   0   0   0   0   7
53    1.7917    0.0072   -0.1585 P   0   0   0   0   0   0   0   0   0   0   8
54    2.8019    0.8979   -0.6131 H   0   0   0   0   0   0   0   0   0   0   9
55    1.8166   -0.2623    1.3448 O   0   0   0   0   0   0   0   0   0   0  10
56    0.4788    0.7372   -0.7743 O   0   0   0   0   0   0   0   0   0   0  11
57   -0.3727    0.1433   -0.7655 H   0   0   0   0   0   0   0   0   0   0  12
58
59     2 1 0 0 0 0
60     3 1 0 0 0 0
61     5 4 0 0 0 0
62     6 4 0 0 0 0
63     8 7 0 0 0 0
64     9 8 0 0 0 0
65    10 8 0 0 0 0
66    11 8 0 0 0 0
67    11 12 0 0 0 0
68
69 M  END
70 $$$$
71 iodoaceticacid-anion.sdf
72 COSMOTHERM      3D                                0
73
74 13 9 0 0 0 0 0 0 0 0 0 V2000
75    1.8087    5.3595    0.5575 O   0   0   0   0   0   0   0   0   0   0   1
76    1.0596    4.8864    0.0933 H   0   0   0   0   0   0   0   0   0   0   2
77    1.5142    5.4326    1.4814 H   0   0   0   0   0   0   0   0   0   0   3
78   -0.1800    4.0882   -0.8141 O   0   0   0   0   0   0   0   0   0   0   4
79   -0.2032    3.0839   -0.6383 H   0   0   0   0   0   0   0   0   0   0   5
80   -1.0636    4.4000   -0.5502 H   0   0   0   0   0   0   0   0   0   0   6
81    0.3701   -1.7677   -0.0153 I   0   0   0   0   0   0   0   0   0   0   7
82   -1.3919   -0.4782    0.3699 C   0   0   0   0   0   0   0   0   0   0   8
83   -1.2348    1.0202    0.0716 C   0   0   0   0   0   0   0   0   0   0   9
84   -0.1517    1.4791   -0.4018 O   0   0   0   0   0   0   0   0   0   0  10
85   -2.2834    1.6638    0.3498 O   0   0   0   0   0   0   0   0   0   0  11
86   -1.6196   -0.6394    1.4278 H   0   0   0   0   0   0   0   0   0   0  12
87   -2.1843   -0.9124   -0.2470 H   0   0   0   0   0   0   0   0   0   0  13
88
89     2 1 0 0 0 0
90     3 1 0 0 0 0
91     5 4 0 0 0 0
92     6 4 0 0 0 0
93     9 8 0 0 0 0
94    12 8 0 0 0 0
95    10 9 0 0 0 0
96    11 9 0 0 0 0
97     8 13 0 0 0 0
98
99 M  END
100 $$$$
101 iodoaceticacid.sdf
102 COSMOTHERM      3D                                0
103
104 14 10 0 0 0 0 0 0 0 0 0 V2000
105   -1.0963    4.4820    0.5820 O   0   0   0   0   0   0   0   0   0   0   1
106   -1.4573    4.5938    1.4795 H   0   0   0   0   0   0   0   0   0   0   2
107   -1.2847    3.5393    0.3371 H   0   0   0   0   0   0   0   0   0   0   3
108    1.4709    3.8353    0.4181 O   0   0   0   0   0   0   0   0   0   0   4
109    0.5640    4.2607    0.5417 H   0   0   0   0   0   0   0   0   0   0   5
110    1.9840    4.4438   -0.1440 H   0   0   0   0   0   0   0   0   0   0   6
111    0.0255   -1.7225    0.2037 I   0   0   0   0   0   0   0   0   0   0   7
112   -0.4033   -0.1853   -1.3108 C   0   0   0   0   0   0   0   0   0   0   8
113   -0.2067    1.1837   -0.7071 C   0   0   0   0   0   0   0   0   0   0   9
114    1.0532    1.5862   -0.7215 O   0   0   0   0   0   0   0   0   0   0  10
115   -1.1624    1.8360   -0.2675 O   0   0   0   0   0   0   0   0   0   0  11
```

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3      -1.4430   -0.3479   -1.5973 H   0   0   0   0   0   0   0   0   0   0   12
4      0.2917   -0.3886   -2.1283 H   0   0   0   0   0   0   0   0   0   0   13
5      1.1879    2.5292   -0.2689 H   0   0   0   0   0   0   0   0   0   0   14
6      2   1   0   0   0   0
7      3   1   0   0   0   0
8      5   4   0   0   0   0
9      6   4   0   0   0   0
10     9   8   0   0   0   0
11    12   8   0   0   0   0
12    13   8   0   0   0   0
13    10   9   0   0   0   0
14    11   9   0   0   0   0
15    10  14   0   0   0   0
16 M   END
17 $$$$
18 maleicacid-anion.sdf
19 COSMOTHERM      3D      0
20
21 17 15   0   0   0   0   0   0   0   0   0   0 V2000
22 -5.5320   -0.0595   -0.8906 O   0   0   0   0   0   0   0   0   0   0   1
23 -4.7551   0.2234   -0.3311 H   0   0   0   0   0   0   0   0   0   0   2
24 -5.2534   0.1277   -1.8032 H   0   0   0   0   0   0   0   0   0   0   3
25 -3.4573   0.6821    0.7408 O   0   0   0   0   0   0   0   0   0   0   4
26 -2.6348   0.1140    0.6042 H   0   0   0   0   0   0   0   0   0   0   5
27 -3.1614   1.5933    0.5692 H   0   0   0   0   0   0   0   0   0   0   6
28 2.2582   -1.0935   -0.0804 C   0   0   0   0   0   0   0   0   0   0   7
29 0.9450   -1.3508    0.1004 C   0   0   0   0   0   0   0   0   0   0   8
30 3.0017    0.2041   -0.1890 C   0   0   0   0   0   0   0   0   0   0   9
31 -0.2184   -0.4102    0.2481 C   0   0   0   0   0   0   0   0   0   0   10
32 2.3362    1.3438   -0.1299 O   0   0   0   0   0   0   0   0   0   0   11
33 4.2328    0.1752   -0.3354 O   0   0   0   0   0   0   0   0   0   0   12
34 -1.3492   -0.9444    0.4182 O   0   0   0   0   0   0   0   0   0   0   13
35 -0.0332    0.8643    0.1977 O   0   0   0   0   0   0   0   0   0   0   14
36 2.9280   -1.9529   -0.1603 H   0   0   0   0   0   0   0   0   0   0   15
37 0.6481   -2.4012    0.1516 H   0   0   0   0   0   0   0   0   0   0   16
38 1.2518    1.1574    0.0164 H   0   0   0   0   0   0   0   0   0   0   17
39
40 2   1   0   0   0   0
41 3   1   0   0   0   0
42 5   4   0   0   0   0
43 6   4   0   0   0   0
44 8   7   0   0   0   0
45 9   7   0   0   0   0
46 15  7   0   0   0   0
47 10  8   0   0   0   0
48 16  8   0   0   0   0
49 11  9   0   0   0   0
50 12  9   0   0   0   0
51 13 10   0   0   0   0
52 14 10   0   0   0   0
53 11 17   0   0   0   0
54 14 17   0   0   0   0
55 M   END
56 $$$$
57 maleicacid.sdf
58 COSMOTHERM      3D      0
59
60 18 17   0   0   0   0   0   0   0   0   0   0 V2000
61 -1.4918   -4.3759    0.7998 O   0   0   0   0   0   0   0   0   0   0   1
62 -1.8234   -5.2489    0.5205 H   0   0   0   0   0   0   0   0   0   0   2
63 -2.2776   -3.7998    0.7798 H   0   0   0   0   0   0   0   0   0   0   3
64 0.5719   -3.5288   -0.6629 O   0   0   0   0   0   0   0   0   0   0   4
65 0.3344   -3.5624   -1.6071 H   0   0   0   0   0   0   0   0   0   0   5
66 -0.2442   -3.8398   -0.1573 H   0   0   0   0   0   0   0   0   0   0   6
67 1.3753    0.9963    0.4119 C   0   0   0   0   0   0   0   0   0   0   7
68 0.8769    2.2499    0.4397 C   0   0   0   0   0   0   0   0   0   0   8
69 0.7268   -0.2541   -0.0598 C   0   0   0   0   0   0   0   0   0   0   9
70 -0.4506    2.8129    0.0283 C   0   0   0   0   0   0   0   0   0   0   10
71 -0.4307   -0.3175   -0.5286 O   0   0   0   0   0   0   0   0   0   0   11
72 1.5047   -1.3060    0.0666 O   0   0   0   0   0   0   0   0   0   0   12
73 -0.6575    4.0193    0.1717 O   0   0   0   0   0   0   0   0   0   0   13
74 -1.3881    2.0164   -0.4841 O   0   0   0   0   0   0   0   0   0   0   14
75 2.3926    0.8530    0.7809 H   0   0   0   0   0   0   0   0   0   0   15
76 1.5323    3.0298    0.8318 H   0   0   0   0   0   0   0   0   0   0   16
77 1.0346   -2.2034   -0.2698 H   0   0   0   0   0   0   0   0   0   0   17
78 -1.0543    1.0349   -0.5322 H   0   0   0   0   0   0   0   0   0   0   18
79
80 2   1   0   0   0   0
81 3   1   0   0   0   0
82 5   4   0   0   0   0
83 6   4   0   0   0   0
84 17  4   0   0   0   0
85 8   7   0   0   0   0
86 9   7   0   0   0   0
87 15  7   0   0   0   0
88 10  8   0   0   0   0
89 16  8   0   0   0   0
90 11  9   0   0   0   0
91 12  9   0   0   0   0
92 13 10   0   0   0   0
93 14 10   0   0   0   0
94 17 12   0   0   0   0
95 11 18   0   0   0   0
96 14 18   0   0   0   0
97 M   END
98 $$$$
99 mandelicacid-anion.sdf
100 COSMOTHERM      3D      0
101
102 24 22   0   0   0   0   0   0   0   0   0   0 V2000
103 -2.5534   -4.5896   -0.3173 O   0   0   0   0   0   0   0   0   0   0   1
104 -1.5905   -4.3335   -0.2303 H   0   0   0   0   0   0   0   0   0   0   2
105 -2.9581   -3.8522   -0.8051 H   0   0   0   0   0   0   0   0   0   0   3
106 0.0816   -3.9628    0.0195 O   0   0   0   0   0   0   0   0   0   0   4
107 0.2152   -2.9851    0.2730 H   0   0   0   0   0   0   0   0   0   0   5
108 0.5992   -4.0778   -0.7967 H   0   0   0   0   0   0   0   0   0   0   6
109 -2.1092    2.9804   -0.3528 C   0   0   0   0   0   0   0   0   0   0   7
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0.0122 -1.6522 0.2832 C 0 0 0 0 0 0 0 0 0 0 0 7
-0.0025 -0.4962 -0.5195 O 0 0 0 0 0 0 0 0 0 0 0 8
-0.6527 -1.5679 1.1723 H 0 0 0 0 0 0 0 0 0 0 0 9
-0.3202 -2.5594 -0.2678 H 0 0 0 0 0 0 0 0 0 0 0 10
1.0286 -1.8789 0.6725 H 0 0 0 0 0 0 0 0 0 0 0 11
2 1 0 0 0 0
3 1 0 0 0 0
8 2 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
8 5 0 0 0 0
8 7 0 0 0 0
9 7 0 0 0 0
10 7 0 0 0 0
7 11 0 0 0 0
M END
$$$$
methanol.sdf
COSMOtherm 3D 0
12 9 0 0 0 0 0 0 0 0 0 V2000
-2.6446 0.7126 0.1548 O 0 0 0 0 0 0 0 0 0 0 0 1
-3.5414 0.3379 0.2246 H 0 0 0 0 0 0 0 0 0 0 0 2
-2.7093 1.3537 -0.5761 H 0 0 0 0 0 0 0 0 0 0 0 3
-0.7133 -1.1887 -0.2139 O 0 0 0 0 0 0 0 0 0 0 0 4
-0.7567 -1.4843 -1.1401 H 0 0 0 0 0 0 0 0 0 0 0 5
-1.4388 -0.5086 -0.1233 H 0 0 0 0 0 0 0 0 0 0 0 6
2.1603 0.8104 -0.3368 C 0 0 0 0 0 0 0 0 0 0 0 7
1.7820 -0.2862 0.5048 O 0 0 0 0 0 0 0 0 0 0 0 8
3.1612 1.1405 -0.0265 H 0 0 0 0 0 0 0 0 0 0 0 9
1.4710 1.6681 -0.2398 H 0 0 0 0 0 0 0 0 0 0 0 10
2.2078 0.5220 -1.4019 H 0 0 0 0 0 0 0 0 0 0 0 11
0.8765 -0.5868 0.2206 H 0 0 0 0 0 0 0 0 0 0 0 12
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
8 7 0 0 0 0
9 7 0 0 0 0
10 7 0 0 0 0
11 7 0 0 0 0
8 12 0 0 0 0
M END
$$$$
methylthiouracil-anion.sdf
COSMOtherm 3D 0
20 18 0 0 0 0 0 0 0 0 0 V2000
-4.5520 0.8673 1.0900 O 0 0 0 0 0 0 0 0 0 0 0 1
-3.9097 0.4665 0.4342 H 0 0 0 0 0 0 0 0 0 0 0 2
-4.0861 0.8260 1.9424 H 0 0 0 0 0 0 0 0 0 0 0 3
-2.8641 -0.1917 -0.7668 O 0 0 0 0 0 0 0 0 0 0 0 4
-1.9148 0.1464 -0.6299 H 0 0 0 0 0 0 0 0 0 0 0 5
-2.7134 -1.1490 -0.6125 H 0 0 0 0 0 0 0 0 0 0 0 6
0.3883 -0.8643 -0.0902 C 0 0 0 0 0 0 0 0 0 0 0 7
1.7378 -0.8684 0.2021 N 0 0 0 0 0 0 0 0 0 0 0 8
2.5625 0.2683 0.2758 C 0 0 0 0 0 0 0 0 0 0 0 9
1.8614 1.4908 0.0146 C 0 0 0 0 0 0 0 0 0 0 0 10
0.5108 1.4655 -0.2763 C 0 0 0 0 0 0 0 0 0 0 0 11
-0.2210 0.3085 -0.3309 N 0 0 0 0 0 0 0 0 0 0 0 12
3.7756 0.1361 0.5482 O 0 0 0 0 0 0 0 0 0 0 0 13
-0.4468 -2.3825 -0.1304 S 0 0 0 0 0 0 0 0 0 0 0 14
2.4183 2.4258 0.0498 H 0 0 0 0 0 0 0 0 0 0 0 15
2.1795 -1.7717 0.3799 H 0 0 0 0 0 0 0 0 0 0 0 16
-0.2583 2.7261 -0.5581 C 0 0 0 0 0 0 0 0 0 0 0 17
-1.0923 2.8298 0.1525 H 0 0 0 0 0 0 0 0 0 0 0 18
0.3812 3.6137 -0.4847 H 0 0 0 0 0 0 0 0 0 0 0 19
-0.6962 2.6869 -1.5671 H 0 0 0 0 0 0 0 0 0 0 0 20
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
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12 7 0 0 0 0
14 7 0 0 0 0
9 8 0 0 0 0
16 8 0 0 0 0
10 9 0 0 0 0
13 9 0 0 0 0
11 10 0 0 0 0
15 10 0 0 0 0
12 11 0 0 0 0
17 11 0 0 0 0
18 17 0 0 0 0
19 17 0 0 0 0
17 20 0 0 0 0
M END
$$$$
methylthiouracil.sdf
COSMOtherm 3D 0
21 19 0 0 0 0 0 0 0 0 0 V2000
-4.6676 1.0172 -0.7490 O 0 0 0 0 0 0 0 0 0 0 0 1
-4.3496 1.9383 -0.7447 H 0 0 0 0 0 0 0 0 0 0 0 2
-5.4383 1.0268 -0.1526 H 0 0 0 0 0 0 0 0 0 0 0 3
-2.7913 -0.8269 0.0031 O 0 0 0 0 0 0 0 0 0 0 0 4
-3.4683 -0.1320 -0.2361 H 0 0 0 0 0 0 0 0 0 0 0 5
-2.5923 -0.6839 0.9554 H 0 0 0 0 0 0 0 0 0 0 0 6
0.4055 -0.0810 0.9003 C 0 0 0 0 0 0 0 0 0 0 0 7
1.7442 0.1910 0.9331 N 0 0 0 0 0 0 0 0 0 0 0 8
2.6153 0.2780 -0.1796 C 0 0 0 0 0 0 0 0 0 0 0 9
1.9682 0.0467 -1.4460 C 0 0 0 0 0 0 0 0 0 0 0 10
0.6285 -0.2243 -1.5077 C 0 0 0 0 0 0 0 0 0 0 0 11
-0.1153 -0.2796 -0.3459 N 0 0 0 0 0 0 0 0 0 0 0 12
3.8139 0.5332 0.0055 O 0 0 0 0 0 0 0 0 0 0 0 13
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URL: <http://mc.manuscriptcentral.com/tandf/tmph>

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5 4 0 0 0 0
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19 9 0 0 0 0
20 9 0 0 0 0
11 10 0 0 0 0
21 10 0 0 0 0
22 10 0 0 0 0
12 11 0 0 0 0
13 11 0 0 0 0
13 23 0 0 0 0
M END
$$$$
nitroaceticacid-anion.sdf
COSMOtherm 3D 0
15 12 0 0 0 0 0 0 0 0 0 V2000
-4.4766 -0.3355 1.4496 O 0 0 0 0 0 0 0 0 0 0 1
-3.9128 -0.0009 0.6957 H 0 0 0 0 0 0 0 0 0 0 2
-4.5251 -1.2962 1.3078 H 0 0 0 0 0 0 0 0 0 0 3
-2.9446 0.7001 -0.5656 O 0 0 0 0 0 0 0 0 0 0 4
-1.9593 0.5091 -0.4213 H 0 0 0 0 0 0 0 0 0 0 5
-3.1490 0.3151 -1.4358 H 0 0 0 0 0 0 0 0 0 0 6
0.3333 -0.1523 -1.0344 C 0 0 0 0 0 0 0 0 0 0 7
1.8656 -0.3766 -0.7708 C 0 0 0 0 0 0 0 0 0 0 8
-0.3638 0.2897 -0.0745 O 0 0 0 0 0 0 0 0 0 0 9
-0.0214 -0.4493 -2.1964 O 0 0 0 0 0 0 0 0 0 0 10
2.2533 -0.0038 0.6191 N 0 0 0 0 0 0 0 0 0 0 11
2.5820 1.1722 0.8383 O 0 0 0 0 0 0 0 0 0 0 12
2.1674 -0.8725 1.5012 O 0 0 0 0 0 0 0 0 0 0 13
2.1060 -1.4357 -0.9050 H 0 0 0 0 0 0 0 0 0 0 14
2.4482 0.2507 -1.4524 H 0 0 0 0 0 0 0 0 0 0 15
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
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8 7 0 0 0 0
9 7 0 0 0 0
10 7 0 0 0 0
11 8 0 0 0 0
14 8 0 0 0 0
12 11 0 0 0 0
13 11 0 0 0 0
8 15 0 0 0 0
M END
$$$$
nitroaceticacid.sdf
COSMOtherm 3D 0
16 14 0 0 0 0 0 0 0 0 0 V2000
1.4238 4.2127 0.1637 O 0 0 0 0 0 0 0 0 0 0 1
1.3770 5.1668 0.3582 H 0 0 0 0 0 0 0 0 0 0 2
2.0406 4.1481 -0.5881 H 0 0 0 0 0 0 0 0 0 0 3
-0.9991 3.1659 -0.2609 O 0 0 0 0 0 0 0 0 0 0 4
-1.2353 3.2805 -1.1991 H 0 0 0 0 0 0 0 0 0 0 5
-0.0805 3.5667 -0.1534 H 0 0 0 0 0 0 0 0 0 0 6
-0.4398 -0.1134 0.0394 C 0 0 0 0 0 0 0 0 0 0 7
-0.7106 -1.4870 0.6707 C 0 0 0 0 0 0 0 0 0 0 8
-1.2509 0.7877 0.5653 O 0 0 0 0 0 0 0 0 0 0 9
0.4095 0.0799 -0.8195 O 0 0 0 0 0 0 0 0 0 0 10
0.2205 -2.5089 0.0823 N 0 0 0 0 0 0 0 0 0 0 11
1.3102 -2.6783 0.6396 O 0 0 0 0 0 0 0 0 0 0 12
-0.1441 -3.0930 -0.9430 O 0 0 0 0 0 0 0 0 0 0 13
-0.5307 -1.4545 1.7500 H 0 0 0 0 0 0 0 0 0 0 14
-1.7359 -1.8095 0.4585 H 0 0 0 0 0 0 0 0 0 0 15
-1.0853 1.7536 0.1614 H 0 0 0 0 0 0 0 0 0 0 16
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
8 7 0 0 0 0
9 7 0 0 0 0
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11 8 0 0 0 0
14 8 0 0 0 0
15 8 0 0 0 0
12 11 0 0 0 0
13 11 0 0 0 0
4 16 0 0 0 0
9 16 0 0 0 0
M END
$$$$
nitromethane-anion.sdf
COSMOtherm 3D 0
12 9 0 0 0 0 0 0 0 0 0 V2000
-3.6863 0.4711 -0.5248 O 0 0 0 0 0 0 0 0 0 0 1
-2.8901 0.0898 -0.0514 H 0 0 0 0 0 0 0 0 0 0 2
-3.5125 1.4271 -0.5613 H 0 0 0 0 0 0 0 0 0 0 3
-1.5699 -0.6739 0.7442 O 0 0 0 0 0 0 0 0 0 0 4
-0.7103 -0.6086 0.1948 H 0 0 0 0 0 0 0 0 0 0 5
-1.3386 -0.2084 1.5677 H 0 0 0 0 0 0 0 0 0 0 6
2.7580 0.2315 -0.6599 C 0 0 0 0 0 0 0 0 0 0 7
1.5786 0.0543 -0.0799 N 0 0 0 0 0 0 0 0 0 0 8
0.6056 -0.5628 -0.7395 O 0 0 0 0 0 0 0 0 0 0 9
1.3259 0.4623 1.1241 O 0 0 0 0 0 0 0 0 0 0 10
3.5305 0.7383 -0.0907 H 0 0 0 0 0 0 0 0 0 0 11
2.8923 -0.1364 -1.6715 H 0 0 0 0 0 0 0 0 0 0 12
```


[illegible]

-4.7815	-2.7214		-1.4584	H	0	0	0	0	0	0	0	0	0	0	0	0	39
-2.5948	-2.6214		-0.3823	H	0	0	0	0	0	0	0	0	0	0	0	0	40
-3.4860	0.0479		-4.5012	H	0	0	0	0	0	0	0	0	0	0	0	0	41
-1.2201	0.9158		-4.4755	H	0	0	0	0	0	0	0	0	0	0	0	0	42
0.8262	-2.6294		-0.2874	H	0	0	0	0	0	0	0	0	0	0	0	0	43
-0.8293	-2.6295		0.2831	H	0	0	0	0	0	0	0	0	0	0	0	0	44
1.2198	0.9107		4.4747	H	0	0	0	0	0	0	0	0	0	0	0	0	45
4.7783	-2.7258		1.4536	H	0	0	0	0	0	0	0	0	0	0	0	0	46
5.2649	-1.4000		3.5199	H	0	0	0	0	0	0	0	0	0	0	0	0	47
3.4842	0.0393		4.5008	H	0	0	0	0	0	0	0	0	0	0	0	0	48
2.5915	-2.6233		0.3777	H	0	0	0	0	0	0	0	0	0	0	0	0	49
-1.7693	2.4543		5.0883	H	0	0	0	0	0	0	0	0	0	0	0	0	50
1.7732	2.4538		-5.0885	H	0	0	0	0	0	0	0	0	0	0	0	0	51
2	1	0	0	0	0												
3	1	0	0	0	0												
5	4	0	0	0	0												
6	4	0	0	0	0												
8	7	0	0	0	0												
12	7	0	0	0	0												
38	7	0	0	0	0												
9	8	0	0	0	0												
39	8	0	0	0	0												
10	9	0	0	0	0												
40	9	0	0	0	0												
11	10	0	0	0	0												
13	10	0	0	0	0												
12	11	0	0	0	0												
16	11	0	0	0	0												
41	12	0	0	0	0												
14	13	0	0	0	0												
17	13	0	0	0	0												
15	14	0	0	0	0												
29	14	0	0	0	0												
16	15	0	0	0	0												
31	15	0	0	0	0												
42	16	0	0	0	0												
18	17	0	0	0	0												
43	17	0	0	0	0												
44	17	0	0	0	0												
19	18	0	0	0	0												
23	18	0	0	0	0												

[illegible]

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3      -0.4108      1.4267      6.7820 H      0      0      0      0      0      0      0      0      0      3
4      1.4251      0.1797      4.4472 O      0      0      0      0      0      0      0      0      0      4
5      0.7447      0.7091      4.9527 H      0      0      0      0      0      0      0      0      0      5
6      2.2444      0.7033      4.4958 H      0      0      0      0      0      0      0      0      0      6
7      0.7459     -0.4230      1.8472 N      0      0      0      0      0      0      0      0      0      7
8      0.8466     -1.7270      1.3234 C      0      0      0      0      0      0      0      0      0      8
9      0.3091      0.4817      0.9183 C      0      0      0      0      0      0      0      0      0      9
10     0.0436     -0.3164     -0.4052 C      0      0      0      0      0      0      0      0      0      10
11     0.3673     -1.6764      0.0448 N      0      0      0      0      0      0      0      0      0      11
12     0.9940      0.1022     -1.5375 C      0      0      0      0      0      0      0      0      0      12
13    -1.4368     -0.1492     -0.7740 C      0      0      0      0      0      0      0      0      0      13
14     1.2797     -2.7078      1.9279 O      0      0      0      0      0      0      0      0      0      14
15     0.1417      1.6839      1.0831 O      0      0      0      0      0      0      0      0      0      15
16    -3.7255     -0.9677     -0.8224 C      0      0      0      0      0      0      0      0      0      16
17    -2.3731     -1.1585     -0.5124 C      0      0      0      0      0      0      0      0      0      17
18    -1.8740      1.0606     -1.3395 C      0      0      0      0      0      0      0      0      0      18
19    -3.2250      1.2526     -1.6402 C      0      0      0      0      0      0      0      0      0      19
20    -4.1560      0.2377     -1.3850 C      0      0      0      0      0      0      0      0      0      20
21     2.1591      0.8452     -1.2961 C      0      0      0      0      0      0      0      0      0      21
22     3.0446      1.1345     -2.3409 C      0      0      0      0      0      0      0      0      0      22
23     2.7802      0.6793     -3.6363 C      0      0      0      0      0      0      0      0      0      23
24     1.6215     -0.0664     -3.8836 C      0      0      0      0      0      0      0      0      0      24
25     0.7331     -0.3487     -2.8425 C      0      0      0      0      0      0      0      0      0      25
26     1.0022     -0.1797      2.8426 H      0      0      0      0      0      0      0      0      0      26
27     0.5318     -2.4441     -0.6010 H      0      0      0      0      0      0      0      0      0      27
28    -4.4422     -1.7659     -0.6209 H      0      0      0      0      0      0      0      0      0      28
29    -2.0450     -2.0992     -0.0689 H      0      0      0      0      0      0      0      0      0      29
30    -1.1552      1.8537     -1.5483 H      0      0      0      0      0      0      0      0      0      30
31    -3.5514      2.1970     -2.0798 H      0      0      0      0      0      0      0      0      0      31
32    -5.2102      0.3864     -1.6260 H      0      0      0      0      0      0      0      0      0      32
33     2.3851      1.2129     -0.2943 H      0      0      0      0      0      0      0      0      0      33
34     3.9435      1.7194     -2.1381 H      0      0      0      0      0      0      0      0      0      34
35     3.4715      0.9061     -4.4499 H      0      0      0      0      0      0      0      0      0      35
36     1.4047     -0.4261     -4.8911 H      0      0      0      0      0      0      0      0      0      36
37    -0.1733     -0.9215     -3.0486 H      0      0      0      0      0      0      0      0      0      37
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2 1 0 0 0 0
3 1 0 0 0 0
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11 8 0 0 0 0
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12 10 0 0 0 0
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27 11 0 0 0 0
21 12 0 0 0 0
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17 13 0 0 0 0
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19 18 0 0 0 0
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31 19 0 0 0 0
32 20 0 0 0 0
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23 22 0 0 0 0
34 22 0 0 0 0
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35 23 0 0 0 0
25 24 0 0 0 0
36 24 0 0 0 0
25 37 0 0 0 0

M END
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phosphoricacid-anion.sdf
COSMOtherm 3D 0

13 10 0 0 0 0 0 0 0 0 0 V2000
-1.2640 0.0167 2.6381 O 0 0 0 0 0 0 0 0 0 0 1
-1.6098 -0.8197 2.9971 H 0 0 0 0 0 0 0 0 0 0 2
-1.3442 -0.0644 1.6314 H 0 0 0 0 0 0 0 0 0 0 3
1.3956 -0.0095 2.3952 O 0 0 0 0 0 0 0 0 0 0 4
0.4190 0.0339 2.6438 H 0 0 0 0 0 0 0 0 0 0 5
1.7632 0.8657 2.6113 H 0 0 0 0 0 0 0 0 0 0 6
-0.0963 -0.0763 -0.9626 P 0 0 0 0 0 0 0 0 0 0 7
0.2371 1.5324 -1.3060 O 0 0 0 0 0 0 0 0 0 0 8
-0.1665 -0.7891 -2.3097 O 0 0 0 0 0 0 0 0 0 0 9
1.2595 -0.6099 -0.1930 O 0 0 0 0 0 0 0 0 0 0 10
-1.3076 -0.1054 0.0020 O 0 0 0 0 0 0 0 0 0 0 11
-0.0244 2.0957 -0.5529 H 0 0 0 0 0 0 0 0 0 0 12
1.3101 -0.3242 0.7807 H 0 0 0 0 0 0 0 0 0 0 13

2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
8 7 0 0 0 0
9 7 0 0 0 0
10 7 0 0 0 0
11 7 0 0 0 0
12 8 0 0 0 0
10 13 0 0 0 0

M END
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phosphoricacid.sdf
COSMOtherm 3D 0

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6 4 0 0 0 0
8 7 0 0 0 0
12 7 0 0 0 0
19 7 0 0 0 0
9 8 0 0 0 0
20 8 0 0 0 0
10 9 0 0 0 0
21 9 0 0 0 0
11 10 0 0 0 0
14 10 0 0 0 0
12 11 0 0 0 0
13 11 0 0 0 0
15 13 0 0 0 0
17 13 0 0 0 0
15 14 0 0 0 0
16 14 0 0 0 0
18 15 0 0 0 0
12 22 0 0 0 0
M END
$$$$
salicylicacid-anion.sdf
COSMOTHERM 3D 0
21 20 0 0 0 0 0 0 0 0 0 V2000
-0.8119 5.5998 -0.9599 O 0 0 0 0 0 0 0 0 0 0 1
-0.2985 4.9326 -0.4202 H 0 0 0 0 0 0 0 0 0 0 2
-1.7306 5.2828 -0.9278 H 0 0 0 0 0 0 0 0 0 0 3
0.6904 3.8210 0.4661 O 0 0 0 0 0 0 0 0 0 0 4
0.5809 2.8706 0.1214 H 0 0 0 0 0 0 0 0 0 0 5
0.4244 3.7717 1.4011 H 0 0 0 0 0 0 0 0 0 0 6
0.0897 -2.6052 -1.9621 C 0 0 0 0 0 0 0 0 0 0 7
-0.1569 -3.6236 -1.0255 C 0 0 0 0 0 0 0 0 0 0 8
-0.2857 -3.3278 0.3306 C 0 0 0 0 0 0 0 0 0 0 9
-0.1692 -1.9976 0.7778 C 0 0 0 0 0 0 0 0 0 0 10
0.0822 -0.9568 -0.1607 C 0 0 0 0 0 0 0 0 0 0 11
0.2070 -1.2873 -1.5214 C 0 0 0 0 0 0 0 0 0 0 12
-0.2978 -1.7248 2.0977 O 0 0 0 0 0 0 0 0 0 0 13
0.2110 0.4647 0.3106 C 0 0 0 0 0 0 0 0 0 0 14
0.4466 1.3802 -0.5350 O 0 0 0 0 0 0 0 0 0 0 15
0.0731 0.6767 1.5760 O 0 0 0 0 0 0 0 0 0 0 16
0.1885 -2.8437 -3.0221 H 0 0 0 0 0 0 0 0 0 0 17
-0.2499 -4.6596 -1.3580 H 0 0 0 0 0 0 0 0 0 0 18
-0.4777 -4.1144 1.0630 H 0 0 0 0 0 0 0 0 0 0 19
0.3995 -0.4784 -2.2287 H 0 0 0 0 0 0 0 0 0 0 20
-0.1696 -0.6841 2.1285 H 0 0 0 0 0 0 0 0 0 0 21
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
8 7 0 0 0 0
12 7 0 0 0 0
17 7 0 0 0 0
9 8 0 0 0 0
18 8 0 0 0 0
10 9 0 0 0 0
19 9 0 0 0 0
11 10 0 0 0 0
13 10 0 0 0 0
12 11 0 0 0 0
14 11 0 0 0 0
20 12 0 0 0 0
15 14 0 0 0 0
16 14 0 0 0 0
13 21 0 0 0 0
16 21 0 0 0 0
M END
$$$$
salicylicacid.sdf
COSMOTHERM 3D 0
22 20 0 0 0 0 0 0 0 0 0 V2000
0.7930 5.0128 -0.7948 O 0 0 0 0 0 0 0 0 0 0 1
1.6519 4.9969 -0.3347 H 0 0 0 0 0 0 0 0 0 0 2
0.5950 5.9607 -0.9050 H 0 0 0 0 0 0 0 0 0 0 3
-1.1974 3.7042 0.4487 O 0 0 0 0 0 0 0 0 0 0 4
-0.4271 4.1991 0.0333 H 0 0 0 0 0 0 0 0 0 0 5
-1.2049 3.9644 1.3871 H 0 0 0 0 0 0 0 0 0 0 6
-1.5297 -2.9927 -0.3039 C 0 0 0 0 0 0 0 0 0 0 7
-0.3457 -3.7511 -0.2744 C 0 0 0 0 0 0 0 0 0 0 8
0.8911 -3.1380 -0.0948 C 0 0 0 0 0 0 0 0 0 0 9
0.9697 -1.7428 0.0618 C 0 0 0 0 0 0 0 0 0 0 10
-0.2221 -0.9633 0.0334 C 0 0 0 0 0 0 0 0 0 0 11
-1.4605 -1.6122 -0.1511 C 0 0 0 0 0 0 0 0 0 0 12
2.1881 -1.1773 0.2360 O 0 0 0 0 0 0 0 0 0 0 13
-0.1246 0.5002 0.1993 C 0 0 0 0 0 0 0 0 0 0 14
0.9778 1.0726 0.3702 O 0 0 0 0 0 0 0 0 0 0 15
-1.2710 1.1635 0.1554 O 0 0 0 0 0 0 0 0 0 0 16
-2.4936 -3.4825 -0.4453 H 0 0 0 0 0 0 0 0 0 0 17
-0.3913 -4.8353 -0.3936 H 0 0 0 0 0 0 0 0 0 0 18
1.8127 -3.7213 -0.0710 H 0 0 0 0 0 0 0 0 0 0 19
-2.3684 -1.0089 -0.1721 H 0 0 0 0 0 0 0 0 0 0 20
2.0060 -0.1842 0.3287 H 0 0 0 0 0 0 0 0 0 0 21
-1.1300 2.1909 0.2870 H 0 0 0 0 0 0 0 0 0 0 22
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
8 7 0 0 0 0
12 7 0 0 0 0
17 7 0 0 0 0
9 8 0 0 0 0
18 8 0 0 0 0
10 9 0 0 0 0
19 9 0 0 0 0
11 10 0 0 0 0
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13 10 0 0 0 0
12 11 0 0 0 0
14 11 0 0 0 0
20 12 0 0 0 0
21 13 0 0 0 0
15 14 0 0 0 0
16 14 0 0 0 0
16 22 0 0 0 0
M END
$$$$
succinimide-anion.sdf
COSMOtherm 3D 0

17 15 0 0 0 0 0 0 0 0 0 V2000
-3.9456 -1.0950 0.0939 O 0 0 0 0 0 0 0 0 0 0 1
-3.3483 -0.2914 0.0405 H 0 0 0 0 0 0 0 0 0 0 2
-4.6745 -0.8156 0.6736 H 0 0 0 0 0 0 0 0 0 0 3
-2.3398 1.0978 -0.0551 O 0 0 0 0 0 0 0 0 0 0 4
-1.3455 0.8180 -0.0171 H 0 0 0 0 0 0 0 0 0 0 5
-2.4479 1.5024 -0.9338 H 0 0 0 0 0 0 0 0 0 0 6
2.3285 -0.5102 -0.7983 C 0 0 0 0 0 0 0 0 0 0 7
0.9302 0.0380 -1.1215 C 0 0 0 0 0 0 0 0 0 0 8
2.3753 -0.4880 0.7300 C 0 0 0 0 0 0 0 0 0 0 9
1.0020 0.0801 1.1227 C 0 0 0 0 0 0 0 0 0 0 10
0.2358 0.3497 0.0187 N 0 0 0 0 0 0 0 0 0 0 11
0.6431 0.2659 2.3004 O 0 0 0 0 0 0 0 0 0 0 12
0.4938 0.1804 -2.2789 O 0 0 0 0 0 0 0 0 0 0 13
3.0871 0.1287 -1.2730 H 0 0 0 0 0 0 0 0 0 0 14
2.4327 -1.5161 -1.2302 H 0 0 0 0 0 0 0 0 0 0 15
3.1664 0.1559 1.1404 H 0 0 0 0 0 0 0 0 0 0 16
2.4978 -1.4829 1.1824 H 0 0 0 0 0 0 0 0 0 0 17
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
8 7 0 0 0 0
9 7 0 0 0 0
14 7 0 0 0 0
15 7 0 0 0 0
11 8 0 0 0 0
13 8 0 0 0 0
10 9 0 0 0 0
16 9 0 0 0 0
11 10 0 0 0 0
12 10 0 0 0 0
9 17 0 0 0 0
M END
$$$$
succinimide.sdf
COSMOtherm 3D 0

18 16 0 0 0 0 0 0 0 0 0 V2000
-4.1741 -0.1825 0.8499 O 0 0 0 0 0 0 0 0 0 0 1
-4.7265 -0.9148 0.5214 H 0 0 0 0 0 0 0 0 0 0 2
-4.8126 0.5193 1.0728 H 0 0 0 0 0 0 0 0 0 0 3
-2.3001 0.7078 -0.9312 O 0 0 0 0 0 0 0 0 0 0 4
-3.0025 0.3545 -0.3150 H 0 0 0 0 0 0 0 0 0 0 5
-2.5349 0.3607 -1.8098 H 0 0 0 0 0 0 0 0 0 0 6
2.5824 0.4000 0.4111 C 0 0 0 0 0 0 0 0 0 0 7
1.2626 1.0820 0.0757 C 0 0 0 0 0 0 0 0 0 0 8
2.2971 -1.1032 0.2838 C 0 0 0 0 0 0 0 0 0 0 9
0.8309 -1.1938 -0.1183 C 0 0 0 0 0 0 0 0 0 0 10
0.3273 0.0969 -0.2111 N 0 0 0 0 0 0 0 0 0 0 11
0.1806 -2.2131 -0.3320 O 0 0 0 0 0 0 0 0 0 0 12
1.0341 2.2885 0.0539 O 0 0 0 0 0 0 0 0 0 0 13
2.8900 0.7016 1.4216 H 0 0 0 0 0 0 0 0 0 0 14
3.3527 0.7577 -0.2859 H 0 0 0 0 0 0 0 0 0 0 15
2.4412 -1.6551 1.2227 H 0 0 0 0 0 0 0 0 0 0 16
2.9060 -1.5994 -0.4843 H 0 0 0 0 0 0 0 0 0 0 17
-0.6689 0.3067 -0.4785 H 0 0 0 0 0 0 0 0 0 0 18
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
8 7 0 0 0 0
9 7 0 0 0 0
14 7 0 0 0 0
15 7 0 0 0 0
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10 9 0 0 0 0
16 9 0 0 0 0
17 9 0 0 0 0
11 10 0 0 0 0
12 10 0 0 0 0
11 18 0 0 0 0
M END
$$$$
sulfurousacid-anion.sdf
COSMOtherm 3D 0

11 8 0 0 0 0 0 0 0 0 0 V2000
-3.7682 -0.7281 0.1816 O 0 0 0 0 0 0 0 0 0 0 1
-3.0049 -0.1079 0.0388 H 0 0 0 0 0 0 0 0 0 0 2
-4.3877 -0.5182 -0.5380 H 0 0 0 0 0 0 0 0 0 0 3
-1.6171 0.9921 -0.0982 O 0 0 0 0 0 0 0 0 0 0 4
0.9773 0.9234 1.2004 O 0 0 0 0 0 0 0 0 0 0 5
1.5855 -0.0960 -0.1274 S 0 0 0 0 0 0 0 0 0 0 6
1.2205 -1.5194 0.3107 O 0 0 0 0 0 0 0 0 0 0 7
0.6494 0.3356 -1.3042 O 0 0 0 0 0 0 0 0 0 0 8
0.0010 1.0059 1.0385 H 0 0 0 0 0 0 0 0 0 0 9
-1.8788 1.8924 -0.3630 H 0 0 0 0 0 0 0 0 0 0 10
-0.8790 0.7246 -0.7334 H 0 0 0 0 0 0 0 0 0 0 11
2 1 0 0 0 0
3 1 0 0 0 0
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10 4 0 0 0 0
6 5 0 0 0 0
9 5 0 0 0 0
7 6 0 0 0 0
8 6 0 0 0 0
4 11 0 0 0 0
M END
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sulfurousacid.sdf
COSMOtherm 3D 0
12 9 0 0 0 0 0 0 0 0 0 V2000
-3.8880 0.2199 -0.0067 O 0 0 0 0 0 0 0 0 0 0 0 1
-4.3854 0.0311 0.8100 H 0 0 0 0 0 0 0 0 0 0 0 2
-4.4501 -0.1287 -0.7225 H 0 0 0 0 0 0 0 0 0 0 0 3
-1.4335 -0.7797 0.0002 O 0 0 0 0 0 0 0 0 0 0 0 4
-1.4810 -1.7529 -0.0031 H 0 0 0 0 0 0 0 0 0 0 0 5
-2.3883 -0.4435 0.0008 H 0 0 0 0 0 0 0 0 0 0 0 6
1.5752 0.3524 0.0007 S 0 0 0 0 0 0 0 0 0 0 0 7
0.5006 0.5595 -1.2814 O 0 0 0 0 0 0 0 0 0 0 0 8
0.5097 0.5394 1.2932 O 0 0 0 0 0 0 0 0 0 0 0 9
1.9930 -1.0982 -0.0125 O 0 0 0 0 0 0 0 0 0 0 0 10
-0.3066 -0.0138 -1.0755 H 0 0 0 0 0 0 0 0 0 0 0 11
-0.3001 -0.0280 1.0835 H 0 0 0 0 0 0 0 0 0 0 0 12
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
8 7 0 0 0 0
9 7 0 0 0 0
10 7 0 0 0 0
11 8 0 0 0 0
9 12 0 0 0 0
M END
$$$$
tert-butanol-anion.sdf
COSMOtherm 3D 0
20 18 0 0 0 0 0 0 0 0 0 V2000
-0.8522 0.0089 3.2856 O 0 0 0 0 0 0 0 0 0 0 0 1
0.0309 -0.0113 2.6918 H 0 0 0 0 0 0 0 0 0 0 0 2
-1.5773 0.0383 2.6392 H 0 0 0 0 0 0 0 0 0 0 0 3
1.2693 -0.0961 1.8939 O 0 0 0 0 0 0 0 0 0 0 0 4
0.7504 -0.5734 0.5361 H 0 0 0 0 0 0 0 0 0 0 0 5
1.5895 0.8131 1.7637 H 0 0 0 0 0 0 0 0 0 0 0 6
-0.0977 0.0182 -1.2269 C 0 0 0 0 0 0 0 0 0 0 0 7
1.0433 0.9770 -1.6194 C 0 0 0 0 0 0 0 0 0 0 0 8
-1.2273 0.7991 -0.5286 C 0 0 0 0 0 0 0 0 0 0 0 9
-0.6392 -0.6933 -2.4730 C 0 0 0 0 0 0 0 0 0 0 0 10
0.6951 1.7604 -2.3107 H 0 0 0 0 0 0 0 0 0 0 0 11
-2.0469 0.1163 -0.2578 H 0 0 0 0 0 0 0 0 0 0 0 12
0.1605 -1.2724 -2.9590 H 0 0 0 0 0 0 0 0 0 0 0 13
-1.6348 1.5893 -1.1786 H 0 0 0 0 0 0 0 0 0 0 0 14
1.4547 1.4686 -0.7248 H 0 0 0 0 0 0 0 0 0 0 0 15
1.8553 0.4189 -2.1096 H 0 0 0 0 0 0 0 0 0 0 0 16
-1.4482 -1.3860 -2.1959 H 0 0 0 0 0 0 0 0 0 0 0 17
-0.8510 1.2687 0.3924 H 0 0 0 0 0 0 0 0 0 0 0 18
-1.0358 0.0289 -3.2023 H 0 0 0 0 0 0 0 0 0 0 0 19
0.4039 -1.0077 -0.3536 O 0 0 0 0 0 0 0 0 0 0 0 20
2 1 0 0 0 0
3 1 0 0 0 0
4 2 0 0 0 0
6 4 0 0 0 0
8 7 0 0 0 0
9 7 0 0 0 0
10 7 0 0 0 0
11 8 0 0 0 0
15 8 0 0 0 0
16 8 0 0 0 0
12 9 0 0 0 0
14 9 0 0 0 0
18 9 0 0 0 0
13 10 0 0 0 0
17 10 0 0 0 0
19 10 0 0 0 0
5 20 0 0 0 0
7 20 0 0 0 0
M END
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tert-butanol.sdf
COSMOtherm 3D 0
21 18 0 0 0 0 0 0 0 0 0 V2000
-3.7549 -0.7955 0.0304 O 0 0 0 0 0 0 0 0 0 0 0 1
-3.8311 -1.2542 -0.8255 H 0 0 0 0 0 0 0 0 0 0 0 2
-4.6589 -0.4832 0.2167 H 0 0 0 0 0 0 0 0 0 0 0 3
-1.9521 1.2682 0.0843 O 0 0 0 0 0 0 0 0 0 0 0 4
-2.6088 0.5203 0.0089 H 0 0 0 0 0 0 0 0 0 0 0 5
-2.0322 1.7616 -0.7505 H 0 0 0 0 0 0 0 0 0 0 0 6
1.4266 -0.1268 -0.0249 C 0 0 0 0 0 0 0 0 0 0 0 7
1.5150 0.5456 -1.4043 C 0 0 0 0 0 0 0 0 0 0 0 8
0.7626 -1.5084 -0.1403 C 0 0 0 0 0 0 0 0 0 0 0 9
2.8158 -0.2456 0.6094 C 0 0 0 0 0 0 0 0 0 0 0 10
2.1217 -0.0538 -2.0999 H 0 0 0 0 0 0 0 0 0 0 0 11
0.6815 -1.9767 0.8521 H 0 0 0 0 0 0 0 0 0 0 0 12
3.2765 0.7483 0.7127 H 0 0 0 0 0 0 0 0 0 0 0 13
1.3455 -2.1759 -0.7929 H 0 0 0 0 0 0 0 0 0 0 0 14
0.5118 0.6614 -1.8430 H 0 0 0 0 0 0 0 0 0 0 0 15
1.9716 1.5423 -1.3144 H 0 0 0 0 0 0 0 0 0 0 0 16
2.7436 -0.7023 1.6074 H 0 0 0 0 0 0 0 0 0 0 0 17
-0.2484 -1.4171 -0.5652 H 0 0 0 0 0 0 0 0 0 0 0 18
3.4746 -0.8705 -0.0108 H 0 0 0 0 0 0 0 0 0 0 0 19
0.6553 0.7103 0.8773 O 0 0 0 0 0 0 0 0 0 0 0 20
-0.2550 0.8326 0.4996 H 0 0 0 0 0 0 0 0 0 0 0 21
2 1 0 0 0 0
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3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
8 7 0 0 0 0
9 7 0 0 0 0
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20 7 0 0 0 0
11 8 0 0 0 0
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16 8 0 0 0 0
12 9 0 0 0 0
14 9 0 0 0 0
18 9 0 0 0 0
13 10 0 0 0 0
17 10 0 0 0 0
19 10 0 0 0 0
20 21 0 0 0 0
M END
$$$$
thymine-anion.sdf
COSMOtherm 3D 0
20 18 0 0 0 0 0 0 0 0 0 V2000
-1.4276 -0.5927 4.5599 O 0 0 0 0 0 0 0 0 0 0 1
-0.6691 -0.1679 4.0618 H 0 0 0 0 0 0 0 0 0 0 2
-2.1384 0.0700 4.5325 H 0 0 0 0 0 0 0 0 0 0 3
0.6958 0.4844 3.2432 O 0 0 0 0 0 0 0 0 0 0 4
0.6193 0.3666 2.2198 H 0 0 0 0 0 0 0 0 0 0 5
0.7584 1.4449 3.3866 H 0 0 0 0 0 0 0 0 0 0 6
-0.8426 0.2191 0.0712 C 0 0 0 0 0 0 0 0 0 0 7
-1.1806 0.1144 -1.2641 C 0 0 0 0 0 0 0 0 0 0 8
-0.1046 -0.0934 -2.2010 C 0 0 0 0 0 0 0 0 0 0 9
1.1627 -0.1587 -1.6085 N 0 0 0 0 0 0 0 0 0 0 10
1.4615 -0.0446 -0.2419 C 0 0 0 0 0 0 0 0 0 0 11
0.4067 0.1471 0.6021 N 0 0 0 0 0 0 0 0 0 0 12
-0.2183 -0.2126 -3.4439 O 0 0 0 0 0 0 0 0 0 0 13
2.6548 -0.1232 0.1336 O 0 0 0 0 0 0 0 0 0 0 14
-2.5935 0.2030 -1.7675 C 0 0 0 0 0 0 0 0 0 0 15
-1.6405 0.3733 0.8069 H 0 0 0 0 0 0 0 0 0 0 16
1.9544 -0.3044 -2.2368 H 0 0 0 0 0 0 0 0 0 0 17
-2.8937 -0.7152 -2.2977 H 0 0 0 0 0 0 0 0 0 0 18
-2.7194 1.0338 -2.4801 H 0 0 0 0 0 0 0 0 0 0 19
-3.2928 0.3599 -0.9345 H 0 0 0 0 0 0 0 0 0 0 20
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
8 7 0 0 0 0
12 7 0 0 0 0
16 7 0 0 0 0
9 8 0 0 0 0
15 8 0 0 0 0
10 9 0 0 0 0
13 9 0 0 0 0
11 10 0 0 0 0
17 10 0 0 0 0
12 11 0 0 0 0
14 11 0 0 0 0
18 15 0 0 0 0
19 15 0 0 0 0
15 20 0 0 0 0
M END
$$$$
thymine.sdf
COSMOtherm 3D 0
21 19 0 0 0 0 0 0 0 0 0 V2000
-4.0896 0.6265 -0.0341 O 0 0 0 0 0 0 0 0 0 0 1
-4.4871 0.8845 -0.8848 H 0 0 0 0 0 0 0 0 0 0 2
-3.1816 1.0344 -0.0343 H 0 0 0 0 0 0 0 0 0 0 3
-2.9755 -1.8287 -0.0091 O 0 0 0 0 0 0 0 0 0 0 4
-3.5485 -1.0052 -0.0162 H 0 0 0 0 0 0 0 0 0 0 5
-3.1871 -2.2833 0.8258 H 0 0 0 0 0 0 0 0 0 0 6
0.6492 -1.3379 -0.0034 C 0 0 0 0 0 0 0 0 0 0 7
1.9044 -0.8048 -0.0151 C 0 0 0 0 0 0 0 0 0 0 8
2.0265 0.6459 -0.0032 C 0 0 0 0 0 0 0 0 0 0 9
0.8010 1.3396 0.0175 N 0 0 0 0 0 0 0 0 0 0 10
-0.4697 0.7975 0.0314 C 0 0 0 0 0 0 0 0 0 0 11
-0.4950 -0.5758 0.0167 N 0 0 0 0 0 0 0 0 0 0 12
3.0913 1.2815 -0.0102 O 0 0 0 0 0 0 0 0 0 0 13
-1.4892 1.5139 0.0550 O 0 0 0 0 0 0 0 0 0 0 14
3.1509 -1.6391 -0.0364 C 0 0 0 0 0 0 0 0 0 0 15
0.4772 -2.4145 -0.0102 H 0 0 0 0 0 0 0 0 0 0 16
0.8531 2.3598 0.0277 H 0 0 0 0 0 0 0 0 0 0 17
-1.4330 -1.0562 0.0349 H 0 0 0 0 0 0 0 0 0 0 18
3.7795 -1.4323 0.8431 H 0 0 0 0 0 0 0 0 0 0 19
3.7601 -1.4166 -0.9253 H 0 0 0 0 0 0 0 0 0 0 20
2.9037 -2.7084 -0.0430 H 0 0 0 0 0 0 0 0 0 0 21
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
8 7 0 0 0 0
12 7 0 0 0 0
16 7 0 0 0 0
9 8 0 0 0 0
15 8 0 0 0 0
10 9 0 0 0 0
13 9 0 0 0 0
11 10 0 0 0 0
17 10 0 0 0 0
12 11 0 0 0 0
14 11 0 0 0 0
18 12 0 0 0 0
19 15 0 0 0 0
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20 15 0 0 0 0
15 21 0 0 0 0
M END
$$$$
trans-5-formyluracil-anion.sdf
COSMOtherm 3D 0

19 17 0 0 0 0 0 0 0 0 0 V2000
1.6722 -4.3871 0.2923 O 0 0 0 0 0 0 0 0 0 0 1
0.7527 -4.0301 0.1286 H 0 0 0 0 0 0 0 0 0 0 2
1.9127 -4.0543 1.1735 H 0 0 0 0 0 0 0 0 0 0 3
-0.8517 -3.4418 -0.1974 O 0 0 0 0 0 0 0 0 0 0 4
-0.8406 -2.4237 -0.1853 H 0 0 0 0 0 0 0 0 0 0 5
-1.1432 -3.6758 -1.0965 H 0 0 0 0 0 0 0 0 0 0 6
0.5335 -0.1585 -0.1234 C 0 0 0 0 0 0 0 0 0 0 7
0.8042 1.2151 -0.0366 C 0 0 0 0 0 0 0 0 0 0 8
-0.3202 2.1265 0.0810 C 0 0 0 0 0 0 0 0 0 0 9
-1.5586 1.4709 0.0915 N 0 0 0 0 0 0 0 0 0 0 10
-1.7842 0.0928 0.0005 C 0 0 0 0 0 0 0 0 0 0 11
-0.6727 -0.7267 -0.1105 N 0 0 0 0 0 0 0 0 0 0 12
-0.2739 3.3677 0.1685 O 0 0 0 0 0 0 0 0 0 0 13
-2.9441 -0.3493 0.0165 O 0 0 0 0 0 0 0 0 0 0 14
2.1551 1.7271 -0.0606 C 0 0 0 0 0 0 0 0 0 0 15
1.3822 -0.8460 -0.2060 H 0 0 0 0 0 0 0 0 0 0 16
-2.3876 2.0620 0.1733 H 0 0 0 0 0 0 0 0 0 0 17
3.1884 1.0415 -0.1591 O 0 0 0 0 0 0 0 0 0 0 18
2.2335 2.8342 0.0172 H 0 0 0 0 0 0 0 0 0 0 19
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
8 7 0 0 0 0
12 7 0 0 0 0
16 7 0 0 0 0
9 8 0 0 0 0
15 8 0 0 0 0
10 9 0 0 0 0
13 9 0 0 0 0
11 10 0 0 0 0
17 10 0 0 0 0
12 11 0 0 0 0
14 11 0 0 0 0
18 15 0 0 0 0
15 19 0 0 0 0
M END
$$$$
trans-5-formyluracil.sdf
COSMOtherm 3D 0

20 18 0 0 0 0 0 0 0 0 0 V2000
-5.0669 -0.4929 0.8925 O 0 0 0 0 0 0 0 0 0 0 1
-5.8675 -1.0385 0.7891 H 0 0 0 0 0 0 0 0 0 0 2
-5.3682 0.4136 0.7006 H 0 0 0 0 0 0 0 0 0 0 3
-3.0247 -1.3378 -0.6807 O 0 0 0 0 0 0 0 0 0 0 4
-3.3180 -1.2981 -1.6084 H 0 0 0 0 0 0 0 0 0 0 5
-3.8024 -1.0086 -0.1408 H 0 0 0 0 0 0 0 0 0 0 6
0.4065 -0.9135 -0.1609 C 0 0 0 0 0 0 0 0 0 0 7
1.6933 -0.4598 0.0437 C 0 0 0 0 0 0 0 0 0 0 8
1.9256 0.9793 0.1344 C 0 0 0 0 0 0 0 0 0 0 9
0.7583 1.7516 -0.0046 N 0 0 0 0 0 0 0 0 0 0 10
-0.5369 1.3027 -0.2106 C 0 0 0 0 0 0 0 0 0 0 11
-0.6510 -0.0900 -0.2815 N 0 0 0 0 0 0 0 0 0 0 12
3.0155 1.5337 0.3144 O 0 0 0 0 0 0 0 0 0 0 13
-1.5047 2.0508 -0.3211 O 0 0 0 0 0 0 0 0 0 0 14
2.8098 -1.3916 0.1663 C 0 0 0 0 0 0 0 0 0 0 15
0.1951 -1.9816 -0.2353 H 0 0 0 0 0 0 0 0 0 0 16
0.8738 2.7654 0.0515 H 0 0 0 0 0 0 0 0 0 0 17
-1.6206 -0.4970 -0.4436 H 0 0 0 0 0 0 0 0 0 0 18
2.7105 -2.6217 0.1009 O 0 0 0 0 0 0 0 0 0 0 19
3.7990 -0.9134 0.3289 H 0 0 0 0 0 0 0 0 0 0 20
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
8 7 0 0 0 0
12 7 0 0 0 0
16 7 0 0 0 0
9 8 0 0 0 0
15 8 0 0 0 0
10 9 0 0 0 0
13 9 0 0 0 0
11 10 0 0 0 0
17 10 0 0 0 0
12 11 0 0 0 0
14 11 0 0 0 0
18 12 0 0 0 0
19 15 0 0 0 0
15 20 0 0 0 0
M END
$$$$
trichloroaceticacid-anion.sdf
COSMOtherm 3D 0

13 10 0 0 0 0 0 0 0 0 0 V2000
-5.5924 0.2214 -0.8335 O 0 0 0 0 0 0 0 0 0 0 1
-4.8803 0.0480 -0.1555 H 0 0 0 0 0 0 0 0 0 0 2
-5.3339 1.0637 -1.2452 H 0 0 0 0 0 0 0 0 0 0 3
-3.6752 -0.3549 1.0409 O 0 0 0 0 0 0 0 0 0 0 4
-2.7427 -0.2861 0.6606 H 0 0 0 0 0 0 0 0 0 0 5
-3.6934 0.2806 1.7776 H 0 0 0 0 0 0 0 0 0 0 6
1.4204 -1.6867 -0.6746 Cl 0 0 0 0 0 0 0 0 0 0 7
1.1345 0.0085 -0.0628 C 0 0 0 0 0 0 0 0 0 0 8
-0.2828 0.0686 0.6862 C 0 0 0 0 0 0 0 0 0 0 9
-0.2725 0.4219 1.8762 O 0 0 0 0 0 0 0 0 0 0 10
-1.2407 -0.2606 -0.0656 O 0 0 0 0 0 0 0 0 0 0 11
```

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1
2
3      1.1093      1.1511      -1.4842 Cl  0  0  0  0  0  0  0  0  0  0  12
4      2.5204      0.4655      1.0074 Cl  0  0  0  0  0  0  0  0  0  0  13
5      2  1  0  0  0  0
6      3  1  0  0  0  0
7      5  4  0  0  0  0
8      6  4  0  0  0  0
9      8  7  0  0  0  0
10     9  8  0  0  0  0
11    12  8  0  0  0  0
12    10  9  0  0  0  0
13    11  9  0  0  0  0
14     8 13  0  0  0  0
15
16 M  END
17 $$$
18 trichloroaceticacid.sdf
19 COSMOTHERM      3D      0
20
21 14 12  0  0  0  0  0  0  0  0  0  0 V2000
22 0.9504 4.8833 -0.3752 O  0  0  0  0  0  0  0  0  0  0  1
23 1.6564 4.9101 0.2959 H  0  0  0  0  0  0  0  0  0  0  2
24 0.7410 5.8195 -0.5476 H  0  0  0  0  0  0  0  0  0  0  3
25 -1.1964 3.4835 0.3072 O  0  0  0  0  0  0  0  0  0  0  4
26 -0.3698 4.0277 0.0952 H  0  0  0  0  0  0  0  0  0  0  5
27 -1.4424 3.7007 1.2245 H  0  0  0  0  0  0  0  0  0  0  6
28 -1.3339 -1.8526 0.8689 Cl  0  0  0  0  0  0  0  0  0  0  7
29 0.0521 -1.0896 -0.0215 C  0  0  0  0  0  0  0  0  0  0  8
30 0.0746 0.4513 0.3094 C  0  0  0  0  0  0  0  0  0  0  9
31 1.0277 0.9581 0.8763 O  0  0  0  0  0  0  0  0  0  0  10
32 -1.0243 1.0324 -0.0979 O  0  0  0  0  0  0  0  0  0  0  11
33 -0.1709 -1.3163 -1.8070 Cl  0  0  0  0  0  0  0  0  0  0  12
34 1.5840 -1.8733 0.4863 Cl  0  0  0  0  0  0  0  0  0  0  13
35 -1.0321 2.0942 0.1203 H  0  0  0  0  0  0  0  0  0  0  14
36
37 2  1  0  0  0  0
38 3  1  0  0  0  0
39 5  4  0  0  0  0
40 6  4  0  0  0  0
41 8  7  0  0  0  0
42 9  8  0  0  0  0
43 12  8  0  0  0  0
44 13  8  0  0  0  0
45 10  9  0  0  0  0
46 11  9  0  0  0  0
47 4 14  0  0  0  0
48 11 14  0  0  0  0
49
50 M  END
51 $$$
52 uracil-anion.sdf
53 COSMOTHERM      3D      0
54
55 17 15  0  0  0  0  0  0  0  0  0  0 V2000
56 4.5904 0.6715 1.1155 O  0  0  0  0  0  0  0  0  0  0  1
57 3.9929 0.1942 0.4684 H  0  0  0  0  0  0  0  0  0  0  2
58 4.5697 0.1215 1.9171 H  0  0  0  0  0  0  0  0  0  0  3
59 3.0115 -0.5688 -0.7199 O  0  0  0  0  0  0  0  0  0  0  4
60 2.0038 -0.4443 -0.5443 H  0  0  0  0  0  0  0  0  0  0  5
61 3.1544 -1.5314 -0.7288 H  0  0  0  0  0  0  0  0  0  0  6
62 -0.0177 -0.3682 1.1153 C  0  0  0  0  0  0  0  0  0  0  7
63 -1.3202 -0.2489 1.5554 C  0  0  0  0  0  0  0  0  0  0  8
64 -2.3474 0.0557 0.6024 C  0  0  0  0  0  0  0  0  0  0  9
65 -1.8599 0.1972 -0.7055 N  0  0  0  0  0  0  0  0  0  0  10
66 -0.5257 0.0717 -1.1253 C  0  0  0  0  0  0  0  0  0  0  11
67 0.4052 -0.2207 -0.1646 N  0  0  0  0  0  0  0  0  0  0  12
68 -3.5723 0.1971 0.8292 O  0  0  0  0  0  0  0  0  0  0  13
69 -0.2476 0.2287 -2.3350 O  0  0  0  0  0  0  0  0  0  0  14
70 -1.5848 -0.3812 2.6027 H  0  0  0  0  0  0  0  0  0  0  15
71 0.7730 -0.6014 1.8357 H  0  0  0  0  0  0  0  0  0  0  16
72 -2.5449 0.4159 -1.4306 H  0  0  0  0  0  0  0  0  0  0  17
73
74 2  1  0  0  0  0
75 3  1  0  0  0  0
76 5  4  0  0  0  0
77 6  4  0  0  0  0
78 8  7  0  0  0  0
79 12  7  0  0  0  0
80 16  7  0  0  0  0
81 9  8  0  0  0  0
82 15  8  0  0  0  0
83 10  9  0  0  0  0
84 13  9  0  0  0  0
85 11 10  0  0  0  0
86 12 11  0  0  0  0
87 14 11  0  0  0  0
88 10 17  0  0  0  0
89
90 M  END
91 $$$
92 uracil.sdf
93 COSMOTHERM      3D      0
94
95 18 16  0  0  0  0  0  0  0  0  0  0 V2000
96 -4.6348 0.9766 0.2501 O  0  0  0  0  0  0  0  0  0  0  1
97 -4.9546 0.6782 1.1209 H  0  0  0  0  0  0  0  0  0  0  2
98 -5.4471 1.1105 -0.2716 H  0  0  0  0  0  0  0  0  0  0  3
99 -2.8979 -0.7432 -0.9545 O  0  0  0  0  0  0  0  0  0  0  4
100 -3.5562 -0.1532 -0.4875 H  0  0  0  0  0  0  0  0  0  0  5
101 -3.1881 -1.6528 -0.7644 H  0  0  0  0  0  0  0  0  0  0  6
102 0.5401 -0.0695 -1.4915 C  0  0  0  0  0  0  0  0  0  0  7
103 1.8769 0.1800 -1.4067 C  0  0  0  0  0  0  0  0  0  0  8
104 2.5119 0.2270 -0.1098 C  0  0  0  0  0  0  0  0  0  0  9
105 1.6307 -0.0061 0.9646 N  0  0  0  0  0  0  0  0  0  0  10
106 0.2671 -0.2666 0.9004 C  0  0  0  0  0  0  0  0  0  0  11
107 -0.2398 -0.2840 -0.3885 N  0  0  0  0  0  0  0  0  0  0  12
108 3.7138 0.4463 0.1147 O  0  0  0  0  0  0  0  0  0  0  13
109 -0.4244 -0.4636 1.9040 O  0  0  0  0  0  0  0  0  0  0  14
110 2.4779 0.3467 -2.2968 H  0  0  0  0  0  0  0  0  0  0  15
111 0.0141 -0.1139 -2.4451 H  0  0  0  0  0  0  0  0  0  0  16
112 2.0351 0.0153 1.9022 H  0  0  0  0  0  0  0  0  0  0  17
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-1.2690 -0.4728 -0.5089 H 0 0 0 0 0 0 0 0 0 0 0 18
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
8 7 0 0 0 0
12 7 0 0 0 0
16 7 0 0 0 0
9 8 0 0 0 0
15 8 0 0 0 0
10 9 0 0 0 0
13 9 0 0 0 0
11 10 0 0 0 0
17 10 0 0 0 0
12 11 0 0 0 0
14 11 0 0 0 0
12 18 0 0 0 0
M END
$$$$
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S4 d) Bare Bases & Cations

```
1,3-dihydro-1-methyl-5-phenyl-1,4-benzodiazepin-2-one.sdf
COSMOTHERM 3D 0

33 35 0 0 0 0 0 0 0 0 0 V2000
-3.1559 0.5382 1.7695 C 0 0 0 0 0 0 0 0 0 0 0 1
-2.5277 -1.8007 0.1659 C 0 0 0 0 0 0 0 0 0 0 0 2
-2.0420 -3.0290 -0.2759 C 0 0 0 0 0 0 0 0 0 0 0 3
-0.7421 -3.1295 -0.7890 C 0 0 0 0 0 0 0 0 0 0 0 4
0.0639 -1.9958 -0.8327 C 0 0 0 0 0 0 0 0 0 0 0 5
-0.4028 -0.7375 -0.3972 C 0 0 0 0 0 0 0 0 0 0 0 6
-1.7307 -0.6423 0.0980 C 0 0 0 0 0 0 0 0 0 0 0 7
0.4987 0.4397 -0.4754 C 0 0 0 0 0 0 0 0 0 0 0 8
-2.2685 0.5788 0.5937 N 0 0 0 0 0 0 0 0 0 0 0 9
0.1203 1.6094 -0.8876 N 0 0 0 0 0 0 0 0 0 0 0 10
-1.2698 1.7572 -1.3165 C 0 0 0 0 0 0 0 0 0 0 0 11
-2.1806 1.7739 -0.0936 C 0 0 0 0 0 0 0 0 0 0 0 12
1.9278 0.2799 -0.0794 C 0 0 0 0 0 0 0 0 0 0 0 13
2.9241 1.0347 -0.7279 C 0 0 0 0 0 0 0 0 0 0 0 14
2.3026 -0.5833 0.9673 C 0 0 0 0 0 0 0 0 0 0 0 15
4.2607 0.9262 -0.3402 C 0 0 0 0 0 0 0 0 0 0 0 16
3.6399 -0.6800 1.3635 C 0 0 0 0 0 0 0 0 0 0 0 17
4.6230 0.0708 0.7091 C 0 0 0 0 0 0 0 0 0 0 0 18
-2.7774 2.7898 0.2833 O 0 0 0 0 0 0 0 0 0 0 0 19
-2.8299 -0.2684 2.4339 H 0 0 0 0 0 0 0 0 0 0 0 20
-3.0800 1.4991 2.2888 H 0 0 0 0 0 0 0 0 0 0 0 21
-4.2057 0.3793 1.4819 H 0 0 0 0 0 0 0 0 0 0 0 22
-3.5437 -1.7313 0.5535 H 0 0 0 0 0 0 0 0 0 0 0 23
-2.6850 -3.9091 -0.2273 H 0 0 0 0 0 0 0 0 0 0 0 24
-0.3608 -4.0869 -1.1462 H 0 0 0 0 0 0 0 0 0 0 0 25
1.0810 -2.0689 -1.2197 H 0 0 0 0 0 0 0 0 0 0 0 26
-1.5852 0.9450 -1.9975 H 0 0 0 0 0 0 0 0 0 0 0 27
-1.3894 2.7175 -1.8290 H 0 0 0 0 0 0 0 0 0 0 0 28
2.6365 1.6991 -1.5437 H 0 0 0 0 0 0 0 0 0 0 0 29
1.5422 -1.1684 1.4868 H 0 0 0 0 0 0 0 0 0 0 0 30
5.0249 1.5065 -0.8606 H 0 0 0 0 0 0 0 0 0 0 0 31
3.9137 -1.3437 2.1856 H 0 0 0 0 0 0 0 0 0 0 0 32
5.6682 -0.0122 1.0125 H 0 0 0 0 0 0 0 0 0 0 0 33

9 1 0 0 0 0
20 1 0 0 0 0
21 1 0 0 0 0
22 1 0 0 0 0
3 2 0 0 0 0
7 2 0 0 0 0
23 2 0 0 0 0
4 3 0 0 0 0
24 3 0 0 0 0
5 4 0 0 0 0
25 4 0 0 0 0
6 5 0 0 0 0
26 5 0 0 0 0
7 6 0 0 0 0
8 6 0 0 0 0
9 7 0 0 0 0
10 8 0 0 0 0
13 8 0 0 0 0
12 9 0 0 0 0
11 10 0 0 0 0
12 11 0 0 0 0
27 11 0 0 0 0
28 11 0 0 0 0
19 12 0 0 0 0
14 13 0 0 0 0
15 13 0 0 0 0
16 14 0 0 0 0
29 14 0 0 0 0
17 15 0 0 0 0
30 15 0 0 0 0
18 16 0 0 0 0
31 16 0 0 0 0
18 17 0 0 0 0
32 17 0 0 0 0
18 33 0 0 0 0
M END
$$$$
1,3-dihydro-1-methyl-5-phenyl-1,4-benzodiazepin-2-one_p1.sdf
COSMOTHERM 3D 0

34 36 0 0 0 0 0 0 0 0 0 V2000
-2.5140 -1.8206 0.0979 C 0 0 0 0 0 0 0 0 0 0 0 1
```

```
1
2
3      -3.2473    0.4462    1.7120 C    0    0    0    0    0    0    0    0    0    2
4      -2.3076    0.5441    0.5763 N    0    0    0    0    0    0    0    0    0    3
5      -2.2551    1.7606   -0.0785 C    0    0    0    0    0    0    0    0    0    4
6      -2.9214    2.7324    0.2729 O    0    0    0    0    0    0    0    0    0    5
7      -1.2814    1.8164   -1.2556 C    0    0    0    0    0    0    0    0    0    6
8      0.0717    1.5726   -0.7731 N    0    0    0    0    0    0    0    0    0    7
9      0.5307    0.3901   -0.4083 C    0    0    0    0    0    0    0    0    0    8
10     -1.7335   -0.6521    0.0691 C    0    0    0    0    0    0    0    0    0    9
11     -0.3761   -0.7474   -0.3718 C    0    0    0    0    0    0    0    0    0    10
12     -1.9968   -3.0434   -0.3204 C    0    0    0    0    0    0    0    0    0    11
13     -0.6721   -3.1418   -0.7679 C    0    0    0    0    0    0    0    0    0    12
14     0.1265   -2.0080   -0.7792 C    0    0    0    0    0    0    0    0    0    13
15     1.9513    0.2727   -0.0635 C    0    0    0    0    0    0    0    0    0    14
16     2.3575   -0.5952    0.9720 C    0    0    0    0    0    0    0    0    0    15
17     3.7005   -0.6596    1.3402 C    0    0    0    0    0    0    0    0    0    16
18     4.6502    0.1245    0.6742 C    0    0    0    0    0    0    0    0    0    17
19     4.2559    0.9800   -0.3629 C    0    0    0    0    0    0    0    0    0    18
20     2.9144    1.0607   -0.7305 C    0    0    0    0    0    0    0    0    0    19
21     -3.5464   -1.7643    0.4391 H    0    0    0    0    0    0    0    0    0    20
22     -4.2770    0.2714    1.3705 H    0    0    0    0    0    0    0    0    0    21
23     -2.9256   -0.3696    2.3662 H    0    0    0    0    0    0    0    0    0    22
24     -3.2153    1.3942    2.2584 H    0    0    0    0    0    0    0    0    0    23
25     -1.3190    2.8129   -1.7004 H    0    0    0    0    0    0    0    0    0    24
26     -1.5434    1.0630   -2.0128 H    0    0    0    0    0    0    0    0    0    25
27     -2.6370   -3.9263   -0.3046 H    0    0    0    0    0    0    0    0    0    26
28     -0.2705   -4.0971   -1.1054 H    0    0    0    0    0    0    0    0    0    27
29     1.1544   -2.0696   -1.1349 H    0    0    0    0    0    0    0    0    0    28
30     1.6164   -1.1905    1.5059 H    0    0    0    0    0    0    0    0    0    29
31     4.0068   -1.3207    2.1517 H    0    0    0    0    0    0    0    0    0    30
32     5.7015    0.0658    0.9600 H    0    0    0    0    0    0    0    0    0    31
33     4.9986    1.5762   -0.8942 H    0    0    0    0    0    0    0    0    0    32
34     2.6211    1.7013   -1.5641 H    0    0    0    0    0    0    0    0    0    33
35     0.6845    2.3849   -0.6783 H    0    0    0    0    0    0    0    0    0    34
36
37 9 1 0 0 0 0
38 11 1 0 0 0 0
39 20 1 0 0 0 0
40 3 2 0 0 0 0
41 21 2 0 0 0 0
42 22 2 0 0 0 0
43 23 2 0 0 0 0
44 4 3 0 0 0 0
45 9 3 0 0 0 0
46 5 4 0 0 0 0
47 6 4 0 0 0 0
48 7 6 0 0 0 0
49 24 6 0 0 0 0
50 25 6 0 0 0 0
51 8 7 0 0 0 0
52 10 8 0 0 0 0
53 14 8 0 0 0 0
54 10 9 0 0 0 0
55 13 10 0 0 0 0
56 12 11 0 0 0 0
57 26 11 0 0 0 0
58 13 12 0 0 0 0
59 27 12 0 0 0 0
60 28 13 0 0 0 0
61 15 14 0 0 0 0
62 19 14 0 0 0 0
63 16 15 0 0 0 0
64 29 15 0 0 0 0
65 17 16 0 0 0 0
66 30 16 0 0 0 0
67 18 17 0 0 0 0
68 31 17 0 0 0 0
69 19 18 0 0 0 0
70 32 18 0 0 0 0
71 33 19 0 0 0 0
72 7 34 0 0 0 0
73
74 M END
75 $$$$
76 1,3-dihydro-3-hydroxy-1-methyl-5-phenyl-1,4-benzodiazepin-2-one.sdf
77 COSMOtherm 3D 0
78
79 34 36 0 0 0 0 0 0 0 0 0 0 V2000
80 1.6969 -3.3157 0.5838 C 0 0 0 0 0 0 0 0 0 0 0 1
81 0.4128 -3.2274 1.1366 C 0 0 0 0 0 0 0 0 0 0 0 2
82 -0.2968 -2.0349 1.0326 C 0 0 0 0 0 0 0 0 0 0 0 3
83 0.2557 -0.8979 0.4059 C 0 0 0 0 0 0 0 0 0 0 0 4
84 1.5682 -0.9932 -0.1280 C 0 0 0 0 0 0 0 0 0 0 0 5
85 2.2661 -2.2110 -0.0453 C 0 0 0 0 0 0 0 0 0 0 0 6
86 -0.5416 0.3532 0.3303 C 0 0 0 0 0 0 0 0 0 0 0 7
87 2.1848 0.0929 -0.8170 N 0 0 0 0 0 0 0 0 0 0 0 8
88 2.1896 1.3702 -0.3311 C 0 0 0 0 0 0 0 0 0 0 0 9
89 1.3555 1.6191 0.9384 C 0 0 0 0 0 0 0 0 0 0 0 10
90 -0.0441 1.5312 0.5493 N 0 0 0 0 0 0 0 0 0 0 0 11
91 2.9974 -0.1884 -2.0154 C 0 0 0 0 0 0 0 0 0 0 0 12
92 2.7804 2.3123 -0.8778 O 0 0 0 0 0 0 0 0 0 0 0 13
93 -1.9915 0.2668 -0.0015 C 0 0 0 0 0 0 0 0 0 0 0 14
94 -2.8905 1.2073 0.5372 C 0 0 0 0 0 0 0 0 0 0 0 15
95 -2.4806 -0.7148 -0.8838 C 0 0 0 0 0 0 0 0 0 0 0 16
96 -3.8354 -0.7481 -1.2265 C 0 0 0 0 0 0 0 0 0 0 0 17
97 -4.7218 0.1872 -0.6811 C 0 0 0 0 0 0 0 0 0 0 0 18
98 -4.2450 1.1635 0.2041 C 0 0 0 0 0 0 0 0 0 0 0 19
99 2.2632 -4.2458 0.6508 H 0 0 0 0 0 0 0 0 0 0 0 20
100 -0.0320 -4.0861 1.6408 H 0 0 0 0 0 0 0 0 0 0 0 21
101 -1.3012 -1.9639 1.4516 H 0 0 0 0 0 0 0 0 0 0 0 22
102 3.2692 -2.2850 -0.4642 H 0 0 0 0 0 0 0 0 0 0 0 23
103 1.6057 0.8738 1.7149 H 0 0 0 0 0 0 0 0 0 0 0 24
104 1.6587 2.8998 1.4460 O 0 0 0 0 0 0 0 0 0 0 0 25
105 2.5609 -1.0390 -2.5484 H 0 0 0 0 0 0 0 0 0 0 0 26
106 4.0402 -0.4116 -1.7496 H 0 0 0 0 0 0 0 0 0 0 0 27
107 2.9796 0.6985 -2.6567 H 0 0 0 0 0 0 0 0 0 0 0 28
108 -2.5143 1.9646 1.2264 H 0 0 0 0 0 0 0 0 0 0 0 29
109 -1.7958 -1.4435 -1.3200 H 0 0 0 0 0 0 0 0 0 0 0 30
```



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15 14 0 0 0 0
16 14 0 0 0 0
19 15 0 0 0 0
29 15 0 0 0 0
17 16 0 0 0 0
30 16 0 0 0 0
18 17 0 0 0 0
31 17 0 0 0 0
19 18 0 0 0 0
32 18 0 0 0 0
33 19 0 0 0 0
34 25 0 0 0 0
11 35 0 0 0 0
M END
$$$$
1,3-dihydro-3-hydroxy-5-phenyl-1,4-benzodiazepin-2-one.sdf
COSMOTHERM 3D 0

31 33 0 0 0 0 0 0 0 0 0 V2000
0.5145 -3.2825 -0.9215 C 0 0 0 0 0 0 0 0 0 0 0 1
-0.1408 -2.0552 -0.9137 C 0 0 0 0 0 0 0 0 0 0 0 2
0.4201 -0.9208 -0.2872 C 0 0 0 0 0 0 0 0 0 0 0 3
1.6892 -1.0618 0.3311 C 0 0 0 0 0 0 0 0 0 0 0 4
2.3275 -2.3139 0.3574 C 0 0 0 0 0 0 0 0 0 0 0 5
1.7462 -3.4150 -0.2641 C 0 0 0 0 0 0 0 0 0 0 0 6
2.3246 0.0097 0.9993 N 0 0 0 0 0 0 0 0 0 0 0 7
-0.3379 0.3568 -0.2491 C 0 0 0 0 0 0 0 0 0 0 0 8
0.1958 1.5303 -0.3966 N 0 0 0 0 0 0 0 0 0 0 0 9
1.6134 1.6188 -0.7086 C 0 0 0 0 0 0 0 0 0 0 0 10
-1.8101 0.3044 -0.0162 C 0 0 0 0 0 0 0 0 0 0 0 11
-2.6479 1.2608 -0.6206 C 0 0 0 0 0 0 0 0 0 0 0 12
-2.3806 -0.6581 0.8378 C 0 0 0 0 0 0 0 0 0 0 0 13
-4.0231 1.2506 -0.3811 C 0 0 0 0 0 0 0 0 0 0 0 14
-4.5814 0.2931 0.4764 C 0 0 0 0 0 0 0 0 0 0 0 15
-3.7559 -0.6572 1.0878 C 0 0 0 0 0 0 0 0 0 0 0 16
2.3914 1.3046 0.5802 C 0 0 0 0 0 0 0 0 0 0 0 17
3.0037 2.1900 1.1890 O 0 0 0 0 0 0 0 0 0 0 0 18
1.9545 2.9130 -1.1531 O 0 0 0 0 0 0 0 0 0 0 0 19
0.0651 -4.1381 -1.4269 H 0 0 0 0 0 0 0 0 0 0 0 20
-1.1093 -1.9558 -1.4050 H 0 0 0 0 0 0 0 0 0 0 0 21
3.2914 -2.4070 0.8609 H 0 0 0 0 0 0 0 0 0 0 0 22
2.2600 -4.3772 -0.2455 H 0 0 0 0 0 0 0 0 0 0 0 23
2.9356 -0.2308 1.7818 H 0 0 0 0 0 0 0 0 0 0 0 24
1.8951 0.8973 -1.4980 H 0 0 0 0 0 0 0 0 0 0 0 25
-2.2080 2.0044 -1.2867 H 0 0 0 0 0 0 0 0 0 0 0 26
-1.7444 -1.3979 1.3254 H 0 0 0 0 0 0 0 0 0 0 0 27
-4.6635 1.9887 -0.8674 H 0 0 0 0 0 0 0 0 0 0 0 28
-5.6564 0.2871 0.6651 H 0 0 0 0 0 0 0 0 0 0 0 29
-4.1830 -1.4009 1.7629 H 0 0 0 0 0 0 0 0 0 0 0 30
2.3465 3.3668 -0.3722 H 0 0 0 0 0 0 0 0 0 0 0 31
2 1 0 0 0 0
6 1 0 0 0 0
20 1 0 0 0 0
3 2 0 0 0 0
21 2 0 0 0 0
4 3 0 0 0 0
8 3 0 0 0 0
5 4 0 0 0 0
7 4 0 0 0 0
6 5 0 0 0 0
22 5 0 0 0 0
23 6 0 0 0 0
17 7 0 0 0 0
24 7 0 0 0 0
9 8 0 0 0 0
11 8 0 0 0 0
10 9 0 0 0 0
17 10 0 0 0 0
19 10 0 0 0 0
25 10 0 0 0 0
12 11 0 0 0 0
13 11 0 0 0 0
14 12 0 0 0 0
26 12 0 0 0 0
16 13 0 0 0 0
27 13 0 0 0 0
15 14 0 0 0 0
28 14 0 0 0 0
16 15 0 0 0 0
29 15 0 0 0 0
30 16 0 0 0 0
18 17 0 0 0 0
19 31 0 0 0 0
M END
$$$$
1,3-dihydro-3-hydroxy-5-phenyl-1,4-benzodiazepin-2-one.pl.sdf
COSMOTHERM 3D 0

32 34 0 0 0 0 0 0 0 0 0 V2000
-3.3101 -0.4252 -0.8747 C 0 0 0 0 0 0 0 0 0 0 0 1
-2.0811 0.2156 -0.8508 C 0 0 0 0 0 0 0 0 0 0 0 2
-0.9402 -0.3940 -0.2697 C 0 0 0 0 0 0 0 0 0 0 0 3
-1.0790 -1.7028 0.2850 C 0 0 0 0 0 0 0 0 0 0 0 4
-2.3414 -2.3165 0.2928 C 0 0 0 0 0 0 0 0 0 0 0 5
-3.4422 -1.6897 -0.2813 C 0 0 0 0 0 0 0 0 0 0 0 6
-0.0328 -2.3972 0.9266 N 0 0 0 0 0 0 0 0 0 0 0 7
0.2947 0.3760 -0.2033 C 0 0 0 0 0 0 0 0 0 0 0 8
1.4605 -0.2324 -0.3137 N 0 0 0 0 0 0 0 0 0 0 0 9
1.6497 -1.6491 -0.6964 C 0 0 0 0 0 0 0 0 0 0 0 10
0.2944 1.8293 -0.0030 C 0 0 0 0 0 0 0 0 0 0 0 11
1.2784 2.6302 -0.6222 C 0 0 0 0 0 0 0 0 0 0 0 12
-0.6585 2.4283 0.8481 C 0 0 0 0 0 0 0 0 0 0 0 13
1.3028 4.0043 -0.3938 C 0 0 0 0 0 0 0 0 0 0 0 14
0.3602 4.5910 0.4608 C 0 0 0 0 0 0 0 0 0 0 0 15
-0.6155 3.8018 1.0819 C 0 0 0 0 0 0 0 0 0 0 0 16
```



```
23 10 0 0 0 0
14 13 0 0 0 0
15 13 0 0 0 0
18 14 0 0 0 0
24 14 0 0 0 0
16 15 0 0 0 0
25 15 0 0 0 0
17 16 0 0 0 0
26 16 0 0 0 0
18 17 0 0 0 0
27 17 0 0 0 0
28 18 0 0 0 0
10 30 0 0 0 0
M END
$$$$
1,3-dihydro-5-phenyl-1,4-benzodiazepin-2-one_p2.sdf
COSMOTHERM 3D 0

31 33 0 0 0 0 0 0 0 0 0 V2000
2.1892 3.0098 -0.1068 C 0 0 0 0 0 0 0 0 0 0 0 1
0.9070 3.0900 -0.6731 C 0 0 0 0 0 0 0 0 0 0 0 2
0.1202 1.9512 -0.7423 C 0 0 0 0 0 0 0 0 0 0 0 3
0.5949 0.6945 -0.2863 C 0 0 0 0 0 0 0 0 0 0 0 4
1.9207 0.6170 0.2408 C 0 0 0 0 0 0 0 0 0 0 0 5
2.6849 1.7923 0.3450 C 0 0 0 0 0 0 0 0 0 0 0 6
-0.3176 -0.4371 -0.3040 C 0 0 0 0 0 0 0 0 0 0 0 7
2.4905 -0.5592 0.7583 N 0 0 0 0 0 0 0 0 0 0 0 8
2.4522 -1.8301 0.2276 C 0 0 0 0 0 0 0 0 0 0 0 9
1.4905 -1.9870 -0.9493 C 0 0 0 0 0 0 0 0 0 0 0 10
0.1337 -1.6573 -0.5327 N 0 0 0 0 0 0 0 0 0 0 0 11
3.1395 -2.7462 0.6696 O 0 0 0 0 0 0 0 0 0 0 0 12
-1.7569 -0.2784 -0.0596 C 0 0 0 0 0 0 0 0 0 0 0 13
-2.6861 -1.0864 -0.7499 C 0 0 0 0 0 0 0 0 0 0 0 14
-2.2168 0.6483 0.8996 C 0 0 0 0 0 0 0 0 0 0 0 15
-3.5804 0.7508 1.1705 C 0 0 0 0 0 0 0 0 0 0 0 16
-4.4969 -0.0513 0.4798 C 0 0 0 0 0 0 0 0 0 0 0 17
-4.0484 -0.9659 -0.4818 C 0 0 0 0 0 0 0 0 0 0 0 18
2.8100 3.9030 -0.0274 H 0 0 0 0 0 0 0 0 0 0 0 19
0.5274 4.0400 -1.0486 H 0 0 0 0 0 0 0 0 0 0 0 20
-0.8785 2.0056 -1.1740 H 0 0 0 0 0 0 0 0 0 0 0 21
3.6846 1.7319 0.7777 H 0 0 0 0 0 0 0 0 0 0 0 22
1.7945 -1.3193 -1.7701 H 0 0 0 0 0 0 0 0 0 0 0 23
-2.3467 -1.7749 -1.5258 H 0 0 0 0 0 0 0 0 0 0 0 24
-1.5032 1.2582 1.4538 H 0 0 0 0 0 0 0 0 0 0 0 25
-3.9292 1.4571 1.9249 H 0 0 0 0 0 0 0 0 0 0 0 26
-5.5640 0.0385 0.6883 H 0 0 0 0 0 0 0 0 0 0 0 27
-4.7637 -1.5775 -1.0328 H 0 0 0 0 0 0 0 0 0 0 0 28
1.5079 -3.0231 -1.2935 H 0 0 0 0 0 0 0 0 0 0 0 29
3.2258 -0.4236 1.4556 H 0 0 0 0 0 0 0 0 0 0 0 30
-0.5072 -2.4414 -0.3954 H 0 0 0 0 0 0 0 0 0 0 0 31
2 1 0 0 0 0
6 1 0 0 0 0
19 1 0 0 0 0
3 2 0 0 0 0
20 2 0 0 0 0
4 3 0 0 0 0
21 3 0 0 0 0
5 4 0 0 0 0
7 4 0 0 0 0
6 5 0 0 0 0
8 5 0 0 0 0
22 6 0 0 0 0
11 7 0 0 0 0
13 7 0 0 0 0
9 8 0 0 0 0
30 8 0 0 0 0
10 9 0 0 0 0
12 9 0 0 0 0
11 10 0 0 0 0
23 10 0 0 0 0
29 10 0 0 0 0
14 13 0 0 0 0
15 13 0 0 0 0
18 14 0 0 0 0
24 14 0 0 0 0
16 15 0 0 0 0
25 15 0 0 0 0
17 16 0 0 0 0
26 16 0 0 0 0
18 17 0 0 0 0
27 17 0 0 0 0
28 18 0 0 0 0
11 31 0 0 0 0
M END
$$$$
1-methylindole-cation0.sdf
COSMOTHERM 3D 0

20 21 0 0 0 0 0 0 0 0 0 V2000
-2.1556 -1.1270 0.0657 C 0 0 0 0 0 0 0 0 0 0 0 1
-2.5622 0.1959 -0.1619 C 0 0 0 0 0 0 0 0 0 0 0 2
-1.6357 1.2459 -0.2123 C 0 0 0 0 0 0 0 0 0 0 0 3
-0.2834 0.9406 -0.0289 C 0 0 0 0 0 0 0 0 0 0 0 4
0.0887 -0.3919 0.1966 C 0 0 0 0 0 0 0 0 0 0 0 5
-0.8002 -1.4481 0.2536 C 0 0 0 0 0 0 0 0 0 0 0 6
1.5647 -0.4426 0.3564 N 0 0 0 0 0 0 0 0 0 0 0 7
0.9277 1.7585 -0.0136 C 0 0 0 0 0 0 0 0 0 0 0 8
1.9942 0.9767 0.2092 C 0 0 0 0 0 0 0 0 0 0 0 9
2.2580 -1.3673 -0.6218 C 0 0 0 0 0 0 0 0 0 0 0 10
-2.8989 -1.9239 0.1000 H 0 0 0 0 0 0 0 0 0 0 0 11
-3.6223 0.4108 -0.3025 H 0 0 0 0 0 0 0 0 0 0 0 12
-1.9594 2.2721 -0.3872 H 0 0 0 0 0 0 0 0 0 0 0 13
-0.4833 -2.4749 0.4354 H 0 0 0 0 0 0 0 0 0 0 0 14
0.9671 2.8353 -0.1596 H 0 0 0 0 0 0 0 0 0 0 0 15
3.0555 1.1836 0.2983 H 0 0 0 0 0 0 0 0 0 0 0 16
```

[illegible]

```
5 4 0 0 0 0
8 4 0 0 0 0
6 5 0 0 0 0
7 5 0 0 0 0
16 6 0 0 0 0
9 7 0 0 0 0
10 7 0 0 0 0
9 8 0 0 0 0
11 8 0 0 0 0
12 8 0 0 0 0
17 9 0 0 0 0
18 10 0 0 0 0
19 10 0 0 0 0
10 20 0 0 0 0
M END
$$$$
1-methylindole.sdf
COSMOTHERM 3D 0
19 20 0 0 0 0 0 0 0 0 V2000
1.4007 -2.4885 0.0000 C 0 0 0 0 0 0 0 0 0 0 1
-1.8514 -0.7865 0.0000 C 0 0 0 0 0 0 0 0 0 0 2
-0.9724 0.3481 0.0000 C 0 0 0 0 0 0 0 0 0 0 3
-1.1675 1.7446 0.0000 C 0 0 0 0 0 0 0 0 0 0 4
-0.0554 2.5850 0.0000 C 0 0 0 0 0 0 0 0 0 0 5
1.2570 2.0575 0.0000 C 0 0 0 0 0 0 0 0 0 0 6
1.4859 0.6809 0.0000 C 0 0 0 0 0 0 0 0 0 0 7
0.3670 -0.1661 0.0000 C 0 0 0 0 0 0 0 0 0 0 8
-1.0522 -1.9113 0.0000 C 0 0 0 0 0 0 0 0 0 0 9
0.2844 -1.5493 0.0000 N 0 0 0 0 0 0 0 0 0 0 10
1.3705 -3.1238 -0.8959 H 0 0 0 0 0 0 0 0 0 0 11
2.3429 -1.9312 0.0002 H 0 0 0 0 0 0 0 0 0 0 12
1.3703 -3.1240 0.8958 H 0 0 0 0 0 0 0 0 0 0 13
-2.9379 -0.7771 -0.0001 H 0 0 0 0 0 0 0 0 0 0 14
-2.1776 2.1606 0.0001 H 0 0 0 0 0 0 0 0 0 0 15
-0.1955 3.6678 0.0000 H 0 0 0 0 0 0 0 0 0 0 16
2.1094 2.7393 0.0001 H 0 0 0 0 0 0 0 0 0 0 17
2.5038 0.2877 -0.0001 H 0 0 0 0 0 0 0 0 0 0 18
-1.3268 -2.9628 0.0000 H 0 0 0 0 0 0 0 0 0 0 19
10 1 0 0 0 0
11 1 0 0 0 0
12 1 0 0 0 0
13 1 0 0 0 0
3 2 0 0 0 0
9 2 0 0 0 0
14 2 0 0 0 0
4 3 0 0 0 0
8 3 0 0 0 0
5 4 0 0 0 0
15 4 0 0 0 0
6 5 0 0 0 0
16 5 0 0 0 0
7 6 0 0 0 0
17 6 0 0 0 0
8 7 0 0 0 0
18 7 0 0 0 0
10 8 0 0 0 0
10 9 0 0 0 0
9 19 0 0 0 0
M END
$$$$
1-methylpyrrole-cation0.sdf
COSMOTHERM 3D 0
14 14 0 0 0 0 0 0 0 0 V2000
-0.7328 1.3841 -0.1824 C 0 0 0 0 0 0 0 0 0 0 1
0.7327 1.3842 -0.1825 C 0 0 0 0 0 0 0 0 0 0 2
-1.1730 0.1660 0.1693 C 0 0 0 0 0 0 0 0 0 0 3
0.0000 -0.7000 0.4220 N 0 0 0 0 0 0 0 0 0 0 4
1.1730 0.1661 0.1693 C 0 0 0 0 0 0 0 0 0 0 5
-1.3612 2.2349 -0.4317 H 0 0 0 0 0 0 0 0 0 0 6
1.3612 2.2349 -0.4318 H 0 0 0 0 0 0 0 0 0 0 7
-2.1601 -0.2646 0.2976 H 0 0 0 0 0 0 0 0 0 0 8
0.0000 -1.9666 -0.4123 C 0 0 0 0 0 0 0 0 0 0 9
2.1601 -0.2647 0.2977 H 0 0 0 0 0 0 0 0 0 0 10
0.0002 -0.9798 1.4184 H 0 0 0 0 0 0 0 0 0 0 11
0.8987 -2.5364 -0.1606 H 0 0 0 0 0 0 0 0 0 0 12
0.0010 -1.6722 -1.4656 H 0 0 0 0 0 0 0 0 0 0 13
-0.8998 -2.5353 -0.1621 H 0 0 0 0 0 0 0 0 0 0 14
2 1 0 0 0 0
3 1 0 0 0 0
6 1 0 0 0 0
5 2 0 0 0 0
7 2 0 0 0 0
4 3 0 0 0 0
8 3 0 0 0 0
5 4 0 0 0 0
9 4 0 0 0 0
11 4 0 0 0 0
10 5 0 0 0 0
12 9 0 0 0 0
13 9 0 0 0 0
9 14 0 0 0 0
M END
$$$$
1-methylpyrrole-cation1.sdf
COSMOTHERM 3D 0
14 14 0 0 0 0 0 0 0 0 V2000
0.6199 1.5303 0.0009 C 0 0 0 0 0 0 0 0 0 0 1
-0.7391 1.4695 0.0010 C 0 0 0 0 0 0 0 0 0 0 2
1.1642 0.1513 -0.0007 C 0 0 0 0 0 0 0 0 0 0 3
-0.0379 -0.6861 -0.0019 N 0 0 0 0 0 0 0 0 0 0 4
-1.1051 0.0794 -0.0009 C 0 0 0 0 0 0 0 0 0 0 5
-0.0033 -2.1517 0.0016 C 0 0 0 0 0 0 0 0 0 0 6
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1.2467 2.4187 0.0012 H 0 0 0 0 0 0 0 0 0 0 0 7
-1.4491 2.2912 0.0017 H 0 0 0 0 0 0 0 0 0 0 0 8
-2.1068 -0.3477 -0.0015 H 0 0 0 0 0 0 0 0 0 0 0 9
1.7792 -0.0742 0.8867 H 0 0 0 0 0 0 0 0 0 0 0 10
1.7790 -0.0723 -0.8888 H 0 0 0 0 0 0 0 0 0 0 0 11
-0.4683 -2.5292 0.9200 H 0 0 0 0 0 0 0 0 0 0 0 12
1.0410 -2.4743 -0.0387 H 0 0 0 0 0 0 0 0 0 0 0 13
-0.5393 -2.5343 -0.8748 H 0 0 0 0 0 0 0 0 0 0 0 14
2 1 0 0 0 0
3 1 0 0 0 0
7 1 0 0 0 0
5 2 0 0 0 0
8 2 0 0 0 0
4 3 0 0 0 0
10 3 0 0 0 0
11 3 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
9 5 0 0 0 0
12 6 0 0 0 0
13 6 0 0 0 0
6 14 0 0 0 0
M END
$$$$
1-methylpyrrole-cation2.sdf
COSMOTHERM 3D 0
14 14 0 0 0 0 0 0 0 0 0 V2000
0.7186 1.4840 0.0001 C 0 0 0 0 0 0 0 0 0 0 0 1
-0.7755 1.4249 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 2
1.1110 0.0612 -0.0001 C 0 0 0 0 0 0 0 0 0 0 0 3
0.0355 -0.6820 0.0000 N 0 0 0 0 0 0 0 0 0 0 0 4
-1.1451 0.1320 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 5
1.1407 2.0114 -0.8754 H 0 0 0 0 0 0 0 0 0 0 0 6
1.1405 2.0109 0.8759 H 0 0 0 0 0 0 0 0 0 0 0 7
-0.0135 -2.1469 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 8
-1.4339 2.2880 0.0000 H 0 0 0 0 0 0 0 0 0 0 0 9
2.1106 -0.3669 0.0000 H 0 0 0 0 0 0 0 0 0 0 0 10
-2.1175 -0.3500 0.0001 H 0 0 0 0 0 0 0 0 0 0 0 11
-0.5490 -2.4817 0.8961 H 0 0 0 0 0 0 0 0 0 0 0 12
1.0080 -2.5369 0.0000 H 0 0 0 0 0 0 0 0 0 0 0 13
-0.5490 -2.4817 -0.8961 H 0 0 0 0 0 0 0 0 0 0 0 14
2 1 0 0 0 0
3 1 0 0 0 0
6 1 0 0 0 0
7 1 0 0 0 0
5 2 0 0 0 0
9 2 0 0 0 0
4 3 0 0 0 0
10 3 0 0 0 0
5 4 0 0 0 0
8 4 0 0 0 0
11 5 0 0 0 0
12 8 0 0 0 0
13 8 0 0 0 0
8 14 0 0 0 0
M END
$$$$
1-methylpyrrole.sdf
COSMOTHERM 3D 0
13 13 0 0 0 0 0 0 0 0 0 V2000
-0.7135 1.4603 -0.0135 C 0 0 0 0 0 0 0 0 0 0 0 1
0.7136 1.4602 -0.0135 C 0 0 0 0 0 0 0 0 0 0 0 2
-1.1240 0.1342 0.0110 C 0 0 0 0 0 0 0 0 0 0 0 3
0.0000 -0.6644 0.0317 N 0 0 0 0 0 0 0 0 0 0 0 4
1.1241 0.1340 0.0111 C 0 0 0 0 0 0 0 0 0 0 0 5
0.0000 -2.1239 -0.0245 C 0 0 0 0 0 0 0 0 0 0 0 6
-1.3679 2.3281 -0.0187 H 0 0 0 0 0 0 0 0 0 0 0 7
1.3681 2.3279 -0.0186 H 0 0 0 0 0 0 0 0 0 0 0 8
-2.1163 -0.3070 0.0199 H 0 0 0 0 0 0 0 0 0 0 0 9
2.1164 -0.3071 0.0198 H 0 0 0 0 0 0 0 0 0 0 0 10
0.0211 -2.4806 -1.0645 H 0 0 0 0 0 0 0 0 0 0 0 11
-0.9025 -2.5066 0.4665 H 0 0 0 0 0 0 0 0 0 0 0 12
0.8800 -2.5095 0.5040 H 0 0 0 0 0 0 0 0 0 0 0 13
2 1 0 0 0 0
3 1 0 0 0 0
7 1 0 0 0 0
5 2 0 0 0 0
8 2 0 0 0 0
4 3 0 0 0 0
9 3 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
10 5 0 0 0 0
11 6 0 0 0 0
12 6 0 0 0 0
6 13 0 0 0 0
M END
$$$$
2,3-dihydro-1-methyl-5-phenyl-1,4-benzodiazepine_new.sdf
COSMOTHERM 3D 0
34 36 0 0 0 0 0 0 0 0 0 V2000
0.9866 3.7460 -1.3608 H 0 0 0 0 0 0 0 0 0 0 0 1
1.2460 2.7785 -0.9292 C 0 0 0 0 0 0 0 0 0 0 0 2
0.3300 1.7264 -0.9514 C 0 0 0 0 0 0 0 0 0 0 0 3
0.6325 0.4629 -0.4126 C 0 0 0 0 0 0 0 0 0 0 0 4
1.9223 0.2397 0.1704 C 0 0 0 0 0 0 0 0 0 0 0 5
2.8235 1.3294 0.2122 C 0 0 0 0 0 0 0 0 0 0 0 6
2.4921 2.5729 -0.3263 C 0 0 0 0 0 0 0 0 0 0 0 7
2.2413 -0.9814 0.7815 N 0 0 0 0 0 0 0 0 0 0 0 8
2.1516 -2.2417 0.0094 C 0 0 0 0 0 0 0 0 0 0 0 9
1.1893 -2.1581 -1.1655 C 0 0 0 0 0 0 0 0 0 0 0 10
-0.1731 -1.8364 -0.7422 N 0 0 0 0 0 0 0 0 0 0 0 11
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URL: <http://mc.manuscriptcentral.com/tandf/tmph>

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4 3 0 0 0 0
5 4 0 0 0 0
9 4 0 0 0 0
6 5 0 0 0 0
10 5 0 0 0 0
3 11 0 0 0 0
M END
$$$$
2-methylimidazole.sdf
COSMOtherm 3D 0
12 12 0 0 0 0 0 0 0 0 0 V2000
-2.1570 0.0029 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 1
-0.6655 -0.0460 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 2
0.1269 1.0717 0.0000 N 0 0 0 0 0 0 0 0 0 0 0 3
1.4490 0.6680 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 4
1.4036 -0.7078 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 5
0.0872 -1.1473 0.0000 N 0 0 0 0 0 0 0 0 0 0 0 6
-2.5447 0.5242 -0.8884 H 0 0 0 0 0 0 0 0 0 0 0 7
-2.5512 -1.0201 0.0006 H 0 0 0 0 0 0 0 0 0 0 0 8
-2.5447 0.5253 0.8877 H 0 0 0 0 0 0 0 0 0 0 0 9
-0.1970 2.0357 0.0002 H 0 0 0 0 0 0 0 0 0 0 0 10
2.2676 1.3795 0.0000 H 0 0 0 0 0 0 0 0 0 0 0 11
2.2357 -1.4064 0.0000 H 0 0 0 0 0 0 0 0 0 0 0 12
2 1 0 0 0 0
7 1 0 0 0 0
8 1 0 0 0 0
9 1 0 0 0 0
3 2 0 0 0 0
6 2 0 0 0 0
4 3 0 0 0 0
10 3 0 0 0 0
5 4 0 0 0 0
11 4 0 0 0 0
6 5 0 0 0 0
5 12 0 0 0 0
M END
$$$$
2-methylimidazole_p2.sdf
COSMOtherm 3D 0
13 13 0 0 0 0 0 0 0 0 0 V2000
-2.1742 -0.0005 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 1
-0.6935 0.0008 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 2
0.1190 1.0751 -0.0001 N 0 0 0 0 0 0 0 0 0 0 0 3
1.4465 0.6818 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 4
1.4457 -0.6839 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 5
0.1170 -1.0736 0.0001 N 0 0 0 0 0 0 0 0 0 0 0 6
-2.5598 0.5151 -0.8904 H 0 0 0 0 0 0 0 0 0 0 0 7
-2.5486 -1.0302 0.0005 H 0 0 0 0 0 0 0 0 0 0 0 8
-2.5598 0.5160 0.8900 H 0 0 0 0 0 0 0 0 0 0 0 9
-0.2055 2.0401 0.0003 H 0 0 0 0 0 0 0 0 0 0 0 10
2.2578 1.3986 0.0003 H 0 0 0 0 0 0 0 0 0 0 0 11
2.2555 -1.4022 0.0000 H 0 0 0 0 0 0 0 0 0 0 0 12
-0.2115 -2.0374 -0.0005 H 0 0 0 0 0 0 0 0 0 0 0 13
2 1 0 0 0 0
7 1 0 0 0 0
8 1 0 0 0 0
9 1 0 0 0 0
3 2 0 0 0 0
6 2 0 0 0 0
4 3 0 0 0 0
10 3 0 0 0 0
5 4 0 0 0 0
11 4 0 0 0 0
6 5 0 0 0 0
12 5 0 0 0 0
6 13 0 0 0 0
M END
$$$$
2-methylindole-cation0.sdf
COSMOtherm 3D 0
20 21 0 0 0 0 0 0 0 0 0 V2000
-2.5979 -0.7246 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 1
-2.6258 0.6777 0.0001 C 0 0 0 0 0 0 0 0 0 0 0 2
-1.4455 1.4338 -0.0001 C 0 0 0 0 0 0 0 0 0 0 0 3
-0.2236 0.7522 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 4
-0.2353 -0.6493 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 5
-1.3783 -1.4239 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 6
1.1699 -1.1103 0.0000 N 0 0 0 0 0 0 0 0 0 0 0 7
1.1664 1.1990 0.0001 C 0 0 0 0 0 0 0 0 0 0 0 8
2.0033 0.1440 0.0001 C 0 0 0 0 0 0 0 0 0 0 0 9
1.3829 -1.6940 -0.8255 H 0 0 0 0 0 0 0 0 0 0 0 10
-3.5325 -1.2860 0.0001 H 0 0 0 0 0 0 0 0 0 0 0 11
-3.5884 1.1911 0.0000 H 0 0 0 0 0 0 0 0 0 0 0 12
-1.4789 2.5236 -0.0002 H 0 0 0 0 0 0 0 0 0 0 0 13
-1.3451 -2.5132 -0.0001 H 0 0 0 0 0 0 0 0 0 0 0 14
1.4923 2.2364 0.0001 H 0 0 0 0 0 0 0 0 0 0 0 15
3.4768 -0.0014 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 16
1.3828 -1.6942 0.8253 H 0 0 0 0 0 0 0 0 0 0 0 17
3.8269 -0.5509 0.8879 H 0 0 0 0 0 0 0 0 0 0 0 18
3.9400 0.9923 0.0013 H 0 0 0 0 0 0 0 0 0 0 0 19
3.8269 -0.5485 -0.8895 H 0 0 0 0 0 0 0 0 0 0 0 20
2 1 0 0 0 0
6 1 0 0 0 0
11 1 0 0 0 0
3 2 0 0 0 0
12 2 0 0 0 0
4 3 0 0 0 0
13 3 0 0 0 0
5 4 0 0 0 0
8 4 0 0 0 0
6 5 0 0 0 0
7 5 0 0 0 0
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14 6 0 0 0 0
9 7 0 0 0 0
10 7 0 0 0 0
17 7 0 0 0 0
9 8 0 0 0 0
15 8 0 0 0 0
16 9 0 0 0 0
18 16 0 0 0 0
19 16 0 0 0 0
16 20 0 0 0 0
M END
$$$$
2-methylindole-cation1.sdf
COSMOtherm 3D 0

20 21 0 0 0 0 0 0 0 0 0 V2000
-2.5038 -0.7501 0.1576 C 0 0 0 0 0 0 0 0 0 0 1
-2.5643 0.6881 0.1656 C 0 0 0 0 0 0 0 0 0 0 2
-1.4320 1.4478 0.0374 C 0 0 0 0 0 0 0 0 0 0 3
-0.1783 0.7692 -0.1072 C 0 0 0 0 0 0 0 0 0 0 4
-0.1405 -0.6937 -0.1071 C 0 0 0 0 0 0 0 0 0 0 5
-1.3281 -1.4547 0.0208 C 0 0 0 0 0 0 0 0 0 0 6
1.1229 -1.0955 -0.2449 N 0 0 0 0 0 0 0 0 0 0 7
1.1124 1.2100 -0.2564 C 0 0 0 0 0 0 0 0 0 0 8
2.0275 0.0449 -0.3688 C 0 0 0 0 0 0 0 0 0 0 9
1.4296 -2.0648 -0.3006 H 0 0 0 0 0 0 0 0 0 0 10
3.1922 0.0094 0.6402 C 0 0 0 0 0 0 0 0 0 0 11
2.4507 0.0372 -1.3938 H 0 0 0 0 0 0 0 0 0 0 12
-3.4388 -1.3028 0.2631 H 0 0 0 0 0 0 0 0 0 0 13
-3.5377 1.1660 0.2775 H 0 0 0 0 0 0 0 0 0 0 14
-1.4660 2.5372 0.0399 H 0 0 0 0 0 0 0 0 0 0 15
-1.3057 -2.5438 0.0177 H 0 0 0 0 0 0 0 0 0 0 16
1.4588 2.2404 -0.3020 H 0 0 0 0 0 0 0 0 0 0 17
3.7924 -0.8940 0.4779 H 0 0 0 0 0 0 0 0 0 0 18
3.8291 0.8882 0.4844 H 0 0 0 0 0 0 0 0 0 0 19
2.8101 0.0153 1.6685 H 0 0 0 0 0 0 0 0 0 0 20
2 1 0 0 0 0
6 1 0 0 0 0
13 1 0 0 0 0
3 2 0 0 0 0
14 2 0 0 0 0
4 3 0 0 0 0
15 3 0 0 0 0
5 4 0 0 0 0
8 4 0 0 0 0
6 5 0 0 0 0
7 5 0 0 0 0
16 6 0 0 0 0
9 7 0 0 0 0
10 7 0 0 0 0
9 8 0 0 0 0
17 8 0 0 0 0
11 9 0 0 0 0
12 9 0 0 0 0
18 11 0 0 0 0
19 11 0 0 0 0
11 20 0 0 0 0
M END
$$$$
2-methylindole-cation2.sdf
COSMOtherm 3D 0

20 21 0 0 0 0 0 0 0 0 0 V2000
-2.5678 -0.7821 -0.0022 C 0 0 0 0 0 0 0 0 0 0 1
-2.6381 0.6201 -0.0024 C 0 0 0 0 0 0 0 0 0 0 2
-1.4779 1.4109 -0.0007 C 0 0 0 0 0 0 0 0 0 0 3
-0.2445 0.7668 0.0004 C 0 0 0 0 0 0 0 0 0 0 4
-0.2031 -0.6365 0.0014 C 0 0 0 0 0 0 0 0 0 0 5
-1.3339 -1.4452 0.0000 C 0 0 0 0 0 0 0 0 0 0 6
1.1644 -1.0207 0.0045 N 0 0 0 0 0 0 0 0 0 0 7
1.1752 1.2665 0.0040 C 0 0 0 0 0 0 0 0 0 0 8
1.9834 0.0057 0.0033 C 0 0 0 0 0 0 0 0 0 0 9
1.4775 -1.9945 0.0054 H 0 0 0 0 0 0 0 0 0 0 10
1.4284 1.8773 0.8871 H 0 0 0 0 0 0 0 0 0 0 11
1.4331 1.8851 -0.8720 H 0 0 0 0 0 0 0 0 0 0 12
-3.4877 -1.3678 -0.0040 H 0 0 0 0 0 0 0 0 0 0 13
-3.6151 1.1055 -0.0038 H 0 0 0 0 0 0 0 0 0 0 14
-1.5467 2.4993 -0.0004 H 0 0 0 0 0 0 0 0 0 0 15
-1.2667 -2.5330 0.0005 H 0 0 0 0 0 0 0 0 0 0 16
3.4516 -0.1103 -0.0063 C 0 0 0 0 0 0 0 0 0 0 17
3.8445 0.3302 -0.9366 H 0 0 0 0 0 0 0 0 0 0 18
3.8762 0.4769 0.8216 H 0 0 0 0 0 0 0 0 0 0 19
3.7828 -1.1520 0.0702 H 0 0 0 0 0 0 0 0 0 0 20
2 1 0 0 0 0
6 1 0 0 0 0
13 1 0 0 0 0
3 2 0 0 0 0
14 2 0 0 0 0
4 3 0 0 0 0
15 3 0 0 0 0
5 4 0 0 0 0
8 4 0 0 0 0
6 5 0 0 0 0
7 5 0 0 0 0
16 6 0 0 0 0
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19 17 0 0 0 0
17 20 0 0 0 0
M END
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$$$$
2-methylindole.sdf
COSMOtherm      3D      0

19 20 0 0 0 0 0 0 0 0 0 V2000
-1.4226 -1.4502 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 1
-0.6554 -2.6157 0.0001 C 0 0 0 0 0 0 0 0 0 0 0 0 2
0.7577 -2.5635 0.0001 C 0 0 0 0 0 0 0 0 0 0 0 0 3
1.4348 -1.3417 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 4
0.6621 -0.1735 -0.0001 C 0 0 0 0 0 0 0 0 0 0 0 0 5
-0.7709 -0.1992 -0.0001 C 0 0 0 0 0 0 0 0 0 0 0 0 6
-1.2098 1.1681 -0.0001 C 0 0 0 0 0 0 0 0 0 0 0 0 7
-0.0814 1.9716 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 8
0.0539 3.4621 0.0002 C 0 0 0 0 0 0 0 0 0 0 0 0 9
1.0406 1.1552 -0.0001 N 0 0 0 0 0 0 0 0 0 0 0 0 10
-2.5136 -1.5062 0.0000 H 0 0 0 0 0 0 0 0 0 0 0 0 11
-1.1525 -3.5880 0.0003 H 0 0 0 0 0 0 0 0 0 0 0 0 12
1.3300 -3.4930 0.0001 H 0 0 0 0 0 0 0 0 0 0 0 0 13
2.5257 -1.2997 0.0000 H 0 0 0 0 0 0 0 0 0 0 0 0 14
-2.2366 1.5246 0.0000 H 0 0 0 0 0 0 0 0 0 0 0 0 15
-0.4235 3.9046 0.8868 H 0 0 0 0 0 0 0 0 0 0 0 0 16
1.1098 3.7639 -0.0003 H 0 0 0 0 0 0 0 0 0 0 0 0 17
-0.4243 3.9050 -0.8858 H 0 0 0 0 0 0 0 0 0 0 0 0 18
1.9983 1.4940 0.0003 H 0 0 0 0 0 0 0 0 0 0 0 0 19

2 1 0 0 0 0 0
6 1 0 0 0 0 0
11 1 0 0 0 0 0
3 2 0 0 0 0 0
12 2 0 0 0 0 0
4 3 0 0 0 0 0
13 3 0 0 0 0 0
5 4 0 0 0 0 0
14 4 0 0 0 0 0
6 5 0 0 0 0 0
10 5 0 0 0 0 0
7 6 0 0 0 0 0
8 7 0 0 0 0 0
15 7 0 0 0 0 0
9 8 0 0 0 0 0
10 8 0 0 0 0 0
16 9 0 0 0 0 0
17 9 0 0 0 0 0
18 9 0 0 0 0 0
10 19 0 0 0 0 0

M END
$$$$
2-methylpyrrole-cation0.sdf
COSMOtherm      3D      0

14 14 0 0 0 0 0 0 0 0 0 V2000
-1.4962 0.7071 -0.0002 C 0 0 0 0 0 0 0 0 0 0 0 0 1
-0.1126 1.1814 0.0004 C 0 0 0 0 0 0 0 0 0 0 0 0 2
-1.5102 -0.6352 -0.0007 C 0 0 0 0 0 0 0 0 0 0 0 0 3
-0.1071 -1.0975 0.0005 N 0 0 0 0 0 0 0 0 0 0 0 0 4
0.7374 0.1351 0.0003 C 0 0 0 0 0 0 0 0 0 0 0 0 5
-2.3770 1.3438 -0.0001 H 0 0 0 0 0 0 0 0 0 0 0 0 6
0.1883 2.2257 0.0003 H 0 0 0 0 0 0 0 0 0 0 0 0 7
-2.2959 -1.3823 -0.0008 H 0 0 0 0 0 0 0 0 0 0 0 0 8
0.0919 -1.6922 -0.8220 H 0 0 0 0 0 0 0 0 0 0 0 0 9
2.2128 -0.0005 -0.0005 C 0 0 0 0 0 0 0 0 0 0 0 0 10
0.0900 -1.6903 0.8249 H 0 0 0 0 0 0 0 0 0 0 0 0 11
2.5681 -0.5430 -0.8904 H 0 0 0 0 0 0 0 0 0 0 0 0 12
2.6669 0.9974 0.0009 H 0 0 0 0 0 0 0 0 0 0 0 0 13
2.5691 -0.5460 0.8872 H 0 0 0 0 0 0 0 0 0 0 0 0 14

2 1 0 0 0 0 0
3 1 0 0 0 0 0
6 1 0 0 0 0 0
5 2 0 0 0 0 0
7 2 0 0 0 0 0
4 3 0 0 0 0 0
8 3 0 0 0 0 0
5 4 0 0 0 0 0
9 4 0 0 0 0 0
11 4 0 0 0 0 0
10 5 0 0 0 0 0
12 10 0 0 0 0 0
13 10 0 0 0 0 0
10 14 0 0 0 0 0

M END
$$$$
2-methylpyrrole-cation1.sdf
COSMOtherm      3D      0

14 14 0 0 0 0 0 0 0 0 0 V2000
-0.1921 -0.1715 1.1906 C 0 0 0 0 0 0 0 0 0 0 0 0 1
-1.4150 0.1916 0.7185 C 0 0 0 0 0 0 0 0 0 0 0 0 2
0.7343 -0.4376 0.0524 C 0 0 0 0 0 0 0 0 0 0 0 0 3
-0.1315 -0.1667 -1.1008 N 0 0 0 0 0 0 0 0 0 0 0 0 4
-1.3344 0.1808 -0.7178 C 0 0 0 0 0 0 0 0 0 0 0 0 5
0.1684 -0.2583 -2.0714 H 0 0 0 0 0 0 0 0 0 0 0 0 6
0.1105 -0.2731 2.2303 H 0 0 0 0 0 0 0 0 0 0 0 0 7
-2.3065 0.4479 1.2827 H 0 0 0 0 0 0 0 0 0 0 0 0 8
-2.1166 0.4087 -1.4401 H 0 0 0 0 0 0 0 0 0 0 0 0 9
0.9863 -1.5148 0.0300 H 0 0 0 0 0 0 0 0 0 0 0 0 10
2.0334 0.3856 0.0299 C 0 0 0 0 0 0 0 0 0 0 0 0 11
2.6274 0.1337 0.9166 H 0 0 0 0 0 0 0 0 0 0 0 0 12
1.8111 1.4598 0.0382 H 0 0 0 0 0 0 0 0 0 0 0 0 13
2.6172 0.1389 -0.8653 H 0 0 0 0 0 0 0 0 0 0 0 0 14

2 1 0 0 0 0 0
3 1 0 0 0 0 0
7 1 0 0 0 0 0
5 2 0 0 0 0 0
8 2 0 0 0 0 0
4 3 0 0 0 0 0
10 3 0 0 0 0 0
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11 3 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
9 5 0 0 0 0
12 11 0 0 0 0
13 11 0 0 0 0
11 14 0 0 0 0
M END
$$$$
2-methylpyrrole-cation2.sdf
COSMOTHERM 3D 0
14 14 0 0 0 0 0 0 0 0 0 V2000
-0.1919 1.2050 0.0034 C 0 0 0 0 0 0 0 0 0 0 1
-1.5597 0.5949 -0.0041 C 0 0 0 0 0 0 0 0 0 0 2
0.7234 0.0283 0.0053 C 0 0 0 0 0 0 0 0 0 0 3
-0.0309 -1.0475 0.0037 N 0 0 0 0 0 0 0 0 0 0 4
-1.4222 -0.7428 -0.0029 C 0 0 0 0 0 0 0 0 0 0 5
0.0048 1.8551 -0.8670 H 0 0 0 0 0 0 0 0 0 0 6
-0.0052 1.8430 0.8854 H 0 0 0 0 0 0 0 0 0 0 7
0.3326 -2.0030 0.0059 H 0 0 0 0 0 0 0 0 0 0 8
-2.4907 1.1527 -0.0066 H 0 0 0 0 0 0 0 0 0 0 9
2.1976 0.0181 -0.0037 C 0 0 0 0 0 0 0 0 0 0 10
-2.1421 -1.5547 -0.0049 H 0 0 0 0 0 0 0 0 0 0 11
2.5605 0.4533 -0.9485 H 0 0 0 0 0 0 0 0 0 0 12
2.5823 0.6553 0.8056 H 0 0 0 0 0 0 0 0 0 0 13
2.5997 -0.9959 0.1015 H 0 0 0 0 0 0 0 0 0 0 14
2 1 0 0 0 0
3 1 0 0 0 0
6 1 0 0 0 0
7 1 0 0 0 0
5 2 0 0 0 0
9 2 0 0 0 0
4 3 0 0 0 0
10 3 0 0 0 0
5 4 0 0 0 0
8 4 0 0 0 0
11 5 0 0 0 0
12 10 0 0 0 0
13 10 0 0 0 0
10 14 0 0 0 0
M END
$$$$
2-methylpyrrole-cation3.sdf
COSMOTHERM 3D 0
14 14 0 0 0 0 0 0 0 0 0 V2000
-1.4475 -0.7307 0.0001 C 0 0 0 0 0 0 0 0 0 0 1
-0.0284 -1.0499 -0.0001 N 0 0 0 0 0 0 0 0 0 0 2
-1.4426 0.7537 0.0000 C 0 0 0 0 0 0 0 0 0 0 3
-0.1589 1.1963 0.0000 C 0 0 0 0 0 0 0 0 0 0 4
0.7147 0.0406 0.0000 C 0 0 0 0 0 0 0 0 0 0 5
2.1970 0.0252 0.0000 C 0 0 0 0 0 0 0 0 0 0 6
-1.9416 -1.1611 0.8874 H 0 0 0 0 0 0 0 0 0 0 7
0.3323 -2.0035 -0.0002 H 0 0 0 0 0 0 0 0 0 0 8
-2.3511 1.3512 -0.0001 H 0 0 0 0 0 0 0 0 0 0 9
0.1948 2.2233 -0.0001 H 0 0 0 0 0 0 0 0 0 0 10
2.5713 -0.5052 0.8880 H 0 0 0 0 0 0 0 0 0 0 11
2.5946 1.0448 -0.0027 H 0 0 0 0 0 0 0 0 0 0 12
2.5715 -0.5103 -0.8848 H 0 0 0 0 0 0 0 0 0 0 13
-1.9418 -1.1613 -0.8871 H 0 0 0 0 0 0 0 0 0 0 14
2 1 0 0 0 0
3 1 0 0 0 0
7 1 0 0 0 0
5 2 0 0 0 0
8 2 0 0 0 0
4 3 0 0 0 0
9 3 0 0 0 0
5 4 0 0 0 0
10 4 0 0 0 0
6 5 0 0 0 0
11 6 0 0 0 0
12 6 0 0 0 0
13 6 0 0 0 0
1 14 0 0 0 0
M END
$$$$
2-methylpyrrole-cation4.sdf
COSMOTHERM 3D 0
14 14 0 0 0 0 0 0 0 0 0 V2000
-1.3621 -0.7884 0.0001 C 0 0 0 0 0 0 0 0 0 0 1
-0.0867 -1.0606 -0.0001 N 0 0 0 0 0 0 0 0 0 0 2
-1.5232 0.6774 0.0001 C 0 0 0 0 0 0 0 0 0 0 3
-0.1147 1.1770 -0.0001 C 0 0 0 0 0 0 0 0 0 0 4
0.7304 0.1215 -0.0003 C 0 0 0 0 0 0 0 0 0 0 5
2.2114 0.0013 0.0002 C 0 0 0 0 0 0 0 0 0 0 6
0.2949 -2.0100 -0.0003 H 0 0 0 0 0 0 0 0 0 0 7
-2.1169 1.0034 0.8747 H 0 0 0 0 0 0 0 0 0 0 8
0.1693 2.2248 -0.0003 H 0 0 0 0 0 0 0 0 0 0 9
2.5645 -0.5373 0.8923 H 0 0 0 0 0 0 0 0 0 0 10
2.6633 0.9997 -0.0055 H 0 0 0 0 0 0 0 0 0 0 11
2.5643 -0.5476 -0.8858 H 0 0 0 0 0 0 0 0 0 0 12
-2.1233 -1.5649 0.0001 H 0 0 0 0 0 0 0 0 0 0 13
-2.1171 1.0033 -0.8744 H 0 0 0 0 0 0 0 0 0 0 14
2 1 0 0 0 0
3 1 0 0 0 0
13 1 0 0 0 0
5 2 0 0 0 0
7 2 0 0 0 0
4 3 0 0 0 0
8 3 0 0 0 0
5 4 0 0 0 0
9 4 0 0 0 0
6 5 0 0 0 0
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10 6 0 0 0 0
11 6 0 0 0 0
12 6 0 0 0 0
3 14 0 0 0 0
M END
$$$$
2-methylpyrrole.sdf
COSMOtherm 3D 0

13 13 0 0 0 0 0 0 0 0 0 V2000
0.1624 -1.1720 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 1
1.5031 -0.6733 -0.0001 C 0 0 0 0 0 0 0 0 0 0 0 2
-0.7011 -0.0818 0.0001 C 0 0 0 0 0 0 0 0 0 0 0 3
0.0891 1.0512 0.0001 N 0 0 0 0 0 0 0 0 0 0 0 4
1.4267 0.7103 -0.0001 C 0 0 0 0 0 0 0 0 0 0 0 5
-2.1950 -0.0100 -0.0001 C 0 0 0 0 0 0 0 0 0 0 0 6
-0.2636 2.0039 -0.0001 H 0 0 0 0 0 0 0 0 0 0 0 7
-0.1456 -2.2148 0.0002 H 0 0 0 0 0 0 0 0 0 0 0 8
2.4184 -1.2597 0.0000 H 0 0 0 0 0 0 0 0 0 0 0 9
2.1979 1.4742 -0.0001 H 0 0 0 0 0 0 0 0 0 0 0 10
-2.5824 0.5172 0.8865 H 0 0 0 0 0 0 0 0 0 0 0 11
-2.6169 -1.0233 0.0019 H 0 0 0 0 0 0 0 0 0 0 0 12
-2.5824 0.5137 -0.8887 H 0 0 0 0 0 0 0 0 0 0 0 13

2 1 0 0 0 0
3 1 0 0 0 0
8 1 0 0 0 0
5 2 0 0 0 0
9 2 0 0 0 0
4 3 0 0 0 0
6 3 0 0 0 0
5 4 0 0 0 0
7 4 0 0 0 0
10 5 0 0 0 0
11 6 0 0 0 0
12 6 0 0 0 0
6 13 0 0 0 0
M END
$$$$
2-methylpyrrole0.sdf
COSMOtherm 3D 0

13 13 0 0 0 0 0 0 0 0 0 V2000
0.0000 1.1720 -0.1624 C 0 0 0 0 0 0 0 0 0 0 0 1
0.0000 0.6733 -1.5031 C 0 0 0 0 0 0 0 0 0 0 0 2
0.0000 0.0818 0.7012 C 0 0 0 0 0 0 0 0 0 0 0 3
0.0000 -1.0512 -0.0892 N 0 0 0 0 0 0 0 0 0 0 0 4
0.0000 -0.7103 -1.4267 C 0 0 0 0 0 0 0 0 0 0 0 5
0.0000 0.0100 2.1950 C 0 0 0 0 0 0 0 0 0 0 0 6
-0.0001 -2.0039 0.2636 H 0 0 0 0 0 0 0 0 0 0 0 7
-0.0001 2.2148 0.1456 H 0 0 0 0 0 0 0 0 0 0 0 8
-0.0001 1.2597 -2.4184 H 0 0 0 0 0 0 0 0 0 0 0 9
0.0000 -1.4742 -2.1979 H 0 0 0 0 0 0 0 0 0 0 0 10
0.8883 -0.5143 2.5825 H 0 0 0 0 0 0 0 0 0 0 0 11
-0.8869 -0.5166 2.5824 H 0 0 0 0 0 0 0 0 0 0 0 12
-0.0014 1.0233 2.6169 H 0 0 0 0 0 0 0 0 0 0 0 13

2 1 0 0 0 0
3 1 0 0 0 0
8 1 0 0 0 0
5 2 0 0 0 0
9 2 0 0 0 0
4 3 0 0 0 0
6 3 0 0 0 0
5 4 0 0 0 0
7 4 0 0 0 0
10 5 0 0 0 0
11 6 0 0 0 0
12 6 0 0 0 0
6 13 0 0 0 0
M END
$$$$
2-methylpyrrole1.sdf
COSMOtherm 3D 0

13 13 0 0 0 0 0 0 0 0 0 V2000
-0.1687 1.1744 -0.0003 C 0 0 0 0 0 0 0 0 0 0 0 1
-1.5057 0.6688 0.0003 C 0 0 0 0 0 0 0 0 0 0 0 2
0.7005 0.0872 -0.0006 C 0 0 0 0 0 0 0 0 0 0 0 3
-0.0854 -1.0479 -0.0003 N 0 0 0 0 0 0 0 0 0 0 0 4
-1.4243 -0.7155 0.0002 C 0 0 0 0 0 0 0 0 0 0 0 5
2.1970 0.0108 0.0004 C 0 0 0 0 0 0 0 0 0 0 0 6
0.2752 -1.9978 -0.0002 H 0 0 0 0 0 0 0 0 0 0 0 7
0.1311 2.2197 -0.0003 H 0 0 0 0 0 0 0 0 0 0 0 8
-2.4236 1.2513 0.0006 H 0 0 0 0 0 0 0 0 0 0 0 9
-2.1915 -1.4831 0.0003 H 0 0 0 0 0 0 0 0 0 0 0 10
2.5369 -1.0342 -0.0134 H 0 0 0 0 0 0 0 0 0 0 0 11
2.6272 0.4880 0.8940 H 0 0 0 0 0 0 0 0 0 0 0 12
2.6289 0.5123 -0.8788 H 0 0 0 0 0 0 0 0 0 0 0 13

2 1 0 0 0 0
3 1 0 0 0 0
8 1 0 0 0 0
5 2 0 0 0 0
9 2 0 0 0 0
4 3 0 0 0 0
6 3 0 0 0 0
5 4 0 0 0 0
7 4 0 0 0 0
10 5 0 0 0 0
11 6 0 0 0 0
12 6 0 0 0 0
6 13 0 0 0 0
M END
$$$$
3-aminopyridine.sdf
COSMOtherm 3D 0
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13 13 0 0 0 0 0 0 0 0 0 V2000
-2.3249 -0.0284 0.0000 N 0 0 0 0 0 0 0 0 0 0 1
-0.9572 0.0159 0.0000 C 0 0 0 0 0 0 0 0 0 0 2
-0.1851 -1.1746 0.0000 C 0 0 0 0 0 0 0 0 0 0 3
1.1546 -1.1985 0.0000 N 0 0 0 0 0 0 0 0 0 0 4
1.8161 -0.0225 0.0000 C 0 0 0 0 0 0 0 0 0 0 5
1.1486 1.2074 0.0000 C 0 0 0 0 0 0 0 0 0 0 6
-0.2436 1.2354 0.0000 C 0 0 0 0 0 0 0 0 0 0 7
-2.8204 -0.9120 0.0003 H 0 0 0 0 0 0 0 0 0 0 8
-2.8772 0.8206 -0.0004 H 0 0 0 0 0 0 0 0 0 0 9
-0.6941 -2.1443 0.0000 H 0 0 0 0 0 0 0 0 0 0 10
2.9074 -0.0733 0.0000 H 0 0 0 0 0 0 0 0 0 0 11
1.7172 2.1391 0.0000 H 0 0 0 0 0 0 0 0 0 0 12
-0.7841 2.1846 0.0000 H 0 0 0 0 0 0 0 0 0 0 13
2 1 0 0 0 0
8 1 0 0 0 0
9 1 0 0 0 0
3 2 0 0 0 0
7 2 0 0 0 0
4 3 0 0 0 0
10 3 0 0 0 0
5 4 0 0 0 0
6 5 0 0 0 0
11 5 0 0 0 0
7 6 0 0 0 0
12 6 0 0 0 0
7 13 0 0 0 0
M END
$$$$
3-aminopyridine_p1.sdf
COSMOTHERM 3D 0
14 14 0 0 0 0 0 0 0 0 0 V2000
-2.3403 -0.0230 -0.0346 N 0 0 0 0 0 0 0 0 0 0 1
-0.9807 0.0114 0.0052 C 0 0 0 0 0 0 0 0 0 0 2
-0.2265 -1.1784 0.0062 C 0 0 0 0 0 0 0 0 0 0 3
1.1195 -1.1169 -0.0002 N 0 0 0 0 0 0 0 0 0 0 4
1.8329 0.0292 -0.0040 C 0 0 0 0 0 0 0 0 0 0 5
1.1322 1.2320 0.0001 C 0 0 0 0 0 0 0 0 0 0 6
-0.2562 1.2316 0.0053 C 0 0 0 0 0 0 0 0 0 0 7
-2.8279 -0.8927 0.1567 H 0 0 0 0 0 0 0 0 0 0 8
-2.8602 0.8264 0.1618 H 0 0 0 0 0 0 0 0 0 0 9
-0.6700 -2.1712 0.0101 H 0 0 0 0 0 0 0 0 0 0 10
2.9150 -0.0622 -0.0082 H 0 0 0 0 0 0 0 0 0 0 11
1.6851 2.1698 0.0014 H 0 0 0 0 0 0 0 0 0 0 12
-0.8028 2.1758 0.0092 H 0 0 0 0 0 0 0 0 0 0 13
1.6294 -2.0028 0.0010 H 0 0 0 0 0 0 0 0 0 0 14
2 1 0 0 0 0
8 1 0 0 0 0
9 1 0 0 0 0
3 2 0 0 0 0
7 2 0 0 0 0
4 3 0 0 0 0
10 3 0 0 0 0
5 4 0 0 0 0
6 5 0 0 0 0
11 5 0 0 0 0
7 6 0 0 0 0
12 6 0 0 0 0
13 7 0 0 0 0
4 14 0 0 0 0
M END
$$$$
3-hydro-2-methylamine-4-oxy-5-phenyl-1,4-benzodiazepine.sdf
COSMOTHERM 3D 0
35 37 0 0 0 0 0 0 0 0 0 V2000
-3.8018 -1.1222 -0.1384 C 0 0 0 0 0 0 0 0 0 0 1
-3.5153 0.1501 -0.6661 C 0 0 0 0 0 0 0 0 0 0 2
-2.1983 0.5832 -0.7209 C 0 0 0 0 0 0 0 0 0 0 3
-1.1154 -0.2276 -0.2911 C 0 0 0 0 0 0 0 0 0 0 4
-1.4091 -1.5355 0.2288 C 0 0 0 0 0 0 0 0 0 0 5
-2.7688 -1.9329 0.3084 C 0 0 0 0 0 0 0 0 0 0 6
0.2261 0.3675 -0.3302 C 0 0 0 0 0 0 0 0 0 0 7
1.2940 -0.3702 -0.6572 N 0 0 0 0 0 0 0 0 0 0 8
1.0852 -1.8004 -1.0280 C 0 0 0 0 0 0 0 0 0 0 9
-0.4850 -2.4291 0.7505 N 0 0 0 0 0 0 0 0 0 0 10
0.7169 -2.5323 0.2399 C 0 0 0 0 0 0 0 0 0 0 11
0.4202 1.8015 -0.0137 C 0 0 0 0 0 0 0 0 0 0 12
1.6568 -3.2715 0.8730 N 0 0 0 0 0 0 0 0 0 0 13
-0.2315 2.3564 1.1052 C 0 0 0 0 0 0 0 0 0 0 14
-0.0803 3.7096 1.4202 C 0 0 0 0 0 0 0 0 0 0 15
0.7106 4.5343 0.6125 C 0 0 0 0 0 0 0 0 0 0 16
1.3558 3.9942 -0.5081 C 0 0 0 0 0 0 0 0 0 0 17
1.2206 2.6390 -0.8159 C 0 0 0 0 0 0 0 0 0 0 18
2.9426 -3.7037 0.3266 C 0 0 0 0 0 0 0 0 0 0 19
2.5230 0.0323 -0.6226 O 0 0 0 0 0 0 0 0 0 0 20
1.3395 -3.7251 1.7280 H 0 0 0 0 0 0 0 0 0 0 21
-4.8339 -1.4725 -0.0755 H 0 0 0 0 0 0 0 0 0 0 22
-4.3183 0.7957 -1.0244 H 0 0 0 0 0 0 0 0 0 0 23
-1.9764 1.5755 -1.1163 H 0 0 0 0 0 0 0 0 0 0 24
-2.9770 -2.9161 0.7348 H 0 0 0 0 0 0 0 0 0 0 25
0.2619 -1.8687 -1.7515 H 0 0 0 0 0 0 0 0 0 0 26
2.0171 -2.1339 -1.4879 H 0 0 0 0 0 0 0 0 0 0 27
-0.8542 1.7193 1.7354 H 0 0 0 0 0 0 0 0 0 0 28
-0.5838 4.1201 2.2973 H 0 0 0 0 0 0 0 0 0 0 29
0.8253 5.5925 0.8542 H 0 0 0 0 0 0 0 0 0 0 30
1.9686 4.6334 -1.1465 H 0 0 0 0 0 0 0 0 0 0 31
1.7343 2.2256 -1.6832 H 0 0 0 0 0 0 0 0 0 0 32
3.4859 -4.2185 1.1259 H 0 0 0 0 0 0 0 0 0 0 33
2.8230 -4.4006 -0.5174 H 0 0 0 0 0 0 0 0 0 0 34
3.5470 -2.8455 0.0054 H 0 0 0 0 0 0 0 0 0 0 35
2 1 0 0 0 0
6 1 0 0 0 0
22 1 0 0 0 0
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3 2 0 0 0 0
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27 9 0 0 0 0
11 10 0 0 0 0
13 11 0 0 0 0
14 12 0 0 0 0
18 12 0 0 0 0
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21 13 0 0 0 0
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28 14 0 0 0 0
16 15 0 0 0 0
29 15 0 0 0 0
17 16 0 0 0 0
30 16 0 0 0 0
18 17 0 0 0 0
31 17 0 0 0 0
32 18 0 0 0 0
33 19 0 0 0 0
34 19 0 0 0 0
19 35 0 0 0 0
M END
$$$$
3-hydro-2-methylamine-4-oxy-5-phenyl-1,4-benzodiazepine_pl.sdf
COSMOTHERM 3D 0
36 38 0 0 0 0 0 0 0 0 0 V2000
1.0299 0.1384 -3.8176 C 0 0 0 0 0 0 0 0 0 0 1
-0.2108 0.7111 -3.5015 C 0 0 0 0 0 0 0 0 0 0 2
-0.6226 0.7834 -2.1766 C 0 0 0 0 0 0 0 0 0 0 3
0.1842 0.3093 -1.1138 C 0 0 0 0 0 0 0 0 0 0 4
1.4548 -0.2279 -1.4572 C 0 0 0 0 0 0 0 0 0 0 5
1.8552 -0.3258 -2.7995 C 0 0 0 0 0 0 0 0 0 0 6
-0.3845 0.3261 0.2424 C 0 0 0 0 0 0 0 0 0 0 7
0.3780 0.6358 1.2967 N 0 0 0 0 0 0 0 0 0 0 8
1.8117 1.0163 1.0629 C 0 0 0 0 0 0 0 0 0 0 9
2.3513 -0.7452 -0.4911 N 0 0 0 0 0 0 0 0 0 0 10
2.5661 -0.2273 0.7258 C 0 0 0 0 0 0 0 0 0 0 11
-1.8133 0.0085 0.4496 C 0 0 0 0 0 0 0 0 0 0 12
3.3846 -0.8145 1.5809 N 0 0 0 0 0 0 0 0 0 0 13
-2.3851 -1.0758 -0.2463 C 0 0 0 0 0 0 0 0 0 0 14
-3.7357 -1.3914 -0.0822 C 0 0 0 0 0 0 0 0 0 0 15
-4.5397 -0.6186 0.7632 C 0 0 0 0 0 0 0 0 0 0 16
-3.9821 0.4667 1.4516 C 0 0 0 0 0 0 0 0 0 0 17
-2.6286 0.7754 1.3063 C 0 0 0 0 0 0 0 0 0 0 18
3.7690 -0.3108 2.9062 C 0 0 0 0 0 0 0 0 0 0 19
0.0094 0.6077 2.5273 O 0 0 0 0 0 0 0 0 0 0 20
3.8481 -1.6707 1.2750 H 0 0 0 0 0 0 0 0 0 0 21
1.3578 0.0649 -4.8550 H 0 0 0 0 0 0 0 0 0 0 22
-0.8571 1.0951 -4.2913 H 0 0 0 0 0 0 0 0 0 0 23
-1.5949 1.2130 -1.9361 H 0 0 0 0 0 0 0 0 0 0 24
2.8287 -0.7615 -3.0302 H 0 0 0 0 0 0 0 0 0 0 25
1.8743 1.7311 0.2317 H 0 0 0 0 0 0 0 0 0 0 26
2.1569 1.4878 1.9834 H 0 0 0 0 0 0 0 0 0 0 27
-1.7652 -1.6799 -0.9105 H 0 0 0 0 0 0 0 0 0 0 28
-4.1607 -2.2415 -0.6184 H 0 0 0 0 0 0 0 0 0 0 29
-5.5967 -0.8610 0.8867 H 0 0 0 0 0 0 0 0 0 0 30
-4.6060 1.0774 2.1066 H 0 0 0 0 0 0 0 0 0 0 31
-2.2022 1.6160 1.8519 H 0 0 0 0 0 0 0 0 0 0 32
4.2496 -1.1362 3.4388 H 0 0 0 0 0 0 0 0 0 0 33
4.4793 0.5218 2.8180 H 0 0 0 0 0 0 0 0 0 0 34
2.8860 0.0034 3.4731 H 0 0 0 0 0 0 0 0 0 0 35
2.9323 -1.5313 -0.7900 H 0 0 0 0 0 0 0 0 0 0 36
2 1 0 0 0 0
6 1 0 0 0 0
22 1 0 0 0 0
3 2 0 0 0 0
23 2 0 0 0 0
4 3 0 0 0 0
24 3 0 0 0 0
5 4 0 0 0 0
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10 5 0 0 0 0
25 6 0 0 0 0
8 7 0 0 0 0
12 7 0 0 0 0
9 8 0 0 0 0
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11 9 0 0 0 0
26 9 0 0 0 0
27 9 0 0 0 0
11 10 0 0 0 0
13 11 0 0 0 0
14 12 0 0 0 0
18 12 0 0 0 0
19 13 0 0 0 0
21 13 0 0 0 0
15 14 0 0 0 0
28 14 0 0 0 0
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29 15 0 0 0 0
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6 1 0 0 0 0
13 1 0 0 0 0
3 2 0 0 0 0
14 2 0 0 0 0
4 3 0 0 0 0
15 3 0 0 0 0
5 4 0 0 0 0
8 4 0 0 0 0
6 5 0 0 0 0
7 5 0 0 0 0
16 6 0 0 0 0
9 7 0 0 0 0
10 7 0 0 0 0
9 8 0 0 0 0
11 8 0 0 0 0
12 8 0 0 0 0
17 9 0 0 0 0
18 11 0 0 0 0
19 11 0 0 0 0
11 20 0 0 0 0
M END
$$$$
3-methylindole.sdf
COSMOtherm 3D 0

19 20 0 0 0 0 0 0 0 0 0 V2000
-0.1901 -0.4240 0.0001 C 0 0 0 0 0 0 0 0 0 0 1
0.6938 -1.5229 0.0000 C 0 0 0 0 0 0 0 0 0 0 2
2.0688 -1.2878 0.0000 C 0 0 0 0 0 0 0 0 0 0 3
2.5850 0.0294 0.0000 C 0 0 0 0 0 0 0 0 0 0 4
1.7384 1.1393 -0.0001 C 0 0 0 0 0 0 0 0 0 0 5
0.3569 0.9005 0.0001 C 0 0 0 0 0 0 0 0 0 0 6
0.3090 -2.5451 0.0000 H 0 0 0 0 0 0 0 0 0 0 7
2.7613 -2.1318 0.0000 H 0 0 0 0 0 0 0 0 0 0 8
3.6661 0.1816 -0.0001 H 0 0 0 0 0 0 0 0 0 0 9
2.1380 2.1553 -0.0002 H 0 0 0 0 0 0 0 0 0 0 10
-1.6277 -0.2968 0.0000 C 0 0 0 0 0 0 0 0 0 0 11
-1.8922 1.0595 0.0000 C 0 0 0 0 0 0 0 0 0 0 12
-2.6308 -1.4112 0.0000 C 0 0 0 0 0 0 0 0 0 0 13
-0.7070 1.7787 0.0000 N 0 0 0 0 0 0 0 0 0 0 14
-2.8458 1.5810 0.0000 H 0 0 0 0 0 0 0 0 0 0 15
-2.5203 -2.0580 0.8852 H 0 0 0 0 0 0 0 0 0 0 16
-3.6568 -1.0183 -0.0006 H 0 0 0 0 0 0 0 0 0 0 17
-2.5195 -2.0587 -0.8847 H 0 0 0 0 0 0 0 0 0 0 18
-0.6405 2.7915 0.0000 H 0 0 0 0 0 0 0 0 0 0 19
2 1 0 0 0 0
6 1 0 0 0 0
11 1 0 0 0 0
3 2 0 0 0 0
7 2 0 0 0 0
4 3 0 0 0 0
8 3 0 0 0 0
5 4 0 0 0 0
9 4 0 0 0 0
6 5 0 0 0 0
10 5 0 0 0 0
14 6 0 0 0 0
12 11 0 0 0 0
13 11 0 0 0 0
14 12 0 0 0 0
15 12 0 0 0 0
16 13 0 0 0 0
17 13 0 0 0 0
18 13 0 0 0 0
14 19 0 0 0 0
M END
$$$$
3-methylpyrrole-cation0.sdf
COSMOtherm 3D 0

14 14 0 0 0 0 0 0 0 0 0 V2000
-1.1699 -0.0939 0.0004 C 0 0 0 0 0 0 0 0 0 0 1
0.0302 0.7632 0.0010 C 0 0 0 0 0 0 0 0 0 0 2
-0.8087 -1.3850 -0.0003 C 0 0 0 0 0 0 0 0 0 0 3
0.6662 -1.4411 -0.0007 N 0 0 0 0 0 0 0 0 0 0 4
1.1155 -0.0365 0.0010 C 0 0 0 0 0 0 0 0 0 0 5
-2.1942 0.2709 0.0014 H 0 0 0 0 0 0 0 0 0 0 6
0.0034 2.2543 -0.0007 C 0 0 0 0 0 0 0 0 0 0 7
-1.3576 -2.3200 0.0003 H 0 0 0 0 0 0 0 0 0 0 8
1.0227 -1.9555 -0.8249 H 0 0 0 0 0 0 0 0 0 0 9
2.1826 0.1577 0.0011 H 0 0 0 0 0 0 0 0 0 0 10
1.0239 -1.9583 0.8212 H 0 0 0 0 0 0 0 0 0 0 11
-0.5111 2.6262 -0.8997 H 0 0 0 0 0 0 0 0 0 0 12
-0.5567 2.6285 0.8694 H 0 0 0 0 0 0 0 0 0 0 13
1.0157 2.6752 0.0241 H 0 0 0 0 0 0 0 0 0 0 14
2 1 0 0 0 0
3 1 0 0 0 0
6 1 0 0 0 0
5 2 0 0 0 0
7 2 0 0 0 0
4 3 0 0 0 0
8 3 0 0 0 0
5 4 0 0 0 0
9 4 0 0 0 0
11 4 0 0 0 0
10 5 0 0 0 0
12 7 0 0 0 0
13 7 0 0 0 0
7 14 0 0 0 0
M END
$$$$
3-methylpyrrole-cation1.sdf
COSMOtherm 3D 0

14 14 0 0 0 0 0 0 0 0 0 V2000
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0.7564 0.0519 -0.0048 C 0 0 0 0 0 0 0 0 0 0 0 1
-0.0388 1.1687 -0.0035 C 0 0 0 0 0 0 0 0 0 0 0 2
-0.1347 -1.1507 -0.0036 C 0 0 0 0 0 0 0 0 0 0 0 3
-1.4709 -0.5724 0.0034 N 0 0 0 0 0 0 0 0 0 0 0 4
-1.4017 0.7393 0.0025 C 0 0 0 0 0 0 0 0 0 0 0 5
-2.3314 -1.1180 0.0040 H 0 0 0 0 0 0 0 0 0 0 0 6
2.2373 -0.0298 0.0032 C 0 0 0 0 0 0 0 0 0 0 0 7
0.2798 2.2070 -0.0056 H 0 0 0 0 0 0 0 0 0 0 0 8
-2.3019 1.3515 0.0058 H 0 0 0 0 0 0 0 0 0 0 0 9
0.0100 -1.7927 0.8802 H 0 0 0 0 0 0 0 0 0 0 0 10
0.0020 -1.7839 -0.8953 H 0 0 0 0 0 0 0 0 0 0 0 11
2.5980 -0.6823 -0.8064 H 0 0 0 0 0 0 0 0 0 0 0 12
2.6918 0.9619 -0.1027 H 0 0 0 0 0 0 0 0 0 0 0 13
2.5879 -0.4785 0.9468 H 0 0 0 0 0 0 0 0 0 0 0 14
2 1 0 0 0 0
3 1 0 0 0 0
7 1 0 0 0 0
5 2 0 0 0 0
8 2 0 0 0 0
4 3 0 0 0 0
10 3 0 0 0 0
11 3 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
9 5 0 0 0 0
12 7 0 0 0 0
13 7 0 0 0 0
7 14 0 0 0 0
M END
$$$$
3-methylpyrrole-cation2.sdf
COSMOTHERM 3D 0
14 14 0 0 0 0 0 0 0 0 0 V2000
-0.0193 0.7566 -0.4119 C 0 0 0 0 0 0 0 0 0 0 0 1
-1.1951 -0.1421 -0.1510 C 0 0 0 0 0 0 0 0 0 0 0 2
1.1327 -0.1438 -0.1635 C 0 0 0 0 0 0 0 0 0 0 0 3
0.6827 -1.3273 0.1501 N 0 0 0 0 0 0 0 0 0 0 0 4
-0.7410 -1.3685 0.1689 C 0 0 0 0 0 0 0 0 0 0 0 5
0.0120 0.9867 -1.4996 H 0 0 0 0 0 0 0 0 0 0 0 6
0.0199 2.1030 0.3494 C 0 0 0 0 0 0 0 0 0 0 0 7
1.2745 -2.1371 0.3509 H 0 0 0 0 0 0 0 0 0 0 0 8
-2.2341 0.1638 -0.2291 H 0 0 0 0 0 0 0 0 0 0 0 9
2.1964 0.0735 -0.2304 H 0 0 0 0 0 0 0 0 0 0 0 10
-1.2425 -2.2987 0.4144 H 0 0 0 0 0 0 0 0 0 0 0 11
0.9236 2.6635 0.0806 H 0 0 0 0 0 0 0 0 0 0 0 12
-0.8592 2.6967 0.0722 H 0 0 0 0 0 0 0 0 0 0 0 13
0.0094 1.9339 1.4328 H 0 0 0 0 0 0 0 0 0 0 0 14
2 1 0 0 0 0
3 1 0 0 0 0
6 1 0 0 0 0
7 1 0 0 0 0
5 2 0 0 0 0
9 2 0 0 0 0
4 3 0 0 0 0
10 3 0 0 0 0
5 4 0 0 0 0
8 4 0 0 0 0
11 5 0 0 0 0
12 7 0 0 0 0
13 7 0 0 0 0
7 14 0 0 0 0
M END
$$$$
3-methylpyrrole-cation3.sdf
COSMOTHERM 3D 0
14 14 0 0 0 0 0 0 0 0 0 V2000
-0.0474 0.7697 0.0001 C 0 0 0 0 0 0 0 0 0 0 0 1
-1.1459 -0.0428 0.0001 C 0 0 0 0 0 0 0 0 0 0 0 2
1.0998 -0.1116 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 3
0.7246 -1.3661 0.0001 N 0 0 0 0 0 0 0 0 0 0 0 4
-0.7276 -1.4656 -0.0001 C 0 0 0 0 0 0 0 0 0 0 0 5
0.0307 2.2621 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 6
-2.1888 0.2658 0.0000 H 0 0 0 0 0 0 0 0 0 0 0 7
2.1548 0.1591 -0.0001 H 0 0 0 0 0 0 0 0 0 0 0 8
1.3540 -2.1683 -0.0003 H 0 0 0 0 0 0 0 0 0 0 0 9
-1.0710 -2.0251 0.8865 H 0 0 0 0 0 0 0 0 0 0 0 10
0.5744 2.6256 0.8843 H 0 0 0 0 0 0 0 0 0 0 0 11
-0.9731 2.7030 0.0032 H 0 0 0 0 0 0 0 0 0 0 0 12
0.5685 2.6256 -0.8880 H 0 0 0 0 0 0 0 0 0 0 0 13
-1.0706 -2.0243 -0.8873 H 0 0 0 0 0 0 0 0 0 0 0 14
2 1 0 0 0 0
3 1 0 0 0 0
6 1 0 0 0 0
5 2 0 0 0 0
7 2 0 0 0 0
4 3 0 0 0 0
8 3 0 0 0 0
5 4 0 0 0 0
9 4 0 0 0 0
10 5 0 0 0 0
11 6 0 0 0 0
12 6 0 0 0 0
13 6 0 0 0 0
5 14 0 0 0 0
M END
$$$$
3-methylpyrrole-cation4.sdf
COSMOTHERM 3D 0
14 14 0 0 0 0 0 0 0 0 0 V2000
0.0392 -0.7597 0.0001 C 0 0 0 0 0 0 0 0 0 0 0 1
-1.1833 0.1180 0.0001 C 0 0 0 0 0 0 0 0 0 0 0 2
1.1176 0.0613 0.0001 C 0 0 0 0 0 0 0 0 0 0 0 3
```

```
0.6627 1.4052 0.0000 N 0 0 0 0 0 0 0 0 0 0 4
-0.6403 1.4900 -0.0002 C 0 0 0 0 0 0 0 0 0 0 5
0.0071 -2.2528 -0.0001 C 0 0 0 0 0 0 0 0 0 0 6
-1.8379 -0.0480 -0.8751 H 0 0 0 0 0 0 0 0 0 0 7
2.1844 -0.1370 0.0001 H 0 0 0 0 0 0 0 0 0 0 8
1.2921 2.2112 -0.0002 H 0 0 0 0 0 0 0 0 0 0 9
0.5200 -2.6572 -0.8851 H 0 0 0 0 0 0 0 0 0 0 10
-1.0241 -2.6259 -0.0015 H 0 0 0 0 0 0 0 0 0 0 11
0.5177 -2.6573 0.8863 H 0 0 0 0 0 0 0 0 0 0 12
-1.1645 2.4421 -0.0002 H 0 0 0 0 0 0 0 0 0 0 13
-1.8372 -0.0476 0.8759 H 0 0 0 0 0 0 0 0 0 0 14
2 1 0 0 0 0
3 1 0 0 0 0
6 1 0 0 0 0
5 2 0 0 0 0
7 2 0 0 0 0
4 3 0 0 0 0
8 3 0 0 0 0
5 4 0 0 0 0
9 4 0 0 0 0
13 5 0 0 0 0
10 6 0 0 0 0
11 6 0 0 0 0
12 6 0 0 0 0
2 14 0 0 0 0
M END
$$$$
3-methylpyrrole.sdf
COSMOTHERM 3D 0
13 13 0 0 0 0 0 0 0 0 0 V2000
-0.6511 -1.4106 0.0000 N 0 0 0 0 0 0 0 0 0 0 1
-1.1067 -0.1084 0.0000 C 0 0 0 0 0 0 0 0 0 0 2
-0.0016 0.7370 0.0000 C 0 0 0 0 0 0 0 0 0 0 3
1.1545 -0.1072 0.0000 C 0 0 0 0 0 0 0 0 0 0 4
0.7237 -1.4275 0.0000 C 0 0 0 0 0 0 0 0 0 0 5
-0.0120 2.2425 0.0000 C 0 0 0 0 0 0 0 0 0 0 6
-1.2446 -2.2344 0.0001 H 0 0 0 0 0 0 0 0 0 0 7
-2.1709 0.1086 0.0000 H 0 0 0 0 0 0 0 0 0 0 8
2.1907 0.2239 -0.0001 H 0 0 0 0 0 0 0 0 0 0 9
1.2735 -2.3634 0.0000 H 0 0 0 0 0 0 0 0 0 0 10
-0.5221 2.6524 0.8858 H 0 0 0 0 0 0 0 0 0 0 11
1.0138 2.6365 -0.0003 H 0 0 0 0 0 0 0 0 0 0 12
-0.5227 2.6526 -0.8853 H 0 0 0 0 0 0 0 0 0 0 13
2 1 0 0 0 0
5 1 0 0 0 0
7 1 0 0 0 0
3 2 0 0 0 0
8 2 0 0 0 0
4 3 0 0 0 0
6 3 0 0 0 0
5 4 0 0 0 0
9 4 0 0 0 0
10 5 0 0 0 0
11 6 0 0 0 0
12 6 0 0 0 0
6 13 0 0 0 0
M END
$$$$
4-aminopyridine.sdf
COSMOTHERM 3D 0
13 13 0 0 0 0 0 0 0 0 0 V2000
1.1542 0.0003 -1.1441 C 0 0 0 0 0 0 0 0 0 0 1
-0.2346 -0.0064 -1.2036 C 0 0 0 0 0 0 0 0 0 0 2
-0.9780 -0.0057 0.0000 C 0 0 0 0 0 0 0 0 0 0 3
-0.2346 -0.0061 1.2035 C 0 0 0 0 0 0 0 0 0 0 4
1.1542 0.0001 1.1441 C 0 0 0 0 0 0 0 0 0 0 5
1.8756 0.0038 0.0000 N 0 0 0 0 0 0 0 0 0 0 6
-2.3477 0.0416 0.0000 N 0 0 0 0 0 0 0 0 0 0 7
-2.8390 -0.2004 0.8557 H 0 0 0 0 0 0 0 0 0 0 8
-2.8390 -0.1998 -0.8559 H 0 0 0 0 0 0 0 0 0 0 9
1.7308 0.0001 -2.0739 H 0 0 0 0 0 0 0 0 0 0 10
-0.7430 -0.0088 -2.1697 H 0 0 0 0 0 0 0 0 0 0 11
-0.7430 -0.0089 2.1697 H 0 0 0 0 0 0 0 0 0 0 12
1.7309 -0.0006 2.0738 H 0 0 0 0 0 0 0 0 0 0 13
2 1 0 0 0 0
6 1 0 0 0 0
10 1 0 0 0 0
3 2 0 0 0 0
11 2 0 0 0 0
4 3 0 0 0 0
7 3 0 0 0 0
5 4 0 0 0 0
12 4 0 0 0 0
6 5 0 0 0 0
8 7 0 0 0 0
9 7 0 0 0 0
5 13 0 0 0 0
M END
$$$$
4-aminopyridine0.sdf
COSMOTHERM 3D 0
13 13 0 0 0 0 0 0 0 0 0 V2000
1.1441 -1.1542 0.0000 C 0 0 0 0 0 0 0 0 0 0 1
1.2036 0.2346 0.0059 C 0 0 0 0 0 0 0 0 0 0 2
0.0000 0.9781 0.0056 C 0 0 0 0 0 0 0 0 0 0 3
-1.2036 0.2346 0.0063 C 0 0 0 0 0 0 0 0 0 0 4
-1.1441 -1.1542 -0.0004 C 0 0 0 0 0 0 0 0 0 0 5
0.0000 -1.8756 -0.0037 N 0 0 0 0 0 0 0 0 0 0 6
0.0000 2.3475 -0.0411 N 0 0 0 0 0 0 0 0 0 0 7
0.8561 2.8395 0.1979 H 0 0 0 0 0 0 0 0 0 0 8
-0.8559 2.8394 0.1989 H 0 0 0 0 0 0 0 0 0 0 9
2.0739 -1.7309 0.0009 H 0 0 0 0 0 0 0 0 0 0 10
```



```

9 2 0 0 0 0
4 3 0 0 0 0
8 3 0 0 0 0
5 4 0 0 0 0
10 4 0 0 0 0
6 5 0 0 0 0
11 5 0 0 0 0
7 6 0 0 0 0
12 7 0 0 0 0
13 8 0 0 0 0
8 14 0 0 0 0
M END
$$$$
4-chloroaniline_pl.sdf
COSMOTHERM 3D 0

15 15 0 0 0 0 0 0 0 0 0 V2000
-3.3292 0.0000 0.0096 N 0 0 0 0 0 0 0 0 0 0 1
-1.1795 -1.2184 -0.0057 C 0 0 0 0 0 0 0 0 0 0 2
-1.8528 0.0000 -0.0065 C 0 0 0 0 0 0 0 0 0 0 3
-1.1795 1.2184 -0.0057 C 0 0 0 0 0 0 0 0 0 0 4
0.2174 1.2206 -0.0013 C 0 0 0 0 0 0 0 0 0 0 5
0.8958 0.0000 0.0011 C 0 0 0 0 0 0 0 0 0 0 6
0.2174 -1.2206 -0.0014 C 0 0 0 0 0 0 0 0 0 0 7
2.6629 0.0000 0.0025 Cl 0 0 0 0 0 0 0 0 0 0 8
-3.7172 -0.8281 -0.4636 H 0 0 0 0 0 0 0 0 0 0 9
-3.7174 0.8251 -0.4688 H 0 0 0 0 0 0 0 0 0 0 10
-1.7257 -2.1626 -0.0090 H 0 0 0 0 0 0 0 0 0 0 11
-1.7256 2.1627 -0.0091 H 0 0 0 0 0 0 0 0 0 0 12
0.7635 2.1630 -0.0035 H 0 0 0 0 0 0 0 0 0 0 13
0.7635 -2.1630 -0.0036 H 0 0 0 0 0 0 0 0 0 0 14
-3.7080 0.0029 0.9688 H 0 0 0 0 0 0 0 0 0 0 15
3 1 0 0 0 0
9 1 0 0 0 0
10 1 0 0 0 0
3 2 0 0 0 0
7 2 0 0 0 0
11 2 0 0 0 0
4 3 0 0 0 0
5 4 0 0 0 0
12 4 0 0 0 0
6 5 0 0 0 0
13 5 0 0 0 0
7 6 0 0 0 0
8 6 0 0 0 0
14 7 0 0 0 0
1 15 0 0 0 0
M END
$$$$
4-methoxyaniline_a.sdf
COSMOTHERM 3D 0

18 18 0 0 0 0 0 0 0 0 0 V2000
-0.1005 -1.3621 -0.0035 C 0 0 0 0 0 0 0 0 0 0 1
1.2815 -1.1858 -0.0062 C 0 0 0 0 0 0 0 0 0 0 2
1.8502 0.1062 -0.0077 C 0 0 0 0 0 0 0 0 0 0 3
0.9771 1.2080 -0.0094 C 0 0 0 0 0 0 0 0 0 0 4
-0.4140 1.0369 -0.0061 C 0 0 0 0 0 0 0 0 0 0 5
-0.9629 -0.2528 -0.0014 C 0 0 0 0 0 0 0 0 0 0 6
-2.3166 -0.5330 0.0025 O 0 0 0 0 0 0 0 0 0 0 7
-3.2191 0.5852 0.0060 C 0 0 0 0 0 0 0 0 0 0 8
3.2435 0.2799 0.0678 N 0 0 0 0 0 0 0 0 0 0 9
3.5752 1.1664 -0.3098 H 0 0 0 0 0 0 0 0 0 0 10
3.7821 -0.4930 -0.3210 H 0 0 0 0 0 0 0 0 0 0 11
-0.5269 -2.3671 -0.0055 H 0 0 0 0 0 0 0 0 0 0 12
1.9340 -2.0622 -0.0057 H 0 0 0 0 0 0 0 0 0 0 13
1.3871 2.2208 -0.0136 H 0 0 0 0 0 0 0 0 0 0 14
-1.0521 1.9202 -0.0102 H 0 0 0 0 0 0 0 0 0 0 15
-4.2260 0.1542 0.0112 H 0 0 0 0 0 0 0 0 0 0 16
-3.0817 1.2081 0.9043 H 0 0 0 0 0 0 0 0 0 0 17
-3.0905 1.2069 -0.8944 H 0 0 0 0 0 0 0 0 0 0 18
2 1 0 0 0 0
6 1 0 0 0 0
12 1 0 0 0 0
3 2 0 0 0 0
13 2 0 0 0 0
4 3 0 0 0 0
9 3 0 0 0 0
5 4 0 0 0 0
14 4 0 0 0 0
6 5 0 0 0 0
15 5 0 0 0 0
7 6 0 0 0 0
8 7 0 0 0 0
16 8 0 0 0 0
17 8 0 0 0 0
10 9 0 0 0 0
11 9 0 0 0 0
8 18 0 0 0 0
M END
$$$$
4-methoxyaniline_pl.sdf
COSMOTHERM 3D 0

19 19 0 0 0 0 0 0 0 0 0 V2000
3.2415 -0.5890 0.0073 C 0 0 0 0 0 0 0 0 0 0 1
-3.2361 -0.2754 -0.0070 N 0 0 0 0 0 0 0 0 0 0 2
-1.7696 -0.0924 0.0082 C 0 0 0 0 0 0 0 0 0 0 3
-1.2462 1.2015 0.0072 C 0 0 0 0 0 0 0 0 0 0 4
0.1340 1.3729 0.0003 C 0 0 0 0 0 0 0 0 0 0 5
0.9879 0.2525 -0.0052 C 0 0 0 0 0 0 0 0 0 0 6
0.4436 -1.0431 -0.0038 C 0 0 0 0 0 0 0 0 0 0 7
-0.9448 -1.2110 0.0036 C 0 0 0 0 0 0 0 0 0 0 8
2.3247 0.5257 -0.0092 O 0 0 0 0 0 0 0 0 0 0 9
4.2410 -0.1435 0.0176 H 0 0 0 0 0 0 0 0 0 0 10
```



```
1
2
3      0.0238      1.2219      1.4173 C      0      0      0      0      0      0      0      0      0      0      2
4      0.0054      0.0002      2.0861 C      0      0      0      0      0      0      0      0      0      0      3
5     -0.0145     -1.2225      1.4175 C      0      0      0      0      0      0      0      0      0      0      4
6     -0.0173     -1.2242      0.0239 C      0      0      0      0      0      0      0      0      0      0      5
7     -0.0018      0.0002     -0.6474 C      0      0      0      0      0      0      0      0      0      0      6
8     -0.0012      0.0001     -2.1295 N      0      0      0      0      0      0      0      0      0      0      7
9     -0.0072      0.0002      3.5603 N      0      0      0      0      0      0      0      0      0      0      8
10    -0.0404      1.0927     -2.7116 O      0      0      0      0      0      0      0      0      0      0      9
11      0.0381     -1.0930     -2.7110 O      0      0      0      0      0      0      0      0      0      0      10
12      0.5614     -0.7654      3.9503 H      0      0      0      0      0      0      0      0      0      0      11
13     -0.9615     -0.1100      3.9370 H      0      0      0      0      0      0      0      0      0      0      12
14      0.0342      2.1603     -0.5315 H      0      0      0      0      0      0      0      0      0      0      13
15      0.0439      2.1632      1.9671 H      0      0      0      0      0      0      0      0      0      0      14
16     -0.0259     -2.1637      1.9675 H      0      0      0      0      0      0      0      0      0      0      15
17     -0.0293     -2.1601     -0.5311 H      0      0      0      0      0      0      0      0      0      0      16
18      0.3672      0.8789      3.9454 H      0      0      0      0      0      0      0      0      0      0      17
19
20 2 1 0 0 0 0
21 6 1 0 0 0 0
22 13 1 0 0 0 0
23 3 2 0 0 0 0
24 14 2 0 0 0 0
25 4 3 0 0 0 0
26 8 3 0 0 0 0
27 5 4 0 0 0 0
28 15 4 0 0 0 0
29 6 5 0 0 0 0
30 16 5 0 0 0 0
31 7 6 0 0 0 0
32 9 7 0 0 0 0
33 10 7 0 0 0 0
34 11 8 0 0 0 0
35 12 8 0 0 0 0
36 8 17 0 0 0 0
37
38 M END
39 $$$$
40 4-nitroaniline1.sdf
41 COSMOtherm 3D 0
42
43 16 16 0 0 0 0 0 0 0 0 0 V2000
44 -0.0573 -0.0207 -1.2179 C 0 0 0 0 0 0 0 0 0 0 0 0 1
45 -1.4319 -0.0241 -1.2199 C 0 0 0 0 0 0 0 0 0 0 0 0 2
46 -2.1502 -0.0077 0.0001 C 0 0 0 0 0 0 0 0 0 0 0 0 3
47 -1.4321 -0.0228 1.2198 C 0 0 0 0 0 0 0 0 0 0 0 0 4
48 -0.0574 -0.0201 1.2178 C 0 0 0 0 0 0 0 0 0 0 0 0 5
49 0.6764 -0.0045 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 6
50 -3.4943 0.0813 0.0000 N 0 0 0 0 0 0 0 0 0 0 0 0 7
51 2.0256 0.0073 -0.0001 N 0 0 0 0 0 0 0 0 0 0 0 0 8
52 2.6590 0.0131 1.0948 O 0 0 0 0 0 0 0 0 0 0 0 0 9
53 2.6588 0.0153 -1.0946 O 0 0 0 0 0 0 0 0 0 0 0 0 10
54 -3.9805 -0.1796 0.8496 H 0 0 0 0 0 0 0 0 0 0 0 0 11
55 -3.9797 -0.1820 -0.8495 H 0 0 0 0 0 0 0 0 0 0 0 0 12
56 0.4783 -0.0300 -2.1636 H 0 0 0 0 0 0 0 0 0 0 0 0 13
57 -1.9693 -0.0380 -2.1671 H 0 0 0 0 0 0 0 0 0 0 0 0 14
58 -1.9696 -0.0353 2.1670 H 0 0 0 0 0 0 0 0 0 0 0 0 15
59 0.4784 -0.0289 2.1633 H 0 0 0 0 0 0 0 0 0 0 0 0 16
60
61 2 1 0 0 0 0
62 6 1 0 0 0 0
63 13 1 0 0 0 0
64 3 2 0 0 0 0
65 14 2 0 0 0 0
66 4 3 0 0 0 0
67 7 3 0 0 0 0
68 5 4 0 0 0 0
69 15 4 0 0 0 0
70 6 5 0 0 0 0
71 8 6 0 0 0 0
72 11 7 0 0 0 0
73 12 7 0 0 0 0
74 9 8 0 0 0 0
75 10 8 0 0 0 0
76 5 16 0 0 0 0
77
78 M END
79 $$$$
80 aniline-cation.sdf
81 COSMOtherm 3D 0
82
83 15 15 0 0 0 0 0 0 0 0 0 V2000
84 -1.1972 -1.2132 -0.0012 C 0 0 0 0 0 0 0 0 0 0 0 0 1
85 0.2015 -1.2207 0.0049 C 0 0 0 0 0 0 0 0 0 0 0 0 2
86 0.8717 0.0000 0.0072 C 0 0 0 0 0 0 0 0 0 0 0 0 3
87 0.2015 1.2206 0.0052 C 0 0 0 0 0 0 0 0 0 0 0 0 4
88 -1.1972 1.2132 -0.0015 C 0 0 0 0 0 0 0 0 0 0 0 0 5
89 -1.8947 0.0000 -0.0052 C 0 0 0 0 0 0 0 0 0 0 0 0 6
90 2.3509 0.0000 -0.0069 N 0 0 0 0 0 0 0 0 0 0 0 0 7
91 -1.7390 -2.1597 0.0004 H 0 0 0 0 0 0 0 0 0 0 0 0 8
92 0.7549 -2.1612 0.0101 H 0 0 0 0 0 0 0 0 0 0 0 0 9
93 0.7549 2.1611 0.0102 H 0 0 0 0 0 0 0 0 0 0 0 0 10
94 -1.7389 2.1598 -0.0003 H 0 0 0 0 0 0 0 0 0 0 0 0 11
95 -2.9855 0.0001 -0.0078 H 0 0 0 0 0 0 0 0 0 0 0 0 12
96 2.7308 0.0028 -0.9655 H 0 0 0 0 0 0 0 0 0 0 0 0 13
97 2.7379 -0.8284 0.4663 H 0 0 0 0 0 0 0 0 0 0 0 0 14
98 2.7380 0.8254 0.4715 H 0 0 0 0 0 0 0 0 0 0 0 0 15
99
100 2 1 0 0 0 0
101 6 1 0 0 0 0
102 8 1 0 0 0 0
103 3 2 0 0 0 0
104 9 2 0 0 0 0
105 4 3 0 0 0 0
106 7 3 0 0 0 0
107 5 4 0 0 0 0
108 10 4 0 0 0 0
109 6 5 0 0 0 0
110 11 5 0 0 0 0
111 12 6 0 0 0 0
112 13 7 0 0 0 0
```

```
14 7 0 0 0 0
7 15 0 0 0 0
M END
$$$$
aniline.sdf
COSMOtherm 3D 0

14 14 0 0 0 0 0 0 0 0 V2000
-1.8803 -0.0001 -0.0043 C 0 0 0 0 0 0 0 0 0 0 0 1
-1.1670 1.2065 0.0002 C 0 0 0 0 0 0 0 0 0 0 0 2
0.2297 1.2131 0.0068 C 0 0 0 0 0 0 0 0 0 0 0 3
0.9533 0.0000 0.0072 C 0 0 0 0 0 0 0 0 0 0 0 4
0.2298 -1.2130 0.0068 C 0 0 0 0 0 0 0 0 0 0 0 5
-1.1668 -1.2065 0.0002 C 0 0 0 0 0 0 0 0 0 0 0 6
-2.9713 -0.0001 -0.0088 H 0 0 0 0 0 0 0 0 0 0 0 7
-1.7035 2.1580 0.0022 H 0 0 0 0 0 0 0 0 0 0 0 8
0.7733 2.1612 0.0103 H 0 0 0 0 0 0 0 0 0 0 0 9
2.3466 0.0001 -0.0568 N 0 0 0 0 0 0 0 0 0 0 0 10
0.7735 -2.1611 0.0105 H 0 0 0 0 0 0 0 0 0 0 0 11
-1.7033 -2.1581 0.0021 H 0 0 0 0 0 0 0 0 0 0 0 12
2.8017 -0.8433 0.2864 H 0 0 0 0 0 0 0 0 0 0 0 13
2.8023 0.8427 0.2870 H 0 0 0 0 0 0 0 0 0 0 0 14
2 1 0 0 0 0
6 1 0 0 0 0
7 1 0 0 0 0
3 2 0 0 0 0
8 2 0 0 0 0
4 3 0 0 0 0
9 3 0 0 0 0
5 4 0 0 0 0
10 4 0 0 0 0
6 5 0 0 0 0
11 5 0 0 0 0
12 6 0 0 0 0
13 10 0 0 0 0
10 14 0 0 0 0
M END
$$$$
benzimidazole.sdf
COSMOtherm 3D 0

15 16 0 0 0 0 0 0 0 0 V2000
-1.4381 -0.9689 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 1
-0.7108 0.2267 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 2
0.7121 0.2562 0.0001 C 0 0 0 0 0 0 0 0 0 0 0 3
1.4362 -0.9467 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 4
0.7165 -2.1426 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 5
-0.6973 -2.1530 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 6
1.1636 1.5764 0.0000 N 0 0 0 0 0 0 0 0 0 0 0 7
-1.0884 1.5589 0.0000 N 0 0 0 0 0 0 0 0 0 0 0 8
0.0599 2.3073 -0.0001 C 0 0 0 0 0 0 0 0 0 0 0 9
-2.5288 -0.9795 -0.0001 H 0 0 0 0 0 0 0 0 0 0 0 10
2.5277 -0.9403 0.0001 H 0 0 0 0 0 0 0 0 0 0 0 11
1.2538 -3.0926 -0.0001 H 0 0 0 0 0 0 0 0 0 0 0 12
-1.2230 -3.1094 -0.0001 H 0 0 0 0 0 0 0 0 0 0 0 13
-2.0368 1.9255 0.0006 H 0 0 0 0 0 0 0 0 0 0 0 14
0.0255 3.3941 -0.0002 H 0 0 0 0 0 0 0 0 0 0 0 15
2 1 0 0 0 0
6 1 0 0 0 0
10 1 0 0 0 0
3 2 0 0 0 0
8 2 0 0 0 0
4 3 0 0 0 0
7 3 0 0 0 0
5 4 0 0 0 0
11 4 0 0 0 0
6 5 0 0 0 0
12 5 0 0 0 0
13 6 0 0 0 0
9 7 0 0 0 0
9 8 0 0 0 0
14 8 0 0 0 0
9 15 0 0 0 0
M END
$$$$
benzimidazole_p1.sdf
COSMOtherm 3D 0

16 17 0 0 0 0 0 0 0 0 V2000
-2.3250 0.0000 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 1
-1.5496 1.0899 0.0001 N 0 0 0 0 0 0 0 0 0 0 0 2
-0.2099 0.7064 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 3
-0.2099 -0.7064 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 4
-1.5496 -1.0899 -0.0001 N 0 0 0 0 0 0 0 0 0 0 0 5
0.9776 1.4425 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 6
2.1617 0.7066 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 7
2.1617 -0.7066 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 8
0.9776 -1.4425 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 9
-3.4092 -0.0001 -0.0001 H 0 0 0 0 0 0 0 0 0 0 0 10
-1.9063 2.0441 -0.0001 H 0 0 0 0 0 0 0 0 0 0 0 11
0.9753 2.5319 0.0001 H 0 0 0 0 0 0 0 0 0 0 0 12
3.1148 1.2365 0.0000 H 0 0 0 0 0 0 0 0 0 0 0 13
3.1148 -1.2365 0.0000 H 0 0 0 0 0 0 0 0 0 0 0 14
0.9752 -2.5319 0.0000 H 0 0 0 0 0 0 0 0 0 0 0 15
-1.9063 -2.0441 0.0002 H 0 0 0 0 0 0 0 0 0 0 0 16
2 1 0 0 0 0
5 1 0 0 0 0
10 1 0 0 0 0
3 2 0 0 0 0
11 2 0 0 0 0
4 3 0 0 0 0
6 3 0 0 0 0
5 4 0 0 0 0
9 4 0 0 0 0
7 6 0 0 0 0
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12 6 0 0 0 0
8 7 0 0 0 0
13 7 0 0 0 0
9 8 0 0 0 0
14 8 0 0 0 0
15 9 0 0 0 0
5 16 0 0 0 0
M END
$$$$
clonidine-cation2.sdf
COSMOtherm 3D 0

24 25 0 0 0 0 0 0 0 0 0 V2000
2.7823 0.9918 0.5509 C 0 0 0 0 0 0 0 0 0 0 1
1.5195 1.1167 -0.0268 C 0 0 0 0 0 0 0 0 0 0 2
0.7357 -0.0120 -0.3359 C 0 0 0 0 0 0 0 0 0 0 3
1.2745 -1.2831 -0.0544 C 0 0 0 0 0 0 0 0 0 0 4
2.5327 -1.4268 0.5294 C 0 0 0 0 0 0 0 0 0 0 5
3.2786 -0.2843 0.8265 C 0 0 0 0 0 0 0 0 0 0 6
0.8910 2.7212 -0.3805 Cl 0 0 0 0 0 0 0 0 0 0 7
0.3468 -2.7219 -0.4560 Cl 0 0 0 0 0 0 0 0 0 0 8
-0.5396 0.1298 -0.9530 N 0 0 0 0 0 0 0 0 0 0 9
-1.6941 0.1355 -0.2665 C 0 0 0 0 0 0 0 0 0 0 10
-3.9581 0.0522 0.1724 C 0 0 0 0 0 0 0 0 0 0 11
-3.1839 0.2225 1.4955 C 0 0 0 0 0 0 0 0 0 0 12
-2.9010 0.3159 -0.8278 N 0 0 0 0 0 0 0 0 0 0 13
-1.7943 -0.0351 1.0609 N 0 0 0 0 0 0 0 0 0 0 14
-3.0556 0.1638 -1.8214 H 0 0 0 0 0 0 0 0 0 0 15
-1.0012 0.0900 1.6849 H 0 0 0 0 0 0 0 0 0 0 16
3.3682 1.8811 0.7796 H 0 0 0 0 0 0 0 0 0 0 17
2.9261 -2.4206 0.7385 H 0 0 0 0 0 0 0 0 0 0 18
4.2650 -0.3899 1.2792 H 0 0 0 0 0 0 0 0 0 0 19
-4.3441 -0.9704 0.0519 H 0 0 0 0 0 0 0 0 0 0 20
-4.7789 0.7686 0.0684 H 0 0 0 0 0 0 0 0 0 0 21
-3.2690 1.2440 1.8935 H 0 0 0 0 0 0 0 0 0 0 22
-3.4903 -0.4967 2.2615 H 0 0 0 0 0 0 0 0 0 0 23
-0.5835 0.2607 -1.9627 H 0 0 0 0 0 0 0 0 0 0 24

2 1 0 0 0 0
6 1 0 0 0 0
17 1 0 0 0 0
3 2 0 0 0 0
7 2 0 0 0 0
4 3 0 0 0 0
9 3 0 0 0 0
5 4 0 0 0 0
8 4 0 0 0 0
6 5 0 0 0 0
18 5 0 0 0 0
19 6 0 0 0 0
10 9 0 0 0 0
13 10 0 0 0 0
14 10 0 0 0 0
12 11 0 0 0 0
13 11 0 0 0 0
20 11 0 0 0 0
21 11 0 0 0 0
14 12 0 0 0 0
22 12 0 0 0 0
23 12 0 0 0 0
15 13 0 0 0 0
16 14 0 0 0 0
9 24 0 0 0 0
M END
$$$$
clonidine.sdf
COSMOtherm 3D 0

23 24 0 0 0 0 0 0 0 0 0 V2000
-0.6414 -2.8298 0.8595 N 0 0 0 0 0 0 0 0 0 0 1
-0.3588 -1.6195 0.2590 C 0 0 0 0 0 0 0 0 0 0 2
-0.0669 -1.8560 -1.0702 N 0 0 0 0 0 0 0 0 0 0 3
-0.5395 2.9761 -0.4990 C 0 0 0 0 0 0 0 0 0 0 4
-0.9229 1.7267 -0.0170 C 0 0 0 0 0 0 0 0 0 0 5
-0.0027 0.6961 0.3045 C 0 0 0 0 0 0 0 0 0 0 6
1.3593 1.0382 0.0978 C 0 0 0 0 0 0 0 0 0 0 7
1.7742 2.2785 -0.3850 C 0 0 0 0 0 0 0 0 0 0 8
0.8182 3.2524 -0.6836 C 0 0 0 0 0 0 0 0 0 0 9
2.6036 -0.1604 0.5041 Cl 0 0 0 0 0 0 0 0 0 0 10
-2.6498 1.4001 0.2048 Cl 0 0 0 0 0 0 0 0 0 0 11
-0.4203 -0.4855 0.8978 N 0 0 0 0 0 0 0 0 0 0 12
-0.8022 -3.8672 -0.1730 C 0 0 0 0 0 0 0 0 0 0 13
0.0846 -3.3044 -1.2950 C 0 0 0 0 0 0 0 0 0 0 14
-1.2746 -2.8158 1.6559 H 0 0 0 0 0 0 0 0 0 0 15
0.5515 -1.2106 -1.5555 H 0 0 0 0 0 0 0 0 0 0 16
-1.2973 3.7250 -0.7290 H 0 0 0 0 0 0 0 0 0 0 17
2.8370 2.4809 -0.5177 H 0 0 0 0 0 0 0 0 0 0 18
1.1310 4.2272 -1.0583 H 0 0 0 0 0 0 0 0 0 0 19
-1.8523 -3.9480 -0.5007 H 0 0 0 0 0 0 0 0 0 0 20
-0.4604 -4.8451 0.1849 H 0 0 0 0 0 0 0 0 0 0 21
-0.2616 -3.5916 -2.2945 H 0 0 0 0 0 0 0 0 0 0 22
1.1338 -3.6198 -1.1701 H 0 0 0 0 0 0 0 0 0 0 23

2 1 0 0 0 0
13 1 0 0 0 0
15 1 0 0 0 0
3 2 0 0 0 0
12 2 0 0 0 0
14 3 0 0 0 0
16 3 0 0 0 0
5 4 0 0 0 0
9 4 0 0 0 0
17 4 0 0 0 0
6 5 0 0 0 0
11 5 0 0 0 0
7 6 0 0 0 0
12 6 0 0 0 0
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  8 7 0 0 0 0
 10 7 0 0 0 0
  9 8 0 0 0 0
 18 8 0 0 0 0
 19 9 0 0 0 0
 14 13 0 0 0 0
 20 13 0 0 0 0
 21 13 0 0 0 0
 22 14 0 0 0 0
 14 23 0 0 0 0
M  END
$$$$
clonidine0.sdf
COSMOtherm      3D      0

23 24 0 0 0 0 0 0 0 0 0 V2000
-1.7913 0.3793 -2.2634 C 0 0 0 0 0 0 0 0 0 0 1
-1.3625 -0.0997 -1.0264 C 0 0 0 0 0 0 0 0 0 0 2
 0.0037 -0.2996 -0.6967 C 0 0 0 0 0 0 0 0 0 0 3
 0.9122 0.0194 -1.7386 C 0 0 0 0 0 0 0 0 0 0 4
 0.5146 0.4970 -2.9853 C 0 0 0 0 0 0 0 0 0 0 5
-0.8463 0.6780 -3.2479 C 0 0 0 0 0 0 0 0 0 0 6
-2.5943 -0.5089 0.1842 C1 0 0 0 0 0 0 0 0 0 0 7
 2.6429 -0.1973 -1.4299 C1 0 0 0 0 0 0 0 0 0 0 8
 0.4381 -0.8875 0.4814 N 0 0 0 0 0 0 0 0 0 0 9
 0.3717 -0.2549 1.6186 C 0 0 0 0 0 0 0 0 0 0 10
 0.8241 0.1742 3.8651 C 0 0 0 0 0 0 0 0 0 0 11
-0.0887 1.2812 3.3149 C 0 0 0 0 0 0 0 0 0 0 12
 0.6745 -0.8561 2.8237 N 0 0 0 0 0 0 0 0 0 0 13
 0.0576 1.0676 1.8642 N 0 0 0 0 0 0 0 0 0 0 14
 1.3220 -1.6407 2.8005 H 0 0 0 0 0 0 0 0 0 0 15
-0.5746 1.5446 1.2261 H 0 0 0 0 0 0 0 0 0 0 16
-2.8566 0.5069 -2.4557 H 0 0 0 0 0 0 0 0 0 0 17
 1.2640 0.7260 -3.7428 H 0 0 0 0 0 0 0 0 0 0 18
-1.1701 1.0493 -4.2204 H 0 0 0 0 0 0 0 0 0 0 19
 1.8683 0.5218 3.9384 H 0 0 0 0 0 0 0 0 0 0 20
 0.4976 -0.1952 4.8440 H 0 0 0 0 0 0 0 0 0 0 21
-1.1330 1.1327 3.6363 H 0 0 0 0 0 0 0 0 0 0 22
 0.2386 2.2860 3.6056 H 0 0 0 0 0 0 0 0 0 0 23

 2 1 0 0 0 0
 6 1 0 0 0 0
17 1 0 0 0 0
 3 2 0 0 0 0
 7 2 0 0 0 0
 4 3 0 0 0 0
 9 3 0 0 0 0
 5 4 0 0 0 0
 8 4 0 0 0 0
 6 5 0 0 0 0
18 5 0 0 0 0
19 6 0 0 0 0
10 9 0 0 0 0
13 10 0 0 0 0
14 10 0 0 0 0
12 11 0 0 0 0
13 11 0 0 0 0
20 11 0 0 0 0
21 11 0 0 0 0
14 12 0 0 0 0
22 12 0 0 0 0
15 13 0 0 0 0
16 14 0 0 0 0
12 23 0 0 0 0
M  END
$$$$
clonidine1.sdf
COSMOtherm      3D      0

23 24 0 0 0 0 0 0 0 0 0 V2000
 1.7883 0.3817 2.2655 C 0 0 0 0 0 0 0 0 0 0 1
 1.3620 -0.1001 1.0286 C 0 0 0 0 0 0 0 0 0 0 2
-0.0036 -0.3005 0.6965 C 0 0 0 0 0 0 0 0 0 0 3
-0.9140 0.0185 1.7367 C 0 0 0 0 0 0 0 0 0 0 4
-0.5190 0.4982 2.9833 C 0 0 0 0 0 0 0 0 0 0 5
 0.8413 0.6802 3.2481 C 0 0 0 0 0 0 0 0 0 0 6
 2.5959 -0.5090 -0.1798 C1 0 0 0 0 0 0 0 0 0 0 7
-2.6441 -0.1992 1.4249 C1 0 0 0 0 0 0 0 0 0 0 8
-0.4349 -0.8894 -0.4822 N 0 0 0 0 0 0 0 0 0 0 9
-0.3698 -0.2557 -1.6189 C 0 0 0 0 0 0 0 0 0 0 10
-0.8202 0.1748 -3.8656 C 0 0 0 0 0 0 0 0 0 0 11
 0.0880 1.2843 -3.3125 C 0 0 0 0 0 0 0 0 0 0 12
-0.6693 -0.8562 -2.8251 N 0 0 0 0 0 0 0 0 0 0 13
-0.0587 1.0680 -1.8624 N 0 0 0 0 0 0 0 0 0 0 14
-1.3147 -1.6426 -2.8037 H 0 0 0 0 0 0 0 0 0 0 15
 0.5717 1.5456 -1.2229 H 0 0 0 0 0 0 0 0 0 0 16
 2.8531 0.5101 2.4595 H 0 0 0 0 0 0 0 0 0 0 17
-1.2697 0.7276 3.7393 H 0 0 0 0 0 0 0 0 0 0 18
 1.1631 1.0535 4.2206 H 0 0 0 0 0 0 0 0 0 0 19
-1.8653 0.5190 -3.9410 H 0 0 0 0 0 0 0 0 0 0 20
-0.4903 -0.1925 -4.8441 H 0 0 0 0 0 0 0 0 0 0 21
 1.1332 1.1405 -3.6333 H 0 0 0 0 0 0 0 0 0 0 22
-0.2429 2.2883 -3.6021 H 0 0 0 0 0 0 0 0 0 0 23

 2 1 0 0 0 0
 6 1 0 0 0 0
17 1 0 0 0 0
 3 2 0 0 0 0
 7 2 0 0 0 0
 4 3 0 0 0 0
 9 3 0 0 0 0
 5 4 0 0 0 0
 8 4 0 0 0 0
 6 5 0 0 0 0
18 5 0 0 0 0
19 6 0 0 0 0
10 9 0 0 0 0
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13 10 0 0 0 0
14 10 0 0 0 0
12 11 0 0 0 0
13 11 0 0 0 0
20 11 0 0 0 0
21 11 0 0 0 0
14 12 0 0 0 0
22 12 0 0 0 0
15 13 0 0 0 0
16 14 0 0 0 0
12 23 0 0 0 0
M END
$$$$
clonidine_pl.sdf
COSMOTHERM 3D 0
24 25 0 0 0 0 0 0 0 0 0 V2000
-2.6479 -0.0153 0.5329 C1 0 0 0 0 0 0 0 0 0 0 1
-0.6424 -3.2432 -0.7885 C 0 0 0 0 0 0 0 0 0 0 2
-1.6704 -2.3535 -0.4699 C 0 0 0 0 0 0 0 0 0 0 3
-1.3491 -1.1188 0.0927 C 0 0 0 0 0 0 0 0 0 0 4
-0.0111 -0.7396 0.3201 C 0 0 0 0 0 0 0 0 0 0 5
0.9978 -1.6653 -0.0103 C 0 0 0 0 0 0 0 0 0 0 6
0.6943 -2.9092 -0.5615 C 0 0 0 0 0 0 0 0 0 0 7
2.6795 -1.2394 0.2783 C1 0 0 0 0 0 0 0 0 0 0 8
0.3155 0.5107 0.9153 N 0 0 0 0 0 0 0 0 0 0 9
0.2889 1.6795 0.2526 C 0 0 0 0 0 0 0 0 0 0 10
0.4971 2.8740 0.8308 N 0 0 0 0 0 0 0 0 0 0 11
0.0619 1.8106 -1.0634 N 0 0 0 0 0 0 0 0 0 0 12
0.6350 3.9114 -0.2141 C 0 0 0 0 0 0 0 0 0 0 13
-0.0744 3.2420 -1.4076 C 0 0 0 0 0 0 0 0 0 0 14
-0.8875 -4.2128 -1.2228 H 0 0 0 0 0 0 0 0 0 0 15
-2.7128 -2.6205 -0.6381 H 0 0 0 0 0 0 0 0 0 0 16
1.4940 -3.6066 -0.8070 H 0 0 0 0 0 0 0 0 0 0 17
0.9580 2.9585 1.7334 H 0 0 0 0 0 0 0 0 0 0 18
-0.3551 1.0728 -1.6245 H 0 0 0 0 0 0 0 0 0 0 19
1.6985 4.0984 -0.4220 H 0 0 0 0 0 0 0 0 0 0 20
0.1516 4.8424 0.0973 H 0 0 0 0 0 0 0 0 0 0 21
0.4097 3.4578 -2.3651 H 0 0 0 0 0 0 0 0 0 0 22
-1.1377 3.5171 -1.4614 H 0 0 0 0 0 0 0 0 0 0 23
0.6007 0.5239 1.8934 H 0 0 0 0 0 0 0 0 0 0 24
4 1 0 0 0 0
3 2 0 0 0 0
7 2 0 0 0 0
15 2 0 0 0 0
4 3 0 0 0 0
16 3 0 0 0 0
5 4 0 0 0 0
6 5 0 0 0 0
9 5 0 0 0 0
7 6 0 0 0 0
8 6 0 0 0 0
17 7 0 0 0 0
10 9 0 0 0 0
11 10 0 0 0 0
12 10 0 0 0 0
13 11 0 0 0 0
18 11 0 0 0 0
14 12 0 0 0 0
19 12 0 0 0 0
14 13 0 0 0 0
20 13 0 0 0 0
21 13 0 0 0 0
22 14 0 0 0 0
23 14 0 0 0 0
9 24 0 0 0 0
M END
$$$$
clonidine_t_p3.sdf
COSMOTHERM 3D 0
24 25 0 0 0 0 0 0 0 0 0 V2000
0.2266 -3.1852 -1.4946 C 0 0 0 0 0 0 0 0 0 0 1
0.0496 -3.9584 -0.1723 C 0 0 0 0 0 0 0 0 0 0 2
-0.0338 -1.7954 -1.0617 N 0 0 0 0 0 0 0 0 0 0 3
2.7209 0.8916 0.3820 C1 0 0 0 0 0 0 0 0 0 0 4
-0.2840 3.2789 -0.8267 C 0 0 0 0 0 0 0 0 0 0 5
0.9919 2.7821 -0.5519 C 0 0 0 0 0 0 0 0 0 0 6
1.1166 1.5200 0.0275 C 0 0 0 0 0 0 0 0 0 0 7
-0.0121 0.7353 0.3342 C 0 0 0 0 0 0 0 0 0 0 8
-1.2831 1.2753 0.0549 C 0 0 0 0 0 0 0 0 0 0 9
-1.4267 2.5326 -0.5309 C 0 0 0 0 0 0 0 0 0 0 10
-2.7220 0.3475 0.4561 C1 0 0 0 0 0 0 0 0 0 0 11
0.1292 -0.5399 0.9519 N 0 0 0 0 0 0 0 0 0 0 12
0.1353 -1.6947 0.2659 C 0 0 0 0 0 0 0 0 0 0 13
0.3141 -2.9015 0.8280 N 0 0 0 0 0 0 0 0 0 0 14
-0.4884 -3.4922 -2.2642 H 0 0 0 0 0 0 0 0 0 0 15
1.2503 -3.2700 -1.8869 H 0 0 0 0 0 0 0 0 0 0 16
0.7627 -4.7818 -0.0657 H 0 0 0 0 0 0 0 0 0 0 17
-0.9748 -4.3404 -0.0545 H 0 0 0 0 0 0 0 0 0 0 18
0.0945 -1.0027 -1.6856 H 0 0 0 0 0 0 0 0 0 0 19
-0.3894 4.2648 -1.2802 H 0 0 0 0 0 0 0 0 0 0 20
1.8812 3.3682 -0.7795 H 0 0 0 0 0 0 0 0 0 0 21
-2.4205 2.9261 -0.7398 H 0 0 0 0 0 0 0 0 0 0 22
0.2606 -0.5830 1.9615 H 0 0 0 0 0 0 0 0 0 0 23
0.1615 -3.0559 1.8216 H 0 0 0 0 0 0 0 0 0 0 24
2 1 0 0 0 0
3 1 0 0 0 0
15 1 0 0 0 0
16 1 0 0 0 0
14 2 0 0 0 0
17 2 0 0 0 0
18 2 0 0 0 0
13 3 0 0 0 0
19 3 0 0 0 0
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18 5 0 0 0 0
19 6 0 0 0 0
8 7 0 0 0 0
9 7 0 0 0 0
6 20 0 0 0 0
M END
$$$$
debrisoquine.sdf
COSMOTHERM 3D 0
26 27 0 0 0 0 0 0 0 0 0 V2000
-0.3155 -3.3905 -0.6126 C 0 0 0 0 0 0 0 0 0 0 1
0.9954 -3.2267 -0.1453 C 0 0 0 0 0 0 0 0 0 0 2
1.3990 -1.9875 0.3573 C 0 0 0 0 0 0 0 0 0 0 3
0.5122 -0.8985 0.3957 C 0 0 0 0 0 0 0 0 0 0 4
-0.8079 -1.0606 -0.0703 C 0 0 0 0 0 0 0 0 0 0 5
-1.2035 -2.3130 -0.5724 C 0 0 0 0 0 0 0 0 0 0 6
0.9814 0.4263 0.9789 C 0 0 0 0 0 0 0 0 0 0 7
-1.7866 0.0970 -0.0308 C 0 0 0 0 0 0 0 0 0 0 8
-1.3228 1.1946 0.9342 C 0 0 0 0 0 0 0 0 0 0 9
0.0835 1.5422 0.6803 N 0 0 0 0 0 0 0 0 0 0 10
0.4490 2.4409 -0.3154 C 0 0 0 0 0 0 0 0 0 0 11
-0.5118 3.4082 -0.6136 N 0 0 0 0 0 0 0 0 0 0 12
1.6042 2.3415 -0.9147 N 0 0 0 0 0 0 0 0 0 0 13
-0.6437 -4.3551 -1.0048 H 0 0 0 0 0 0 0 0 0 0 14
1.6988 -4.0612 -0.1735 H 0 0 0 0 0 0 0 0 0 0 15
2.4212 -1.8577 0.7235 H 0 0 0 0 0 0 0 0 0 0 16
-2.2286 -2.4412 -0.9306 H 0 0 0 0 0 0 0 0 0 0 17
1.9754 0.6810 0.5943 H 0 0 0 0 0 0 0 0 0 0 18
1.0574 0.3305 2.0768 H 0 0 0 0 0 0 0 0 0 0 19
-2.7849 -0.2632 0.2631 H 0 0 0 0 0 0 0 0 0 0 20
-1.8956 0.5291 -1.0404 H 0 0 0 0 0 0 0 0 0 0 21
-1.3853 0.8389 1.9743 H 0 0 0 0 0 0 0 0 0 0 22
-1.9678 2.0758 0.8596 H 0 0 0 0 0 0 0 0 0 0 23
-0.1499 4.1870 -1.1598 H 0 0 0 0 0 0 0 0 0 0 24
-1.0876 3.7329 0.1611 H 0 0 0 0 0 0 0 0 0 0 25
1.7486 3.1609 -1.5153 H 0 0 0 0 0 0 0 0 0 0 26
2 1 0 0 0 0
6 1 0 0 0 0
14 1 0 0 0 0
3 2 0 0 0 0
15 2 0 0 0 0
4 3 0 0 0 0
16 3 0 0 0 0
5 4 0 0 0 0
7 4 0 0 0 0
6 5 0 0 0 0
8 5 0 0 0 0
17 6 0 0 0 0
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19 7 0 0 0 0
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21 8 0 0 0 0
10 9 0 0 0 0
22 9 0 0 0 0
23 9 0 0 0 0
11 10 0 0 0 0
12 11 0 0 0 0
13 11 0 0 0 0
24 12 0 0 0 0
25 12 0 0 0 0
13 26 0 0 0 0
M END
$$$$
debrisoquine_a.sdf
COSMOTHERM 3D 0
26 27 0 0 0 0 0 0 0 0 0 V2000
-0.3158 -3.3907 -0.6122 C 0 0 0 0 0 0 0 0 0 0 1
0.9952 -3.2269 -0.1450 C 0 0 0 0 0 0 0 0 0 0 2
1.3989 -1.9876 0.3573 C 0 0 0 0 0 0 0 0 0 0 3
0.5123 -0.8985 0.3954 C 0 0 0 0 0 0 0 0 0 0 4
-0.8078 -1.0606 -0.0705 C 0 0 0 0 0 0 0 0 0 0 5
-1.2037 -2.3130 -0.5723 C 0 0 0 0 0 0 0 0 0 0 6
0.9816 0.4261 0.9784 C 0 0 0 0 0 0 0 0 0 0 7
-1.7862 0.0973 -0.0313 C 0 0 0 0 0 0 0 0 0 0 8
-1.3227 1.1945 0.9342 C 0 0 0 0 0 0 0 0 0 0 9
0.0837 1.5423 0.6806 N 0 0 0 0 0 0 0 0 0 0 10
0.4489 2.4410 -0.3153 C 0 0 0 0 0 0 0 0 0 0 11
-0.5116 3.4087 -0.6126 N 0 0 0 0 0 0 0 0 0 0 12
1.6037 2.3412 -0.9154 N 0 0 0 0 0 0 0 0 0 0 13
-0.6441 -4.3553 -1.0041 H 0 0 0 0 0 0 0 0 0 0 14
1.6985 -4.0615 -0.1730 H 0 0 0 0 0 0 0 0 0 0 15
2.4212 -1.8578 0.7234 H 0 0 0 0 0 0 0 0 0 0 16
-2.2288 -2.4412 -0.9302 H 0 0 0 0 0 0 0 0 0 0 17
1.9754 0.6808 0.5935 H 0 0 0 0 0 0 0 0 0 0 18
1.0581 0.3301 2.0763 H 0 0 0 0 0 0 0 0 0 0 19
-2.7849 -0.2627 0.2619 H 0 0 0 0 0 0 0 0 0 0 20
-1.8945 0.5297 -1.0409 H 0 0 0 0 0 0 0 0 0 0 21
-1.3852 0.8382 1.9741 H 0 0 0 0 0 0 0 0 0 0 22
-1.9677 2.0757 0.8600 H 0 0 0 0 0 0 0 0 0 0 23
-0.1497 4.1878 -1.1584 H 0 0 0 0 0 0 0 0 0 0 24
-1.0872 3.7330 0.1625 H 0 0 0 0 0 0 0 0 0 0 25
1.7481 3.1608 -1.5158 H 0 0 0 0 0 0 0 0 0 0 26
2 1 0 0 0 0
6 1 0 0 0 0
14 1 0 0 0 0
3 2 0 0 0 0
15 2 0 0 0 0
4 3 0 0 0 0
16 3 0 0 0 0
5 4 0 0 0 0
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6 5 0 0 0 0
8 5 0 0 0 0
17 6 0 0 0 0
10 7 0 0 0 0
18 7 0 0 0 0
19 7 0 0 0 0
9 8 0 0 0 0
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21 8 0 0 0 0
10 9 0 0 0 0
22 9 0 0 0 0
23 9 0 0 0 0
11 10 0 0 0 0
12 11 0 0 0 0
13 11 0 0 0 0
24 12 0 0 0 0
25 12 0 0 0 0
13 26 0 0 0 0
M END
$$$$
debrisoquine_a_p2.sdf
COSMOtherm 3D 0
27 28 0 0 0 0 0 0 0 0 0 V2000
-0.1971 -3.5846 -0.4254 C 0 0 0 0 0 0 0 0 0 0 1
1.1205 -3.3048 -0.0393 C 0 0 0 0 0 0 0 0 0 0 2
1.4740 -2.0019 0.3156 C 0 0 0 0 0 0 0 0 0 0 3
0.5245 -0.9679 0.2854 C 0 0 0 0 0 0 0 0 0 0 4
-0.7999 -1.2433 -0.0981 C 0 0 0 0 0 0 0 0 0 0 5
-1.1436 -2.5588 -0.4542 C 0 0 0 0 0 0 0 0 0 0 6
0.9480 0.4233 0.7167 C 0 0 0 0 0 0 0 0 0 0 7
-1.8334 -0.1388 -0.1458 C 0 0 0 0 0 0 0 0 0 0 8
-1.4179 1.0861 0.6726 C 0 0 0 0 0 0 0 0 0 0 9
-0.0316 1.4515 0.3330 N 0 0 0 0 0 0 0 0 0 0 10
0.3177 2.6416 -0.1852 C 0 0 0 0 0 0 0 0 0 0 11
-0.5515 3.6685 -0.1955 N 0 0 0 0 0 0 0 0 0 0 12
1.5458 2.8371 -0.7037 N 0 0 0 0 0 0 0 0 0 0 13
-0.4844 -4.6002 -0.7038 H 0 0 0 0 0 0 0 0 0 0 14
1.8687 -4.0990 -0.0152 H 0 0 0 0 0 0 0 0 0 0 15
2.5012 -1.7805 0.6168 H 0 0 0 0 0 0 0 0 0 0 16
-2.1723 -2.7767 -0.7521 H 0 0 0 0 0 0 0 0 0 0 17
1.9338 0.6606 0.3049 H 0 0 0 0 0 0 0 0 0 0 18
1.0524 0.4556 1.8162 H 0 0 0 0 0 0 0 0 0 0 19
-2.7990 -0.5056 0.2329 H 0 0 0 0 0 0 0 0 0 0 20
-2.0015 0.1679 -1.1915 H 0 0 0 0 0 0 0 0 0 0 21
-1.4601 0.8746 1.7524 H 0 0 0 0 0 0 0 0 0 0 22
-2.0952 1.9189 0.4648 H 0 0 0 0 0 0 0 0 0 0 23
-0.3021 4.5281 -0.6742 H 0 0 0 0 0 0 0 0 0 0 24
-1.2941 3.7348 0.4923 H 0 0 0 0 0 0 0 0 0 0 25
1.8012 3.7632 -1.0320 H 0 0 0 0 0 0 0 0 0 0 26
2.0735 2.0655 -1.0977 H 0 0 0 0 0 0 0 0 0 0 27
2 1 0 0 0 0
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26 13 0 0 0 0
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debrisoquine_p2.sdf
COSMOtherm 3D 0
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-1.1679 -2.5717 0.3303 C 0 0 0 0 0 0 0 0 0 0 1
-0.7914 -1.2492 0.0383 C 0 0 0 0 0 0 0 0 0 0 2
0.5664 -0.9637 -0.1920 C 0 0 0 0 0 0 0 0 0 0 3
1.5156 -1.9977 -0.1353 C 0 0 0 0 0 0 0 0 0 0 4
1.1296 -3.3068 0.1563 C 0 0 0 0 0 0 0 0 0 0 5
-0.2212 -3.5954 0.3922 C 0 0 0 0 0 0 0 0 0 0 6
-1.8308 -0.1500 -0.0301 C 0 0 0 0 0 0 0 0 0 0 7
-1.3170 1.0363 -0.8414 C 0 0 0 0 0 0 0 0 0 0 8
1.0595 0.4393 -0.5108 C 0 0 0 0 0 0 0 0 0 0 9
0.0061 1.4475 -0.3417 N 0 0 0 0 0 0 0 0 0 0 10
0.2561 2.6597 0.1798 C 0 0 0 0 0 0 0 0 0 0 11
-0.7528 3.4708 0.5516 N 0 0 0 0 0 0 0 0 0 0 12
1.5229 3.0846 0.3381 N 0 0 0 0 0 0 0 0 0 0 13
-2.2233 -2.7955 0.5053 H 0 0 0 0 0 0 0 0 0 0 14
2.5692 -1.7706 -0.3177 H 0 0 0 0 0 0 0 0 0 0 15
1.8788 -4.0992 0.1999 H 0 0 0 0 0 0 0 0 0 0 16
-0.5342 -4.6161 0.6192 H 0 0 0 0 0 0 0 0 0 0 17
-2.0987 0.1830 0.9867 H 0 0 0 0 0 0 0 0 0 0 18
-2.7542 -0.5298 -0.4915 H 0 0 0 0 0 0 0 0 0 0 19
-2.0065 1.8855 -0.8157 H 0 0 0 0 0 0 0 0 0 0 20
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URL: <http://mc.manuscriptcentral.com/tandf/tmph>

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26 20 0 0 0 0
27 20 0 0 0 0
28 20 0 0 0 0
2 29 0 0 0 0
M END
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di-n-butylamine.sdf
COSMOTHERM 3D 0
28 27 0 0 0 0 0 0 0 0 0 V2000
1.2254 -0.0132 0.5100 C 0 0 0 0 0 0 0 0 0 0 1
0.0000 -0.0702 -0.3018 N 0 0 0 0 0 0 0 0 0 0 2
-1.2254 -0.0132 0.5099 C 0 0 0 0 0 0 0 0 0 0 3
2.4814 -0.0266 -0.3624 C 0 0 0 0 0 0 0 0 0 0 4
1.2290 -0.8929 1.1768 H 0 0 0 0 0 0 0 0 0 0 5
1.2450 0.8826 1.1701 H 0 0 0 0 0 0 0 0 0 0 6
0.0000 0.7377 -0.9342 H 0 0 0 0 0 0 0 0 0 0 7
-1.2294 -0.8935 1.1761 H 0 0 0 0 0 0 0 0 0 0 8
-1.2446 0.8820 1.1708 H 0 0 0 0 0 0 0 0 0 0 9
-2.4814 -0.0254 -0.3625 C 0 0 0 0 0 0 0 0 0 0 10
3.7820 0.0326 0.4492 C 0 0 0 0 0 0 0 0 0 0 11
2.4477 0.8326 -1.0568 H 0 0 0 0 0 0 0 0 0 0 12
2.4734 -0.9361 -0.9872 H 0 0 0 0 0 0 0 0 0 0 13
-3.7820 0.0317 0.4492 C 0 0 0 0 0 0 0 0 0 0 14
-2.4481 0.8350 -1.0554 H 0 0 0 0 0 0 0 0 0 0 15
-2.4730 -0.9339 -0.9888 H 0 0 0 0 0 0 0 0 0 0 16
5.0386 0.0138 -0.4279 C 0 0 0 0 0 0 0 0 0 0 17
3.8109 -0.8190 1.1509 H 0 0 0 0 0 0 0 0 0 0 18
3.7816 0.9441 1.0711 H 0 0 0 0 0 0 0 0 0 0 19
-5.0386 0.0139 -0.4278 C 0 0 0 0 0 0 0 0 0 0 20
-3.8105 -0.8212 1.1493 H 0 0 0 0 0 0 0 0 0 0 21
-3.7820 0.9422 1.0727 H 0 0 0 0 0 0 0 0 0 0 22
5.9542 0.0575 0.1805 H 0 0 0 0 0 0 0 0 0 0 23
5.0542 0.8725 -1.1175 H 0 0 0 0 0 0 0 0 0 0 24
5.0842 -0.9031 -1.0362 H 0 0 0 0 0 0 0 0 0 0 25
-5.9542 0.0576 0.1805 H 0 0 0 0 0 0 0 0 0 0 26
-5.0539 0.8730 -1.1170 H 0 0 0 0 0 0 0 0 0 0 27
-5.0846 -0.9027 -1.0367 H 0 0 0 0 0 0 0 0 0 0 28
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di-n-propylamine-cation.sdf
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1.2701 0.0005 -0.3947 C 0 0 0 0 0 0 0 0 0 0 1
0.0000 0.0006 0.4196 N 0 0 0 0 0 0 0 0 0 0 2
-1.2701 0.0005 -0.3947 C 0 0 0 0 0 0 0 0 0 0 3
2.5021 -0.0006 0.5026 C 0 0 0 0 0 0 0 0 0 0 4
1.2295 -0.8921 -1.0319 H 0 0 0 0 0 0 0 0 0 0 5
1.2304 0.8937 -1.0312 H 0 0 0 0 0 0 0 0 0 0 6
0.0000 0.8206 1.0430 H 0 0 0 0 0 0 0 0 0 0 7
-1.2298 -0.8922 -1.0317 H 0 0 0 0 0 0 0 0 0 0 8
-1.2301 0.8935 -1.0314 H 0 0 0 0 0 0 0 0 0 0 9
-2.5021 0.0002 0.5026 C 0 0 0 0 0 0 0 0 0 0 10
3.7917 -0.0003 -0.3262 C 0 0 0 0 0 0 0 0 0 0 11
2.4785 0.8857 1.1569 H 0 0 0 0 0 0 0 0 0 0 12
2.4778 -0.8882 1.1552 H 0 0 0 0 0 0 0 0 0 0 13
-3.7917 -0.0008 -0.3261 C 0 0 0 0 0 0 0 0 0 0 14
-2.4786 0.8873 1.1558 H 0 0 0 0 0 0 0 0 0 0 15
-2.4777 -0.8866 1.1562 H 0 0 0 0 0 0 0 0 0 0 16
4.6706 -0.0031 0.3325 H 0 0 0 0 0 0 0 0 0 0 17
3.8509 -0.8892 -0.9715 H 0 0 0 0 0 0 0 0 0 0 18
3.8532 0.8916 -0.9671 H 0 0 0 0 0 0 0 0 0 0 19
-4.6706 -0.0001 0.3326 H 0 0 0 0 0 0 0 0 0 0 20
-3.8520 -0.8919 -0.9683 H 0 0 0 0 0 0 0 0 0 0 21
-3.8522 0.8889 -0.9703 H 0 0 0 0 0 0 0 0 0 0 22
0.0000 -0.8194 1.0430 H 0 0 0 0 0 0 0 0 0 0 23
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19 11 0 0 0 0
20 14 0 0 0 0
21 14 0 0 0 0
22 14 0 0 0 0
2 23 0 0 0 0
M END
$$$$
di-n-propylamine.sdf
COSMOtherm 3D 0
22 21 0 0 0 0 0 0 0 0 0 V2000
1.2255 0.0141 -0.3703 C 0 0 0 0 0 0 0 0 0 0 1
0.0000 0.0586 0.4414 N 0 0 0 0 0 0 0 0 0 0 2
-1.2255 0.0134 -0.3703 C 0 0 0 0 0 0 0 0 0 0 3
2.4820 0.0181 0.5018 C 0 0 0 0 0 0 0 0 0 0 4
1.2288 0.9023 -1.0260 H 0 0 0 0 0 0 0 0 0 0 5
1.2478 -0.8730 -1.0423 H 0 0 0 0 0 0 0 0 0 0 6
0.0003 -0.7581 1.0623 H 0 0 0 0 0 0 0 0 0 0 7
-1.2295 0.9018 -1.0256 H 0 0 0 0 0 0 0 0 0 0 8
-1.2472 -0.8735 -1.0427 H 0 0 0 0 0 0 0 0 0 0 9
-2.4820 0.0161 0.5018 C 0 0 0 0 0 0 0 0 0 0 10
3.7744 -0.0313 -0.3202 C 0 0 0 0 0 0 0 0 0 0 11
2.4468 -0.8483 1.1853 H 0 0 0 0 0 0 0 0 0 0 12
2.4713 0.9194 1.1363 H 0 0 0 0 0 0 0 0 0 0 13
-3.7744 -0.0299 -0.3203 C 0 0 0 0 0 0 0 0 0 0 14
-2.4475 -0.8518 1.1834 H 0 0 0 0 0 0 0 0 0 0 15
-2.4705 0.9160 1.1384 H 0 0 0 0 0 0 0 0 0 0 16
4.6606 -0.0251 0.3307 H 0 0 0 0 0 0 0 0 0 0 17
3.8503 0.8353 -0.9956 H 0 0 0 0 0 0 0 0 0 0 18
3.8200 -0.9417 -0.9378 H 0 0 0 0 0 0 0 0 0 0 19
-4.6606 -0.0258 0.3308 H 0 0 0 0 0 0 0 0 0 0 20
-3.8501 0.8392 -0.9924 H 0 0 0 0 0 0 0 0 0 0 21
-3.8204 -0.9380 -0.9412 H 0 0 0 0 0 0 0 0 0 0 22
2 1 0 0 0 0
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19 11 0 0 0 0
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21 14 0 0 0 0
14 22 0 0 0 0
M END
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di-sec-butylamine-cation.sdf
COSMOtherm 3D 0
29 28 0 0 0 0 0 0 0 0 0 V2000
-0.0212 0.6220 -0.5114 N 0 0 0 0 0 0 0 0 0 0 1
1.3787 0.4070 0.0707 C 0 0 0 0 0 0 0 0 0 0 2
-1.1996 -0.0229 0.2194 C 0 0 0 0 0 0 0 0 0 0 3
-1.4818 0.7540 1.4985 C 0 0 0 0 0 0 0 0 0 0 4
-2.3812 -0.0737 -0.7572 C 0 0 0 0 0 0 0 0 0 0 5
2.2783 1.5244 -0.4468 C 0 0 0 0 0 0 0 0 0 0 6
1.8577 -1.0022 -0.2928 C 0 0 0 0 0 0 0 0 0 0 7
-0.2008 1.6352 -0.5735 H 0 0 0 0 0 0 0 0 0 0 8
1.2573 0.4962 1.1585 H 0 0 0 0 0 0 0 0 0 0 9
-0.8723 -1.0455 0.4531 H 0 0 0 0 0 0 0 0 0 0 10
-1.8022 1.7824 1.2709 H 0 0 0 0 0 0 0 0 0 0 11
-2.2901 0.2613 2.0527 H 0 0 0 0 0 0 0 0 0 0 12
-0.6094 0.7917 2.1641 H 0 0 0 0 0 0 0 0 0 0 13
-2.0395 -0.5387 -1.6964 H 0 0 0 0 0 0 0 0 0 0 14
-3.5755 -0.8657 -0.2141 C 0 0 0 0 0 0 0 0 0 0 15
-2.6909 0.9559 -1.0027 H 0 0 0 0 0 0 0 0 0 0 16
3.2793 1.4255 -0.0094 H 0 0 0 0 0 0 0 0 0 0 17
1.8902 2.5135 -0.1643 H 0 0 0 0 0 0 0 0 0 0 18
2.3771 1.4784 -1.5414 H 0 0 0 0 0 0 0 0 0 0 19
3.1388 -1.4043 0.4473 C 0 0 0 0 0 0 0 0 0 0 20
1.0684 -1.7306 -0.0515 H 0 0 0 0 0 0 0 0 0 0 21
2.0186 -1.0514 -1.3831 H 0 0 0 0 0 0 0 0 0 0 22
-4.3592 -0.9365 -0.9807 H 0 0 0 0 0 0 0 0 0 0 23
-4.0182 -0.3865 0.6697 H 0 0 0 0 0 0 0 0 0 0 24
-3.2803 -1.8891 0.0613 H 0 0 0 0 0 0 0 0 0 0 25
3.4142 -2.4355 0.1885 H 0 0 0 0 0 0 0 0 0 0 26
3.9870 -0.7577 0.1829 H 0 0 0 0 0 0 0 0 0 0 27
2.9978 -1.3562 1.5373 H 0 0 0 0 0 0 0 0 0 0 28
-0.0162 0.2881 -1.4875 H 0 0 0 0 0 0 0 0 0 0 29
2 1 0 0 0 0
3 1 0 0 0 0
8 1 0 0 0 0
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23 15 0 0 0 0
24 15 0 0 0 0
25 15 0 0 0 0
26 20 0 0 0 0
27 20 0 0 0 0
28 20 0 0 0 0
1 29 0 0 0 0
M END
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di-sec-butylamine.sdf
COSMOtherm 3D 0

28 27 0 0 0 0 0 0 0 0 0 V2000
-0.0130 0.6223 -0.5377 N 0 0 0 0 0 0 0 0 0 0 1
1.3284 0.4125 0.0522 C 0 0 0 0 0 0 0 0 0 0 2
-1.1469 -0.0029 0.1839 C 0 0 0 0 0 0 0 0 0 0 3
-1.4850 0.7107 1.5043 C 0 0 0 0 0 0 0 0 0 0 4
-2.3555 -0.0710 -0.7664 C 0 0 0 0 0 0 0 0 0 0 5
2.2506 1.5376 -0.4260 C 0 0 0 0 0 0 0 0 0 0 6
1.8657 -0.9774 -0.3390 C 0 0 0 0 0 0 0 0 0 0 7
-0.1902 1.6316 -0.5823 H 0 0 0 0 0 0 0 0 0 0 8
1.2883 0.4552 1.1621 H 0 0 0 0 0 0 0 0 0 0 9
-0.8449 -1.0393 0.4134 H 0 0 0 0 0 0 0 0 0 0 10
-1.8552 1.7298 1.3021 H 0 0 0 0 0 0 0 0 0 0 11
-2.2601 0.1755 2.0723 H 0 0 0 0 0 0 0 0 0 0 12
-0.6000 0.7910 2.1525 H 0 0 0 0 0 0 0 0 0 0 13
-2.0114 -0.5303 -1.7065 H 0 0 0 0 0 0 0 0 0 0 14
-3.5580 -0.8513 -0.2220 C 0 0 0 0 0 0 0 0 0 0 15
-2.6638 0.9600 -1.0179 H 0 0 0 0 0 0 0 0 0 0 16
3.2714 1.4101 -0.0411 H 0 0 0 0 0 0 0 0 0 0 17
1.8854 2.5189 -0.0856 H 0 0 0 0 0 0 0 0 0 0 18
2.2968 1.5500 -1.5268 H 0 0 0 0 0 0 0 0 0 0 19
3.1049 -1.4154 0.4508 C 0 0 0 0 0 0 0 0 0 0 20
1.0668 -1.7207 -0.1859 H 0 0 0 0 0 0 0 0 0 0 21
2.0825 -0.9728 -1.4211 H 0 0 0 0 0 0 0 0 0 0 22
-4.3523 -0.9239 -0.9796 H 0 0 0 0 0 0 0 0 0 0 23
-3.9937 -0.3723 0.6667 H 0 0 0 0 0 0 0 0 0 0 24
-3.2697 -1.8772 0.0573 H 0 0 0 0 0 0 0 0 0 0 25
3.4207 -2.4270 0.1566 H 0 0 0 0 0 0 0 0 0 0 26
3.9597 -0.7430 0.2842 H 0 0 0 0 0 0 0 0 0 0 27
2.8993 -1.4320 1.5329 H 0 0 0 0 0 0 0 0 0 0 28

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23 15 0 0 0 0
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25 15 0 0 0 0
26 20 0 0 0 0
27 20 0 0 0 0
20 28 0 0 0 0
M END
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diethylamine-cation.sdf
COSMOtherm 3D 0

17 16 0 0 0 0 0 0 0 0 0 V2000
1.2712 -0.0047 0.5410 C 0 0 0 0 0 0 0 0 0 0 1
0.0000 0.0005 -0.2740 N 0 0 0 0 0 0 0 0 0 0 2
-1.2712 0.0047 0.5410 C 0 0 0 0 0 0 0 0 0 0 3
2.4951 0.0019 -0.3587 C 0 0 0 0 0 0 0 0 0 0 4
1.2278 0.8832 1.1829 H 0 0 0 0 0 0 0 0 0 0 5
1.2281 -0.9010 1.1710 H 0 0 0 0 0 0 0 0 0 0 6
-0.0030 -0.8190 -0.8980 H 0 0 0 0 0 0 0 0 0 0 7
-1.2286 0.9008 1.1714 H 0 0 0 0 0 0 0 0 0 0 8
-1.2273 -0.8835 1.1826 H 0 0 0 0 0 0 0 0 0 0 9
-2.4951 -0.0024 -0.3587 C 0 0 0 0 0 0 0 0 0 0 10
3.3966 -0.0049 0.2678 H 0 0 0 0 0 0 0 0 0 0 11
2.5251 -0.8870 -1.0047 H 0 0 0 0 0 0 0 0 0 0 12
2.5270 0.9025 -0.9882 H 0 0 0 0 0 0 0 0 0 0 13
-3.3966 0.0022 0.2678 H 0 0 0 0 0 0 0 0 0 0 14
-2.5256 -0.9020 -0.9896 H 0 0 0 0 0 0 0 0 0 0 15
-2.5264 0.8874 -1.0034 H 0 0 0 0 0 0 0 0 0 0 16
0.0030 0.8205 -0.8972 H 0 0 0 0 0 0 0 0 0 0 17
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dimethyl-iso-butylamine.sdf
COSMOtherm      3D      0

22 21 0 0 0 0 0 0 0 0 0 V2000
1.2288 -0.1570 0.1768 N 0 0 0 0 0 0 0 0 0 0 0 1
1.6285 -0.7790 -1.0875 C 0 0 0 0 0 0 0 0 0 0 0 2
2.3258 0.6573 0.7050 C 0 0 0 0 0 0 0 0 0 0 0 3
0.0141 0.6583 0.0280 C 0 0 0 0 0 0 0 0 0 0 0 4
-1.2770 -0.1351 -0.2402 C 0 0 0 0 0 0 0 0 0 0 0 5
-2.4442 0.8425 -0.4454 C 0 0 0 0 0 0 0 0 0 0 0 6
-1.5761 -1.1306 0.8883 C 0 0 0 0 0 0 0 0 0 0 0 7
2.5377 -1.3771 -0.9319 H 0 0 0 0 0 0 0 0 0 0 0 8
0.8415 -1.4508 -1.4547 H 0 0 0 0 0 0 0 0 0 0 0 9
1.8401 -0.0265 -1.8809 H 0 0 0 0 0 0 0 0 0 0 0 10
2.0400 1.0849 1.6769 H 0 0 0 0 0 0 0 0 0 0 0 11
2.6042 1.4959 0.0267 H 0 0 0 0 0 0 0 0 0 0 0 12
3.2174 0.0305 0.8512 H 0 0 0 0 0 0 0 0 0 0 0 13
0.1498 1.4131 -0.7829 H 0 0 0 0 0 0 0 0 0 0 0 14
-0.1187 1.2223 0.9671 H 0 0 0 0 0 0 0 0 0 0 0 15
-1.1515 -0.7023 -1.1789 H 0 0 0 0 0 0 0 0 0 0 0 16
-3.3749 0.3014 -0.6726 H 0 0 0 0 0 0 0 0 0 0 0 17
-2.2458 1.5382 -1.2749 H 0 0 0 0 0 0 0 0 0 0 0 18
-2.6183 1.4416 0.4636 H 0 0 0 0 0 0 0 0 0 0 0 19
-2.4768 -1.7223 0.6649 H 0 0 0 0 0 0 0 0 0 0 0 20
-0.7351 -1.8216 1.0405 H 0 0 0 0 0 0 0 0 0 0 0 21
-1.7490 -0.5969 1.8377 H 0 0 0 0 0 0 0 0 0 0 0 22

2 1 0 0 0 0
3 1 0 0 0 0
4 1 0 0 0 0
8 2 0 0 0 0
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18 6 0 0 0 0
19 6 0 0 0 0
20 7 0 0 0 0
21 7 0 0 0 0
7 22 0 0 0 0

M END
$$$$
dimethyl-iso-propylamine-cation.sdf
COSMOtherm      3D      0

20 19 0 0 0 0 0 0 0 0 0 V2000
0.6794 -0.0013 0.2861 N 0 0 0 0 0 0 0 0 0 0 0 1
1.4703 -1.2293 -0.0709 C 0 0 0 0 0 0 0 0 0 0 0 2
1.4680 1.2306 -0.0630 C 0 0 0 0 0 0 0 0 0 0 0 3
-0.7319 -0.0013 -0.3377 C 0 0 0 0 0 0 0 0 0 0 0 4
-1.4873 1.2631 0.0652 C 0 0 0 0 0 0 0 0 0 0 0 5
-1.4897 -1.2619 0.0729 C 0 0 0 0 0 0 0 0 0 0 0 6
2.4676 -1.1304 0.3678 H 0 0 0 0 0 0 0 0 0 0 0 7
0.9768 -2.1148 0.3348 H 0 0 0 0 0 0 0 0 0 0 0 8
1.5386 -1.2893 -1.1622 H 0 0 0 0 0 0 0 0 0 0 0 9
2.4676 1.1274 0.3696 H 0 0 0 0 0 0 0 0 0 0 0 10
0.9763 2.1115 0.3548 H 0 0 0 0 0 0 0 0 0 0 0 11
1.5304 1.3018 -1.1539 H 0 0 0 0 0 0 0 0 0 0 0 12
-0.5428 -0.0046 -1.4205 H 0 0 0 0 0 0 0 0 0 0 0 13
-2.5064 1.1940 -0.3363 H 0 0 0 0 0 0 0 0 0 0 0 14
-1.0382 2.1780 -0.3382 H 0 0 0 0 0 0 0 0 0 0 0 15
-1.5635 1.3503 1.1596 H 0 0 0 0 0 0 0 0 0 0 0 16
-2.5083 -1.1941 -0.3300 H 0 0 0 0 0 0 0 0 0 0 0 17
-1.0417 -2.1803 -0.3235 H 0 0 0 0 0 0 0 0 0 0 0 18
-1.5670 -1.3412 1.1679 H 0 0 0 0 0 0 0 0 0 0 0 19
0.5521 -0.0047 1.3085 H 0 0 0 0 0 0 0 0 0 0 0 20

2 1 0 0 0 0
3 1 0 0 0 0
4 1 0 0 0 0
7 2 0 0 0 0
8 2 0 0 0 0
9 2 0 0 0 0
10 3 0 0 0 0
11 3 0 0 0 0
12 3 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
13 4 0 0 0 0
14 5 0 0 0 0
15 5 0 0 0 0
16 5 0 0 0 0
17 6 0 0 0 0
18 6 0 0 0 0
19 6 0 0 0 0
1 20 0 0 0 0

M END
$$$$
dimethyl-iso-propylamine.sdf
COSMOtherm      3D      0

19 18 0 0 0 0 0 0 0 0 0 V2000
0.6711 -0.0003 0.3162 N 0 0 0 0 0 0 0 0 0 0 0 1
1.4477 -1.1939 -0.0461 C 0 0 0 0 0 0 0 0 0 0 0 2
1.4473 1.1939 -0.0448 C 0 0 0 0 0 0 0 0 0 0 0 3
-0.6737 -0.0003 -0.3167 C 0 0 0 0 0 0 0 0 0 0 0 4
-1.4724 1.2525 0.0696 C 0 0 0 0 0 0 0 0 0 0 0 5
-1.4733 -1.2520 0.0709 C 0 0 0 0 0 0 0 0 0 0 0 6
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[illegible]

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11 4 0 0 0 0
12 4 0 0 0 0
13 4 0 0 0 0
14 9 0 0 0 0
15 9 0 0 0 0
16 9 0 0 0 0
17 14 0 0 0 0
18 14 0 0 0 0
14 19 0 0 0 0
M END
$$$$
dimethyl-sec-butylamine-cation.sdf
COSMOtherm 3D 0
23 22 0 0 0 0 0 0 0 0 V2000
1.0889 0.2264 0.2810 N 0 0 0 0 0 0 0 0 0 1
2.2339 -0.6965 -0.0296 C 0 0 0 0 0 0 0 0 0 2
1.4104 1.6028 -0.2338 C 0 0 0 0 0 0 0 0 0 3
-0.2844 -0.2720 -0.2306 C 0 0 0 0 0 0 0 0 0 4
-1.3989 0.5010 0.4918 C 0 0 0 0 0 0 0 0 0 5
-0.4279 -1.7791 -0.0499 C 0 0 0 0 0 0 0 0 0 6
3.1520 -0.2225 0.3309 H 0 0 0 0 0 0 0 0 0 7
2.0864 -1.6501 0.4820 H 0 0 0 0 0 0 0 0 0 8
2.2813 -0.8387 -1.1139 H 0 0 0 0 0 0 0 0 0 9
2.3306 1.9446 0.2491 H 0 0 0 0 0 0 0 0 0 10
0.5925 2.2867 0.0035 H 0 0 0 0 0 0 0 0 0 11
1.5494 1.5334 -1.3174 H 0 0 0 0 0 0 0 0 0 12
-0.2744 -0.0166 -1.3006 H 0 0 0 0 0 0 0 0 0 13
-1.1321 1.5633 0.5816 H 0 0 0 0 0 0 0 0 0 14
-2.7479 0.4068 -0.2317 C 0 0 0 0 0 0 0 0 0 15
-1.4905 0.1079 1.5176 H 0 0 0 0 0 0 0 0 0 16
-1.4442 -2.0655 -0.3491 H 0 0 0 0 0 0 0 0 0 17
0.2668 -2.3514 -0.6755 H 0 0 0 0 0 0 0 0 0 18
-0.2970 -2.0706 1.0026 H 0 0 0 0 0 0 0 0 0 19
-3.5062 0.9871 0.3112 H 0 0 0 0 0 0 0 0 0 20
-3.1103 -0.6283 -0.3015 H 0 0 0 0 0 0 0 0 0 21
-2.6773 0.8138 -1.2511 H 0 0 0 0 0 0 0 0 0 22
1.0178 0.2865 1.3068 H 0 0 0 0 0 0 0 0 0 23
2 1 0 0 0 0
3 1 0 0 0 0
4 1 0 0 0 0
7 2 0 0 0 0
8 2 0 0 0 0
9 2 0 0 0 0
10 3 0 0 0 0
11 3 0 0 0 0
12 3 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
13 4 0 0 0 0
14 5 0 0 0 0
15 5 0 0 0 0
16 5 0 0 0 0
17 6 0 0 0 0
18 6 0 0 0 0
19 6 0 0 0 0
20 15 0 0 0 0
21 15 0 0 0 0
22 15 0 0 0 0
1 23 0 0 0 0
M END
$$$$
dimethyl-sec-butylamine.sdf
COSMOtherm 3D 0
22 21 0 0 0 0 0 0 0 0 V2000
1.0908 0.2134 0.3103 N 0 0 0 0 0 0 0 0 0 1
2.2061 -0.6565 -0.0869 C 0 0 0 0 0 0 0 0 0 2
1.3878 1.5764 -0.1530 C 0 0 0 0 0 0 0 0 0 3
-0.2252 -0.2610 -0.2007 C 0 0 0 0 0 0 0 0 0 4
-1.3813 0.5106 0.4722 C 0 0 0 0 0 0 0 0 0 5
-0.4106 -1.7678 0.0203 C 0 0 0 0 0 0 0 0 0 6
3.1433 -0.2250 0.2916 H 0 0 0 0 0 0 0 0 0 7
2.1008 -1.6581 0.3457 H 0 0 0 0 0 0 0 0 0 8
2.3003 -0.7586 -1.1915 H 0 0 0 0 0 0 0 0 0 9
2.3574 1.8944 0.2551 H 0 0 0 0 0 0 0 0 0 10
0.6314 2.2911 0.1920 H 0 0 0 0 0 0 0 0 0 11
1.4433 1.6402 -1.2630 H 0 0 0 0 0 0 0 0 0 12
-0.2717 -0.0651 -1.2992 H 0 0 0 0 0 0 0 0 0 13
-1.1256 1.5767 0.5486 H 0 0 0 0 0 0 0 0 0 14
-2.7201 0.3925 -0.2671 C 0 0 0 0 0 0 0 0 0 15
-1.4854 0.1419 1.5069 H 0 0 0 0 0 0 0 0 0 16
0.2557 -2.3748 -0.6059 H 0 0 0 0 0 0 0 0 0 17
-1.4408 -2.0559 -0.2285 H 0 0 0 0 0 0 0 0 0 18
-0.2317 -2.0256 1.0763 H 0 0 0 0 0 0 0 0 0 19
-3.4988 0.9779 0.2434 H 0 0 0 0 0 0 0 0 0 20
-3.0758 -0.6470 -0.3233 H 0 0 0 0 0 0 0 0 0 21
-2.6371 0.7735 -1.2968 H 0 0 0 0 0 0 0 0 0 22
2 1 0 0 0 0
3 1 0 0 0 0
4 1 0 0 0 0
7 2 0 0 0 0
8 2 0 0 0 0
9 2 0 0 0 0
10 3 0 0 0 0
11 3 0 0 0 0
12 3 0 0 0 0
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13 4 0 0 0 0
14 5 0 0 0 0
15 5 0 0 0 0
16 5 0 0 0 0
17 6 0 0 0 0
18 6 0 0 0 0
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19 6 0 0 0 0
20 15 0 0 0 0
21 15 0 0 0 0
15 22 0 0 0 0
M END
$$$$
dimethyl-tert-butylamine-cation.sdf
COSMOtherm 3D 0

23 22 0 0 0 0 0 0 0 0 0 V2000
1.5905 -1.2243 -0.0043 C 0 0 0 0 0 0 0 0 0 0 0 1
0.8265 0.0035 0.4073 N 0 0 0 0 0 0 0 0 0 0 0 2
1.5941 1.2284 -0.0061 C 0 0 0 0 0 0 0 0 0 0 0 3
-0.6863 -0.0018 -0.0240 C 0 0 0 0 0 0 0 0 0 0 0 4
-1.2932 1.3429 0.3930 C 0 0 0 0 0 0 0 0 0 0 0 5
-1.3676 -1.1368 0.7504 C 0 0 0 0 0 0 0 0 0 0 0 6
-0.7897 -0.2127 -1.5343 C 0 0 0 0 0 0 0 0 0 0 0 7
2.5590 -1.2006 0.5043 H 0 0 0 0 0 0 0 0 0 0 0 8
1.0416 -2.1209 0.2922 H 0 0 0 0 0 0 0 0 0 0 0 9
1.7387 -1.2018 -1.0875 H 0 0 0 0 0 0 0 0 0 0 0 10
2.6238 1.1096 0.3455 H 0 0 0 0 0 0 0 0 0 0 0 11
1.1501 2.1142 0.4522 H 0 0 0 0 0 0 0 0 0 0 0 12
1.5803 1.3070 -1.0971 H 0 0 0 0 0 0 0 0 0 0 0 13
-2.3814 1.2810 0.2629 H 0 0 0 0 0 0 0 0 0 0 0 14
-0.9335 2.1758 -0.2241 H 0 0 0 0 0 0 0 0 0 0 0 15
-1.0967 1.5666 1.4520 H 0 0 0 0 0 0 0 0 0 0 0 16
-2.4434 -1.1034 0.5349 H 0 0 0 0 0 0 0 0 0 0 0 17
-1.0063 -2.1300 0.4565 H 0 0 0 0 0 0 0 0 0 0 0 18
-1.2402 -1.0145 1.8366 H 0 0 0 0 0 0 0 0 0 0 0 19
-1.8490 -0.1364 -1.8139 H 0 0 0 0 0 0 0 0 0 0 0 20
-0.4374 -1.2054 -1.8424 H 0 0 0 0 0 0 0 0 0 0 0 21
-0.2460 0.5553 -2.1012 H 0 0 0 0 0 0 0 0 0 0 0 22
0.8011 0.0050 1.4369 H 0 0 0 0 0 0 0 0 0 0 0 23

2 1 0 0 0 0
8 1 0 0 0 0
9 1 0 0 0 0
10 1 0 0 0 0
3 2 0 0 0 0
4 2 0 0 0 0
11 3 0 0 0 0
12 3 0 0 0 0
13 3 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
7 4 0 0 0 0
14 5 0 0 0 0
15 5 0 0 0 0
16 5 0 0 0 0
17 6 0 0 0 0
18 6 0 0 0 0
19 6 0 0 0 0
20 7 0 0 0 0
21 7 0 0 0 0
22 7 0 0 0 0
2 23 0 0 0 0
M END
$$$$
dimethyl-tert-butylamine.sdf
COSMOtherm 3D 0

22 21 0 0 0 0 0 0 0 0 0 V2000
1.5723 -1.1946 0.0173 C 0 0 0 0 0 0 0 0 0 0 0 1
0.8227 0.0009 0.4211 N 0 0 0 0 0 0 0 0 0 0 0 2
1.5766 1.1925 0.0151 C 0 0 0 0 0 0 0 0 0 0 0 3
-0.6202 -0.0010 -0.0046 C 0 0 0 0 0 0 0 0 0 0 0 4
-1.2877 1.2963 0.4910 C 0 0 0 0 0 0 0 0 0 0 0 5
-1.3336 -1.1827 0.6808 C 0 0 0 0 0 0 0 0 0 0 0 6
-0.8002 -0.1114 -1.5366 C 0 0 0 0 0 0 0 0 0 0 0 7
2.5632 -1.1660 0.4938 H 0 0 0 0 0 0 0 0 0 0 0 8
1.0689 -2.1085 0.3545 H 0 0 0 0 0 0 0 0 0 0 0 9
1.7334 -1.2714 -1.0794 H 0 0 0 0 0 0 0 0 0 0 0 10
2.5935 1.1177 0.4271 H 0 0 0 0 0 0 0 0 0 0 0 11
1.1220 2.1047 0.4189 H 0 0 0 0 0 0 0 0 0 0 0 12
1.6740 1.3088 -1.0862 H 0 0 0 0 0 0 0 0 0 0 0 13
-2.3764 1.2218 0.3590 H 0 0 0 0 0 0 0 0 0 0 0 14
-0.9493 2.1808 -0.0659 H 0 0 0 0 0 0 0 0 0 0 0 15
-1.0795 1.4553 1.5599 H 0 0 0 0 0 0 0 0 0 0 0 16
-2.4128 -1.1329 0.4759 H 0 0 0 0 0 0 0 0 0 0 0 17
-0.9779 -2.1566 0.3182 H 0 0 0 0 0 0 0 0 0 0 0 18
-1.1847 -1.1411 1.7703 H 0 0 0 0 0 0 0 0 0 0 0 19
-1.8678 -0.0587 -1.7966 H 0 0 0 0 0 0 0 0 0 0 0 20
-0.4105 -1.0645 -1.9226 H 0 0 0 0 0 0 0 0 0 0 0 21
-0.2890 0.7085 -2.0626 H 0 0 0 0 0 0 0 0 0 0 0 22

2 1 0 0 0 0
8 1 0 0 0 0
9 1 0 0 0 0
10 1 0 0 0 0
3 2 0 0 0 0
4 2 0 0 0 0
11 3 0 0 0 0
12 3 0 0 0 0
13 3 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
7 4 0 0 0 0
14 5 0 0 0 0
15 5 0 0 0 0
16 5 0 0 0 0
17 6 0 0 0 0
18 6 0 0 0 0
19 6 0 0 0 0
20 7 0 0 0 0
21 7 0 0 0 0
7 22 0 0 0 0
M END
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$$$$
dimethylamine-cation.sdf
COSMOTHERM      3D      0

11 10 0 0 0 0 0 0 0 0 0 V2000
1.2556 0.0000 -0.2861 C 0 0 0 0 0 0 0 0 0 0 1
0.0000 0.0000 0.5299 N 0 0 0 0 0 0 0 0 0 0 2
-1.2556 0.0000 -0.2861 C 0 0 0 0 0 0 0 0 0 0 3
2.1129 -0.0009 0.3934 H 0 0 0 0 0 0 0 0 0 0 4
1.2614 -0.8988 -0.9100 H 0 0 0 0 0 0 0 0 0 0 5
1.2623 0.8997 -0.9088 H 0 0 0 0 0 0 0 0 0 0 6
-0.0001 0.8178 1.1531 H 0 0 0 0 0 0 0 0 0 0 7
-2.1128 0.0014 0.3935 H 0 0 0 0 0 0 0 0 0 0 8
-1.2626 -0.8998 -0.9086 H 0 0 0 0 0 0 0 0 0 0 9
-1.2612 0.8986 -0.9102 H 0 0 0 0 0 0 0 0 0 0 10
0.0001 -0.8177 1.1532 H 0 0 0 0 0 0 0 0 0 0 11

2 1 0 0 0 0
4 1 0 0 0 0
5 1 0 0 0 0
6 1 0 0 0 0
3 2 0 0 0 0
7 2 0 0 0 0
8 3 0 0 0 0
9 3 0 0 0 0
10 3 0 0 0 0
2 11 0 0 0 0

M  END
$$$$
dimethylamine.sdf
COSMOTHERM      3D      0

10 9 0 0 0 0 0 0 0 0 V2000
1.2168 0.0159 -0.2573 C 0 0 0 0 0 0 0 0 0 0 1
0.0000 -0.0882 0.5567 N 0 0 0 0 0 0 0 0 0 0 2
-1.2168 0.0159 -0.2573 C 0 0 0 0 0 0 0 0 0 0 3
2.1018 0.0109 0.3942 H 0 0 0 0 0 0 0 0 0 0 4
1.2859 -0.8543 -0.9284 H 0 0 0 0 0 0 0 0 0 0 5
1.2527 0.9295 -0.8875 H 0 0 0 0 0 0 0 0 0 0 6
0.0000 0.6739 1.2394 H 0 0 0 0 0 0 0 0 0 0 7
-2.1018 0.0106 0.3943 H 0 0 0 0 0 0 0 0 0 0 8
-1.2858 -0.8541 -0.9286 H 0 0 0 0 0 0 0 0 0 0 9
-1.2529 0.9296 -0.8873 H 0 0 0 0 0 0 0 0 0 0 10

2 1 0 0 0 0
4 1 0 0 0 0
5 1 0 0 0 0
6 1 0 0 0 0
3 2 0 0 0 0
7 2 0 0 0 0
8 3 0 0 0 0
9 3 0 0 0 0
3 10 0 0 0 0

M  END
$$$$
dimethylethylamine-cation.sdf
COSMOTHERM      3D      0

17 16 0 0 0 0 0 0 0 0 V2000
1.6899 0.8096 -0.0063 C 0 0 0 0 0 0 0 0 0 0 1
0.4590 -0.0005 -0.2935 N 0 0 0 0 0 0 0 0 0 0 2
-0.7718 0.6486 0.3187 C 0 0 0 0 0 0 0 0 0 0 3
0.6416 -1.4260 0.1394 C 0 0 0 0 0 0 0 0 0 0 4
2.5434 0.3342 -0.4992 H 0 0 0 0 0 0 0 0 0 0 5
1.5414 1.8216 -0.3951 H 0 0 0 0 0 0 0 0 0 0 6
1.8401 0.8335 1.0780 H 0 0 0 0 0 0 0 0 0 0 7
-0.7299 1.7015 0.0143 H 0 0 0 0 0 0 0 0 0 0 8
-2.0701 0.0032 -0.1335 C 0 0 0 0 0 0 0 0 0 0 9
-0.6334 0.5918 1.4060 H 0 0 0 0 0 0 0 0 0 0 10
1.5370 -1.8224 -0.3487 H 0 0 0 0 0 0 0 0 0 0 11
-0.2332 -2.0099 -0.1586 H 0 0 0 0 0 0 0 0 0 0 12
0.7608 -1.4400 1.2280 H 0 0 0 0 0 0 0 0 0 0 13
-2.9033 0.5960 0.2674 H 0 0 0 0 0 0 0 0 0 0 14
-2.1855 -1.0232 0.2370 H 0 0 0 0 0 0 0 0 0 0 15
-2.1571 0.0032 -1.2295 H 0 0 0 0 0 0 0 0 0 0 16
0.3236 -0.0019 -1.3139 H 0 0 0 0 0 0 0 0 0 0 17

2 1 0 0 0 0
5 1 0 0 0 0
6 1 0 0 0 0
7 1 0 0 0 0
3 2 0 0 0 0
4 2 0 0 0 0
8 3 0 0 0 0
9 3 0 0 0 0
10 3 0 0 0 0
11 4 0 0 0 0
12 4 0 0 0 0
13 4 0 0 0 0
14 9 0 0 0 0
15 9 0 0 0 0
16 9 0 0 0 0
2 17 0 0 0 0

M  END
$$$$
dimethylethylamine.sdf
COSMOTHERM      3D      0

16 15 0 0 0 0 0 0 0 0 V2000
1.6571 0.7843 -0.0278 C 0 0 0 0 0 0 0 0 0 0 1
0.4542 0.0010 -0.3233 N 0 0 0 0 0 0 0 0 0 0 2
-0.7258 0.6265 0.2987 C 0 0 0 0 0 0 0 0 0 0 3
0.6378 -1.3846 0.1174 C 0 0 0 0 0 0 0 0 0 0 4
2.5247 0.3400 -0.5365 H 0 0 0 0 0 0 0 0 0 0 5
1.5316 1.8140 -0.3924 H 0 0 0 0 0 0 0 0 0 0 6
1.8830 0.8282 1.0616 H 0 0 0 0 0 0 0 0 0 0 7
-0.7135 1.6901 0.0134 H 0 0 0 0 0 0 0 0 0 0 8
-2.0533 0.0084 -0.1372 C 0 0 0 0 0 0 0 0 0 0 9
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-0.6444    0.5937    1.4106 H    0    0    0    0    0    0    0    0    0    0    10
1.5290    -1.8084   -0.3668 H    0    0    0    0    0    0    0    0    0    0    11
-0.2257    -1.9997   -0.1671 H    0    0    0    0    0    0    0    0    0    0    12
0.7730    -1.4635    1.2203 H    0    0    0    0    0    0    0    0    0    0    13
-2.8888    0.5958    0.2708 H    0    0    0    0    0    0    0    0    0    0    14
-2.1718    -1.0240    0.2209 H    0    0    0    0    0    0    0    0    0    0    15
-2.1393     0.0056   -1.2342 H    0    0    0    0    0    0    0    0    0    0    16
2  1  0  0  0  0
5  1  0  0  0  0
6  1  0  0  0  0
7  1  0  0  0  0
3  2  0  0  0  0
4  2  0  0  0  0
8  3  0  0  0  0
9  3  0  0  0  0
10 3  0  0  0  0
11 4  0  0  0  0
12 4  0  0  0  0
13 4  0  0  0  0
14 9  0  0  0  0
15 9  0  0  0  0
9 16 0  0  0  0
M  END
$$$$
ethylamine-cation.sdf
COSMOTHERM      3D      0
11 10 0 0 0 0 0 0 0 0 0 0 V2000
1.3011    0.0000   -0.2769 C    0    0    0    0    0    0    0    0    0    0    1
0.0590    0.0000    0.5959 C    0    0    0    0    0    0    0    0    0    0    2
-1.1924    0.0000   -0.2466 N    0    0    0    0    0    0    0    0    0    0    3
-2.0411    0.0126    0.3332 H    0    0    0    0    0    0    0    0    0    0    4
-1.2464   -0.8343   -0.8457 H    0    0    0    0    0    0    0    0    0    0    5
2.1896   -0.0024    0.3681 H    0    0    0    0    0    0    0    0    0    0    6
1.3442   -0.8932   -0.9164 H    0    0    0    0    0    0    0    0    0    0    7
1.3461    0.8959   -0.9124 H    0    0    0    0    0    0    0    0    0    0    8
0.0015    0.8915    1.2303 H    0    0    0    0    0    0    0    0    0    0    9
0.0010   -0.8907    1.2315 H    0    0    0    0    0    0    0    0    0    0    10
-1.2340    0.8221   -0.8634 H    0    0    0    0    0    0    0    0    0    0    11
2  1  0  0  0  0
6  1  0  0  0  0
7  1  0  0  0  0
8  1  0  0  0  0
3  2  0  0  0  0
9  2  0  0  0  0
10 2  0  0  0  0
4  3  0  0  0  0
5  3  0  0  0  0
3 11 0  0  0  0
M  END
$$$$
ethylamine.sdf
COSMOTHERM      3D      0
10 9 0 0 0 0 0 0 0 0 0 0 V2000
1.2758    0.0160   -0.2572 C    0    0    0    0    0    0    0    0    0    0    1
-0.0054   -0.0334    0.5710 C    0    0    0    0    0    0    0    0    0    0    2
-1.1983    0.0724   -0.2982 N    0    0    0    0    0    0    0    0    0    0    3
-2.0440    0.0061    0.2757 H    0    0    0    0    0    0    0    0    0    0    4
-1.2295   -0.7435   -0.9182 H    0    0    0    0    0    0    0    0    0    0    5
2.1629   -0.0340    0.3910 H    0    0    0    0    0    0    0    0    0    0    6
1.3258   -0.8337   -0.9566 H    0    0    0    0    0    0    0    0    0    0    7
1.3284    0.9447   -0.8451 H    0    0    0    0    0    0    0    0    0    0    8
-0.0263    0.8158    1.2724 H    0    0    0    0    0    0    0    0    0    0    9
-0.0048   -0.9545    1.1863 H    0    0    0    0    0    0    0    0    0    0    10
2  1  0  0  0  0
6  1  0  0  0  0
7  1  0  0  0  0
8  1  0  0  0  0
3  2  0  0  0  0
9  2  0  0  0  0
4  3  0  0  0  0
5  3  0  0  0  0
2 10 0  0  0  0
M  END
$$$$
guanidine_a.sdf
COSMOTHERM      3D      0
9  8 0 0 0 0 0 0 0 0 0 0 V2000
-0.7948   -1.0826   -0.0500 N    0    0    0    0    0    0    0    0    0    0    1
0.0866   -0.0108    0.0019 C    0    0    0    0    0    0    0    0    0    0    2
-0.5356    1.2292    0.0530 N    0    0    0    0    0    0    0    0    0    0    3
1.3855   -0.0876   -0.0063 N    0    0    0    0    0    0    0    0    0    0    4
-0.3975   -1.9865    0.1941 H    0    0    0    0    0    0    0    0    0    0    5
-1.7164   -0.9376    0.3590 H    0    0    0    0    0    0    0    0    0    0    6
-1.4443    1.2969   -0.4012 H    0    0    0    0    0    0    0    0    0    0    7
0.0796    2.0051   -0.1819 H    0    0    0    0    0    0    0    0    0    0    8
1.6800   -1.0689    0.0535 H    0    0    0    0    0    0    0    0    0    0    9
2  1  0  0  0  0
5  1  0  0  0  0
6  1  0  0  0  0
3  2  0  0  0  0
4  2  0  0  0  0
7  3  0  0  0  0
8  3  0  0  0  0
4  9  0  0  0  0
M  END
$$$$
guanidine_a_p2.sdf
COSMOTHERM      3D      0
10 9 0 0 0 0 0 0 0 0 0 0 V2000
-1.3381   -0.0340    0.0073 N    0    0    0    0    0    0    0    0    0    0    1
0.0000    0.0001   -0.0014 C    0    0    0    0    0    0    0    0    0    0    2
```

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1
2
3      0.6396      1.1760      0.0081 N      0      0      0      0      0      0      0      0      0      0      0      0      3
4      0.6986     -1.1420     -0.0096 N      0      0      0      0      0      0      0      0      0      0      0      0      4
5     -1.8388     -0.9153     -0.0270 H      0      0      0      0      0      0      0      0      0      0      0      0      5
6     -1.8833      0.8196     -0.0447 H      0      0      0      0      0      0      0      0      0      0      0      0      6
7      0.1272      2.0497     -0.0438 H      0      0      0      0      0      0      0      0      0      0      0      0      7
8      1.6517      1.2206     -0.0366 H      0      0      0      0      0      0      0      0      0      0      0      0      8
9      0.2309     -2.0407      0.0406 H      0      0      0      0      0      0      0      0      0      0      0      0      9
10     1.7112     -1.1352      0.0468 H      0      0      0      0      0      0      0      0      0      0      0      0      10
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M END
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h2o.sdf
COSMOtherm 3D 0

```
3 2 0 0 0 0 0 0 0 0 0 V2000
0.0000 0.0000 0.0674 O 0 0 0 0 0 0 0 0 0 0 0 0 0 1
-0.7649 0.0000 -0.5349 H 0 0 0 0 0 0 0 0 0 0 0 0 0 2
0.7648 0.0000 -0.5349 H 0 0 0 0 0 0 0 0 0 0 0 0 0 3
2 1 0 0 0 0
1 3 0 0 0 0
```

M END
\$\$\$\$
hydroxyimidazo(2,3-a)isoindol_e-cation.sdf
COSMOtherm 3D 0

```
27 29 0 0 0 0 0 0 0 0 0 V2000
0.9004 0.2373 4.0032 C 0 0 0 0 0 0 0 0 0 0 0 0 0 1
1.8771 0.2080 2.9717 C 0 0 0 0 0 0 0 0 0 0 0 0 0 2
1.5273 0.0809 1.6351 C 0 0 0 0 0 0 0 0 0 0 0 0 0 3
0.1576 -0.0307 1.3023 C 0 0 0 0 0 0 0 0 0 0 0 0 0 4
-0.8330 0.0166 2.3529 C 0 0 0 0 0 0 0 0 0 0 0 0 0 5
-0.4488 0.1463 3.7080 C 0 0 0 0 0 0 0 0 0 0 0 0 0 6
-2.0990 -0.0817 1.7379 C 0 0 0 0 0 0 0 0 0 0 0 0 0 7
-0.5569 -0.1578 0.0747 C 0 0 0 0 0 0 0 0 0 0 0 0 0 8
-1.9083 -0.1707 0.4067 N 0 0 0 0 0 0 0 0 0 0 0 0 0 9
-0.1086 -0.2589 -1.2648 C 0 0 0 0 0 0 0 0 0 0 0 0 0 10
-0.0732 -0.1020 -3.5923 C 0 0 0 0 0 0 0 0 0 0 0 0 0 11
1.2662 -0.6599 -3.0856 C 0 0 0 0 0 0 0 0 0 0 0 0 0 12
-0.8971 -0.1915 -2.3676 N 0 0 0 0 0 0 0 0 0 0 0 0 0 13
1.1705 -0.4552 -1.6335 N 0 0 0 0 0 0 0 0 0 0 0 0 0 14
0.1075 1.2411 -4.0169 O 0 0 0 0 0 0 0 0 0 0 0 0 0 15
1.2249 0.3381 5.0398 H 0 0 0 0 0 0 0 0 0 0 0 0 0 16
2.9314 0.2944 3.2393 H 0 0 0 0 0 0 0 0 0 0 0 0 0 17
2.3087 0.0816 0.8744 H 0 0 0 0 0 0 0 0 0 0 0 0 0 18
-1.2028 0.1799 4.4961 H 0 0 0 0 0 0 0 0 0 0 0 0 0 19
-3.0974 -0.1049 2.1627 H 0 0 0 0 0 0 0 0 0 0 0 0 0 20
-2.6722 -0.2969 -0.2550 H 0 0 0 0 0 0 0 0 0 0 0 0 0 21
-0.5235 -0.7057 -4.3885 H 0 0 0 0 0 0 0 0 0 0 0 0 0 22
2.1124 -0.1117 -3.5147 H 0 0 0 0 0 0 0 0 0 0 0 0 0 23
1.3633 -1.7306 -3.3133 H 0 0 0 0 0 0 0 0 0 0 0 0 0 24
-1.8170 0.2422 -2.3494 H 0 0 0 0 0 0 0 0 0 0 0 0 0 25
-0.6516 1.4939 -4.5749 H 0 0 0 0 0 0 0 0 0 0 0 0 0 26
1.8606 -0.8492 -1.0012 H 0 0 0 0 0 0 0 0 0 0 0 0 0 27
2 1 0 0 0 0
6 1 0 0 0 0
16 1 0 0 0 0
3 2 0 0 0 0
17 2 0 0 0 0
4 3 0 0 0 0
18 3 0 0 0 0
5 4 0 0 0 0
8 4 0 0 0 0
6 5 0 0 0 0
7 5 0 0 0 0
19 6 0 0 0 0
9 7 0 0 0 0
20 7 0 0 0 0
9 8 0 0 0 0
10 8 0 0 0 0
21 9 0 0 0 0
13 10 0 0 0 0
14 10 0 0 0 0
12 11 0 0 0 0
13 11 0 0 0 0
15 11 0 0 0 0
22 11 0 0 0 0
14 12 0 0 0 0
23 12 0 0 0 0
24 12 0 0 0 0
25 13 0 0 0 0
26 15 0 0 0 0
14 27 0 0 0 0
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M END
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hydroxyimidazo(2,3-a)isoindol_e0.sdf
COSMOtherm 3D 0

```
26 28 0 0 0 0 0 0 0 0 0 V2000
-3.8960 1.0816 -0.0210 C 0 0 0 0 0 0 0 0 0 0 0 0 0 1
-2.8081 1.9677 0.2320 C 0 0 0 0 0 0 0 0 0 0 0 0 0 2
-1.5002 1.5168 0.2814 C 0 0 0 0 0 0 0 0 0 0 0 0 0 3
-1.2410 0.1370 0.0700 C 0 0 0 0 0 0 0 0 0 0 0 0 0 4
-2.3554 -0.7659 -0.1715 C 0 0 0 0 0 0 0 0 0 0 0 0 0 5
-3.6836 -0.2702 -0.2186 C 0 0 0 0 0 0 0 0 0 0 0 0 0 6
-1.8189 -2.0580 -0.3140 C 0 0 0 0 0 0 0 0 0 0 0 0 0 7
-0.0657 -0.6539 0.0569 C 0 0 0 0 0 0 0 0 0 0 0 0 0 8
-0.4724 -1.9532 -0.1693 N 0 0 0 0 0 0 0 0 0 0 0 0 0 9
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20 7 0 0 0 0
9 8 0 0 0 0
10 8 0 0 0 0
21 9 0 0 0 0
13 10 0 0 0 0
14 10 0 0 0 0
12 11 0 0 0 0
13 11 0 0 0 0
15 11 0 0 0 0
22 11 0 0 0 0
14 12 0 0 0 0
23 12 0 0 0 0
24 12 0 0 0 0
25 13 0 0 0 0
15 26 0 0 0 0
M END
$$$$
imidazo-(2,3-b)-thioxazole_b-cation1.sdf
COSMOtherm 3D 0

18 19 0 0 0 0 0 0 0 0 0 V2000
3.1474 0.2861 0.6727 C 0 0 0 0 0 0 0 0 0 0 1
1.7392 0.2360 1.1207 N 0 0 0 0 0 0 0 0 0 0 2
3.0564 -0.3060 -0.7545 C 0 0 0 0 0 0 0 0 0 0 3
1.6033 -0.2502 -1.0222 N 0 0 0 0 0 0 0 0 0 0 4
0.9200 -0.0105 0.0981 C 0 0 0 0 0 0 0 0 0 0 5
-2.6315 -0.2097 1.1747 N 0 0 0 0 0 0 0 0 0 0 6
-1.2745 -0.2280 1.3476 C 0 0 0 0 0 0 0 0 0 0 7
-2.9389 0.0093 -0.0833 C 0 0 0 0 0 0 0 0 0 0 8
-1.5847 0.2110 -1.1676 S 0 0 0 0 0 0 0 0 0 0 9
-0.5223 -0.0192 0.2063 C 0 0 0 0 0 0 0 0 0 0 10
3.4885 1.3301 0.6701 H 0 0 0 0 0 0 0 0 0 0 11
3.7863 -0.3039 1.3379 H 0 0 0 0 0 0 0 0 0 0 12
1.4271 0.6756 1.9825 H 0 0 0 0 0 0 0 0 0 0 13
3.3914 -1.3512 -0.7931 H 0 0 0 0 0 0 0 0 0 0 14
3.6086 0.2808 -1.4959 H 0 0 0 0 0 0 0 0 0 0 15
-0.8622 -0.4250 2.3364 H 0 0 0 0 0 0 0 0 0 0 16
-3.9547 0.0813 -0.4683 H 0 0 0 0 0 0 0 0 0 0 17
1.1874 -0.6914 -1.8388 H 0 0 0 0 0 0 0 0 0 0 18

2 1 0 0 0 0
3 1 0 0 0 0
11 1 0 0 0 0
12 1 0 0 0 0
5 2 0 0 0 0
13 2 0 0 0 0
4 3 0 0 0 0
14 3 0 0 0 0
15 3 0 0 0 0
5 4 0 0 0 0
10 5 0 0 0 0
7 6 0 0 0 0
8 6 0 0 0 0
10 7 0 0 0 0
16 7 0 0 0 0
9 8 0 0 0 0
17 8 0 0 0 0
10 9 0 0 0 0
4 18 0 0 0 0
M END
$$$$
imidazo-(2,3-b)-thioxazole_b.sdf
COSMOtherm 3D 0

17 18 0 0 0 0 0 0 0 0 0 V2000
3.0440 0.7249 -0.3622 C 0 0 0 0 0 0 0 0 0 0 1
1.6115 1.0503 -0.1741 N 0 0 0 0 0 0 0 0 0 0 2
3.1096 -0.6878 0.2711 C 0 0 0 0 0 0 0 0 0 0 3
1.7128 -1.1909 0.2911 N 0 0 0 0 0 0 0 0 0 0 4
0.9616 -0.1654 0.0230 C 0 0 0 0 0 0 0 0 0 0 5
-2.6451 -1.1464 -0.2095 N 0 0 0 0 0 0 0 0 0 0 6
-1.2864 -1.3535 -0.2230 C 0 0 0 0 0 0 0 0 0 0 7
-2.9235 0.1184 0.0001 C 0 0 0 0 0 0 0 0 0 0 8
-1.5315 1.1620 0.2024 S 0 0 0 0 0 0 0 0 0 0 9
-0.4988 -0.2401 -0.0205 C 0 0 0 0 0 0 0 0 0 0 10
3.2971 0.7077 -1.4345 H 0 0 0 0 0 0 0 0 0 0 11
3.6880 1.4548 0.1438 H 0 0 0 0 0 0 0 0 0 0 12
1.1959 1.7072 -0.8339 H 0 0 0 0 0 0 0 0 0 0 13
3.4799 -0.6441 1.3094 H 0 0 0 0 0 0 0 0 0 0 14
3.7630 -1.3753 -0.2829 H 0 0 0 0 0 0 0 0 0 0 15
-0.8932 -2.3534 -0.3971 H 0 0 0 0 0 0 0 0 0 0 16
-3.9291 0.5313 0.0577 H 0 0 0 0 0 0 0 0 0 0 17

2 1 0 0 0 0
3 1 0 0 0 0
11 1 0 0 0 0
12 1 0 0 0 0
5 2 0 0 0 0
13 2 0 0 0 0
4 3 0 0 0 0
14 3 0 0 0 0
15 3 0 0 0 0
5 4 0 0 0 0
10 5 0 0 0 0
7 6 0 0 0 0
8 6 0 0 0 0
10 7 0 0 0 0
16 7 0 0 0 0
9 8 0 0 0 0
10 9 0 0 0 0
8 17 0 0 0 0
M END
$$$$
imidazole-cation.sdf
COSMOtherm 3D 0

10 10 0 0 0 0 0 0 0 0 0 V2000
```

-0.9778	0.6844	0.0000	C	0	0	0	0	0	0	0	0	1
0.3480	1.0767	0.0000	N	0	0	0	0	0	0	0	0	2
-0.9779	-0.6842	0.0000	C	0	0	0	0	0	0	0	0	3
0.3477	-1.0767	0.0000	N	0	0	0	0	0	0	0	0	4
1.1436	-0.0001	0.0000	C	0	0	0	0	0	0	0	0	5
-1.7895	1.4006	0.0002	H	0	0	0	0	0	0	0	0	6
-1.7898	-1.4002	-0.0001	H	0	0	0	0	0	0	0	0	7
2.2266	-0.0003	0.0002	H	0	0	0	0	0	0	0	0	8
0.6814	-2.0391	0.0001	H	0	0	0	0	0	0	0	0	9
0.6818	2.0389	-0.0002	H	0	0	0	0	0	0	0	0	10
2	1	0	0	0	0							
3	1	0	0	0	0							
6	1	0	0	0	0							
5	2	0	0	0	0							
4	3	0	0	0	0							
7	3	0	0	0	0							
5	4	0	0	0	0							
9	4	0	0	0	0							
8	5	0	0	0	0							
2	10	0	0	0	0							
M END												
\$\$\$\$												
imidazole.sdf												
COSMOTHERM 3D 0												
9	9	0	0	0	0	0	0	0	0	0	0	0
-0.9869	0.6303	0.0000	C	0	0	0	0	0	0	0	0	1
0.2879	1.1767	0.0000	N	0	0	0	0	0	0	0	0	2
-0.9196	-0.7471	0.0000	C	0	0	0	0	0	0	0	0	3
0.4282	-1.0439	0.0000	N	0	0	0	0	0	0	0	0	4
1.1148	0.1348	0.0000	C	0	0	0	0	0	0	0	0	5
-1.8741	1.2574	0.0000	H	0	0	0	0	0	0	0	0	6
-1.6790	-1.5213	-0.0001	H	0	0	0	0	0	0	0	0	7
2.2001	0.1779	0.0000	H	0	0	0	0	0	0	0	0	8
0.8360	-1.9758	-0.0002	H	0	0	0	0	0	0	0	0	9
2	1	0	0	0	0							
3	1	0	0	0	0							
6	1	0	0	0	0							
5	2	0	0	0	0							
4	3	0	0	0	0							
7	3	0	0	0	0							
5	4	0	0	0	0							
8	5	0	0	0	0							
4	9	0	0	0	0							
M END												
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indole-cation0.sdf												
COSMOTHERM 3D 0												
17	18	0	0	0	0	0	0	0	0	0	0	0
-2.1686	-0.7238	0.0004	C	0	0	0	0	0	0	0	0	1
-2.1977	0.6790	0.0001	C	0	0	0	0	0	0	0	0	2
-1.0181	1.4347	-0.0003	C	0	0	0	0	0	0	0	0	3
0.2022	0.7511	-0.0003	C	0	0	0	0	0	0	0	0	4
0.1934	-0.6510	-0.0004	C	0	0	0	0	0	0	0	0	5
-0.9506	-1.4248	0.0002	C	0	0	0	0	0	0	0	0	6
1.5998	-1.1121	-0.0005	N	0	0	0	0	0	0	0	0	7


```
14 13 0 0 0 0 0 0 0 0 0 V2000
0.0008 0.0746 0.3767 C 0 0 0 0 0 0 0 0 0 0 1
-0.0135 -1.3717 -0.0933 N 0 0 0 0 0 0 0 0 0 0 2
1.2843 0.7340 -0.1113 C 0 0 0 0 0 0 0 0 0 0 3
-1.2696 0.7589 -0.1113 C 0 0 0 0 0 0 0 0 0 0 4
-0.8517 -1.8696 0.2342 H 0 0 0 0 0 0 0 0 0 0 5
0.8032 -1.8923 0.2528 H 0 0 0 0 0 0 0 0 0 0 6
-0.0001 0.0085 1.4724 H 0 0 0 0 0 0 0 0 0 0 7
2.1750 0.1982 0.2462 H 0 0 0 0 0 0 0 0 0 0 8
1.3292 1.7607 0.2742 H 0 0 0 0 0 0 0 0 0 0 9
1.3134 0.7800 -1.2101 H 0 0 0 0 0 0 0 0 0 0 10
-2.1705 0.2426 0.2495 H 0 0 0 0 0 0 0 0 0 0 11
-1.2928 1.7874 0.2711 H 0 0 0 0 0 0 0 0 0 0 12
-1.3000 0.8022 -1.2102 H 0 0 0 0 0 0 0 0 0 0 13
-0.0027 -1.4348 -1.1209 H 0 0 0 0 0 0 0 0 0 0 14
2 1 0 0 0 0
3 1 0 0 0 0
4 1 0 0 0 0
7 1 0 0 0 0
5 2 0 0 0 0
6 2 0 0 0 0
8 3 0 0 0 0
9 3 0 0 0 0
10 3 0 0 0 0
11 4 0 0 0 0
12 4 0 0 0 0
13 4 0 0 0 0
2 14 0 0 0 0
M END
$$$$
iso-propylamine.sdf
COSMOTHERM 3D 0
13 12 0 0 0 0 0 0 0 0 0 V2000
0.0002 0.0080 0.3648 C 0 0 0 0 0 0 0 0 0 0 1
-0.0031 -1.3751 -0.1702 N 0 0 0 0 0 0 0 0 0 0 2
1.2685 0.7231 -0.1049 C 0 0 0 0 0 0 0 0 0 0 3
-1.2649 0.7291 -0.1046 C 0 0 0 0 0 0 0 0 0 0 4
-0.8227 -1.8736 0.1910 H 0 0 0 0 0 0 0 0 0 0 5
0.8074 -1.8817 0.1999 H 0 0 0 0 0 0 0 0 0 0 6
0.0001 0.0086 1.4741 H 0 0 0 0 0 0 0 0 0 0 7
2.1717 0.1927 0.2351 H 0 0 0 0 0 0 0 0 0 0 8
1.3093 1.7472 0.2939 H 0 0 0 0 0 0 0 0 0 0 9
1.2954 0.7759 -1.2047 H 0 0 0 0 0 0 0 0 0 0 10
-2.1707 0.2054 0.2386 H 0 0 0 0 0 0 0 0 0 0 11
-1.2990 1.7548 0.2911 H 0 0 0 0 0 0 0 0 0 0 12
-1.2936 0.7790 -1.2045 H 0 0 0 0 0 0 0 0 0 0 13
2 1 0 0 0 0
3 1 0 0 0 0
4 1 0 0 0 0
7 1 0 0 0 0
5 2 0 0 0 0
6 2 0 0 0 0
8 3 0 0 0 0
9 3 0 0 0 0
10 3 0 0 0 0
11 4 0 0 0 0
12 4 0 0 0 0
4 13 0 0 0 0
M END
$$$$
isoquinoline.sdf
COSMOTHERM 3D 0
17 18 0 0 0 0 0 0 0 0 0 V2000
-1.4145 -1.2319 0.0001 C 0 0 0 0 0 0 0 0 0 0 1
-0.6949 -0.0067 0.0000 C 0 0 0 0 0 0 0 0 0 0 2
0.7395 -0.0248 0.0000 C 0 0 0 0 0 0 0 0 0 0 3
1.4112 -1.2778 -0.0001 C 0 0 0 0 0 0 0 0 0 0 4
0.6858 -2.4545 -0.0001 C 0 0 0 0 0 0 0 0 0 0 5
-0.7339 -2.4344 0.0001 C 0 0 0 0 0 0 0 0 0 0 6
1.4065 1.2295 0.0001 C 0 0 0 0 0 0 0 0 0 0 7
0.6661 2.3934 0.0001 C 0 0 0 0 0 0 0 0 0 0 8
-1.3409 1.2613 -0.0001 C 0 0 0 0 0 0 0 0 0 0 9
-0.7037 2.4251 -0.0001 N 0 0 0 0 0 0 0 0 0 0 10
-2.5065 -1.2083 0.0001 H 0 0 0 0 0 0 0 0 0 0 11
2.5030 -1.2971 0.0000 H 0 0 0 0 0 0 0 0 0 0 12
1.2068 -3.4137 -0.0002 H 0 0 0 0 0 0 0 0 0 0 13
-1.2848 -3.3763 0.0001 H 0 0 0 0 0 0 0 0 0 0 14
2.4975 1.2703 0.0001 H 0 0 0 0 0 0 0 0 0 0 15
1.1605 3.3676 0.0001 H 0 0 0 0 0 0 0 0 0 0 16
-2.4359 1.2978 -0.0002 H 0 0 0 0 0 0 0 0 0 0 17
2 1 0 0 0 0
6 1 0 0 0 0
11 1 0 0 0 0
3 2 0 0 0 0
9 2 0 0 0 0
4 3 0 0 0 0
7 3 0 0 0 0
5 4 0 0 0 0
12 4 0 0 0 0
6 5 0 0 0 0
13 5 0 0 0 0
14 6 0 0 0 0
8 7 0 0 0 0
15 7 0 0 0 0
10 8 0 0 0 0
16 8 0 0 0 0
10 9 0 0 0 0
9 17 0 0 0 0
M END
$$$$
isoquinoline_p1.sdf
COSMOTHERM 3D 0
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18 19 0 0 0 0 0 0 0 0 0 V2000
-2.3422 -0.6622 -0.0003 N 0 0 0 0 0 0 0 0 0 1
-2.3854 0.7092 0.0002 C 0 0 0 0 0 0 0 0 0 2
-1.2133 1.4185 0.0004 C 0 0 0 0 0 0 0 0 0 3
0.0359 0.7403 0.0001 C 0 0 0 0 0 0 0 0 0 4
0.0321 -0.7002 0.0001 C 0 0 0 0 0 0 0 0 0 5
-1.2061 -1.3642 -0.0002 C 0 0 0 0 0 0 0 0 0 6
1.2806 1.4171 -0.0003 C 0 0 0 0 0 0 0 0 0 7
2.4598 0.6946 -0.0003 C 0 0 0 0 0 0 0 0 0 8
1.2594 -1.4180 0.0003 C 0 0 0 0 0 0 0 0 0 9
2.4518 -0.7247 0.0001 C 0 0 0 0 0 0 0 0 0 10
-3.3757 1.1563 0.0003 H 0 0 0 0 0 0 0 0 0 11
-1.2483 2.5074 0.0006 H 0 0 0 0 0 0 0 0 0 12
-1.2981 -2.4489 -0.0007 H 0 0 0 0 0 0 0 0 0 13
1.2946 2.5078 -0.0006 H 0 0 0 0 0 0 0 0 0 14
3.4153 1.2212 -0.0006 H 0 0 0 0 0 0 0 0 0 15
1.2415 -2.5086 0.0004 H 0 0 0 0 0 0 0 0 0 16
3.3980 -1.2666 0.0004 H 0 0 0 0 0 0 0 0 0 17
-3.2280 -1.1720 -0.0009 H 0 0 0 0 0 0 0 0 0 18
2 1 0 0 0 0
6 1 0 0 0 0
3 2 0 0 0 0
11 2 0 0 0 0
4 3 0 0 0 0
12 3 0 0 0 0
5 4 0 0 0 0
7 4 0 0 0 0
6 5 0 0 0 0
9 5 0 0 0 0
13 6 0 0 0 0
8 7 0 0 0 0
14 7 0 0 0 0
10 8 0 0 0 0
15 8 0 0 0 0
10 9 0 0 0 0
16 9 0 0 0 0
17 10 0 0 0 0
1 18 0 0 0 0
M END
$$$$
melamine.sdf
COSMOTHERM 3D 0
15 15 0 0 0 0 0 0 0 0 V2000
1.2183 0.6718 0.0062 N 0 0 0 0 0 0 0 0 0 1
1.1212 -0.6772 0.0037 C 0 0 0 0 0 0 0 0 0 2
-0.0279 -1.3913 0.0066 N 0 0 0 0 0 0 0 0 0 3
-1.1469 -0.6323 0.0045 C 0 0 0 0 0 0 0 0 0 4
-1.1906 0.7191 0.0072 N 0 0 0 0 0 0 0 0 0 5
0.0261 1.3097 0.0040 C 0 0 0 0 0 0 0 0 0 6
0.0528 2.6675 -0.0315 N 0 0 0 0 0 0 0 0 0 7
-2.3363 -1.2876 -0.0319 N 0 0 0 0 0 0 0 0 0 8
2.2835 -1.3796 -0.0311 N 0 0 0 0 0 0 0 0 0 9
-0.8071 3.1756 0.1483 H 0 0 0 0 0 0 0 0 0 10
0.9322 3.1415 0.1474 H 0 0 0 0 0 0 0 0 0 11
-2.3469 -2.2862 0.1476 H 0 0 0 0 0 0 0 0 0 12
-3.1866 -0.7635 0.1477 H 0 0 0 0 0 0 0 0 0 13
3.1535 -0.8892 0.1479 H 0 0 0 0 0 0 0 0 0 14
2.2542 -2.3781 0.1483 H 0 0 0 0 0 0 0 0 0 15
2 1 0 0 0 0
6 1 0 0 0 0
3 2 0 0 0 0
9 2 0 0 0 0
4 3 0 0 0 0
5 4 0 0 0 0
8 4 0 0 0 0
6 5 0 0 0 0
7 6 0 0 0 0
10 7 0 0 0 0
11 7 0 0 0 0
12 8 0 0 0 0
13 8 0 0 0 0
14 9 0 0 0 0
9 15 0 0 0 0
M END
$$$$
melamine_p2.sdf
COSMOTHERM 3D 0
16 16 0 0 0 0 0 0 0 0 V2000
-1.2123 -0.7058 -0.0001 N 0 0 0 0 0 0 0 0 0 1
-1.1903 0.6213 -0.0003 C 0 0 0 0 0 0 0 0 0 2
-0.0003 1.3180 -0.0006 N 0 0 0 0 0 0 0 0 0 3
1.1900 0.6219 -0.0003 C 0 0 0 0 0 0 0 0 0 4
1.2127 -0.7052 0.0002 N 0 0 0 0 0 0 0 0 0 5
0.0004 -1.3198 -0.0001 C 0 0 0 0 0 0 0 0 0 6
0.0007 -2.6581 0.0004 N 0 0 0 0 0 0 0 0 0 7
-2.3244 1.3239 0.0013 N 0 0 0 0 0 0 0 0 0 8
2.3237 1.3251 0.0011 N 0 0 0 0 0 0 0 0 0 9
0.8774 -3.1692 -0.0022 H 0 0 0 0 0 0 0 0 0 10
-0.8756 -3.1698 -0.0035 H 0 0 0 0 0 0 0 0 0 11
-3.2098 0.8266 -0.0031 H 0 0 0 0 0 0 0 0 0 12
-2.3379 2.3389 -0.0048 H 0 0 0 0 0 0 0 0 0 13
2.3364 2.3402 -0.0054 H 0 0 0 0 0 0 0 0 0 14
3.2094 0.8284 -0.0032 H 0 0 0 0 0 0 0 0 0 15
-0.0005 2.3377 -0.0010 H 0 0 0 0 0 0 0 0 0 16
2 1 0 0 0 0
6 1 0 0 0 0
3 2 0 0 0 0
8 2 0 0 0 0
4 3 0 0 0 0
5 4 0 0 0 0
9 4 0 0 0 0
6 5 0 0 0 0
```

```
7 6 0 0 0 0
10 7 0 0 0 0
11 7 0 0 0 0
12 8 0 0 0 0
13 8 0 0 0 0
14 9 0 0 0 0
15 9 0 0 0 0
3 16 0 0 0 0
M END
$$$$
methylamine-cation.sdf
COSMOtherm 3D 0

8 7 0 0 0 0 0 0 0 0 0 V2000
0.7980 0.0000 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 1
-0.6985 0.0000 0.0000 N 0 0 0 0 0 0 0 0 0 0 0 2
-1.0778 0.4774 0.8272 H 0 0 0 0 0 0 0 0 0 0 0 3
-1.0780 -0.9550 -0.0002 H 0 0 0 0 0 0 0 0 0 0 0 4
1.1435 -0.5207 -0.8970 H 0 0 0 0 0 0 0 0 0 0 0 5
1.1435 1.0372 -0.0024 H 0 0 0 0 0 0 0 0 0 0 0 6
1.1435 -0.5166 0.8994 H 0 0 0 0 0 0 0 0 0 0 0 7
-1.0780 0.4778 -0.8269 H 0 0 0 0 0 0 0 0 0 0 0 8
2 1 0 0 0 0
5 1 0 0 0 0
6 1 0 0 0 0
7 1 0 0 0 0
3 2 0 0 0 0
4 2 0 0 0 0
2 8 0 0 0 0
M END
$$$$
methylamine.sdf
COSMOtherm 3D 0

7 6 0 0 0 0 0 0 0 0 0 V2000
0.7456 -0.0001 -0.0133 C 0 0 0 0 0 0 0 0 0 0 0 1
-0.7283 -0.0001 0.0751 N 0 0 0 0 0 0 0 0 0 0 0 2
-1.0989 -0.8135 -0.4232 H 0 0 0 0 0 0 0 0 0 0 0 3
-1.0970 0.8146 -0.4227 H 0 0 0 0 0 0 0 0 0 0 0 4
1.1415 0.8889 0.4982 H 0 0 0 0 0 0 0 0 0 0 0 5
1.1427 -0.8837 0.5066 H 0 0 0 0 0 0 0 0 0 0 0 6
1.1468 -0.0047 -1.0441 H 0 0 0 0 0 0 0 0 0 0 0 7
2 1 0 0 0 0
5 1 0 0 0 0
6 1 0 0 0 0
3 2 0 0 0 0
4 2 0 0 0 0
1 7 0 0 0 0
M END
$$$$
methylguanidine.sdf
COSMOtherm 3D 0

12 11 0 0 0 0 0 0 0 0 0 V2000
-0.6504 -0.6692 0.0000 N 0 0 0 0 0 0 0 0 0 0 0 1
0.0778 0.4923 0.0001 C 0 0 0 0 0 0 0 0 0 0 0 2
-0.6786 1.6457 0.0005 N 0 0 0 0 0 0 0 0 0 0 0 3
1.3865 0.4454 -0.0001 N 0 0 0 0 0 0 0 0 0 0 0 4
-0.0255 -1.9799 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 5
-1.6620 -0.6167 0.0002 H 0 0 0 0 0 0 0 0 0 0 0 6
-0.2214 2.5488 -0.0029 H 0 0 0 0 0 0 0 0 0 0 0 7
-1.6922 1.6312 -0.0028 H 0 0 0 0 0 0 0 0 0 0 0 8
1.7615 1.4004 0.0004 H 0 0 0 0 0 0 0 0 0 0 0 9
-0.8189 -2.7366 -0.0006 H 0 0 0 0 0 0 0 0 0 0 0 10
0.6058 -2.1288 -0.8901 H 0 0 0 0 0 0 0 0 0 0 0 11
0.6051 -2.1292 0.8904 H 0 0 0 0 0 0 0 0 0 0 0 12
2 1 0 0 0 0
5 1 0 0 0 0
6 1 0 0 0 0
3 2 0 0 0 0
4 2 0 0 0 0
7 3 0 0 0 0
8 3 0 0 0 0
9 4 0 0 0 0
10 5 0 0 0 0
11 5 0 0 0 0
5 12 0 0 0 0
M END
$$$$
methylguanidine_a.sdf
COSMOtherm 3D 0

12 11 0 0 0 0 0 0 0 0 0 V2000
-0.6610 -0.6699 -0.0903 N 0 0 0 0 0 0 0 0 0 0 0 1
0.0855 0.4897 -0.0139 C 0 0 0 0 0 0 0 0 0 0 0 2
-0.6839 1.6484 0.0833 N 0 0 0 0 0 0 0 0 0 0 0 3
1.3858 0.5751 -0.0155 N 0 0 0 0 0 0 0 0 0 0 0 4
-0.0347 -1.9794 0.0440 C 0 0 0 0 0 0 0 0 0 0 0 5
-1.6155 -0.6037 0.2553 H 0 0 0 0 0 0 0 0 0 0 0 6
-1.5733 1.6306 -0.4132 H 0 0 0 0 0 0 0 0 0 0 0 7
-0.1522 2.4933 -0.1164 H 0 0 0 0 0 0 0 0 0 0 0 8
1.8080 -0.3582 0.0252 H 0 0 0 0 0 0 0 0 0 0 0 9
-0.8142 -2.7442 -0.0458 H 0 0 0 0 0 0 0 0 0 0 0 10
0.6940 -2.1435 -0.7629 H 0 0 0 0 0 0 0 0 0 0 0 11
0.4781 -2.1116 1.0130 H 0 0 0 0 0 0 0 0 0 0 0 12
2 1 0 0 0 0
5 1 0 0 0 0
6 1 0 0 0 0
3 2 0 0 0 0
4 2 0 0 0 0
7 3 0 0 0 0
8 3 0 0 0 0
9 4 0 0 0 0
10 5 0 0 0 0
11 5 0 0 0 0
```

```

5 12 0 0 0 0
M END
$$$$
methylguanidine_a_p2.sdf
COSMOtherm 3D 0

13 12 0 0 0 0 0 0 0 0 0 V2000
-0.6695 -0.6749 -0.0045 N 0 0 0 0 0 0 0 0 0 0 0 1
-0.0029 0.4848 -0.0019 C 0 0 0 0 0 0 0 0 0 0 0 2
-0.6781 1.6487 0.0299 N 0 0 0 0 0 0 0 0 0 0 0 3
1.3377 0.4923 -0.0194 N 0 0 0 0 0 0 0 0 0 0 0 4
-0.0297 -1.9884 0.0017 C 0 0 0 0 0 0 0 0 0 0 0 5
-1.6840 -0.6353 0.0081 H 0 0 0 0 0 0 0 0 0 0 0 6
-1.6757 1.6593 -0.1577 H 0 0 0 0 0 0 0 0 0 0 0 7
-0.1831 2.5225 -0.1181 H 0 0 0 0 0 0 0 0 0 0 0 8
1.8669 -0.3621 0.1171 H 0 0 0 0 0 0 0 0 0 0 0 9
-0.8199 -2.7443 -0.0086 H 0 0 0 0 0 0 0 0 0 0 0 10
0.5982 -2.1285 -0.8899 H 0 0 0 0 0 0 0 0 0 0 0 11
0.5773 -2.1338 0.9074 H 0 0 0 0 0 0 0 0 0 0 0 12
1.8478 1.3656 0.0611 H 0 0 0 0 0 0 0 0 0 0 0 13

2 1 0 0 0 0
5 1 0 0 0 0
6 1 0 0 0 0
3 2 0 0 0 0
4 2 0 0 0 0
7 3 0 0 0 0
8 3 0 0 0 0
9 4 0 0 0 0
10 5 0 0 0 0
11 5 0 0 0 0
12 5 0 0 0 0
4 13 0 0 0 0
M END
$$$$
methylguanidine_p2.sdf
COSMOtherm 3D 0

13 12 0 0 0 0 0 0 0 0 0 V2000
-0.6250 -0.6987 0.0008 N 0 0 0 0 0 0 0 0 0 0 0 1
-0.0111 -2.0235 -0.0004 C 0 0 0 0 0 0 0 0 0 0 0 2
-1.6414 -0.6741 -0.0019 H 0 0 0 0 0 0 0 0 0 0 0 3
1.0808 -1.9560 0.0027 H 0 0 0 0 0 0 0 0 0 0 0 4
-0.3217 -2.5801 0.8936 H 0 0 0 0 0 0 0 0 0 0 0 5
-0.3174 -2.5768 -0.8980 H 0 0 0 0 0 0 0 0 0 0 0 6
-0.0011 0.4858 -0.0001 C 0 0 0 0 0 0 0 0 0 0 0 7
-0.7348 1.6116 -0.0009 N 0 0 0 0 0 0 0 0 0 0 0 8
-0.2926 2.5239 -0.0012 H 0 0 0 0 0 0 0 0 0 0 0 9
-1.7482 1.5787 0.0050 H 0 0 0 0 0 0 0 0 0 0 0 10
1.3357 0.5808 0.0016 N 0 0 0 0 0 0 0 0 0 0 0 11
1.7885 1.4881 -0.0041 H 0 0 0 0 0 0 0 0 0 0 0 12
1.9332 -0.2366 -0.0101 H 0 0 0 0 0 0 0 0 0 0 0 13

2 1 0 0 0 0
3 1 0 0 0 0
7 1 0 0 0 0
4 2 0 0 0 0
5 2 0 0 0 0
6 2 0 0 0 0
8 7 0 0 0 0
11 7 0 0 0 0
9 8 0 0 0 0
10 8 0 0 0 0
12 11 0 0 0 0
11 13 0 0 0 0
M END
$$$$
methylguanidine_t.sdf
COSMOtherm 3D 0

12 11 0 0 0 0 0 0 0 0 0 V2000
0.0582 -1.9380 -0.0001 C 0 0 0 0 0 0 0 0 0 0 0 1
0.7703 -0.6643 0.0003 N 0 0 0 0 0 0 0 0 0 0 0 2
0.0386 0.4167 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 3
0.6491 1.6502 -0.0006 N 0 0 0 0 0 0 0 0 0 0 0 4
-1.3355 0.4486 0.0001 N 0 0 0 0 0 0 0 0 0 0 0 5
0.7896 -2.7581 0.0008 H 0 0 0 0 0 0 0 0 0 0 0 6
-0.5864 -2.0809 0.8909 H 0 0 0 0 0 0 0 0 0 0 0 7
-0.5845 -2.0813 -0.8924 H 0 0 0 0 0 0 0 0 0 0 0 8
0.1248 2.5158 0.0043 H 0 0 0 0 0 0 0 0 0 0 0 9
1.6604 1.6919 0.0015 H 0 0 0 0 0 0 0 0 0 0 0 10
-1.8551 1.3184 -0.0010 H 0 0 0 0 0 0 0 0 0 0 0 11
-1.8679 -0.4117 0.0004 H 0 0 0 0 0 0 0 0 0 0 0 12

2 1 0 0 0 0
6 1 0 0 0 0
7 1 0 0 0 0
8 1 0 0 0 0
3 2 0 0 0 0
4 3 0 0 0 0
5 3 0 0 0 0
9 4 0 0 0 0
10 4 0 0 0 0
11 5 0 0 0 0
5 12 0 0 0 0
M END
$$$$
methylguanidine_t_p2.sdf
COSMOtherm 3D 0

13 12 0 0 0 0 0 0 0 0 0 V2000
0.0292 -1.9881 -0.0001 C 0 0 0 0 0 0 0 0 0 0 0 1
0.6698 -0.6755 0.0003 N 0 0 0 0 0 0 0 0 0 0 0 2
0.0032 0.4859 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 3
0.6767 1.6467 -0.0003 N 0 0 0 0 0 0 0 0 0 0 0 4
-1.3368 0.4930 0.0004 N 0 0 0 0 0 0 0 0 0 0 0 5
0.8191 -2.7446 0.0006 H 0 0 0 0 0 0 0 0 0 0 0 6
-0.5888 -2.1315 0.8983 H 0 0 0 0 0 0 0 0 0 0 0 7
```

```
1
2
3      -0.5875   -2.1317   -0.8994 H   0   0   0   0   0   0   0   0   0   0   8
4      0.1881    2.5352   -0.0004 H   0   0   0   0   0   0   0   0   0   0   9
5      1.6905    1.6648    0.0019 H   0   0   0   0   0   0   0   0   0   0  10
6     -1.8540    1.3654   -0.0009 H   0   0   0   0   0   0   0   0   0   0  11
7     -1.8718   -0.3678   -0.0023 H   0   0   0   0   0   0   0   0   0   0  12
8      1.6843   -0.6363   -0.0014 H   0   0   0   0   0   0   0   0   0   0  13
9
10     2  1  0  0  0  0
11     6  1  0  0  0  0
12     7  1  0  0  0  0
13     8  1  0  0  0  0
14     3  2  0  0  0  0
15     4  3  0  0  0  0
16     5  3  0  0  0  0
17     9  4  0  0  0  0
18    10  4  0  0  0  0
19    11  5  0  0  0  0
20    12  5  0  0  0  0
21     2 13  0  0  0  0
22
23 M   END
24 $$$$
25 n-butylamine-cation.sdf
26 COSMOtherm      3D      0
27
28 17 16  0  0  0  0  0  0  0  0  0  0 V2000
29 2.6046  0.0002  -0.3317 C   0  0  0  0  0  0  0  0  0  0  0  1
30 1.3307  0.0000  0.5192 C   0  0  0  0  0  0  0  0  0  0  0  2
31 0.0526 -0.0004  -0.3317 C   0  0  0  0  0  0  0  0  0  0  0  3
32 -1.1973 -0.0001  0.5378 C   0  0  0  0  0  0  0  0  0  0  0  4
33 -2.4473  0.0002  -0.3038 N   0  0  0  0  0  0  0  0  0  0  0  5
34 -3.2958  0.0054  0.2767 H   0  0  0  0  0  0  0  0  0  0  0  6
35 -2.4984 -0.8306  -0.9081 H   0  0  0  0  0  0  0  0  0  0  0  7
36 3.5030  0.0016  0.3022 H   0  0  0  0  0  0  0  0  0  0  0  8
37 2.6509 -0.8900  -0.9778 H   0  0  0  0  0  0  0  0  0  0  0  9
38 2.6494  0.8890  -0.9797 H   0  0  0  0  0  0  0  0  0  0  0 10
39 1.3264  0.8837  1.1789 H   0  0  0  0  0  0  0  0  0  0  0 11
40 1.3269 -0.8832  1.1794 H   0  0  0  0  0  0  0  0  0  0  0 12
41 0.0451 -0.8882  -0.9863 H   0  0  0  0  0  0  0  0  0  0  0 13
42 0.0450  0.8871  -0.9868 H   0  0  0  0  0  0  0  0  0  0  0 14
43 -1.2523  0.8919  1.1733 H   0  0  0  0  0  0  0  0  0  0  0 15
44 -1.2529 -0.8917  1.1738 H   0  0  0  0  0  0  0  0  0  0  0 16
45 -2.4930  0.8262  -0.9150 H   0  0  0  0  0  0  0  0  0  0  0 17
46
47 2  1  0  0  0  0
48 8  1  0  0  0  0
49 9  1  0  0  0  0
50 10 1  0  0  0  0
51 3  2  0  0  0  0
52 11 2  0  0  0  0
53 12 2  0  0  0  0
54 4  3  0  0  0  0
55 13 3  0  0  0  0
56 14 3  0  0  0  0
57 5  4  0  0  0  0
58 15 4  0  0  0  0
59 16 4  0  0  0  0
60 6  5  0  0  0  0
61 7  5  0  0  0  0
62 5 17  0  0  0  0
63
64 M   END
65 $$$$
66 n-butylamine.sdf
67 COSMOtherm      3D      0
68
69 16 15  0  0  0  0  0  0  0  0  0  0 V2000
70 2.5761  0.0047  -0.3223 C   0  0  0  0  0  0  0  0  0  0  0  1
71 1.2946 -0.0251  0.5179 C   0  0  0  0  0  0  0  0  0  0  0  2
72 0.0164  0.0326  -0.3284 C   0  0  0  0  0  0  0  0  0  0  0  3
73 -1.2629 -0.0080  0.5082 C   0  0  0  0  0  0  0  0  0  0  0  4
74 -2.4656  0.0520  -0.3511 N   0  0  0  0  0  0  0  0  0  0  0  5
75 -3.3034  0.0201  0.2372 H   0  0  0  0  0  0  0  0  0  0  0  6
76 -2.5073 -0.7985  -0.9220 H   0  0  0  0  0  0  0  0  0  0  0  7
77 3.4738 -0.0398  0.3121 H   0  0  0  0  0  0  0  0  0  0  0  8
78 2.6152 -0.8494  -1.0167 H   0  0  0  0  0  0  0  0  0  0  0  9
79 2.6359  0.9257  -0.9230 H   0  0  0  0  0  0  0  0  0  0  0 10
80 1.2993  0.8218  1.2259 H   0  0  0  0  0  0  0  0  0  0  0 11
81 1.2811 -0.9406  1.1339 H   0  0  0  0  0  0  0  0  0  0  0 12
82 0.0105 -0.8175  -1.0354 H   0  0  0  0  0  0  0  0  0  0  0 13
83 0.0150  0.9505  -0.9414 H   0  0  0  0  0  0  0  0  0  0  0 14
84 -1.2876  0.8641  1.1822 H   0  0  0  0  0  0  0  0  0  0  0 15
85 -1.2410 -0.9091  1.1538 H   0  0  0  0  0  0  0  0  0  0  0 16
86
87 2  1  0  0  0  0
88 8  1  0  0  0  0
89 9  1  0  0  0  0
90 10 1  0  0  0  0
91 3  2  0  0  0  0
92 11 2  0  0  0  0
93 12 2  0  0  0  0
94 4  3  0  0  0  0
95 13 3  0  0  0  0
96 14 3  0  0  0  0
97 5  4  0  0  0  0
98 15 4  0  0  0  0
99 16 4  0  0  0  0
100 6  5  0  0  0  0
101 7  5  0  0  0  0
102 4 16  0  0  0  0
103
104 M   END
105 $$$$
106 n-heptylamine-cation.sdf
107 COSMOtherm      3D      0
108
109 26 25  0  0  0  0  0  0  0  0  0  0 V2000
110 3.2538  0.0006  -0.5336 C   0  0  0  0  0  0  0  0  0  0  0  1
111 1.9982 -0.0010  0.3478 C   0  0  0  0  0  0  0  0  0  0  0  2
112 0.6878 -0.0007  -0.4493 C   0  0  0  0  0  0  0  0  0  0  0  3
113 -0.5614 -0.0017  0.4405 C   0  0  0  0  0  0  0  0  0  0  0  4
114 -1.8697 -0.0013  -0.3628 C   0  0  0  0  0  0  0  0  0  0  0  5
```



```
23 22 0 0 0 0 0 0 0 0 0 V2000
  3.9012 -0.0004 0.3550 C 0 0 0 0 0 0 0 0 0 0 1
  2.6224 -0.0003 -0.4898 C 0 0 0 0 0 0 0 0 0 0 2
  1.3409 0.0002 0.3536 C 0 0 0 0 0 0 0 0 0 0 3
  0.0601 0.0008 -0.4902 C 0 0 0 0 0 0 0 0 0 0 4
  -1.2180 0.0007 0.3603 C 0 0 0 0 0 0 0 0 0 0 5
  -2.4661 -0.0004 -0.5120 C 0 0 0 0 0 0 0 0 0 0 6
  -3.7182 -0.0004 0.3267 N 0 0 0 0 0 0 0 0 0 0 7
  -4.5652 -0.0027 -0.2560 H 0 0 0 0 0 0 0 0 0 0 8
  -3.7693 0.8291 0.9327 H 0 0 0 0 0 0 0 0 0 0 9
  4.8013 -0.0026 -0.2775 H 0 0 0 0 0 0 0 0 0 0 10
  3.9497 0.8896 1.0020 H 0 0 0 0 0 0 0 0 0 0 11
  3.9475 -0.8882 1.0051 H 0 0 0 0 0 0 0 0 0 0 12
  2.6185 -0.8833 -1.1521 H 0 0 0 0 0 0 0 0 0 0 13
  2.6190 0.8822 -1.1528 H 0 0 0 0 0 0 0 0 0 0 14
  1.3416 0.8840 1.0162 H 0 0 0 0 0 0 0 0 0 0 15
  1.3408 -0.8838 1.0160 H 0 0 0 0 0 0 0 0 0 0 16
  0.0578 -0.8834 -1.1509 H 0 0 0 0 0 0 0 0 0 0 17
  0.0582 0.8854 -1.1504 H 0 0 0 0 0 0 0 0 0 0 18
  -1.2276 0.8887 1.0144 H 0 0 0 0 0 0 0 0 0 0 19
  -1.2267 -0.8867 1.0153 H 0 0 0 0 0 0 0 0 0 0 20
  -2.5196 -0.8927 -1.1472 H 0 0 0 0 0 0 0 0 0 0 21
  -2.5203 0.8910 -1.1483 H 0 0 0 0 0 0 0 0 0 0 22
  -3.7671 -0.8278 0.9358 H 0 0 0 0 0 0 0 0 0 0 23
2 1 0 0 0 0
10 1 0 0 0 0
11 1 0 0 0 0
12 1 0 0 0 0
3 2 0 0 0 0
13 2 0 0 0 0
14 2 0 0 0 0
4 3 0 0 0 0
15 3 0 0 0 0
16 3 0 0 0 0
5 4 0 0 0 0
17 4 0 0 0 0
18 4 0 0 0 0
6 5 0 0 0 0
19 5 0 0 0 0
20 5 0 0 0 0
7 6 0 0 0 0
21 6 0 0 0 0
22 6 0 0 0 0
8 7 0 0 0 0
9 7 0 0 0 0
7 23 0 0 0 0
M END
$$$$
n-hexylamine.sdf
COSMOtherm 3D 0
22 21 0 0 0 0 0 0 0 0 0 V2000
  3.8687 -0.0078 -0.3493 C 0 0 0 0 0 0 0 0 0 0 1
  2.5877 -0.0264 0.4919 C 0 0 0 0 0 0 0 0 0 0 2
  1.3070 0.0258 -0.3514 C 0 0 0 0 0 0 0 0 0 0 3
  0.0207 0.0014 0.4840 C 0 0 0 0 0 0 0 0 0 0 4
  -1.2600 0.0421 -0.3590 C 0 0 0 0 0 0 0 0 0 0 5
  -2.5355 -0.0058 0.4834 C 0 0 0 0 0 0 0 0 0 0 6
  -3.7422 0.0306 -0.3715 N 0 0 0 0 0 0 0 0 0 0 7
  -4.5770 -0.0053 0.2209 H 0 0 0 0 0 0 0 0 0 0 8
  -3.7759 -0.8266 -0.9328 H 0 0 0 0 0 0 0 0 0 0 9
  4.7678 -0.0484 0.2836 H 0 0 0 0 0 0 0 0 0 0 10
  3.9050 -0.8682 -1.0362 H 0 0 0 0 0 0 0 0 0 0 11
  3.9299 0.9075 -0.9589 H 0 0 0 0 0 0 0 0 0 0 12
  2.5947 0.8271 1.1923 H 0 0 0 0 0 0 0 0 0 0 13
  2.5710 -0.9360 1.1170 H 0 0 0 0 0 0 0 0 0 0 14
  1.3006 -0.8275 -1.0538 H 0 0 0 0 0 0 0 0 0 0 15
  1.3203 0.9374 -0.9755 H 0 0 0 0 0 0 0 0 0 0 16
  0.0250 0.8577 1.1824 H 0 0 0 0 0 0 0 0 0 0 17
  0.0149 -0.9077 1.1116 H 0 0 0 0 0 0 0 0 0 0 18
  -1.2615 -0.8126 -1.0601 H 0 0 0 0 0 0 0 0 0 0 19
  -1.2737 0.9560 -0.9775 H 0 0 0 0 0 0 0 0 0 0 20
  -2.5687 0.8722 1.1493 H 0 0 0 0 0 0 0 0 0 0 21
  -2.4995 -0.9004 1.1375 H 0 0 0 0 0 0 0 0 0 0 22
2 1 0 0 0 0
10 1 0 0 0 0
11 1 0 0 0 0
12 1 0 0 0 0
3 2 0 0 0 0
13 2 0 0 0 0
14 2 0 0 0 0
4 3 0 0 0 0
15 3 0 0 0 0
16 3 0 0 0 0
5 4 0 0 0 0
17 4 0 0 0 0
18 4 0 0 0 0
6 5 0 0 0 0
19 5 0 0 0 0
20 5 0 0 0 0
7 6 0 0 0 0
21 6 0 0 0 0
8 7 0 0 0 0
9 7 0 0 0 0
6 22 0 0 0 0
M END
$$$$
n-octylamine-cation.sdf
COSMOtherm 3D 0
29 28 0 0 0 0 0 0 0 0 0 V2000
  2.6318 0.0002 0.3668 C 0 0 0 0 0 0 0 0 0 0 1
  1.3458 0.0014 -0.4692 C 0 0 0 0 0 0 0 0 0 0 2
  0.0645 0.0016 0.3742 C 0 0 0 0 0 0 0 0 0 0 3
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21 6 0 0 0 0
22 6 0 0 0 0
8 7 0 0 0 0
9 7 0 0 0 0
23 10 0 0 0 0
24 10 0 0 0 0
25 10 0 0 0 0
26 23 0 0 0 0
27 23 0 0 0 0
23 28 0 0 0 0
M END
$$$$
n-pentylamine-cation.sdf
COSMOtherm 3D 0
20 19 0 0 0 0 0 0 0 0 0 V2000
3.2728 0.0009 0.2228 C 0 0 0 0 0 0 0 0 0 1
1.9469 -0.0002 -0.5457 C 0 0 0 0 0 0 0 0 0 2
0.7220 -0.0008 0.3777 C 0 0 0 0 0 0 0 0 0 3
-0.6076 -0.0009 -0.3895 C 0 0 0 0 0 0 0 0 0 4
-1.7981 -0.0003 0.5596 C 0 0 0 0 0 0 0 0 0 5
-3.1007 0.0009 -0.1984 N 0 0 0 0 0 0 0 0 0 6
-3.9091 0.0036 0.4368 H 0 0 0 0 0 0 0 0 0 7
-3.1908 -0.8282 -0.8003 H 0 0 0 0 0 0 0 0 0 8
4.1331 0.0006 -0.4627 H 0 0 0 0 0 0 0 0 0 9
3.3579 0.8906 0.8662 H 0 0 0 0 0 0 0 0 0 10
3.3584 -0.8874 0.8678 H 0 0 0 0 0 0 0 0 0 11
1.9028 -0.8833 -1.2057 H 0 0 0 0 0 0 0 0 0 12
1.9016 0.8826 -1.2061 H 0 0 0 0 0 0 0 0 0 13
0.7629 0.8834 1.0373 H 0 0 0 0 0 0 0 0 0 14
0.7634 -0.8852 1.0370 H 0 0 0 0 0 0 0 0 0 15
-0.6586 -0.8887 -1.0420 H 0 0 0 0 0 0 0 0 0 16
-0.6583 0.8865 -1.0425 H 0 0 0 0 0 0 0 0 0 17
-1.8111 0.8915 1.1977 H 0 0 0 0 0 0 0 0 0 18
-1.8125 -0.8923 1.1974 H 0 0 0 0 0 0 0 0 0 19
-3.1874 0.8286 -0.8028 H 0 0 0 0 0 0 0 0 0 20
2 1 0 0 0 0
9 1 0 0 0 0
10 1 0 0 0 0
11 1 0 0 0 0
3 2 0 0 0 0
12 2 0 0 0 0
13 2 0 0 0 0
4 3 0 0 0 0
14 3 0 0 0 0
15 3 0 0 0 0
5 4 0 0 0 0
16 4 0 0 0 0
17 4 0 0 0 0
6 5 0 0 0 0
18 5 0 0 0 0
19 5 0 0 0 0
7 6 0 0 0 0
8 6 0 0 0 0
6 20 0 0 0 0
M END
$$$$
n-pentylamine.sdf
COSMOtherm 3D 0
19 18 0 0 0 0 0 0 0 0 V2000
3.2401 -0.0309 0.2271 C 0 0 0 0 0 0 0 0 0 1
1.9152 0.0218 -0.5417 C 0 0 0 0 0 0 0 0 0 2
0.6845 0.0003 0.3739 C 0 0 0 0 0 0 0 0 0 3
-0.6473 0.0406 -0.3857 C 0 0 0 0 0 0 0 0 0 4
-1.8670 0.0006 0.5359 C 0 0 0 0 0 0 0 0 0 5
-3.1250 0.0290 -0.2419 N 0 0 0 0 0 0 0 0 0 6
-3.9208 -0.0036 0.4021 H 0 0 0 0 0 0 0 0 0 7
-3.1920 -0.8322 -0.7939 H 0 0 0 0 0 0 0 0 0 8
4.1034 -0.0142 -0.4548 H 0 0 0 0 0 0 0 0 0 9
3.3375 0.8277 0.9101 H 0 0 0 0 0 0 0 0 0 10
3.3103 -0.9479 0.8331 H 0 0 0 0 0 0 0 0 0 11
1.8603 -0.8315 -1.2399 H 0 0 0 0 0 0 0 0 0 12
1.8868 0.9318 -1.1657 H 0 0 0 0 0 0 0 0 0 13
0.7354 0.8578 1.0691 H 0 0 0 0 0 0 0 0 0 14
0.7189 -0.9075 1.0027 H 0 0 0 0 0 0 0 0 0 15
-0.6957 -0.8179 -1.0804 H 0 0 0 0 0 0 0 0 0 16
-0.6978 0.9511 -1.0072 H 0 0 0 0 0 0 0 0 0 17
-1.8585 0.8847 1.1945 H 0 0 0 0 0 0 0 0 0 18
-1.7892 -0.8880 1.1944 H 0 0 0 0 0 0 0 0 0 19
2 1 0 0 0 0
9 1 0 0 0 0
10 1 0 0 0 0
11 1 0 0 0 0
3 2 0 0 0 0
12 2 0 0 0 0
13 2 0 0 0 0
4 3 0 0 0 0
14 3 0 0 0 0
15 3 0 0 0 0
5 4 0 0 0 0
16 4 0 0 0 0
17 4 0 0 0 0
6 5 0 0 0 0
18 5 0 0 0 0
7 6 0 0 0 0
8 6 0 0 0 0
5 19 0 0 0 0
M END
$$$$
n-propylamine-cation.sdf
COSMOtherm 3D 0
14 13 0 0 0 0 0 0 0 0 V2000
1.9973 -0.0002 0.1345 C 0 0 0 0 0 0 0 0 0 1
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0.6126 0.0002 -0.5230 C 0 0 0 0 0 0 0 0 0 0 0 2
-0.4934 0.0002 0.5243 C 0 0 0 0 0 0 0 0 0 0 0 3
-1.8560 -0.0002 -0.1195 N 0 0 0 0 0 0 0 0 0 0 0 4
-2.6070 0.0078 0.5826 H 0 0 0 0 0 0 0 0 0 0 0 5
-1.9985 -0.8325 -0.7067 H 0 0 0 0 0 0 0 0 0 0 0 6
2.7861 0.0016 -0.6301 H 0 0 0 0 0 0 0 0 0 0 0 7
2.1383 0.8888 0.7667 H 0 0 0 0 0 0 0 0 0 0 0 8
2.1392 -0.8913 0.7636 H 0 0 0 0 0 0 0 0 0 0 0 9
0.5042 -0.8859 -1.1688 H 0 0 0 0 0 0 0 0 0 0 0 10
0.5044 0.8870 -1.1678 H 0 0 0 0 0 0 0 0 0 0 0 11
-0.4516 0.8924 1.1606 H 0 0 0 0 0 0 0 0 0 0 0 12
-0.4514 -0.8913 1.1615 H 0 0 0 0 0 0 0 0 0 0 0 13
-1.9927 0.8242 -0.7191 H 0 0 0 0 0 0 0 0 0 0 0 14
2 1 0 0 0 0
7 1 0 0 0 0
8 1 0 0 0 0
9 1 0 0 0 0
3 2 0 0 0 0
10 2 0 0 0 0
11 2 0 0 0 0
4 3 0 0 0 0
12 3 0 0 0 0
13 3 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
4 14 0 0 0 0
M END
$$$$
n-propylamine.sdf
COSMOTHERM 3D 0
13 12 0 0 0 0 0 0 0 0 0 V2000
1.9655 -0.0207 0.1392 C 0 0 0 0 0 0 0 0 0 0 0 1
0.5809 0.0402 -0.5150 C 0 0 0 0 0 0 0 0 0 0 0 2
-0.5582 -0.0114 0.5042 C 0 0 0 0 0 0 0 0 0 0 0 3
-1.8767 0.0498 -0.1633 N 0 0 0 0 0 0 0 0 0 0 0 4
-2.6160 0.0224 0.5451 H 0 0 0 0 0 0 0 0 0 0 0 5
-2.0067 -0.8018 -0.7188 H 0 0 0 0 0 0 0 0 0 0 0 6
2.7653 0.0170 -0.6147 H 0 0 0 0 0 0 0 0 0 0 0 7
2.1172 0.8238 0.8294 H 0 0 0 0 0 0 0 0 0 0 0 8
2.0933 -0.9501 0.7157 H 0 0 0 0 0 0 0 0 0 0 0 9
0.4679 -0.8025 -1.2193 H 0 0 0 0 0 0 0 0 0 0 0 10
0.4830 0.9623 -1.1116 H 0 0 0 0 0 0 0 0 0 0 0 11
-0.4821 0.8562 1.1802 H 0 0 0 0 0 0 0 0 0 0 0 12
-0.4350 -0.9163 1.1331 H 0 0 0 0 0 0 0 0 0 0 0 13
2 1 0 0 0 0
7 1 0 0 0 0
8 1 0 0 0 0
9 1 0 0 0 0
3 2 0 0 0 0
10 2 0 0 0 0
11 2 0 0 0 0
4 3 0 0 0 0
12 3 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
3 13 0 0 0 0
M END
$$$$
neo-pentylamine-cation.sdf
COSMOTHERM 3D 0
20 19 0 0 0 0 0 0 0 0 0 V2000
1.6474 -0.0100 -0.9834 C 0 0 0 0 0 0 0 0 0 0 0 1
0.4710 0.0000 0.0128 C 0 0 0 0 0 0 0 0 0 0 0 2
0.5434 1.2704 0.8824 C 0 0 0 0 0 0 0 0 0 0 0 3
0.5355 -1.2592 0.8990 C 0 0 0 0 0 0 0 0 0 0 0 4
-0.8093 -0.0014 -0.8412 C 0 0 0 0 0 0 0 0 0 0 0 5
-2.0732 0.0002 -0.0194 N 0 0 0 0 0 0 0 0 0 0 0 6
-2.9072 -0.0021 -0.6208 H 0 0 0 0 0 0 0 0 0 0 0 7
-2.1407 0.8311 0.5833 H 0 0 0 0 0 0 0 0 0 0 0 8
2.6021 -0.0044 -0.4382 H 0 0 0 0 0 0 0 0 0 0 0 9
1.6239 -0.9085 -1.6187 H 0 0 0 0 0 0 0 0 0 0 0 10
1.6239 0.8754 -1.6368 H 0 0 0 0 0 0 0 0 0 0 0 11
1.4972 1.2970 1.4286 H 0 0 0 0 0 0 0 0 0 0 0 12
-0.2562 1.3097 1.6397 H 0 0 0 0 0 0 0 0 0 0 0 13
0.4790 2.1795 0.2658 H 0 0 0 0 0 0 0 0 0 0 0 14
1.4924 -1.2885 1.4398 H 0 0 0 0 0 0 0 0 0 0 0 15
-0.2594 -1.2798 1.6619 H 0 0 0 0 0 0 0 0 0 0 0 16
0.4582 -2.1760 0.2953 H 0 0 0 0 0 0 0 0 0 0 0 17
-0.8599 -0.8950 -1.4754 H 0 0 0 0 0 0 0 0 0 0 0 18
-0.8596 0.8892 -1.4795 H 0 0 0 0 0 0 0 0 0 0 0 19
-2.1392 -0.8275 0.5879 H 0 0 0 0 0 0 0 0 0 0 0 20
2 1 0 0 0 0
9 1 0 0 0 0
10 1 0 0 0 0
11 1 0 0 0 0
3 2 0 0 0 0
4 2 0 0 0 0
5 2 0 0 0 0
12 3 0 0 0 0
13 3 0 0 0 0
14 3 0 0 0 0
15 4 0 0 0 0
16 4 0 0 0 0
17 4 0 0 0 0
6 5 0 0 0 0
18 5 0 0 0 0
19 5 0 0 0 0
7 6 0 0 0 0
8 6 0 0 0 0
6 20 0 0 0 0
M END
$$$$
neo-pentylamine.sdf
```

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1
2
3 COSMOTHERM 3D 0
4
5 19 18 0 0 0 0 0 0 0 0 0 V2000
6 1.6166 0.5264 -0.8427 C 0 0 0 0 0 0 0 0 0 0 0 1
7 0.4452 -0.0054 0.0041 C 0 0 0 0 0 0 0 0 0 0 0 2
8 0.4873 0.6509 1.3979 C 0 0 0 0 0 0 0 0 0 0 0 3
9 0.5637 -1.5334 0.1438 C 0 0 0 0 0 0 0 0 0 0 0 4
10 -0.8681 0.3705 -0.7225 C 0 0 0 0 0 0 0 0 0 0 0 5
11 -2.0840 -0.0560 -0.0006 N 0 0 0 0 0 0 0 0 0 0 0 6
12 -2.8999 0.1258 -0.5916 H 0 0 0 0 0 0 0 0 0 0 0 7
13 -2.2158 0.5352 0.8249 H 0 0 0 0 0 0 0 0 0 0 0 8
14 2.5813 0.2750 -0.3756 H 0 0 0 0 0 0 0 0 0 0 0 9
15 1.6059 0.0882 -1.8532 H 0 0 0 0 0 0 0 0 0 0 0 10
16 1.5668 1.6219 -0.9470 H 0 0 0 0 0 0 0 0 0 0 0 11
17 1.4513 0.4511 1.8914 H 0 0 0 0 0 0 0 0 0 0 0 12
18 -0.3051 0.2593 2.0543 H 0 0 0 0 0 0 0 0 0 0 0 13
19 0.3658 1.7435 1.3254 H 0 0 0 0 0 0 0 0 0 0 0 14
20 1.4868 -1.8052 0.6794 H 0 0 0 0 0 0 0 0 0 0 0 15
21 -0.2927 -1.9424 0.6985 H 0 0 0 0 0 0 0 0 0 0 0 16
22 0.5905 -2.0172 -0.8456 H 0 0 0 0 0 0 0 0 0 0 0 17
23 -0.8746 -0.1266 -1.7061 H 0 0 0 0 0 0 0 0 0 0 0 18
24 -0.8485 1.4628 -0.9152 H 0 0 0 0 0 0 0 0 0 0 0 19
25
26 2 1 0 0 0 0
27 9 1 0 0 0 0
28 10 1 0 0 0 0
29 11 1 0 0 0 0
30 3 2 0 0 0 0
31 4 2 0 0 0 0
32 5 2 0 0 0 0
33 12 3 0 0 0 0
34 13 3 0 0 0 0
35 14 3 0 0 0 0
36 15 4 0 0 0 0
37 16 4 0 0 0 0
38 17 4 0 0 0 0
39 6 5 0 0 0 0
40 18 5 0 0 0 0
41 7 6 0 0 0 0
42 8 6 0 0 0 0
43 5 19 0 0 0 0
44 M END
45 $$$$
46 p-toluidine-cation0.sdf
47 COSMOTHERM 3D 0
48
49 18 18 0 0 0 0 0 0 0 0 0 V2000
50 -0.0102 1.2067 -0.7365 C 0 0 0 0 0 0 0 0 0 0 0 1
51 -0.0043 1.2154 0.6614 C 0 0 0 0 0 0 0 0 0 0 0 2
52 0.0007 -0.0002 1.3376 C 0 0 0 0 0 0 0 0 0 0 0 3
53 -0.0041 -1.2177 0.6611 C 0 0 0 0 0 0 0 0 0 0 0 4
54 -0.0104 -1.2065 -0.7354 C 0 0 0 0 0 0 0 0 0 0 0 5
55 -0.0097 0.0008 -1.4572 C 0 0 0 0 0 0 0 0 0 0 0 6
56 0.0114 0.0002 2.8164 N 0 0 0 0 0 0 0 0 0 0 0 7
57 0.0167 0.0000 -2.9647 C 0 0 0 0 0 0 0 0 0 0 0 8
58 -0.7741 -0.5365 3.2118 H 0 0 0 0 0 0 0 0 0 0 0 9
59 -0.0627 0.9558 3.1918 H 0 0 0 0 0 0 0 0 0 0 0 10
60 -0.0185 2.1579 -1.2719 H 0 0 0 0 0 0 0 0 0 0 0 11
-0.0066 2.1595 1.2096 H 0 0 0 0 0 0 0 0 0 0 0 12
-0.0066 -2.1617 1.2085 H 0 0 0 0 0 0 0 0 0 0 0 13
-0.0188 -2.1570 -1.2723 H 0 0 0 0 0 0 0 0 0 0 0 14
1.0553 -0.0113 -3.3331 H 0 0 0 0 0 0 0 0 0 0 0 15
-0.4665 0.8974 -3.3739 H 0 0 0 0 0 0 0 0 0 0 0 16
-0.4853 -0.8872 -3.3735 H 0 0 0 0 0 0 0 0 0 0 0 17
0.8790 -0.4030 3.1995 H 0 0 0 0 0 0 0 0 0 0 0 18
2 1 0 0 0 0
6 1 0 0 0 0
11 1 0 0 0 0
3 2 0 0 0 0
12 2 0 0 0 0
4 3 0 0 0 0
7 3 0 0 0 0
5 4 0 0 0 0
13 4 0 0 0 0
6 5 0 0 0 0
14 5 0 0 0 0
8 6 0 0 0 0
9 7 0 0 0 0
10 7 0 0 0 0
15 8 0 0 0 0
16 8 0 0 0 0
17 8 0 0 0 0
7 18 0 0 0 0
M END
$$$$
p-toluidine-cation1.sdf
COSMOTHERM 3D 0
18 18 0 0 0 0 0 0 0 0 0 V2000
-0.0087 1.2066 -0.7359 C 0 0 0 0 0 0 0 0 0 0 0 1
0.0033 1.2166 0.6613 C 0 0 0 0 0 0 0 0 0 0 0 2
0.0105 0.0001 1.3375 C 0 0 0 0 0 0 0 0 0 0 0 3
0.0035 -1.2165 0.6612 C 0 0 0 0 0 0 0 0 0 0 0 4
-0.0089 -1.2065 -0.7359 C 0 0 0 0 0 0 0 0 0 0 0 5
-0.0125 0.0001 -1.4571 C 0 0 0 0 0 0 0 0 0 0 0 6
-0.0013 -0.0002 2.8162 N 0 0 0 0 0 0 0 0 0 0 0 7
0.0098 -0.0001 -2.9647 C 0 0 0 0 0 0 0 0 0 0 0 8
-0.9583 -0.0045 3.1998 H 0 0 0 0 0 0 0 0 0 0 0 9
0.4720 0.8286 3.2022 H 0 0 0 0 0 0 0 0 0 0 0 10
-0.0145 2.1575 -1.2721 H 0 0 0 0 0 0 0 0 0 0 0 11
0.0059 2.1605 1.2092 H 0 0 0 0 0 0 0 0 0 0 0 12
0.0060 -2.1605 1.2091 H 0 0 0 0 0 0 0 0 0 0 0 13
-0.0150 -2.1574 -1.2721 H 0 0 0 0 0 0 0 0 0 0 0 14
1.0472 -0.0093 -3.3362 H 0 0 0 0 0 0 0 0 0 0 0 15
-0.4763 0.8965 -3.3723 H 0 0 0 0 0 0 0 0 0 0 0 16
-0.4917 -0.8883 -3.3722 H 0 0 0 0 0 0 0 0 0 0 0 17
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0.4800 -0.8244 3.2021 H 0 0 0 0 0 0 0 0 0 0 0 18
2 1 0 0 0 0
6 1 0 0 0 0
11 1 0 0 0 0
3 2 0 0 0 0
12 2 0 0 0 0
4 3 0 0 0 0
7 3 0 0 0 0
5 4 0 0 0 0
13 4 0 0 0 0
6 5 0 0 0 0
14 5 0 0 0 0
8 6 0 0 0 0
9 7 0 0 0 0
10 7 0 0 0 0
15 8 0 0 0 0
16 8 0 0 0 0
17 8 0 0 0 0
7 18 0 0 0 0
M END
$$$$
p-toluidine.sdf
COSMOTHERM 3D 0
17 17 0 0 0 0 0 0 0 0 0 V2000
-2.9502 0.0012 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 1
-1.4387 -0.0022 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 2
-0.7030 1.1978 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 3
0.6920 1.2093 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 4
1.4255 -0.0011 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 5
-0.7028 -1.1988 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 6
0.6949 -1.2104 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 7
2.8031 0.0024 0.0000 N 0 0 0 0 0 0 0 0 0 0 0 8
-3.3560 0.5166 -0.8852 H 0 0 0 0 0 0 0 0 0 0 0 9
-3.3469 -1.0236 0.0001 H 0 0 0 0 0 0 0 0 0 0 0 10
-3.3561 0.5169 0.8849 H 0 0 0 0 0 0 0 0 0 0 0 11
-1.2345 2.1538 0.0000 H 0 0 0 0 0 0 0 0 0 0 0 12
1.2294 2.1612 -0.0001 H 0 0 0 0 0 0 0 0 0 0 0 13
-1.2350 -2.1542 0.0001 H 0 0 0 0 0 0 0 0 0 0 0 14
1.2318 -2.1624 0.0001 H 0 0 0 0 0 0 0 0 0 0 0 15
3.3240 0.8704 0.0003 H 0 0 0 0 0 0 0 0 0 0 0 16
3.3286 -0.8628 -0.0005 H 0 0 0 0 0 0 0 0 0 0 0 17
2 1 0 0 0 0
9 1 0 0 0 0
10 1 0 0 0 0
11 1 0 0 0 0
3 2 0 0 0 0
6 2 0 0 0 0
4 3 0 0 0 0
12 3 0 0 0 0
5 4 0 0 0 0
13 4 0 0 0 0
7 5 0 0 0 0
8 5 0 0 0 0
7 6 0 0 0 0
14 6 0 0 0 0
15 7 0 0 0 0
16 8 0 0 0 0
8 17 0 0 0 0
M END
$$$$
p-toluidine0.sdf
COSMOTHERM 3D 0
17 17 0 0 0 0 0 0 0 0 0 V2000
-1.1983 -0.7030 0.0108 C 0 0 0 0 0 0 0 0 0 0 0 1
-1.2099 0.6933 0.0029 C 0 0 0 0 0 0 0 0 0 0 0 2
0.0000 1.4253 -0.0040 C 0 0 0 0 0 0 0 0 0 0 0 3
1.2099 0.6933 0.0027 C 0 0 0 0 0 0 0 0 0 0 0 4
1.1983 -0.7030 0.0110 C 0 0 0 0 0 0 0 0 0 0 0 5
-0.0001 -1.4387 0.0119 C 0 0 0 0 0 0 0 0 0 0 0 6
0.0000 2.8030 -0.0102 N 0 0 0 0 0 0 0 0 0 0 0 7
0.0001 -2.9497 -0.0181 C 0 0 0 0 0 0 0 0 0 0 0 8
0.8667 3.3261 -0.0122 H 0 0 0 0 0 0 0 0 0 0 0 9
-0.8666 3.3262 -0.0106 H 0 0 0 0 0 0 0 0 0 0 0 10
-2.1540 -1.2348 0.0188 H 0 0 0 0 0 0 0 0 0 0 0 11
-2.1617 1.2306 0.0061 H 0 0 0 0 0 0 0 0 0 0 0 12
2.1617 1.2306 0.0062 H 0 0 0 0 0 0 0 0 0 0 0 13
2.1539 -1.2349 0.0190 H 0 0 0 0 0 0 0 0 0 0 0 14
0.0030 -3.3355 -1.0515 H 0 0 0 0 0 0 0 0 0 0 0 15
-0.8913 -3.3606 0.4777 H 0 0 0 0 0 0 0 0 0 0 0 16
0.8886 -3.3606 0.4827 H 0 0 0 0 0 0 0 0 0 0 0 17
2 1 0 0 0 0
6 1 0 0 0 0
11 1 0 0 0 0
3 2 0 0 0 0
12 2 0 0 0 0
4 3 0 0 0 0
7 3 0 0 0 0
5 4 0 0 0 0
13 4 0 0 0 0
6 5 0 0 0 0
14 5 0 0 0 0
8 6 0 0 0 0
9 7 0 0 0 0
10 7 0 0 0 0
15 8 0 0 0 0
16 8 0 0 0 0
8 17 0 0 0 0
M END
$$$$
p-toluidine1.sdf
COSMOTHERM 3D 0
17 17 0 0 0 0 0 0 0 0 0 V2000
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6 1 0 0 0 0
3 2 0 0 0 0
7 2 0 0 0 0
4 3 0 0 0 0
5 4 0 0 0 0
8 4 0 0 0 0
5 9 0 0 0 0
M END
$$$$
pyrazole_p2.sdf
COSMOTHERM 3D 0
10 10 0 0 0 0 0 0 0 0 V2000
-0.3985 -1.1151 -0.0001 C 0 0 0 0 0 0 0 0 0 0 1
-1.2372 0.0010 0.0000 C 0 0 0 0 0 0 0 0 0 0 2
-0.3968 1.1157 0.0001 C 0 0 0 0 0 0 0 0 0 0 3
0.8736 0.6733 -0.0001 N 0 0 0 0 0 0 0 0 0 0 4
0.8726 -0.6746 0.0001 N 0 0 0 0 0 0 0 0 0 0 5
-0.6116 -2.1785 0.0000 H 0 0 0 0 0 0 0 0 0 0 6
-2.3204 0.0019 0.0001 H 0 0 0 0 0 0 0 0 0 0 7
-0.6082 2.1794 0.0000 H 0 0 0 0 0 0 0 0 0 0 8
1.7464 -1.1993 0.0004 H 0 0 0 0 0 0 0 0 0 0 9
1.7483 1.1965 -0.0004 H 0 0 0 0 0 0 0 0 0 0 10
2 1 0 0 0 0
5 1 0 0 0 0
6 1 0 0 0 0
3 2 0 0 0 0
7 2 0 0 0 0
4 3 0 0 0 0
8 3 0 0 0 0
5 4 0 0 0 0
9 5 0 0 0 0
4 10 0 0 0 0
M END
$$$$
pyridine.sdf
COSMOTHERM 3D 0
11 11 0 0 0 0 0 0 0 0 V2000
-1.1501 -0.6948 0.0000 C 0 0 0 0 0 0 0 0 0 0 1
-1.2019 0.7023 0.0000 C 0 0 0 0 0 0 0 0 0 0 2
-0.0001 1.4160 0.0001 C 0 0 0 0 0 0 0 0 0 0 3
1.2018 0.7025 0.0000 C 0 0 0 0 0 0 0 0 0 0 4
1.1502 -0.6946 0.0000 C 0 0 0 0 0 0 0 0 0 0 5
0.0001 -1.3983 0.0000 N 0 0 0 0 0 0 0 0 0 0 6
-2.0729 -1.2817 -0.0001 H 0 0 0 0 0 0 0 0 0 0 7
-2.1649 1.2148 -0.0001 H 0 0 0 0 0 0 0 0 0 0 8
-0.0001 2.5072 0.0001 H 0 0 0 0 0 0 0 0 0 0 9
2.1647 1.2151 -0.0002 H 0 0 0 0 0 0 0 0 0 0 10
2.0730 -1.2814 0.0000 H 0 0 0 0 0 0 0 0 0 0 11
2 1 0 0 0 0
6 1 0 0 0 0
7 1 0 0 0 0
3 2 0 0 0 0
8 2 0 0 0 0
4 3 0 0 0 0
9 3 0 0 0 0
5 4 0 0 0 0
10 4 0 0 0 0
6 5 0 0 0 0
5 11 0 0 0 0
M END
$$$$
pyridine_p1.sdf
COSMOTHERM 3D 0
12 12 0 0 0 0 0 0 0 0 V2000
-1.2112 -0.7187 0.0000 C 0 0 0 0 0 0 0 0 0 0 1
-1.1899 0.6674 0.0000 C 0 0 0 0 0 0 0 0 0 0 2
0.0000 1.3094 0.0000 N 0 0 0 0 0 0 0 0 0 0 3
1.1899 0.6674 0.0000 C 0 0 0 0 0 0 0 0 0 0 4
1.2112 -0.7187 0.0001 C 0 0 0 0 0 0 0 0 0 0 5
0.0000 -1.4188 0.0000 C 0 0 0 0 0 0 0 0 0 0 6
-2.1677 -1.2380 0.0000 H 0 0 0 0 0 0 0 0 0 0 7
-2.0793 1.2929 0.0000 H 0 0 0 0 0 0 0 0 0 0 8
2.0793 1.2929 0.0000 H 0 0 0 0 0 0 0 0 0 0 9
2.1677 -1.2379 0.0000 H 0 0 0 0 0 0 0 0 0 0 10
0.0000 -2.5088 -0.0001 H 0 0 0 0 0 0 0 0 0 0 11
-0.0001 2.3319 -0.0003 H 0 0 0 0 0 0 0 0 0 0 12
2 1 0 0 0 0
6 1 0 0 0 0
7 1 0 0 0 0
3 2 0 0 0 0
8 2 0 0 0 0
4 3 0 0 0 0
5 4 0 0 0 0
9 4 0 0 0 0
6 5 0 0 0 0
10 5 0 0 0 0
11 6 0 0 0 0
3 12 0 0 0 0
M END
$$$$
pyrimidine.sdf
COSMOTHERM 3D 0
10 10 0 0 0 0 0 0 0 0 V2000
-0.6564 -1.1881 0.0000 C 0 0 0 0 0 0 0 0 0 0 1
0.6912 -1.2024 0.0000 N 0 0 0 0 0 0 0 0 0 0 2
1.2903 0.0001 0.0000 C 0 0 0 0 0 0 0 0 0 0 3
0.6910 1.2025 0.0000 N 0 0 0 0 0 0 0 0 0 0 4
-0.6566 1.1880 0.0000 C 0 0 0 0 0 0 0 0 0 0 5
-1.3873 -0.0001 0.0000 C 0 0 0 0 0 0 0 0 0 0 6
-1.1562 -2.1601 0.0001 H 0 0 0 0 0 0 0 0 0 0 7
2.3839 0.0002 0.0000 H 0 0 0 0 0 0 0 0 0 0 8
```

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1
2
3      -1.1566    2.1600    0.0000 H    0    0    0    0    0    0    0    0    0    9
4      -2.4769   -0.0002    0.0000 H    0    0    0    0    0    0    0    0    0    10
5
6      2  1  0  0  0  0
7      6  1  0  0  0  0
8      7  1  0  0  0  0
9      3  2  0  0  0  0
10     4  3  0  0  0  0
11     8  3  0  0  0  0
12     5  4  0  0  0  0
13     6  5  0  0  0  0
14     9  5  0  0  0  0
15     6 10  0  0  0  0
16
17 M  END
18 $$$
19 pyrimidine_p1.sdf
20 COSMOTHERM      3D      0
21
22 11 11  0  0  0  0  0  0  0  0  0  0 V2000
23 -0.7982 -1.1061    0.0000 C    0    0    0    0    0    0    0    0    0    1
24 -1.3940  0.1580    0.0000 C    0    0    0    0    0    0    0    0    0    2
25 -0.5567  1.2603    0.0000 C    0    0    0    0    0    0    0    0    0    3
26  0.7766  1.0443    0.0000 N    0    0    0    0    0    0    0    0    0    4
27  1.2964 -0.2050    0.0000 C    0    0    0    0    0    0    0    0    0    5
28  0.5393 -1.2892    0.0000 N    0    0    0    0    0    0    0    0    0    6
29 -1.4091 -2.0104    0.0000 H    0    0    0    0    0    0    0    0    0    7
30 -2.4747  0.2819   -0.0001 H    0    0    0    0    0    0    0    0    0    8
31 -0.8916  2.2951    0.0000 H    0    0    0    0    0    0    0    0    0    9
32  2.3827 -0.2851   -0.0001 H    0    0    0    0    0    0    0    0    0    10
33  1.4162  1.8440    0.0000 H    0    0    0    0    0    0    0    0    0    11
34
35  2  1  0  0  0  0
36  6  1  0  0  0  0
37  7  1  0  0  0  0
38  3  2  0  0  0  0
39  8  2  0  0  0  0
40  4  3  0  0  0  0
41  9  3  0  0  0  0
42  5  4  0  0  0  0
43  6  5  0  0  0  0
44 10  5  0  0  0  0
45  4 11  0  0  0  0
46
47 M  END
48 $$$
49 pyrrole-cation0.sdf
50 COSMOTHERM      3D      0
51
52 11 11  0  0  0  0  0  0  0  0  0  0 V2000
53 -0.7253  1.0037    0.0000 C    0    0    0    0    0    0    0    0    0    1
54  0.7402  0.9928    0.0000 C    0    0    0    0    0    0    0    0    0    2
55 -1.1784 -0.2604    0.0000 C    0    0    0    0    0    0    0    0    0    3
56 -0.0087 -1.1603    0.0000 N    0    0    0    0    0    0    0    0    0    4
57  1.1744 -0.2781    0.0000 C    0    0    0    0    0    0    0    0    0    5
58 -1.3458  1.8956    0.0001 H    0    0    0    0    0    0    0    0    0    6
59  1.3740  1.8752   -0.0001 H    0    0    0    0    0    0    0    0    0    7
60 -2.1671 -0.7054    0.0001 H    0    0    0    0    0    0    0    0    0    8
    -0.0134 -1.7885   -0.8228 H    0    0    0    0    0    0    0    0    0    9
    2.1564 -0.7379   -0.0001 H    0    0    0    0    0    0    0    0    0    10
    -0.0133 -1.7886    0.8228 H    0    0    0    0    0    0    0    0    0    11
    2  1  0  0  0  0
    3  1  0  0  0  0
    6  1  0  0  0  0
    5  2  0  0  0  0
    7  2  0  0  0  0
    4  3  0  0  0  0
    8  3  0  0  0  0
    5  4  0  0  0  0
    9  4  0  0  0  0
   10  5  0  0  0  0
    4 11  0  0  0  0
    11
    M  END
    $$$
    pyrrole-cation1.sdf
    COSMOTHERM      3D      0
    11 11  0  0  0  0  0  0  0  0  0  0 V2000
    0.6758  0.0000    1.0240 C    0    0    0    0    0    0    0    0    0    1
    -0.6860  0.0000    1.0408 C    0    0    0    0    0    0    0    0    0    2
    1.1485  0.0000   -0.3821 C    0    0    0    0    0    0    0    0    0    3
    -0.0964  0.0000   -1.1364 N    0    0    0    0    0    0    0    0    0    4
    -1.1277  0.0000   -0.3272 C    0    0    0    0    0    0    0    0    0    5
    -0.1477  0.0000   -2.1547 H    0    0    0    0    0    0    0    0    0    6
    1.3497 -0.0001    1.8772 H    0    0    0    0    0    0    0    0    0    7
    -1.3478  0.0000    1.9014 H    0    0    0    0    0    0    0    0    0    8
    -2.1472 -0.0002   -0.7087 H    0    0    0    0    0    0    0    0    0    9
    1.7534 -0.8866   -0.6379 H    0    0    0    0    0    0    0    0    0    10
    1.7535  0.8863   -0.6382 H    0    0    0    0    0    0    0    0    0    11
    2  1  0  0  0  0
    3  1  0  0  0  0
    7  1  0  0  0  0
    5  2  0  0  0  0
    8  2  0  0  0  0
    4  3  0  0  0  0
   10  3  0  0  0  0
    5  4  0  0  0  0
    6  4  0  0  0  0
    9  5  0  0  0  0
    3 11  0  0  0  0
    11
    M  END
    $$$
    pyrrole-cation2.sdf
    COSMOTHERM      3D      0
    11 11  0  0  0  0  0  0  0  0  0  0 V2000
    1.0729  0.6260    0.0000 C    0    0    0    0    0    0    0    0    0    1
    -0.3101  1.1955    0.0000 C    0    0    0    0    0    0    0    0    0    2
    0.8423 -0.8313    0.0000 C    0    0    0    0    0    0    0    0    0    3
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-0.4462 -1.0429 0.0000 N 0 0 0 0 0 0 0 0 0 0 4
-1.1876 0.1728 0.0000 C 0 0 0 0 0 0 0 0 0 0 5
1.6792 0.9284 -0.8742 H 0 0 0 0 0 0 0 0 0 0 6
1.6795 0.9285 0.8740 H 0 0 0 0 0 0 0 0 0 0 7
-0.8798 -1.9693 -0.0001 H 0 0 0 0 0 0 0 0 0 0 8
-0.5474 2.2546 0.0000 H 0 0 0 0 0 0 0 0 0 0 9
1.5657 -1.6427 0.0002 H 0 0 0 0 0 0 0 0 0 0 10
-2.2717 0.1347 -0.0001 H 0 0 0 0 0 0 0 0 0 0 11
2 1 0 0 0 0
3 1 0 0 0 0
6 1 0 0 0 0
7 1 0 0 0 0
5 2 0 0 0 0
9 2 0 0 0 0
4 3 0 0 0 0
10 3 0 0 0 0
5 4 0 0 0 0
8 4 0 0 0 0
5 11 0 0 0 0
M END
$$$$
pyrrole.sdf
COSMOTHERM 3D 0
10 10 0 0 0 0 0 0 0 0 V2000
-0.9895 -0.7145 0.0000 C 0 0 0 0 0 0 0 0 0 0 1
-0.9895 0.7146 0.0000 C 0 0 0 0 0 0 0 0 0 0 2
0.3351 1.1286 0.0000 C 0 0 0 0 0 0 0 0 0 0 3
1.1240 0.0000 0.0000 N 0 0 0 0 0 0 0 0 0 0 4
0.3351 -1.1286 0.0000 C 0 0 0 0 0 0 0 0 0 0 5
-1.8588 -1.3668 0.0000 H 0 0 0 0 0 0 0 0 0 0 6
-1.8588 1.3669 0.0000 H 0 0 0 0 0 0 0 0 0 0 7
0.7775 2.1198 0.0000 H 0 0 0 0 0 0 0 0 0 0 8
2.1396 -0.0001 -0.0001 H 0 0 0 0 0 0 0 0 0 0 9
0.7774 -2.1198 0.0000 H 0 0 0 0 0 0 0 0 0 0 10
2 1 0 0 0 0
5 1 0 0 0 0
6 1 0 0 0 0
3 2 0 0 0 0
7 2 0 0 0 0
4 3 0 0 0 0
8 3 0 0 0 0
5 4 0 0 0 0
9 4 0 0 0 0
5 10 0 0 0 0
M END
$$$$
quinoline.sdf
COSMOTHERM 3D 0
17 18 0 0 0 0 0 0 0 0 V2000
0.0244 -0.6934 -0.0001 C 0 0 0 0 0 0 0 0 0 0 1
1.1994 -1.4043 0.0000 N 0 0 0 0 0 0 0 0 0 0 2
2.3361 -0.7179 0.0001 C 0 0 0 0 0 0 0 0 0 0 3
2.4131 0.6978 0.0000 C 0 0 0 0 0 0 0 0 0 0 4
1.2426 1.4273 -0.0001 C 0 0 0 0 0 0 0 0 0 0 5
-0.0024 0.7446 0.0000 C 0 0 0 0 0 0 0 0 0 0 6
-1.2057 -1.4049 -0.0001 C 0 0 0 0 0 0 0 0 0 0 7
-2.4084 -0.7235 0.0000 C 0 0 0 0 0 0 0 0 0 0 8
-2.4351 0.6951 0.0001 C 0 0 0 0 0 0 0 0 0 0 9
-1.2559 1.4156 0.0001 C 0 0 0 0 0 0 0 0 0 0 10
3.2575 -1.3082 0.0003 H 0 0 0 0 0 0 0 0 0 0 11
3.3880 1.1866 0.0000 H 0 0 0 0 0 0 0 0 0 0 12
1.2580 2.5195 -0.0002 H 0 0 0 0 0 0 0 0 0 0 13
-1.1709 -2.4959 -0.0001 H 0 0 0 0 0 0 0 0 0 0 14
-3.3482 -1.2785 -0.0001 H 0 0 0 0 0 0 0 0 0 0 15
-3.3942 1.2157 0.0002 H 0 0 0 0 0 0 0 0 0 0 16
-1.2705 2.5079 0.0001 H 0 0 0 0 0 0 0 0 0 0 17
2 1 0 0 0 0
6 1 0 0 0 0
7 1 0 0 0 0
3 2 0 0 0 0
4 3 0 0 0 0
11 3 0 0 0 0
5 4 0 0 0 0
12 4 0 0 0 0
6 5 0 0 0 0
13 5 0 0 0 0
10 6 0 0 0 0
8 7 0 0 0 0
14 7 0 0 0 0
9 8 0 0 0 0
15 8 0 0 0 0
10 9 0 0 0 0
16 9 0 0 0 0
10 17 0 0 0 0
M END
$$$$
quinoline_pl.sdf
COSMOTHERM 3D 0
18 19 0 0 0 0 0 0 0 0 V2000
-1.4219 -1.2739 0.0003 C 0 0 0 0 0 0 0 0 0 0 1
-0.6955 -2.4478 0.0000 C 0 0 0 0 0 0 0 0 0 0 2
0.7222 -2.4193 -0.0002 C 0 0 0 0 0 0 0 0 0 0 3
1.4124 -1.2207 -0.0002 C 0 0 0 0 0 0 0 0 0 0 4
0.6782 -0.0185 0.0002 C 0 0 0 0 0 0 0 0 0 0 5
-0.7525 -0.0208 0.0002 C 0 0 0 0 0 0 0 0 0 0 6
-1.4294 1.2233 -0.0002 C 0 0 0 0 0 0 0 0 0 0 7
-0.7213 2.4140 -0.0003 C 0 0 0 0 0 0 0 0 0 0 8
0.6766 2.3763 0.0000 C 0 0 0 0 0 0 0 0 0 0 9
1.3166 1.2013 0.0003 N 0 0 0 0 0 0 0 0 0 0 10
-2.5125 -1.2872 0.0003 H 0 0 0 0 0 0 0 0 0 0 11
-1.2113 -3.4084 0.0000 H 0 0 0 0 0 0 0 0 0 0 12
1.2777 -3.3577 -0.0006 H 0 0 0 0 0 0 0 0 0 0 13
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2.5029 -1.1936 -0.0005 H 0 0 0 0 0 0 0 0 0 0 14
-2.5206 1.2333 -0.0005 H 0 0 0 0 0 0 0 0 0 0 15
-1.2250 3.3783 -0.0006 H 0 0 0 0 0 0 0 0 0 0 16
1.3006 3.2674 0.0000 H 0 0 0 0 0 0 0 0 0 0 17
2.3395 1.2050 0.0004 H 0 0 0 0 0 0 0 0 0 0 18
2 1 0 0 0 0
6 1 0 0 0 0
11 1 0 0 0 0
3 2 0 0 0 0
12 2 0 0 0 0
4 3 0 0 0 0
13 3 0 0 0 0
5 4 0 0 0 0
14 4 0 0 0 0
6 5 0 0 0 0
10 5 0 0 0 0
7 6 0 0 0 0
8 7 0 0 0 0
15 7 0 0 0 0
9 8 0 0 0 0
16 8 0 0 0 0
10 9 0 0 0 0
17 9 0 0 0 0
10 18 0 0 0 0
M END
$$$$
sec-butylamine-cation.sdf
COSMOtherm 3D 0
17 16 0 0 0 0 0 0 0 0 0 V2000
0.4666 0.0762 0.3399 C 0 0 0 0 0 0 0 0 0 0 1
1.7549 0.8090 -0.0110 C 0 0 0 0 0 0 0 0 0 0 2
0.5951 -1.3689 -0.1180 N 0 0 0 0 0 0 0 0 0 0 3
-0.7844 0.6996 -0.2826 C 0 0 0 0 0 0 0 0 0 0 4
-2.1013 0.0227 0.1126 C 0 0 0 0 0 0 0 0 0 0 5
1.3881 -1.8400 0.3364 H 0 0 0 0 0 0 0 0 0 0 6
-0.2461 -1.9190 0.1015 H 0 0 0 0 0 0 0 0 0 0 7
0.3493 0.0108 1.4304 H 0 0 0 0 0 0 0 0 0 0 8
2.6315 0.3216 0.4386 H 0 0 0 0 0 0 0 0 0 0 9
1.7025 1.8346 0.3759 H 0 0 0 0 0 0 0 0 0 0 10
1.8977 0.8605 -1.1007 H 0 0 0 0 0 0 0 0 0 0 11
-0.7984 1.7505 0.0425 H 0 0 0 0 0 0 0 0 0 0 12
-0.6714 0.7169 -1.3796 H 0 0 0 0 0 0 0 0 0 0 13
-2.9544 0.5850 -0.2908 H 0 0 0 0 0 0 0 0 0 0 14
-2.1847 -1.0022 -0.2812 H 0 0 0 0 0 0 0 0 0 0 15
-2.2138 -0.0213 1.2063 H 0 0 0 0 0 0 0 0 0 0 16
0.7464 -1.4300 -1.1345 H 0 0 0 0 0 0 0 0 0 0 17
2 1 0 0 0 0
3 1 0 0 0 0
4 1 0 0 0 0
8 1 0 0 0 0
9 2 0 0 0 0
10 2 0 0 0 0
11 2 0 0 0 0
6 3 0 0 0 0
7 3 0 0 0 0
5 4 0 0 0 0
12 4 0 0 0 0
13 4 0 0 0 0
14 5 0 0 0 0
15 5 0 0 0 0
16 5 0 0 0 0
3 17 0 0 0 0
M END
$$$$
sec-butylamine.sdf
COSMOtherm 3D 0
16 15 0 0 0 0 0 0 0 0 0 V2000
0.4785 0.0085 0.3293 C 0 0 0 0 0 0 0 0 0 0 1
1.7562 0.7776 -0.0113 C 0 0 0 0 0 0 0 0 0 0 2
0.5980 -1.3732 -0.1943 N 0 0 0 0 0 0 0 0 0 0 3
-0.7620 0.6916 -0.2647 C 0 0 0 0 0 0 0 0 0 0 4
-2.0912 0.0231 0.1055 C 0 0 0 0 0 0 0 0 0 0 5
1.4078 -1.8264 0.2401 H 0 0 0 0 0 0 0 0 0 0 6
-0.2109 -1.9263 0.1035 H 0 0 0 0 0 0 0 0 0 0 7
0.3613 0.0102 1.4340 H 0 0 0 0 0 0 0 0 0 0 8
2.6417 0.2851 0.4196 H 0 0 0 0 0 0 0 0 0 0 9
1.7133 1.8018 0.3870 H 0 0 0 0 0 0 0 0 0 0 10
1.8933 0.8334 -1.1028 H 0 0 0 0 0 0 0 0 0 0 11
-0.7716 1.7370 0.0852 H 0 0 0 0 0 0 0 0 0 0 12
-0.6505 0.7249 -1.3625 H 0 0 0 0 0 0 0 0 0 0 13
-2.9442 0.6047 -0.2741 H 0 0 0 0 0 0 0 0 0 0 14
-2.1758 -0.9886 -0.3199 H 0 0 0 0 0 0 0 0 0 0 15
-2.2033 -0.0584 1.1984 H 0 0 0 0 0 0 0 0 0 0 16
2 1 0 0 0 0
3 1 0 0 0 0
4 1 0 0 0 0
8 1 0 0 0 0
9 2 0 0 0 0
10 2 0 0 0 0
11 2 0 0 0 0
6 3 0 0 0 0
7 3 0 0 0 0
5 4 0 0 0 0
12 4 0 0 0 0
13 4 0 0 0 0
14 5 0 0 0 0
15 5 0 0 0 0
5 16 0 0 0 0
M END
$$$$
tert-butylamine-cation.sdf
COSMOtherm 3D 0
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[illegible]

URL: <http://mc.manuscriptcentral.com/tandf/tmph>

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30 10 0 0 0 0
31 11 0 0 0 0
11 32 0 0 0 0
M END
$$$$
tetrahydrozoline-cation2.sdf
COSMOTHERM 3D 0

32 34 0 0 0 0 0 0 0 0 0 V2000
3.0694 -0.1025 1.8534 C 0 0 0 0 0 0 0 0 0 1
1.8934 0.4494 2.3770 C 0 0 0 0 0 0 0 0 0 2
0.8030 0.6650 1.5338 C 0 0 0 0 0 0 0 0 0 3
0.8571 0.3274 0.1688 C 0 0 0 0 0 0 0 0 0 4
2.0450 -0.2126 -0.3655 C 0 0 0 0 0 0 0 0 0 5
3.1374 -0.4210 0.4965 C 0 0 0 0 0 0 0 0 0 6
-0.3517 0.6267 -0.7219 C 0 0 0 0 0 0 0 0 0 7
-0.2533 -0.0070 -2.1376 C 0 0 0 0 0 0 0 0 0 8
1.1541 0.1817 -2.7044 C 0 0 0 0 0 0 0 0 0 9
2.1724 -0.5603 -1.8354 C 0 0 0 0 0 0 0 0 0 10
-1.6462 0.1946 -0.0978 C 0 0 0 0 0 0 0 0 0 11
-3.2183 -1.0660 1.0572 C 0 0 0 0 0 0 0 0 0 12
-1.8425 -0.9620 0.5267 N 0 0 0 0 0 0 0 0 0 13
-2.7730 0.8919 -0.1682 N 0 0 0 0 0 0 0 0 0 14
-3.9225 0.1239 0.3550 C 0 0 0 0 0 0 0 0 0 15
-1.0827 -1.5723 0.8151 H 0 0 0 0 0 0 0 0 0 16
3.9327 -0.2733 2.4992 H 0 0 0 0 0 0 0 0 0 17
1.8289 0.7173 3.4328 H 0 0 0 0 0 0 0 0 0 18
-0.1080 1.1089 1.9437 H 0 0 0 0 0 0 0 0 0 19
4.0602 -0.8364 0.0837 H 0 0 0 0 0 0 0 0 0 20
-0.4192 1.7198 -0.8492 H 0 0 0 0 0 0 0 0 0 21
-0.4802 -1.0834 -2.0775 H 0 0 0 0 0 0 0 0 0 22
-1.0116 0.4518 -2.7874 H 0 0 0 0 0 0 0 0 0 23
1.4003 1.2558 -2.7454 H 0 0 0 0 0 0 0 0 0 24
1.1893 -0.1966 -3.7364 H 0 0 0 0 0 0 0 0 0 25
2.0298 -1.6486 -1.9611 H 0 0 0 0 0 0 0 0 0 26
3.1993 -0.3478 -2.1694 H 0 0 0 0 0 0 0 0 0 27
-3.6613 -2.0327 0.7962 H 0 0 0 0 0 0 0 0 0 28
-3.2014 -0.9579 2.1502 H 0 0 0 0 0 0 0 0 0 29
-4.5144 0.7355 1.0438 H 0 0 0 0 0 0 0 0 0 30
-4.5573 -0.2013 -0.4804 H 0 0 0 0 0 0 0 0 0 31
-2.8641 1.7593 -0.6899 H 0 0 0 0 0 0 0 0 0 32
2 1 0 0 0 0
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17 1 0 0 0 0
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31 15 0 0 0 0
14 32 0 0 0 0
M END
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tetrahydrozoline-cation3.sdf
COSMOTHERM 3D 0

32 34 0 0 0 0 0 0 0 0 0 V2000
3.0626 -0.1063 1.8598 C 0 0 0 0 0 0 0 0 0 1
1.8861 0.4472 2.3804 C 0 0 0 0 0 0 0 0 0 2
0.7984 0.6652 1.5343 C 0 0 0 0 0 0 0 0 0 3
0.8562 0.3285 0.1692 C 0 0 0 0 0 0 0 0 0 4
2.0447 -0.2127 -0.3623 C 0 0 0 0 0 0 0 0 0 5
3.1339 -0.4245 0.5030 C 0 0 0 0 0 0 0 0 0 6
-0.3508 0.6299 -0.7237 C 0 0 0 0 0 0 0 0 0 7
-0.2487 -0.0005 -2.1405 C 0 0 0 0 0 0 0 0 0 8
1.1607 0.1875 -2.7025 C 0 0 0 0 0 0 0 0 0 9
2.1754 -0.5583 -1.8324 C 0 0 0 0 0 0 0 0 0 10
-1.6453 0.1947 -0.1014 C 0 0 0 0 0 0 0 0 0 11
-3.2195 -1.0820 1.0341 C 0 0 0 0 0 0 0 0 0 12
-1.8452 -0.9730 0.5012 N 0 0 0 0 0 0 0 0 0 13
-2.7673 0.9010 -0.1495 N 0 0 0 0 0 0 0 0 0 14
-3.9185 0.1327 0.3693 C 0 0 0 0 0 0 0 0 0 15
-1.0885 -1.5967 0.7685 H 0 0 0 0 0 0 0 0 0 16
3.9234 -0.2799 2.5081 H 0 0 0 0 0 0 0 0 0 17
1.8190 0.7144 3.4362 H 0 0 0 0 0 0 0 0 0 18
-0.1135 1.1094 1.9419 H 0 0 0 0 0 0 0 0 0 19
4.0573 -0.8407 0.0925 H 0 0 0 0 0 0 0 0 0 20
-0.4184 1.7232 -0.8480 H 0 0 0 0 0 0 0 0 0 21
-0.4772 -1.0768 -2.0840 H 0 0 0 0 0 0 0 0 0 22
-1.0046 0.4607 -2.7915 H 0 0 0 0 0 0 0 0 0 23
1.4087 1.2612 -2.7402 H 0 0 0 0 0 0 0 0 0 24
```

[illegible]

URL: <http://mc.manuscriptcentral.com/tandf/tmph>

URL: <http://mc.manuscriptcentral.com/tandf/tmph>


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-4.6405 -0.3750 0.1880 H 0 0 0 0 0 0 0 0 0 0 21
-2.9429 0.0612 -1.8378 H 0 0 0 0 0 0 0 0 0 0 22
-3.0446 -0.8739 1.9314 H 0 0 0 0 0 0 0 0 0 0 23
-3.0138 0.8877 2.1562 H 0 0 0 0 0 0 0 0 0 0 24
2 1 0 0 0 0
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13 1 0 0 0 0
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17 6 0 0 0 0
8 7 0 0 0 0
18 7 0 0 0 0
19 7 0 0 0 0
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12 8 0 0 0 0
10 9 0 0 0 0
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22 10 0 0 0 0
12 11 0 0 0 0
23 11 0 0 0 0
11 24 0 0 0 0
M END
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tolazoline_t_p1.sdf
COSMOtherm 3D 0
25 26 0 0 0 0 0 0 0 0 0 0 V2000
1.4254 0.5986 0.1393 H 0 0 0 0 0 0 0 0 0 0 1
0.2990 -1.6835 -1.2043 C 0 0 0 0 0 0 0 0 0 0 2
-0.5802 -1.0272 -0.3281 C 0 0 0 0 0 0 0 0 0 0 3
-0.8832 -1.6210 0.9079 C 0 0 0 0 0 0 0 0 0 0 4
-0.3144 -2.8482 1.2625 C 0 0 0 0 0 0 0 0 0 0 5
0.5654 -3.4948 0.3857 C 0 0 0 0 0 0 0 0 0 0 6
0.8707 -2.9106 -0.8482 C 0 0 0 0 0 0 0 0 0 0 7
-1.1898 0.3076 -0.7060 C 0 0 0 0 0 0 0 0 0 0 8
-0.3964 1.4923 -0.2423 C 0 0 0 0 0 0 0 0 0 0 9
0.8606 1.4435 0.1765 N 0 0 0 0 0 0 0 0 0 0 10
1.4036 2.7937 0.4314 C 0 0 0 0 0 0 0 0 0 0 11
0.1282 3.6745 0.3523 C 0 0 0 0 0 0 0 0 0 0 12
-0.8585 2.7361 -0.2235 N 0 0 0 0 0 0 0 0 0 0 13
0.5319 -1.2370 -2.1738 H 0 0 0 0 0 0 0 0 0 0 14
-1.5726 -1.1227 1.5932 H 0 0 0 0 0 0 0 0 0 0 15
-0.5614 -3.3018 2.2240 H 0 0 0 0 0 0 0 0 0 0 16
1.0076 -4.4534 0.6626 H 0 0 0 0 0 0 0 0 0 0 17
1.5500 -3.4124 -1.5395 H 0 0 0 0 0 0 0 0 0 0 18
-2.2081 0.4057 -0.3023 H 0 0 0 0 0 0 0 0 0 0 19
-1.2803 0.3958 -1.8006 H 0 0 0 0 0 0 0 0 0 0 20
2.1357 3.0476 -0.3465 H 0 0 0 0 0 0 0 0 0 0 21
1.8880 2.8346 1.4128 H 0 0 0 0 0 0 0 0 0 0 22
0.2573 4.5464 -0.2976 H 0 0 0 0 0 0 0 0 0 0 23
-0.2132 4.0066 1.3417 H 0 0 0 0 0 0 0 0 0 0 24
-1.8317 2.9751 -0.3909 H 0 0 0 0 0 0 0 0 0 0 25
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13 25 0 0 0 0
M END
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tri-n-butylamine-cation.sdf
COSMOtherm 3D 0
41 40 0 0 0 0 0 0 0 0 0 0 V2000
2.5400 0.8979 -0.2947 C 0 0 0 0 0 0 0 0 0 0 1
1.2514 1.0242 0.5103 C 0 0 0 0 0 0 0 0 0 0 2
0.0035 0.6792 -0.2860 N 0 0 0 0 0 0 0 0 0 0 3
-1.2428 1.0325 0.5090 C 0 0 0 0 0 0 0 0 0 0 4
-2.5326 0.9047 -0.2938 C 0 0 0 0 0 0 0 0 0 0 5
-0.0009 -0.7378 -0.8428 C 0 0 0 0 0 0 0 0 0 0 6
-0.0118 -1.8352 0.2123 C 0 0 0 0 0 0 0 0 0 0 7
3.7345 1.4642 0.4896 C 0 0 0 0 0 0 0 0 0 0 8
2.7430 -0.1547 -0.5450 H 0 0 0 0 0 0 0 0 0 0 9
2.4344 1.4459 -1.2463 H 0 0 0 0 0 0 0 0 0 0 10
1.1055 2.0606 0.8410 H 0 0 0 0 0 0 0 0 0 0 11
1.2509 0.3804 1.3979 H 0 0 0 0 0 0 0 0 0 0 12
-1.0936 2.0706 0.8332 H 0 0 0 0 0 0 0 0 0 0 13
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1
2
3      -1.2433    0.3942    1.4005 H    0    0    0    0    0    0    0    0    0    14
4      -2.7411   -0.1495   -0.5327 H    0    0    0    0    0    0    0    0    0    15
5      -3.7232    1.4858    0.4855 C    0    0    0    0    0    0    0    0    0    16
6      -2.4252    1.4420   -1.2512 H    0    0    0    0    0    0    0    0    0    17
7      0.8849   -0.8112   -1.4852 H    0    0    0    0    0    0    0    0    0    18
8     -0.8808   -0.8021   -1.4942 H    0    0    0    0    0    0    0    0    0    19
9     -0.9036   -1.7481    0.8523 H    0    0    0    0    0    0    0    0    0    20
10    0.8682   -1.7504    0.8687 H    0    0    0    0    0    0    0    0    0    21
11   -0.0071   -3.2215   -0.4544 C    0    0    0    0    0    0    0    0    0    22
12    5.0500    1.3537   -0.2880 C    0    0    0    0    0    0    0    0    0    23
13    3.5372    2.5200    0.7378 H    0    0    0    0    0    0    0    0    0    24
14    3.8253    0.9288    1.4491 H    0    0    0    0    0    0    0    0    0    25
15   -5.0414    1.3675   -0.2867 C    0    0    0    0    0    0    0    0    0    26
16   -3.5220    2.5445    0.7174 H    0    0    0    0    0    0    0    0    0    27
17   -3.8130    0.9649    1.4530 H    0    0    0    0    0    0    0    0    0    28
18   -0.0193   -4.3626    0.5671 C    0    0    0    0    0    0    0    0    0    29
19    0.8828   -3.3106   -1.0991 H    0    0    0    0    0    0    0    0    0    30
20   -0.8835   -3.3082   -1.1176 H    0    0    0    0    0    0    0    0    0    31
21    5.8876    1.7645    0.2938 H    0    0    0    0    0    0    0    0    0    32
22    5.2865    0.3043   -0.5223 H    0    0    0    0    0    0    0    0    0    33
23    4.9968    1.9067   -1.2381 H    0    0    0    0    0    0    0    0    0    34
24   -5.8754    1.7929    0.2898 H    0    0    0    0    0    0    0    0    0    35
25   -5.2834    0.3153   -0.5013 H    0    0    0    0    0    0    0    0    0    36
26   -4.9881    1.9032   -1.2467 H    0    0    0    0    0    0    0    0    0    37
27   -0.0146   -5.3410    0.0655 H    0    0    0    0    0    0    0    0    0    38
28   -0.9157   -4.3156    1.2043 H    0    0    0    0    0    0    0    0    0    39
29    0.8631   -4.3172    1.2238 H    0    0    0    0    0    0    0    0    0    40
30    0.0060    1.2978   -1.1098 H    0    0    0    0    0    0    0    0    0    41
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36 26 0 0 0 0
37 26 0 0 0 0
38 29 0 0 0 0
39 29 0 0 0 0
40 29 0 0 0 0
3 41 0 0 0 0

M END
\$\$\$\$
tri-n-butylamine.sdf
COSMOtherm 3D 0

40 39 0 0 0 0 0 0 0 0 0 V2000
2.5136 0.9254 -0.3024 C 0 0 0 0 0 0 0 0 0 0 0 1
1.2140 1.0053 0.5054 C 0 0 0 0 0 0 0 0 0 0 0 2
0.0024 0.6637 -0.2606 N 0 0 0 0 0 0 0 0 0 0 0 3
-1.2079 1.0109 0.5050 C 0 0 0 0 0 0 0 0 0 0 0 4
-2.5084 0.9300 -0.3013 C 0 0 0 0 0 0 0 0 0 0 0 5
-0.0008 -0.7166 -0.7866 C 0 0 0 0 0 0 0 0 0 0 0 6
-0.0050 -1.8720 0.2324 C 0 0 0 0 0 0 0 0 0 0 0 7
3.7093 1.5123 0.4605 C 0 0 0 0 0 0 0 0 0 0 0 8
2.7409 -0.1210 -0.5655 H 0 0 0 0 0 0 0 0 0 0 0 9
2.3764 1.4689 -1.2533 H 0 0 0 0 0 0 0 0 0 0 0 10
1.0832 2.0444 0.8509 H 0 0 0 0 0 0 0 0 0 0 0 11
1.3169 0.3865 1.4247 H 0 0 0 0 0 0 0 0 0 0 0 12
-1.0747 2.0512 0.8461 H 0 0 0 0 0 0 0 0 0 0 0 13
-1.3114 0.3961 1.4269 H 0 0 0 0 0 0 0 0 0 0 0 14
-2.7407 -0.1176 -0.5550 H 0 0 0 0 0 0 0 0 0 0 0 15
-3.7008 1.5292 0.4573 C 0 0 0 0 0 0 0 0 0 0 0 16
-2.3696 1.4646 -1.2570 H 0 0 0 0 0 0 0 0 0 0 0 17
0.8773 -0.8233 -1.4425 H 0 0 0 0 0 0 0 0 0 0 0 18
-0.8781 -0.8186 -1.4442 H 0 0 0 0 0 0 0 0 0 0 0 19
-0.8895 -1.7948 0.8874 H 0 0 0 0 0 0 0 0 0 0 0 20
0.8786 -1.8000 0.8892 H 0 0 0 0 0 0 0 0 0 0 0 21
-0.0084 -3.2432 -0.4571 C 0 0 0 0 0 0 0 0 0 0 0 22
5.0278 1.4028 -0.3138 C 0 0 0 0 0 0 0 0 0 0 0 23
3.5060 2.5713 0.6948 H 0 0 0 0 0 0 0 0 0 0 0 24
3.8101 0.9965 1.4309 H 0 0 0 0 0 0 0 0 0 0 0 25
-5.0214 1.4133 -0.3123 C 0 0 0 0 0 0 0 0 0 0 0 26
-3.4941 2.5905 0.6778 H 0 0 0 0 0 0 0 0 0 0 0 27
-3.8005 1.0259 1.4344 H 0 0 0 0 0 0 0 0 0 0 0 28
-0.0138 -4.4182 0.5268 C 0 0 0 0 0 0 0 0 0 0 0 29
0.8744 -3.3199 -1.1154 H 0 0 0 0 0 0 0 0 0 0 0 30
-0.8897 -3.3141 -1.1181 H 0 0 0 0 0 0 0 0 0 0 0 31

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5.8646 1.8356 0.2544 H 0 0 0 0 0 0 0 0 0 0 0 0 32
5.2763 0.3512 -0.5268 H 0 0 0 0 0 0 0 0 0 0 0 0 33
4.9675 1.9327 -1.2772 H 0 0 0 0 0 0 0 0 0 0 0 0 34
-5.8549 1.8593 0.2504 H 0 0 0 0 0 0 0 0 0 0 0 0 35
-5.2751 0.3595 -0.5077 H 0 0 0 0 0 0 0 0 0 0 0 0 36
-4.9606 1.9272 -1.2843 H 0 0 0 0 0 0 0 0 0 0 0 0 37
-0.0162 -5.3846 0.0005 H 0 0 0 0 0 0 0 0 0 0 0 0 38
-0.9034 -4.3881 1.1753 H 0 0 0 0 0 0 0 0 0 0 0 0 39
0.8741 -4.3943 1.1780 H 0 0 0 0 0 0 0 0 0 0 0 0 40
2 1 0 0 0 0
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33 23 0 0 0 0
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35 26 0 0 0 0
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37 26 0 0 0 0
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39 29 0 0 0 0
29 40 0 0 0 0
M END
$$$$
tri-n-propylamine-cation.sdf
COSMOtherm 3D 0
32 31 0 0 0 0 0 0 0 0 0 V2000
2.5484 0.6533 -0.4199 C 0 0 0 0 0 0 0 0 0 0 0 0 1
1.2587 0.9238 0.3471 C 0 0 0 0 0 0 0 0 0 0 0 0 2
0.0090 0.4560 -0.3800 N 0 0 0 0 0 0 0 0 0 0 0 0 3
-1.2339 0.9500 0.3415 C 0 0 0 0 0 0 0 0 0 0 0 0 4
-2.5288 0.6812 -0.4168 C 0 0 0 0 0 0 0 0 0 0 0 0 5
-0.0057 -1.0360 -0.6852 C 0 0 0 0 0 0 0 0 0 0 0 0 6
-0.0354 -1.9358 0.5438 C 0 0 0 0 0 0 0 0 0 0 0 0 7
3.7365 1.3336 0.2728 C 0 0 0 0 0 0 0 0 0 0 0 0 8
2.7397 -0.4273 -0.4902 H 0 0 0 0 0 0 0 0 0 0 0 0 9
2.4492 1.0355 -1.4487 H 0 0 0 0 0 0 0 0 0 0 0 0 10
1.1203 2.0028 0.4947 H 0 0 0 0 0 0 0 0 0 0 0 0 11
1.2541 0.4422 1.3321 H 0 0 0 0 0 0 0 0 0 0 0 0 12
-1.0825 2.0295 0.4713 H 0 0 0 0 0 0 0 0 0 0 0 0 13
-1.2321 0.4844 1.3344 H 0 0 0 0 0 0 0 0 0 0 0 0 14
-2.7319 -0.3984 -0.4684 H 0 0 0 0 0 0 0 0 0 0 0 0 15
-3.7069 1.3860 0.2686 C 0 0 0 0 0 0 0 0 0 0 0 0 16
-2.4294 1.0450 -1.4522 H 0 0 0 0 0 0 0 0 0 0 0 0 17
0.8834 -1.2276 -1.2977 H 0 0 0 0 0 0 0 0 0 0 0 0 18
-0.8813 -1.2047 -1.3233 H 0 0 0 0 0 0 0 0 0 0 0 0 19
-0.9290 -1.7288 1.1509 H 0 0 0 0 0 0 0 0 0 0 0 0 20
0.8401 -1.7456 1.1819 H 0 0 0 0 0 0 0 0 0 0 0 0 21
-0.0419 -3.4102 0.1167 C 0 0 0 0 0 0 0 0 0 0 0 0 22
4.6650 1.1343 -0.2789 H 0 0 0 0 0 0 0 0 0 0 0 0 23
3.5980 2.4235 0.3229 H 0 0 0 0 0 0 0 0 0 0 0 0 24
3.8671 0.9590 1.2990 H 0 0 0 0 0 0 0 0 0 0 0 0 25
-4.6398 1.1866 -0.2757 H 0 0 0 0 0 0 0 0 0 0 0 0 26
-3.5568 2.4751 0.2988 H 0 0 0 0 0 0 0 0 0 0 0 0 27
-3.8371 1.0310 1.3018 H 0 0 0 0 0 0 0 0 0 0 0 0 28
-0.0665 -4.0626 0.9997 H 0 0 0 0 0 0 0 0 0 0 0 0 29
0.8575 -3.6606 -0.4649 H 0 0 0 0 0 0 0 0 0 0 0 0 30
-0.9218 -3.6424 -0.5011 H 0 0 0 0 0 0 0 0 0 0 0 0 31
0.0162 0.9236 -1.2979 H 0 0 0 0 0 0 0 0 0 0 0 0 32
2 1 0 0 0 0
8 1 0 0 0 0
9 1 0 0 0 0
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13 4 0 0 0 0
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31 22 0 0 0 0
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M END
$$$$
tri-n-propylamine.sdf
COSMOtherm 3D 0

31 30 0 0 0 0 0 0 0 0 0 V2000
2.5169 0.6977 -0.4412 C 0 0 0 0 0 0 0 0 0 1
1.2164 0.9080 0.3413 C 0 0 0 0 0 0 0 0 0 2
0.0041 0.4473 -0.3581 N 0 0 0 0 0 0 0 0 0 3
-1.2046 0.9202 0.3396 C 0 0 0 0 0 0 0 0 0 4
-2.5076 0.7095 -0.4384 C 0 0 0 0 0 0 0 0 0 5
-0.0030 -1.0005 -0.6487 C 0 0 0 0 0 0 0 0 0 6
-0.0165 -1.9733 0.5472 C 0 0 0 0 0 0 0 0 0 7
3.7084 1.3811 0.2407 C 0 0 0 0 0 0 0 0 0 8
2.7318 -0.3774 -0.5472 H 0 0 0 0 0 0 0 0 0 9
2.3849 1.0966 -1.4606 H 0 0 0 0 0 0 0 0 0 10
1.0874 1.9896 0.5142 H 0 0 0 0 0 0 0 0 0 11
1.3208 0.4467 1.3491 H 0 0 0 0 0 0 0 0 0 12
-1.0696 2.0024 0.5033 H 0 0 0 0 0 0 0 0 0 13
-1.3095 0.4676 1.3514 H 0 0 0 0 0 0 0 0 0 14
-2.7294 -0.3653 -0.5320 H 0 0 0 0 0 0 0 0 0 15
-3.6935 1.4080 0.2379 C 0 0 0 0 0 0 0 0 0 16
-2.3751 1.0962 -1.4625 H 0 0 0 0 0 0 0 0 0 17
0.8766 -1.2189 -1.2740 H 0 0 0 0 0 0 0 0 0 18
-0.8775 -1.2083 -1.2847 H 0 0 0 0 0 0 0 0 0 19
-0.9031 -1.7856 1.1739 H 0 0 0 0 0 0 0 0 0 20
0.8624 -1.7942 1.1872 H 0 0 0 0 0 0 0 0 0 21
-0.0202 -3.4339 0.0808 C 0 0 0 0 0 0 0 0 0 22
4.6392 1.2074 -0.3184 H 0 0 0 0 0 0 0 0 0 23
3.5569 2.4694 0.3116 H 0 0 0 0 0 0 0 0 0 24
3.8565 0.9976 1.2624 H 0 0 0 0 0 0 0 0 0 25
-4.6268 1.2323 -0.3164 H 0 0 0 0 0 0 0 0 0 26
-3.5360 2.4963 0.2946 H 0 0 0 0 0 0 0 0 0 27
-3.8409 1.0383 1.2648 H 0 0 0 0 0 0 0 0 0 28
-0.0323 -4.1288 0.9335 H 0 0 0 0 0 0 0 0 0 29
0.8726 -3.6605 -0.5229 H 0 0 0 0 0 0 0 0 0 30
-0.9038 -3.6505 -0.5399 H 0 0 0 0 0 0 0 0 0 31
2 1 0 0 0 0
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9 1 0 0 0 0
10 1 0 0 0 0
3 2 0 0 0 0
11 2 0 0 0 0
12 2 0 0 0 0
4 3 0 0 0 0
6 3 0 0 0 0
5 4 0 0 0 0
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14 4 0 0 0 0
15 5 0 0 0 0
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17 5 0 0 0 0
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19 6 0 0 0 0
20 7 0 0 0 0
21 7 0 0 0 0
22 7 0 0 0 0
23 8 0 0 0 0
24 8 0 0 0 0
25 8 0 0 0 0
26 16 0 0 0 0
27 16 0 0 0 0
28 16 0 0 0 0
29 22 0 0 0 0
30 22 0 0 0 0
22 31 0 0 0 0
M END
$$$$
triethylamine-cation.sdf
COSMOtherm 3D 0

23 22 0 0 0 0 0 0 0 0 0 V2000
2.5323 0.5836 -0.2812 C 0 0 0 0 0 0 0 0 0 1
1.2514 0.7976 0.5080 C 0 0 0 0 0 0 0 0 0 2
0.0029 0.3797 -0.2523 N 0 0 0 0 0 0 0 0 0 3
-1.2432 0.8082 0.5058 C 0 0 0 0 0 0 0 0 0 4
-2.5254 0.5967 -0.2821 C 0 0 0 0 0 0 0 0 0 5
-0.0028 -1.0861 -0.6666 C 0 0 0 0 0 0 0 0 0 6
-0.0150 -2.0607 0.4971 C 0 0 0 0 0 0 0 0 0 7
3.3592 1.0347 0.2837 H 0 0 0 0 0 0 0 0 0 8
2.7717 -0.4776 -0.4267 H 0 0 0 0 0 0 0 0 0 9
2.4878 1.0792 -1.2616 H 0 0 0 0 0 0 0 0 0 10
1.1072 1.8604 0.7366 H 0 0 0 0 0 0 0 0 0 11
1.2469 0.2423 1.4527 H 0 0 0 0 0 0 0 0 0 12
-1.0932 1.8715 0.7287 H 0 0 0 0 0 0 0 0 0 13
-1.2416 0.2578 1.4533 H 0 0 0 0 0 0 0 0 0 14
-3.3495 1.0564 0.2798 H 0 0 0 0 0 0 0 0 0 15
-2.7707 -0.4640 -0.4207 H 0 0 0 0 0 0 0 0 0 16
-2.4781 1.0857 -1.2657 H 0 0 0 0 0 0 0 0 0 17
0.8820 -1.2227 -1.2981 H 0 0 0 0 0 0 0 0 0 18
-0.8820 -1.2127 -1.3082 H 0 0 0 0 0 0 0 0 0 19
-0.0159 -3.0769 0.0803 H 0 0 0 0 0 0 0 0 0 20
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-0.9124 -1.9604 1.1215 H 0 0 0 0 0 0 0 0 0 0 0 21
0.8739 -1.9675 1.1345 H 0 0 0 0 0 0 0 0 0 0 0 22
0.0061 0.9145 -1.1325 H 0 0 0 0 0 0 0 0 0 0 0 23
2 1 0 0 0 0
8 1 0 0 0 0
9 1 0 0 0 0
10 1 0 0 0 0
3 2 0 0 0 0
11 2 0 0 0 0
12 2 0 0 0 0
4 3 0 0 0 0
6 3 0 0 0 0
5 4 0 0 0 0
13 4 0 0 0 0
14 4 0 0 0 0
15 5 0 0 0 0
16 5 0 0 0 0
17 5 0 0 0 0
7 6 0 0 0 0
18 6 0 0 0 0
19 6 0 0 0 0
20 7 0 0 0 0
21 7 0 0 0 0
22 7 0 0 0 0
3 23 0 0 0 0
M END
$$$$
triethylamine.sdf
COSMOtherm 3D 0
22 21 0 0 0 0 0 0 0 0 0 0 V2000
-0.0001 -0.0001 0.0243 N 0 0 0 0 0 0 0 0 0 0 0 1
-0.6369 1.2532 -0.4228 C 0 0 0 0 0 0 0 0 0 0 0 2
-0.7665 -1.1783 -0.4235 C 0 0 0 0 0 0 0 0 0 0 0 3
1.4037 -0.0746 -0.4234 C 0 0 0 0 0 0 0 0 0 0 0 4
-0.9148 1.1903 -1.4994 H 0 0 0 0 0 0 0 0 0 0 0 5
-0.4968 -2.4300 0.4115 C 0 0 0 0 0 0 0 0 0 0 0 6
2.3538 0.7849 0.4115 C 0 0 0 0 0 0 0 0 0 0 0 7
-0.5718 -1.3877 -1.4997 H 0 0 0 0 0 0 0 0 0 0 0 8
-1.8573 1.6449 0.4112 C 0 0 0 0 0 0 0 0 0 0 0 9
0.1103 2.0558 -0.3439 H 0 0 0 0 0 0 0 0 0 0 0 10
1.7247 -1.1231 -0.3461 H 0 0 0 0 0 0 0 0 0 0 0 11
-1.8351 -0.9325 -0.3459 H 0 0 0 0 0 0 0 0 0 0 0 12
1.4877 0.1987 -1.4999 H 0 0 0 0 0 0 0 0 0 0 0 13
-1.1068 -3.2692 0.0448 H 0 0 0 0 0 0 0 0 0 0 0 14
-0.7513 -2.2513 1.4664 H 0 0 0 0 0 0 0 0 0 0 0 15
0.5566 -2.7427 0.3636 H 0 0 0 0 0 0 0 0 0 0 0 16
3.3855 0.6751 0.0444 H 0 0 0 0 0 0 0 0 0 0 0 17
2.3265 0.4752 1.4663 H 0 0 0 0 0 0 0 0 0 0 0 18
2.0990 1.8535 0.3631 H 0 0 0 0 0 0 0 0 0 0 0 19
-2.2781 2.5933 0.0446 H 0 0 0 0 0 0 0 0 0 0 0 20
-1.5763 1.7747 1.4664 H 0 0 0 0 0 0 0 0 0 0 0 21
-2.6548 0.8894 0.3615 H 0 0 0 0 0 0 0 0 0 0 0 22
2 1 0 0 0 0
3 1 0 0 0 0
4 1 0 0 0 0
5 2 0 0 0 0
9 2 0 0 0 0
10 2 0 0 0 0
6 3 0 0 0 0
8 3 0 0 0 0
12 3 0 0 0 0
7 4 0 0 0 0
11 4 0 0 0 0
13 4 0 0 0 0
14 6 0 0 0 0
15 6 0 0 0 0
16 6 0 0 0 0
17 7 0 0 0 0
18 7 0 0 0 0
19 7 0 0 0 0
20 9 0 0 0 0
21 9 0 0 0 0
9 22 0 0 0 0
M END
$$$$
trimethylamine-cation.sdf
COSMOtherm 3D 0
14 13 0 0 0 0 0 0 0 0 0 0 V2000
0.3748 1.3828 -0.1133 C 0 0 0 0 0 0 0 0 0 0 0 1
0.0000 0.0000 0.3347 N 0 0 0 0 0 0 0 0 0 0 0 2
1.0104 -1.0159 -0.1133 C 0 0 0 0 0 0 0 0 0 0 0 3
-1.3851 -0.3669 -0.1133 C 0 0 0 0 0 0 0 0 0 0 0 4
-0.3648 2.0884 0.2768 H 0 0 0 0 0 0 0 0 0 0 0 5
1.3696 1.6183 0.2770 H 0 0 0 0 0 0 0 0 0 0 0 6
0.3792 1.3986 -1.2082 H 0 0 0 0 0 0 0 0 0 0 0 7
0.7150 -1.9959 0.2733 H 0 0 0 0 0 0 0 0 0 0 0 8
1.9905 -0.7304 0.2806 H 0 0 0 0 0 0 0 0 0 0 0 9
1.0251 -1.0245 -1.2081 H 0 0 0 0 0 0 0 0 0 0 0 10
-1.6259 -1.3607 0.2758 H 0 0 0 0 0 0 0 0 0 0 0 11
-2.0868 0.3760 0.2781 H 0 0 0 0 0 0 0 0 0 0 0 12
-1.4013 -0.3699 -1.2083 H 0 0 0 0 0 0 0 0 0 0 0 13
0.0001 0.0001 1.3628 H 0 0 0 0 0 0 0 0 0 0 0 14
2 1 0 0 0 0
5 1 0 0 0 0
6 1 0 0 0 0
7 1 0 0 0 0
3 2 0 0 0 0
4 2 0 0 0 0
8 3 0 0 0 0
9 3 0 0 0 0
10 3 0 0 0 0
11 4 0 0 0 0
12 4 0 0 0 0
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13 4 0 0 0 0
2 14 0 0 0 0
M END
$$$$
trimethylamine.sdf
COSMOtherm 3D 0

13 12 0 0 0 0 0 0 0 0 V2000
0.7878 1.1467 -0.0906 C 0 0 0 0 0 0 0 0 0 0 0 1
0.0000 0.0000 0.3668 N 0 0 0 0 0 0 0 0 0 0 0 2
0.5992 -1.2556 -0.0906 C 0 0 0 0 0 0 0 0 0 0 0 3
-1.3871 0.1089 -0.0906 C 0 0 0 0 0 0 0 0 0 0 0 4
0.3467 2.0787 0.2909 H 0 0 0 0 0 0 0 0 0 0 0 5
1.8162 1.0688 0.2906 H 0 0 0 0 0 0 0 0 0 0 0 6
0.8350 1.2152 -1.2013 H 0 0 0 0 0 0 0 0 0 0 0 7
0.0177 -2.1073 0.2905 H 0 0 0 0 0 0 0 0 0 0 0 8
1.6270 -1.3393 0.2908 H 0 0 0 0 0 0 0 0 0 0 0 9
0.6352 -1.3306 -1.2010 H 0 0 0 0 0 0 0 0 0 0 0 10
-1.9736 -0.7393 0.2908 H 0 0 0 0 0 0 0 0 0 0 0 11
-1.8338 1.0385 0.2904 H 0 0 0 0 0 0 0 0 0 0 0 12
-1.4700 0.1152 -1.2010 H 0 0 0 0 0 0 0 0 0 0 0 13
2 1 0 0 0 0
5 1 0 0 0 0
6 1 0 0 0 0
7 1 0 0 0 0
3 2 0 0 0 0
4 2 0 0 0 0
8 3 0 0 0 0
9 3 0 0 0 0
10 3 0 0 0 0
11 4 0 0 0 0
12 4 0 0 0 0
4 13 0 0 0 0
M END
$$$$
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S4 e) Mono-solvated Bases & Cations

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1,3-dihydro-1-methyl-5-phenyl-1,4-benzodiazepin-2-one.sdf
COSMOtherm 3D 0

36 37 0 0 0 0 0 0 0 0 V2000
-3.6952 1.7533 -0.3767 O 0 0 0 0 0 0 0 0 0 0 0 1
-2.8296 1.2610 -0.4899 H 0 0 0 0 0 0 0 0 0 0 0 2
-3.5129 2.4029 0.3236 H 0 0 0 0 0 0 0 0 0 0 0 3
-0.5794 -3.2399 1.7782 C 0 0 0 0 0 0 0 0 0 0 0 4
1.7270 -2.8586 0.0630 C 0 0 0 0 0 0 0 0 0 0 0 5
2.9816 -2.5173 -0.4357 C 0 0 0 0 0 0 0 0 0 0 0 6
3.2167 -1.2289 -0.9331 C 0 0 0 0 0 0 0 0 0 0 0 7
2.1913 -0.2898 -0.9046 C 0 0 0 0 0 0 0 0 0 0 0 8
0.9077 -0.6088 -0.4116 C 0 0 0 0 0 0 0 0 0 0 0 9
0.6730 -1.9257 0.0693 C 0 0 0 0 0 0 0 0 0 0 0 10
-0.1425 0.4362 -0.4108 C 0 0 0 0 0 0 0 0 0 0 0 11
-0.5751 -2.3205 0.6262 N 0 0 0 0 0 0 0 0 0 0 0 12
-1.3749 0.2083 -0.7507 N 0 0 0 0 0 0 0 0 0 0 0 13
-1.7290 -1.1397 -1.1920 C 0 0 0 0 0 0 0 0 0 0 0 14
-1.7887 -2.0718 0.0135 C 0 0 0 0 0 0 0 0 0 0 0 15
0.2259 1.8250 -0.0195 C 0 0 0 0 0 0 0 0 0 0 0 16
-0.3767 2.9240 -0.6610 C 0 0 0 0 0 0 0 0 0 0 0 17
1.1534 2.0616 1.0130 C 0 0 0 0 0 0 0 0 0 0 0 18
-0.0624 4.2281 -0.2740 C 0 0 0 0 0 0 0 0 0 0 0 19
1.4568 3.3677 1.4065 C 0 0 0 0 0 0 0 0 0 0 0 20
0.8527 4.4539 0.7625 C 0 0 0 0 0 0 0 0 0 0 0 21
-2.8462 -2.5506 0.4370 O 0 0 0 0 0 0 0 0 0 0 0 22
0.2970 -3.0346 2.4008 H 0 0 0 0 0 0 0 0 0 0 0 23
-1.4928 -3.0606 2.3545 H 0 0 0 0 0 0 0 0 0 0 0 24
-0.5692 -4.2920 1.4582 H 0 0 0 0 0 0 0 0 0 0 0 25
1.5537 -3.8666 0.4386 H 0 0 0 0 0 0 0 0 0 0 0 26
3.7767 -3.2644 -0.4435 H 0 0 0 0 0 0 0 0 0 0 0 27
4.1947 -0.9599 -1.3338 H 0 0 0 0 0 0 0 0 0 0 0 28
2.3696 0.7188 -1.2794 H 0 0 0 0 0 0 0 0 0 0 0 29
-1.0061 -1.5329 -1.9293 H 0 0 0 0 0 0 0 0 0 0 0 30
-2.7252 -1.1202 -1.6455 H 0 0 0 0 0 0 0 0 0 0 0 31
-1.0846 2.7462 -1.4712 H 0 0 0 0 0 0 0 0 0 0 0 32
1.6246 1.2198 1.5226 H 0 0 0 0 0 0 0 0 0 0 0 33
-0.5262 5.0724 -0.7871 H 0 0 0 0 0 0 0 0 0 0 0 34
2.1668 3.5374 2.2177 H 0 0 0 0 0 0 0 0 0 0 0 35
1.0970 5.4739 1.0643 H 0 0 0 0 0 0 0 0 0 0 0 36
2 1 0 0 0 0
3 1 0 0 0 0
12 4 0 0 0 0
23 4 0 0 0 0
24 4 0 0 0 0
25 4 0 0 0 0
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16 11 0 0 0 0
15 12 0 0 0 0
14 13 0 0 0 0
15 14 0 0 0 0
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30 14 0 0 0 0
31 14 0 0 0 0
22 15 0 0 0 0
17 16 0 0 0 0
18 16 0 0 0 0
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32 17 0 0 0 0
20 18 0 0 0 0
33 18 0 0 0 0
21 19 0 0 0 0
34 19 0 0 0 0
21 20 0 0 0 0
35 20 0 0 0 0
21 36 0 0 0 0
M END
$$$$
1,3-dihydro-1-methyl-5-phenyl-1,4-benzodiazepin-2-one.cation.sdf
COSMOTHERM 3D 0

37 38 0 0 0 0 0 0 0 0 0 V2000
-3.6426 -0.2738 -1.5991 O 0 0 0 0 0 0 0 0 0 0 1
-3.9990 -1.0038 -2.1372 H 0 0 0 0 0 0 0 0 0 0 2
-3.7093 0.5123 -2.1710 H 0 0 0 0 0 0 0 0 0 0 3
1.7804 0.0243 2.8210 C 0 0 0 0 0 0 0 0 0 0 4
-0.4914 1.7163 3.3295 C 0 0 0 0 0 0 0 0 0 0 5
-0.5268 0.5995 2.3641 N 0 0 0 0 0 0 0 0 0 0 6
-1.7559 0.0027 2.1552 C 0 0 0 0 0 0 0 0 0 0 7
-2.7842 0.3927 2.7070 O 0 0 0 0 0 0 0 0 0 0 8
-1.7474 -1.1599 1.1639 C 0 0 0 0 0 0 0 0 0 0 9
-1.3448 -0.6757 -0.1505 N 0 0 0 0 0 0 0 0 0 0 10
-0.1040 -0.3618 -0.4572 C 0 0 0 0 0 0 0 0 0 0 11
0.7040 0.0502 1.9165 C 0 0 0 0 0 0 0 0 0 0 12
0.9275 -0.3858 0.5737 C 0 0 0 0 0 0 0 0 0 0 13
3.0338 -0.4433 2.4370 C 0 0 0 0 0 0 0 0 0 0 14
3.2566 -0.8886 1.1270 C 0 0 0 0 0 0 0 0 0 0 15
2.2171 -0.8444 0.2098 C 0 0 0 0 0 0 0 0 0 0 16
0.2093 -0.0100 -1.8497 C 0 0 0 0 0 0 0 0 0 0 17
1.1430 1.0106 -2.1268 C 0 0 0 0 0 0 0 0 0 0 18
1.4075 1.3750 -3.4466 C 0 0 0 0 0 0 0 0 0 0 19
0.7622 0.7160 -4.5002 C 0 0 0 0 0 0 0 0 0 0 20
-0.1549 -0.3087 -4.2331 C 0 0 0 0 0 0 0 0 0 0 21
-0.4371 -0.6695 -2.9165 C 0 0 0 0 0 0 0 0 0 0 22
1.6255 0.3614 3.8448 H 0 0 0 0 0 0 0 0 0 0 23
-0.4523 1.3530 4.3659 H 0 0 0 0 0 0 0 0 0 0 24
0.3828 2.3389 3.1176 H 0 0 0 0 0 0 0 0 0 0 25
-1.4053 2.3044 3.1988 H 0 0 0 0 0 0 0 0 0 0 26
-2.7592 -1.5660 1.0910 H 0 0 0 0 0 0 0 0 0 0 27
-1.0581 -1.9492 1.4991 H 0 0 0 0 0 0 0 0 0 0 28
3.8411 -0.4679 3.1701 H 0 0 0 0 0 0 0 0 0 0 29
4.2346 -1.2650 0.8277 H 0 0 0 0 0 0 0 0 0 0 30
2.3774 -1.1928 -0.8102 H 0 0 0 0 0 0 0 0 0 0 31
1.6350 1.5348 -1.3072 H 0 0 0 0 0 0 0 0 0 0 32
2.1184 2.1758 -3.6540 H 0 0 0 0 0 0 0 0 0 0 33
0.9789 0.9965 -5.5321 H 0 0 0 0 0 0 0 0 0 0 34
-0.6429 -0.8351 -5.0543 H 0 0 0 0 0 0 0 0 0 0 35
-1.1272 -1.4892 -2.7141 H 0 0 0 0 0 0 0 0 0 0 36
-2.1280 -0.5262 -0.8408 H 0 0 0 0 0 0 0 0 0 0 37
2 1 0 0 0 0
3 1 0 0 0 0
12 4 0 0 0 0
14 4 0 0 0 0
23 4 0 0 0 0
6 5 0 0 0 0
24 5 0 0 0 0
25 5 0 0 0 0
26 5 0 0 0 0
7 6 0 0 0 0
12 6 0 0 0 0
8 7 0 0 0 0
9 7 0 0 0 0
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28 9 0 0 0 0
11 10 0 0 0 0
13 11 0 0 0 0
17 11 0 0 0 0
13 12 0 0 0 0
16 13 0 0 0 0
15 14 0 0 0 0
29 14 0 0 0 0
16 15 0 0 0 0
30 15 0 0 0 0
31 16 0 0 0 0
18 17 0 0 0 0
22 17 0 0 0 0
19 18 0 0 0 0
32 18 0 0 0 0
20 19 0 0 0 0
33 19 0 0 0 0
21 20 0 0 0 0
34 20 0 0 0 0
22 21 0 0 0 0
35 21 0 0 0 0
36 22 0 0 0 0
10 37 0 0 0 0
M END
$$$$
1,3-dihydro-3-hydroxy-1-methyl-5-phenyl-1,4-benzodiazepin-2-one.sdf
COSMOTHERM 3D 0

37 38 0 0 0 0 0 0 0 0 0 V2000
-3.6233 0.2305 -1.5383 O 0 0 0 0 0 0 0 0 0 0 1
-2.7994 -0.0815 -1.0710 H 0 0 0 0 0 0 0 0 0 0 2
-3.2911 0.7969 -2.2561 H 0 0 0 0 0 0 0 0 0 0 3
3.3277 -0.5131 2.1869 C 0 0 0 0 0 0 0 0 0 0 4
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1
2
3      3.4105   -1.0596   0.8997 C   0   0   0   0   0   0   0   0   0   0   5
4      2.3097   -0.9834   0.0526 C   0   0   0   0   0   0   0   0   0   0   6
5      1.0962   -0.3938   0.4676 C   0   0   0   0   0   0   0   0   0   0   7
6      1.0178   0.1366   1.7840 C   0   0   0   0   0   0   0   0   0   0   8
7      2.1462   0.0828   2.6214 C   0   0   0   0   0   0   0   0   0   0   9
8     -0.0426  -0.3433  -0.4804 C   0   0   0   0   0   0   0   0   0   0  10
9     -0.1506   0.7939   2.2704 N   0   0   0   0   0   0   0   0   0   0  11
10    -1.4075   0.2794   2.1192 C   0   0   0   0   0   0   0   0   0   0  12
11    -1.5243  -0.9866   1.2510 C   0   0   0   0   0   0   0   0   0   0  13
12    -1.2705  -0.5804  -0.1284 N   0   0   0   0   0   0   0   0   0   0  14
13     0.0037   1.9866   3.1258 C   0   0   0   0   0   0   0   0   0   0  15
14    -2.4264   0.7938   2.5996 O   0   0   0   0   0   0   0   0   0   0  16
15     0.2242  -0.0178  -1.9076 C   0   0   0   0   0   0   0   0   0   0  17
16    -0.5238  -0.6412  -2.9247 C   0   0   0   0   0   0   0   0   0   0  18
17     1.2002   0.9333  -2.2615 C   0   0   0   0   0   0   0   0   0   0  19
18     1.4106   1.2653  -3.6024 C   0   0   0   0   0   0   0   0   0   0  20
19     0.6633   0.6393  -4.6068 C   0   0   0   0   0   0   0   0   0   0  21
20    -0.3019  -0.3167  -4.2643 C   0   0   0   0   0   0   0   0   0   0  22
21     4.1846  -0.5582   2.8605 H   0   0   0   0   0   0   0   0   0   0  23
22     4.3304  -1.5360   0.5593 H   0   0   0   0   0   0   0   0   0   0  24
23     2.3709  -1.3968  -0.9545 H   0   0   0   0   0   0   0   0   0   0  25
24     2.0892   0.4976   3.6271 H   0   0   0   0   0   0   0   0   0   0  26
25    -0.7936  -1.7475   1.5774 H   0   0   0   0   0   0   0   0   0   0  27
26    -2.8171  -1.5249   1.3871 O   0   0   0   0   0   0   0   0   0   0  28
27     0.8871   2.5448   2.8000 H   0   0   0   0   0   0   0   0   0   0  29
28     0.1076   1.7093   4.1841 H   0   0   0   0   0   0   0   0   0   0  30
29    -0.8899   2.6079   3.0100 H   0   0   0   0   0   0   0   0   0   0  31
30    -1.2687  -1.3912  -2.6564 H   0   0   0   0   0   0   0   0   0   0  32
31     1.7831   1.4288  -1.4837 H   0   0   0   0   0   0   0   0   0   0  33
32     2.1602   2.0144  -3.8628 H   0   0   0   0   0   0   0   0   0   0  34
33     0.8352   0.8920  -5.6546 H   0   0   0   0   0   0   0   0   0   0  35
34    -0.8778  -0.8161  -5.0452 H   0   0   0   0   0   0   0   0   0   0  36
35    -3.3694  -0.7924   1.7471 H   0   0   0   0   0   0   0   0   0   0  37
36
37  2  1  0  0  0  0
38  3  1  0  0  0  0
39  5  4  0  0  0  0
40  9  4  0  0  0  0
41  23 4  0  0  0  0
42  6  5  0  0  0  0
43  24 5  0  0  0  0
44  7  6  0  0  0  0
45  25 6  0  0  0  0
46  8  7  0  0  0  0
47  10 7  0  0  0  0
48  9  8  0  0  0  0
49  11 8  0  0  0  0
50  26 9  0  0  0  0
51  14 10 0  0  0  0
52  17 10 0  0  0  0
53  12 11 0  0  0  0
54  15 11 0  0  0  0
55  13 12 0  0  0  0
56  16 12 0  0  0  0
57  14 13 0  0  0  0
58  27 13 0  0  0  0
59  28 13 0  0  0  0
60  29 15 0  0  0  0
61  30 15 0  0  0  0
62  31 15 0  0  0  0
63  18 17 0  0  0  0
64  19 17 0  0  0  0
65  22 18 0  0  0  0
66  32 18 0  0  0  0
67  20 19 0  0  0  0
68  33 19 0  0  0  0
69  21 20 0  0  0  0
70  34 20 0  0  0  0
71  22 21 0  0  0  0
72  35 21 0  0  0  0
73  36 22 0  0  0  0
74  28 37 0  0  0  0
75
76 M  END
77 $$$
78 1,3-dihydro-3-hydroxy-1-methyl-5-phenyl-1,4-benzodiazepin-2-one-cation.sdf
79 COSMOtherm 3D 0
80
81 38 39 0 0 0 0 0 0 0 0 V2000
82 -3.5131 0.2785 -1.3959 O 0 0 0 0 0 0 0 0 0 0 0 1
83 -4.0854 -0.4027 -1.7936 H 0 0 0 0 0 0 0 0 0 0 0 2
84 -3.4378 0.9697 -2.0788 H 0 0 0 0 0 0 0 0 0 0 0 3
85 3.3716 -0.5273 2.0958 C 0 0 0 0 0 0 0 0 0 0 0 4
86 3.4393 -1.0276 0.7888 C 0 0 0 0 0 0 0 0 0 0 0 5
87 2.3249 -0.9381 -0.0331 C 0 0 0 0 0 0 0 0 0 0 0 6
88 1.1096 -0.3781 0.4297 C 0 0 0 0 0 0 0 0 0 0 0 7
89 1.0449 0.1115 1.7710 C 0 0 0 0 0 0 0 0 0 0 0 8
90 2.1937 0.0399 2.5753 C 0 0 0 0 0 0 0 0 0 0 0 9
91 -0.0092 -0.3002 -0.5074 C 0 0 0 0 0 0 0 0 0 0 0 10
92 -0.1028 0.7595 2.3116 N 0 0 0 0 0 0 0 0 0 0 0 11
93 -1.3666 0.2522 2.2126 C 0 0 0 0 0 0 0 0 0 0 0 12
94 -1.5325 -0.9750 1.2934 C 0 0 0 0 0 0 0 0 0 0 0 13
95 -1.2352 -0.5101 -0.0783 N 0 0 0 0 0 0 0 0 0 0 0 14
96 0.0896 1.9253 3.2003 C 0 0 0 0 0 0 0 0 0 0 0 15
97 -2.3602 0.7338 2.7633 O 0 0 0 0 0 0 0 0 0 0 0 16
98 0.2024 -0.0024 -1.9302 C 0 0 0 0 0 0 0 0 0 0 0 17
99 -0.5868 -0.6345 -2.9146 C 0 0 0 0 0 0 0 0 0 0 0 18
100 1.1819 0.9354 -2.3193 C 0 0 0 0 0 0 0 0 0 0 0 19
101 1.3517 1.2472 -3.6677 C 0 0 0 0 0 0 0 0 0 0 0 20
102 0.5666 0.6145 -4.6392 C 0 0 0 0 0 0 0 0 0 0 0 21
103 -0.3977 -0.3287 -4.2611 C 0 0 0 0 0 0 0 0 0 0 0 22
104 4.2404 -0.5871 2.7522 H 0 0 0 0 0 0 0 0 0 0 0 23
105 4.3573 -1.4821 0.4166 H 0 0 0 0 0 0 0 0 0 0 0 24
106 2.3656 -1.3280 -1.0496 H 0 0 0 0 0 0 0 0 0 0 0 25
107 2.1566 0.4194 3.5952 H 0 0 0 0 0 0 0 0 0 0 0 26
108 -0.8079 -1.7649 1.5471 H 0 0 0 0 0 0 0 0 0 0 0 27
109 -2.8297 -1.4605 1.3682 O 0 0 0 0 0 0 0 0 0 0 0 28
```


[illegible]

```
12 11 0 0 0 0
14 11 0 0 0 0
13 12 0 0 0 0
20 13 0 0 0 0
22 13 0 0 0 0
28 13 0 0 0 0
15 14 0 0 0 0
16 14 0 0 0 0
17 15 0 0 0 0
29 15 0 0 0 0
19 16 0 0 0 0
30 16 0 0 0 0
18 17 0 0 0 0
31 17 0 0 0 0
19 18 0 0 0 0
32 18 0 0 0 0
33 19 0 0 0 0
21 20 0 0 0 0
22 34 0 0 0 0
M END
$$$$
1,3-dihydro-3-hydroxy-5-phenyl-1,4-benzodiazepin-2-one-cation.sdf
COSMOTHERM 3D 0
35 36 0 0 0 0 0 0 0 0 0 V2000
-3.4973 -0.4119 -1.2084 O 0 0 0 0 0 0 0 0 0 0 1
-3.3989 -1.0856 -1.9056 H 0 0 0 0 0 0 0 0 0 0 2
-4.0827 0.2639 -1.5958 H 0 0 0 0 0 0 0 0 0 0 3
3.4965 0.7857 0.9172 C 0 0 0 0 0 0 0 0 0 0 4
2.3507 0.8126 0.1363 C 0 0 0 0 0 0 0 0 0 0 5
1.1277 0.2646 0.5975 C 0 0 0 0 0 0 0 0 0 0 6
1.0944 -0.3119 1.9034 C 0 0 0 0 0 0 0 0 0 0 7
2.2749 -0.3739 2.6610 C 0 0 0 0 0 0 0 0 0 0 8
3.4600 0.1700 2.1776 C 0 0 0 0 0 0 0 0 0 0 9
-0.0502 -0.9207 2.4588 N 0 0 0 0 0 0 0 0 0 0 10
-0.0125 0.2391 -0.3143 C 0 0 0 0 0 0 0 0 0 0 11
-1.2399 0.3833 0.1408 N 0 0 0 0 0 0 0 0 0 0 12
-1.5522 0.7779 1.5306 C 0 0 0 0 0 0 0 0 0 0 13
0.1742 0.0403 -1.7592 C 0 0 0 0 0 0 0 0 0 0 14
-0.6355 0.7377 -2.6805 C 0 0 0 0 0 0 0 0 0 0 15
1.1441 -0.8681 -2.2324 C 0 0 0 0 0 0 0 0 0 0 16
-0.4749 0.5264 -4.0489 C 0 0 0 0 0 0 0 0 0 0 17
0.4798 -0.3881 -4.5113 C 0 0 0 0 0 0 0 0 0 0 18
1.2850 -1.0854 -3.6024 C 0 0 0 0 0 0 0 0 0 0 19
-1.3342 -0.4689 2.4100 C 0 0 0 0 0 0 0 0 0 0 20
-2.2832 -0.9984 2.9883 O 0 0 0 0 0 0 0 0 0 0 21
-2.8640 1.2172 1.6254 O 0 0 0 0 0 0 0 0 0 0 22
4.4197 1.2315 0.5473 H 0 0 0 0 0 0 0 0 0 0 23
2.3743 1.2792 -0.8480 H 0 0 0 0 0 0 0 0 0 0 24
2.2455 -0.8458 3.6442 H 0 0 0 0 0 0 0 0 0 0 25
4.3602 0.1234 2.7914 H 0 0 0 0 0 0 0 0 0 0 26
0.1195 -1.6699 3.1334 H 0 0 0 0 0 0 0 0 0 0 27
-0.8512 1.5792 1.8173 H 0 0 0 0 0 0 0 0 0 0 28
-1.3584 1.4723 -2.3240 H 0 0 0 0 0 0 0 0 0 0 29
1.7607 -1.4243 -1.5258 H 0 0 0 0 0 0 0 0 0 0 30
-1.0892 1.0834 -4.7575 H 0 0 0 0 0 0 0 0 0 0 31
0.6003 -0.5532 -5.5831 H 0 0 0 0 0 0 0 0 0 0 32
2.0245 -1.8020 -3.9622 H 0 0 0 0 0 0 0 0 0 0 33
-3.3647 0.4965 2.0764 H 0 0 0 0 0 0 0 0 0 0 34
-2.0802 0.1606 -0.4670 H 0 0 0 0 0 0 0 0 0 0 35
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
9 4 0 0 0 0
23 4 0 0 0 0
6 5 0 0 0 0
24 5 0 0 0 0
7 6 0 0 0 0
11 6 0 0 0 0
8 7 0 0 0 0
10 7 0 0 0 0
9 8 0 0 0 0
25 8 0 0 0 0
26 9 0 0 0 0
20 10 0 0 0 0
27 10 0 0 0 0
12 11 0 0 0 0
14 11 0 0 0 0
13 12 0 0 0 0
20 13 0 0 0 0
22 13 0 0 0 0
28 13 0 0 0 0
15 14 0 0 0 0
16 14 0 0 0 0
17 15 0 0 0 0
29 15 0 0 0 0
19 16 0 0 0 0
30 16 0 0 0 0
18 17 0 0 0 0
31 17 0 0 0 0
19 18 0 0 0 0
32 18 0 0 0 0
33 19 0 0 0 0
21 20 0 0 0 0
34 22 0 0 0 0
12 35 0 0 0 0
M END
$$$$
1,3-dihydro-5-phenyl-1,4-benzodiazepin-2-one.sdf
COSMOTHERM 3D 0
33 34 0 0 0 0 0 0 0 0 0 V2000
-1.7446 -3.6345 -0.1202 O 0 0 0 0 0 0 0 0 0 0 1
-1.1984 -2.8103 -0.2830 H 0 0 0 0 0 0 0 0 0 0 2
-2.4296 -3.3492 0.5085 H 0 0 0 0 0 0 0 0 0 0 3
```



```
1
2
3      3  1  0  0  0  0
4      5  4  0  0  0  0
5      9  4  0  0  0  0
6      22 4  0  0  0  0
7      6  5  0  0  0  0
8      23 5  0  0  0  0
9      7  6  0  0  0  0
10     24 6  0  0  0  0
11      8  7  0  0  0  0
12     10 7  0  0  0  0
13      9  8  0  0  0  0
14     11 8  0  0  0  0
15     25 9  0  0  0  0
16     14 10 0  0  0  0
17     16 10 0  0  0  0
18     12 11 0  0  0  0
19     33 11 0  0  0  0
20     13 12 0  0  0  0
21     15 12 0  0  0  0
22     14 13 0  0  0  0
23     26 13 0  0  0  0
24     32 13 0  0  0  0
25     17 16 0  0  0  0
26     18 16 0  0  0  0
27     21 17 0  0  0  0
28     27 17 0  0  0  0
29     19 18 0  0  0  0
30     28 18 0  0  0  0
31     20 19 0  0  0  0
32     29 19 0  0  0  0
33     21 20 0  0  0  0
34     30 20 0  0  0  0
35     31 21 0  0  0  0
36     14 34 0  0  0  0
37
38 M   END
39 $$$
40 1-methylindole-cation0.sdf
41 COSMOtherm      3D      0
42
43 23 23  0  0  0  0  0  0  0  0  0  0 V2000
44 1.2462  0.2039 -0.6915 O  0  0  0  0  0  0  0  0  0  0  0  1
45 0.3770 -0.2263 -0.5874 H  0  0  0  0  0  0  0  0  0  0  0  2
46 1.0583  1.1596 -0.6363 H  0  0  0  0  0  0  0  0  0  0  0  3
47 4.8260 -3.2872 -1.1738 C  0  0  0  0  0  0  0  0  0  0  0  4
48 6.0932 -2.6874 -1.2319 C  0  0  0  0  0  0  0  0  0  0  0  5
49 6.3569 -1.4766 -0.5788 C  0  0  0  0  0  0  0  0  0  0  0  6
50 5.3180 -0.8746  0.1400 C  0  0  0  0  0  0  0  0  0  0  0  7
51 4.0610 -1.4991  0.1807 C  0  0  0  0  0  0  0  0  0  0  0  8
52 3.7739 -2.6928 -0.4576 C  0  0  0  0  0  0  0  0  0  0  0  9
53 3.1442 -0.6562  0.9727 N  0  0  0  0  0  0  0  0  0  0  0 10
54 5.2292  0.3579  0.9185 C  0  0  0  0  0  0  0  0  0  0  0 11
55 3.9832  0.4832  1.4056 C  0  0  0  0  0  0  0  0  0  0  0 12
56 2.4629 -1.3631  2.1189 C  0  0  0  0  0  0  0  0  0  0  0 13
57 4.6487 -4.2298 -1.6923 H  0  0  0  0  0  0  0  0  0  0  0 14
58 6.8884 -3.1749 -1.7976 H  0  0  0  0  0  0  0  0  0  0  0 15
59 7.3436 -1.0151 -0.6305 H  0  0  0  0  0  0  0  0  0  0  0 16
60 2.7898 -3.1597 -0.4153 H  0  0  0  0  0  0  0  0  0  0  0 17
61 6.0374  1.0665  1.0827 H  0  0  0  0  0  0  0  0  0  0  0 18
62 3.5164  1.2429  2.0240 H  0  0  0  0  0  0  0  0  0  0  0 19
63 2.3555 -0.2791  0.3144 H  0  0  0  0  0  0  0  0  0  0  0 20
64 1.8532 -2.1755  1.7116 H  0  0  0  0  0  0  0  0  0  0  0 21
65 1.8256 -0.6372  2.6333 H  0  0  0  0  0  0  0  0  0  0  0 22
66 3.2290 -1.7545  2.7951 H  0  0  0  0  0  0  0  0  0  0  0 23
67
68 2  1  0  0  0  0
69 3  1  0  0  0  0
70 5  4  0  0  0  0
71 9  4  0  0  0  0
72 14 4  0  0  0  0
73 6  5  0  0  0  0
74 15 5  0  0  0  0
75 7  6  0  0  0  0
76 16 6  0  0  0  0
77 8  7  0  0  0  0
78 11 7  0  0  0  0
79 9  8  0  0  0  0
80 10 8  0  0  0  0
81 17 9  0  0  0  0
82 12 10 0  0  0  0
83 13 10 0  0  0  0
84 20 10 0  0  0  0
85 12 11 0  0  0  0
86 18 11 0  0  0  0
87 19 12 0  0  0  0
88 21 13 0  0  0  0
89 22 13 0  0  0  0
90 13 23 0  0  0  0
91
92 M   END
93 $$$
94 1-methylindole-cation1.sdf
95 COSMOtherm      3D      0
96
97 23 23  0  0  0  0  0  0  0  0  0  0 V2000
98 0.4865 -0.1995  0.2488 O  0  0  0  0  0  0  0  0  0  0  0  1
99 0.1818 -0.8389 -0.4203 H  0  0  0  0  0  0  0  0  0  0  0  2
100 -0.1009 0.5679  0.1255 H  0  0  0  0  0  0  0  0  0  0  0  3
101 5.5162  4.4930  0.6148 C  0  0  0  0  0  0  0  0  0  0  0  4
102 6.1017  3.7036  1.6644 C  0  0  0  0  0  0  0  0  0  0  0  5
103 5.8064  2.3720  1.8021 C  0  0  0  0  0  0  0  0  0  0  0  6
104 4.8972  1.7814  0.8672 C  0  0  0  0  0  0  0  0  0  0  0  7
105 4.3160  2.6008 -0.1929 C  0  0  0  0  0  0  0  0  0  0  0  8
106 4.6338  3.9776 -0.3094 C  0  0  0  0  0  0  0  0  0  0  0  9
107 3.5029  1.8509 -0.9459 N  0  0  0  0  0  0  0  0  0  0  0 10
108 4.3950  0.5088  0.7232 C  0  0  0  0  0  0  0  0  0  0  0 11
109 3.4708  0.4917 -0.4231 C  0  0  0  0  0  0  0  0  0  0  0 12
110 2.7162  2.2989 -2.0908 C  0  0  0  0  0  0  0  0  0  0  0 13
```

[illegible]

```
1
2
3      -1.4299    2.6039    1.1771 H    0    0    0    0    0    0    0    0    0    0    15
4      -0.1795    2.6583    2.4475 H    0    0    0    0    0    0    0    0    0    0    16
5       1.8080   -1.6064    1.4104 H    0    0    0    0    0    0    0    0    0    0    17
6       1.1478   -2.3669   -1.4655 H    0    0    0    0    0    0    0    0    0    0    18
7      -0.0074   -1.5034   -3.4946 H    0    0    0    0    0    0    0    0    0    0    19
8      -1.1382    0.7072   -3.4764 H    0    0    0    0    0    0    0    0    0    0    20
9      -1.1437    2.1275   -1.4299 H    0    0    0    0    0    0    0    0    0    0    21
10     1.1161    0.6349    2.7841 H    0    0    0    0    0    0    0    0    0    0    22
11
12     2  1  0  0  0  0
13     3  1  0  0  0  0
14     4  0  0  0  0  0
15     4  0  0  0  0  0
16     4  0  0  0  0  0
17     6  5  0  0  0  0
18     12  5  0  0  0  0
19     17  5  0  0  0  0
20     7  6  0  0  0  0
21     11  6  0  0  0  0
22     8  7  0  0  0  0
23     18  7  0  0  0  0
24     9  8  0  0  0  0
25     19  8  0  0  0  0
26     10  9  0  0  0  0
27     20  9  0  0  0  0
28     11  10  0  0  0  0
29     21  10  0  0  0  0
30     13  11  0  0  0  0
31     13  12  0  0  0  0
32     12  22  0  0  0  0
33
34 M  END
35 $$$$
36 1-methylpyrrole-cation0.sdf
37 COSMOtherm 3D 0
38
39 17 16 0 0 0 0 0 0 0 0 0 V2000
40 -2.4045 -0.0292 1.1089 O 0 0 0 0 0 0 0 0 0 0 0 0 1
41 -3.1849 -0.4535 0.7060 H 0 0 0 0 0 0 0 0 0 0 0 0 2
42 -2.7165 0.8473 1.4020 H 0 0 0 0 0 0 0 0 0 0 0 0 3
43 1.6966 0.7229 0.5710 C 0 0 0 0 0 0 0 0 0 0 0 0 4
44 1.6886 -0.7392 0.5668 C 0 0 0 0 0 0 0 0 0 0 0 0 5
45 0.5706 1.1641 -0.0205 C 0 0 0 0 0 0 0 0 0 0 0 0 6
46 -0.2397 0.0053 -0.4126 N 0 0 0 0 0 0 0 0 0 0 0 0 7
47 0.5586 -1.1641 -0.0289 C 0 0 0 0 0 0 0 0 0 0 0 0 8
48 2.4825 1.3490 0.9850 H 0 0 0 0 0 0 0 0 0 0 0 0 9
49 2.4677 -1.3764 0.9765 H 0 0 0 0 0 0 0 0 0 0 0 0 10
50 0.1861 2.1575 -0.2252 H 0 0 0 0 0 0 0 0 0 0 0 0 11
51 -0.6851 0.0132 -1.8547 C 0 0 0 0 0 0 0 0 0 0 0 0 12
52 0.1626 -2.1517 -0.2384 H 0 0 0 0 0 0 0 0 0 0 0 0 13
53 -1.1569 0.0085 0.2062 H 0 0 0 0 0 0 0 0 0 0 0 0 14
54 -1.2863 -0.8839 -2.0314 H 0 0 0 0 0 0 0 0 0 0 0 0 15
55 0.2015 0.0173 -2.4960 H 0 0 0 0 0 0 0 0 0 0 0 0 16
56 -1.2874 0.9114 -2.0205 H 0 0 0 0 0 0 0 0 0 0 0 0 17
57
58 2  1  0  0  0  0
59 3  1  0  0  0  0
60 5  4  0  0  0  0
61 6  4  0  0  0  0
62 9  4  0  0  0  0
63 8  5  0  0  0  0
64 10  5  0  0  0  0
65 7  6  0  0  0  0
66 11  6  0  0  0  0
67 8  7  0  0  0  0
68 12  7  0  0  0  0
69 14  7  0  0  0  0
70 13  8  0  0  0  0
71 15  12  0  0  0  0
72 16  12  0  0  0  0
73 12  17  0  0  0  0
74
75 M  END
76 $$$$
77 1-methylpyrrole-cation1.sdf
78 COSMOtherm 3D 0
79
80 17 16 0 0 0 0 0 0 0 0 0 V2000
81 -3.3810 -0.0118 0.5310 O 0 0 0 0 0 0 0 0 0 0 0 0 1
82 -3.7804 -0.7405 0.0228 H 0 0 0 0 0 0 0 0 0 0 0 0 2
83 -3.7953 0.7876 0.1592 H 0 0 0 0 0 0 0 0 0 0 0 0 3
84 2.0049 -0.0064 0.9686 C 0 0 0 0 0 0 0 0 0 0 0 0 4
85 0.7705 0.0055 1.5375 C 0 0 0 0 0 0 0 0 0 0 0 0 5
86 1.8562 -0.0088 -0.5085 C 0 0 0 0 0 0 0 0 0 0 0 0 6
87 0.4025 0.0026 -0.6969 N 0 0 0 0 0 0 0 0 0 0 0 0 7
88 -0.1983 0.0121 0.4714 C 0 0 0 0 0 0 0 0 0 0 0 0 8
89 -0.2347 0.0055 -2.0113 C 0 0 0 0 0 0 0 0 0 0 0 0 9
90 2.9698 -0.0136 1.4699 H 0 0 0 0 0 0 0 0 0 0 0 0 10
91 0.5191 0.0108 2.5940 H 0 0 0 0 0 0 0 0 0 0 0 0 11
92 -1.2939 0.0193 0.5412 H 0 0 0 0 0 0 0 0 0 0 0 0 12
93 2.2919 -0.9017 -0.9866 H 0 0 0 0 0 0 0 0 0 0 0 0 13
94 2.3073 0.8739 -0.9916 H 0 0 0 0 0 0 0 0 0 0 0 0 14
95 0.0545 -0.8999 -2.5594 H 0 0 0 0 0 0 0 0 0 0 0 0 15
96 0.0901 0.8913 -2.5715 H 0 0 0 0 0 0 0 0 0 0 0 0 16
97 -1.3204 0.0287 -1.8764 H 0 0 0 0 0 0 0 0 0 0 0 0 17
98
99 2  1  0  0  0  0
100 3  1  0  0  0  0
101 5  4  0  0  0  0
102 6  4  0  0  0  0
103 10  4  0  0  0  0
104 8  5  0  0  0  0
105 11  5  0  0  0  0
106 7  6  0  0  0  0
107 13  6  0  0  0  0
108 14  6  0  0  0  0
109 8  7  0  0  0  0
110 9  7  0  0  0  0
111 12  8  0  0  0  0
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```
15 9 0 0 0 0
16 9 0 0 0 0
9 17 0 0 0 0
M END
$$$$
1-methylpyrrole-cation2.sdf
COSMOtherm 3D 0

17 16 0 0 0 0 0 0 0 0 0 V2000
-3.3699 0.0024 0.5250 O 0 0 0 0 0 0 0 0 0 0 1
-3.7638 -0.8037 0.1459 H 0 0 0 0 0 0 0 0 0 0 2
-3.7876 0.7257 0.0241 H 0 0 0 0 0 0 0 0 0 0 3
0.8005 0.0031 1.5424 C 0 0 0 0 0 0 0 0 0 0 4
2.0981 -0.0023 0.7987 C 0 0 0 0 0 0 0 0 0 0 5
-0.2105 0.0040 0.4647 C 0 0 0 0 0 0 0 0 0 0 6
0.4030 0.0007 -0.6912 N 0 0 0 0 0 0 0 0 0 0 7
1.8265 -0.0037 -0.5181 C 0 0 0 0 0 0 0 0 0 0 8
0.6689 -0.8704 2.2073 H 0 0 0 0 0 0 0 0 0 0 9
0.6738 0.8803 2.2034 H 0 0 0 0 0 0 0 0 0 0 10
-0.2337 0.0007 -2.0117 C 0 0 0 0 0 0 0 0 0 0 11
3.0819 -0.0049 1.2582 H 0 0 0 0 0 0 0 0 0 0 12
-1.3052 0.0086 0.5382 H 0 0 0 0 0 0 0 0 0 0 13
2.4651 -0.0072 -1.3957 H 0 0 0 0 0 0 0 0 0 0 14
0.0866 0.8948 -2.5596 H 0 0 0 0 0 0 0 0 0 0 15
-1.3195 0.0049 -1.8813 H 0 0 0 0 0 0 0 0 0 0 16
0.0801 -0.8976 -2.5565 H 0 0 0 0 0 0 0 0 0 0 17
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
9 4 0 0 0 0
10 4 0 0 0 0
8 5 0 0 0 0
12 5 0 0 0 0
7 6 0 0 0 0
13 6 0 0 0 0
8 7 0 0 0 0
11 7 0 0 0 0
14 8 0 0 0 0
15 11 0 0 0 0
16 11 0 0 0 0
11 17 0 0 0 0
M END
$$$$
1-methylpyrrole.sdf
COSMOtherm 3D 0

16 15 0 0 0 0 0 0 0 0 0 V2000
-2.7239 -1.1023 0.3805 O 0 0 0 0 0 0 0 0 0 0 1
-2.7295 -1.8131 -0.2846 H 0 0 0 0 0 0 0 0 0 0 2
-2.0259 -0.4877 0.0628 H 0 0 0 0 0 0 0 0 0 0 3
-0.3490 1.4611 0.4504 C 0 0 0 0 0 0 0 0 0 0 4
-0.6113 0.9852 -0.8716 C 0 0 0 0 0 0 0 0 0 0 5
0.7114 0.7190 0.9498 C 0 0 0 0 0 0 0 0 0 0 6
1.1044 -0.1792 -0.0203 N 0 0 0 0 0 0 0 0 0 0 7
0.3031 -0.0308 -1.1295 C 0 0 0 0 0 0 0 0 0 0 8
2.1284 -1.2082 0.1476 C 0 0 0 0 0 0 0 0 0 0 9
-0.8666 2.2622 0.9712 H 0 0 0 0 0 0 0 0 0 0 10
-1.3526 1.3656 -1.5698 H 0 0 0 0 0 0 0 0 0 0 11
1.2181 0.7528 1.9095 H 0 0 0 0 0 0 0 0 0 0 12
0.4524 -0.6492 -2.0095 H 0 0 0 0 0 0 0 0 0 0 13
1.6956 -2.1322 0.5565 H 0 0 0 0 0 0 0 0 0 0 14
2.9027 -0.8411 0.8312 H 0 0 0 0 0 0 0 0 0 0 15
2.5874 -1.4255 -0.8242 H 0 0 0 0 0 0 0 0 0 0 16
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
10 4 0 0 0 0
8 5 0 0 0 0
11 5 0 0 0 0
7 6 0 0 0 0
12 6 0 0 0 0
8 7 0 0 0 0
9 7 0 0 0 0
13 8 0 0 0 0
14 9 0 0 0 0
15 9 0 0 0 0
9 16 0 0 0 0
M END
$$$$
2,3-dihydro-1-methyl-5-phenyl-1,4-benzodiazepine_new.sdf
COSMOtherm 3D 0

37 38 0 0 0 0 0 0 0 0 0 V2000
-2.1123 -3.6017 -0.1734 O 0 0 0 0 0 0 0 0 0 0 1
-1.5060 -2.8126 -0.3282 H 0 0 0 0 0 0 0 0 0 0 2
-2.7501 -3.2898 0.4914 H 0 0 0 0 0 0 0 0 0 0 3
1.6521 3.7835 -1.4585 H 0 0 0 0 0 0 0 0 0 0 4
1.7763 2.8003 -1.0032 C 0 0 0 0 0 0 0 0 0 0 5
0.7185 1.8925 -0.9834 C 0 0 0 0 0 0 0 0 0 0 6
0.8461 0.6109 -0.4154 C 0 0 0 0 0 0 0 0 0 0 7
2.1004 0.2178 0.1578 C 0 0 0 0 0 0 0 0 0 0 8
3.1486 1.1683 0.1573 C 0 0 0 0 0 0 0 0 0 0 9
2.9903 2.4315 -0.4117 C 0 0 0 0 0 0 0 0 0 0 10
2.2528 -1.0166 0.8031 N 0 0 0 0 0 0 0 0 0 0 11
1.9693 -2.2759 0.0786 C 0 0 0 0 0 0 0 0 0 0 12
1.0021 -2.0936 -1.0797 C 0 0 0 0 0 0 0 0 0 0 13
-0.2860 -1.5513 -0.6456 N 0 0 0 0 0 0 0 0 0 0 14
-0.3397 -0.2816 -0.3848 C 0 0 0 0 0 0 0 0 0 0 15
-1.6660 0.3009 -0.0291 C 0 0 0 0 0 0 0 0 0 0 16
-2.8385 -0.1794 -0.6426 C 0 0 0 0 0 0 0 0 0 0 17
-4.0870 0.3364 -0.2885 C 0 0 0 0 0 0 0 0 0 0 18
-4.1845 1.3350 0.6891 C 0 0 0 0 0 0 0 0 0 0 19
-3.0249 1.8186 1.3063 C 0 0 0 0 0 0 0 0 0 0 20
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[illegible]

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23 5 0 0 0 0
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24 6 0 0 0 0
8 7 0 0 0 0
10 7 0 0 0 0
9 8 0 0 0 0
11 8 0 0 0 0
25 9 0 0 0 0
14 10 0 0 0 0
15 10 0 0 0 0
12 11 0 0 0 0
21 11 0 0 0 0
13 12 0 0 0 0
26 12 0 0 0 0
27 12 0 0 0 0
14 13 0 0 0 0
28 13 0 0 0 0
29 13 0 0 0 0
16 15 0 0 0 0
20 15 0 0 0 0
17 16 0 0 0 0
30 16 0 0 0 0
18 17 0 0 0 0
31 17 0 0 0 0
19 18 0 0 0 0
32 18 0 0 0 0
20 19 0 0 0 0
33 19 0 0 0 0
34 20 0 0 0 0
35 21 0 0 0 0
36 21 0 0 0 0
37 21 0 0 0 0
14 38 0 0 0 0
M END
$$$$
2-aminopyridine0.sdf
COSMOtherm 3D 0

16 15 0 0 0 0 0 0 0 0 0 V2000
-3.1787 0.7279 0.0496 O 0 0 0 0 0 0 0 0 0 0 1
-2.1731 0.7593 -0.0068 H 0 0 0 0 0 0 0 0 0 0 2
-3.3753 0.8918 0.9883 H 0 0 0 0 0 0 0 0 0 0 3
0.5287 1.4578 -0.0791 C 0 0 0 0 0 0 0 0 0 0 4
1.8899 1.1872 0.0067 C 0 0 0 0 0 0 0 0 0 0 5
2.2841 -0.1601 0.0871 C 0 0 0 0 0 0 0 0 0 0 6
1.3253 -1.1622 0.0709 C 0 0 0 0 0 0 0 0 0 0 7
-0.0400 -0.7970 -0.0276 C 0 0 0 0 0 0 0 0 0 0 8
-0.4227 0.5014 -0.0968 N 0 0 0 0 0 0 0 0 0 0 9
-1.0349 -1.7410 -0.1125 N 0 0 0 0 0 0 0 0 0 0 10
-1.9868 -1.4145 0.0520 H 0 0 0 0 0 0 0 0 0 0 11
-0.8328 -2.6780 0.2235 H 0 0 0 0 0 0 0 0 0 0 12
0.1628 2.4860 -0.1362 H 0 0 0 0 0 0 0 0 0 0 13
2.6172 1.9980 0.0166 H 0 0 0 0 0 0 0 0 0 0 14
3.3408 -0.4223 0.1627 H 0 0 0 0 0 0 0 0 0 0 15
1.6050 -2.2147 0.1294 H 0 0 0 0 0 0 0 0 0 0 16

2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
9 4 0 0 0 0
13 4 0 0 0 0
6 5 0 0 0 0
14 5 0 0 0 0
7 6 0 0 0 0
15 6 0 0 0 0
8 7 0 0 0 0
9 8 0 0 0 0
10 8 0 0 0 0
11 10 0 0 0 0
12 10 0 0 0 0
7 16 0 0 0 0
M END
$$$$
2-aminopyridine1.sdf
COSMOtherm 3D 0

16 15 0 0 0 0 0 0 0 0 0 V2000
-3.2025 -0.1015 -0.7335 O 0 0 0 0 0 0 0 0 0 0 1
-2.1987 -0.0183 -0.7201 H 0 0 0 0 0 0 0 0 0 0 2
-3.5222 0.8162 -0.6877 H 0 0 0 0 0 0 0 0 0 0 3
0.4760 0.0355 -1.4565 C 0 0 0 0 0 0 0 0 0 0 4
1.8481 0.0020 -1.2339 C 0 0 0 0 0 0 0 0 0 0 5
2.2923 -0.0355 0.0995 C 0 0 0 0 0 0 0 0 0 0 6
1.3692 -0.0321 1.1346 C 0 0 0 0 0 0 0 0 0 0 7
-0.0109 0.0086 0.8171 C 0 0 0 0 0 0 0 0 0 0 8
-0.4418 0.0370 -0.4674 N 0 0 0 0 0 0 0 0 0 0 9
-0.9730 0.0721 1.7960 N 0 0 0 0 0 0 0 0 0 0 10
-1.9267 -0.1472 1.5124 H 0 0 0 0 0 0 0 0 0 0 11
-0.7209 -0.2316 2.7319 H 0 0 0 0 0 0 0 0 0 0 12
0.0728 0.0595 -2.4721 H 0 0 0 0 0 0 0 0 0 0 13
2.5462 0.0009 -2.0701 H 0 0 0 0 0 0 0 0 0 0 14
3.3597 -0.0688 0.3252 H 0 0 0 0 0 0 0 0 0 0 15
1.6877 -0.0595 2.1774 H 0 0 0 0 0 0 0 0 0 0 16

2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
9 4 0 0 0 0
13 4 0 0 0 0
6 5 0 0 0 0
14 5 0 0 0 0
7 6 0 0 0 0
15 6 0 0 0 0
8 7 0 0 0 0
9 8 0 0 0 0
10 8 0 0 0 0
11 10 0 0 0 0
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12 10 0 0 0 0
7 16 0 0 0 0
M END
$$$$
2-aminopyridine-cation.sdf
COSMOtherm 3D 0

17 16 0 0 0 0 0 0 0 0 V2000
-3.0795 -0.0051 0.6722 O 0 0 0 0 0 0 0 0 0 0 0 0 1
-3.5594 -0.7885 0.9976 H 0 0 0 0 0 0 0 0 0 0 0 0 2
-3.5735 0.7595 1.0201 H 0 0 0 0 0 0 0 0 0 0 0 0 3
0.7113 0.0038 1.4876 C 0 0 0 0 0 0 0 0 0 0 0 0 4
2.0190 -0.0010 1.0660 C 0 0 0 0 0 0 0 0 0 0 0 0 5
2.2734 -0.0047 -0.3254 C 0 0 0 0 0 0 0 0 0 0 0 0 6
1.2369 -0.0035 -1.2368 C 0 0 0 0 0 0 0 0 0 0 0 0 7
-0.1026 0.0022 -0.7715 C 0 0 0 0 0 0 0 0 0 0 0 0 8
-0.3051 0.0051 0.5813 N 0 0 0 0 0 0 0 0 0 0 0 0 9
-1.1776 0.0046 -1.5732 N 0 0 0 0 0 0 0 0 0 0 0 0 10
-1.0635 0.0035 -2.5807 H 0 0 0 0 0 0 0 0 0 0 0 0 11
-2.1197 0.0104 -1.1770 H 0 0 0 0 0 0 0 0 0 0 0 0 12
0.4070 0.0070 2.5321 H 0 0 0 0 0 0 0 0 0 0 0 0 13
2.8273 -0.0019 1.7937 H 0 0 0 0 0 0 0 0 0 0 0 0 14
3.3023 -0.0086 -0.6868 H 0 0 0 0 0 0 0 0 0 0 0 0 15
1.4199 -0.0056 -2.3104 H 0 0 0 0 0 0 0 0 0 0 0 0 16
-1.2979 0.0077 0.9044 H 0 0 0 0 0 0 0 0 0 0 0 0 17
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
9 4 0 0 0 0
13 4 0 0 0 0
6 5 0 0 0 0
14 5 0 0 0 0
7 6 0 0 0 0
15 6 0 0 0 0
8 7 0 0 0 0
16 7 0 0 0 0
9 8 0 0 0 0
10 8 0 0 0 0
11 10 0 0 0 0
12 10 0 0 0 0
9 17 0 0 0 0
M END
$$$$
2-aminothiazole.sdf
COSMOtherm 3D 0

13 12 0 0 0 0 0 0 0 0 V2000
-3.4875 -0.1000 -0.3146 O 0 0 0 0 0 0 0 0 0 0 0 0 1
-2.4920 -0.0241 -0.3843 H 0 0 0 0 0 0 0 0 0 0 0 0 2
-3.7896 0.8150 -0.1812 H 0 0 0 0 0 0 0 0 0 0 0 0 3
0.0548 0.0068 0.6698 C 0 0 0 0 0 0 0 0 0 0 0 0 4
-0.6821 0.0423 -0.4242 N 0 0 0 0 0 0 0 0 0 0 0 0 5
-0.4456 0.0741 1.9368 N 0 0 0 0 0 0 0 0 0 0 0 0 6
0.1078 0.0385 -1.5626 C 0 0 0 0 0 0 0 0 0 0 0 0 7
1.4550 -0.0012 -1.3671 C 0 0 0 0 0 0 0 0 0 0 0 0 8
1.8062 -0.0309 0.3574 S 0 0 0 0 0 0 0 0 0 0 0 0 9
-1.4377 -0.1368 2.0317 H 0 0 0 0 0 0 0 0 0 0 0 0 10
0.1296 -0.2666 2.7023 H 0 0 0 0 0 0 0 0 0 0 0 0 11
-0.3756 0.0612 -2.5381 H 0 0 0 0 0 0 0 0 0 0 0 0 12
2.2595 -0.0198 -2.0955 H 0 0 0 0 0 0 0 0 0 0 0 0 13
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
9 4 0 0 0 0
7 5 0 0 0 0
10 6 0 0 0 0
11 6 0 0 0 0
8 7 0 0 0 0
12 7 0 0 0 0
9 8 0 0 0 0
8 13 0 0 0 0
M END
$$$$
2-aminothiazole_p2.sdf
COSMOtherm 3D 0

14 13 0 0 0 0 0 0 0 0 V2000
-3.1994 -0.3561 0.0027 O 0 0 0 0 0 0 0 0 0 0 0 0 1
-3.7488 -0.5743 0.7775 H 0 0 0 0 0 0 0 0 0 0 0 0 2
-3.7547 -0.5677 -0.7697 H 0 0 0 0 0 0 0 0 0 0 0 0 3
-0.9849 1.5491 -0.0043 N 0 0 0 0 0 0 0 0 0 0 0 0 4
-0.1082 0.5497 -0.0007 C 0 0 0 0 0 0 0 0 0 0 0 0 5
-0.4631 -0.7497 -0.0019 N 0 0 0 0 0 0 0 0 0 0 0 0 6
0.5953 -1.6490 -0.0020 C 0 0 0 0 0 0 0 0 0 0 0 0 7
1.8044 -1.0476 0.0011 C 0 0 0 0 0 0 0 0 0 0 0 0 8
1.6370 0.7115 0.0015 S 0 0 0 0 0 0 0 0 0 0 0 0 9
-1.9853 1.3239 -0.0001 H 0 0 0 0 0 0 0 0 0 0 0 0 10
-0.6885 2.5192 0.0110 H 0 0 0 0 0 0 0 0 0 0 0 0 11
0.3823 -2.7138 -0.0048 H 0 0 0 0 0 0 0 0 0 0 0 0 12
2.7915 -1.4964 0.0015 H 0 0 0 0 0 0 0 0 0 0 0 0 13
-1.4731 -0.9963 -0.0029 H 0 0 0 0 0 0 0 0 0 0 0 0 14
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
10 4 0 0 0 0
11 4 0 0 0 0
6 5 0 0 0 0
9 5 0 0 0 0
7 6 0 0 0 0
8 7 0 0 0 0
12 7 0 0 0 0
9 8 0 0 0 0
13 8 0 0 0 0
6 14 0 0 0 0
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14 4 0 0 0 0
6 5 0 0 0 0
15 5 0 0 0 0
7 6 0 0 0 0
16 6 0 0 0 0
8 7 0 0 0 0
11 7 0 0 0 0
9 8 0 0 0 0
10 8 0 0 0 0
17 9 0 0 0 0
12 10 0 0 0 0
13 10 0 0 0 0
20 10 0 0 0 0
12 11 0 0 0 0
18 11 0 0 0 0
19 12 0 0 0 0
21 19 0 0 0 0
22 19 0 0 0 0
19 23 0 0 0 0
M END
$$$$
2-methylindole-cation1.sdf
COSMOtherm 3D 0
23 23 0 0 0 0 0 0 0 0 0 V2000
-3.0723 -0.1149 -2.1235 O 0 0 0 0 0 0 0 0 0 0 1
-3.0625 -0.8501 -2.7630 H 0 0 0 0 0 0 0 0 0 0 2
-3.1223 0.6891 -2.6716 H 0 0 0 0 0 0 0 0 0 0 3
2.3194 0.1988 -1.4919 C 0 0 0 0 0 0 0 0 0 0 4
3.0229 0.1156 -0.2375 C 0 0 0 0 0 0 0 0 0 0 5
2.3522 -0.0507 0.9446 C 0 0 0 0 0 0 0 0 0 0 6
0.9222 -0.1412 0.9016 C 0 0 0 0 0 0 0 0 0 0 7
0.2246 -0.0515 -0.3836 C 0 0 0 0 0 0 0 0 0 0 8
0.9495 0.1169 -1.5929 C 0 0 0 0 0 0 0 0 0 0 9
-1.0872 -0.1571 -0.1881 N 0 0 0 0 0 0 0 0 0 0 10
-0.0359 -0.3026 1.8698 C 0 0 0 0 0 0 0 0 0 0 11
-1.3790 -0.3367 1.2322 C 0 0 0 0 0 0 0 0 0 0 12
-1.8203 -0.1385 -0.9388 H 0 0 0 0 0 0 0 0 0 0 13
-2.4023 0.6799 1.7749 C 0 0 0 0 0 0 0 0 0 0 14
-1.7947 -1.3561 1.3699 H 0 0 0 0 0 0 0 0 0 0 15
2.9078 0.3312 -2.4014 H 0 0 0 0 0 0 0 0 0 0 16
4.1105 0.1881 -0.2472 H 0 0 0 0 0 0 0 0 0 0 17
2.8758 -0.1163 1.8986 H 0 0 0 0 0 0 0 0 0 0 18
0.4397 0.1824 -2.5536 H 0 0 0 0 0 0 0 0 0 0 19
0.1157 -0.4065 2.9423 H 0 0 0 0 0 0 0 0 0 0 20
-3.3503 0.5771 1.2331 H 0 0 0 0 0 0 0 0 0 0 21
-2.5821 0.4788 2.8380 H 0 0 0 0 0 0 0 0 0 0 22
-2.0252 1.7036 1.6592 H 0 0 0 0 0 0 0 0 0 0 23
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
9 4 0 0 0 0
16 4 0 0 0 0
6 5 0 0 0 0
17 5 0 0 0 0
7 6 0 0 0 0
18 6 0 0 0 0
8 7 0 0 0 0
11 7 0 0 0 0
9 8 0 0 0 0
10 8 0 0 0 0
19 9 0 0 0 0
12 10 0 0 0 0
13 10 0 0 0 0
12 11 0 0 0 0
20 11 0 0 0 0
14 12 0 0 0 0
15 12 0 0 0 0
21 14 0 0 0 0
22 14 0 0 0 0
14 23 0 0 0 0
M END
$$$$
2-methylindole-cation2.sdf
COSMOtherm 3D 0
23 23 0 0 0 0 0 0 0 0 0 V2000
-2.9036 0.0044 -2.2117 O 0 0 0 0 0 0 0 0 0 0 1
-2.8905 -0.7612 -2.8148 H 0 0 0 0 0 0 0 0 0 0 2
-2.8973 0.7848 -2.7956 H 0 0 0 0 0 0 0 0 0 0 3
2.4642 -0.0021 -1.3987 C 0 0 0 0 0 0 0 0 0 0 4
3.0703 0.0017 -0.1328 C 0 0 0 0 0 0 0 0 0 0 5
2.3038 0.0038 1.0439 C 0 0 0 0 0 0 0 0 0 0 6
0.9175 0.0016 0.9252 C 0 0 0 0 0 0 0 0 0 0 7
0.3337 -0.0019 -0.3526 C 0 0 0 0 0 0 0 0 0 0 8
1.0696 -0.0043 -1.5333 C 0 0 0 0 0 0 0 0 0 0 9
-1.0778 -0.0032 -0.1902 N 0 0 0 0 0 0 0 0 0 0 10
-0.1999 0.0020 1.9327 C 0 0 0 0 0 0 0 0 0 0 11
-1.4290 -0.0011 1.0740 C 0 0 0 0 0 0 0 0 0 0 12
-1.7652 -0.0034 -1.0007 H 0 0 0 0 0 0 0 0 0 0 13
-0.1999 0.8831 2.5963 H 0 0 0 0 0 0 0 0 0 0 14
-0.1976 -0.8769 2.5991 H 0 0 0 0 0 0 0 0 0 0 15
3.0865 -0.0039 -2.2944 H 0 0 0 0 0 0 0 0 0 0 16
4.1589 0.0030 -0.0615 H 0 0 0 0 0 0 0 0 0 0 17
2.7872 0.0063 2.0218 H 0 0 0 0 0 0 0 0 0 0 18
0.5911 -0.0070 -2.5129 H 0 0 0 0 0 0 0 0 0 0 19
-2.8284 -0.0030 1.5422 C 0 0 0 0 0 0 0 0 0 0 20
-3.0038 -0.8866 2.1751 H 0 0 0 0 0 0 0 0 0 0 21
-3.0058 0.8776 2.1785 H 0 0 0 0 0 0 0 0 0 0 22
-3.5405 -0.0026 0.7095 H 0 0 0 0 0 0 0 0 0 0 23
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
9 4 0 0 0 0
16 4 0 0 0 0
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6 5 0 0 0 0
17 5 0 0 0 0
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18 6 0 0 0 0
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19 9 0 0 0 0
12 10 0 0 0 0
13 10 0 0 0 0
12 11 0 0 0 0
14 11 0 0 0 0
15 11 0 0 0 0
20 12 0 0 0 0
21 20 0 0 0 0
22 20 0 0 0 0
20 23 0 0 0 0
M END
$$$$
2-methylindole.sdf
COSMOtherm 3D 0
22 22 0 0 0 0 0 0 0 0 0 V2000
-3.0510 -2.2527 0.0235 O 0 0 0 0 0 0 0 0 0 0 1
-2.9347 -2.9000 0.7422 H 0 0 0 0 0 0 0 0 0 0 2
-3.0829 -2.7954 -0.7848 H 0 0 0 0 0 0 0 0 0 0 3
2.3322 1.0011 0.0123 C 0 0 0 0 0 0 0 0 0 0 4
3.0682 -0.1851 0.0061 C 0 0 0 0 0 0 0 0 0 0 5
2.4261 -1.4445 -0.0072 C 0 0 0 0 0 0 0 0 0 0 6
1.0325 -1.5448 -0.0150 C 0 0 0 0 0 0 0 0 0 0 7
0.2940 -0.3536 -0.0086 C 0 0 0 0 0 0 0 0 0 0 8
0.9237 0.9348 0.0052 C 0 0 0 0 0 0 0 0 0 0 9
-0.1349 1.9060 0.0094 C 0 0 0 0 0 0 0 0 0 0 10
-1.3359 1.2151 -0.0018 C 0 0 0 0 0 0 0 0 0 0 11
-2.7379 1.7307 -0.0089 C 0 0 0 0 0 0 0 0 0 0 12
-1.0722 -0.1470 -0.0146 N 0 0 0 0 0 0 0 0 0 0 13
2.8416 1.9677 0.0227 H 0 0 0 0 0 0 0 0 0 0 14
4.1594 -0.1427 0.0111 H 0 0 0 0 0 0 0 0 0 0 15
3.0284 -2.3550 -0.0119 H 0 0 0 0 0 0 0 0 0 0 16
0.5380 -2.5181 -0.0256 H 0 0 0 0 0 0 0 0 0 0 17
-0.0326 2.9883 0.0192 H 0 0 0 0 0 0 0 0 0 0 18
-3.2702 1.4416 -0.9291 H 0 0 0 0 0 0 0 0 0 0 19
-3.3178 1.3380 0.8409 H 0 0 0 0 0 0 0 0 0 0 20
-2.7380 2.8260 0.0541 H 0 0 0 0 0 0 0 0 0 0 21
-1.7863 -0.8950 -0.0088 H 0 0 0 0 0 0 0 0 0 0 22
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
9 4 0 0 0 0
14 4 0 0 0 0
6 5 0 0 0 0
15 5 0 0 0 0
7 6 0 0 0 0
16 6 0 0 0 0
8 7 0 0 0 0
17 7 0 0 0 0
9 8 0 0 0 0
13 8 0 0 0 0
10 9 0 0 0 0
11 10 0 0 0 0
18 10 0 0 0 0
12 11 0 0 0 0
13 11 0 0 0 0
19 12 0 0 0 0
20 12 0 0 0 0
21 12 0 0 0 0
13 22 0 0 0 0
M END
$$$$
2-methylpyrrole-cation0.sdf
COSMOtherm 3D 0
17 16 0 0 0 0 0 0 0 0 0 V2000
-2.6590 0.4143 -0.4713 O 0 0 0 0 0 0 0 0 0 0 1
-3.2414 -0.0140 -1.1262 H 0 0 0 0 0 0 0 0 0 0 2
-2.6620 1.3602 -0.7096 H 0 0 0 0 0 0 0 0 0 0 3
1.6220 0.3213 -1.1109 C 0 0 0 0 0 0 0 0 0 0 4
1.5638 0.5509 0.3296 C 0 0 0 0 0 0 0 0 0 0 5
0.5606 -0.4194 -1.4817 C 0 0 0 0 0 0 0 0 0 0 6
-0.2539 -0.6730 -0.2889 N 0 0 0 0 0 0 0 0 0 0 7
0.4670 -0.0498 0.8432 C 0 0 0 0 0 0 0 0 0 0 8
2.3992 0.6882 -1.7762 H 0 0 0 0 0 0 0 0 0 0 9
2.2921 1.1172 0.9045 H 0 0 0 0 0 0 0 0 0 0 10
0.2238 -0.8114 -2.4350 H 0 0 0 0 0 0 0 0 0 0 11
-0.4149 -1.6815 -0.1393 H 0 0 0 0 0 0 0 0 0 0 12
-0.0925 -0.1596 2.2129 C 0 0 0 0 0 0 0 0 0 0 13
-1.2582 -0.2228 -0.4003 H 0 0 0 0 0 0 0 0 0 0 14
-0.1810 -1.2104 2.5299 H 0 0 0 0 0 0 0 0 0 0 15
0.5656 0.3601 2.9193 H 0 0 0 0 0 0 0 0 0 0 16
-1.0954 0.2905 2.2791 H 0 0 0 0 0 0 0 0 0 0 17
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
9 4 0 0 0 0
8 5 0 0 0 0
10 5 0 0 0 0
7 6 0 0 0 0
11 6 0 0 0 0
8 7 0 0 0 0
12 7 0 0 0 0
14 7 0 0 0 0
13 8 0 0 0 0
15 13 0 0 0 0
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16 13 0 0 0 0
13 17 0 0 0 0
M END
$$$$
2-methylpyrrole-cation1.sdf
COSMOtherm 3D 0
17 16 0 0 0 0 0 0 0 0 V2000
-3.0859 0.0803 -0.2013 O 0 0 0 0 0 0 0 0 0 0 0 0 1
-3.5024 -0.7927 -0.3217 H 0 0 0 0 0 0 0 0 0 0 0 0 2
-3.5248 0.6549 -0.8549 H 0 0 0 0 0 0 0 0 0 0 0 0 3
1.8722 0.2611 0.1714 C 0 0 0 0 0 0 0 0 0 0 0 0 4
1.7627 -0.1384 -1.1230 C 0 0 0 0 0 0 0 0 0 0 0 0 5
0.5127 0.4235 0.7644 C 0 0 0 0 0 0 0 0 0 0 0 0 6
-0.3591 0.0594 -0.3595 N 0 0 0 0 0 0 0 0 0 0 0 0 7
0.3546 -0.2502 -1.4110 C 0 0 0 0 0 0 0 0 0 0 0 0 8
-1.4170 0.0615 -0.3176 H 0 0 0 0 0 0 0 0 0 0 0 0 9
2.7865 0.4507 0.7292 H 0 0 0 0 0 0 0 0 0 0 0 0 10
2.5568 -0.3435 -1.8350 H 0 0 0 0 0 0 0 0 0 0 0 0 11
-0.1129 -0.5399 -2.3513 H 0 0 0 0 0 0 0 0 0 0 0 0 12
0.3365 1.4932 0.9857 H 0 0 0 0 0 0 0 0 0 0 0 0 13
0.2278 -0.4041 2.0290 C 0 0 0 0 0 0 0 0 0 0 0 0 14
0.9111 -0.0851 2.8253 H 0 0 0 0 0 0 0 0 0 0 0 0 15
0.3782 -1.4734 1.8339 H 0 0 0 0 0 0 0 0 0 0 0 0 16
-0.8028 -0.2362 2.3648 H 0 0 0 0 0 0 0 0 0 0 0 0 17
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
10 4 0 0 0 0
8 5 0 0 0 0
11 5 0 0 0 0
7 6 0 0 0 0
13 6 0 0 0 0
14 6 0 0 0 0
8 7 0 0 0 0
9 7 0 0 0 0
12 8 0 0 0 0
15 14 0 0 0 0
16 14 0 0 0 0
14 17 0 0 0 0
M END
$$$$
2-methylpyrrole-cation2.sdf
COSMOtherm 3D 0
17 16 0 0 0 0 0 0 0 0 V2000
-3.0247 0.0031 0.4992 O 0 0 0 0 0 0 0 0 0 0 0 0 1
-3.4819 -0.8048 0.2025 H 0 0 0 0 0 0 0 0 0 0 0 0 2
-3.5044 0.7350 0.0706 H 0 0 0 0 0 0 0 0 0 0 0 0 3
1.8678 -0.0030 -0.3720 C 0 0 0 0 0 0 0 0 0 0 0 0 4
1.8102 0.0004 1.1249 C 0 0 0 0 0 0 0 0 0 0 0 0 5
0.4315 -0.0012 -0.7768 C 0 0 0 0 0 0 0 0 0 0 0 0 6
-0.2929 0.0017 0.3181 N 0 0 0 0 0 0 0 0 0 0 0 0 7
0.5156 0.0030 1.4909 C 0 0 0 0 0 0 0 0 0 0 0 0 8
2.3956 0.8713 -0.7921 H 0 0 0 0 0 0 0 0 0 0 0 0 9
2.3912 -0.8822 -0.7875 H 0 0 0 0 0 0 0 0 0 0 0 0 10
-1.3514 0.0021 0.3395 H 0 0 0 0 0 0 0 0 0 0 0 0 11
2.6738 0.0001 1.7826 H 0 0 0 0 0 0 0 0 0 0 0 0 12
-0.1222 0.0002 -2.1461 C 0 0 0 0 0 0 0 0 0 0 0 0 13
0.0387 0.0051 2.4659 H 0 0 0 0 0 0 0 0 0 0 0 0 14
0.2162 0.9001 -2.6827 H 0 0 0 0 0 0 0 0 0 0 0 0 15
0.2632 -0.8650 -2.7063 H 0 0 0 0 0 0 0 0 0 0 0 0 16
-1.2178 -0.0271 -2.1439 H 0 0 0 0 0 0 0 0 0 0 0 0 17
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
9 4 0 0 0 0
10 4 0 0 0 0
8 5 0 0 0 0
12 5 0 0 0 0
7 6 0 0 0 0
13 6 0 0 0 0
8 7 0 0 0 0
11 7 0 0 0 0
14 8 0 0 0 0
15 13 0 0 0 0
16 13 0 0 0 0
13 17 0 0 0 0
M END
$$$$
2-methylpyrrole-cation3.sdf
COSMOtherm 3D 0
17 16 0 0 0 0 0 0 0 0 V2000
3.0451 -0.4770 -0.0009 O 0 0 0 0 0 0 0 0 0 0 0 0 1
3.4928 -0.1628 0.8056 H 0 0 0 0 0 0 0 0 0 0 0 0 2
3.5211 -0.0464 -0.7339 H 0 0 0 0 0 0 0 0 0 0 0 0 3
-0.5326 -1.5166 -0.0032 C 0 0 0 0 0 0 0 0 0 0 0 0 4
0.2949 -0.3175 -0.0063 N 0 0 0 0 0 0 0 0 0 0 0 0 5
-1.9133 -0.9656 0.0030 C 0 0 0 0 0 0 0 0 0 0 0 0 6
-1.8506 0.3890 0.0038 C 0 0 0 0 0 0 0 0 0 0 0 0 7
-0.4482 0.7688 -0.0016 C 0 0 0 0 0 0 0 0 0 0 0 0 8
0.1008 2.1440 0.0001 C 0 0 0 0 0 0 0 0 0 0 0 0 9
-0.3132 -2.1361 0.8824 H 0 0 0 0 0 0 0 0 0 0 0 0 10
1.3476 -0.3335 -0.0080 H 0 0 0 0 0 0 0 0 0 0 0 0 11
-2.8044 -1.5888 0.0058 H 0 0 0 0 0 0 0 0 0 0 0 0 12
-2.6748 1.0971 0.0076 H 0 0 0 0 0 0 0 0 0 0 0 0 13
-0.2419 2.6733 0.9021 H 0 0 0 0 0 0 0 0 0 0 0 0 14
-0.2951 2.6991 -0.8632 H 0 0 0 0 0 0 0 0 0 0 0 0 15
1.1959 2.1517 -0.0313 H 0 0 0 0 0 0 0 0 0 0 0 0 16
-0.3207 -2.1359 -0.8907 H 0 0 0 0 0 0 0 0 0 0 0 0 17
2 1 0 0 0 0
3 1 0 0 0 0
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5 4 0 0 0 0
6 4 0 0 0 0
10 4 0 0 0 0
8 5 0 0 0 0
11 5 0 0 0 0
7 6 0 0 0 0
12 6 0 0 0 0
8 7 0 0 0 0
13 7 0 0 0 0
9 8 0 0 0 0
14 9 0 0 0 0
15 9 0 0 0 0
16 9 0 0 0 0
4 17 0 0 0 0
M END
$$$$
2-methylpyrrole-cation4.sdf
COSMOtherm 3D 0
17 16 0 0 0 0 0 0 0 0 0 V2000
-3.0040 -0.4190 0.0159 O 0 0 0 0 0 0 0 0 0 0 1
-3.3964 -1.0518 0.6449 H 0 0 0 0 0 0 0 0 0 0 2
-3.4136 -0.6353 -0.8418 H 0 0 0 0 0 0 0 0 0 0 3
0.4695 -1.4531 -0.0051 C 0 0 0 0 0 0 0 0 0 0 4
-0.2833 -0.3892 -0.0048 N 0 0 0 0 0 0 0 0 0 0 5
1.8872 -1.0392 -0.0004 C 0 0 0 0 0 0 0 0 0 0 6
1.8000 0.4530 0.0033 C 0 0 0 0 0 0 0 0 0 0 7
0.4976 0.8174 0.0009 C 0 0 0 0 0 0 0 0 0 0 8
-0.1812 2.1408 0.0022 C 0 0 0 0 0 0 0 0 0 0 9
-1.3477 -0.4101 -0.0061 H 0 0 0 0 0 0 0 0 0 0 10
2.4193 -1.4568 -0.8753 H 0 0 0 0 0 0 0 0 0 0 11
2.6544 1.1231 0.0074 H 0 0 0 0 0 0 0 0 0 0 12
-0.8164 2.2618 -0.8879 H 0 0 0 0 0 0 0 0 0 0 13
0.5668 2.9420 0.0065 H 0 0 0 0 0 0 0 0 0 0 14
-0.8218 2.2572 0.8890 H 0 0 0 0 0 0 0 0 0 0 15
0.0568 -2.4595 -0.0091 H 0 0 0 0 0 0 0 0 0 0 16
2.4149 -1.4612 0.8750 H 0 0 0 0 0 0 0 0 0 0 17
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
16 4 0 0 0 0
8 5 0 0 0 0
10 5 0 0 0 0
7 6 0 0 0 0
11 6 0 0 0 0
8 7 0 0 0 0
12 7 0 0 0 0
9 8 0 0 0 0
13 9 0 0 0 0
14 9 0 0 0 0
15 9 0 0 0 0
6 17 0 0 0 0
M END
$$$$
2-methylpyrrole.sdf
COSMOtherm 3D 0
16 15 0 0 0 0 0 0 0 0 0 V2000
-3.1515 0.0009 0.4699 O 0 0 0 0 0 0 0 0 0 0 1
-3.5751 -0.7676 0.0472 H 0 0 0 0 0 0 0 0 0 0 2
-3.5727 0.7694 0.0446 H 0 0 0 0 0 0 0 0 0 0 3
1.8655 0.0011 -0.3578 C 0 0 0 0 0 0 0 0 0 0 4
1.8749 0.0008 1.0723 C 0 0 0 0 0 0 0 0 0 0 5
0.5376 -0.0003 -0.7750 C 0 0 0 0 0 0 0 0 0 0 6
-0.2450 -0.0015 0.3622 N 0 0 0 0 0 0 0 0 0 0 7
0.5520 -0.0008 1.4887 C 0 0 0 0 0 0 0 0 0 0 8
-0.0562 -0.0004 -2.1487 C 0 0 0 0 0 0 0 0 0 0 9
-1.2777 -0.0016 0.3688 H 0 0 0 0 0 0 0 0 0 0 10
2.7310 0.0021 -1.0164 H 0 0 0 0 0 0 0 0 0 0 11
2.7476 0.0015 1.7207 H 0 0 0 0 0 0 0 0 0 0 12
0.1153 -0.0016 2.4829 H 0 0 0 0 0 0 0 0 0 0 13
-0.6864 -0.8865 -2.3265 H 0 0 0 0 0 0 0 0 0 0 14
0.7433 -0.0026 -2.9010 H 0 0 0 0 0 0 0 0 0 0 15
-0.6830 0.8878 -2.3282 H 0 0 0 0 0 0 0 0 0 0 16
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
11 4 0 0 0 0
8 5 0 0 0 0
12 5 0 0 0 0
7 6 0 0 0 0
9 6 0 0 0 0
8 7 0 0 0 0
10 7 0 0 0 0
13 8 0 0 0 0
14 9 0 0 0 0
15 9 0 0 0 0
9 16 0 0 0 0
M END
$$$$
2-methylpyrrole_90.sdf
COSMOtherm 3D 0
16 15 0 0 0 0 0 0 0 0 0 V2000
-3.1515 0.0009 0.4699 O 0 0 0 0 0 0 0 0 0 0 1
-3.5751 -0.7676 0.0472 H 0 0 0 0 0 0 0 0 0 0 2
-3.5727 0.7694 0.0446 H 0 0 0 0 0 0 0 0 0 0 3
1.8655 0.0011 -0.3578 C 0 0 0 0 0 0 0 0 0 0 4
1.8749 0.0008 1.0723 C 0 0 0 0 0 0 0 0 0 0 5
0.5376 -0.0003 -0.7750 C 0 0 0 0 0 0 0 0 0 0 6
-0.2450 -0.0015 0.3622 N 0 0 0 0 0 0 0 0 0 0 7
0.5520 -0.0008 1.4887 C 0 0 0 0 0 0 0 0 0 0 8
-0.0562 -0.0004 -2.1487 C 0 0 0 0 0 0 0 0 0 0 9
```

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1
2
3      -1.2777      -0.0016      0.3688 H      0      0      0      0      0      0      0      0      0      0      10
4      2.7310      0.0021     -1.0164 H      0      0      0      0      0      0      0      0      0      0      11
5      2.7476      0.0015      1.7207 H      0      0      0      0      0      0      0      0      0      0      12
6      0.1153     -0.0016      2.4829 H      0      0      0      0      0      0      0      0      0      0      13
7     -0.6864     -0.8865     -2.3265 H      0      0      0      0      0      0      0      0      0      0      14
8      0.7433     -0.0026     -2.9010 H      0      0      0      0      0      0      0      0      0      0      15
9     -0.6830      0.8878     -2.3282 H      0      0      0      0      0      0      0      0      0      0      16
10
11      2      1      0      0      0      0
12      3      1      0      0      0      0
13      5      4      0      0      0      0
14      6      4      0      0      0      0
15     11      4      0      0      0      0
16      8      5      0      0      0      0
17     12      5      0      0      0      0
18      7      6      0      0      0      0
19      9      6      0      0      0      0
20      8      7      0      0      0      0
21     10      7      0      0      0      0
22     13      8      0      0      0      0
23     14      9      0      0      0      0
24     15      9      0      0      0      0
25      9     16      0      0      0      0
26
27 M      END
28 $$$
29 3-aminopyridine.sdf
30 COSMOTHERM      3D      0
31
32 16 15      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0
33     -3.6378      0.6632     -0.0544 O      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0
34     -2.6709      0.3789     -0.0212 H      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0
35     -3.8323      0.9639      0.8499 H      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0
36      2.2989      1.5481     -0.0048 N      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0
37      1.3698      0.5464      0.0003 C      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0
38     -0.0178      0.8346     -0.0024 C      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0
39     -0.9676     -0.1109     -0.0016 N      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0
40     -0.6045     -1.4102      0.0020 C      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0
41      0.7407     -1.7933      0.0038 C      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0
42      1.7351     -0.8194      0.0029 C      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0
43      2.0202      2.5218      0.0202 H      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0
44      3.2907      1.3426      0.0152 H      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0
45     -0.3590      1.8739     -0.0056 H      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0
46     -1.4114     -2.1453      0.0039 H      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0
47      1.0076     -2.8512      0.0066 H      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0
48      2.7903     -1.1000      0.0045 H      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0
49
50      2      1      0      0      0      0
51      3      1      0      0      0      0
52      5      4      0      0      0      0
53     11      4      0      0      0      0
54     12      4      0      0      0      0
55      6      5      0      0      0      0
56     10      5      0      0      0      0
57      7      6      0      0      0      0
58     13      6      0      0      0      0
59      8      7      0      0      0      0
60      9      8      0      0      0      0
61     14      8      0      0      0      0
62     10      9      0      0      0      0
63     15      9      0      0      0      0
64     10     16      0      0      0      0
65
66 M      END
67 $$$
68 3-aminopyridine-cation.sdf
69 COSMOTHERM      3D      0
70
71 17 16      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0
72     -3.5120     -0.0007      0.7133 O      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0
73     -4.0281     -0.7757      0.4250 H      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0
74     -4.0343      0.7683      0.4202 H      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0
75      2.3385      0.0386      1.5211 N      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0
76      1.3876     -0.0065      0.5446 C      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0
77      0.0162     -0.0057      0.8681 C      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0
78     -0.9110      0.0014     -0.1076 N      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0
79     -0.6145      0.0052     -1.4237 C      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0
80      0.7260     -0.0003     -1.8017 C      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0
81      1.7218     -0.0070     -0.8334 C      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0
82      2.0768     -0.1743      2.4791 H      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0
83      3.2990     -0.1816      1.2753 H      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0
84     -0.3517     -0.0093      1.8922 H      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0
85     -1.4500      0.0105     -2.1188 H      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0
86      0.9834     -0.0012     -2.8597 H      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0
87      2.7722     -0.0122     -1.1282 H      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0
88     -1.9315      0.0013      0.1819 H      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0
89
90      2      1      0      0      0      0
91      3      1      0      0      0      0
92      5      4      0      0      0      0
93     11      4      0      0      0      0
94     12      4      0      0      0      0
95      6      5      0      0      0      0
96     10      5      0      0      0      0
97      7      6      0      0      0      0
98     13      6      0      0      0      0
99      8      7      0      0      0      0
100      9      8      0      0      0      0
101     14      8      0      0      0      0
102     10      9      0      0      0      0
103     15      9      0      0      0      0
104     16     10      0      0      0      0
105      7     17      0      0      0      0
106
107 M      END
108 $$$
109 3-hydro-2-methylamine-4-oxy-5-phenyl-1,4-benzodiazepine.sdf
110 COSMOTHERM      3D      0
111
112 38 39      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0
113     -2.3433      0.3376     -4.0730 O      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0
114
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[illegible]

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2
3 -3.7180 -1.3219 1.0429 H 0 0 0 0 0 0 0 0 0 0 0 24
4 -1.1844 4.7894 -0.4666 H 0 0 0 0 0 0 0 0 0 0 0 25
5 1.1506 4.2792 -1.2244 H 0 0 0 0 0 0 0 0 0 0 0 26
6 1.9632 1.9455 -1.2143 H 0 0 0 0 0 0 0 0 0 0 0 27
7 -2.6903 2.9337 0.2085 H 0 0 0 0 0 0 0 0 0 0 0 28
8 -1.3405 -0.3533 -2.1034 H 0 0 0 0 0 0 0 0 0 0 0 29
9 -1.5998 -2.1075 -1.8475 H 0 0 0 0 0 0 0 0 0 0 0 30
10 1.8121 1.0100 1.6861 H 0 0 0 0 0 0 0 0 0 0 0 31
11 4.1207 0.8016 2.5592 H 0 0 0 0 0 0 0 0 0 0 0 32
12 5.7528 -0.7180 1.4359 H 0 0 0 0 0 0 0 0 0 0 0 33
13 5.0449 -2.0322 -0.5638 H 0 0 0 0 0 0 0 0 0 0 0 34
14 2.7257 -1.8602 -1.4135 H 0 0 0 0 0 0 0 0 0 0 0 35
15 -4.0116 -3.5388 0.5190 H 0 0 0 0 0 0 0 0 0 0 0 36
16 -4.0358 -2.9617 -1.1693 H 0 0 0 0 0 0 0 0 0 0 0 37
17 -2.5141 -3.5759 -0.4366 H 0 0 0 0 0 0 0 0 0 0 0 38
18 -2.8497 0.6682 1.0100 H 0 0 0 0 0 0 0 0 0 0 0 39
19
20 2 1 0 0 0 0
21 3 1 0 0 0 0
22 5 4 0 0 0 0
23 9 4 0 0 0 0
24 25 4 0 0 0 0
25 6 5 0 0 0 0
26 26 5 0 0 0 0
27 7 6 0 0 0 0
28 27 6 0 0 0 0
29 8 7 0 0 0 0
30 10 7 0 0 0 0
31 9 8 0 0 0 0
32 13 8 0 0 0 0
33 28 9 0 0 0 0
34 11 10 0 0 0 0
35 15 10 0 0 0 0
36 12 11 0 0 0 0
37 23 11 0 0 0 0
38 14 12 0 0 0 0
39 29 12 0 0 0 0
40 30 12 0 0 0 0
41 14 13 0 0 0 0
42 16 14 0 0 0 0
43 17 15 0 0 0 0
44 21 15 0 0 0 0
45 22 16 0 0 0 0
46 24 16 0 0 0 0
47 18 17 0 0 0 0
48 31 17 0 0 0 0
49 19 18 0 0 0 0
50 32 18 0 0 0 0
51 20 19 0 0 0 0
52 33 19 0 0 0 0
53 21 20 0 0 0 0
54 34 20 0 0 0 0
55 35 21 0 0 0 0
56 36 22 0 0 0 0
57 37 22 0 0 0 0
58 38 22 0 0 0 0
59 13 39 0 0 0 0
60 M END
$$$
3-hydro-2-methylamine-4-oxy-5-phenyl-1,4-benzodiazepine_t-cation.sdf
COSMOtherm 3D 0
39 40 0 0 0 0 0 0 0 0 0 V2000
-4.2085 -2.1613 0.2194 O 0 0 0 0 0 0 0 0 0 0 0 1
-4.0185 -3.1169 0.2414 H 0 0 0 0 0 0 0 0 0 0 0 2
-5.0919 -2.0639 0.6190 H 0 0 0 0 0 0 0 0 0 0 0 3
-0.8129 0.4811 3.7652 C 0 0 0 0 0 0 0 0 0 0 0 4
0.4935 0.9025 3.4769 C 0 0 0 0 0 0 0 0 0 0 0 5
0.9448 0.9049 2.1629 C 0 0 0 0 0 0 0 0 0 0 0 6
0.1157 0.5112 1.0844 C 0 0 0 0 0 0 0 0 0 0 0 7
-1.2194 0.1317 1.3960 C 0 0 0 0 0 0 0 0 0 0 0 8
-1.6600 0.1015 2.7302 C 0 0 0 0 0 0 0 0 0 0 0 9
0.7206 0.4304 -0.2544 C 0 0 0 0 0 0 0 0 0 0 0 10
0.0301 0.8005 -1.3385 N 0 0 0 0 0 0 0 0 0 0 0 11
-1.3487 1.3647 -1.1590 C 0 0 0 0 0 0 0 0 0 0 0 12
-2.1447 -0.2881 0.4157 N 0 0 0 0 0 0 0 0 0 0 0 13
-2.2647 0.2364 -0.8125 C 0 0 0 0 0 0 0 0 0 0 0 14
2.1020 -0.0720 -0.4127 C 0 0 0 0 0 0 0 0 0 0 0 15
-3.1465 -0.2590 -1.6649 N 0 0 0 0 0 0 0 0 0 0 0 16
2.5176 -1.1911 0.3367 C 0 0 0 0 0 0 0 0 0 0 0 17
3.8191 -1.6833 0.2170 C 0 0 0 0 0 0 0 0 0 0 0 18
4.7311 -1.0556 -0.6387 C 0 0 0 0 0 0 0 0 0 0 0 19
4.3307 0.0638 -1.3795 C 0 0 0 0 0 0 0 0 0 0 0 20
3.0256 0.5486 -1.2780 C 0 0 0 0 0 0 0 0 0 0 0 21
-3.4404 0.2571 -3.0060 C 0 0 0 0 0 0 0 0 0 0 0 22
0.4254 0.6900 -2.5570 O 0 0 0 0 0 0 0 0 0 0 0 23
-1.1739 0.4610 4.7941 H 0 0 0 0 0 0 0 0 0 0 0 24
1.1592 1.2217 4.2795 H 0 0 0 0 0 0 0 0 0 0 0 25
1.9667 1.2148 1.9439 H 0 0 0 0 0 0 0 0 0 0 0 26
-2.6832 -0.2136 2.9409 H 0 0 0 0 0 0 0 0 0 0 0 27
-1.3416 2.1055 -0.3481 H 0 0 0 0 0 0 0 0 0 0 0 28
-1.6056 1.8493 -2.1017 H 0 0 0 0 0 0 0 0 0 0 0 29
1.8132 -1.6840 1.0085 H 0 0 0 0 0 0 0 0 0 0 0 30
4.1206 -2.5584 0.7950 H 0 0 0 0 0 0 0 0 0 0 0 31
5.7497 -1.4368 -0.7291 H 0 0 0 0 0 0 0 0 0 0 0 32
5.0395 0.5622 -2.0431 H 0 0 0 0 0 0 0 0 0 0 0 33
2.7212 1.4132 -1.8659 H 0 0 0 0 0 0 0 0 0 0 0 34
-4.0555 -0.4911 -3.5143 H 0 0 0 0 0 0 0 0 0 0 0 35
-3.9996 1.2010 -2.9532 H 0 0 0 0 0 0 0 0 0 0 0 36
-2.5187 0.3992 -3.5814 H 0 0 0 0 0 0 0 0 0 0 0 37
-2.8465 -1.0114 0.6736 H 0 0 0 0 0 0 0 0 0 0 0 38
-3.7216 -1.0406 -1.3130 H 0 0 0 0 0 0 0 0 0 0 0 39
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
9 4 0 0 0 0
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24 4 0 0 0 0
6 5 0 0 0 0
25 5 0 0 0 0
7 6 0 0 0 0
26 6 0 0 0 0
8 7 0 0 0 0
10 7 0 0 0 0
9 8 0 0 0 0
13 8 0 0 0 0
27 9 0 0 0 0
11 10 0 0 0 0
15 10 0 0 0 0
12 11 0 0 0 0
23 11 0 0 0 0
14 12 0 0 0 0
28 12 0 0 0 0
29 12 0 0 0 0
14 13 0 0 0 0
38 13 0 0 0 0
16 14 0 0 0 0
17 15 0 0 0 0
21 15 0 0 0 0
22 16 0 0 0 0
18 17 0 0 0 0
30 17 0 0 0 0
19 18 0 0 0 0
31 18 0 0 0 0
20 19 0 0 0 0
32 19 0 0 0 0
21 20 0 0 0 0
33 20 0 0 0 0
34 21 0 0 0 0
35 22 0 0 0 0
36 22 0 0 0 0
37 22 0 0 0 0
16 39 0 0 0 0
M END
$$$$
3-methylindole-cation0.sdf
COSMOtherm 3D 0
23 23 0 0 0 0 0 0 0 0 0 V2000
1.4088 0.2248 -0.5581 O 0 0 0 0 0 0 0 0 0 0 1
0.5021 -0.0947 -0.7229 H 0 0 0 0 0 0 0 0 0 0 2
1.3007 1.1602 -0.3040 H 0 0 0 0 0 0 0 0 0 0 3
4.5367 -3.6329 -1.2507 C 0 0 0 0 0 0 0 0 0 0 4
5.8553 -3.2897 -0.9131 C 0 0 0 0 0 0 0 0 0 0 5
6.1299 -2.3282 0.0685 C 0 0 0 0 0 0 0 0 0 0 6
5.0504 -1.7114 0.7112 C 0 0 0 0 0 0 0 0 0 0 7
3.7454 -2.0756 0.3494 C 0 0 0 0 0 0 0 0 0 0 8
3.4438 -3.0205 -0.6152 C 0 0 0 0 0 0 0 0 0 0 9
2.8080 -1.2683 1.1442 N 0 0 0 0 0 0 0 0 0 0 10
4.9721 -0.6855 1.7625 C 0 0 0 0 0 0 0 0 0 0 11
3.6690 -0.4419 2.0132 C 0 0 0 0 0 0 0 0 0 0 12
2.1647 -1.8528 1.7002 H 0 0 0 0 0 0 0 0 0 0 13
4.3528 -4.3863 -2.0171 H 0 0 0 0 0 0 0 0 0 0 14
6.6827 -3.7822 -1.4260 H 0 0 0 0 0 0 0 0 0 0 15
7.1589 -2.0707 0.3228 H 0 0 0 0 0 0 0 0 0 0 16
2.4175 -3.2832 -0.8724 H 0 0 0 0 0 0 0 0 0 0 17
6.1460 -0.0453 2.4247 C 0 0 0 0 0 0 0 0 0 0 18
3.1817 0.2295 2.7128 H 0 0 0 0 0 0 0 0 0 0 19
2.1826 -0.6442 0.4955 H 0 0 0 0 0 0 0 0 0 0 20
6.7817 0.4609 1.6823 H 0 0 0 0 0 0 0 0 0 0 21
6.7690 -0.8052 2.9208 H 0 0 0 0 0 0 0 0 0 0 22
5.8301 0.6904 3.1740 H 0 0 0 0 0 0 0 0 0 0 23
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
9 4 0 0 0 0
14 4 0 0 0 0
6 5 0 0 0 0
15 5 0 0 0 0
7 6 0 0 0 0
16 6 0 0 0 0
8 7 0 0 0 0
11 7 0 0 0 0
9 8 0 0 0 0
10 8 0 0 0 0
17 9 0 0 0 0
12 10 0 0 0 0
13 10 0 0 0 0
20 10 0 0 0 0
12 11 0 0 0 0
18 11 0 0 0 0
19 12 0 0 0 0
21 18 0 0 0 0
22 18 0 0 0 0
18 23 0 0 0 0
M END
$$$$
3-methylindole-cation1.sdf
COSMOtherm 3D 0
23 23 0 0 0 0 0 0 0 0 0 V2000
0.8175 0.0068 -0.2490 O 0 0 0 0 0 0 0 0 0 0 1
0.3335 -0.7595 0.1086 H 0 0 0 0 0 0 0 0 0 0 2
0.3367 0.7838 0.0895 H 0 0 0 0 0 0 0 0 0 0 3
4.9342 -0.0407 3.4195 C 0 0 0 0 0 0 0 0 0 0 4
6.3305 -0.0700 3.0818 C 0 0 0 0 0 0 0 0 0 0 5
6.7425 -0.0813 1.7728 C 0 0 0 0 0 0 0 0 0 0 6
5.7454 -0.0620 0.7486 C 0 0 0 0 0 0 0 0 0 0 7
4.3345 -0.0320 1.1104 C 0 0 0 0 0 0 0 0 0 0 8
3.9344 -0.0221 2.4720 C 0 0 0 0 0 0 0 0 0 0 9
3.5827 -0.0164 0.0072 N 0 0 0 0 0 0 0 0 0 0 10
5.8264 -0.0625 -0.6354 C 0 0 0 0 0 0 0 0 0 0 11
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1
2
3      4.4347   -0.0389   -1.1649 C   0   0   0   0   0   0   0   0   0   0   12
4      2.5374   -0.0029   -0.0304 H   0   0   0   0   0   0   0   0   0   0   13
5      4.2295   -0.9264   -1.7901 H   0   0   0   0   0   0   0   0   0   0   14
6      4.2572    0.8407   -1.8090 H   0   0   0   0   0   0   0   0   0   0   15
7      4.6601   -0.0334   4.4759 H   0   0   0   0   0   0   0   0   0   0   16
8      7.0628   -0.0838   3.8893 H   0   0   0   0   0   0   0   0   0   0   17
9      7.8010   -0.1036   1.5117 H   0   0   0   0   0   0   0   0   0   0   18
10     2.8815   -0.0005   2.7508 H   0   0   0   0   0   0   0   0   0   0   19
11     7.0294   -0.0652   -1.5013 C   0   0   0   0   0   0   0   0   0   0   20
12     7.7552   -0.8217   -1.1687 H   0   0   0   0   0   0   0   0   0   0   21
13     7.5379    0.9120   -1.4403 H   0   0   0   0   0   0   0   0   0   0   22
14     6.7734   -0.2492   -2.5515 H   0   0   0   0   0   0   0   0   0   0   23
15
16     2   1   0   0   0   0
17     3   1   0   0   0   0
18     5   4   0   0   0   0
19     9   4   0   0   0   0
20     16  4   0   0   0   0
21     6   5   0   0   0   0
22     17  5   0   0   0   0
23     7   6   0   0   0   0
24     18  6   0   0   0   0
25     8   7   0   0   0   0
26     11  7   0   0   0   0
27     9   8   0   0   0   0
28     10  8   0   0   0   0
29     19  9   0   0   0   0
30     12 10   0   0   0   0
31     13 10   0   0   0   0
32     12 11   0   0   0   0
33     20 11   0   0   0   0
34     14 12   0   0   0   0
35     15 12   0   0   0   0
36     21 20   0   0   0   0
37     22 20   0   0   0   0
38     20 23   0   0   0   0
39
40 M   END
41 $$$$
42 3-methylindole-cation2.sdf
43 COSMOTHERM      3D      0
44
45 23 23   0   0   0   0   0   0   0   0   0   0 V2000
46 1.2525   -0.4529   -0.8008 O   0   0   0   0   0   0   0   0   0   0   1
47 0.6379   -1.1429   -0.4899 H   0   0   0   0   0   0   0   0   0   0   2
48 0.6974   0.1644   -1.3118 H   0   0   0   0   0   0   0   0   0   0   3
49 6.3816   0.3414   0.4727 C   0   0   0   0   0   0   0   0   0   0   4
50 6.8243   1.0293   1.6141 C   0   0   0   0   0   0   0   0   0   0   5
51 5.9186   1.5731   2.5389 C   0   0   0   0   0   0   0   0   0   0   6
52 4.5574   1.4162   2.2957 C   0   0   0   0   0   0   0   0   0   0   7
53 4.1401   0.7253   1.1450 C   0   0   0   0   0   0   0   0   0   0   8
54 5.0155   0.1739   0.2143 C   0   0   0   0   0   0   0   0   0   0   9
55 2.7177   0.7147   1.1362 N   0   0   0   0   0   0   0   0   0   0   10
56 3.3243   1.8562   3.0522 C   0   0   0   0   0   0   0   0   0   0   11
57 2.2351   1.3350   2.1745 C   0   0   0   0   0   0   0   0   0   0   12
58 2.1200   0.2545   0.3763 H   0   0   0   0   0   0   0   0   0   0   13
59 3.2048   3.3670   3.3574 C   0   0   0   0   0   0   0   0   0   0   14
60 3.2466   1.3072   4.0114 H   0   0   0   0   0   0   0   0   0   0   15
61 7.1115   -0.0695   -0.2254 H   0   0   0   0   0   0   0   0   0   0   16
62 7.8956   1.1425   1.7863 H   0   0   0   0   0   0   0   0   0   0   17
63 6.2803   2.1017   3.4219 H   0   0   0   0   0   0   0   0   0   0   18
64 4.6614   -0.3597   -0.6677 H   0   0   0   0   0   0   0   0   0   0   19
65 1.1621   1.4272   2.3344 H   0   0   0   0   0   0   0   0   0   0   20
66 2.2584   3.5795   3.8707 H   0   0   0   0   0   0   0   0   0   0   21
67 4.0310   3.6696   4.0124 H   0   0   0   0   0   0   0   0   0   0   22
68 3.2516   3.9553   2.4324 H   0   0   0   0   0   0   0   0   0   0   23
69
70     2   1   0   0   0   0
71     3   1   0   0   0   0
72     5   4   0   0   0   0
73     9   4   0   0   0   0
74     16  4   0   0   0   0
75     6   5   0   0   0   0
76     17  5   0   0   0   0
77     7   6   0   0   0   0
78     18  6   0   0   0   0
79     8   7   0   0   0   0
80     11  7   0   0   0   0
81     9   8   0   0   0   0
82     10  8   0   0   0   0
83     19  9   0   0   0   0
84     12 10   0   0   0   0
85     13 10   0   0   0   0
86     12 11   0   0   0   0
87     14 11   0   0   0   0
88     15 11   0   0   0   0
89     20 12   0   0   0   0
90     21 14   0   0   0   0
91     22 14   0   0   0   0
92     14 23   0   0   0   0
93
94 M   END
95 $$$$
96 3-methylindole.sdf
97 COSMOTHERM      3D      0
98
99 22 22   0   0   0   0   0   0   0   0   0   0 V2000
100 -4.0948   0.0052   -0.5293 O   0   0   0   0   0   0   0   0   0   0   1
101 -4.3574   -0.7628   -1.0677 H   0   0   0   0   0   0   0   0   0   0   2
102 -4.3486   0.7751   -1.0692 H   0   0   0   0   0   0   0   0   0   0   3
103 0.9313   0.0001   0.3719 C   0   0   0   0   0   0   0   0   0   0   4
104 2.2160   0.0026   -0.2101 C   0   0   0   0   0   0   0   0   0   0   5
105 2.3309   0.0025   -1.6005 C   0   0   0   0   0   0   0   0   0   0   6
106 1.1836   -0.0004   -2.4287 C   0   0   0   0   0   0   0   0   0   0   7
107 -0.1019   -0.0030   -1.8849 C   0   0   0   0   0   0   0   0   0   0   8
108 -0.2175   -0.0028   -0.4866 C   0   0   0   0   0   0   0   0   0   0   9
109 3.1103   0.0048   0.4172 H   0   0   0   0   0   0   0   0   0   0   10
110 3.3210   0.0048   -2.0613 H   0   0   0   0   0   0   0   0   0   0   11
111 1.3057   -0.0005   -3.5136 H   0   0   0   0   0   0   0   0   0   0   12
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9 7 0 0 0 0
12 8 0 0 0 0
15 10 0 0 0 0
16 10 0 0 0 0
10 17 0 0 0 0
M END
$$$$
3-methylpyrrole-cation2.sdf
COSMOtherm 3D 0

17 16 0 0 0 0 0 0 0 0 0 V2000
0.6594 0.2895 -0.6696 O 0 0 0 0 0 0 0 0 0 0 1
0.1119 -0.3142 -1.2047 H 0 0 0 0 0 0 0 0 0 0 2
0.0195 0.8590 -0.2043 H 0 0 0 0 0 0 0 0 0 0 3
3.3615 -2.2364 2.6033 C 0 0 0 0 0 0 0 0 0 0 4
4.4315 -1.5289 1.8212 C 0 0 0 0 0 0 0 0 0 0 5
2.1210 -1.7475 1.9489 C 0 0 0 0 0 0 0 0 0 0 6
2.4320 -0.9436 0.9708 N 0 0 0 0 0 0 0 0 0 0 7
3.8446 -0.7859 0.8634 C 0 0 0 0 0 0 0 0 0 0 8
3.4157 -3.3224 2.3701 H 0 0 0 0 0 0 0 0 0 0 9
3.4000 -2.0871 4.1415 C 0 0 0 0 0 0 0 0 0 0 10
1.7249 -0.4692 0.3298 H 0 0 0 0 0 0 0 0 0 0 11
5.4975 -1.6268 2.0048 H 0 0 0 0 0 0 0 0 0 0 12
1.0900 -1.9981 2.1896 H 0 0 0 0 0 0 0 0 0 0 13
4.2528 -0.1442 0.0893 H 0 0 0 0 0 0 0 0 0 0 14
2.5658 -2.6351 4.5967 H 0 0 0 0 0 0 0 0 0 0 15
4.3420 -2.5016 4.5204 H 0 0 0 0 0 0 0 0 0 0 16
3.3343 -1.0305 4.4293 H 0 0 0 0 0 0 0 0 0 0 17
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
9 4 0 0 0 0
10 4 0 0 0 0
8 5 0 0 0 0
12 5 0 0 0 0
7 6 0 0 0 0
13 6 0 0 0 0
8 7 0 0 0 0
11 7 0 0 0 0
14 8 0 0 0 0
15 10 0 0 0 0
16 10 0 0 0 0
10 17 0 0 0 0
M END
$$$$
3-methylpyrrole-cation3.sdf
COSMOtherm 3D 0

17 16 0 0 0 0 0 0 0 0 0 V2000
-0.4357 0.0030 3.4680 O 0 0 0 0 0 0 0 0 0 0 1
-0.8860 -0.7997 3.7886 H 0 0 0 0 0 0 0 0 0 0 2
-0.9981 0.7390 3.7712 H 0 0 0 0 0 0 0 0 0 0 3
-0.1922 -0.0004 -1.4806 C 0 0 0 0 0 0 0 0 0 0 4
1.1529 0.0001 -1.2473 C 0 0 0 0 0 0 0 0 0 0 5
-0.8207 0.0001 -0.1746 C 0 0 0 0 0 0 0 0 0 0 6
0.0701 0.0012 0.7835 N 0 0 0 0 0 0 0 0 0 0 7
1.4115 0.0013 0.2140 C 0 0 0 0 0 0 0 0 0 0 8
-0.9334 -0.0013 -2.7784 C 0 0 0 0 0 0 0 0 0 0 9
1.9463 -0.0001 -1.9914 H 0 0 0 0 0 0 0 0 0 0 10
-1.8874 -0.0007 0.0482 H 0 0 0 0 0 0 0 0 0 0 11
-0.1432 0.0011 1.8201 H 0 0 0 0 0 0 0 0 0 0 12
1.9713 -0.8843 0.5595 H 0 0 0 0 0 0 0 0 0 0 13
-1.5827 -0.8857 -2.8583 H 0 0 0 0 0 0 0 0 0 0 14
-0.2365 -0.0047 -3.6250 H 0 0 0 0 0 0 0 0 0 0 15
-1.5781 0.8862 -2.8619 H 0 0 0 0 0 0 0 0 0 0 16
1.9709 0.8876 0.5582 H 0 0 0 0 0 0 0 0 0 0 17
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
9 4 0 0 0 0
8 5 0 0 0 0
10 5 0 0 0 0
7 6 0 0 0 0
11 6 0 0 0 0
8 7 0 0 0 0
12 7 0 0 0 0
13 8 0 0 0 0
14 9 0 0 0 0
15 9 0 0 0 0
16 9 0 0 0 0
8 17 0 0 0 0
M END
$$$$
3-methylpyrrole-cation4.sdf
COSMOtherm 3D 0

17 16 0 0 0 0 0 0 0 0 0 V2000
-3.4628 0.4141 -0.0012 O 0 0 0 0 0 0 0 0 0 0 1
-3.7790 0.9214 -0.7711 H 0 0 0 0 0 0 0 0 0 0 2
-3.7874 0.9095 0.7730 H 0 0 0 0 0 0 0 0 0 0 3
1.4422 0.2532 -0.0007 C 0 0 0 0 0 0 0 0 0 0 4
1.1686 -1.2279 -0.0018 C 0 0 0 0 0 0 0 0 0 0 5
0.2407 0.8778 -0.0008 C 0 0 0 0 0 0 0 0 0 0 6
-0.7928 -0.0977 0.0022 N 0 0 0 0 0 0 0 0 0 0 7
-0.3084 -1.3089 0.0011 C 0 0 0 0 0 0 0 0 0 0 8
2.7998 0.8634 0.0006 C 0 0 0 0 0 0 0 0 0 0 9
1.5895 -1.7501 -0.8802 H 0 0 0 0 0 0 0 0 0 0 10
-0.0198 1.9315 0.0006 H 0 0 0 0 0 0 0 0 0 0 11
-1.8300 0.1386 0.0047 H 0 0 0 0 0 0 0 0 0 0 12
2.7441 1.9588 -0.0199 H 0 0 0 0 0 0 0 0 0 0 13
3.3809 0.5252 -0.8712 H 0 0 0 0 0 0 0 0 0 0 14
3.3627 0.5587 0.8967 H 0 0 0 0 0 0 0 0 0 0 15
-0.9419 -2.1926 0.0020 H 0 0 0 0 0 0 0 0 0 0 16
```

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1
2
3      1.5944      -1.7538      0.8719 H      0      0      0      0      0      0      0      0      0      0      0      0      17
4      2      1      0      0      0      0
5      3      1      0      0      0      0
6      5      4      0      0      0      0
7      6      4      0      0      0      0
8      9      4      0      0      0      0
9      8      5      0      0      0      0
10     10     5      0      0      0      0
11     7      6      0      0      0      0
12     11     6      0      0      0      0
13     8      7      0      0      0      0
14     12     7      0      0      0      0
15     16     8      0      0      0      0
16     13     9      0      0      0      0
17     14     9      0      0      0      0
18     15     9      0      0      0      0
19     5      17     0      0      0      0
20 M      END
21 $$$$
22 3-methylpyrrole.sdf
23 COSMOTHERM      3D      0
24
25 16 15      0      0      0      0      0      0      0      0      0      0 V2000
26 -3.6033      0.0063      -0.3908 O      0      0      0      0      0      0      0      0      0      0      0      0      1
27 -3.9116      -0.7672      -0.8966 H      0      0      0      0      0      0      0      0      0      0      0      0      2
28 -3.8889      0.7692      -0.9251 H      0      0      0      0      0      0      0      0      0      0      0      0      3
29 -0.7499      -0.0077      0.1104 N      0      0      0      0      0      0      0      0      0      0      0      0      4
30 0.2380      -0.0068      -0.8523 C      0      0      0      0      0      0      0      0      0      0      0      0      5
31 1.4759      0.0003      -0.2147 C      0      0      0      0      0      0      0      0      0      0      0      0      6
32 1.2040      0.0036      1.1905 C      0      0      0      0      0      0      0      0      0      0      0      0      7
33 -0.1758      -0.0013      1.3593 C      0      0      0      0      0      0      0      0      0      0      0      0      8
34 2.8332      0.0043      -0.8662 C      0      0      0      0      0      0      0      0      0      0      0      0      9
35 -1.7648      -0.0087      -0.0821 H      0      0      0      0      0      0      0      0      0      0      0      0      10
36 -0.0149      -0.0107      -1.9090 H      0      0      0      0      0      0      0      0      0      0      0      0      11
37 1.9441      0.0086      1.9881 H      0      0      0      0      0      0      0      0      0      0      0      0      12
38 -0.7856      -0.0010      2.2578 H      0      0      0      0      0      0      0      0      0      0      0      0      13
39 2.9858      0.8918      -1.5002 H      0      0      0      0      0      0      0      0      0      0      0      0      14
40 3.6275      0.0032      -0.1065 H      0      0      0      0      0      0      0      0      0      0      0      0      15
41 2.9885      -0.8786      -1.5059 H      0      0      0      0      0      0      0      0      0      0      0      0      16
42
43 2      1      0      0      0      0
44 3      1      0      0      0      0
45 5      4      0      0      0      0
46 8      4      0      0      0      0
47 10     4      0      0      0      0
48 6      5      0      0      0      0
49 11     5      0      0      0      0
50 7      6      0      0      0      0
51 9      6      0      0      0      0
52 8      7      0      0      0      0
53 12     7      0      0      0      0
54 13     8      0      0      0      0
55 14     9      0      0      0      0
56 15     9      0      0      0      0
57 9      16     0      0      0      0
58 M      END
59 $$$$
60 4-aminopyridine0.sdf
    COSMOTHERM      3D      0
    16 15      0      0      0      0      0      0      0      0      0      0 V2000
    -3.8873      -0.0703      -0.0014 O      0      0      0      0      0      0      0      0      0      0      0      0      1
    -2.8765      -0.0252      0.0001 H      0      0      0      0      0      0      0      0      0      0      0      0      2
    -4.1698      0.8601      0.0143 H      0      0      0      0      0      0      0      0      0      0      0      0      3
    -0.4166      0.0091      1.1499 C      0      0      0      0      0      0      0      0      0      0      0      0      4
    0.9696      0.0070      1.2058 C      0      0      0      0      0      0      0      0      0      0      0      0      5
    1.7125      0.0027      -0.0001 C      0      0      0      0      0      0      0      0      0      0      0      0      6
    0.9690      0.0072      -1.2057 C      0      0      0      0      0      0      0      0      0      0      0      0      7
    -0.4172      0.0097      -1.1491 C      0      0      0      0      0      0      0      0      0      0      0      0      8
    -1.1294      0.0091      0.0006 N      0      0      0      0      0      0      0      0      0      0      0      0      9
    3.0766      -0.0449      -0.0007 N      0      0      0      0      0      0      0      0      0      0      0      0      10
    3.5796      0.1556      0.8583 H      0      0      0      0      0      0      0      0      0      0      0      0      11
    3.5788      0.1561      -0.8600 H      0      0      0      0      0      0      0      0      0      0      0      0      12
    -0.9976      0.0128      2.0758 H      0      0      0      0      0      0      0      0      0      0      0      0      13
    1.4789      0.0077      2.1711 H      0      0      0      0      0      0      0      0      0      0      0      0      14
    1.4777      0.0080      -2.1713 H      0      0      0      0      0      0      0      0      0      0      0      0      15
    -0.9994      0.0138      -2.0742 H      0      0      0      0      0      0      0      0      0      0      0      0      16
    2      1      0      0      0      0
    3      1      0      0      0      0
    5      4      0      0      0      0
    9      4      0      0      0      0
    13     4      0      0      0      0
    6      5      0      0      0      0
    14     5      0      0      0      0
    7      6      0      0      0      0
    10     6      0      0      0      0
    8      7      0      0      0      0
    15     7      0      0      0      0
    9      8      0      0      0      0
    11     10     0      0      0      0
    12     10     0      0      0      0
    8      16     0      0      0      0
    M      END
    $$$$
    4-aminopyridine-cation.sdf
    COSMOTHERM      3D      0
    17 16      0      0      0      0      0      0      0      0      0      0 V2000
    -3.8167      -0.0059      0.0561 O      0      0      0      0      0      0      0      0      0      0      0      0      1
    -4.2321      -0.7324      -0.4432 H      0      0      0      0      0      0      0      0      0      0      0      0      2
    -4.2352      0.8025      -0.2918 H      0      0      0      0      0      0      0      0      0      0      0      0      3
    -0.3895      -0.0007      1.1760 C      0      0      0      0      0      0      0      0      0      0      0      0      4
    0.9828      -0.0002      1.2167 C      0      0      0      0      0      0      0      0      0      0      0      0      5
    1.7277      -0.0001      0.0021 C      0      0      0      0      0      0      0      0      0      0      0      0      6
    0.9921      0.0019      -1.2181 C      0      0      0      0      0      0      0      0      0      0      0      0      7
    -0.3803      0.0017      -1.1876 C      0      0      0      0      0      0      0      0      0      0      0      0      8
```

```
1
2
3      -1.0557    0.0003   -0.0084 N    0  0  0  0  0  0  0  0  0  0  9
4      3.0708   -0.0012    0.0072 N    0  0  0  0  0  0  0  0  0  0 10
5      3.6012   -0.0001   -0.8581 H    0  0  0  0  0  0  0  0  0  0 11
6      3.5946   -0.0032    0.8767 H    0  0  0  0  0  0  0  0  0  0 12
7     -1.0025   -0.0006    2.0752 H    0  0  0  0  0  0  0  0  0  0 13
8      1.4921   -0.0006    2.1797 H    0  0  0  0  0  0  0  0  0  0 14
9      1.5087    0.0032   -2.1771 H    0  0  0  0  0  0  0  0  0  0 15
10     -0.9863    0.0040   -2.0917 H    0  0  0  0  0  0  0  0  0  0 16
11     -2.1072    0.0019   -0.0127 H    0  0  0  0  0  0  0  0  0  0 17
12
13  2  1  0  0  0  0
14  3  1  0  0  0  0
15  5  4  0  0  0  0
16  9  4  0  0  0  0
17 13  4  0  0  0  0
18  6  5  0  0  0  0
19 14  5  0  0  0  0
20  7  6  0  0  0  0
21 10  6  0  0  0  0
22  8  7  0  0  0  0
23 15  7  0  0  0  0
24  9  8  0  0  0  0
25 16  8  0  0  0  0
26 11 10  0  0  0  0
27 12 10  0  0  0  0
28  9 17  0  0  0  0
29
30 M  END
31 $$$
32 4-chloroaniline.sdf
33 COSMOtherm      3D      0
34
35 17 16  0  0  0  0  0  0  0  0  0  0 V2000
36   -1.4769    0.1059    4.2036 O    0  0  0  0  0  0  0  0  0  0  0  1
37   -1.6555   -0.8058    4.4923 H    0  0  0  0  0  0  0  0  0  0  2
38   -0.6364    0.0352    3.6725 H    0  0  0  0  0  0  0  0  0  0  3
39   -0.4385    0.0151   -3.1610 Cl   0  0  0  0  0  0  0  0  0  0  4
40    0.4686   -1.2285    0.5821 C    0  0  0  0  0  0  0  0  0  0  5
41    0.6764   -0.0236    1.2794 C    0  0  0  0  0  0  0  0  0  0  6
42    0.5337    1.1934    0.5867 C    0  0  0  0  0  0  0  0  0  0  7
43    0.1933    1.2094   -0.7676 C    0  0  0  0  0  0  0  0  0  0  8
44   -0.0078    0.0001   -1.4350 C    0  0  0  0  0  0  0  0  0  0  9
45    0.1277   -1.2208   -0.7723 C    0  0  0  0  0  0  0  0  0  0 10
46    0.9500   -0.0333    2.6621 N    0  0  0  0  0  0  0  0  0  0 11
47    0.5756   -2.1829    1.1017 H    0  0  0  0  0  0  0  0  0  0 12
48    0.6922    2.1385    1.1101 H    0  0  0  0  0  0  0  0  0  0 13
49    0.0901    2.1584   -1.2941 H    0  0  0  0  0  0  0  0  0  0 14
50   -0.0265   -2.1608   -1.3025 H    0  0  0  0  0  0  0  0  0  0 15
51    1.4190   -0.8825    2.9801 H    0  0  0  0  0  0  0  0  0  0 16
52    1.4698    0.7847    2.9824 H    0  0  0  0  0  0  0  0  0  0 17
53
54  2  1  0  0  0  0
55  3  1  0  0  0  0
56  9  4  0  0  0  0
57  6  5  0  0  0  0
58 10  5  0  0  0  0
59 12  5  0  0  0  0
60  7  6  0  0  0  0
61 11  6  0  0  0  0
62  8  7  0  0  0  0
63 13  7  0  0  0  0
64  9  8  0  0  0  0
65 14  8  0  0  0  0
66 10  9  0  0  0  0
67 15 10  0  0  0  0
68 16 11  0  0  0  0
69 11 17  0  0  0  0
70
71 M  END
72 $$$
73 4-chloroaniline-cation.sdf
74 COSMOtherm      3D      0
75
76 18 17  0  0  0  0  0  0  0  0  0  0 V2000
77    0.9729    0.9306    4.0910 O    0  0  0  0  0  0  0  0  0  0  0  1
78    1.0138    0.6913    5.0355 H    0  0  0  0  0  0  0  0  0  0  2
79    0.7405    1.8775    4.0857 H    0  0  0  0  0  0  0  0  0  0  3
80   -0.7009   -0.6293    2.6632 N    0  0  0  0  0  0  0  0  0  0  4
81   -1.4476    0.1708    0.4466 C    0  0  0  0  0  0  0  0  0  0  5
82   -0.4583   -0.4205    1.2283 C    0  0  0  0  0  0  0  0  0  0  6
83    0.7695   -0.8024    0.6882 C    0  0  0  0  0  0  0  0  0  0  7
84    1.0126   -0.5919   -0.6708 C    0  0  0  0  0  0  0  0  0  0  8
85    0.0180   -0.0005   -1.4533 C    0  0  0  0  0  0  0  0  0  0  9
86   -1.2099    0.3847   -0.9140 C    0  0  0  0  0  0  0  0  0  0 10
87    0.3235    0.2642   -3.1754 Cl   0  0  0  0  0  0  0  0  0  0 11
88   -1.6781   -0.4249    2.9082 H    0  0  0  0  0  0  0  0  0  0 12
89   -0.0705    0.0014    3.2740 H    0  0  0  0  0  0  0  0  0  0 13
90   -2.4042    0.4629    0.8825 H    0  0  0  0  0  0  0  0  0  0 14
91    1.5358   -1.2652    1.3111 H    0  0  0  0  0  0  0  0  0  0 15
92    1.9650   -0.8873   -1.1092 H    0  0  0  0  0  0  0  0  0  0 16
93   -1.9755    0.8426   -1.5388 H    0  0  0  0  0  0  0  0  0  0 17
94   -0.5293   -1.6061    2.9373 H    0  0  0  0  0  0  0  0  0  0 18
95
96  2  1  0  0  0  0
97  3  1  0  0  0  0
98  6  4  0  0  0  0
99 12  4  0  0  0  0
100 13  4  0  0  0  0
101  6  5  0  0  0  0
102 10  5  0  0  0  0
103 14  5  0  0  0  0
104  7  6  0  0  0  0
105  8  7  0  0  0  0
106 15  7  0  0  0  0
107  9  8  0  0  0  0
108 16  8  0  0  0  0
109 10  9  0  0  0  0
110 11  9  0  0  0  0
111 17 10  0  0  0  0
112  4 18  0  0  0  0
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1
2
3      3.2225      0.0231      0.0052 C      0      0      0      0      0      0      0      0      0      4
4      1.7186      0.0037      0.0006 C      0      0      0      0      0      0      0      0      0      5
5      0.9721      1.1951      0.0014 C      0      0      0      0      0      0      0      0      0      6
6     -0.4198      1.1371     -0.0017 C      0      0      0      0      0      0      0      0      0      7
7     -1.1118     -0.0212     -0.0068 N      0      0      0      0      0      0      0      0      0      8
8     -0.4011     -1.1652     -0.0079 C      0      0      0      0      0      0      0      0      0      9
9      0.9940     -1.1979     -0.0046 C      0      0      0      0      0      0      0      0      0     10
10     3.6025      0.5452      0.8964 H      0      0      0      0      0      0      0      0      0     11
11     3.6373     -0.9927     -0.0038 H      0      0      0      0      0      0      0      0      0     12
12     3.6084      0.5640     -0.8720 H      0      0      0      0      0      0      0      0      0     13
13     1.4712      2.1660      0.0052 H      0      0      0      0      0      0      0      0      0     14
14     -1.0145      2.0539      0.0003 H      0      0      0      0      0      0      0      0      0     15
15     -0.9786     -2.0929     -0.0119 H      0      0      0      0      0      0      0      0      0     16
16      1.5114     -2.1590     -0.0053 H      0      0      0      0      0      0      0      0      0     17
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M END
\$\$\$\$
4-methylpyridine-cation.sdf
COSMOTHERM 3D 0

18 17 0 0 0 0 0 0 0 0 0 V2000
-3.7695 -0.0586 0.0092 O 0 0 0 0 0 0 0 0 0 0 0 1
-4.1810 0.2255 -0.8275 H 0 0 0 0 0 0 0 0 0 0 0 2
-4.2034 0.4805 0.6956 H 0 0 0 0 0 0 0 0 0 0 0 3
-0.4038 -1.1692 0.0028 C 0 0 0 0 0 0 0 0 0 0 0 4
0.9809 -1.2055 -0.0037 C 0 0 0 0 0 0 0 0 0 0 0 5
1.7195 -0.0085 -0.0075 C 0 0 0 0 0 0 0 0 0 0 0 6
1.0017 1.2034 -0.0079 C 0 0 0 0 0 0 0 0 0 0 0 7
-0.3816 1.1920 -0.0009 C 0 0 0 0 0 0 0 0 0 0 0 8
-1.0495 0.0168 0.0047 N 0 0 0 0 0 0 0 0 0 0 0 9
3.2176 -0.0155 0.0060 C 0 0 0 0 0 0 0 0 0 0 0 10
-1.0260 -2.0621 0.0044 H 0 0 0 0 0 0 0 0 0 0 0 11
1.4840 -2.1719 -0.0078 H 0 0 0 0 0 0 0 0 0 0 0 12
1.5218 2.1609 -0.0155 H 0 0 0 0 0 0 0 0 0 0 0 13
-0.9876 2.0959 -0.0010 H 0 0 0 0 0 0 0 0 0 0 0 14
-2.1106 0.0250 0.0064 H 0 0 0 0 0 0 0 0 0 0 0 15
3.6202 0.7133 -0.7112 H 0 0 0 0 0 0 0 0 0 0 0 16
3.6189 -1.0095 -0.2243 H 0 0 0 0 0 0 0 0 0 0 0 17
3.5826 0.2794 1.0028 H 0 0 0 0 0 0 0 0 0 0 0 18
2 1 0 0 0 0 0
3 1 0 0 0 0 0
5 4 0 0 0 0 0
9 4 0 0 0 0 0
11 4 0 0 0 0 0
6 5 0 0 0 0 0
12 5 0 0 0 0 0
7 6 0 0 0 0 0
10 6 0 0 0 0 0
8 7 0 0 0 0 0
13 7 0 0 0 0 0
9 8 0 0 0 0 0
14 8 0 0 0 0 0
15 9 0 0 0 0 0
16 10 0 0 0 0 0
17 10 0 0 0 0 0
10 18 0 0 0 0 0
M END
\$\$\$\$
4-nitroaniline-cation1.sdf
COSMOTHERM 3D 0

20 19 0 0 0 0 0 0 0 0 0 V2000
-1.3645 4.2122 -0.4517 O 0 0 0 0 0 0 0 0 0 0 0 1
-1.2480 4.7864 -1.2315 H 0 0 0 0 0 0 0 0 0 0 0 2
-1.7344 4.7970 0.2357 H 0 0 0 0 0 0 0 0 0 0 0 3
-0.0340 -0.5776 1.2644 C 0 0 0 0 0 0 0 0 0 0 0 4
0.2390 0.7854 1.3632 C 0 0 0 0 0 0 0 0 0 0 0 5
0.5918 1.4922 0.2134 C 0 0 0 0 0 0 0 0 0 0 0 6
0.6786 0.8771 -1.0367 C 0 0 0 0 0 0 0 0 0 0 0 7
0.4041 -0.4846 -1.1415 C 0 0 0 0 0 0 0 0 0 0 0 8
0.0527 -1.1890 0.0124 C 0 0 0 0 0 0 0 0 0 0 0 9
-0.2320 -2.6365 -0.0950 N 0 0 0 0 0 0 0 0 0 0 0 10
0.8474 2.9311 0.3128 N 0 0 0 0 0 0 0 0 0 0 0 11
-0.4979 -3.2577 0.9441 O 0 0 0 0 0 0 0 0 0 0 0 12
-0.1911 -3.1575 -1.2189 O 0 0 0 0 0 0 0 0 0 0 0 13
1.6342 3.2187 -0.2848 H 0 0 0 0 0 0 0 0 0 0 0 14
1.0929 3.2048 1.2734 H 0 0 0 0 0 0 0 0 0 0 0 15
-0.3068 -1.1555 2.1451 H 0 0 0 0 0 0 0 0 0 0 0 16
0.1802 1.2867 2.3298 H 0 0 0 0 0 0 0 0 0 0 0 17
0.9609 1.4474 -1.9219 H 0 0 0 0 0 0 0 0 0 0 0 18
0.4668 -0.9926 -2.1017 H 0 0 0 0 0 0 0 0 0 0 0 19
-0.0263 3.5135 0.0154 H 0 0 0 0 0 0 0 0 0 0 0 20
2 1 0 0 0 0 0
3 1 0 0 0 0 0
5 4 0 0 0 0 0
9 4 0 0 0 0 0
16 4 0 0 0 0 0
6 5 0 0 0 0 0
17 5 0 0 0 0 0
7 6 0 0 0 0 0

```
11 6 0 0 0 0
8 7 0 0 0 0
18 7 0 0 0 0
9 8 0 0 0 0
19 8 0 0 0 0
10 9 0 0 0 0
12 10 0 0 0 0
13 10 0 0 0 0
14 11 0 0 0 0
15 11 0 0 0 0
11 20 0 0 0 0
M END
$$$$
4-nitroaniline1.sdf
COSMOTHERM 3D 0

19 18 0 0 0 0 0 0 0 0 0 V2000
-1.0217 0.0017 4.9205 O 0 0 0 0 0 0 0 0 0 0 1
-1.5558 -0.8099 4.9918 H 0 0 0 0 0 0 0 0 0 0 2
-1.6792 0.7200 4.8989 H 0 0 0 0 0 0 0 0 0 0 3
1.3461 0.0056 -0.8656 C 0 0 0 0 0 0 0 0 0 0 4
1.6665 0.0069 0.4769 C 0 0 0 0 0 0 0 0 0 0 5
0.6441 0.0019 1.4715 C 0 0 0 0 0 0 0 0 0 0 6
-0.7167 -0.0044 1.0423 C 0 0 0 0 0 0 0 0 0 0 7
-1.0338 -0.0039 -0.3011 C 0 0 0 0 0 0 0 0 0 0 8
-0.0058 0.0001 -1.2660 C 0 0 0 0 0 0 0 0 0 0 9
0.9522 0.0023 2.7864 N 0 0 0 0 0 0 0 0 0 0 10
-0.3367 -0.0008 -2.6607 N 0 0 0 0 0 0 0 0 0 0 11
-1.5459 0.0135 -3.0015 O 0 0 0 0 0 0 0 0 0 0 12
0.5915 -0.0165 -3.5079 O 0 0 0 0 0 0 0 0 0 0 13
0.2233 0.0021 3.5151 H 0 0 0 0 0 0 0 0 0 0 14
1.9231 0.0084 3.0834 H 0 0 0 0 0 0 0 0 0 0 15
2.1306 0.0098 -1.6208 H 0 0 0 0 0 0 0 0 0 0 16
2.7125 0.0124 0.7878 H 0 0 0 0 0 0 0 0 0 0 17
-1.5115 -0.0093 1.7899 H 0 0 0 0 0 0 0 0 0 0 18
-2.0741 -0.0084 -0.6226 H 0 0 0 0 0 0 0 0 0 0 19

2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
9 4 0 0 0 0
16 4 0 0 0 0
6 5 0 0 0 0
17 5 0 0 0 0
7 6 0 0 0 0
10 6 0 0 0 0
8 7 0 0 0 0
18 7 0 0 0 0
9 8 0 0 0 0
11 9 0 0 0 0
14 10 0 0 0 0
15 10 0 0 0 0
12 11 0 0 0 0
13 11 0 0 0 0
8 19 0 0 0 0
M END
$$$$
aniline-cation.sdf
COSMOTHERM 3D 0

18 17 0 0 0 0 0 0 0 0 0 V2000
-0.9194 -0.3289 -3.2766 O 0 0 0 0 0 0 0 0 0 0 1
-0.5812 -0.9004 -3.9908 H 0 0 0 0 0 0 0 0 0 0 2
-1.3774 0.3981 -3.7378 H 0 0 0 0 0 0 0 0 0 0 3
-0.4874 1.0331 1.8729 C 0 0 0 0 0 0 0 0 0 0 4
0.0025 1.2827 0.5862 C 0 0 0 0 0 0 0 0 0 0 5
0.4900 0.2156 -0.1660 C 0 0 0 0 0 0 0 0 0 0 6
0.5032 -1.0890 0.3271 C 0 0 0 0 0 0 0 0 0 0 7
0.0115 -1.3259 1.6143 C 0 0 0 0 0 0 0 0 0 0 8
-0.4831 -0.2680 2.3867 C 0 0 0 0 0 0 0 0 0 0 9
0.9804 0.4670 -1.5304 N 0 0 0 0 0 0 0 0 0 0 10
-0.8706 1.8601 2.4717 H 0 0 0 0 0 0 0 0 0 0 11
0.0041 2.2954 0.1783 H 0 0 0 0 0 0 0 0 0 0 12
0.8962 -1.9075 -0.2779 H 0 0 0 0 0 0 0 0 0 0 13
0.0203 -2.3408 2.0138 H 0 0 0 0 0 0 0 0 0 0 14
-0.8610 -0.4585 3.3922 H 0 0 0 0 0 0 0 0 0 0 15
1.8495 -0.0493 -1.7224 H 0 0 0 0 0 0 0 0 0 0 16
1.1970 1.4620 -1.6724 H 0 0 0 0 0 0 0 0 0 0 17
0.2566 0.1775 -2.2779 H 0 0 0 0 0 0 0 0 0 0 18

2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
9 4 0 0 0 0
11 4 0 0 0 0
6 5 0 0 0 0
12 5 0 0 0 0
7 6 0 0 0 0
10 6 0 0 0 0
8 7 0 0 0 0
13 7 0 0 0 0
9 8 0 0 0 0
14 8 0 0 0 0
15 9 0 0 0 0
16 10 0 0 0 0
17 10 0 0 0 0
10 18 0 0 0 0
M END
$$$$
aniline.sdf
COSMOTHERM 3D 0

17 16 0 0 0 0 0 0 0 0 0 V2000
-3.4772 0.9917 -0.0927 O 0 0 0 0 0 0 0 0 0 0 1
-2.7842 0.2776 -0.0125 H 0 0 0 0 0 0 0 0 0 0 2
-3.4177 1.4813 0.7459 H 0 0 0 0 0 0 0 0 0 0 3
1.7135 0.2509 -1.2279 C 0 0 0 0 0 0 0 0 0 0 4
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0.4379 -0.3194 -1.1983 C 0 0 0 0 0 0 0 0 0 0 0 5
-0.1963 -0.5777 0.0315 C 0 0 0 0 0 0 0 0 0 0 0 6
0.4742 -0.2532 1.2257 C 0 0 0 0 0 0 0 0 0 0 0 7
1.7494 0.3175 1.1858 C 0 0 0 0 0 0 0 0 0 0 0 8
2.3798 0.5743 -0.0386 C 0 0 0 0 0 0 0 0 0 0 0 9
-1.5133 -1.0891 0.0649 N 0 0 0 0 0 0 0 0 0 0 0 10
2.1912 0.4400 -2.1914 H 0 0 0 0 0 0 0 0 0 0 0 11
-0.0732 -0.5692 -2.1310 H 0 0 0 0 0 0 0 0 0 0 0 12
-0.0081 -0.4520 2.1858 H 0 0 0 0 0 0 0 0 0 0 0 13
2.2557 0.5577 2.1230 H 0 0 0 0 0 0 0 0 0 0 0 14
3.3762 1.0178 -0.0655 H 0 0 0 0 0 0 0 0 0 0 0 15
-1.7275 -1.6034 0.9204 H 0 0 0 0 0 0 0 0 0 0 0 16
-1.7446 -1.6669 -0.7447 H 0 0 0 0 0 0 0 0 0 0 0 17
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
9 4 0 0 0 0
11 4 0 0 0 0
6 5 0 0 0 0
12 5 0 0 0 0
7 6 0 0 0 0
10 6 0 0 0 0
8 7 0 0 0 0
13 7 0 0 0 0
9 8 0 0 0 0
14 8 0 0 0 0
15 9 0 0 0 0
16 10 0 0 0 0
10 17 0 0 0 0
M END
$$$$
benzimidazole.sdf
COSMOtherm 3D 0
18 18 0 0 0 0 0 0 0 0 0 V2000
-3.7844 1.1119 -0.0707 O 0 0 0 0 0 0 0 0 0 0 0 1
-2.9237 0.5993 -0.0261 H 0 0 0 0 0 0 0 0 0 0 0 2
-3.8689 1.5177 0.8092 H 0 0 0 0 0 0 0 0 0 0 0 3
2.2409 -0.6270 -0.0113 C 0 0 0 0 0 0 0 0 0 0 0 4
0.8601 -0.8534 -0.0019 C 0 0 0 0 0 0 0 0 0 0 0 5
-0.0860 0.2076 0.0088 C 0 0 0 0 0 0 0 0 0 0 0 6
0.3517 1.5410 0.0104 C 0 0 0 0 0 0 0 0 0 0 0 7
1.7278 1.7723 0.0013 C 0 0 0 0 0 0 0 0 0 0 0 8
2.6564 0.7062 -0.0090 C 0 0 0 0 0 0 0 0 0 0 0 9
-1.3781 -0.3182 0.0174 N 0 0 0 0 0 0 0 0 0 0 0 10
0.0956 -2.0091 -0.0004 N 0 0 0 0 0 0 0 0 0 0 0 11
-1.2177 -1.6339 0.0110 C 0 0 0 0 0 0 0 0 0 0 0 12
2.9586 -1.4482 -0.0198 H 0 0 0 0 0 0 0 0 0 0 0 13
-0.3639 2.3646 0.0179 H 0 0 0 0 0 0 0 0 0 0 0 14
2.0988 2.7986 0.0025 H 0 0 0 0 0 0 0 0 0 0 0 15
3.7243 0.9306 -0.0160 H 0 0 0 0 0 0 0 0 0 0 0 16
0.4365 -2.9672 -0.0057 H 0 0 0 0 0 0 0 0 0 0 0 17
-2.0214 -2.3653 0.0146 H 0 0 0 0 0 0 0 0 0 0 0 18
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
9 4 0 0 0 0
13 4 0 0 0 0
6 5 0 0 0 0
11 5 0 0 0 0
7 6 0 0 0 0
10 6 0 0 0 0
8 7 0 0 0 0
14 7 0 0 0 0
9 8 0 0 0 0
15 8 0 0 0 0
16 9 0 0 0 0
12 10 0 0 0 0
12 11 0 0 0 0
17 11 0 0 0 0
12 18 0 0 0 0
M END
$$$$
benzimidazole-cation.sdf
COSMOtherm 3D 0
19 19 0 0 0 0 0 0 0 0 0 V2000
-3.7170 0.0009 -1.0375 O 0 0 0 0 0 0 0 0 0 0 0 1
-3.9078 -0.7689 -1.6039 H 0 0 0 0 0 0 0 0 0 0 0 2
-3.9155 0.7769 -1.5926 H 0 0 0 0 0 0 0 0 0 0 0 3
-1.2673 -0.0008 1.5890 C 0 0 0 0 0 0 0 0 0 0 0 4
-1.3327 -0.0014 0.2548 N 0 0 0 0 0 0 0 0 0 0 0 5
-0.0364 -0.0008 -0.2579 C 0 0 0 0 0 0 0 0 0 0 0 6
0.8358 -0.0005 0.8545 C 0 0 0 0 0 0 0 0 0 0 0 7
0.0153 0.0006 1.9795 N 0 0 0 0 0 0 0 0 0 0 0 8
0.4503 -0.0002 -1.5690 C 0 0 0 0 0 0 0 0 0 0 0 9
1.8365 -0.0006 -1.7180 C 0 0 0 0 0 0 0 0 0 0 0 10
2.7067 0.0004 -0.6044 C 0 0 0 0 0 0 0 0 0 0 0 11
2.2251 0.0015 0.7041 C 0 0 0 0 0 0 0 0 0 0 0 12
-2.1178 -0.0008 2.2616 H 0 0 0 0 0 0 0 0 0 0 0 13
-2.2358 0.0000 -0.2996 H 0 0 0 0 0 0 0 0 0 0 0 14
-0.2191 -0.0004 -2.4286 H 0 0 0 0 0 0 0 0 0 0 0 15
2.2621 -0.0001 -2.7221 H 0 0 0 0 0 0 0 0 0 0 0 16
3.7841 0.0022 -0.7733 H 0 0 0 0 0 0 0 0 0 0 0 17
2.8938 0.0028 1.5643 H 0 0 0 0 0 0 0 0 0 0 0 18
0.3190 -0.0010 2.9515 H 0 0 0 0 0 0 0 0 0 0 0 19
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
8 4 0 0 0 0
13 4 0 0 0 0
6 5 0 0 0 0
14 5 0 0 0 0
7 6 0 0 0 0
9 6 0 0 0 0
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  8  7  0  0  0  0
 12  7  0  0  0  0
 10  9  0  0  0  0
 15  9  0  0  0  0
 11 10  0  0  0  0
 16 10  0  0  0  0
 12 11  0  0  0  0
 17 11  0  0  0  0
 18 12  0  0  0  0
  8 19  0  0  0  0
M  END
$$$$
clonidine-cation2.sdf
COSMOtherm          3D          0

27 27  0  0  0  0  0  0  0  0  0  0 V2000
 1.8027 -1.9601  2.4012 O  0  0  0  0  0  0  0  0  0  0  1
 1.8325 -1.6945  3.3384 H  0  0  0  0  0  0  0  0  0  0  2
 1.7088 -2.9297  2.4184 H  0  0  0  0  0  0  0  0  0  0  3
-2.6505  1.6329 -0.0583 C  0  0  0  0  0  0  0  0  0  0  4
-1.3378  1.3127  0.2870 C  0  0  0  0  0  0  0  0  0  0  5
-0.8399 -0.0010  0.1692 C  0  0  0  0  0  0  0  0  0  0  6
-1.7333 -0.9926 -0.2840 C  0  0  0  0  0  0  0  0  0  0  7
-3.0548 -0.6965 -0.6141 C  0  0  0  0  0  0  0  0  0  0  8
-3.5034  0.6215 -0.5045 C  0  0  0  0  0  0  0  0  0  0  9
-0.2865  2.5852  0.9040 Cl  0  0  0  0  0  0  0  0  0  0 10
-1.1642 -2.6522 -0.4315 Cl  0  0  0  0  0  0  0  0  0  0 11
 0.4874 -0.3341  0.5391 N  0  0  0  0  0  0  0  0  0  0 12
 1.5747  0.0058 -0.1736 C  0  0  0  0  0  0  0  0  0  0 13
 3.7745  0.0016 -0.8620 C  0  0  0  0  0  0  0  0  0  0 14
 2.9643  0.9787 -1.7387 C  0  0  0  0  0  0  0  0  0  0 15
 2.8265 -0.2620  0.2385 N  0  0  0  0  0  0  0  0  0  0 16
 1.5779  0.6241 -1.3664 N  0  0  0  0  0  0  0  0  0  0 17
 2.9807 -0.9616  0.9697 H  0  0  0  0  0  0  0  0  0  0 18
 0.7714  1.1243 -1.7293 H  0  0  0  0  0  0  0  0  0  0 19
-3.0036  2.6585  0.0402 H  0  0  0  0  0  0  0  0  0  0 20
-3.7206 -1.4866 -0.9586 H  0  0  0  0  0  0  0  0  0  0 21
-4.5336  0.8635 -0.7666 H  0  0  0  0  0  0  0  0  0  0 22
 4.0064 -0.9311 -1.3977 H  0  0  0  0  0  0  0  0  0  0 23
 4.7004  0.4452 -0.4824 H  0  0  0  0  0  0  0  0  0  0 24
 3.1692  2.0283 -1.4814 H  0  0  0  0  0  0  0  0  0  0 25
 3.1290  0.8249 -2.8097 H  0  0  0  0  0  0  0  0  0  0 26
 0.6673 -0.9771  1.3349 H  0  0  0  0  0  0  0  0  0  0 27
 2  1  0  0  0  0
 3  1  0  0  0  0
 5  4  0  0  0  0
 9  4  0  0  0  0
20  4  0  0  0  0
 6  5  0  0  0  0
10  5  0  0  0  0
 7  6  0  0  0  0
12  6  0  0  0  0
 8  7  0  0  0  0
11  7  0  0  0  0
 9  8  0  0  0  0
21  8  0  0  0  0
22  9  0  0  0  0
13 12  0  0  0  0
16 13  0  0  0  0
17 13  0  0  0  0
15 14  0  0  0  0
16 14  0  0  0  0
23 14  0  0  0  0
24 14  0  0  0  0
17 15  0  0  0  0
25 15  0  0  0  0
26 15  0  0  0  0
18 16  0  0  0  0
19 17  0  0  0  0
12 27  0  0  0  0
M  END
$$$$
clonidine.sdf
COSMOtherm          3D          0

26 26  0  0  0  0  0  0  0  0  0  0 V2000
-2.2157  2.4338  1.3631 O  0  0  0  0  0  0  0  0  0  0  1
-1.5941  1.7934  0.9011 H  0  0  0  0  0  0  0  0  0  0  2
-3.1023  2.0588  1.2213 H  0  0  0  0  0  0  0  0  0  0  3
-0.3167  0.3478  2.8317 N  0  0  0  0  0  0  0  0  0  0  4
-0.0339 -0.1052  1.5653 C  0  0  0  0  0  0  0  0  0  0  5
 0.5724 -1.3349  1.6623 N  0  0  0  0  0  0  0  0  0  0  6
-0.5847 -0.6395 -3.0386 C  0  0  0  0  0  0  0  0  0  0  7
-0.9176 -0.3132 -1.7255 C  0  0  0  0  0  0  0  0  0  0  8
 0.0274  0.1485 -0.7760 C  0  0  0  0  0  0  0  0  0  0  9
 1.3536  0.2655 -1.2634 C  0  0  0  0  0  0  0  0  0  0 10
 1.7183 -0.0597 -2.5693 C  0  0  0  0  0  0  0  0  0  0 11
 0.7420 -0.5127 -3.4597 C  0  0  0  0  0  0  0  0  0  0 12
 2.6075  0.8817 -0.1719 Cl  0  0  0  0  0  0  0  0  0  0 13
-2.6030 -0.4876 -1.2128 Cl  0  0  0  0  0  0  0  0  0  0 14
-0.3683  0.5677  0.4912 N  0  0  0  0  0  0  0  0  0  0 15
-0.1294 -0.7461  3.7990 C  0  0  0  0  0  0  0  0  0  0 16
 0.9152 -1.6085  3.0705 C  0  0  0  0  0  0  0  0  0  0 17
-1.0953  1.0015  2.9273 H  0  0  0  0  0  0  0  0  0  0 18
 1.1985 -1.6406  0.9219 H  0  0  0  0  0  0  0  0  0  0 19
-1.3561 -0.9912 -3.7233 H  0  0  0  0  0  0  0  0  0  0 20
 2.7545  0.0527 -2.8871 H  0  0  0  0  0  0  0  0  0  0 21
 1.0147 -0.7644 -4.4847 H  0  0  0  0  0  0  0  0  0  0 22
-1.0671 -1.3049  3.9559 H  0  0  0  0  0  0  0  0  0  0 23
 0.2317 -0.3705  4.7629 H  0  0  0  0  0  0  0  0  0  0 24
 0.8209 -2.6754  3.3014 H  0  0  0  0  0  0  0  0  0  0 25
 1.9404 -1.2757  3.3004 H  0  0  0  0  0  0  0  0  0  0 26
 2  1  0  0  0  0
 3  1  0  0  0  0
 5  4  0  0  0  0
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16 4 0 0 0 0
18 4 0 0 0 0
6 5 0 0 0 0
15 5 0 0 0 0
17 6 0 0 0 0
19 6 0 0 0 0
8 7 0 0 0 0
12 7 0 0 0 0
20 7 0 0 0 0
9 8 0 0 0 0
14 8 0 0 0 0
10 9 0 0 0 0
15 9 0 0 0 0
11 10 0 0 0 0
13 10 0 0 0 0
12 11 0 0 0 0
21 11 0 0 0 0
22 12 0 0 0 0
17 16 0 0 0 0
23 16 0 0 0 0
24 16 0 0 0 0
25 17 0 0 0 0
17 26 0 0 0 0
M END
$$$$
clonidine-cation.sdf
COSMOtherm 3D 0
27 27 0 0 0 0 0 0 0 0 0 V2000
-1.7823 2.3939 -1.9839 O 0 0 0 0 0 0 0 0 0 0 1
-1.6918 2.3996 -2.9540 H 0 0 0 0 0 0 0 0 0 0 2
-1.8014 3.3341 -1.7285 H 0 0 0 0 0 0 0 0 0 0 3
0.2524 0.9052 2.5799 Cl 0 0 0 0 0 0 0 0 0 0 4
3.4986 -0.4944 0.6585 C 0 0 0 0 0 0 0 0 0 0 5
2.6315 -0.0499 1.6585 C 0 0 0 0 0 0 0 0 0 0 6
1.3213 0.2890 1.3213 C 0 0 0 0 0 0 0 0 0 0 7
0.8397 0.1660 0.0018 C 0 0 0 0 0 0 0 0 0 0 8
1.7474 -0.2846 -0.9778 C 0 0 0 0 0 0 0 0 0 0 9
3.0664 -0.6087 -0.6646 C 0 0 0 0 0 0 0 0 0 0 10
1.1989 -0.4382 -2.6437 Cl 0 0 0 0 0 0 0 0 0 0 11
-0.4843 0.5308 -0.3484 N 0 0 0 0 0 0 0 0 0 0 12
-1.5749 -0.1765 -0.0093 C 0 0 0 0 0 0 0 0 0 0 13
-2.8243 0.2388 -0.2828 N 0 0 0 0 0 0 0 0 0 0 14
-1.5844 -1.3676 0.6129 N 0 0 0 0 0 0 0 0 0 0 15
-3.7782 -0.8553 -0.0145 C 0 0 0 0 0 0 0 0 0 0 16
-2.9733 -1.7310 0.9680 C 0 0 0 0 0 0 0 0 0 0 17
4.5269 -0.7518 0.9135 H 0 0 0 0 0 0 0 0 0 0 18
2.9712 0.0522 2.6884 H 0 0 0 0 0 0 0 0 0 0 19
3.7431 -0.9520 -1.4459 H 0 0 0 0 0 0 0 0 0 0 20
-2.9753 0.9700 -0.9830 H 0 0 0 0 0 0 0 0 0 0 21
-0.7817 -1.7292 1.1201 H 0 0 0 0 0 0 0 0 0 0 22
-4.0116 -1.3947 -0.9447 H 0 0 0 0 0 0 0 0 0 0 23
-4.7027 -0.4686 0.4260 H 0 0 0 0 0 0 0 0 0 0 24
-3.1433 -2.8019 0.8194 H 0 0 0 0 0 0 0 0 0 0 25
-3.1780 -1.4671 2.0160 H 0 0 0 0 0 0 0 0 0 0 26
-0.6590 1.3256 -0.9944 H 0 0 0 0 0 0 0 0 0 0 27
2 1 0 0 0 0
3 1 0 0 0 0
7 4 0 0 0 0
6 5 0 0 0 0
10 5 0 0 0 0
18 5 0 0 0 0
7 6 0 0 0 0
19 6 0 0 0 0
8 7 0 0 0 0
9 8 0 0 0 0
12 8 0 0 0 0
10 9 0 0 0 0
11 9 0 0 0 0
20 10 0 0 0 0
13 12 0 0 0 0
14 13 0 0 0 0
15 13 0 0 0 0
16 14 0 0 0 0
21 14 0 0 0 0
17 15 0 0 0 0
22 15 0 0 0 0
17 16 0 0 0 0
23 16 0 0 0 0
24 16 0 0 0 0
25 17 0 0 0 0
26 17 0 0 0 0
12 27 0 0 0 0
M END
$$$$
clonidine_t_p3.sdf
COSMOtherm 3D 0
27 27 0 0 0 0 0 0 0 0 0 V2000
-2.4431 1.8145 1.8993 O 0 0 0 0 0 0 0 0 0 0 1
-2.4633 1.7240 2.8692 H 0 0 0 0 0 0 0 0 0 0 2
-3.3796 1.8275 1.6304 H 0 0 0 0 0 0 0 0 0 0 3
1.7686 2.9508 -0.9573 C 0 0 0 0 0 0 0 0 0 0 4
0.8684 3.7714 -0.0109 C 0 0 0 0 0 0 0 0 0 0 5
1.3801 1.5689 -0.6042 N 0 0 0 0 0 0 0 0 0 0 6
-0.8934 -0.3148 -2.5923 Cl 0 0 0 0 0 0 0 0 0 0 7
0.5153 -3.5059 -0.5874 C 0 0 0 0 0 0 0 0 0 0 8
0.0689 -2.6662 -1.6097 C 0 0 0 0 0 0 0 0 0 0 9
-0.2816 -1.3513 -1.3055 C 0 0 0 0 0 0 0 0 0 0 10
-0.1718 -0.8390 0.0035 C 0 0 0 0 0 0 0 0 0 0 11
0.2802 -1.7196 1.0067 C 0 0 0 0 0 0 0 0 0 0 12
0.6189 -3.0424 0.7260 C 0 0 0 0 0 0 0 0 0 0 13
0.4183 -1.1320 2.6605 Cl 0 0 0 0 0 0 0 0 0 0 14
-0.5474 0.4909 0.3193 N 0 0 0 0 0 0 0 0 0 0 15
0.1743 1.5737 -0.0137 C 0 0 0 0 0 0 0 0 0 0 16
```

[illegible]

		1.7285	0.0694	-1.2808	C	0	0	0	0	0	0	0	0	0	0	9
		-1.6660	-1.1297	0.0598	N	0	0	0	0	0	0	0	0	0	0	10
		-1.9406	-1.7243	-0.7292	H	0	0	0	0	0	0	0	0	0	0	11
		-1.9280	-1.6530	0.9018	H	0	0	0	0	0	0	0	0	0	0	12
		1.7197	1.8670	-0.0711	H	0	0	0	0	0	0	0	0	0	0	13
		3.2664	1.0071	-0.0565	H	0	0	0	0	0	0	0	0	0	0	14
		2.2993	-0.7997	1.3453	H	0	0	0	0	0	0	0	0	0	0	15
		2.0287	0.7609	2.1316	H	0	0	0	0	0	0	0	0	0	0	16
		-0.3156	0.8266	1.2838	H	0	0	0	0	0	0	0	0	0	0	17
		-0.0386	-0.6720	2.1898	H	0	0	0	0	0	0	0	0	0	0	18
		0.3284	-1.9065	0.0705	H	0	0	0	0	0	0	0	0	0	0	19
		-0.3416	0.7349	-1.3197	H	0	0	0	0	0	0	0	0	0	0	20
		-0.0751	-0.8222	-2.1247	H	0	0	0	0	0	0	0	0	0	0	21
		2.2778	-0.8876	-1.3175	H	0	0	0	0	0	0	0	0	0	0	22
		1.9889	0.6167	-2.2006	H	0	0	0	0	0	0	0	0	0	0	23
	2	1	0	0	0											
	3	1	0	0	0											
	5	4	0	0	0											
	9	4	0	0	0											
	13	4	0	0	0											
	14	4	0	0	0											
	6	5	0	0	0											
	15	5	0	0	0											
	16	5	0	0	0											
	7	6	0	0	0											
	17	6	0	0	0											
	18	6	0	0	0											
	8	7	0	0	0											
	10	7	0	0	0											
	19	7	0	0	0											
	9	8	0	0	0											
	20	8	0	0	0											
	21	8	0	0	0											
	22	9	0	0	0											
	11	10	0	0	0											
	12	10	0	0	0											
	9	23	0	0	0											
M																
\$\$\$\$																
debrisoquine.sdf																
COSMOTHERM					3D											0
29	29	0	0	0	0	0	0	0	0	V2000						
-3.3937			0.4642		-0.5125	O	0	0	0	0	0	0	0	0	0	1

29	29	0	0	0	0	0	0	0	V2000											
-3.0390	-0.0050	-0.7814	O	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	
-2.4539	-0.8002	-0.5493	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	2		
-2.4706	0.7652	-0.5984	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	3		
0.3613	3.3672	-0.6303	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	4		
-0.6758	3.2120	0.2984	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	5		
-0.8492	1.9819	0.9391	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	6		
-0.0035	0.8955	0.6571	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	7		
1.0449	1.0500	-0.2713	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	8		
1.2104	2.2928	-0.9066	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	9		
-0.2059	-0.4234	1.3858	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	10		
1.9737	-0.1059	-0.5916	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	11		
1.8874	-1.2226	0.4564	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	12		
0.4787	-1.5447	0.7417	N	0	0	0	0	0	0	0	0	0	0	0	0	0	0	13		
-0.2436	-2.4075	-0.0648	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	14		
0.4953	-3.4272	-0.6467	N	0	0	0	0	0	0	0	0	0	0	0	0	0	0	15		
-1.5281	-2.2391	-0.2574	N	0	0	0	0	0	0	0	0	0	0	0	0	0	0	16		
0.5086	4.3235	-1.1357	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	17		
-1.3446	4.0449	0.5235	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	18		
-1.6519	1.8595	1.6714	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	19		
2.0243	2.4173	-1.6258	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	20		
-1.2726	-0.6627	1.4643	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	21		
0.1885	-0.3351	2.4133	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	22		
3.0115	0.2545	-0.6671	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	23		
1.7169	-0.5215	-1.5813	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	24		
2.3423	-0.8979	1.4045	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	25		
2.4336	-2.1106	0.1229	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	26		
-0.0608	-4.1553	-1.0886	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	27		
1.2703	-3.8066	-0.1062	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	28		
-1.9243	-3.0472	-0.7479	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	29		
2	1	0	0	0	0															
3	1	0	0	0	0															

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8 7 0 0 0 0
10 7 0 0 0 0
9 8 0 0 0 0
11 8 0 0 0 0
20 9 0 0 0 0
13 10 0 0 0 0
21 10 0 0 0 0
22 10 0 0 0 0
12 11 0 0 0 0
23 11 0 0 0 0
24 11 0 0 0 0
13 12 0 0 0 0
25 12 0 0 0 0
26 12 0 0 0 0
14 13 0 0 0 0
15 14 0 0 0 0
16 14 0 0 0 0
27 15 0 0 0 0
28 15 0 0 0 0
29 16 0 0 0 0
16 30 0 0 0 0
M END
$$$$
debrisoquine_p2.sdf
COSMOTHERM 3D 0

30 30 0 0 0 0 0 0 0 0 0 V2000
-5.3329 0.7293 -0.5254 O 0 0 0 0 0 0 0 0 0 0 1
-6.1068 0.1406 -0.5842 H 0 0 0 0 0 0 0 0 0 0 2
-5.6819 1.6247 -0.6848 H 0 0 0 0 0 0 0 0 0 0 3
3.1833 0.5324 0.9989 C 0 0 0 0 0 0 0 0 0 0 4
1.8590 0.1344 0.7455 C 0 0 0 0 0 0 0 0 0 0 5
1.4918 -0.2101 -0.5676 C 0 0 0 0 0 0 0 0 0 0 6
2.4479 -0.1567 -1.5956 C 0 0 0 0 0 0 0 0 0 0 7
3.7589 0.2418 -1.3320 C 0 0 0 0 0 0 0 0 0 0 8
4.1288 0.5903 -0.0260 C 0 0 0 0 0 0 0 0 0 0 9
0.8439 0.0718 1.8667 C 0 0 0 0 0 0 0 0 0 0 10
-0.3085 -0.8605 1.5059 C 0 0 0 0 0 0 0 0 0 0 11
0.0819 -0.6498 -0.9289 C 0 0 0 0 0 0 0 0 0 0 12
-0.8551 -0.4923 0.1893 N 0 0 0 0 0 0 0 0 0 0 13
-2.1413 -0.1527 -0.0095 C 0 0 0 0 0 0 0 0 0 0 14
-2.9561 0.1407 1.0245 N 0 0 0 0 0 0 0 0 0 0 15
-2.6541 -0.0929 -1.2540 N 0 0 0 0 0 0 0 0 0 0 16
3.4711 0.7949 2.0201 H 0 0 0 0 0 0 0 0 0 0 17
2.1573 -0.4278 -2.6139 H 0 0 0 0 0 0 0 0 0 0 18
4.4898 0.2815 -2.1415 H 0 0 0 0 0 0 0 0 0 0 19
5.1523 0.9010 0.1914 H 0 0 0 0 0 0 0 0 0 0 20
0.4510 1.0799 2.0805 H 0 0 0 0 0 0 0 0 0 0 21
1.3217 -0.2844 2.7912 H 0 0 0 0 0 0 0 0 0 0 22
-1.1006 -0.8426 2.2606 H 0 0 0 0 0 0 0 0 0 0 23
0.0486 -1.9008 1.4354 H 0 0 0 0 0 0 0 0 0 0 24
0.0914 -1.7025 -1.2630 H 0 0 0 0 0 0 0 0 0 0 25
-0.2710 -0.0381 -1.7698 H 0 0 0 0 0 0 0 0 0 0 26
-3.9189 0.4122 0.7919 H 0 0 0 0 0 0 0 0 0 0 27
-2.5736 0.5027 1.8918 H 0 0 0 0 0 0 0 0 0 0 28
-3.6386 0.1871 -1.3412 H 0 0 0 0 0 0 0 0 0 0 29
-2.2638 -0.6592 -2.0001 H 0 0 0 0 0 0 0 0 0 0 30
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
9 4 0 0 0 0
17 4 0 0 0 0
6 5 0 0 0 0
10 5 0 0 0 0
7 6 0 0 0 0
12 6 0 0 0 0
8 7 0 0 0 0
18 7 0 0 0 0
9 8 0 0 0 0
19 8 0 0 0 0
20 9 0 0 0 0
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21 10 0 0 0 0
22 10 0 0 0 0
13 11 0 0 0 0
23 11 0 0 0 0
24 11 0 0 0 0
13 12 0 0 0 0
25 12 0 0 0 0
26 12 0 0 0 0
14 13 0 0 0 0
15 14 0 0 0 0
16 14 0 0 0 0
27 15 0 0 0 0
28 15 0 0 0 0
29 16 0 0 0 0
16 30 0 0 0 0
M END
$$$$
di-iso-butylamine-cation.sdf
COSMOTHERM 3D 0

32 30 0 0 0 0 0 0 0 0 0 V2000
-2.4904 0.0684 -0.6627 O 0 0 0 0 0 0 0 0 0 0 1
-3.2283 0.1954 -0.0393 H 0 0 0 0 0 0 0 0 0 0 2
-2.7771 -0.6687 -1.2319 H 0 0 0 0 0 0 0 0 0 0 3
1.2532 3.6910 -0.2243 C 0 0 0 0 0 0 0 0 0 0 4
0.5186 2.5003 0.4124 C 0 0 0 0 0 0 0 0 0 0 5
-0.9681 2.8159 0.6252 C 0 0 0 0 0 0 0 0 0 0 6
0.7587 1.2629 -0.4600 C 0 0 0 0 0 0 0 0 0 0 7
0.1842 -0.0011 0.1383 N 0 0 0 0 0 0 0 0 0 0 8
0.7611 -1.2697 -0.4485 C 0 0 0 0 0 0 0 0 0 0 9
0.4889 -2.5064 0.4158 C 0 0 0 0 0 0 0 0 0 0 10
1.2758 -3.6902 -0.1696 C 0 0 0 0 0 0 0 0 0 0 11
-1.0028 -2.8444 0.5426 C 0 0 0 0 0 0 0 0 0 0 12
```



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23 9 0 0 0 0
24 9 0 0 0 0
11 10 0 0 0 0
12 10 0 0 0 0
25 10 0 0 0 0
26 11 0 0 0 0
27 11 0 0 0 0
28 11 0 0 0 0
29 12 0 0 0 0
30 12 0 0 0 0
12 31 0 0 0 0
M END
$$$$
di-iso-propylamine-cation.sdf
COSMOTHERM 3D 0
26 24 0 0 0 0 0 0 0 0 0 V2000
-2.5346 0.2190 -1.0061 O 0 0 0 0 0 0 0 0 0 0 1
-2.9874 1.0395 -0.7396 H 0 0 0 0 0 0 0 0 0 0 2
-3.2134 -0.4756 -0.9257 H 0 0 0 0 0 0 0 0 0 0 3
-0.0240 -0.4241 0.0653 N 0 0 0 0 0 0 0 0 0 0 4
0.1294 0.2545 1.4209 C 0 0 0 0 0 0 0 0 0 0 5
1.0113 -0.1278 -1.0144 C 0 0 0 0 0 0 0 0 0 0 6
0.7034 -1.0221 -2.2135 C 0 0 0 0 0 0 0 0 0 0 7
1.0116 1.3563 -1.3623 C 0 0 0 0 0 0 0 0 0 0 8
1.4835 -0.0699 2.0403 C 0 0 0 0 0 0 0 0 0 0 9
-1.0415 -0.1874 2.2973 C 0 0 0 0 0 0 0 0 0 0 10
-0.0255 -1.4416 0.2240 H 0 0 0 0 0 0 0 0 0 0 11
0.0506 1.3306 1.2195 H 0 0 0 0 0 0 0 0 0 0 12
1.9794 -0.4168 -0.5855 H 0 0 0 0 0 0 0 0 0 0 13
1.4813 -0.8838 -2.9756 H 0 0 0 0 0 0 0 0 0 0 14
0.6931 -2.0849 -1.9312 H 0 0 0 0 0 0 0 0 0 0 15
-0.2666 -0.7644 -2.6639 H 0 0 0 0 0 0 0 0 0 0 16
1.7486 1.5300 -2.1575 H 0 0 0 0 0 0 0 0 0 0 17
1.2924 1.9889 -0.5096 H 0 0 0 0 0 0 0 0 0 0 18
0.0278 1.6789 -1.7342 H 0 0 0 0 0 0 0 0 0 0 19
1.5345 0.3930 3.0347 H 0 0 0 0 0 0 0 0 0 0 20
2.3238 0.3196 1.4509 H 0 0 0 0 0 0 0 0 0 0 21
1.6111 -1.1560 2.1651 H 0 0 0 0 0 0 0 0 0 0 22
-0.9889 0.3378 3.2596 H 0 0 0 0 0 0 0 0 0 0 23
-2.0086 0.0503 1.8329 H 0 0 0 0 0 0 0 0 0 0 24
-1.0008 -1.2691 2.4964 H 0 0 0 0 0 0 0 0 0 0 25
-0.9808 -0.1852 -0.3194 H 0 0 0 0 0 0 0 0 0 0 26
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
11 4 0 0 0 0
9 5 0 0 0 0
10 5 0 0 0 0
12 5 0 0 0 0
7 6 0 0 0 0
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15 7 0 0 0 0
16 7 0 0 0 0
17 8 0 0 0 0
18 8 0 0 0 0
19 8 0 0 0 0
20 9 0 0 0 0
21 9 0 0 0 0
22 9 0 0 0 0
23 10 0 0 0 0
24 10 0 0 0 0
25 10 0 0 0 0
4 26 0 0 0 0
M END
$$$$
di-iso-propylamine.sdf
COSMOTHERM 3D 0
25 23 0 0 0 0 0 0 0 0 0 V2000
-0.3136 -0.0152 0.1632 O 0 0 0 0 0 0 0 0 0 0 1
0.6973 0.0054 0.0870 H 0 0 0 0 0 0 0 0 0 0 2
-0.5107 0.6012 0.8899 H 0 0 0 0 0 0 0 0 0 0 3
2.4800 0.0292 -0.0402 N 0 0 0 0 0 0 0 0 0 0 4
2.9773 1.2355 -0.7614 C 0 0 0 0 0 0 0 0 0 0 5
2.9551 -1.2833 -0.5598 C 0 0 0 0 0 0 0 0 0 0 6
2.7938 -2.3327 0.5425 C 0 0 0 0 0 0 0 0 0 0 7
2.1795 -1.6735 -1.8227 C 0 0 0 0 0 0 0 0 0 0 8
4.4863 1.4690 -0.5862 C 0 0 0 0 0 0 0 0 0 0 9
2.1786 2.4577 -0.2964 C 0 0 0 0 0 0 0 0 0 0 10
2.7879 0.1114 0.9362 H 0 0 0 0 0 0 0 0 0 0 11
2.7661 1.0698 -1.8297 H 0 0 0 0 0 0 0 0 0 0 12
4.0294 -1.2249 -0.8190 H 0 0 0 0 0 0 0 0 0 0 13
3.1270 -3.3180 0.1877 H 0 0 0 0 0 0 0 0 0 0 14
3.3925 -2.0728 1.4294 H 0 0 0 0 0 0 0 0 0 0 15
1.7395 -2.4147 0.8490 H 0 0 0 0 0 0 0 0 0 0 16
1.1134 -1.8212 -1.5922 H 0 0 0 0 0 0 0 0 0 0 17
2.5781 -2.6104 -2.2381 H 0 0 0 0 0 0 0 0 0 0 18
2.2577 -0.9054 -2.6060 H 0 0 0 0 0 0 0 0 0 0 19
4.8115 2.3467 -1.1646 H 0 0 0 0 0 0 0 0 0 0 20
5.0811 0.6087 -0.9247 H 0 0 0 0 0 0 0 0 0 0 21
4.7236 1.6561 0.4736 H 0 0 0 0 0 0 0 0 0 0 22
2.5198 3.3639 -0.8172 H 0 0 0 0 0 0 0 0 0 0 23
1.1055 2.3262 -0.4925 H 0 0 0 0 0 0 0 0 0 0 24
2.3142 2.6204 0.7852 H 0 0 0 0 0 0 0 0 0 0 25
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
11 4 0 0 0 0
9 5 0 0 0 0
10 5 0 0 0 0
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0.9720 -0.2577 -2.4890 H 0 0 0 0 0 0 0 0 0 0 16
-0.6839 0.2849 3.7921 C 0 0 0 0 0 0 0 0 0 0 17
-0.3147 -1.3713 2.4466 H 0 0 0 0 0 0 0 0 0 0 18
1.0044 -0.1919 2.5145 H 0 0 0 0 0 0 0 0 0 0 19
-0.1732 -0.4034 -5.0303 C 0 0 0 0 0 0 0 0 0 0 20
-0.4291 1.3686 -3.8096 H 0 0 0 0 0 0 0 0 0 0 21
-1.7919 0.2488 -3.7462 H 0 0 0 0 0 0 0 0 0 0 22
-0.1367 -0.3936 5.0527 C 0 0 0 0 0 0 0 0 0 0 23
-0.4749 1.3675 3.8364 H 0 0 0 0 0 0 0 0 0 0 24
-1.7824 0.1838 3.7672 H 0 0 0 0 0 0 0 0 0 0 25
-0.5895 0.0516 -5.9413 H 0 0 0 0 0 0 0 0 0 0 26
-0.4480 -1.4697 -5.0325 H 0 0 0 0 0 0 0 0 0 0 27
0.9244 -0.3418 -5.0965 H 0 0 0 0 0 0 0 0 0 0 28
-0.5773 0.0376 5.9639 H 0 0 0 0 0 0 0 0 0 0 29
-0.3592 -1.4721 5.0510 H 0 0 0 0 0 0 0 0 0 0 30
0.9563 -0.2787 5.1224 H 0 0 0 0 0 0 0 0 0 0 31
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
7 4 0 0 0 0
8 4 0 0 0 0
9 4 0 0 0 0
6 5 0 0 0 0
10 5 0 0 0 0
11 6 0 0 0 0
12 6 0 0 0 0
13 6 0 0 0 0
14 7 0 0 0 0
15 7 0 0 0 0
16 7 0 0 0 0
17 13 0 0 0 0
18 13 0 0 0 0
19 13 0 0 0 0
20 14 0 0 0 0
21 14 0 0 0 0
22 14 0 0 0 0
23 17 0 0 0 0
24 17 0 0 0 0
25 17 0 0 0 0
26 20 0 0 0 0
27 20 0 0 0 0
28 20 0 0 0 0
29 23 0 0 0 0
30 23 0 0 0 0
23 31 0 0 0 0
M END
$$$$
di-n-propylamine-cation.sdf
COSMOtherm 3D 0
26 24 0 0 0 0 0 0 0 0 0 0 V2000
-2.6078 0.1605 0.0341 O 0 0 0 0 0 0 0 0 0 0 1
-3.1653 -0.4383 -0.4949 H 0 0 0 0 0 0 0 0 0 0 2
-2.9130 1.0546 -0.2040 H 0 0 0 0 0 0 0 0 0 0 3
0.7153 0.2713 -1.2628 C 0 0 0 0 0 0 0 0 0 0 4
0.1332 -0.3055 0.0010 N 0 0 0 0 0 0 0 0 0 0 5
0.7130 0.2695 1.2668 C 0 0 0 0 0 0 0 0 0 0 6
0.1268 -0.3944 -2.5028 C 0 0 0 0 0 0 0 0 0 0 7
0.5043 1.3486 -1.2433 H 0 0 0 0 0 0 0 0 0 0 8
1.8026 0.1276 -1.2088 H 0 0 0 0 0 0 0 0 0 0 9
0.2872 -1.3228 0.0005 H 0 0 0 0 0 0 0 0 0 0 10
0.4976 1.3460 1.2502 H 0 0 0 0 0 0 0 0 0 0 11
1.8009 0.1300 1.2128 H 0 0 0 0 0 0 0 0 0 0 12
0.1266 -0.4021 2.5048 C 0 0 0 0 0 0 0 0 0 0 13
0.7438 0.1746 -3.7855 C 0 0 0 0 0 0 0 0 0 0 14
0.3055 -1.4807 -2.4529 H 0 0 0 0 0 0 0 0 0 0 15
-0.9645 -0.2457 -2.5161 H 0 0 0 0 0 0 0 0 0 0 16
0.7298 0.1780 3.7895 C 0 0 0 0 0 0 0 0 0 0 17
0.3229 -1.4855 2.4578 H 0 0 0 0 0 0 0 0 0 0 18
-0.9665 -0.2693 2.5117 H 0 0 0 0 0 0 0 0 0 0 19
0.3068 -0.3086 -4.6700 H 0 0 0 0 0 0 0 0 0 0 20
0.5630 1.2567 -3.8687 H 0 0 0 0 0 0 0 0 0 0 21
1.8310 0.0082 -3.8116 H 0 0 0 0 0 0 0 0 0 0 22
0.3004 -0.3141 4.6727 H 0 0 0 0 0 0 0 0 0 0 23
0.5276 1.2563 3.8731 H 0 0 0 0 0 0 0 0 0 0 24
1.8200 0.0330 3.8182 H 0 0 0 0 0 0 0 0 0 0 25
-0.9160 -0.1545 -0.0004 H 0 0 0 0 0 0 0 0 0 0 26
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
7 4 0 0 0 0
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9 4 0 0 0 0
6 5 0 0 0 0
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13 6 0 0 0 0
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17 13 0 0 0 0
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20 14 0 0 0 0
21 14 0 0 0 0
22 14 0 0 0 0
23 17 0 0 0 0
24 17 0 0 0 0
25 17 0 0 0 0
5 26 0 0 0 0
M END
$$$$
di-n-propylamine.sdf
COSMOtherm 3D 0
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URL: <http://mc.manuscriptcentral.com/tandf/tmph>

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20 9 0 0 0 0
21 9 0 0 0 0
22 9 0 0 0 0
23 10 0 0 0 0
24 10 0 0 0 0
25 10 0 0 0 0
26 18 0 0 0 0
27 18 0 0 0 0
28 18 0 0 0 0
29 23 0 0 0 0
30 23 0 0 0 0
31 23 0 0 0 0
4 32 0 0 0 0
M END
$$$$
di-sec-butylamine.sdf
COSMOtherm 3D 0

31 29 0 0 0 0 0 0 0 0 0 V2000
2.9090 0.0161 0.1899 O 0 0 0 0 0 0 0 0 0 0 1
1.9140 0.1882 0.1003 H 0 0 0 0 0 0 0 0 0 0 2
2.9849 -0.9536 0.2057 H 0 0 0 0 0 0 0 0 0 0 3
0.1758 0.6115 -0.0287 N 0 0 0 0 0 0 0 0 0 0 4
-0.4587 0.4130 1.3051 C 0 0 0 0 0 0 0 0 0 0 5
-0.5443 -0.0076 -1.1793 C 0 0 0 0 0 0 0 0 0 0 6
-1.8534 0.7236 -1.5135 C 0 0 0 0 0 0 0 0 0 0 7
0.4073 -0.0727 -2.3867 C 0 0 0 0 0 0 0 0 0 0 8
-0.0052 1.5426 2.2336 C 0 0 0 0 0 0 0 0 0 0 9
-0.1006 -0.9780 1.8600 C 0 0 0 0 0 0 0 0 0 0 10
0.2231 1.6216 -0.2071 H 0 0 0 0 0 0 0 0 0 0 11
-1.5616 0.4664 1.2138 H 0 0 0 0 0 0 0 0 0 0 12
-0.7812 -1.0422 -0.8796 H 0 0 0 0 0 0 0 0 0 0 13
-1.6392 1.7388 -1.8866 H 0 0 0 0 0 0 0 0 0 0 14
-2.4238 0.1917 -2.2880 H 0 0 0 0 0 0 0 0 0 0 15
-2.5044 0.8123 -0.6320 H 0 0 0 0 0 0 0 0 0 0 16
1.3438 -0.5476 -2.0559 H 0 0 0 0 0 0 0 0 0 0 17
-0.1521 -0.8337 -3.5947 C 0 0 0 0 0 0 0 0 0 0 18
0.6702 0.9581 -2.6851 H 0 0 0 0 0 0 0 0 0 0 19
-0.4356 1.4263 3.2371 H 0 0 0 0 0 0 0 0 0 0 20
-0.3216 2.5233 1.8468 H 0 0 0 0 0 0 0 0 0 0 21
1.0920 1.5446 2.3284 H 0 0 0 0 0 0 0 0 0 0 22
-0.9471 -1.4013 3.0658 C 0 0 0 0 0 0 0 0 0 0 23
-0.2277 -1.7232 1.0581 H 0 0 0 0 0 0 0 0 0 0 24
0.9701 -0.9837 2.1247 H 0 0 0 0 0 0 0 0 0 0 25
0.6094 -0.9222 -4.3834 H 0 0 0 0 0 0 0 0 0 0 26
-1.0248 -0.3301 -4.0342 H 0 0 0 0 0 0 0 0 0 0 27
-0.4588 -1.8533 -3.3125 H 0 0 0 0 0 0 0 0 0 0 28
-0.6790 -2.4159 3.3940 H 0 0 0 0 0 0 0 0 0 0 29
-0.8054 -0.7295 3.9254 H 0 0 0 0 0 0 0 0 0 0 30
-2.0197 -1.4036 2.8157 H 0 0 0 0 0 0 0 0 0 0 31
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
11 4 0 0 0 0
9 5 0 0 0 0
10 5 0 0 0 0
12 5 0 0 0 0
7 6 0 0 0 0
8 6 0 0 0 0
13 6 0 0 0 0
14 7 0 0 0 0
15 7 0 0 0 0
16 7 0 0 0 0
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18 8 0 0 0 0
19 8 0 0 0 0
20 9 0 0 0 0
21 9 0 0 0 0
22 9 0 0 0 0
23 10 0 0 0 0
24 10 0 0 0 0
25 10 0 0 0 0
26 18 0 0 0 0
27 18 0 0 0 0
28 18 0 0 0 0
29 23 0 0 0 0
30 23 0 0 0 0
23 31 0 0 0 0
M END
$$$$
diethylamine-cation.sdf
COSMOtherm 3D 0

20 18 0 0 0 0 0 0 0 0 0 V2000
2.3726 -0.0864 -0.1217 O 0 0 0 0 0 0 0 0 0 0 1
2.9207 0.3783 0.5364 H 0 0 0 0 0 0 0 0 0 0 2
2.7376 0.1848 -0.9836 H 0 0 0 0 0 0 0 0 0 0 3
-0.9245 1.2804 -0.3813 C 0 0 0 0 0 0 0 0 0 0 4
-0.3845 0.0093 0.2229 N 0 0 0 0 0 0 0 0 0 0 5
-0.9414 -1.2524 -0.3848 C 0 0 0 0 0 0 0 0 0 0 6
-0.3523 2.5042 0.3164 C 0 0 0 0 0 0 0 0 0 0 7
-0.6598 1.2559 -1.4453 H 0 0 0 0 0 0 0 0 0 0 8
-2.0169 1.2357 -0.2923 H 0 0 0 0 0 0 0 0 0 0 9
-0.5912 0.0096 1.2307 H 0 0 0 0 0 0 0 0 0 0 10
-0.6647 -1.2344 -1.4463 H 0 0 0 0 0 0 0 0 0 0 11
-2.0338 -1.1859 -0.3073 H 0 0 0 0 0 0 0 0 0 0 12
-0.4016 -2.4864 0.3220 C 0 0 0 0 0 0 0 0 0 0 13
-0.7632 3.4079 -0.1521 H 0 0 0 0 0 0 0 0 0 0 14
-0.6233 2.5222 1.3817 H 0 0 0 0 0 0 0 0 0 0 15
0.7423 2.5458 0.2276 H 0 0 0 0 0 0 0 0 0 0 16
-0.8262 -3.3826 -0.1493 H 0 0 0 0 0 0 0 0 0 0 17
-0.6859 -2.4960 1.3840 H 0 0 0 0 0 0 0 0 0 0 18
0.6930 -2.5492 0.2464 H 0 0 0 0 0 0 0 0 0 0 19
0.6708 0.0035 0.1253 H 0 0 0 0 0 0 0 0 0 0 20
```



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2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
7 4 0 0 0 0
8 4 0 0 0 0
9 4 0 0 0 0
6 5 0 0 0 0
10 5 0 0 0 0
11 6 0 0 0 0
12 6 0 0 0 0
13 6 0 0 0 0
14 7 0 0 0 0
15 7 0 0 0 0
16 7 0 0 0 0
17 13 0 0 0 0
18 13 0 0 0 0
19 13 0 0 0 0
5 20 0 0 0 0
M END
$$$$
diethylamine.sdf
COSMOTHERM 3D 0
19 17 0 0 0 0 0 0 0 0 0 V2000
-2.4197 0.0798 -0.0748 O 0 0 0 0 0 0 0 0 0 0 1
-1.4092 -0.0328 -0.0391 H 0 0 0 0 0 0 0 0 0 0 2
-2.5526 0.9671 -0.4501 H 0 0 0 0 0 0 0 0 0 0 3
0.9245 0.3815 -1.2014 C 0 0 0 0 0 0 0 0 0 0 4
0.3344 -0.2104 0.0180 N 0 0 0 0 0 0 0 0 0 0 5
0.8648 0.3898 1.2599 C 0 0 0 0 0 0 0 0 0 0 6
0.4372 -0.3320 -2.4590 C 0 0 0 0 0 0 0 0 0 0 7
0.6313 1.4434 -1.2290 H 0 0 0 0 0 0 0 0 0 0 8
2.0313 0.3567 -1.1564 H 0 0 0 0 0 0 0 0 0 0 9
0.5555 -1.2127 0.0263 H 0 0 0 0 0 0 0 0 0 0 10
0.5621 1.4493 1.2713 H 0 0 0 0 0 0 0 0 0 0 11
1.9729 0.3734 1.2642 H 0 0 0 0 0 0 0 0 0 0 12
0.3281 -0.3241 2.4971 C 0 0 0 0 0 0 0 0 0 0 13
0.8698 0.1333 -3.3561 H 0 0 0 0 0 0 0 0 0 0 14
0.7356 -1.3917 -2.4532 H 0 0 0 0 0 0 0 0 0 0 15
-0.6585 -0.2845 -2.5395 H 0 0 0 0 0 0 0 0 0 0 16
0.7217 0.1442 3.4104 H 0 0 0 0 0 0 0 0 0 0 17
0.6309 -1.3825 2.5055 H 0 0 0 0 0 0 0 0 0 0 18
-0.7702 -0.2798 2.5326 H 0 0 0 0 0 0 0 0 0 0 19
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
7 4 0 0 0 0
8 4 0 0 0 0
9 4 0 0 0 0
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10 5 0 0 0 0
11 6 0 0 0 0
12 6 0 0 0 0
13 6 0 0 0 0
14 7 0 0 0 0
15 7 0 0 0 0
16 7 0 0 0 0
17 13 0 0 0 0
18 13 0 0 0 0
13 19 0 0 0 0
M END
$$$$
dimethyl-iso-butylamine-cation.sdf
COSMOTHERM 3D 0
26 24 0 0 0 0 0 0 0 0 0 V2000
-1.8809 0.2729 2.1334 O 0 0 0 0 0 0 0 0 0 0 1
-2.4047 -0.5181 2.3558 H 0 0 0 0 0 0 0 0 0 0 2
-2.5334 0.9092 1.7892 H 0 0 0 0 0 0 0 0 0 0 3
0.5848 -0.0270 0.8766 N 0 0 0 0 0 0 0 0 0 0 4
0.9713 -1.4680 1.0099 C 0 0 0 0 0 0 0 0 0 0 5
1.3776 0.8235 1.8260 C 0 0 0 0 0 0 0 0 0 0 6
0.7353 0.4977 -0.5377 C 0 0 0 0 0 0 0 0 0 0 7
-0.0392 -0.2629 -1.6190 C 0 0 0 0 0 0 0 0 0 0 8
0.3027 0.3783 -2.9751 C 0 0 0 0 0 0 0 0 0 0 9
-1.5551 -0.2690 -1.3804 C 0 0 0 0 0 0 0 0 0 0 10
0.8772 -1.7557 2.0620 H 0 0 0 0 0 0 0 0 0 0 11
0.3063 -2.0844 0.3983 H 0 0 0 0 0 0 0 0 0 0 12
2.0091 -1.5868 0.6787 H 0 0 0 0 0 0 0 0 0 0 13
1.0468 1.8613 1.7286 H 0 0 0 0 0 0 0 0 0 0 14
2.4400 0.7382 1.5725 H 0 0 0 0 0 0 0 0 0 0 15
1.2021 0.4660 2.8457 H 0 0 0 0 0 0 0 0 0 0 16
1.8135 0.4790 -0.7491 H 0 0 0 0 0 0 0 0 0 0 17
0.4093 1.5467 -0.5022 H 0 0 0 0 0 0 0 0 0 0 18
0.3226 -1.3034 -1.6473 H 0 0 0 0 0 0 0 0 0 0 19
-0.1955 -0.1687 -3.7877 H 0 0 0 0 0 0 0 0 0 0 20
1.3853 0.3631 -3.1681 H 0 0 0 0 0 0 0 0 0 0 21
-0.0381 1.4248 -3.0129 H 0 0 0 0 0 0 0 0 0 0 22
-2.0652 -0.7871 -2.2048 H 0 0 0 0 0 0 0 0 0 0 23
-1.8374 -0.7829 -0.4497 H 0 0 0 0 0 0 0 0 0 0 24
-1.9479 0.7592 -1.3330 H 0 0 0 0 0 0 0 0 0 0 25
-0.4215 0.0625 1.1859 H 0 0 0 0 0 0 0 0 0 0 26
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
7 4 0 0 0 0
11 5 0 0 0 0
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9 8 0 0 0 0
10 8 0 0 0 0
19 8 0 0 0 0
20 9 0 0 0 0
21 9 0 0 0 0
22 9 0 0 0 0
23 10 0 0 0 0
24 10 0 0 0 0
25 10 0 0 0 0
4 26 0 0 0 0
M END
$$$$
dimethyl-iso-butylamine.sdf
COSMOTHERM 3D 0
25 23 0 0 0 0 0 0 0 0 0 V2000
1.9439 -2.1351 -0.1430 O 0 0 0 0 0 0 0 0 0 0 1
1.0813 -1.6050 -0.1073 H 0 0 0 0 0 0 0 0 0 0 2
2.4712 -1.6915 -0.8293 H 0 0 0 0 0 0 0 0 0 0 3
-0.5494 -0.8933 0.0095 N 0 0 0 0 0 0 0 0 0 0 4
-0.9866 -1.0649 1.4052 C 0 0 0 0 0 0 0 0 0 0 5
-1.3050 -1.8098 -0.8639 C 0 0 0 0 0 0 0 0 0 0 6
-0.7472 0.4978 -0.4607 C 0 0 0 0 0 0 0 0 0 0 7
0.0577 1.5859 0.2689 C 0 0 0 0 0 0 0 0 0 0 8
-0.3547 2.9603 -0.2839 C 0 0 0 0 0 0 0 0 0 0 9
1.5733 1.3823 0.1498 C 0 0 0 0 0 0 0 0 0 0 10
-0.8665 -2.1178 1.6949 H 0 0 0 0 0 0 0 0 0 0 11
-0.3735 -0.4529 2.0782 H 0 0 0 0 0 0 0 0 0 0 12
-2.0506 -0.7829 1.5420 H 0 0 0 0 0 0 0 0 0 0 13
-0.9519 -1.7079 -1.8992 H 0 0 0 0 0 0 0 0 0 0 14
-2.3936 -1.6005 -0.8407 H 0 0 0 0 0 0 0 0 0 0 15
-1.1426 -2.8465 -0.5389 H 0 0 0 0 0 0 0 0 0 0 16
-1.8279 0.7526 -0.3979 H 0 0 0 0 0 0 0 0 0 0 17
-0.4754 0.5174 -1.5295 H 0 0 0 0 0 0 0 0 0 0 18
-0.2141 1.5666 1.3380 H 0 0 0 0 0 0 0 0 0 0 19
0.1756 3.7668 0.2434 H 0 0 0 0 0 0 0 0 0 0 20
-1.4354 3.1344 -0.1699 H 0 0 0 0 0 0 0 0 0 0 21
-0.1095 3.0421 -1.3554 H 0 0 0 0 0 0 0 0 0 0 22
2.1150 2.1892 0.6663 H 0 0 0 0 0 0 0 0 0 0 23
1.8959 0.4263 0.5849 H 0 0 0 0 0 0 0 0 0 0 24
1.8827 1.3925 -0.9084 H 0 0 0 0 0 0 0 0 0 0 25
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
7 4 0 0 0 0
11 5 0 0 0 0
12 5 0 0 0 0
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16 6 0 0 0 0
8 7 0 0 0 0
17 7 0 0 0 0
18 7 0 0 0 0
9 8 0 0 0 0
10 8 0 0 0 0
19 8 0 0 0 0
20 9 0 0 0 0
21 9 0 0 0 0
22 9 0 0 0 0
23 10 0 0 0 0
24 10 0 0 0 0
10 25 0 0 0 0
M END
$$$$
dimethyl-iso-propylamine-cation.sdf
COSMOTHERM 3D 0
23 21 0 0 0 0 0 0 0 0 0 V2000
-1.9862 1.6111 0.0008 O 0 0 0 0 0 0 0 0 0 0 1
-2.4674 1.7752 0.8322 H 0 0 0 0 0 0 0 0 0 0 2
-2.6824 1.5866 -0.6809 H 0 0 0 0 0 0 0 0 0 0 3
-0.2710 -0.5930 0.0024 N 0 0 0 0 0 0 0 0 0 0 4
-0.6014 -1.3877 -1.2267 C 0 0 0 0 0 0 0 0 0 0 5
-0.5846 -1.4046 1.2253 C 0 0 0 0 0 0 0 0 0 0 6
1.1756 -0.0694 -0.0037 C 0 0 0 0 0 0 0 0 0 0 7
1.4524 0.7491 1.2573 C 0 0 0 0 0 0 0 0 0 0 8
1.4431 0.7500 -1.2662 C 0 0 0 0 0 0 0 0 0 0 9
-1.6236 -1.7659 -1.1269 H 0 0 0 0 0 0 0 0 0 0 10
-0.5337 -0.7484 -2.1099 H 0 0 0 0 0 0 0 0 0 0 11
0.1011 -2.2249 -1.3067 H 0 0 0 0 0 0 0 0 0 0 12
-1.6085 -1.7804 1.1340 H 0 0 0 0 0 0 0 0 0 0 13
-0.5041 -0.7779 2.1164 H 0 0 0 0 0 0 0 0 0 0 14
0.1186 -2.2429 1.2834 H 0 0 0 0 0 0 0 0 0 0 15
1.7955 -0.9780 -0.0060 H 0 0 0 0 0 0 0 0 0 0 16
2.4716 1.1510 1.1878 H 0 0 0 0 0 0 0 0 0 0 17
1.3991 0.1529 2.1759 H 0 0 0 0 0 0 0 0 0 0 18
0.7618 1.6013 1.3407 H 0 0 0 0 0 0 0 0 0 0 19
2.4605 1.1572 -1.2007 H 0 0 0 0 0 0 0 0 0 0 20
1.3895 0.1525 -2.1838 H 0 0 0 0 0 0 0 0 0 0 21
0.7470 1.5979 -1.3467 H 0 0 0 0 0 0 0 0 0 0 22
-0.9135 0.2489 0.0117 H 0 0 0 0 0 0 0 0 0 0 23
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
7 4 0 0 0 0
10 5 0 0 0 0
11 5 0 0 0 0
12 5 0 0 0 0
13 6 0 0 0 0
14 6 0 0 0 0
15 6 0 0 0 0
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  8 7 0 0 0 0
  9 7 0 0 0 0
16 7 0 0 0 0
17 8 0 0 0 0
18 8 0 0 0 0
19 8 0 0 0 0
20 9 0 0 0 0
21 9 0 0 0 0
22 9 0 0 0 0
  4 23 0 0 0 0
M  END
$$$$
dimethyl-iso-propylamine.sdf
COSMOTHERM      3D      0

22 20 0 0 0 0 0 0 0 0 0 V2000
-2.0223 -0.1972 1.6354 O 0 0 0 0 0 0 0 0 0 0 1
-1.3685 -0.1031 0.8635 H 0 0 0 0 0 0 0 0 0 0 2
-2.1600 0.7131 1.9490 H 0 0 0 0 0 0 0 0 0 0 3
-0.3056 0.0265 -0.5381 N 0 0 0 0 0 0 0 0 0 0 4
-0.6807 1.2690 -1.2396 C 0 0 0 0 0 0 0 0 0 0 5
-0.6142 -1.1228 -1.4106 C 0 0 0 0 0 0 0 0 0 0 6
 1.1313 0.0393 -0.1207 C 0 0 0 0 0 0 0 0 0 0 7
 1.5196 -1.2687 0.5799 C 0 0 0 0 0 0 0 0 0 0 8
 1.4286 1.2272 0.8045 C 0 0 0 0 0 0 0 0 0 0 9
-1.7242 1.1895 -1.5712 H 0 0 0 0 0 0 0 0 0 0 10
-0.6036 2.1330 -0.5699 H 0 0 0 0 0 0 0 0 0 0 11
-0.0440 1.4522 -2.1287 H 0 0 0 0 0 0 0 0 0 0 12
-1.6565 -1.0437 -1.7466 H 0 0 0 0 0 0 0 0 0 0 13
-0.5058 -2.0669 -0.8646 H 0 0 0 0 0 0 0 0 0 0 14
 0.0396 -1.1524 -2.3056 H 0 0 0 0 0 0 0 0 0 0 15
 1.7528 0.1433 -1.0371 H 0 0 0 0 0 0 0 0 0 0 16
 2.5534 -1.1916 0.9445 H 0 0 0 0 0 0 0 0 0 0 17
 1.4712 -2.1396 -0.0859 H 0 0 0 0 0 0 0 0 0 0 18
 0.8645 -1.4530 1.4453 H 0 0 0 0 0 0 0 0 0 0 19
 2.4677 1.1639 1.1563 H 0 0 0 0 0 0 0 0 0 0 20
 1.3106 2.1975 0.3055 H 0 0 0 0 0 0 0 0 0 0 21
 0.7685 1.2038 1.6854 H 0 0 0 0 0 0 0 0 0 0 22

 2 1 0 0 0 0
 3 1 0 0 0 0
 5 4 0 0 0 0
 6 4 0 0 0 0
 7 4 0 0 0 0
10 5 0 0 0 0
11 5 0 0 0 0
12 5 0 0 0 0
13 6 0 0 0 0
14 6 0 0 0 0
15 6 0 0 0 0
 8 7 0 0 0 0
 9 7 0 0 0 0
16 7 0 0 0 0
17 8 0 0 0 0
18 8 0 0 0 0
19 8 0 0 0 0
20 9 0 0 0 0
21 9 0 0 0 0
 9 22 0 0 0 0
M  END
$$$$
dimethyl-n-butylamine-cation.sdf
COSMOTHERM      3D      0

26 24 0 0 0 0 0 0 0 0 0 V2000
-2.3073 -0.0874 1.8174 O 0 0 0 0 0 0 0 0 0 0 1
-2.7885 -0.8790 1.5149 H 0 0 0 0 0 0 0 0 0 0 2
-2.8614 0.6612 1.5308 H 0 0 0 0 0 0 0 0 0 0 3
 1.0157 -0.8509 2.3666 C 0 0 0 0 0 0 0 0 0 0 4
 0.4180 0.0214 1.3040 N 0 0 0 0 0 0 0 0 0 0 5
 0.7360 -0.5229 -0.0727 C 0 0 0 0 0 0 0 0 0 0 6
 0.8464 1.4460 1.4814 C 0 0 0 0 0 0 0 0 0 0 7
 0.7328 -0.4547 3.3471 H 0 0 0 0 0 0 0 0 0 0 8
 0.6303 -1.8684 2.2456 H 0 0 0 0 0 0 0 0 0 0 9
 2.1056 -0.8439 2.2571 H 0 0 0 0 0 0 0 0 0 0 10
 0.4279 -1.5769 -0.0538 H 0 0 0 0 0 0 0 0 0 0 11
 0.0343 0.2192 -1.2054 C 0 0 0 0 0 0 0 0 0 0 12
 1.8293 -0.4859 -0.1783 H 0 0 0 0 0 0 0 0 0 0 13
 0.6024 1.7566 2.5024 H 0 0 0 0 0 0 0 0 0 0 14
 0.3139 2.0787 0.7661 H 0 0 0 0 0 0 0 0 0 0 15
 1.9277 1.5118 1.3151 H 0 0 0 0 0 0 0 0 0 0 16
 0.2601 -0.4922 -2.5491 C 0 0 0 0 0 0 0 0 0 0 17
 0.4084 1.2514 -1.2801 H 0 0 0 0 0 0 0 0 0 0 18
-1.0475 0.2767 -0.9985 H 0 0 0 0 0 0 0 0 0 0 19
-0.4020 0.2414 -3.7198 C 0 0 0 0 0 0 0 0 0 0 20
-0.1316 -1.5205 -2.4853 H 0 0 0 0 0 0 0 0 0 0 21
 1.3436 -0.5810 -2.7341 H 0 0 0 0 0 0 0 0 0 0 22
-0.2265 -0.2883 -4.6673 H 0 0 0 0 0 0 0 0 0 0 23
-0.0025 1.2617 -3.8258 H 0 0 0 0 0 0 0 0 0 0 24
-1.4904 0.3201 -3.5750 H 0 0 0 0 0 0 0 0 0 0 25
-0.6336 -0.0144 1.4289 H 0 0 0 0 0 0 0 0 0 0 26

 2 1 0 0 0 0
 3 1 0 0 0 0
 5 4 0 0 0 0
 8 4 0 0 0 0
 9 4 0 0 0 0
10 4 0 0 0 0
 6 5 0 0 0 0
 7 5 0 0 0 0
11 6 0 0 0 0
12 6 0 0 0 0
13 6 0 0 0 0
14 7 0 0 0 0
15 7 0 0 0 0
16 7 0 0 0 0
17 12 0 0 0 0
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18 12 0 0 0 0
19 12 0 0 0 0
20 17 0 0 0 0
21 17 0 0 0 0
22 17 0 0 0 0
23 20 0 0 0 0
24 20 0 0 0 0
25 20 0 0 0 0
5 26 0 0 0 0
M END
$$$$
dimethyl-n-butylamine.sdf
COSMOtherm 3D 0
25 23 0 0 0 0 0 0 0 0 0 V2000
-2.3702 -0.1655 1.7031 O 0 0 0 0 0 0 0 0 0 0 1
-1.3704 -0.0821 1.5374 H 0 0 0 0 0 0 0 0 0 0 2
-2.7564 0.6011 1.2458 H 0 0 0 0 0 0 0 0 0 0 3
0.9598 -0.8337 2.3738 C 0 0 0 0 0 0 0 0 0 0 4
0.3687 0.0201 1.3295 N 0 0 0 0 0 0 0 0 0 0 5
0.7571 -0.4744 -0.0116 C 0 0 0 0 0 0 0 0 0 0 6
0.7726 1.4211 1.5393 C 0 0 0 0 0 0 0 0 0 0 7
0.6341 -0.4826 3.3626 H 0 0 0 0 0 0 0 0 0 0 8
0.6207 -1.8700 2.2400 H 0 0 0 0 0 0 0 0 0 0 9
2.0680 -0.8193 2.3443 H 0 0 0 0 0 0 0 0 0 0 10
0.5454 -1.5555 -0.0264 H 0 0 0 0 0 0 0 0 0 0 11
0.0089 0.1931 -1.1678 C 0 0 0 0 0 0 0 0 0 0 12
1.8535 -0.3580 -0.1543 H 0 0 0 0 0 0 0 0 0 0 13
0.4707 1.7375 2.5468 H 0 0 0 0 0 0 0 0 0 0 14
0.2775 2.0757 0.8117 H 0 0 0 0 0 0 0 0 0 0 15
1.8698 1.5519 1.4431 H 0 0 0 0 0 0 0 0 0 0 16
0.3454 -0.4476 -2.5216 C 0 0 0 0 0 0 0 0 0 0 17
0.2499 1.2675 -1.2133 H 0 0 0 0 0 0 0 0 0 0 18
-1.0762 0.1163 -0.9835 H 0 0 0 0 0 0 0 0 0 0 19
-0.3842 0.2175 -3.6941 C 0 0 0 0 0 0 0 0 0 0 20
0.0903 -1.5205 -2.4891 H 0 0 0 0 0 0 0 0 0 0 21
1.4348 -0.3943 -2.6886 H 0 0 0 0 0 0 0 0 0 0 22
-0.1338 -0.2682 -4.6488 H 0 0 0 0 0 0 0 0 0 0 23
-0.1133 1.2815 -3.7779 H 0 0 0 0 0 0 0 0 0 0 24
-1.4763 0.1606 -3.5649 H 0 0 0 0 0 0 0 0 0 0 25
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
8 4 0 0 0 0
9 4 0 0 0 0
10 4 0 0 0 0
6 5 0 0 0 0
7 5 0 0 0 0
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12 6 0 0 0 0
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16 7 0 0 0 0
17 12 0 0 0 0
18 12 0 0 0 0
19 12 0 0 0 0
20 17 0 0 0 0
21 17 0 0 0 0
22 17 0 0 0 0
23 20 0 0 0 0
24 20 0 0 0 0
20 25 0 0 0 0
M END
$$$$
dimethyl-n-propylamine-cation.sdf
COSMOtherm 3D 0
23 21 0 0 0 0 0 0 0 0 0 V2000
2.1357 1.6551 -0.0453 O 0 0 0 0 0 0 0 0 0 0 1
2.7386 1.2710 -0.7073 H 0 0 0 0 0 0 0 0 0 0 2
2.6354 1.6268 0.7908 H 0 0 0 0 0 0 0 0 0 0 3
-1.1816 1.6297 -0.9989 C 0 0 0 0 0 0 0 0 0 0 4
-0.4844 0.7376 -0.0173 N 0 0 0 0 0 0 0 0 0 0 5
-0.5481 -0.7063 -0.4675 C 0 0 0 0 0 0 0 0 0 0 6
-1.0234 0.9421 1.3652 C 0 0 0 0 0 0 0 0 0 0 7
-1.0696 2.6681 -0.6706 H 0 0 0 0 0 0 0 0 0 0 8
-0.7255 1.4949 -1.9848 H 0 0 0 0 0 0 0 0 0 0 9
-2.2423 1.3578 -1.0324 H 0 0 0 0 0 0 0 0 0 0 10
-0.1880 -0.7115 -1.5047 H 0 0 0 0 0 0 0 0 0 0 11
0.2826 -1.6567 0.3897 C 0 0 0 0 0 0 0 0 0 0 12
-1.6108 -0.9865 -0.4709 H 0 0 0 0 0 0 0 0 0 0 13
-0.9567 2.0067 1.6097 H 0 0 0 0 0 0 0 0 0 0 14
-0.4310 0.3620 2.0781 H 0 0 0 0 0 0 0 0 0 0 15
-2.0695 0.6162 1.3875 H 0 0 0 0 0 0 0 0 0 0 16
0.2985 -3.0617 -0.2268 C 0 0 0 0 0 0 0 0 0 0 17
-0.1270 -1.7123 1.4085 H 0 0 0 0 0 0 0 0 0 0 18
1.3128 -1.2751 0.4715 H 0 0 0 0 0 0 0 0 0 0 19
0.8846 -3.7481 0.3989 H 0 0 0 0 0 0 0 0 0 0 20
0.7468 -3.0514 -1.2309 H 0 0 0 0 0 0 0 0 0 0 21
-0.7194 -3.4699 -0.3121 H 0 0 0 0 0 0 0 0 0 0 22
0.5354 1.0252 -0.0085 H 0 0 0 0 0 0 0 0 0 0 23
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
8 4 0 0 0 0
9 4 0 0 0 0
10 4 0 0 0 0
6 5 0 0 0 0
7 5 0 0 0 0
11 6 0 0 0 0
12 6 0 0 0 0
13 6 0 0 0 0
14 7 0 0 0 0
15 7 0 0 0 0
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16 7 0 0 0 0
17 12 0 0 0 0
18 12 0 0 0 0
19 12 0 0 0 0
20 17 0 0 0 0
21 17 0 0 0 0
22 17 0 0 0 0
5 23 0 0 0 0
M END
$$$$
dimethyl-n-propylamine.sdf
COSMOtherm 3D 0

22 20 0 0 0 0 0 0 0 0 0 V2000
-2.1982 -0.1277 1.5878 O 0 0 0 0 0 0 0 0 0 0 1
-1.2380 -0.0725 1.2573 H 0 0 0 0 0 0 0 0 0 0 2
-2.5764 0.7431 1.3757 H 0 0 0 0 0 0 0 0 0 0 3
1.1621 -0.9576 1.6330 C 0 0 0 0 0 0 0 0 0 0 4
0.4427 -0.0151 0.7600 N 0 0 0 0 0 0 0 0 0 0 5
0.5793 -0.4269 -0.6557 C 0 0 0 0 0 0 0 0 0 0 6
0.9339 1.3542 0.9863 C 0 0 0 0 0 0 0 0 0 0 7
1.0167 -0.6706 2.6835 H 0 0 0 0 0 0 0 0 0 0 8
0.7653 -1.9717 1.4889 H 0 0 0 0 0 0 0 0 0 0 9
2.2507 -0.9721 1.4224 H 0 0 0 0 0 0 0 0 0 0 10
0.3213 -1.4967 -0.7033 H 0 0 0 0 0 0 0 0 0 0 11
-0.3207 0.3443 -1.6245 C 0 0 0 0 0 0 0 0 0 0 12
1.6401 -0.3366 -0.9765 H 0 0 0 0 0 0 0 0 0 0 13
0.8243 1.6081 2.0494 H 0 0 0 0 0 0 0 0 0 0 14
0.3483 2.0739 0.4010 H 0 0 0 0 0 0 0 0 0 0 15
2.0022 1.4601 0.7081 H 0 0 0 0 0 0 0 0 0 0 16
-0.2239 -0.2101 -3.0505 C 0 0 0 0 0 0 0 0 0 0 17
-0.0479 1.4109 -1.6326 H 0 0 0 0 0 0 0 0 0 0 18
-1.3614 0.2833 -1.2664 H 0 0 0 0 0 0 0 0 0 0 19
-0.8709 0.3535 -3.7378 H 0 0 0 0 0 0 0 0 0 0 20
-0.5310 -1.2666 -3.0896 H 0 0 0 0 0 0 0 0 0 0 21
0.8063 -0.1458 -3.4341 H 0 0 0 0 0 0 0 0 0 0 22

2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
8 4 0 0 0 0
9 4 0 0 0 0
10 4 0 0 0 0
6 5 0 0 0 0
7 5 0 0 0 0
11 6 0 0 0 0
12 6 0 0 0 0
13 6 0 0 0 0
14 7 0 0 0 0
15 7 0 0 0 0
16 7 0 0 0 0
17 12 0 0 0 0
18 12 0 0 0 0
19 12 0 0 0 0
20 17 0 0 0 0
21 17 0 0 0 0
17 22 0 0 0 0
M END
$$$$
dimethyl-sec-butylamine-cation.sdf
COSMOtherm 3D 0

26 24 0 0 0 0 0 0 0 0 0 V2000
-1.7263 -2.0925 0.5418 O 0 0 0 0 0 0 0 0 0 0 1
-1.7437 -2.7917 -0.1370 H 0 0 0 0 0 0 0 0 0 0 2
-2.6268 -2.0960 0.9149 H 0 0 0 0 0 0 0 0 0 0 3
-0.8199 0.4144 -0.2831 N 0 0 0 0 0 0 0 0 0 0 4
-1.7298 1.3964 0.3942 C 0 0 0 0 0 0 0 0 0 0 5
-1.0121 0.5168 -1.7685 C 0 0 0 0 0 0 0 0 0 0 6
0.6614 0.5646 0.1178 C 0 0 0 0 0 0 0 0 0 0 7
1.4490 -0.6804 -0.3260 C 0 0 0 0 0 0 0 0 0 0 8
0.8037 0.8121 1.6177 C 0 0 0 0 0 0 0 0 0 0 9
-2.7405 1.2499 -0.0006 H 0 0 0 0 0 0 0 0 0 0 10
-1.7291 1.2204 1.4724 H 0 0 0 0 0 0 0 0 0 0 11
-1.3871 2.4128 0.1713 H 0 0 0 0 0 0 0 0 0 0 12
-2.0617 0.3055 -1.9962 H 0 0 0 0 0 0 0 0 0 0 13
-0.3741 -0.2066 -2.2817 H 0 0 0 0 0 0 0 0 0 0 14
-0.7565 1.5347 -2.0832 H 0 0 0 0 0 0 0 0 0 0 15
1.0059 1.4469 -0.4435 H 0 0 0 0 0 0 0 0 0 0 16
1.1204 -1.0095 -1.3215 H 0 0 0 0 0 0 0 0 0 0 17
2.9616 -0.4309 -0.3825 C 0 0 0 0 0 0 0 0 0 0 18
1.2276 -1.5052 0.3702 H 0 0 0 0 0 0 0 0 0 0 19
1.8719 0.8114 1.8688 H 0 0 0 0 0 0 0 0 0 0 20
0.3983 1.7812 1.9308 H 0 0 0 0 0 0 0 0 0 0 21
0.3253 0.0124 2.2028 H 0 0 0 0 0 0 0 0 0 0 22
3.4808 -1.3393 -0.7178 H 0 0 0 0 0 0 0 0 0 0 23
3.3738 -0.1570 0.5988 H 0 0 0 0 0 0 0 0 0 0 24
3.2020 0.3762 -1.0905 H 0 0 0 0 0 0 0 0 0 0 25
-1.1361 -0.5513 0.0148 H 0 0 0 0 0 0 0 0 0 0 26

2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
7 4 0 0 0 0
10 5 0 0 0 0
11 5 0 0 0 0
12 5 0 0 0 0
13 6 0 0 0 0
14 6 0 0 0 0
15 6 0 0 0 0
8 7 0 0 0 0
9 7 0 0 0 0
16 7 0 0 0 0
17 8 0 0 0 0
18 8 0 0 0 0
19 8 0 0 0 0
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20 9 0 0 0 0
21 9 0 0 0 0
22 9 0 0 0 0
23 18 0 0 0 0
24 18 0 0 0 0
25 18 0 0 0 0
4 26 0 0 0 0
M END
$$$$
dimethyl-sec-butylamine.sdf
COSMOtherm 3D 0
25 23 0 0 0 0 0 0 0 0 0 V2000
2.0780 -1.8077 0.6067 O 0 0 0 0 0 0 0 0 0 0 0 1
1.1979 -1.4148 0.2853 H 0 0 0 0 0 0 0 0 0 0 0 2
2.7576 -1.2685 0.1671 H 0 0 0 0 0 0 0 0 0 0 0 3
-0.3686 -0.8310 -0.2756 N 0 0 0 0 0 0 0 0 0 0 0 4
-1.3774 -1.7204 0.3309 C 0 0 0 0 0 0 0 0 0 0 0 5
-0.4146 -1.0172 -1.7391 C 0 0 0 0 0 0 0 0 0 0 0 6
-0.5596 0.6073 0.0975 C 0 0 0 0 0 0 0 0 0 0 0 7
0.6713 1.4431 -0.3149 C 0 0 0 0 0 0 0 0 0 0 0 8
-0.8231 0.7723 1.5987 C 0 0 0 0 0 0 0 0 0 0 0 9
-1.1938 -2.7462 -0.0161 H 0 0 0 0 0 0 0 0 0 0 0 10
-1.2988 -1.7130 1.4235 H 0 0 0 0 0 0 0 0 0 0 0 11
-2.4104 -1.4373 0.0445 H 0 0 0 0 0 0 0 0 0 0 0 12
-0.2459 -2.0769 -1.9718 H 0 0 0 0 0 0 0 0 0 0 0 13
0.3674 -0.4339 -2.2379 H 0 0 0 0 0 0 0 0 0 0 0 14
-1.3967 -0.7178 -2.1583 H 0 0 0 0 0 0 0 0 0 0 0 15
-1.4445 0.9902 -0.4582 H 0 0 0 0 0 0 0 0 0 0 0 16
1.0300 1.1224 -1.3029 H 0 0 0 0 0 0 0 0 0 0 0 17
0.4000 2.9516 -0.3714 C 0 0 0 0 0 0 0 0 0 0 0 18
1.4875 1.2322 0.3964 H 0 0 0 0 0 0 0 0 0 0 0 19
-1.7984 0.3746 1.9064 H 0 0 0 0 0 0 0 0 0 0 0 20
-0.8108 1.8391 1.8586 H 0 0 0 0 0 0 0 0 0 0 0 21
-0.0368 0.2723 2.1856 H 0 0 0 0 0 0 0 0 0 0 0 22
1.2986 3.4940 -0.6995 H 0 0 0 0 0 0 0 0 0 0 0 23
0.1088 3.3594 0.6076 H 0 0 0 0 0 0 0 0 0 0 0 24
-0.4077 3.1808 -1.0838 H 0 0 0 0 0 0 0 0 0 0 0 25
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
7 4 0 0 0 0
10 5 0 0 0 0
11 5 0 0 0 0
12 5 0 0 0 0
13 6 0 0 0 0
14 6 0 0 0 0
15 6 0 0 0 0
8 7 0 0 0 0
9 7 0 0 0 0
16 7 0 0 0 0
17 8 0 0 0 0
18 8 0 0 0 0
19 8 0 0 0 0
20 9 0 0 0 0
21 9 0 0 0 0
22 9 0 0 0 0
23 18 0 0 0 0
24 18 0 0 0 0
18 25 0 0 0 0
M END
$$$$
dimethyl-tert-butylamine-cation.sdf
COSMOtherm 3D 0
26 24 0 0 0 0 0 0 0 0 0 V2000
-2.6947 0.0177 0.8570 O 0 0 0 0 0 0 0 0 0 0 0 1
-3.2957 -0.7298 0.6839 H 0 0 0 0 0 0 0 0 0 0 0 2
-3.2556 0.8080 0.7539 H 0 0 0 0 0 0 0 0 0 0 0 3
-0.3618 1.2116 -1.4980 C 0 0 0 0 0 0 0 0 0 0 0 4
-0.3108 0.0016 -0.6121 N 0 0 0 0 0 0 0 0 0 0 0 5
-0.4083 -1.2341 -1.4580 C 0 0 0 0 0 0 0 0 0 0 0 6
0.8784 -0.0002 0.4060 C 0 0 0 0 0 0 0 0 0 0 0 7
0.8150 -1.3124 1.1996 C 0 0 0 0 0 0 0 0 0 0 0 8
0.6689 1.1844 1.3602 C 0 0 0 0 0 0 0 0 0 0 0 9
2.2078 0.1251 -0.3411 C 0 0 0 0 0 0 0 0 0 0 0 10
-1.3212 1.2006 -2.0259 H 0 0 0 0 0 0 0 0 0 0 0 11
-0.2872 2.1202 -0.8962 H 0 0 0 0 0 0 0 0 0 0 0 12
0.4558 1.1666 -2.2241 H 0 0 0 0 0 0 0 0 0 0 0 13
-1.2626 -1.1125 -2.1321 H 0 0 0 0 0 0 0 0 0 0 0 14
-0.5682 -2.1077 -0.8222 H 0 0 0 0 0 0 0 0 0 0 0 15
0.5074 -1.3509 -2.0458 H 0 0 0 0 0 0 0 0 0 0 0 16
1.5393 -1.2507 2.0226 H 0 0 0 0 0 0 0 0 0 0 0 17
1.0817 -2.1850 0.5902 H 0 0 0 0 0 0 0 0 0 0 0 18
-0.1789 -1.4719 1.6429 H 0 0 0 0 0 0 0 0 0 0 0 19
1.4368 1.1347 2.1438 H 0 0 0 0 0 0 0 0 0 0 0 20
0.7761 2.1558 0.8615 H 0 0 0 0 0 0 0 0 0 0 0 21
-0.3141 1.1375 1.8505 H 0 0 0 0 0 0 0 0 0 0 0 22
3.0199 0.0666 0.3964 H 0 0 0 0 0 0 0 0 0 0 0 23
2.3035 1.0873 -0.8611 H 0 0 0 0 0 0 0 0 0 0 0 24
2.3614 -0.6897 -1.0617 H 0 0 0 0 0 0 0 0 0 0 0 25
-1.1897 0.0234 -0.0247 H 0 0 0 0 0 0 0 0 0 0 0 26
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
11 4 0 0 0 0
12 4 0 0 0 0
13 4 0 0 0 0
6 5 0 0 0 0
7 5 0 0 0 0
14 6 0 0 0 0
15 6 0 0 0 0
16 6 0 0 0 0
8 7 0 0 0 0
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9 7 0 0 0 0
10 7 0 0 0 0
17 8 0 0 0 0
18 8 0 0 0 0
19 8 0 0 0 0
20 9 0 0 0 0
21 9 0 0 0 0
22 9 0 0 0 0
23 10 0 0 0 0
24 10 0 0 0 0
25 10 0 0 0 0
5 26 0 0 0 0
M END
$$$$
dimethyl-tert-butylamine.sdf
COSMOTHERM 3D 0

25 23 0 0 0 0 0 0 0 0 0 V2000
-2.7239 -0.0870 -0.8895 O 0 0 0 0 0 0 0 0 0 0 1
-1.8341 -0.0470 -0.3972 H 0 0 0 0 0 0 0 0 0 0 2
-2.9288 0.8408 -1.0980 H 0 0 0 0 0 0 0 0 0 0 3
-0.4497 -1.1757 1.4474 C 0 0 0 0 0 0 0 0 0 0 4
-0.3594 -0.0008 0.5598 N 0 0 0 0 0 0 0 0 0 0 5
-0.5027 1.2192 1.3773 C 0 0 0 0 0 0 0 0 0 0 6
0.8559 -0.0015 -0.3447 C 0 0 0 0 0 0 0 0 0 0 7
0.7991 1.2464 -1.2462 C 0 0 0 0 0 0 0 0 0 0 8
0.7915 -1.2450 -1.2519 C 0 0 0 0 0 0 0 0 0 0 9
2.1840 -0.0058 0.4408 C 0 0 0 0 0 0 0 0 0 0 10
-1.4148 -1.1407 1.9716 H 0 0 0 0 0 0 0 0 0 0 11
-0.4147 -2.1056 0.8691 H 0 0 0 0 0 0 0 0 0 0 12
0.3501 -1.2033 2.2121 H 0 0 0 0 0 0 0 0 0 0 13
-1.4424 1.1472 1.9424 H 0 0 0 0 0 0 0 0 0 0 14
-0.5601 2.1105 0.7426 H 0 0 0 0 0 0 0 0 0 0 15
0.3200 1.3539 2.1052 H 0 0 0 0 0 0 0 0 0 0 16
1.5630 1.1624 -2.0322 H 0 0 0 0 0 0 0 0 0 0 17
0.9990 2.1737 -0.6924 H 0 0 0 0 0 0 0 0 0 0 18
-0.1836 1.3322 -1.7333 H 0 0 0 0 0 0 0 0 0 0 19
1.5905 -1.1879 -2.0050 H 0 0 0 0 0 0 0 0 0 0 20
0.9360 -2.1802 -0.6943 H 0 0 0 0 0 0 0 0 0 0 21
-0.1739 -1.2941 -1.7767 H 0 0 0 0 0 0 0 0 0 0 22
3.0294 0.0219 -0.2622 H 0 0 0 0 0 0 0 0 0 0 23
2.2928 -0.9121 1.0539 H 0 0 0 0 0 0 0 0 0 0 24
2.2726 0.8714 1.0983 H 0 0 0 0 0 0 0 0 0 0 25
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
11 4 0 0 0 0
12 4 0 0 0 0
13 4 0 0 0 0
6 5 0 0 0 0
7 5 0 0 0 0
14 6 0 0 0 0
15 6 0 0 0 0
16 6 0 0 0 0
8 7 0 0 0 0
9 7 0 0 0 0
10 7 0 0 0 0
17 8 0 0 0 0
18 8 0 0 0 0
19 8 0 0 0 0
20 9 0 0 0 0
21 9 0 0 0 0
22 9 0 0 0 0
23 10 0 0 0 0
24 10 0 0 0 0
10 25 0 0 0 0
M END
$$$$
dimethylamine-cation.sdf
COSMOTHERM 3D 0

14 12 0 0 0 0 0 0 0 0 0 V2000
2.1938 -0.0026 -0.1109 O 0 0 0 0 0 0 0 0 0 0 1
2.6814 -0.7814 0.2143 H 0 0 0 0 0 0 0 0 0 0 2
2.6869 0.7580 0.2475 H 0 0 0 0 0 0 0 0 0 0 3
-1.0662 1.2544 -0.1830 C 0 0 0 0 0 0 0 0 0 0 4
-0.5225 -0.0002 0.4215 N 0 0 0 0 0 0 0 0 0 0 5
-1.0776 -1.2500 -0.1824 C 0 0 0 0 0 0 0 0 0 0 6
-0.6124 2.1129 0.3220 H 0 0 0 0 0 0 0 0 0 0 7
-0.8142 1.2649 -1.2480 H 0 0 0 0 0 0 0 0 0 0 8
-2.1530 1.2715 -0.0514 H 0 0 0 0 0 0 0 0 0 0 9
-0.7141 0.0009 1.4309 H 0 0 0 0 0 0 0 0 0 0 10
-0.6320 -2.1124 0.3231 H 0 0 0 0 0 0 0 0 0 0 11
-0.8252 -1.2639 -1.2475 H 0 0 0 0 0 0 0 0 0 0 12
-2.1644 -1.2561 -0.0516 H 0 0 0 0 0 0 0 0 0 0 13
0.5333 -0.0041 0.3181 H 0 0 0 0 0 0 0 0 0 0 14
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
7 4 0 0 0 0
8 4 0 0 0 0
9 4 0 0 0 0
6 5 0 0 0 0
10 5 0 0 0 0
11 6 0 0 0 0
12 6 0 0 0 0
13 6 0 0 0 0
5 14 0 0 0 0
M END
$$$$
dimethylamine.sdf
COSMOTHERM 3D 0

13 11 0 0 0 0 0 0 0 0 0 V2000
-2.2579 0.0129 0.0035 O 0 0 0 0 0 0 0 0 0 0 1
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1
2
3      -1.2483   -0.1319    0.0034 H   0   0   0   0   0   0   0   0   0   0   2
4      -2.3678    0.9792    0.0028 H   0   0   0   0   0   0   0   0   0   0   3
5       1.0521    0.1655   -1.2258 C   0   0   0   0   0   0   0   0   0   0   4
6       0.4627   -0.3972    0.0005 N   0   0   0   0   0   0   0   0   0   0   5
7       1.0628    0.1662    1.2214 C   0   0   0   0   0   0   0   0   0   0   6
8       0.6182   -0.3312   -2.1037 H   0   0   0   0   0   0   0   0   0   0   7
9       0.8147    1.2379   -1.2843 H   0   0   0   0   0   0   0   0   0   0   8
10      2.1522    0.0548   -1.2634 H   0   0   0   0   0   0   0   0   0   0   9
11      0.6131   -1.4097    0.0000 H   0   0   0   0   0   0   0   0   0   0   10
12      0.6425   -0.3361    2.1028 H   0   0   0   0   0   0   0   0   0   0   11
13      0.8189    1.2367    1.2859 H   0   0   0   0   0   0   0   0   0   0   12
14      2.1640    0.0624    1.2455 H   0   0   0   0   0   0   0   0   0   0   13
15
16      2   1   0   0   0   0
17      3   1   0   0   0   0
18      5   4   0   0   0   0
19      7   4   0   0   0   0
20      8   4   0   0   0   0
21      9   4   0   0   0   0
22      6   5   0   0   0   0
23     10   5   0   0   0   0
24     11   6   0   0   0   0
25     12   6   0   0   0   0
26     6  13   0   0   0   0
27
28 M   END
29 $$$$
30 dimethylethylamine-cation.sdf
31 COSMOtherm      3D      0
32
33 20 18   0   0   0   0   0   0   0   0   0   0 V2000
34 -2.2949   -0.0076   -0.9361 O   0   0   0   0   0   0   0   0   0   0   0   1
35 -2.4286   -0.7089   -1.5993 H   0   0   0   0   0   0   0   0   0   0   0   2
36 -2.5544    0.8139   -1.3916 H   0   0   0   0   0   0   0   0   0   0   0   3
37 -0.2441   -0.7953    1.7321 C   0   0   0   0   0   0   0   0   0   0   0   4
38  0.0790    0.0004    0.5050 N   0   0   0   0   0   0   0   0   0   0   0   5
39  1.1884   -0.6631   -0.2861 C   0   0   0   0   0   0   0   0   0   0   0   6
40  0.3866    1.4231    0.8574 C   0   0   0   0   0   0   0   0   0   0   0   7
41 -1.0797   -0.3161    2.2523 H   0   0   0   0   0   0   0   0   0   0   0   8
42 -0.5199   -1.8113    1.4319 H   0   0   0   0   0   0   0   0   0   0   0   9
43  0.6390   -0.8201    2.3805 H   0   0   0   0   0   0   0   0   0   0   0   10
44  0.8730   -1.7054   -0.4201 H   0   0   0   0   0   0   0   0   0   0   0   11
45  1.4510    0.0003   -1.6287 C   0   0   0   0   0   0   0   0   0   0   0   12
46  2.0782   -0.6525    0.3575 H   0   0   0   0   0   0   0   0   0   0   0   13
47 -0.4545    1.8289    1.4286 H   0   0   0   0   0   0   0   0   0   0   0   14
48  0.5242    2.0044   -0.0585 H   0   0   0   0   0   0   0   0   0   0   0   15
49  1.2996    1.4463    1.4627 H   0   0   0   0   0   0   0   0   0   0   0   16
50  2.1790   -0.6129   -2.1768 H   0   0   0   0   0   0   0   0   0   0   0   17
51  1.8762    1.0069   -1.5267 H   0   0   0   0   0   0   0   0   0   0   0   18
52  0.5375    0.0575   -2.2372 H   0   0   0   0   0   0   0   0   0   0   0   19
53 -0.7893    0.0022   -0.1016 H   0   0   0   0   0   0   0   0   0   0   0   20
54
55      2   1   0   0   0   0
56      3   1   0   0   0   0
57      5   4   0   0   0   0
58      8   4   0   0   0   0
59      9   4   0   0   0   0
60     10   4   0   0   0   0
61      6   5   0   0   0   0
62      7   5   0   0   0   0
63     11   6   0   0   0   0
64     12   6   0   0   0   0
65     13   6   0   0   0   0
66     14   7   0   0   0   0
67     15   7   0   0   0   0
68     16   7   0   0   0   0
69     17  12   0   0   0   0
70     18  12   0   0   0   0
71     19  12   0   0   0   0
72     5  20   0   0   0   0
73
74 M   END
75 $$$$
76 dimethylethylamine.sdf
77 COSMOtherm      3D      0
78
79 19 17   0   0   0   0   0   0   0   0   0   0 V2000
80 -2.2735    1.0303   -0.0564 O   0   0   0   0   0   0   0   0   0   0   0   1
81 -1.4097    0.4953   -0.0195 H   0   0   0   0   0   0   0   0   0   0   0   2
82 -2.2147    1.6389    0.7000 H   0   0   0   0   0   0   0   0   0   0   0   3
83 -0.2761   -1.7040   -0.7762 C   0   0   0   0   0   0   0   0   0   0   0   4
84  0.0398   -0.4951    0.0018 N   0   0   0   0   0   0   0   0   0   0   0   5
85  1.1651    0.2342   -0.6282 C   0   0   0   0   0   0   0   0   0   0   0   6
86  0.3308   -0.8575    1.3986 C   0   0   0   0   0   0   0   0   0   0   0   7
87 -1.1374   -2.2165   -0.3261 H   0   0   0   0   0   0   0   0   0   0   0   8
88 -0.5339   -1.4239   -1.8068 H   0   0   0   0   0   0   0   0   0   0   0   9
89  0.5762   -2.4130   -0.8079 H   0   0   0   0   0   0   0   0   0   0   0   10
90  0.9096    0.3523   -1.6922 H   0   0   0   0   0   0   0   0   0   0   0   11
91  1.4284    1.6088   -0.0174 C   0   0   0   0   0   0   0   0   0   0   0   12
92  2.0861   -0.3849   -0.5839 H   0   0   0   0   0   0   0   0   0   0   0   13
93 -0.5258   -1.4025    1.8175 H   0   0   0   0   0   0   0   0   0   0   0   14
94  0.4910    0.0439    2.0029 H   0   0   0   0   0   0   0   0   0   0   0   15
95  1.2305   -1.5008    1.4782 H   0   0   0   0   0   0   0   0   0   0   0   16
96  2.2050    2.1255   -0.5992 H   0   0   0   0   0   0   0   0   0   0   0   17
97  1.7826    1.5457    1.0209 H   0   0   0   0   0   0   0   0   0   0   0   18
98  0.5192    2.2271   -0.0380 H   0   0   0   0   0   0   0   0   0   0   0   19
99
100      2   1   0   0   0   0
101      3   1   0   0   0   0
102      5   4   0   0   0   0
103      8   4   0   0   0   0
104      9   4   0   0   0   0
105     10   4   0   0   0   0
106      6   5   0   0   0   0
107      7   5   0   0   0   0
108     11   6   0   0   0   0
109     12   6   0   0   0   0
110     13   6   0   0   0   0
111     14   7   0   0   0   0
112     15   7   0   0   0   0
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16 7 0 0 0 0
17 12 0 0 0 0
18 12 0 0 0 0
12 19 0 0 0 0
M END
$$$$
ethylamine-cation.sdf
COSMOTHERM 3D 0

14 12 0 0 0 0 0 0 0 0 0 V2000
-2.3013 0.0579 -0.3158 O 0 0 0 0 0 0 0 0 0 0 1
-2.4642 -0.5444 -1.0644 H 0 0 0 0 0 0 0 0 0 0 2
-2.4905 0.9467 -0.6675 H 0 0 0 0 0 0 0 0 0 0 3
1.4879 -0.1765 -1.0412 C 0 0 0 0 0 0 0 0 0 0 4
1.2615 0.4106 0.3421 C 0 0 0 0 0 0 0 0 0 0 5
0.1047 -0.2611 1.0335 N 0 0 0 0 0 0 0 0 0 0 6
-0.0375 0.1229 1.9756 H 0 0 0 0 0 0 0 0 0 0 7
0.2751 -1.2682 1.1468 H 0 0 0 0 0 0 0 0 0 0 8
2.3441 0.3272 -1.5088 H 0 0 0 0 0 0 0 0 0 0 9
1.7140 -1.2512 -0.9887 H 0 0 0 0 0 0 0 0 0 0 10
0.6129 -0.0303 -1.6899 H 0 0 0 0 0 0 0 0 0 0 11
1.0198 1.4789 0.2975 H 0 0 0 0 0 0 0 0 0 0 12
2.1376 0.2792 0.9875 H 0 0 0 0 0 0 0 0 0 0 13
-0.7998 -0.1412 0.4940 H 0 0 0 0 0 0 0 0 0 0 14
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
9 4 0 0 0 0
10 4 0 0 0 0
11 4 0 0 0 0
6 5 0 0 0 0
12 5 0 0 0 0
13 5 0 0 0 0
7 6 0 0 0 0
8 6 0 0 0 0
6 14 0 0 0 0
M END
$$$$
ethylamine.sdf
COSMOTHERM 3D 0

13 11 0 0 0 0 0 0 0 0 0 V2000
-2.3162 0.3514 0.1253 O 0 0 0 0 0 0 0 0 0 0 1
-1.4362 -0.1324 -0.0385 H 0 0 0 0 0 0 0 0 0 0 2
-2.3691 1.0057 -0.5925 H 0 0 0 0 0 0 0 0 0 0 3
1.4519 1.0325 -0.1578 C 0 0 0 0 0 0 0 0 0 0 4
1.2252 -0.3749 0.3862 C 0 0 0 0 0 0 0 0 0 0 5
0.0571 -1.0126 -0.2689 N 0 0 0 0 0 0 0 0 0 0 6
-0.0680 -1.9618 0.0956 H 0 0 0 0 0 0 0 0 0 0 7
0.2480 -1.1258 -1.2698 H 0 0 0 0 0 0 0 0 0 0 8
2.3052 1.5088 0.3457 H 0 0 0 0 0 0 0 0 0 0 9
1.6694 1.0083 -1.2371 H 0 0 0 0 0 0 0 0 0 0 10
0.5631 1.6613 -0.0013 H 0 0 0 0 0 0 0 0 0 0 11
1.0146 -0.3312 1.4655 H 0 0 0 0 0 0 0 0 0 0 12
2.1436 -0.9757 0.2597 H 0 0 0 0 0 0 0 0 0 0 13
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
9 4 0 0 0 0
10 4 0 0 0 0
11 4 0 0 0 0
6 5 0 0 0 0
12 5 0 0 0 0
7 6 0 0 0 0
8 6 0 0 0 0
5 13 0 0 0 0
M END
$$$$
guanidine_a.sdf
COSMOTHERM 3D 0

12 10 0 0 0 0 0 0 0 0 0 V2000
-2.7623 -0.1144 -0.0128 O 0 0 0 0 0 0 0 0 0 0 1
-1.8265 -0.0146 -0.4001 H 0 0 0 0 0 0 0 0 0 0 2
-3.0212 0.7905 0.2325 H 0 0 0 0 0 0 0 0 0 0 3
2.1109 -0.1222 -0.3647 N 0 0 0 0 0 0 0 0 0 0 4
0.7760 0.0238 -0.0488 C 0 0 0 0 0 0 0 0 0 0 5
0.4993 0.0855 1.3036 N 0 0 0 0 0 0 0 0 0 0 6
-0.2014 0.0944 -0.9124 N 0 0 0 0 0 0 0 0 0 0 7
2.3720 0.0900 -1.3240 H 0 0 0 0 0 0 0 0 0 0 8
2.7918 0.2004 0.3197 H 0 0 0 0 0 0 0 0 0 0 9
1.1460 -0.3915 1.9279 H 0 0 0 0 0 0 0 0 0 0 10
-0.4789 -0.0745 1.5373 H 0 0 0 0 0 0 0 0 0 0 11
0.1420 0.1312 -1.8761 H 0 0 0 0 0 0 0 0 0 0 12
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
8 4 0 0 0 0
9 4 0 0 0 0
6 5 0 0 0 0
7 5 0 0 0 0
10 6 0 0 0 0
11 6 0 0 0 0
7 12 0 0 0 0
M END
$$$$
guanidine_a_p2.sdf
COSMOTHERM 3D 0

13 11 0 0 0 0 0 0 0 0 0 V2000
-2.5414 0.0064 0.0002 O 0 0 0 0 0 0 0 0 0 0 1
-3.1398 -0.7618 -0.0216 H 0 0 0 0 0 0 0 0 0 0 2
-3.1286 0.7834 0.0188 H 0 0 0 0 0 0 0 0 0 0 3
2.1277 0.0154 0.0002 N 0 0 0 0 0 0 0 0 0 0 4
0.7873 -0.0026 0.0001 C 0 0 0 0 0 0 0 0 0 0 5
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1
2
3      0.1081  -0.0044   1.1543 N   0   0   0   0   0   0   0   0   0   0   6
4      0.1086  -0.0150  -1.1547 N   0   0   0   0   0   0   0   0   0   0   7
5      2.6505  -0.0184  -0.8679 H   0   0   0   0   0   0   0   0   0   0   8
6      2.6507  -0.0172   0.8682 H   0   0   0   0   0   0   0   0   0   0   9
7      0.5885  -0.0378   2.0465 H   0   0   0   0   0   0   0   0   0   0  10
8     -0.9162  -0.0195   1.1254 H   0   0   0   0   0   0   0   0   0   0  11
9      0.5886   0.0435  -2.0457 H   0   0   0   0   0   0   0   0   0   0  12
10     -0.9155   0.0122  -1.1256 H   0   0   0   0   0   0   0   0   0   0  13
11
12      2   1   0   0   0   0
13      3   1   0   0   0   0
14      5   4   0   0   0   0
15      8   4   0   0   0   0
16      9   4   0   0   0   0
17      6   5   0   0   0   0
18      7   5   0   0   0   0
19     10   6   0   0   0   0
20     11   6   0   0   0   0
21     12   7   0   0   0   0
22     7  13   0   0   0   0
23
24 M   END
25 $$$
26 hydroxyimidazo(2,3-a)isoindol_e-cation.sdf
27 COSMOtherm      3D      0
28
29 30 31   0   0   0   0   0   0   0   0   0   0 V2000
30 -3.1366  -2.0486   0.0671 O   0   0   0   0   0   0   0   0   0   0   1
31 -3.6931  -2.3306   0.8158 H   0   0   0   0   0   0   0   0   0   0   2
32 -3.6503  -2.2579  -0.7342 H   0   0   0   0   0   0   0   0   0   0   3
33   0.6687   4.2929  -0.1892 C   0   0   0   0   0   0   0   0   0   0   4
34   1.7742   3.4033  -0.1318 C   0   0   0   0   0   0   0   0   0   0   5
35   1.6049   2.0299  -0.0265 C   0   0   0   0   0   0   0   0   0   0   6
36   0.2910   1.5087   0.0270 C   0   0   0   0   0   0   0   0   0   0   7
37  -0.8296   2.4186  -0.0396 C   0   0   0   0   0   0   0   0   0   0   8
38  -0.6299   3.8141  -0.1462 C   0   0   0   0   0   0   0   0   0   0   9
39  -2.0036   1.6358   0.0149 C   0   0   0   0   0   0   0   0   0   0  10
40  -0.2599   0.1952   0.1254 C   0   0   0   0   0   0   0   0   0   0  11
41  -1.6438   0.3425   0.1081 N   0   0   0   0   0   0   0   0   0   0  12
42   0.3571  -1.0786   0.2210 C   0   0   0   0   0   0   0   0   0   0  13
43   0.6580  -3.3872   0.1815 C   0   0   0   0   0   0   0   0   0   0  14
44   1.9872  -2.6969   0.5260 C   0   0   0   0   0   0   0   0   0   0  15
45  -0.2869  -2.2663   0.2950 N   0   0   0   0   0   0   0   0   0   0  16
46   1.6904  -1.2844   0.2527 N   0   0   0   0   0   0   0   0   0   0  17
47   0.7310  -3.9012  -1.1463 O   0   0   0   0   0   0   0   0   0   0  18
48   0.8520   5.3653  -0.2722 H   0   0   0   0   0   0   0   0   0   0  19
49   2.7854   3.8118  -0.1748 H   0   0   0   0   0   0   0   0   0   0  20
50   2.4876   1.3903  -0.0011 H   0   0   0   0   0   0   0   0   0   0  21
51  -1.4831   4.4926  -0.1963 H   0   0   0   0   0   0   0   0   0   0  22
52  -3.0490   1.9272  -0.0071 H   0   0   0   0   0   0   0   0   0   0  23
53  -2.3195  -0.4458   0.1508 H   0   0   0   0   0   0   0   0   0   0  24
54   0.3836  -4.1810   0.8864 H   0   0   0   0   0   0   0   0   0   0  25
55   2.8015  -3.0661  -0.1079 H   0   0   0   0   0   0   0   0   0   0  26
56   2.2483  -2.8379   1.5845 H   0   0   0   0   0   0   0   0   0   0  27
57  -1.3016  -2.3757   0.1456 H   0   0   0   0   0   0   0   0   0   0  28
58  -0.0036  -4.5303  -1.2728 H   0   0   0   0   0   0   0   0   0   0  29
59   2.3487  -0.5519   0.4981 H   0   0   0   0   0   0   0   0   0   0  30
60
61      2   1   0   0   0   0
62      3   1   0   0   0   0
63      5   4   0   0   0   0
64      9   4   0   0   0   0
65     19   4   0   0   0   0
66      6   5   0   0   0   0
67     20   5   0   0   0   0
68      7   6   0   0   0   0
69     21   6   0   0   0   0
70      8   7   0   0   0   0
71     11   7   0   0   0   0
72      9   8   0   0   0   0
73     10   8   0   0   0   0
74     22   9   0   0   0   0
75     12  10   0   0   0   0
76     23  10   0   0   0   0
77     12  11   0   0   0   0
78     13  11   0   0   0   0
79     24  12   0   0   0   0
80     16  13   0   0   0   0
81     17  13   0   0   0   0
82     15  14   0   0   0   0
83     16  14   0   0   0   0
84     18  14   0   0   0   0
85     25  14   0   0   0   0
86     17  15   0   0   0   0
87     26  15   0   0   0   0
88     27  15   0   0   0   0
89     28  16   0   0   0   0
90     29  18   0   0   0   0
91     17  30   0   0   0   0
92
93 M   END
94 $$$
95 hydroxyimidazo(2,3-a)isoindol_e0.sdf
96 COSMOtherm      3D      0
97
98 29 30   0   0   0   0   0   0   0   0   0   0 V2000
99 -2.7912  -0.6123  -4.2850 O   0   0   0   0   0   0   0   0   0   0   1
100 -3.2833  -1.4150  -4.0339 H   0   0   0   0   0   0   0   0   0   0   2
101 -2.8960  -0.5582  -5.2523 H   0   0   0   0   0   0   0   0   0   0   3
102  -1.7206   0.0858   3.9144 C   0   0   0   0   0   0   0   0   0   0   4
103  -2.2680   0.5198   2.6715 C   0   0   0   0   0   0   0   0   0   0   5
104  -1.5127   0.5378   1.5113 C   0   0   0   0   0   0   0   0   0   0   6
105  -0.1594   0.1115   1.5642 C   0   0   0   0   0   0   0   0   0   0   7
106   0.3993  -0.3164   2.8374 C   0   0   0   0   0   0   0   0   0   0   8
107  -0.4034  -0.3249   4.0082 C   0   0   0   0   0   0   0   0   0   0   9
108   1.7439  -0.6578   2.6065 C   0   0   0   0   0   0   0   0   0   0  10
109   0.8795   0.0037   0.6066 C   0   0   0   0   0   0   0   0   0   0  11
110   1.9901  -0.4534   1.2863 N   0   0   0   0   0   0   0   0   0   0  12
111   0.9704   0.2754  -0.8110 C   0   0   0   0   0   0   0   0   0   0  13
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25 14 0 0 0 0
17 15 0 0 0 0
26 15 0 0 0 0
27 15 0 0 0 0
28 16 0 0 0 0
18 29 0 0 0 0
M END
$$$$
hydroxyimidazo(2,3-a)isoindol_e3.sdf
COSMOtherm 3D 0

29 30 0 0 0 0 0 0 0 0 0 V2000
-2.2940 1.4137 3.2645 O 0 0 0 0 0 0 0 0 0 0 0 1
-2.8339 0.6269 3.4597 H 0 0 0 0 0 0 0 0 0 0 0 2
-2.5480 1.6615 2.3575 H 0 0 0 0 0 0 0 0 0 0 0 3
0.0342 1.3645 -4.0355 C 0 0 0 0 0 0 0 0 0 0 0 4
0.4040 2.0875 -2.8632 C 0 0 0 0 0 0 0 0 0 0 0 5
0.4550 1.4797 -1.6207 C 0 0 0 0 0 0 0 0 0 0 0 6
0.1335 0.1009 -1.5185 C 0 0 0 0 0 0 0 0 0 0 0 7
-0.2578 -0.6295 -2.7137 C 0 0 0 0 0 0 0 0 0 0 0 8
-0.2976 0.0238 -3.9721 C 0 0 0 0 0 0 0 0 0 0 0 9
-0.5438 -1.9487 -2.3184 C 0 0 0 0 0 0 0 0 0 0 0 10
0.0705 -0.8159 -0.4410 C 0 0 0 0 0 0 0 0 0 0 0 11
-0.3403 -2.0197 -0.9765 N 0 0 0 0 0 0 0 0 0 0 0 12
0.3301 -0.7114 0.9783 C 0 0 0 0 0 0 0 0 0 0 0 13
1.0966 0.2355 2.9577 C 0 0 0 0 0 0 0 0 0 0 0 14
0.4928 -1.1899 3.1474 C 0 0 0 0 0 0 0 0 0 0 0 15
0.9535 0.4126 1.5103 N 0 0 0 0 0 0 0 0 0 0 0 16
-0.0259 -1.6279 1.8391 N 0 0 0 0 0 0 0 0 0 0 0 17
0.4460 1.2593 3.7072 O 0 0 0 0 0 0 0 0 0 0 0 18
0.0086 1.8859 -4.9942 H 0 0 0 0 0 0 0 0 0 0 0 19
0.6474 3.1482 -2.9511 H 0 0 0 0 0 0 0 0 0 0 0 20
0.7246 2.0621 -0.7385 H 0 0 0 0 0 0 0 0 0 0 0 21
-0.5890 -0.5246 -4.8702 H 0 0 0 0 0 0 0 0 0 0 0 22
-0.8597 -2.8164 -2.8878 H 0 0 0 0 0 0 0 0 0 0 0 23
-0.4686 -2.8539 -0.4052 H 0 0 0 0 0 0 0 0 0 0 0 24
2.1513 0.2982 3.2559 H 0 0 0 0 0 0 0 0 0 0 0 25
1.2497 -1.9035 3.5110 H 0 0 0 0 0 0 0 0 0 0 0 26
-0.3115 -1.1604 3.9001 H 0 0 0 0 0 0 0 0 0 0 0 27
1.6781 0.8994 0.9893 H 0 0 0 0 0 0 0 0 0 0 0 28
-0.5265 1.2407 3.4950 H 0 0 0 0 0 0 0 0 0 0 0 29
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
9 4 0 0 0 0
19 4 0 0 0 0
6 5 0 0 0 0
20 5 0 0 0 0
7 6 0 0 0 0
21 6 0 0 0 0
8 7 0 0 0 0
11 7 0 0 0 0
9 8 0 0 0 0
10 8 0 0 0 0
22 9 0 0 0 0
12 10 0 0 0 0
23 10 0 0 0 0
12 11 0 0 0 0
13 11 0 0 0 0
24 12 0 0 0 0
16 13 0 0 0 0
17 13 0 0 0 0
15 14 0 0 0 0
16 14 0 0 0 0
18 14 0 0 0 0
25 14 0 0 0 0
17 15 0 0 0 0
26 15 0 0 0 0
27 15 0 0 0 0
28 16 0 0 0 0
18 29 0 0 0 0
M END
$$$$
imidazo-(2,3-b)-thioxazole_b-cation1.sdf
COSMOtherm 3D 0

21 21 0 0 0 0 0 0 0 0 0 V2000
-3.1554 0.4583 1.0941 O 0 0 0 0 0 0 0 0 0 0 0 1
-3.7273 -0.2466 0.7414 H 0 0 0 0 0 0 0 0 0 0 0 2
-3.3956 1.2528 0.5849 H 0 0 0 0 0 0 0 0 0 0 0 3
1.4840 -0.1992 2.9072 C 0 0 0 0 0 0 0 0 0 0 0 4
1.7209 -0.0035 1.4614 N 0 0 0 0 0 0 0 0 0 0 0 5
-0.0458 0.0117 3.0132 C 0 0 0 0 0 0 0 0 0 0 0 6
-0.4818 -0.0779 1.6028 N 0 0 0 0 0 0 0 0 0 0 0 7
0.5653 -0.0241 0.7861 C 0 0 0 0 0 0 0 0 0 0 0 8
1.1616 0.4131 -2.8591 N 0 0 0 0 0 0 0 0 0 0 0 9
1.4766 0.4629 -1.5283 C 0 0 0 0 0 0 0 0 0 0 0 10
-0.0501 -0.0636 -3.0328 C 0 0 0 0 0 0 0 0 0 0 0 11
-0.9113 -0.4866 -1.5741 S 0 0 0 0 0 0 0 0 0 0 0 12
0.4951 0.0212 -0.6603 C 0 0 0 0 0 0 0 0 0 0 0 13
1.7857 -1.2166 3.1919 H 0 0 0 0 0 0 0 0 0 0 0 14
2.0548 0.5266 3.4961 H 0 0 0 0 0 0 0 0 0 0 0 15
2.6124 -0.2252 1.0266 H 0 0 0 0 0 0 0 0 0 0 0 16
-0.2996 1.0053 3.4081 H 0 0 0 0 0 0 0 0 0 0 0 17
-0.5401 -0.7540 3.6209 H 0 0 0 0 0 0 0 0 0 0 0 18
2.4449 0.8574 -1.2225 H 0 0 0 0 0 0 0 0 0 0 0 19
-0.5247 -0.2069 -4.0022 H 0 0 0 0 0 0 0 0 0 0 0 20
-1.4682 0.1150 1.3172 H 0 0 0 0 0 0 0 0 0 0 0 21
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
14 4 0 0 0 0
15 4 0 0 0 0
8 5 0 0 0 0
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16 5 0 0 0 0
7 6 0 0 0 0
17 6 0 0 0 0
18 6 0 0 0 0
8 7 0 0 0 0
13 8 0 0 0 0
10 9 0 0 0 0
11 9 0 0 0 0
13 10 0 0 0 0
19 10 0 0 0 0
12 11 0 0 0 0
20 11 0 0 0 0
13 12 0 0 0 0
7 21 0 0 0 0
M END
$$$$
imidazo-(2,3-b)-thioxazole_b.sdf
COSMOTHERM 3D 0
20 20 0 0 0 0 0 0 0 0 0 V2000
-3.2274 -1.7469 0.2047 O 0 0 0 0 0 0 0 0 0 0 1
-2.2208 -1.7171 0.1851 H 0 0 0 0 0 0 0 0 0 0 2
-3.4712 -1.2515 1.0054 H 0 0 0 0 0 0 0 0 0 0 3
1.7649 -2.6115 -0.2912 C 0 0 0 0 0 0 0 0 0 0 4
1.7429 -1.1514 -0.0457 N 0 0 0 0 0 0 0 0 0 0 5
0.3183 -2.9995 0.1032 C 0 0 0 0 0 0 0 0 0 0 6
-0.4566 -1.7352 0.0588 N 0 0 0 0 0 0 0 0 0 0 7
0.4127 -0.7693 -0.0338 C 0 0 0 0 0 0 0 0 0 0 8
-1.2688 2.5596 -0.3487 N 0 0 0 0 0 0 0 0 0 0 9
-1.1872 1.1891 -0.3913 C 0 0 0 0 0 0 0 0 0 0 10
-0.1191 3.0860 0.0015 C 0 0 0 0 0 0 0 0 0 0 11
1.1628 1.9352 0.3122 S 0 0 0 0 0 0 0 0 0 0 12
0.0378 0.6429 -0.0698 C 0 0 0 0 0 0 0 0 0 0 13
1.9738 -2.8177 -1.3529 H 0 0 0 0 0 0 0 0 0 0 14
2.5257 -3.1061 0.3246 H 0 0 0 0 0 0 0 0 0 0 15
2.4079 -0.5750 -0.5592 H 0 0 0 0 0 0 0 0 0 0 16
0.2752 -3.4022 1.1288 H 0 0 0 0 0 0 0 0 0 0 17
-0.1221 -3.7490 -0.5676 H 0 0 0 0 0 0 0 0 0 0 18
-2.0620 0.6025 -0.6690 H 0 0 0 0 0 0 0 0 0 0 19
0.0675 4.1531 0.1093 H 0 0 0 0 0 0 0 0 0 0 20
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
14 4 0 0 0 0
15 4 0 0 0 0
8 5 0 0 0 0
16 5 0 0 0 0
7 6 0 0 0 0
17 6 0 0 0 0
18 6 0 0 0 0
8 7 0 0 0 0
13 8 0 0 0 0
10 9 0 0 0 0
11 9 0 0 0 0
13 10 0 0 0 0
19 10 0 0 0 0
12 11 0 0 0 0
13 12 0 0 0 0
11 20 0 0 0 0
M END
$$$$
imidazole-cation.sdf
COSMOTHERM 3D 0
13 12 0 0 0 0 0 0 0 0 0 V2000
-3.0497 0.0014 -0.0593 O 0 0 0 0 0 0 0 0 0 0 1
-3.4650 -0.7808 0.3480 H 0 0 0 0 0 0 0 0 0 0 2
-3.4666 0.7619 0.3856 H 0 0 0 0 0 0 0 0 0 0 3
0.4820 -0.0005 1.1468 C 0 0 0 0 0 0 0 0 0 0 4
-0.3294 -0.0002 0.0268 N 0 0 0 0 0 0 0 0 0 0 5
1.7775 -0.0002 0.7025 C 0 0 0 0 0 0 0 0 0 0 6
1.7146 0.0003 -0.6781 N 0 0 0 0 0 0 0 0 0 0 7
0.4329 0.0004 -1.0728 C 0 0 0 0 0 0 0 0 0 0 8
0.0771 -0.0007 2.1511 H 0 0 0 0 0 0 0 0 0 0 9
2.7199 -0.0005 1.2354 H 0 0 0 0 0 0 0 0 0 0 10
0.0850 0.0009 -2.0986 H 0 0 0 0 0 0 0 0 0 0 11
2.5138 0.0006 -1.3090 H 0 0 0 0 0 0 0 0 0 0 12
-1.3881 0.0005 0.0272 H 0 0 0 0 0 0 0 0 0 0 13
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
9 4 0 0 0 0
8 5 0 0 0 0
7 6 0 0 0 0
10 6 0 0 0 0
8 7 0 0 0 0
12 7 0 0 0 0
11 8 0 0 0 0
5 13 0 0 0 0
M END
$$$$
imidazole.sdf
COSMOTHERM 3D 0
12 11 0 0 0 0 0 0 0 0 0 V2000
-3.1604 -0.0441 0.0048 O 0 0 0 0 0 0 0 0 0 0 1
-2.1542 -0.0284 0.0025 H 0 0 0 0 0 0 0 0 0 0 2
-3.4155 0.8941 0.0270 H 0 0 0 0 0 0 0 0 0 0 3
0.4514 -0.0083 -1.1154 C 0 0 0 0 0 0 0 0 0 0 4
-0.3795 -0.0233 -0.0065 N 0 0 0 0 0 0 0 0 0 0 5
1.7688 0.0142 -0.7141 C 0 0 0 0 0 0 0 0 0 0 6
1.7310 0.0127 0.6659 N 0 0 0 0 0 0 0 0 0 0 7
0.4268 -0.0098 1.0524 C 0 0 0 0 0 0 0 0 0 0 8
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15 12 0 0 0 0
11 20 0 0 0 0
M END
$$$$
indole-cation2.sdf
COSMOtherm 3D 0

20 20 0 0 0 0 0 0 0 0 0 V2000
-3.5645 -0.0006 1.2070 O 0 0 0 0 0 0 0 0 0 0 0 0 1
-4.1290 -0.7873 1.0935 H 0 0 0 0 0 0 0 0 0 0 0 0 2
-4.1607 0.7575 1.0651 H 0 0 0 0 0 0 0 0 0 0 0 0 3
1.7683 0.0011 1.7535 C 0 0 0 0 0 0 0 0 0 0 0 0 4
2.6785 -0.0007 0.6837 C 0 0 0 0 0 0 0 0 0 0 0 0 5
2.2415 -0.0028 -0.6499 C 0 0 0 0 0 0 0 0 0 0 0 0 6
0.8709 -0.0010 -0.8912 C 0 0 0 0 0 0 0 0 0 0 0 0 7
-0.0210 0.0007 0.1968 C 0 0 0 0 0 0 0 0 0 0 0 0 8
0.3864 0.0026 1.5278 C 0 0 0 0 0 0 0 0 0 0 0 0 9
-1.3436 0.0011 -0.3248 N 0 0 0 0 0 0 0 0 0 0 0 0 10
0.0503 0.0007 -2.1526 C 0 0 0 0 0 0 0 0 0 0 0 0 11
-1.3389 0.0014 -1.6284 C 0 0 0 0 0 0 0 0 0 0 0 0 12
-2.2298 0.0002 0.2749 H 0 0 0 0 0 0 0 0 0 0 0 0 13
0.2161 -0.8775 -2.8013 H 0 0 0 0 0 0 0 0 0 0 0 0 14
0.2184 0.8787 -2.8015 H 0 0 0 0 0 0 0 0 0 0 0 0 15
2.1421 -0.0006 2.7777 H 0 0 0 0 0 0 0 0 0 0 0 0 16
3.7489 0.0014 0.8942 H 0 0 0 0 0 0 0 0 0 0 0 0 17
2.9594 -0.0058 -1.4707 H 0 0 0 0 0 0 0 0 0 0 0 0 18
-0.3278 0.0055 2.3513 H 0 0 0 0 0 0 0 0 0 0 0 0 19
-2.2632 0.0009 -2.2027 H 0 0 0 0 0 0 0 0 0 0 0 0 20
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
9 4 0 0 0 0
16 4 0 0 0 0
6 5 0 0 0 0
17 5 0 0 0 0
7 6 0 0 0 0
18 6 0 0 0 0
8 7 0 0 0 0
11 7 0 0 0 0
9 8 0 0 0 0
10 8 0 0 0 0
19 9 0 0 0 0
12 10 0 0 0 0
13 10 0 0 0 0
12 11 0 0 0 0
14 11 0 0 0 0
15 11 0 0 0 0
12 20 0 0 0 0
M END
$$$$
indole.sdf
COSMOtherm 3D 0

19 19 0 0 0 0 0 0 0 0 0 V2000
-3.8057 0.0054 -1.0505 O 0 0 0 0 0 0 0 0 0 0 0 0 1
-3.9527 -0.7649 -1.6290 H 0 0 0 0 0 0 0 0 0 0 0 0 2
-3.9413 0.7734 -1.6345 H 0 0 0 0 0 0 0 0 0 0 0 0 3
-0.0409 -0.0029 -0.1758 C 0 0 0 0 0 0 0 0 0 0 0 0 4
-1.3072 -0.0047 0.3754 N 0 0 0 0 0 0 0 0 0 0 0 0 5
-1.1981 -0.0026 1.7528 C 0 0 0 0 0 0 0 0 0 0 0 0 6
0.1337 0.0011 2.1206 C 0 0 0 0 0 0 0 0 0 0 0 0 7
0.9013 0.0011 0.9058 C 0 0 0 0 0 0 0 0 0 0 0 0 8
0.3653 -0.0043 -1.5188 C 0 0 0 0 0 0 0 0 0 0 0 0 9
1.7359 -0.0013 -1.7803 C 0 0 0 0 0 0 0 0 0 0 0 0 10
2.6832 0.0028 -0.7289 C 0 0 0 0 0 0 0 0 0 0 0 0 11
2.2801 0.0039 0.6058 C 0 0 0 0 0 0 0 0 0 0 0 0 12
-2.1952 -0.0058 -0.1556 H 0 0 0 0 0 0 0 0 0 0 0 0 13
-2.0913 -0.0034 2.3713 H 0 0 0 0 0 0 0 0 0 0 0 0 14
0.5138 0.0036 3.1385 H 0 0 0 0 0 0 0 0 0 0 0 0 15
-0.3637 -0.0072 -2.3315 H 0 0 0 0 0 0 0 0 0 0 0 0 16
2.0833 -0.0024 -2.8151 H 0 0 0 0 0 0 0 0 0 0 0 0 17
3.7478 0.0051 -0.9712 H 0 0 0 0 0 0 0 0 0 0 0 0 18
3.0213 0.0069 1.4083 H 0 0 0 0 0 0 0 0 0 0 0 0 19
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
8 4 0 0 0 0
9 4 0 0 0 0
6 5 0 0 0 0
13 5 0 0 0 0
7 6 0 0 0 0
14 6 0 0 0 0
8 7 0 0 0 0
15 7 0 0 0 0
12 8 0 0 0 0
10 9 0 0 0 0
16 9 0 0 0 0
11 10 0 0 0 0
17 10 0 0 0 0
12 11 0 0 0 0
18 11 0 0 0 0
12 19 0 0 0 0
M END
$$$$
iso-propylamine-cation.sdf
COSMOtherm 3D 0

17 15 0 0 0 0 0 0 0 0 0 V2000
-2.4596 -0.4111 -0.0012 O 0 0 0 0 0 0 0 0 0 0 0 0 1
-3.0174 -0.2708 -0.7881 H 0 0 0 0 0 0 0 0 0 0 0 0 2
-3.0507 -0.2290 0.7522 H 0 0 0 0 0 0 0 0 0 0 0 0 3
1.0978 0.2901 0.0007 C 0 0 0 0 0 0 0 0 0 0 0 0 4
-0.1520 1.1497 0.0198 N 0 0 0 0 0 0 0 0 0 0 0 0 5
1.1293 -0.5585 1.2666 C 0 0 0 0 0 0 0 0 0 0 0 0 6
1.1165 -0.5273 -1.2858 C 0 0 0 0 0 0 0 0 0 0 0 0 7
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13 12 0 0 0 0
12 20 0 0 0 0
M END
$$$$
isoquinoline-cation.sdf
COSMOTHERM 3D 0

21 21 0 0 0 0 0 0 0 0 V2000
-4.4219 0.0021 0.7252 O 0 0 0 0 0 0 0 0 0 0 1
-4.9554 -0.7444 0.3963 H 0 0 0 0 0 0 0 0 0 0 2
-4.9228 0.7982 0.4693 H 0 0 0 0 0 0 0 0 0 0 3
-1.8212 -0.0037 -0.0637 N 0 0 0 0 0 0 0 0 0 0 4
-1.4970 -0.0018 -1.3959 C 0 0 0 0 0 0 0 0 0 0 5
-0.1812 0.0001 -1.7808 C 0 0 0 0 0 0 0 0 0 0 6
0.8493 0.0001 -0.8016 C 0 0 0 0 0 0 0 0 0 0 7
0.4695 -0.0018 0.5875 C 0 0 0 0 0 0 0 0 0 0 8
-0.9019 -0.0040 0.9024 C 0 0 0 0 0 0 0 0 0 0 9
2.2281 0.0025 -1.1312 C 0 0 0 0 0 0 0 0 0 0 10
3.1784 0.0027 -0.1268 C 0 0 0 0 0 0 0 0 0 0 11
1.4677 -0.0014 1.5996 C 0 0 0 0 0 0 0 0 0 0 12
2.8001 0.0009 1.2414 C 0 0 0 0 0 0 0 0 0 0 13
-2.3330 -0.0015 -2.0913 H 0 0 0 0 0 0 0 0 0 0 14
0.0679 0.0016 -2.8416 H 0 0 0 0 0 0 0 0 0 0 15
-1.2665 -0.0058 1.9291 H 0 0 0 0 0 0 0 0 0 0 16
2.5252 0.0039 -2.1808 H 0 0 0 0 0 0 0 0 0 0 17
4.2382 0.0045 -0.3858 H 0 0 0 0 0 0 0 0 0 0 18
1.1669 -0.0028 2.6482 H 0 0 0 0 0 0 0 0 0 0 19
3.5724 0.0014 2.0113 H 0 0 0 0 0 0 0 0 0 0 20
-2.8480 -0.0035 0.2091 H 0 0 0 0 0 0 0 0 0 0 21
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
9 4 0 0 0 0
6 5 0 0 0 0
14 5 0 0 0 0
7 6 0 0 0 0
15 6 0 0 0 0
8 7 0 0 0 0
10 7 0 0 0 0
9 8 0 0 0 0
12 8 0 0 0 0
16 9 0 0 0 0
11 10 0 0 0 0
17 10 0 0 0 0
13 11 0 0 0 0
18 11 0 0 0 0
13 12 0 0 0 0
19 12 0 0 0 0
20 13 0 0 0 0
4 21 0 0 0 0
M END
$$$$
melamine.sdf
COSMOTHERM 3D 0

18 17 0 0 0 0 0 0 0 0 V2000
-3.6154 0.0731 0.0149 O 0 0 0 0 0 0 0 0 0 0 1
-2.6488 0.0436 -0.2507 H 0 0 0 0 0 0 0 0 0 0 2
-3.8783 1.0013 -0.1128 H 0 0 0 0 0 0 0 0 0 0 3
0.9759 0.0077 1.3137 N 0 0 0 0 0 0 0 0 0 0 4
-0.3367 -0.0445 1.0069 C 0 0 0 0 0 0 0 0 0 0 5
-0.8497 -0.0642 -0.2497 N 0 0 0 0 0 0 0 0 0 0 6
0.0748 -0.0303 -1.2387 C 0 0 0 0 0 0 0 0 0 0 7
1.4110 0.0207 -1.0580 N 0 0 0 0 0 0 0 0 0 0 8
1.7973 0.0343 0.2386 C 0 0 0 0 0 0 0 0 0 0 9
3.1304 0.0516 0.4831 N 0 0 0 0 0 0 0 0 0 0 10
-0.3796 -0.0779 -2.5140 N 0 0 0 0 0 0 0 0 0 0 11
-1.2223 -0.1080 2.0300 N 0 0 0 0 0 0 0 0 0 0 12
3.7694 0.2313 -0.2845 H 0 0 0 0 0 0 0 0 0 0 13
3.4553 0.2191 1.4296 H 0 0 0 0 0 0 0 0 0 0 14
-1.3712 0.0342 -2.6959 H 0 0 0 0 0 0 0 0 0 0 15
0.2703 0.0976 -3.2732 H 0 0 0 0 0 0 0 0 0 0 16
-0.8933 0.0600 2.9749 H 0 0 0 0 0 0 0 0 0 0 17
-2.2154 0.0005 1.8252 H 0 0 0 0 0 0 0 0 0 0 18
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
9 4 0 0 0 0
6 5 0 0 0 0
12 5 0 0 0 0
7 6 0 0 0 0
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11 7 0 0 0 0
9 8 0 0 0 0
10 9 0 0 0 0
13 10 0 0 0 0
14 10 0 0 0 0
15 11 0 0 0 0
16 11 0 0 0 0
17 12 0 0 0 0
12 18 0 0 0 0
M END
$$$$
melamine_p2.sdf
COSMOTHERM 3D 0

19 18 0 0 0 0 0 0 0 0 V2000
-3.5159 -0.0198 0.0039 O 0 0 0 0 0 0 0 0 0 0 1
-4.0535 0.2262 -0.7708 H 0 0 0 0 0 0 0 0 0 0 2
-4.0507 0.2321 0.7787 H 0 0 0 0 0 0 0 0 0 0 3
0.9467 -1.3383 0.0003 N 0 0 0 0 0 0 0 0 0 0 4
-0.3474 -1.0322 -0.0015 C 0 0 0 0 0 0 0 0 0 0 5
-0.7835 0.2751 -0.0039 N 0 0 0 0 0 0 0 0 0 0 6
0.1456 1.2864 -0.0015 C 0 0 0 0 0 0 0 0 0 0 7
1.4518 1.0339 0.0003 N 0 0 0 0 0 0 0 0 0 0 8
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6 5 0 0 0 0
7 5 0 0 0 0
10 6 0 0 0 0
11 6 0 0 0 0
12 7 0 0 0 0
13 8 0 0 0 0
14 8 0 0 0 0
8 15 0 0 0 0
M END
$$$$
methylguanidine_a.sdf
COSMOTHERM 3D 0

15 13 0 0 0 0 0 0 0 0 0 V2000
-3.1365 -0.4868 0.0980 O 0 0 0 0 0 0 0 0 0 0 1
-2.1347 -0.6502 0.0176 H 0 0 0 0 0 0 0 0 0 0 2
-3.4346 -0.3531 -0.8182 H 0 0 0 0 0 0 0 0 0 0 3
1.6711 0.3347 0.1015 N 0 0 0 0 0 0 0 0 0 0 4
0.3051 0.3088 -0.0088 C 0 0 0 0 0 0 0 0 0 0 5
-0.2993 1.5563 -0.0874 N 0 0 0 0 0 0 0 0 0 0 6
-0.4371 -0.7678 -0.0611 N 0 0 0 0 0 0 0 0 0 0 7
2.4771 -0.8744 -0.0129 C 0 0 0 0 0 0 0 0 0 0 8
2.1299 1.2077 -0.1449 H 0 0 0 0 0 0 0 0 0 0 9
0.1629 2.3112 0.4162 H 0 0 0 0 0 0 0 0 0 0 10
-1.3030 1.5288 0.0874 H 0 0 0 0 0 0 0 0 0 0 11
0.1203 -1.6242 -0.1069 H 0 0 0 0 0 0 0 0 0 0 12
3.5267 -0.6034 0.1448 H 0 0 0 0 0 0 0 0 0 0 13
2.1955 -1.6018 0.7621 H 0 0 0 0 0 0 0 0 0 0 14
2.3825 -1.3552 -1.0017 H 0 0 0 0 0 0 0 0 0 0 15
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
8 4 0 0 0 0
9 4 0 0 0 0
6 5 0 0 0 0
7 5 0 0 0 0
10 6 0 0 0 0
11 6 0 0 0 0
12 7 0 0 0 0
13 8 0 0 0 0
14 8 0 0 0 0
8 15 0 0 0 0
M END
$$$$
methylguanidine_a_p2.sdf
COSMOTHERM 3D 0

16 14 0 0 0 0 0 0 0 0 0 V2000
-2.6771 -0.2274 -0.0472 O 0 0 0 0 0 0 0 0 0 0 1
-3.2134 -0.4016 -0.8414 H 0 0 0 0 0 0 0 0 0 0 2
-3.2773 -0.3862 0.7034 H 0 0 0 0 0 0 0 0 0 0 3
0.1584 -0.7409 0.0347 N 0 0 0 0 0 0 0 0 0 0 4
0.5650 0.5331 0.0076 C 0 0 0 0 0 0 0 0 0 0 5
-0.3503 1.5187 0.0972 N 0 0 0 0 0 0 0 0 0 0 6
1.8697 0.8341 -0.0858 N 0 0 0 0 0 0 0 0 0 0 7
1.0590 -1.8880 0.0214 C 0 0 0 0 0 0 0 0 0 0 8
-0.8590 -0.8889 0.0272 H 0 0 0 0 0 0 0 0 0 0 9
-1.3380 1.2574 0.0154 H 0 0 0 0 0 0 0 0 0 0 10
-0.0884 2.4682 -0.1476 H 0 0 0 0 0 0 0 0 0 0 11
2.5790 0.1097 -0.0659 H 0 0 0 0 0 0 0 0 0 0 12
0.4502 -2.7940 0.0950 H 0 0 0 0 0 0 0 0 0 0 13
1.6409 -1.9371 -0.9116 H 0 0 0 0 0 0 0 0 0 0 14
1.7470 -1.8654 0.8799 H 0 0 0 0 0 0 0 0 0 0 15
2.1861 1.7933 0.0080 H 0 0 0 0 0 0 0 0 0 0 16
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
8 4 0 0 0 0
9 4 0 0 0 0
6 5 0 0 0 0
7 5 0 0 0 0
10 6 0 0 0 0
11 6 0 0 0 0
12 7 0 0 0 0
13 8 0 0 0 0
14 8 0 0 0 0
15 8 0 0 0 0
7 16 0 0 0 0
M END
$$$$
methylguanidine_p2.sdf
COSMOTHERM 3D 0

16 14 0 0 0 0 0 0 0 0 0 V2000
-2.8995 -0.5713 -0.1202 O 0 0 0 0 0 0 0 0 0 0 1
-3.1864 -0.3855 -1.0324 H 0 0 0 0 0 0 0 0 0 0 2
-3.4080 0.0555 0.4250 H 0 0 0 0 0 0 0 0 0 0 3
0.8883 1.0506 -0.1003 N 0 0 0 0 0 0 0 0 0 0 4
-0.3290 1.8265 0.1178 C 0 0 0 0 0 0 0 0 0 0 5
1.7238 1.5473 -0.3940 H 0 0 0 0 0 0 0 0 0 0 6
-1.0625 1.6697 -0.6860 H 0 0 0 0 0 0 0 0 0 0 7
-0.7856 1.5663 1.0829 H 0 0 0 0 0 0 0 0 0 0 8
-0.0511 2.8845 0.1382 H 0 0 0 0 0 0 0 0 0 0 9
0.9720 -0.2818 0.0111 C 0 0 0 0 0 0 0 0 0 0 10
2.1725 -0.8780 -0.1419 N 0 0 0 0 0 0 0 0 0 0 11
2.2571 -1.8806 -0.0094 H 0 0 0 0 0 0 0 0 0 0 12
3.0247 -0.3355 -0.0415 H 0 0 0 0 0 0 0 0 0 0 13
-0.1149 -1.0189 0.2699 N 0 0 0 0 0 0 0 0 0 0 14
-0.0052 -2.0221 0.3824 H 0 0 0 0 0 0 0 0 0 0 15
-1.0814 -0.6785 0.1226 H 0 0 0 0 0 0 0 0 0 0 16
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
10 4 0 0 0 0
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7 5 0 0 0 0
8 5 0 0 0 0
9 5 0 0 0 0
11 10 0 0 0 0
14 10 0 0 0 0
12 11 0 0 0 0
13 11 0 0 0 0
15 14 0 0 0 0
14 16 0 0 0 0
M END
$$$$
methylguanidine_t.sdf
COSMOtherm 3D 0
15 13 0 0 0 0 0 0 0 0 V2000
-2.7457 -0.1051 -0.1285 O 0 0 0 0 0 0 0 0 0 0 1
-1.7898 -0.0336 0.2286 H 0 0 0 0 0 0 0 0 0 0 2
-3.0345 0.8175 -0.2382 H 0 0 0 0 0 0 0 0 0 0 3
0.4076 0.0365 1.9650 C 0 0 0 0 0 0 0 0 0 0 4
-0.1477 0.0281 0.6149 N 0 0 0 0 0 0 0 0 0 0 5
0.6779 0.0070 -0.3943 C 0 0 0 0 0 0 0 0 0 0 6
0.1802 0.1136 -1.6869 N 0 0 0 0 0 0 0 0 0 0 7
2.0466 -0.1132 -0.3005 N 0 0 0 0 0 0 0 0 0 0 8
-0.4150 0.1274 2.6859 H 0 0 0 0 0 0 0 0 0 0 9
0.9560 -0.8935 2.2046 H 0 0 0 0 0 0 0 0 0 0 10
1.0947 0.8860 2.1415 H 0 0 0 0 0 0 0 0 0 0 11
0.6990 -0.3905 -2.4041 H 0 0 0 0 0 0 0 0 0 0 12
-0.8250 -0.0555 -1.7417 H 0 0 0 0 0 0 0 0 0 0 13
2.6024 0.2179 -1.0854 H 0 0 0 0 0 0 0 0 0 0 14
2.4676 0.0784 0.6042 H 0 0 0 0 0 0 0 0 0 0 15
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
9 4 0 0 0 0
10 4 0 0 0 0
11 4 0 0 0 0
6 5 0 0 0 0
7 6 0 0 0 0
8 6 0 0 0 0
12 7 0 0 0 0
13 7 0 0 0 0
14 8 0 0 0 0
8 15 0 0 0 0
M END
$$$$
methylguanidine_t_p2.sdf
COSMOtherm 3D 0
16 14 0 0 0 0 0 0 0 0 V2000
-2.9205 -0.0019 0.5632 O 0 0 0 0 0 0 0 0 0 0 1
-3.3293 -0.8743 0.4220 H 0 0 0 0 0 0 0 0 0 0 2
-3.3523 0.5744 -0.0920 H 0 0 0 0 0 0 0 0 0 0 3
-0.3478 0.0334 -1.8100 C 0 0 0 0 0 0 0 0 0 0 4
0.9008 -0.0488 -1.0574 N 0 0 0 0 0 0 0 0 0 0 5
0.9846 -0.0082 0.2798 C 0 0 0 0 0 0 0 0 0 0 6
2.1986 0.0187 0.8643 N 0 0 0 0 0 0 0 0 0 0 7
-0.1170 0.0360 1.0361 N 0 0 0 0 0 0 0 0 0 0 8
-0.1018 -0.0483 -2.8727 H 0 0 0 0 0 0 0 0 0 0 9
-1.0260 -0.7901 -1.5471 H 0 0 0 0 0 0 0 0 0 0 10
-0.8564 0.9937 -1.6394 H 0 0 0 0 0 0 0 0 0 0 11
2.2844 -0.1030 1.8676 H 0 0 0 0 0 0 0 0 0 0 12
3.0389 -0.1129 0.3115 H 0 0 0 0 0 0 0 0 0 0 13
-0.0211 0.0551 2.0463 H 0 0 0 0 0 0 0 0 0 0 14
-1.0814 0.0147 0.6653 H 0 0 0 0 0 0 0 0 0 0 15
1.7710 -0.0625 -1.5801 H 0 0 0 0 0 0 0 0 0 0 16
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
9 4 0 0 0 0
10 4 0 0 0 0
11 4 0 0 0 0
6 5 0 0 0 0
7 6 0 0 0 0
8 6 0 0 0 0
12 7 0 0 0 0
13 7 0 0 0 0
14 8 0 0 0 0
15 8 0 0 0 0
5 16 0 0 0 0
M END
$$$$
n-butylamine-cation.sdf
COSMOtherm 3D 0
20 18 0 0 0 0 0 0 0 0 V2000
-1.3036 0.1207 2.9363 O 0 0 0 0 0 0 0 0 0 0 1
-2.0105 -0.5279 2.7651 H 0 0 0 0 0 0 0 0 0 0 2
-1.7274 0.9885 2.8076 H 0 0 0 0 0 0 0 0 0 0 3
-0.9142 -0.1954 -3.0163 C 0 0 0 0 0 0 0 0 0 0 4
0.1530 0.3639 -2.0699 C 0 0 0 0 0 0 0 0 0 0 5
0.0915 -0.2652 -0.6706 C 0 0 0 0 0 0 0 0 0 0 6
1.1534 0.3185 0.2537 C 0 0 0 0 0 0 0 0 0 0 7
1.1005 -0.3119 1.6188 N 0 0 0 0 0 0 0 0 0 0 8
1.8321 0.0699 2.2305 H 0 0 0 0 0 0 0 0 0 0 9
1.2593 -1.3257 1.5648 H 0 0 0 0 0 0 0 0 0 0 10
-0.8452 0.2705 -4.0099 H 0 0 0 0 0 0 0 0 0 0 11
-0.8001 -1.2826 -3.1458 H 0 0 0 0 0 0 0 0 0 0 12
-1.9268 -0.0082 -2.6271 H 0 0 0 0 0 0 0 0 0 0 13
0.0324 1.4562 -1.9812 H 0 0 0 0 0 0 0 0 0 0 14
1.1545 0.1948 -2.4996 H 0 0 0 0 0 0 0 0 0 0 15
0.2331 -1.3561 -0.7502 H 0 0 0 0 0 0 0 0 0 0 16
-0.9083 -0.1004 -0.2353 H 0 0 0 0 0 0 0 0 0 0 17
1.0126 1.3965 0.4004 H 0 0 0 0 0 0 0 0 0 0 18
2.1641 0.1498 -0.1382 H 0 0 0 0 0 0 0 0 0 0 19
0.1659 -0.1512 2.0931 H 0 0 0 0 0 0 0 0 0 0 20
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2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
11 4 0 0 0 0
12 4 0 0 0 0
13 4 0 0 0 0
6 5 0 0 0 0
14 5 0 0 0 0
15 5 0 0 0 0
7 6 0 0 0 0
16 6 0 0 0 0
17 6 0 0 0 0
8 7 0 0 0 0
18 7 0 0 0 0
19 7 0 0 0 0
9 8 0 0 0 0
10 8 0 0 0 0
8 20 0 0 0 0
M END
$$$$
n-butylamine.sdf
COSMOTHERM 3D 0
19 17 0 0 0 0 0 0 0 0 0 V2000
1.3689 -2.9093 -0.1854 O 0 0 0 0 0 0 0 0 0 0 1
0.4930 -2.4341 0.0206 H 0 0 0 0 0 0 0 0 0 0 2
1.9715 -2.6228 0.5222 H 0 0 0 0 0 0 0 0 0 0 3
0.8944 2.9876 0.1905 C 0 0 0 0 0 0 0 0 0 0 4
-0.1688 2.0329 -0.3637 C 0 0 0 0 0 0 0 0 0 0 5
-0.0981 0.6308 0.2545 C 0 0 0 0 0 0 0 0 0 0 6
-1.1650 -0.3178 -0.2923 C 0 0 0 0 0 0 0 0 0 0 7
-1.0469 -1.6655 0.3150 N 0 0 0 0 0 0 0 0 0 0 8
-1.7805 -2.2759 -0.0575 H 0 0 0 0 0 0 0 0 0 0 9
-1.2289 -1.6017 1.3217 H 0 0 0 0 0 0 0 0 0 0 10
0.8348 3.9762 -0.2884 H 0 0 0 0 0 0 0 0 0 0 11
0.7712 3.1324 1.2752 H 0 0 0 0 0 0 0 0 0 0 12
1.9084 2.5933 0.0202 H 0 0 0 0 0 0 0 0 0 0 13
-0.0551 1.9509 -1.4581 H 0 0 0 0 0 0 0 0 0 0 14
-1.1721 2.4583 -0.1896 H 0 0 0 0 0 0 0 0 0 0 15
-0.2115 0.7092 1.3505 H 0 0 0 0 0 0 0 0 0 0 16
0.8982 0.1927 0.0717 H 0 0 0 0 0 0 0 0 0 0 17
-1.0385 -0.4317 -1.3804 H 0 0 0 0 0 0 0 0 0 0 18
-2.1667 0.1209 -0.1269 H 0 0 0 0 0 0 0 0 0 0 19
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
11 4 0 0 0 0
12 4 0 0 0 0
13 4 0 0 0 0
6 5 0 0 0 0
14 5 0 0 0 0
15 5 0 0 0 0
7 6 0 0 0 0
16 6 0 0 0 0
17 6 0 0 0 0
8 7 0 0 0 0
18 7 0 0 0 0
9 8 0 0 0 0
10 8 0 0 0 0
7 19 0 0 0 0
M END
$$$$
n-heptylamine-cation.sdf
COSMOTHERM 3D 0
29 27 0 0 0 0 0 0 0 0 0 V2000
-1.7848 -0.1888 4.3958 O 0 0 0 0 0 0 0 0 0 0 1
-2.0781 -1.1158 4.3306 H 0 0 0 0 0 0 0 0 0 0 2
-2.4740 0.3221 3.9338 H 0 0 0 0 0 0 0 0 0 0 3
-0.5953 0.3770 -3.8375 C 0 0 0 0 0 0 0 0 0 0 4
0.1851 -0.2628 -2.6813 C 0 0 0 0 0 0 0 0 0 0 5
-0.1288 0.3533 -1.3121 C 0 0 0 0 0 0 0 0 0 0 6
0.6609 -0.2889 -0.1639 C 0 0 0 0 0 0 0 0 0 0 7
0.3429 0.3296 1.2044 C 0 0 0 0 0 0 0 0 0 0 8
1.1587 -0.3219 2.3151 C 0 0 0 0 0 0 0 0 0 0 9
0.8505 0.2897 3.6543 N 0 0 0 0 0 0 0 0 0 0 10
1.4484 -0.1087 4.3886 H 0 0 0 0 0 0 0 0 0 0 11
-0.1583 0.1284 3.9362 H 0 0 0 0 0 0 0 0 0 0 12
-0.2749 -0.2469 -5.2004 C 0 0 0 0 0 0 0 0 0 0 13
-1.6771 0.2878 -3.6365 H 0 0 0 0 0 0 0 0 0 0 14
-0.3766 1.4584 -3.8663 H 0 0 0 0 0 0 0 0 0 0 15
1.2680 -0.1726 -2.8814 H 0 0 0 0 0 0 0 0 0 0 16
-0.0329 -1.3454 -2.6524 H 0 0 0 0 0 0 0 0 0 0 17
-1.2101 0.2584 -1.1084 H 0 0 0 0 0 0 0 0 0 0 18
0.0870 1.4358 -1.3407 H 0 0 0 0 0 0 0 0 0 0 19
1.7417 -0.1905 -0.3650 H 0 0 0 0 0 0 0 0 0 0 20
0.4462 -1.3710 -0.1335 H 0 0 0 0 0 0 0 0 0 0 21
-0.7326 0.2170 1.4199 H 0 0 0 0 0 0 0 0 0 0 22
0.5567 1.4114 1.1805 H 0 0 0 0 0 0 0 0 0 0 23
2.2357 -0.1976 2.1464 H 0 0 0 0 0 0 0 0 0 0 24
0.9411 -1.3936 2.4027 H 0 0 0 0 0 0 0 0 0 0 25
-0.8486 0.2314 -6.0084 H 0 0 0 0 0 0 0 0 0 0 26
0.7945 -0.1425 -5.4423 H 0 0 0 0 0 0 0 0 0 0 27
-0.5148 -1.3218 -5.2108 H 0 0 0 0 0 0 0 0 0 0 28
1.0248 1.3027 3.6485 H 0 0 0 0 0 0 0 0 0 0 29
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
13 4 0 0 0 0
14 4 0 0 0 0
15 4 0 0 0 0
6 5 0 0 0 0
16 5 0 0 0 0
17 5 0 0 0 0
7 6 0 0 0 0
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18 6 0 0 0 0
19 6 0 0 0 0
8 7 0 0 0 0
20 7 0 0 0 0
21 7 0 0 0 0
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25 9 0 0 0 0
11 10 0 0 0 0
12 10 0 0 0 0
26 13 0 0 0 0
27 13 0 0 0 0
28 13 0 0 0 0
10 29 0 0 0 0
M END
$$$$
n-heptylamine.sdf
COSMOtherm 3D 0
28 26 0 0 0 0 0 0 0 0 0 V2000
-1.8357 -0.2676 -4.3924 O 0 0 0 0 0 0 0 0 0 0 1
-0.8844 -0.0394 -4.1133 H 0 0 0 0 0 0 0 0 0 0 2
-2.3808 0.4242 -3.9798 H 0 0 0 0 0 0 0 0 0 0 3
-0.6195 0.3486 3.8005 C 0 0 0 0 0 0 0 0 0 0 4
0.2064 -0.2473 2.6525 C 0 0 0 0 0 0 0 0 0 0 5
-0.1395 0.3358 1.2766 C 0 0 0 0 0 0 0 0 0 0 6
0.6889 -0.2626 0.1319 C 0 0 0 0 0 0 0 0 0 0 7
0.3325 0.3121 -1.2449 C 0 0 0 0 0 0 0 0 0 0 8
1.1713 -0.2854 -2.3751 C 0 0 0 0 0 0 0 0 0 0 9
0.7812 0.2806 -3.6888 N 0 0 0 0 0 0 0 0 0 0 10
1.3713 -0.1182 -4.4251 H 0 0 0 0 0 0 0 0 0 0 11
0.9748 1.2872 -3.6972 H 0 0 0 0 0 0 0 0 0 0 12
-0.2613 -0.2369 5.1712 C 0 0 0 0 0 0 0 0 0 0 13
-0.4763 1.4429 3.8186 H 0 0 0 0 0 0 0 0 0 0 14
-1.6919 0.1829 3.5981 H 0 0 0 0 0 0 0 0 0 0 15
0.0600 -1.3423 2.6316 H 0 0 0 0 0 0 0 0 0 0 16
1.2801 -0.0853 2.8567 H 0 0 0 0 0 0 0 0 0 0 17
0.0071 1.4305 1.2975 H 0 0 0 0 0 0 0 0 0 0 18
-1.2128 0.1730 1.0722 H 0 0 0 0 0 0 0 0 0 0 19
0.5485 -1.3580 0.1164 H 0 0 0 0 0 0 0 0 0 0 20
1.7615 -0.0918 0.3324 H 0 0 0 0 0 0 0 0 0 0 21
0.4731 1.4077 -1.2318 H 0 0 0 0 0 0 0 0 0 0 22
-0.7350 0.1332 -1.4587 H 0 0 0 0 0 0 0 0 0 0 23
1.0101 -1.3739 -2.4218 H 0 0 0 0 0 0 0 0 0 0 24
2.2445 -0.1255 -2.1608 H 0 0 0 0 0 0 0 0 0 0 25
-0.8734 0.2051 5.9716 H 0 0 0 0 0 0 0 0 0 0 26
-0.4209 -1.3266 5.1910 H 0 0 0 0 0 0 0 0 0 0 27
0.7960 -0.0512 5.4170 H 0 0 0 0 0 0 0 0 0 0 28
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
13 4 0 0 0 0
14 4 0 0 0 0
15 4 0 0 0 0
6 5 0 0 0 0
16 5 0 0 0 0
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21 7 0 0 0 0
9 8 0 0 0 0
22 8 0 0 0 0
23 8 0 0 0 0
10 9 0 0 0 0
24 9 0 0 0 0
25 9 0 0 0 0
11 10 0 0 0 0
12 10 0 0 0 0
26 13 0 0 0 0
27 13 0 0 0 0
13 28 0 0 0 0
M END
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n-hexylamine-cation.sdf
COSMOtherm 3D 0
26 24 0 0 0 0 0 0 0 0 0 V2000
-1.7287 0.2071 -3.7423 O 0 0 0 0 0 0 0 0 0 0 1
-2.2914 -0.5721 -3.9039 H 0 0 0 0 0 0 0 0 0 0 2
-1.7896 0.7274 -4.5643 H 0 0 0 0 0 0 0 0 0 0 3
-0.7365 -0.2228 4.4406 C 0 0 0 0 0 0 0 0 0 0 4
0.0749 0.3898 3.2934 C 0 0 0 0 0 0 0 0 0 0 5
-0.2007 -0.2727 1.9376 C 0 0 0 0 0 0 0 0 0 0 6
0.6136 0.3358 0.7886 C 0 0 0 0 0 0 0 0 0 0 7
0.3272 -0.3248 -0.5667 C 0 0 0 0 0 0 0 0 0 0 8
1.1667 0.2932 -1.6794 C 0 0 0 0 0 0 0 0 0 0 9
0.8829 -0.3542 -3.0074 N 0 0 0 0 0 0 0 0 0 0 10
1.5016 0.0161 -3.7390 H 0 0 0 0 0 0 0 0 0 0 11
-0.1194 -0.1900 -3.3183 H 0 0 0 0 0 0 0 0 0 0 12
-0.5194 0.2755 5.3970 H 0 0 0 0 0 0 0 0 0 0 13
-1.8182 -0.1325 4.2542 H 0 0 0 0 0 0 0 0 0 0 14
-0.5074 -1.2932 4.5610 H 0 0 0 0 0 0 0 0 0 0 15
1.1519 0.3122 3.5214 H 0 0 0 0 0 0 0 0 0 0 16
-0.1468 1.4682 3.2203 H 0 0 0 0 0 0 0 0 0 0 17
-1.2773 -0.1907 1.7052 H 0 0 0 0 0 0 0 0 0 0 18
0.0189 -1.3526 2.0082 H 0 0 0 0 0 0 0 0 0 0 19
1.6894 0.2448 1.0174 H 0 0 0 0 0 0 0 0 0 0 20
0.3993 1.4162 0.7205 H 0 0 0 0 0 0 0 0 0 0 21
-0.7429 -0.2197 -0.8095 H 0 0 0 0 0 0 0 0 0 0 22
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0.5406 -1.4052 -0.5052 H 0 0 0 0 0 0 0 0 0 0 23
2.2397 0.1707 -1.4857 H 0 0 0 0 0 0 0 0 0 0 24
0.9556 1.3629 -1.8012 H 0 0 0 0 0 0 0 0 0 0 25
1.0469 -1.3679 -2.9681 H 0 0 0 0 0 0 0 0 0 0 26
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
13 4 0 0 0 0
14 4 0 0 0 0
15 4 0 0 0 0
6 5 0 0 0 0
16 5 0 0 0 0
17 5 0 0 0 0
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22 8 0 0 0 0
23 8 0 0 0 0
10 9 0 0 0 0
24 9 0 0 0 0
25 9 0 0 0 0
11 10 0 0 0 0
12 10 0 0 0 0
10 26 0 0 0 0
M END
$$$$
n-hexylamine.sdf
COSMOTHERM 3D 0
25 23 0 0 0 0 0 0 0 0 0 0 V2000
-1.7758 -0.2420 -3.8114 O 0 0 0 0 0 0 0 0 0 0 1
-0.8328 -0.0080 -3.5098 H 0 0 0 0 0 0 0 0 0 0 2
-2.3323 0.4561 -3.4254 H 0 0 0 0 0 0 0 0 0 0 3
-0.7583 0.1983 4.4017 C 0 0 0 0 0 0 0 0 0 0 4
0.1195 -0.3499 3.2708 C 0 0 0 0 0 0 0 0 0 0 5
-0.2208 0.2435 1.8975 C 0 0 0 0 0 0 0 0 0 0 6
0.6534 -0.3009 0.7601 C 0 0 0 0 0 0 0 0 0 0 7
0.3109 0.2939 -0.6115 C 0 0 0 0 0 0 0 0 0 0 8
1.1947 -0.2496 -1.7346 C 0 0 0 0 0 0 0 0 0 0 9
0.8171 0.3346 -3.0440 N 0 0 0 0 0 0 0 0 0 0 10
1.4326 -0.0324 -3.7761 H 0 0 0 0 0 0 0 0 0 0 11
0.9840 1.3459 -3.0268 H 0 0 0 0 0 0 0 0 0 0 12
-0.4899 -0.2459 5.3719 H 0 0 0 0 0 0 0 0 0 0 13
-0.6512 1.2907 4.4930 H 0 0 0 0 0 0 0 0 0 0 14
-1.8228 -0.0174 4.2181 H 0 0 0 0 0 0 0 0 0 0 15
0.0178 -1.4480 3.2252 H 0 0 0 0 0 0 0 0 0 0 16
1.1807 -0.1493 3.4978 H 0 0 0 0 0 0 0 0 0 0 17
-0.1180 1.3425 1.9415 H 0 0 0 0 0 0 0 0 0 0 18
-1.2829 0.0431 1.6689 H 0 0 0 0 0 0 0 0 0 0 19
0.5501 -1.3997 0.7167 H 0 0 0 0 0 0 0 0 0 0 20
1.7147 -0.0998 0.9901 H 0 0 0 0 0 0 0 0 0 0 21
0.4154 1.3929 -0.5700 H 0 0 0 0 0 0 0 0 0 0 22
-0.7448 0.0863 -0.8553 H 0 0 0 0 0 0 0 0 0 0 23
1.0701 -1.3413 -1.8099 H 0 0 0 0 0 0 0 0 0 0 24
2.2570 -0.0607 -1.4913 H 0 0 0 0 0 0 0 0 0 0 25
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
13 4 0 0 0 0
14 4 0 0 0 0
15 4 0 0 0 0
6 5 0 0 0 0
16 5 0 0 0 0
17 5 0 0 0 0
7 6 0 0 0 0
18 6 0 0 0 0
19 6 0 0 0 0
8 7 0 0 0 0
20 7 0 0 0 0
21 7 0 0 0 0
9 8 0 0 0 0
22 8 0 0 0 0
23 8 0 0 0 0
10 9 0 0 0 0
24 9 0 0 0 0
11 10 0 0 0 0
12 10 0 0 0 0
9 25 0 0 0 0
M END
$$$$
n-octylamine-cation.sdf
COSMOTHERM 3D 0
32 30 0 0 0 0 0 0 0 0 0 0 V2000
-1.9226 -4.9259 -0.2235 O 0 0 0 0 0 0 0 0 0 0 1
-2.2177 -4.7328 -1.1319 H 0 0 0 0 0 0 0 0 0 0 2
-2.6042 -4.5282 0.3479 H 0 0 0 0 0 0 0 0 0 0 3
-0.3277 3.2564 0.2666 C 0 0 0 0 0 0 0 0 0 0 4
0.4065 2.0480 -0.3288 C 0 0 0 0 0 0 0 0 0 0 5
0.0119 0.7111 0.3119 C 0 0 0 0 0 0 0 0 0 0 6
0.7590 -0.4881 -0.2860 C 0 0 0 0 0 0 0 0 0 0 7
0.3527 -1.8272 0.3451 C 0 0 0 0 0 0 0 0 0 0 8
1.1266 -2.9893 -0.2666 C 0 0 0 0 0 0 0 0 0 0 9
0.7240 -4.3022 0.3477 N 0 0 0 0 0 0 0 0 0 0 10
1.2902 -5.0736 -0.0259 H 0 0 0 0 0 0 0 0 0 0 11
-0.2939 -4.5281 0.1590 H 0 0 0 0 0 0 0 0 0 0 12
0.0571 4.5910 -0.3854 C 0 0 0 0 0 0 0 0 0 0 13
-1.4178 3.1057 0.1672 H 0 0 0 0 0 0 0 0 0 0 14
-0.1226 3.3097 1.3509 H 0 0 0 0 0 0 0 0 0 0 15
1.4960 2.1955 -0.2202 H 0 0 0 0 0 0 0 0 0 0 16
0.2090 2.0018 -1.4146 H 0 0 0 0 0 0 0 0 0 0 17
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1
2
3 -1.0755 0.5576 0.1959 H 0 0 0 0 0 0 0 0 0 0 18
4 0.2045 0.7552 1.3983 H 0 0 0 0 0 0 0 0 0 0 19
5 1.8454 -0.3407 -0.1594 H 0 0 0 0 0 0 0 0 0 0 20
6 0.5739 -0.5278 -1.3733 H 0 0 0 0 0 0 0 0 0 0 21
7 -0.7291 -1.9885 0.2052 H 0 0 0 0 0 0 0 0 0 0 22
8 0.5376 -1.7962 1.4320 H 0 0 0 0 0 0 0 0 0 0 23
9 2.2066 -2.8794 -0.1084 H 0 0 0 0 0 0 0 0 0 0 24
10 0.9392 -3.0770 -1.3441 H 0 0 0 0 0 0 0 0 0 0 25
11 -0.6774 5.7940 0.2174 C 0 0 0 0 0 0 0 0 0 0 26
12 1.1467 4.7391 -0.2892 H 0 0 0 0 0 0 0 0 0 0 27
13 -0.1507 4.5372 -1.4680 H 0 0 0 0 0 0 0 0 0 0 28
14 -0.3809 6.7340 -0.2715 H 0 0 0 0 0 0 0 0 0 0 29
15 -1.7682 5.6888 0.1064 H 0 0 0 0 0 0 0 0 0 0 30
16 -0.4605 5.8932 1.2926 H 0 0 0 0 0 0 0 0 0 0 31
17 0.8680 -4.2958 1.3653 H 0 0 0 0 0 0 0 0 0 0 32
18
19 2 1 0 0 0 0
20 3 1 0 0 0 0
21 5 4 0 0 0 0
22 13 4 0 0 0 0
23 14 4 0 0 0 0
24 15 4 0 0 0 0
25 6 5 0 0 0 0
26 16 5 0 0 0 0
27 17 5 0 0 0 0
28 7 6 0 0 0 0
29 18 6 0 0 0 0
30 19 6 0 0 0 0
31 8 7 0 0 0 0
32 20 7 0 0 0 0
33 21 7 0 0 0 0
34 9 8 0 0 0 0
35 22 8 0 0 0 0
36 23 8 0 0 0 0
37 10 9 0 0 0 0
38 24 9 0 0 0 0
39 25 9 0 0 0 0
40 11 10 0 0 0 0
41 12 10 0 0 0 0
42 26 13 0 0 0 0
43 27 13 0 0 0 0
44 28 13 0 0 0 0
45 29 26 0 0 0 0
46 30 26 0 0 0 0
47 31 26 0 0 0 0
48 10 32 0 0 0 0
49
50 M END
51 $$$
52 n-octylamine.sdf
53 COSMOTHERM 3D 0
54
55 31 29 0 0 0 0 0 0 0 0 0 0 V2000
56 -1.9624 -0.2928 -4.9311 O 0 0 0 0 0 0 0 0 0 0 1
57 -1.0072 -0.0398 -4.6883 H 0 0 0 0 0 0 0 0 0 0 2
58 -2.5079 0.3928 -4.5086 H 0 0 0 0 0 0 0 0 0 0 3
59 -0.3750 0.2079 3.2171 C 0 0 0 0 0 0 0 0 0 0 4
60 0.4541 -0.2834 2.0236 C 0 0 0 0 0 0 0 0 0 0 5
-0.0405 0.2444 0.6702 C 0 0 0 0 0 0 0 0 0 0 6
0.7898 -0.2533 -0.5202 C 0 0 0 0 0 0 0 0 0 0 7
0.3113 0.2944 -1.8710 C 0 0 0 0 0 0 0 0 0 0 8
1.1461 -0.2121 -3.0478 C 0 0 0 0 0 0 0 0 0 0 9
0.6586 0.3471 -4.3318 N 0 0 0 0 0 0 0 0 0 0 10
1.2377 -0.0017 -5.1015 H 0 0 0 0 0 0 0 0 0 0 11
0.7887 1.3638 -4.3305 H 0 0 0 0 0 0 0 0 0 0 12
0.1302 -0.3064 4.5720 C 0 0 0 0 0 0 0 0 0 0 13
-0.3782 1.3127 3.2281 H 0 0 0 0 0 0 0 0 0 0 14
-1.4274 -0.1002 3.0817 H 0 0 0 0 0 0 0 0 0 0 15
0.4483 -1.3879 2.0070 H 0 0 0 0 0 0 0 0 0 0 16
1.5079 0.0159 2.1661 H 0 0 0 0 0 0 0 0 0 0 17
-0.0290 1.3489 0.6849 H 0 0 0 0 0 0 0 0 0 0 18
-1.0953 -0.0502 0.5267 H 0 0 0 0 0 0 0 0 0 0 19
0.7644 -1.3572 -0.5445 H 0 0 0 0 0 0 0 0 0 0 20
1.8469 0.0273 -0.3673 H 0 0 0 0 0 0 0 0 0 0 21
0.3494 1.3982 -1.8506 H 0 0 0 0 0 0 0 0 0 0 22
-0.7440 0.0181 -2.0352 H 0 0 0 0 0 0 0 0 0 0 23
1.0699 -1.3089 -3.1129 H 0 0 0 0 0 0 0 0 0 0 24
2.2114 0.0288 -2.8736 H 0 0 0 0 0 0 0 0 0 0 25
-0.7030 0.1914 5.7583 C 0 0 0 0 0 0 0 0 0 0 26
0.1330 -1.4101 4.5611 H 0 0 0 0 0 0 0 0 0 0 27
1.1818 0.0013 4.7056 H 0 0 0 0 0 0 0 0 0 0 28
-0.3172 -0.1953 6.7135 H 0 0 0 0 0 0 0 0 0 0 29
-0.6946 1.2913 5.8150 H 0 0 0 0 0 0 0 0 0 0 30
-1.7529 -0.1285 5.6675 H 0 0 0 0 0 0 0 0 0 0 31
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
13 4 0 0 0 0
14 4 0 0 0 0
15 4 0 0 0 0
16 5 0 0 0 0
17 5 0 0 0 0
18 6 0 0 0 0
19 6 0 0 0 0
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22 8 0 0 0 0
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25 9 0 0 0 0
11 10 0 0 0 0
12 10 0 0 0 0
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26 13 0 0 0 0
27 13 0 0 0 0
28 13 0 0 0 0
29 26 0 0 0 0
30 26 0 0 0 0
26 31 0 0 0 0
M END
$$$$
n-pentylamine-cation.sdf
COSMOtherm 3D 0

23 21 0 0 0 0 0 0 0 0 0 V2000
-1.4802 0.1347 3.4282 O 0 0 0 0 0 0 0 0 0 0 1
-2.2034 -0.4255 3.0927 H 0 0 0 0 0 0 0 0 0 0 2
-1.8329 1.0423 3.3915 H 0 0 0 0 0 0 0 0 0 0 3
-0.4255 0.2035 -3.8838 C 0 0 0 0 0 0 0 0 0 0 4
-0.5724 -0.3896 -2.4787 C 0 0 0 0 0 0 0 0 0 0 5
0.3622 0.2653 -1.4532 C 0 0 0 0 0 0 0 0 0 0 6
0.2205 -0.3286 -0.0454 C 0 0 0 0 0 0 0 0 0 0 7
1.1661 0.3429 0.9435 C 0 0 0 0 0 0 0 0 0 0 8
1.0349 -0.2526 2.3190 N 0 0 0 0 0 0 0 0 0 0 9
1.7043 0.1736 2.9713 H 0 0 0 0 0 0 0 0 0 0 10
1.2338 -1.2608 2.3075 H 0 0 0 0 0 0 0 0 0 0 11
-1.1049 -0.2847 -4.5980 H 0 0 0 0 0 0 0 0 0 0 12
-0.6545 1.2806 -3.8859 H 0 0 0 0 0 0 0 0 0 0 13
0.6019 0.0803 -4.2610 H 0 0 0 0 0 0 0 0 0 0 14
-0.3698 -1.4735 -2.5121 H 0 0 0 0 0 0 0 0 0 0 15
-1.6162 -0.2808 -2.1383 H 0 0 0 0 0 0 0 0 0 0 16
0.1584 1.3492 -1.4149 H 0 0 0 0 0 0 0 0 0 0 17
1.4073 0.1565 -1.7913 H 0 0 0 0 0 0 0 0 0 0 18
0.4324 -1.4104 -0.0774 H 0 0 0 0 0 0 0 0 0 0 19
-0.8197 -0.2130 0.3018 H 0 0 0 0 0 0 0 0 0 0 20
0.9525 1.4142 1.0440 H 0 0 0 0 0 0 0 0 0 0 21
2.2139 0.2237 0.6411 H 0 0 0 0 0 0 0 0 0 0 22
0.0625 -0.1135 2.7175 H 0 0 0 0 0 0 0 0 0 0 23

2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
12 4 0 0 0 0
13 4 0 0 0 0
14 4 0 0 0 0
6 5 0 0 0 0
15 5 0 0 0 0
16 5 0 0 0 0
7 6 0 0 0 0
17 6 0 0 0 0
18 6 0 0 0 0
8 7 0 0 0 0
19 7 0 0 0 0
20 7 0 0 0 0
9 8 0 0 0 0
21 8 0 0 0 0
22 8 0 0 0 0
10 9 0 0 0 0
11 9 0 0 0 0
9 23 0 0 0 0
M END
$$$$
n-pentylamine.sdf
COSMOtherm 3D 0

22 20 0 0 0 0 0 0 0 0 0 V2000
1.5564 -3.3717 -0.2059 O 0 0 0 0 0 0 0 0 0 0 1
0.6290 -2.9940 -0.0242 H 0 0 0 0 0 0 0 0 0 0 2
2.1170 -2.9775 0.4842 H 0 0 0 0 0 0 0 0 0 0 3
0.3989 3.8482 -0.1921 C 0 0 0 0 0 0 0 0 0 0 4
0.5807 2.4321 0.3647 C 0 0 0 0 0 0 0 0 0 0 5
-0.3890 1.4128 -0.2480 C 0 0 0 0 0 0 0 0 0 0 6
-0.2107 -0.0069 0.3029 C 0 0 0 0 0 0 0 0 0 0 7
-1.1894 -1.0113 -0.3065 C 0 0 0 0 0 0 0 0 0 0 8
-0.9794 -2.3696 0.2498 N 0 0 0 0 0 0 0 0 0 0 9
-1.6527 -3.0201 -0.1664 H 0 0 0 0 0 0 0 0 0 0 10
-1.1903 -2.3624 1.2529 H 0 0 0 0 0 0 0 0 0 0 11
1.1062 4.5555 0.2666 H 0 0 0 0 0 0 0 0 0 0 12
0.5620 3.8706 -1.2813 H 0 0 0 0 0 0 0 0 0 0 13
-0.6195 4.2218 -0.0005 H 0 0 0 0 0 0 0 0 0 0 14
0.4455 2.4462 1.4600 H 0 0 0 0 0 0 0 0 0 0 15
1.6171 2.0962 0.1873 H 0 0 0 0 0 0 0 0 0 0 16
-0.2551 1.3992 -1.3444 H 0 0 0 0 0 0 0 0 0 0 17
-1.4265 1.7473 -0.0687 H 0 0 0 0 0 0 0 0 0 0 18
-0.3455 0.0069 1.3994 H 0 0 0 0 0 0 0 0 0 0 19
0.8203 -0.3534 0.1162 H 0 0 0 0 0 0 0 0 0 0 20
-1.0327 -1.0707 -1.3951 H 0 0 0 0 0 0 0 0 0 0 21
-2.2252 -0.6579 -0.1471 H 0 0 0 0 0 0 0 0 0 0 22

2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
12 4 0 0 0 0
13 4 0 0 0 0
14 4 0 0 0 0
6 5 0 0 0 0
15 5 0 0 0 0
16 5 0 0 0 0
7 6 0 0 0 0
17 6 0 0 0 0
18 6 0 0 0 0
8 7 0 0 0 0
19 7 0 0 0 0
20 7 0 0 0 0
9 8 0 0 0 0
21 8 0 0 0 0
10 9 0 0 0 0
11 9 0 0 0 0
8 22 0 0 0 0
M END
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$$$$
n-propylamine-cation.sdf
COSMOTHERM      3D      0

17 15 0 0 0 0 0 0 0 0 0 V2000
-0.8461 -0.0751 2.6731 O 0 0 0 0 0 0 0 0 0 0 0 1
-1.2714 -0.9507 2.7204 H 0 0 0 0 0 0 0 0 0 0 0 2
-1.5852 0.5580 2.6161 H 0 0 0 0 0 0 0 0 0 0 0 3
-0.7132 -0.1377 -2.5359 C 0 0 0 0 0 0 0 0 0 0 0 4
-0.3372 0.4136 -1.1559 C 0 0 0 0 0 0 0 0 0 0 0 5
0.8180 -0.3695 -0.5425 C 0 0 0 0 0 0 0 0 0 0 0 6
1.1958 0.1792 0.8069 N 0 0 0 0 0 0 0 0 0 0 0 7
2.0019 -0.3229 1.1981 H 0 0 0 0 0 0 0 0 0 0 0 8
0.3982 0.0991 1.5002 H 0 0 0 0 0 0 0 0 0 0 0 9
-1.5439 0.4364 -2.9682 H 0 0 0 0 0 0 0 0 0 0 0 10
0.1365 -0.0786 -3.2325 H 0 0 0 0 0 0 0 0 0 0 0 11
-1.0274 -1.1900 -2.4719 H 0 0 0 0 0 0 0 0 0 0 0 12
-1.2100 0.3669 -0.4854 H 0 0 0 0 0 0 0 0 0 0 0 13
-0.0519 1.4746 -1.2418 H 0 0 0 0 0 0 0 0 0 0 0 14
1.7145 -0.3198 -1.1726 H 0 0 0 0 0 0 0 0 0 0 0 15
0.5568 -1.4242 -0.3906 H 0 0 0 0 0 0 0 0 0 0 0 16
1.4652 1.1688 0.7421 H 0 0 0 0 0 0 0 0 0 0 0 17

2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
10 4 0 0 0 0
11 4 0 0 0 0
12 4 0 0 0 0
6 5 0 0 0 0
13 5 0 0 0 0
14 5 0 0 0 0
7 6 0 0 0 0
15 6 0 0 0 0
16 6 0 0 0 0
8 7 0 0 0 0
9 7 0 0 0 0
7 17 0 0 0 0

M END
$$$$
n-propylamine.sdf
COSMOTHERM      3D      0

16 14 0 0 0 0 0 0 0 0 0 V2000
-2.6711 -0.9029 -0.1455 O 0 0 0 0 0 0 0 0 0 0 0 1
-1.9895 -0.1610 -0.0037 H 0 0 0 0 0 0 0 0 0 0 0 2
-2.5588 -1.4845 0.6259 H 0 0 0 0 0 0 0 0 0 0 0 3
2.5110 -0.6923 -0.1328 C 0 0 0 0 0 0 0 0 0 0 0 4
1.1063 -0.3532 0.3773 C 0 0 0 0 0 0 0 0 0 0 0 5
0.5023 0.8612 -0.3286 C 0 0 0 0 0 0 0 0 0 0 0 6
-0.8571 1.1583 0.1830 N 0 0 0 0 0 0 0 0 0 0 0 7
-1.2383 1.9746 -0.3043 H 0 0 0 0 0 0 0 0 0 0 0 8
-0.7974 1.4312 1.1693 H 0 0 0 0 0 0 0 0 0 0 0 9
2.9232 -1.5671 0.3903 H 0 0 0 0 0 0 0 0 0 0 0 10
2.4984 -0.9213 -1.2097 H 0 0 0 0 0 0 0 0 0 0 0 11
3.2051 0.1482 0.0226 H 0 0 0 0 0 0 0 0 0 0 0 12
1.1445 -0.1553 1.4625 H 0 0 0 0 0 0 0 0 0 0 0 13
0.4345 -1.2158 0.2380 H 0 0 0 0 0 0 0 0 0 0 0 14
0.4144 0.6569 -1.4074 H 0 0 0 0 0 0 0 0 0 0 0 15
1.1825 1.7262 -0.2172 H 0 0 0 0 0 0 0 0 0 0 0 16

2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
10 4 0 0 0 0
11 4 0 0 0 0
12 4 0 0 0 0
6 5 0 0 0 0
13 5 0 0 0 0
14 5 0 0 0 0
7 6 0 0 0 0
15 6 0 0 0 0
8 7 0 0 0 0
9 7 0 0 0 0
6 16 0 0 0 0

M END
$$$$
neo-pentylamine-cation.sdf
COSMOTHERM      3D      0

23 21 0 0 0 0 0 0 0 0 0 V2000
-3.2209 0.5099 -0.0040 O 0 0 0 0 0 0 0 0 0 0 0 1
-3.3762 1.0261 -0.8158 H 0 0 0 0 0 0 0 0 0 0 0 2
-3.3301 1.1514 0.7211 H 0 0 0 0 0 0 0 0 0 0 0 3
2.3008 0.3561 -0.8711 C 0 0 0 0 0 0 0 0 0 0 0 4
1.0520 0.1469 0.0091 C 0 0 0 0 0 0 0 0 0 0 0 5
0.3118 1.4872 0.1753 C 0 0 0 0 0 0 0 0 0 0 0 6
1.4820 -0.3971 1.3859 C 0 0 0 0 0 0 0 0 0 0 0 7
0.1784 -0.8823 -0.7327 C 0 0 0 0 0 0 0 0 0 0 0 8
-1.0835 -1.2589 -0.0003 N 0 0 0 0 0 0 0 0 0 0 0 9
-1.5265 -2.0667 -0.4549 H 0 0 0 0 0 0 0 0 0 0 0 10
-1.8109 -0.4896 0.0250 H 0 0 0 0 0 0 0 0 0 0 0 11
2.9721 1.0911 -0.4036 H 0 0 0 0 0 0 0 0 0 0 0 12
2.8605 -0.5828 -0.9996 H 0 0 0 0 0 0 0 0 0 0 0 13
2.0270 0.7330 -1.8685 H 0 0 0 0 0 0 0 0 0 0 0 14
0.9778 2.2284 0.6410 H 0 0 0 0 0 0 0 0 0 0 0 15
-0.5744 1.3955 0.8208 H 0 0 0 0 0 0 0 0 0 0 0 16
-0.0125 1.8855 -0.7979 H 0 0 0 0 0 0 0 0 0 0 0 17
2.1843 0.3023 1.8621 H 0 0 0 0 0 0 0 0 0 0 0 18
0.6320 -0.5110 2.0780 H 0 0 0 0 0 0 0 0 0 0 0 19
1.9844 -1.3718 1.2919 H 0 0 0 0 0 0 0 0 0 0 0 20
0.7366 -1.8147 -0.8855 H 0 0 0 0 0 0 0 0 0 0 0 21
-0.1346 -0.4993 -1.7122 H 0 0 0 0 0 0 0 0 0 0 0 22
-0.8823 -1.5474 0.9660 H 0 0 0 0 0 0 0 0 0 0 0 23

2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
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12 4 0 0 0 0
13 4 0 0 0 0
14 4 0 0 0 0
6 5 0 0 0 0
7 5 0 0 0 0
8 5 0 0 0 0
15 6 0 0 0 0
16 6 0 0 0 0
17 6 0 0 0 0
18 7 0 0 0 0
19 7 0 0 0 0
20 7 0 0 0 0
9 8 0 0 0 0
21 8 0 0 0 0
22 8 0 0 0 0
10 9 0 0 0 0
11 9 0 0 0 0
9 23 0 0 0 0
M END
$$$$
neo-pentylamine.sdf
COSMOTHERM 3D 0
22 20 0 0 0 0 0 0 0 0 0 V2000
-3.2339 -0.0394 -0.5574 O 0 0 0 0 0 0 0 0 0 0 1
-2.4133 0.0039 0.0382 H 0 0 0 0 0 0 0 0 0 0 2
-3.0788 0.6384 -1.2373 H 0 0 0 0 0 0 0 0 0 0 3
2.3551 0.7584 -0.2400 C 0 0 0 0 0 0 0 0 0 0 4
1.0205 -0.0060 -0.1372 C 0 0 0 0 0 0 0 0 0 0 5
1.3081 -1.4789 0.2152 C 0 0 0 0 0 0 0 0 0 0 6
0.2853 0.0741 -1.4879 C 0 0 0 0 0 0 0 0 0 0 7
0.1938 0.6656 0.9833 C 0 0 0 0 0 0 0 0 0 0 8
-1.1173 0.0204 1.2387 N 0 0 0 0 0 0 0 0 0 0 9
-1.5720 0.5081 2.0166 H 0 0 0 0 0 0 0 0 0 0 10
-0.9682 -0.9351 1.5775 H 0 0 0 0 0 0 0 0 0 0 11
2.9895 0.3239 -1.0276 H 0 0 0 0 0 0 0 0 0 0 12
2.1871 1.8185 -0.4883 H 0 0 0 0 0 0 0 0 0 0 13
2.9131 0.7145 0.7081 H 0 0 0 0 0 0 0 0 0 0 14
1.9635 -1.9334 -0.5435 H 0 0 0 0 0 0 0 0 0 0 15
0.3866 -2.0801 0.2504 H 0 0 0 0 0 0 0 0 0 0 16
1.8124 -1.5631 1.1910 H 0 0 0 0 0 0 0 0 0 0 17
0.8985 -0.3724 -2.2862 H 0 0 0 0 0 0 0 0 0 0 18
-0.6739 -0.4611 -1.4573 H 0 0 0 0 0 0 0 0 0 0 19
0.0833 1.1215 -1.7630 H 0 0 0 0 0 0 0 0 0 0 20
-0.0043 1.7116 0.6995 H 0 0 0 0 0 0 0 0 0 0 21
0.8132 0.6890 1.8999 H 0 0 0 0 0 0 0 0 0 0 22
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
12 4 0 0 0 0
13 4 0 0 0 0
14 4 0 0 0 0
6 5 0 0 0 0
7 5 0 0 0 0
8 5 0 0 0 0
15 6 0 0 0 0
16 6 0 0 0 0
17 6 0 0 0 0
18 7 0 0 0 0
19 7 0 0 0 0
20 7 0 0 0 0
9 8 0 0 0 0
21 8 0 0 0 0
10 9 0 0 0 0
11 9 0 0 0 0
8 22 0 0 0 0
M END
$$$$
p-toluidine-cation0.sdf
COSMOTHERM 3D 0
21 20 0 0 0 0 0 0 0 0 0 V2000
-0.8053 -3.8126 -0.6898 O 0 0 0 0 0 0 0 0 0 0 1
-1.5602 -4.1324 -0.1627 H 0 0 0 0 0 0 0 0 0 0 2
-1.1938 -3.5239 -1.5358 H 0 0 0 0 0 0 0 0 0 0 3
-1.1625 1.0994 0.3811 C 0 0 0 0 0 0 0 0 0 0 4
-0.8157 -0.2364 0.5992 C 0 0 0 0 0 0 0 0 0 0 5
0.4869 -0.6478 0.3197 C 0 0 0 0 0 0 0 0 0 0 6
1.4378 0.2416 -0.1738 C 0 0 0 0 0 0 0 0 0 0 7
1.0739 1.5745 -0.3863 C 0 0 0 0 0 0 0 0 0 0 8
-0.2269 2.0275 -0.1092 C 0 0 0 0 0 0 0 0 0 0 9
0.8599 -2.0551 0.5494 N 0 0 0 0 0 0 0 0 0 0 10
-0.6022 3.4748 -0.3079 C 0 0 0 0 0 0 0 0 0 0 11
1.8036 -2.2492 0.1906 H 0 0 0 0 0 0 0 0 0 0 12
0.1843 -2.7359 0.0692 H 0 0 0 0 0 0 0 0 0 0 13
-2.1827 1.4233 0.5959 H 0 0 0 0 0 0 0 0 0 0 14
-1.5542 -0.9436 0.9799 H 0 0 0 0 0 0 0 0 0 0 15
2.4522 -0.0962 -0.3945 H 0 0 0 0 0 0 0 0 0 0 16
1.8183 2.2715 -0.7760 H 0 0 0 0 0 0 0 0 0 0 17
-0.3923 4.0585 0.6029 H 0 0 0 0 0 0 0 0 0 0 18
-1.6729 3.5841 -0.5276 H 0 0 0 0 0 0 0 0 0 0 19
-0.0281 3.9286 -1.1272 H 0 0 0 0 0 0 0 0 0 0 20
0.8781 -2.2833 1.5530 H 0 0 0 0 0 0 0 0 0 0 21
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
9 4 0 0 0 0
14 4 0 0 0 0
6 5 0 0 0 0
15 5 0 0 0 0
7 6 0 0 0 0
10 6 0 0 0 0
8 7 0 0 0 0
16 7 0 0 0 0
9 8 0 0 0 0
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17 8 0 0 0 0
11 9 0 0 0 0
12 10 0 0 0 0
13 10 0 0 0 0
18 11 0 0 0 0
19 11 0 0 0 0
20 11 0 0 0 0
10 21 0 0 0 0
M END
$$$$
p-toluidine.sdf
COSMOtherm 3D 0
20 19 0 0 0 0 0 0 0 0 0 V2000
0.1002 1.3000 -3.7656 O 0 0 0 0 0 0 0 0 0 0 1
-0.8257 1.5460 -3.9342 H 0 0 0 0 0 0 0 0 0 0 2
0.0381 0.4944 -3.1768 H 0 0 0 0 0 0 0 0 0 0 3
0.0270 0.6835 3.4364 C 0 0 0 0 0 0 0 0 0 0 4
0.0060 0.2214 1.9982 C 0 0 0 0 0 0 0 0 0 0 5
1.1996 -0.0318 1.2975 C 0 0 0 0 0 0 0 0 0 0 6
1.1918 -0.4566 -0.0326 C 0 0 0 0 0 0 0 0 0 0 7
-0.0247 -0.6458 -0.7145 C 0 0 0 0 0 0 0 0 0 0 8
-1.2003 0.0266 1.3063 C 0 0 0 0 0 0 0 0 0 0 9
-1.2239 -0.3989 -0.0263 C 0 0 0 0 0 0 0 0 0 0 10
-0.0347 -1.0068 -2.0840 N 0 0 0 0 0 0 0 0 0 0 11
0.5306 1.6577 3.5391 H 0 0 0 0 0 0 0 0 0 0 12
-0.9918 0.7893 3.8335 H 0 0 0 0 0 0 0 0 0 0 13
0.5683 -0.0266 4.0807 H 0 0 0 0 0 0 0 0 0 0 14
2.1595 0.1031 1.8027 H 0 0 0 0 0 0 0 0 0 0 15
2.1356 -0.6439 -0.5504 H 0 0 0 0 0 0 0 0 0 0 16
-2.1482 0.2064 1.8198 H 0 0 0 0 0 0 0 0 0 0 17
-2.1799 -0.5430 -0.5354 H 0 0 0 0 0 0 0 0 0 0 18
0.7798 -1.5580 -2.3593 H 0 0 0 0 0 0 0 0 0 0 19
-0.8829 -1.5025 -2.3628 H 0 0 0 0 0 0 0 0 0 0 20
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
12 4 0 0 0 0
13 4 0 0 0 0
14 4 0 0 0 0
6 5 0 0 0 0
9 5 0 0 0 0
7 6 0 0 0 0
15 6 0 0 0 0
8 7 0 0 0 0
16 7 0 0 0 0
10 8 0 0 0 0
11 8 0 0 0 0
10 9 0 0 0 0
17 9 0 0 0 0
18 10 0 0 0 0
19 11 0 0 0 0
11 20 0 0 0 0
M END
$$$$
p-toluidine0.sdf
COSMOtherm 3D 0
20 19 0 0 0 0 0 0 0 0 0 V2000
-1.2986 0.1085 -3.7746 O 0 0 0 0 0 0 0 0 0 0 1
-1.5119 -0.8113 -4.0086 H 0 0 0 0 0 0 0 0 0 0 2
-0.4972 0.0341 -3.1825 H 0 0 0 0 0 0 0 0 0 0 3
0.0451 1.1999 1.3012 C 0 0 0 0 0 0 0 0 0 0 4
0.4649 1.1894 -0.0319 C 0 0 0 0 0 0 0 0 0 0 5
0.6429 -0.0277 -0.7129 C 0 0 0 0 0 0 0 0 0 0 6
0.3939 -1.2261 -0.0212 C 0 0 0 0 0 0 0 0 0 0 7
-0.0251 -1.1999 1.3120 C 0 0 0 0 0 0 0 0 0 0 8
-0.2132 0.0098 2.0029 C 0 0 0 0 0 0 0 0 0 0 9
0.9999 -0.0436 -2.0835 N 0 0 0 0 0 0 0 0 0 0 10
-0.6985 0.0308 3.4332 C 0 0 0 0 0 0 0 0 0 0 11
1.4923 -0.8943 -2.3605 H 0 0 0 0 0 0 0 0 0 0 12
1.5532 0.7681 -2.3626 H 0 0 0 0 0 0 0 0 0 0 13
-0.0777 2.1603 1.8083 H 0 0 0 0 0 0 0 0 0 0 14
0.6604 2.1321 -0.5489 H 0 0 0 0 0 0 0 0 0 0 15
0.5337 -2.1833 -0.5295 H 0 0 0 0 0 0 0 0 0 0 16
-0.2045 -2.1467 1.8278 H 0 0 0 0 0 0 0 0 0 0 17
-1.7996 0.0628 3.4818 H 0 0 0 0 0 0 0 0 0 0 18
-0.3240 0.9135 3.9707 H 0 0 0 0 0 0 0 0 0 0 19
-0.3755 -0.8668 3.9795 H 0 0 0 0 0 0 0 0 0 0 20
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
9 4 0 0 0 0
14 4 0 0 0 0
6 5 0 0 0 0
15 5 0 0 0 0
7 6 0 0 0 0
10 6 0 0 0 0
8 7 0 0 0 0
16 7 0 0 0 0
9 8 0 0 0 0
17 8 0 0 0 0
11 9 0 0 0 0
12 10 0 0 0 0
13 10 0 0 0 0
18 11 0 0 0 0
19 11 0 0 0 0
11 20 0 0 0 0
M END
$$$$
p-toluidine1.sdf
COSMOtherm 3D 0
20 19 0 0 0 0 0 0 0 0 0 V2000
-3.7656 -1.3067 0.0814 O 0 0 0 0 0 0 0 0 0 0 1
```

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-3.1790 -0.4993 0.0237 H 0 0 0 0 0 0 0 0 0 0 2
-4.0171 -1.4867 -0.8409 H 0 0 0 0 0 0 0 0 0 0 3
1.3026 0.0271 1.1997 C 0 0 0 0 0 0 0 0 0 0 4
-0.0302 0.4475 1.1991 C 0 0 0 0 0 0 0 0 0 0 5
-0.7141 0.6455 -0.0136 C 0 0 0 0 0 0 0 0 0 0 6
-0.0248 0.4151 -1.2171 C 0 0 0 0 0 0 0 0 0 0 7
1.3079 -0.0058 -1.2005 C 0 0 0 0 0 0 0 0 0 0 8
2.0014 -0.2134 0.0042 C 0 0 0 0 0 0 0 0 0 0 9
-2.0844 1.0027 -0.0206 N 0 0 0 0 0 0 0 0 0 0 10
3.4312 -0.7007 0.0146 C 0 0 0 0 0 0 0 0 0 0 11
-2.3623 1.5108 -0.8616 H 0 0 0 0 0 0 0 0 0 0 12
-2.3630 1.5408 0.8014 H 0 0 0 0 0 0 0 0 0 0 13
1.8116 -0.1114 2.1570 H 0 0 0 0 0 0 0 0 0 0 14
-0.5448 0.6289 2.1458 H 0 0 0 0 0 0 0 0 0 0 15
-0.5352 0.5705 -2.1708 H 0 0 0 0 0 0 0 0 0 0 16
1.8213 -0.1699 -2.1513 H 0 0 0 0 0 0 0 0 0 0 17
3.4787 -1.8022 0.0292 H 0 0 0 0 0 0 0 0 0 0 18
3.9707 -0.3408 0.9022 H 0 0 0 0 0 0 0 0 0 0 19
3.9758 -0.3638 -0.8788 H 0 0 0 0 0 0 0 0 0 0 20
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
9 4 0 0 0 0
14 4 0 0 0 0
6 5 0 0 0 0
15 5 0 0 0 0
7 6 0 0 0 0
10 6 0 0 0 0
8 7 0 0 0 0
16 7 0 0 0 0
9 8 0 0 0 0
17 8 0 0 0 0
11 9 0 0 0 0
12 10 0 0 0 0
13 10 0 0 0 0
18 11 0 0 0 0
19 11 0 0 0 0
11 20 0 0 0 0
M END
$$$$
pyrazine.sdf
COSMOTHERM 3D 0
13 12 0 0 0 0 0 0 0 0 0 V2000
-3.4665 -0.0478 -0.0042 O 0 0 0 0 0 0 0 0 0 0 1
-2.4676 -0.0340 0.0043 H 0 0 0 0 0 0 0 0 0 0 2
-3.7188 0.8897 0.0535 H 0 0 0 0 0 0 0 0 0 0 3
1.4739 0.0036 1.1381 C 0 0 0 0 0 0 0 0 0 0 4
2.1789 0.0100 -0.0067 N 0 0 0 0 0 0 0 0 0 0 5
0.0759 -0.0075 1.1483 C 0 0 0 0 0 0 0 0 0 0 6
-0.6340 -0.0121 0.0069 N 0 0 0 0 0 0 0 0 0 0 7
0.0650 -0.0062 -1.1413 C 0 0 0 0 0 0 0 0 0 0 8
1.4628 0.0050 -1.1446 C 0 0 0 0 0 0 0 0 0 0 9
2.0372 0.0071 2.0738 H 0 0 0 0 0 0 0 0 0 0 10
-0.4821 -0.0126 2.0866 H 0 0 0 0 0 0 0 0 0 0 11
-0.5019 -0.0103 -2.0743 H 0 0 0 0 0 0 0 0 0 0 12
2.0171 0.0096 -2.0857 H 0 0 0 0 0 0 0 0 0 0 13
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
10 4 0 0 0 0
9 5 0 0 0 0
7 6 0 0 0 0
11 6 0 0 0 0
8 7 0 0 0 0
9 8 0 0 0 0
12 8 0 0 0 0
9 13 0 0 0 0
M END
$$$$
pyrazine-cation.sdf
COSMOTHERM 3D 0
14 13 0 0 0 0 0 0 0 0 0 V2000
-3.2535 0.0515 0.0028 O 0 0 0 0 0 0 0 0 0 0 1
-3.6709 -0.3104 0.8063 H 0 0 0 0 0 0 0 0 0 0 2
-3.6985 -0.3974 -0.7395 H 0 0 0 0 0 0 0 0 0 0 3
0.0369 1.1570 -0.0051 C 0 0 0 0 0 0 0 0 0 0 4
-0.5974 -0.0292 -0.0084 N 0 0 0 0 0 0 0 0 0 0 5
0.0855 -1.1880 -0.0044 C 0 0 0 0 0 0 0 0 0 0 6
1.4782 -1.1341 0.0033 C 0 0 0 0 0 0 0 0 0 0 7
2.1514 0.0282 0.0064 N 0 0 0 0 0 0 0 0 0 0 8
1.4307 1.1614 0.0006 C 0 0 0 0 0 0 0 0 0 0 9
-1.6778 -0.0455 -0.0121 H 0 0 0 0 0 0 0 0 0 0 10
-0.5737 2.0575 -0.0077 H 0 0 0 0 0 0 0 0 0 0 11
-0.4858 -2.1139 -0.0074 H 0 0 0 0 0 0 0 0 0 0 12
2.0598 -2.0562 0.0072 H 0 0 0 0 0 0 0 0 0 0 13
1.9735 2.1069 0.0031 H 0 0 0 0 0 0 0 0 0 0 14
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
9 4 0 0 0 0
11 4 0 0 0 0
6 5 0 0 0 0
10 5 0 0 0 0
7 6 0 0 0 0
12 6 0 0 0 0
8 7 0 0 0 0
13 7 0 0 0 0
9 8 0 0 0 0
9 14 0 0 0 0
M END
$$$$
pyrazole.sdf
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2.0158 2.1518 0.0047 H 0 0 0 0 0 0 0 0 0 0 0 10
-0.5110 2.0965 -0.0019 H 0 0 0 0 0 0 0 0 0 0 0 11
-0.5661 -2.0602 -0.0067 H 0 0 0 0 0 0 0 0 0 0 0 12
1.9589 -2.1823 0.0009 H 0 0 0 0 0 0 0 0 0 0 0 13
3.2600 -0.0319 0.0064 H 0 0 0 0 0 0 0 0 0 0 0 14
-1.6322 0.0305 -0.0065 H 0 0 0 0 0 0 0 0 0 0 0 15
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
9 4 0 0 0 0
10 4 0 0 0 0
6 5 0 0 0 0
11 5 0 0 0 0
7 6 0 0 0 0
8 7 0 0 0 0
12 7 0 0 0 0
9 8 0 0 0 0
13 8 0 0 0 0
14 9 0 0 0 0
6 15 0 0 0 0
M END
$$$$
pyrimidine.sdf
COSMOTHERM 3D 0
13 12 0 0 0 0 0 0 0 0 0 V2000
-3.4437 -0.0635 -0.0158 O 0 0 0 0 0 0 0 0 0 0 0 1
-2.4456 -0.0214 -0.0028 H 0 0 0 0 0 0 0 0 0 0 0 2
-3.7230 0.8679 0.0117 H 0 0 0 0 0 0 0 0 0 0 0 3
2.1191 -0.0047 -0.0414 C 0 0 0 0 0 0 0 0 0 0 0 4
1.4422 -0.0010 -1.2070 N 0 0 0 0 0 0 0 0 0 0 0 5
0.1049 0.0056 -1.1102 C 0 0 0 0 0 0 0 0 0 0 0 6
-0.6138 0.0093 0.0254 N 0 0 0 0 0 0 0 0 0 0 0 7
0.0811 0.0047 1.1798 C 0 0 0 0 0 0 0 0 0 0 0 8
1.4744 -0.0018 1.1957 C 0 0 0 0 0 0 0 0 0 0 0 9
3.2096 -0.0103 -0.1099 H 0 0 0 0 0 0 0 0 0 0 0 10
-0.4597 0.0091 -2.0459 H 0 0 0 0 0 0 0 0 0 0 0 11
-0.5016 0.0069 2.1036 H 0 0 0 0 0 0 0 0 0 0 0 12
2.0333 -0.0051 2.1308 H 0 0 0 0 0 0 0 0 0 0 0 13
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
9 4 0 0 0 0
10 4 0 0 0 0
6 5 0 0 0 0
7 6 0 0 0 0
11 6 0 0 0 0
8 7 0 0 0 0
9 8 0 0 0 0
12 8 0 0 0 0
9 13 0 0 0 0
M END
$$$$
pyrimidine-cation.sdf
COSMOTHERM 3D 0
14 13 0 0 0 0 0 0 0 0 0 V2000
-3.2426 -0.0636 -0.0007 O 0 0 0 0 0 0 0 0 0 0 0 1
-3.6753 0.3787 -0.7542 H 0 0 0 0 0 0 0 0 0 0 0 2
-3.6684 0.3114 0.7922 H 0 0 0 0 0 0 0 0 0 0 0 3
2.0974 -0.0533 0.0016 C 0 0 0 0 0 0 0 0 0 0 0 4
1.4717 1.1959 0.0010 C 0 0 0 0 0 0 0 0 0 0 0 5
0.0865 1.2148 -0.0005 C 0 0 0 0 0 0 0 0 0 0 0 6
-0.5773 0.0398 -0.0022 N 0 0 0 0 0 0 0 0 0 0 0 7
0.0907 -1.1343 -0.0019 C 0 0 0 0 0 0 0 0 0 0 0 8
1.4137 -1.2168 0.0001 N 0 0 0 0 0 0 0 0 0 0 0 9
3.1860 -0.1325 0.0033 H 0 0 0 0 0 0 0 0 0 0 0 10
2.0428 2.1219 0.0023 H 0 0 0 0 0 0 0 0 0 0 0 11
-0.5131 2.1235 -0.0005 H 0 0 0 0 0 0 0 0 0 0 0 12
-0.5116 -2.0427 -0.0033 H 0 0 0 0 0 0 0 0 0 0 0 13
-1.6549 0.0316 -0.0028 H 0 0 0 0 0 0 0 0 0 0 0 14
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
9 4 0 0 0 0
10 4 0 0 0 0
6 5 0 0 0 0
11 5 0 0 0 0
7 6 0 0 0 0
12 6 0 0 0 0
8 7 0 0 0 0
9 8 0 0 0 0
13 8 0 0 0 0
7 14 0 0 0 0
M END
$$$$
pyrrole-cation0.sdf
COSMOTHERM 3D 0
14 13 0 0 0 0 0 0 0 0 0 V2000
-2.6041 0.0101 0.4602 O 0 0 0 0 0 0 0 0 0 0 0 1
-3.0592 -0.8531 0.4655 H 0 0 0 0 0 0 0 0 0 0 0 2
-3.2471 0.6318 0.0700 H 0 0 0 0 0 0 0 0 0 0 0 3
1.5369 0.7370 0.4344 C 0 0 0 0 0 0 0 0 0 0 0 4
1.5485 -0.7243 0.4312 C 0 0 0 0 0 0 0 0 0 0 0 5
0.4751 1.1657 -0.2759 C 0 0 0 0 0 0 0 0 0 0 0 6
-0.2692 -0.0054 -0.7396 N 0 0 0 0 0 0 0 0 0 0 0 7
0.4929 -1.1669 -0.2799 C 0 0 0 0 0 0 0 0 0 0 0 8
2.2651 1.3730 0.9304 H 0 0 0 0 0 0 0 0 0 0 0 9
2.2875 -1.3507 0.9235 H 0 0 0 0 0 0 0 0 0 0 0 10
0.0998 2.1530 -0.5224 H 0 0 0 0 0 0 0 0 0 0 0 11
-0.4145 -0.0058 -1.7618 H 0 0 0 0 0 0 0 0 0 0 0 12
0.1350 -2.1588 -0.5336 H 0 0 0 0 0 0 0 0 0 0 0 13
-1.2922 -0.0131 -0.2895 H 0 0 0 0 0 0 0 0 0 0 0 14
2 1 0 0 0 0
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3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
9 4 0 0 0 0
8 5 0 0 0 0
10 5 0 0 0 0
7 6 0 0 0 0
11 6 0 0 0 0
8 7 0 0 0 0
12 7 0 0 0 0
13 8 0 0 0 0
7 14 0 0 0 0
M END
$$$$
pyrrole-cation1.sdf
COSMOTHERM 3D 0
14 13 0 0 0 0 0 0 0 0 0 V2000
-3.0547 -0.0450 0.0199 O 0 0 0 0 0 0 0 0 0 0 1
-3.4484 -0.0111 -0.8712 H 0 0 0 0 0 0 0 0 0 0 2
-3.4901 0.6769 0.5091 H 0 0 0 0 0 0 0 0 0 0 3
1.8833 -0.6195 -0.0011 C 0 0 0 0 0 0 0 0 0 0 4
1.8266 0.7402 -0.0089 C 0 0 0 0 0 0 0 0 0 0 5
0.5013 -1.1625 0.0094 C 0 0 0 0 0 0 0 0 0 0 6
-0.3255 0.0376 0.0073 N 0 0 0 0 0 0 0 0 0 0 7
0.4333 1.1047 -0.0045 C 0 0 0 0 0 0 0 0 0 0 8
-1.3837 0.0340 0.0071 H 0 0 0 0 0 0 0 0 0 0 9
2.7711 -1.2471 -0.0021 H 0 0 0 0 0 0 0 0 0 0 10
2.6504 1.4475 -0.0175 H 0 0 0 0 0 0 0 0 0 0 11
0.0050 2.1058 -0.0090 H 0 0 0 0 0 0 0 0 0 0 12
0.2855 -1.7775 0.8995 H 0 0 0 0 0 0 0 0 0 0 13
0.2753 -1.7867 -0.8717 H 0 0 0 0 0 0 0 0 0 0 14
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
10 4 0 0 0 0
8 5 0 0 0 0
11 5 0 0 0 0
7 6 0 0 0 0
13 6 0 0 0 0
8 7 0 0 0 0
9 7 0 0 0 0
12 8 0 0 0 0
6 14 0 0 0 0
M END
$$$$
pyrrole-cation2.sdf
COSMOTHERM 3D 0
14 13 0 0 0 0 0 0 0 0 0 V2000
-3.0354 0.0436 -0.0056 O 0 0 0 0 0 0 0 0 0 0 1
-3.4467 -0.2946 0.8108 H 0 0 0 0 0 0 0 0 0 0 2
-3.4554 -0.4630 -0.7247 H 0 0 0 0 0 0 0 0 0 0 3
1.8228 0.7342 -0.0008 C 0 0 0 0 0 0 0 0 0 0 4
1.7899 -0.7614 0.0013 C 0 0 0 0 0 0 0 0 0 0 5
0.3911 1.1000 -0.0019 C 0 0 0 0 0 0 0 0 0 0 6
-0.3255 0.0094 -0.0002 N 0 0 0 0 0 0 0 0 0 0 7
0.4997 -1.1514 0.0021 C 0 0 0 0 0 0 0 0 0 0 8
2.3417 1.1690 0.8736 H 0 0 0 0 0 0 0 0 0 0 9
2.3423 1.1669 -0.8759 H 0 0 0 0 0 0 0 0 0 0 10
-1.3908 -0.0170 -0.0013 H 0 0 0 0 0 0 0 0 0 0 11
2.6645 -1.4045 0.0030 H 0 0 0 0 0 0 0 0 0 0 12
-0.0556 2.0916 -0.0041 H 0 0 0 0 0 0 0 0 0 0 13
0.0390 -2.1340 0.0036 H 0 0 0 0 0 0 0 0 0 0 14
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
9 4 0 0 0 0
10 4 0 0 0 0
8 5 0 0 0 0
12 5 0 0 0 0
7 6 0 0 0 0
13 6 0 0 0 0
8 7 0 0 0 0
11 7 0 0 0 0
8 14 0 0 0 0
M END
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pyrrole.sdf
COSMOTHERM 3D 0
13 12 0 0 0 0 0 0 0 0 0 V2000
-3.1605 0.0125 0.0535 O 0 0 0 0 0 0 0 0 0 0 1
-3.5334 -0.8583 -0.1739 H 0 0 0 0 0 0 0 0 0 0 2
-3.5513 0.6172 -0.6028 H 0 0 0 0 0 0 0 0 0 0 3
1.8445 -0.0065 -0.7257 C 0 0 0 0 0 0 0 0 0 0 4
1.8594 -0.0011 0.7028 C 0 0 0 0 0 0 0 0 0 0 5
0.5370 0.0064 1.1279 C 0 0 0 0 0 0 0 0 0 0 6
-0.2675 0.0058 0.0107 N 0 0 0 0 0 0 0 0 0 0 7
0.5135 -0.0021 -1.1228 C 0 0 0 0 0 0 0 0 0 0 8
2.7066 -0.0130 -1.3877 H 0 0 0 0 0 0 0 0 0 0 9
2.7352 -0.0025 1.3468 H 0 0 0 0 0 0 0 0 0 0 10
0.1089 0.0123 2.1257 H 0 0 0 0 0 0 0 0 0 0 11
-1.3011 0.0083 0.0182 H 0 0 0 0 0 0 0 0 0 0 12
0.0645 -0.0044 -2.1115 H 0 0 0 0 0 0 0 0 0 0 13
2 1 0 0 0 0
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10 5 0 0 0 0
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11 6 0 0 0 0
8 7 0 0 0 0
12 7 0 0 0 0
8 13 0 0 0 0
M END
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quinoline.sdf
COSMOTHERM 3D 0
20 20 0 0 0 0 0 0 0 0 0 V2000
-3.4690 1.7152 -0.0583 O 0 0 0 0 0 0 0 0 0 0 1
-2.7048 1.0658 -0.0173 H 0 0 0 0 0 0 0 0 0 0 2
-3.5114 2.0931 0.8371 H 0 0 0 0 0 0 0 0 0 0 3
-0.0379 0.2273 0.0014 C 0 0 0 0 0 0 0 0 0 0 4
-1.3609 -0.1421 0.0038 N 0 0 0 0 0 0 0 0 0 0 5
-1.6564 -1.4374 0.0043 C 0 0 0 0 0 0 0 0 0 0 6
-0.6842 -2.4659 0.0019 C 0 0 0 0 0 0 0 0 0 0 7
0.6514 -2.1193 -0.0003 C 0 0 0 0 0 0 0 0 0 0 8
1.0182 -0.7478 -0.0002 C 0 0 0 0 0 0 0 0 0 0 9
0.2933 1.6082 0.0009 C 0 0 0 0 0 0 0 0 0 0 10
1.6171 2.0060 -0.0005 C 0 0 0 0 0 0 0 0 0 0 11
2.6616 1.0459 -0.0015 C 0 0 0 0 0 0 0 0 0 0 12
2.3691 -0.3044 -0.0016 C 0 0 0 0 0 0 0 0 0 0 13
-2.7199 -1.6913 0.0070 H 0 0 0 0 0 0 0 0 0 0 14
-1.0018 -3.5086 0.0019 H 0 0 0 0 0 0 0 0 0 0 15
1.4311 -2.8844 -0.0021 H 0 0 0 0 0 0 0 0 0 0 16
-0.5176 2.3388 -0.0002 H 0 0 0 0 0 0 0 0 0 0 17
1.8645 3.0689 -0.0007 H 0 0 0 0 0 0 0 0 0 0 18
3.7001 1.3805 -0.0023 H 0 0 0 0 0 0 0 0 0 0 19
3.1687 -1.0484 -0.0027 H 0 0 0 0 0 0 0 0 0 0 20
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
9 4 0 0 0 0
10 4 0 0 0 0
6 5 0 0 0 0
7 6 0 0 0 0
14 6 0 0 0 0
8 7 0 0 0 0
15 7 0 0 0 0
9 8 0 0 0 0
16 8 0 0 0 0
13 9 0 0 0 0
11 10 0 0 0 0
17 10 0 0 0 0
12 11 0 0 0 0
18 11 0 0 0 0
13 12 0 0 0 0
19 12 0 0 0 0
13 20 0 0 0 0
M END
$$$$
quinoline-cation.sdf
COSMOTHERM 3D 0
21 21 0 0 0 0 0 0 0 0 0 V2000
-3.2512 1.7780 0.0135 O 0 0 0 0 0 0 0 0 0 0 1
-3.9725 1.6523 0.6570 H 0 0 0 0 0 0 0 0 0 0 2
-3.6997 1.9148 -0.8412 H 0 0 0 0 0 0 0 0 0 0 3
2.3653 -0.3586 0.0014 C 0 0 0 0 0 0 0 0 0 0 4
2.6872 0.9840 0.0016 C 0 0 0 0 0 0 0 0 0 0 5
1.6678 1.9697 0.0014 C 0 0 0 0 0 0 0 0 0 0 6
0.3311 1.6146 0.0003 C 0 0 0 0 0 0 0 0 0 0 7
-0.0093 0.2449 -0.0023 C 0 0 0 0 0 0 0 0 0 0 8
1.0042 -0.7665 -0.0013 C 0 0 0 0 0 0 0 0 0 0 9
0.5998 -2.1248 -0.0004 C 0 0 0 0 0 0 0 0 0 0 10
-0.7436 -2.4594 -0.0011 C 0 0 0 0 0 0 0 0 0 0 11
-1.6997 -1.4360 -0.0016 C 0 0 0 0 0 0 0 0 0 0 12
-1.3265 -0.1531 -0.0012 N 0 0 0 0 0 0 0 0 0 0 13
3.1436 -1.1232 0.0017 H 0 0 0 0 0 0 0 0 0 0 14
3.7324 1.2946 0.0033 H 0 0 0 0 0 0 0 0 0 0 15
1.9423 3.0251 0.0030 H 0 0 0 0 0 0 0 0 0 0 16
-0.4553 2.3702 0.0023 H 0 0 0 0 0 0 0 0 0 0 17
1.3620 -2.9060 0.0021 H 0 0 0 0 0 0 0 0 0 0 18
-1.0737 -3.4962 -0.0001 H 0 0 0 0 0 0 0 0 0 0 19
-2.7714 -1.6285 -0.0017 H 0 0 0 0 0 0 0 0 0 0 20
-2.0826 0.5924 -0.0010 H 0 0 0 0 0 0 0 0 0 0 21
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
9 4 0 0 0 0
14 4 0 0 0 0
6 5 0 0 0 0
15 5 0 0 0 0
7 6 0 0 0 0
16 6 0 0 0 0
8 7 0 0 0 0
17 7 0 0 0 0
9 8 0 0 0 0
13 8 0 0 0 0
10 9 0 0 0 0
11 10 0 0 0 0
18 10 0 0 0 0
12 11 0 0 0 0
19 11 0 0 0 0
13 12 0 0 0 0
20 12 0 0 0 0
13 21 0 0 0 0
M END
$$$$
sec-butylamine-cation.sdf
COSMOTHERM 3D 0
20 18 0 0 0 0 0 0 0 0 0 V2000
-2.5056 0.4073 0.9056 O 0 0 0 0 0 0 0 0 0 0 1
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2
3 -2.6773 0.3192 1.8609 H 0 0 0 0 0 0 0 0 0 0 0 2
4 -3.3654 0.2216 0.4860 H 0 0 0 0 0 0 0 0 0 0 0 3
5 0.5942 -0.2765 -0.7790 C 0 0 0 0 0 0 0 0 0 0 0 4
6 -0.0817 0.4322 -1.9477 C 0 0 0 0 0 0 0 0 0 0 0 5
7 -0.4309 -1.1524 -0.0818 N 0 0 0 0 0 0 0 0 0 0 0 6
8 1.2249 0.6846 0.2322 C 0 0 0 0 0 0 0 0 0 0 0 7
9 1.9820 0.0042 1.3790 C 0 0 0 0 0 0 0 0 0 0 0 8
10 -0.8163 -1.8527 -0.7277 H 0 0 0 0 0 0 0 0 0 0 0 9
11 -0.0080 -1.6773 0.6938 H 0 0 0 0 0 0 0 0 0 0 0 10
12 1.3586 -0.9725 -1.1534 H 0 0 0 0 0 0 0 0 0 0 0 11
13 -0.5600 -0.2849 -2.6302 H 0 0 0 0 0 0 0 0 0 0 0 12
14 0.6727 0.9892 -2.5189 H 0 0 0 0 0 0 0 0 0 0 0 13
15 -0.8407 1.1462 -1.5957 H 0 0 0 0 0 0 0 0 0 0 0 14
16 1.9191 1.3208 -0.3374 H 0 0 0 0 0 0 0 0 0 0 0 15
17 0.4451 1.3568 0.6278 H 0 0 0 0 0 0 0 0 0 0 0 16
18 2.4847 0.7563 2.0027 H 0 0 0 0 0 0 0 0 0 0 0 17
19 1.3171 -0.5668 2.0463 H 0 0 0 0 0 0 0 0 0 0 0 18
20 2.7500 -0.6844 0.9956 H 0 0 0 0 0 0 0 0 0 0 0 19
21 -1.2426 -0.5864 0.3039 H 0 0 0 0 0 0 0 0 0 0 0 20
22 2 1 0 0 0 0 0
23 3 1 0 0 0 0 0
24 5 4 0 0 0 0 0
25 6 4 0 0 0 0 0
26 7 4 0 0 0 0 0
27 11 4 0 0 0 0 0
28 12 5 0 0 0 0 0
29 13 5 0 0 0 0 0
30 14 5 0 0 0 0 0
31 9 6 0 0 0 0 0
32 10 6 0 0 0 0 0
33 8 7 0 0 0 0 0
34 15 7 0 0 0 0 0
35 16 7 0 0 0 0 0
36 17 8 0 0 0 0 0
37 18 8 0 0 0 0 0
38 19 8 0 0 0 0 0
39 6 20 0 0 0 0 0
40 M END
41 $$$$
42 sec-butylamine.sdf
43 COSMOtherm 3D 0
44 19 17 0 0 0 0 0 0 0 0 0 0 V2000
45 -2.6012 -0.9728 0.3938 O 0 0 0 0 0 0 0 0 0 0 0 1
46 -1.8215 -0.5798 -0.1233 H 0 0 0 0 0 0 0 0 0 0 0 2
47 -3.2525 -0.2515 0.4336 H 0 0 0 0 0 0 0 0 0 0 0 3
48 0.5784 0.7544 -0.3142 C 0 0 0 0 0 0 0 0 0 0 0 4
49 -0.0337 1.9538 0.4113 C 0 0 0 0 0 0 0 0 0 0 0 5
50 -0.4899 0.0670 -1.0882 N 0 0 0 0 0 0 0 0 0 0 0 6
51 1.2331 -0.2287 0.6660 C 0 0 0 0 0 0 0 0 0 0 0 7
52 1.9557 -1.4049 -0.0020 C 0 0 0 0 0 0 0 0 0 0 0 8
53 -0.8898 0.7226 -1.7675 H 0 0 0 0 0 0 0 0 0 0 0 9
54 -0.0837 -0.6881 -1.6488 H 0 0 0 0 0 0 0 0 0 0 0 10
55 1.3672 1.1259 -0.9982 H 0 0 0 0 0 0 0 0 0 0 0 11
56 -0.4949 2.6550 -0.3010 H 0 0 0 0 0 0 0 0 0 0 0 12
57 0.7374 2.5013 0.9721 H 0 0 0 0 0 0 0 0 0 0 0 13
58 -0.8096 1.6235 1.1189 H 0 0 0 0 0 0 0 0 0 0 0 14
59 1.9532 0.3392 1.2768 H 0 0 0 0 0 0 0 0 0 0 0 15
60 0.4581 -0.6038 1.3561 H 0 0 0 0 0 0 0 0 0 0 0 16
61 2.4647 -2.0283 0.7474 H 0 0 0 0 0 0 0 0 0 0 0 17
62 1.2615 -2.0616 -0.5486 H 0 0 0 0 0 0 0 0 0 0 0 18
63 2.7169 -1.0505 -0.7147 H 0 0 0 0 0 0 0 0 0 0 0 19
64 2 1 0 0 0 0 0
65 3 1 0 0 0 0 0
66 5 4 0 0 0 0 0
67 6 4 0 0 0 0 0
68 7 4 0 0 0 0 0
69 11 4 0 0 0 0 0
70 12 5 0 0 0 0 0
71 13 5 0 0 0 0 0
72 14 5 0 0 0 0 0
73 9 6 0 0 0 0 0
74 10 6 0 0 0 0 0
75 8 7 0 0 0 0 0
76 15 7 0 0 0 0 0
77 16 7 0 0 0 0 0
78 17 8 0 0 0 0 0
79 18 8 0 0 0 0 0
80 8 19 0 0 0 0 0
81 M END
82 $$$$
83 tert-butylamine-cation.sdf
84 COSMOtherm 3D 0
85 20 18 0 0 0 0 0 0 0 0 0 0 V2000
86 -2.8548 0.0010 0.0347 O 0 0 0 0 0 0 0 0 0 0 0 1
87 -3.3787 -0.7799 -0.2221 H 0 0 0 0 0 0 0 0 0 0 0 2
88 -3.4030 0.7606 -0.2347 H 0 0 0 0 0 0 0 0 0 0 0 3
89 2.1301 0.0061 -0.6321 C 0 0 0 0 0 0 0 0 0 0 0 4
90 0.7611 -0.0017 0.0538 C 0 0 0 0 0 0 0 0 0 0 0 5
91 0.5557 1.2451 0.9189 C 0 0 0 0 0 0 0 0 0 0 0 6
92 0.5368 -1.2896 0.8514 C 0 0 0 0 0 0 0 0 0 0 0 7
93 -0.2985 0.0354 -1.0476 N 0 0 0 0 0 0 0 0 0 0 0 8
94 -1.2865 0.0235 -0.6566 H 0 0 0 0 0 0 0 0 0 0 0 9
95 -0.1998 -0.7698 -1.6795 H 0 0 0 0 0 0 0 0 0 0 0 10
96 2.2552 -0.8716 -1.2831 H 0 0 0 0 0 0 0 0 0 0 0 11
97 2.2692 0.9158 -1.2347 H 0 0 0 0 0 0 0 0 0 0 0 12
98 2.9199 -0.0210 0.1305 H 0 0 0 0 0 0 0 0 0 0 0 13
99 -0.4424 1.2524 1.3792 H 0 0 0 0 0 0 0 0 0 0 0 14
100 0.6814 2.1646 0.3286 H 0 0 0 0 0 0 0 0 0 0 0 15
101 1.3025 1.2536 1.7239 H 0 0 0 0 0 0 0 0 0 0 0 16
102 -0.4579 -1.3023 1.3190 H 0 0 0 0 0 0 0 0 0 0 0 17
103 0.6397 -2.1779 0.2112 H 0 0 0 0 0 0 0 0 0 0 0 18
104 1.2890 -1.3568 1.6484 H 0 0 0 0 0 0 0 0 0 0 0 19
105 -0.1982 0.8792 -1.6265 H 0 0 0 0 0 0 0 0 0 0 0 20
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2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
11 4 0 0 0 0
12 4 0 0 0 0
13 4 0 0 0 0
6 5 0 0 0 0
7 5 0 0 0 0
8 5 0 0 0 0
14 6 0 0 0 0
15 6 0 0 0 0
16 6 0 0 0 0
17 7 0 0 0 0
18 7 0 0 0 0
19 7 0 0 0 0
9 8 0 0 0 0
10 8 0 0 0 0
8 20 0 0 0 0
M END
$$$$
tert-butylamine.sdf
COSMOTHERM 3D 0
19 17 0 0 0 0 0 0 0 0 0 V2000
-2.9674 -0.0574 0.0093 O 0 0 0 0 0 0 0 0 0 0 1
-2.0076 -0.0630 0.3412 H 0 0 0 0 0 0 0 0 0 0 2
-3.1629 0.8819 -0.1509 H 0 0 0 0 0 0 0 0 0 0 3
0.5937 -1.1746 -0.9956 C 0 0 0 0 0 0 0 0 0 0 4
0.7309 0.0027 -0.0190 C 0 0 0 0 0 0 0 0 0 0 5
0.5422 1.3364 -0.7572 C 0 0 0 0 0 0 0 0 0 0 6
2.1107 -0.0336 0.6661 C 0 0 0 0 0 0 0 0 0 0 7
-0.3704 -0.1149 0.9845 N 0 0 0 0 0 0 0 0 0 0 8
-0.2771 0.6380 1.6756 H 0 0 0 0 0 0 0 0 0 0 9
-0.2526 -0.9856 1.5146 H 0 0 0 0 0 0 0 0 0 0 10
0.6892 -2.1356 -0.4664 H 0 0 0 0 0 0 0 0 0 0 11
-0.3853 -1.1519 -1.4960 H 0 0 0 0 0 0 0 0 0 0 12
1.3789 -1.1324 -1.7643 H 0 0 0 0 0 0 0 0 0 0 13
0.6205 2.1854 -0.0601 H 0 0 0 0 0 0 0 0 0 0 14
-0.4451 1.3757 -1.2403 H 0 0 0 0 0 0 0 0 0 0 15
1.3126 1.4627 -1.5312 H 0 0 0 0 0 0 0 0 0 0 16
2.2107 0.7955 1.3840 H 0 0 0 0 0 0 0 0 0 0 17
2.2488 -0.9794 1.2128 H 0 0 0 0 0 0 0 0 0 0 18
2.9230 0.0558 -0.0715 H 0 0 0 0 0 0 0 0 0 0 19
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
11 4 0 0 0 0
12 4 0 0 0 0
13 4 0 0 0 0
6 5 0 0 0 0
7 5 0 0 0 0
8 5 0 0 0 0
14 6 0 0 0 0
15 6 0 0 0 0
16 6 0 0 0 0
17 7 0 0 0 0
18 7 0 0 0 0
9 8 0 0 0 0
10 8 0 0 0 0
7 19 0 0 0 0
M END
$$$$
tert-butylcyclohexylamine-cation.sdf
COSMOTHERM 3D 0
36 35 0 0 0 0 0 0 0 0 0 V2000
-2.8269 1.1312 -0.7075 O 0 0 0 0 0 0 0 0 0 0 1
-3.3907 1.1957 0.0845 H 0 0 0 0 0 0 0 0 0 0 2
-3.1605 1.8269 -1.3028 H 0 0 0 0 0 0 0 0 0 0 3
-0.0254 0.8387 -0.5273 N 0 0 0 0 0 0 0 0 0 0 4
0.6057 2.0559 0.1867 C 0 0 0 0 0 0 0 0 0 0 5
2.1257 1.9840 0.0155 C 0 0 0 0 0 0 0 0 0 0 6
0.0411 3.2912 -0.5264 C 0 0 0 0 0 0 0 0 0 0 7
0.1955 2.0375 1.6601 C 0 0 0 0 0 0 0 0 0 0 8
0.3149 -0.5627 -0.0168 C 0 0 0 0 0 0 0 0 0 0 9
-0.8615 -1.1730 0.7509 C 0 0 0 0 0 0 0 0 0 0 10
-0.5016 -2.5881 1.2345 C 0 0 0 0 0 0 0 0 0 0 11
-0.0742 -3.4896 0.0679 C 0 0 0 0 0 0 0 0 0 0 12
1.0822 -2.8628 -0.7232 C 0 0 0 0 0 0 0 0 0 0 13
0.7355 -1.4429 -1.1991 C 0 0 0 0 0 0 0 0 0 0 14
0.2714 0.8961 -1.5117 H 0 0 0 0 0 0 0 0 0 0 15
2.5741 2.8784 0.4679 H 0 0 0 0 0 0 0 0 0 0 16
2.5640 1.1084 0.5132 H 0 0 0 0 0 0 0 0 0 0 17
2.4068 1.9675 -1.0479 H 0 0 0 0 0 0 0 0 0 0 18
0.4772 4.1944 -0.0797 H 0 0 0 0 0 0 0 0 0 0 19
-1.0511 3.3523 -0.4191 H 0 0 0 0 0 0 0 0 0 0 20
0.2941 3.2864 -1.5969 H 0 0 0 0 0 0 0 0 0 0 21
-0.8974 2.0635 1.7757 H 0 0 0 0 0 0 0 0 0 0 22
0.5910 1.1599 2.1894 H 0 0 0 0 0 0 0 0 0 0 23
0.6063 2.9312 2.1484 H 0 0 0 0 0 0 0 0 0 0 24
1.1697 -0.4428 0.6633 H 0 0 0 0 0 0 0 0 0 0 25
-1.7381 -1.2255 0.0838 H 0 0 0 0 0 0 0 0 0 0 26
-1.1378 -0.5372 1.6054 H 0 0 0 0 0 0 0 0 0 0 27
0.3187 -2.5235 1.9705 H 0 0 0 0 0 0 0 0 0 0 28
-1.3650 -3.0202 1.7618 H 0 0 0 0 0 0 0 0 0 0 29
-0.9345 -3.6469 -0.6058 H 0 0 0 0 0 0 0 0 0 0 30
0.2199 -4.4814 0.4441 H 0 0 0 0 0 0 0 0 0 0 31
1.9829 -2.8214 -0.0868 H 0 0 0 0 0 0 0 0 0 0 32
1.3399 -3.4843 -1.5939 H 0 0 0 0 0 0 0 0 0 0 33
-0.0948 -1.4896 -1.9255 H 0 0 0 0 0 0 0 0 0 0 34
1.5983 -0.9914 -1.7147 H 0 0 0 0 0 0 0 0 0 0 35
-1.0740 0.9682 -0.5453 H 0 0 0 0 0 0 0 0 0 0 36
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
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34 14 0 0 0 0
14 35 0 0 0 0
M END
$$$$
tetrahydrozoline-cation2.sdf
COSMOtherm 3D 0

35 36 0 0 0 0 0 0 0 0 0 V2000
-3.0467 0.3542 -0.4084 O 0 0 0 0 0 0 0 0 0 0 0 1
-3.8612 0.2818 -0.9384 H 0 0 0 0 0 0 0 0 0 0 0 2
-3.1617 1.1749 0.1034 H 0 0 0 0 0 0 0 0 0 0 0 3
0.2010 1.9286 3.0281 C 0 0 0 0 0 0 0 0 0 0 0 4
0.7194 2.3907 1.8122 C 0 0 0 0 0 0 0 0 0 0 0 5
0.8957 1.4946 0.7570 C 0 0 0 0 0 0 0 0 0 0 0 6
0.5508 0.1378 0.8868 C 0 0 0 0 0 0 0 0 0 0 0 7
0.0352 -0.3335 2.1111 C 0 0 0 0 0 0 0 0 0 0 0 8
-0.1291 0.5797 3.1682 C 0 0 0 0 0 0 0 0 0 0 0 9
0.8193 -0.8228 -0.2787 C 0 0 0 0 0 0 0 0 0 0 0 10
0.1081 -2.1898 -0.1210 C 0 0 0 0 0 0 0 0 0 0 0 11
0.3149 -2.7236 1.2970 C 0 0 0 0 0 0 0 0 0 0 0 12
-0.3455 -1.7875 2.3127 C 0 0 0 0 0 0 0 0 0 0 0 13
0.4717 -0.2131 -1.6070 C 0 0 0 0 0 0 0 0 0 0 0 14
-0.7081 0.7983 -3.3206 C 0 0 0 0 0 0 0 0 0 0 0 15
-0.7366 0.1897 -1.9727 N 0 0 0 0 0 0 0 0 0 0 0 16
1.3569 -0.0435 -2.5861 N 0 0 0 0 0 0 0 0 0 0 0 17
0.7086 0.4241 -3.8275 C 0 0 0 0 0 0 0 0 0 0 0 18
-1.5656 0.2515 -1.3418 H 0 0 0 0 0 0 0 0 0 0 0 19
0.0637 2.6152 3.8655 H 0 0 0 0 0 0 0 0 0 0 0 20
0.9918 3.4404 1.6889 H 0 0 0 0 0 0 0 0 0 0 0 21
1.3129 1.8580 -0.1859 H 0 0 0 0 0 0 0 0 0 0 0 22
-0.5214 0.2148 4.1209 H 0 0 0 0 0 0 0 0 0 0 0 23
1.9050 -1.0153 -0.3071 H 0 0 0 0 0 0 0 0 0 0 0 24
-0.9699 -2.0727 -0.3139 H 0 0 0 0 0 0 0 0 0 0 0 25
0.5025 -2.8879 -0.8731 H 0 0 0 0 0 0 0 0 0 0 0 26
1.3937 -2.8140 1.5079 H 0 0 0 0 0 0 0 0 0 0 0 27
-0.1138 -3.7332 1.3806 H 0 0 0 0 0 0 0 0 0 0 0 28
-1.4430 -1.8807 2.2274 H 0 0 0 0 0 0 0 0 0 0 0 29
-0.0942 -2.0890 3.3409 H 0 0 0 0 0 0 0 0 0 0 0 30
-1.5033 0.3831 -3.9497 H 0 0 0 0 0 0 0 0 0 0 0 31
-0.8482 1.8854 -3.2391 H 0 0 0 0 0 0 0 0 0 0 0 32
1.2487 1.2783 -4.2494 H 0 0 0 0 0 0 0 0 0 0 0 33
0.6895 -0.3915 -4.5636 H 0 0 0 0 0 0 0 0 0 0 0 34
2.3137 -0.3817 -2.5401 H 0 0 0 0 0 0 0 0 0 0 0 35

2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
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23 9 0 0 0 0
11 10 0 0 0 0
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25 11 0 0 0 0
26 11 0 0 0 0
13 12 0 0 0 0
27 12 0 0 0 0
28 12 0 0 0 0
29 13 0 0 0 0
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16 14 0 0 0 0
17 14 0 0 0 0
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31 15 0 0 0 0
32 15 0 0 0 0
19 16 0 0 0 0
18 17 0 0 0 0
33 18 0 0 0 0
34 18 0 0 0 0
17 35 0 0 0 0
M END
$$$$
tetrahydrozoline-cation3.sdf
COSMOtherm 3D 0

35 36 0 0 0 0 0 0 0 0 0 V2000
-3.0142 0.4468 -0.3537 O 0 0 0 0 0 0 0 0 0 0 0 1
-3.8306 0.4936 -0.8838 H 0 0 0 0 0 0 0 0 0 0 0 2
-3.0520 1.2376 0.2133 H 0 0 0 0 0 0 0 0 0 0 0 3
0.2427 1.9205 3.0210 C 0 0 0 0 0 0 0 0 0 0 0 4
0.7684 2.3726 1.8045 C 0 0 0 0 0 0 0 0 0 0 0 5
0.9262 1.4731 0.7491 C 0 0 0 0 0 0 0 0 0 0 0 6
0.5598 0.1220 0.8809 C 0 0 0 0 0 0 0 0 0 0 0 7
0.0374 -0.3395 2.1064 C 0 0 0 0 0 0 0 0 0 0 0 8
-0.1108 0.5779 3.1626 C 0 0 0 0 0 0 0 0 0 0 0 9
0.8027 -0.8425 -0.2864 C 0 0 0 0 0 0 0 0 0 0 0 10
0.0593 -2.1922 -0.1270 C 0 0 0 0 0 0 0 0 0 0 0 11
0.2637 -2.7346 1.2883 C 0 0 0 0 0 0 0 0 0 0 0 12
-0.3681 -1.7863 2.3110 C 0 0 0 0 0 0 0 0 0 0 0 13
0.4610 -0.2243 -1.6122 C 0 0 0 0 0 0 0 0 0 0 0 14
-0.7082 0.8176 -3.3146 C 0 0 0 0 0 0 0 0 0 0 0 15
-0.7389 0.2136 -1.9648 N 0 0 0 0 0 0 0 0 0 0 0 16
1.3409 -0.0801 -2.6007 N 0 0 0 0 0 0 0 0 0 0 0 17
0.6907 0.3988 -3.8371 C 0 0 0 0 0 0 0 0 0 0 0 18
-1.5555 0.3000 -1.3210 H 0 0 0 0 0 0 0 0 0 0 0 19
0.1165 2.6104 3.8576 H 0 0 0 0 0 0 0 0 0 0 0 20
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15 8 0 0 0 0
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18 9 0 0 0 0
11 10 0 0 0 0
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12 11 0 0 0 0
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13 12 0 0 0 0
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30 13 0 0 0 0
16 15 0 0 0 0
31 15 0 0 0 0
17 16 0 0 0 0
32 16 0 0 0 0
18 17 0 0 0 0
33 17 0 0 0 0
18 34 0 0 0 0
M END
$$$$
tetrahydrozoline_p2.sdf
COSMOTHERM 3D 0
35 36 0 0 0 0 0 0 0 0 0 V2000
-1.0162 -2.0946 3.9019 O 0 0 0 0 0 0 0 0 0 1
-0.8552 -3.0160 3.6294 H 0 0 0 0 0 0 0 0 0 2
-1.9856 -2.0231 3.9666 H 0 0 0 0 0 0 0 0 0 3
0.3036 0.1814 1.2406 C 0 0 0 0 0 0 0 0 0 4
0.3989 -0.1108 2.5289 N 0 0 0 0 0 0 0 0 0 5
1.2105 0.8965 3.2456 C 0 0 0 0 0 0 0 0 0 6
1.8383 1.7069 2.0811 C 0 0 0 0 0 0 0 0 0 7
1.0357 1.2489 0.9279 N 0 0 0 0 0 0 0 0 0 8
-0.5669 -0.5766 0.2717 C 0 0 0 0 0 0 0 0 0 9
0.0006 -0.5305 -1.1454 C 0 0 0 0 0 0 0 0 0 10
-0.6097 0.2334 -2.1604 C 0 0 0 0 0 0 0 0 0 11
-1.8901 1.0112 -1.9230 C 0 0 0 0 0 0 0 0 0 12
-2.2029 1.2409 -0.4412 C 0 0 0 0 0 0 0 0 0 13
-2.0290 -0.0586 0.3470 C 0 0 0 0 0 0 0 0 0 14
1.1586 -1.2763 -1.4335 C 0 0 0 0 0 0 0 0 0 15
1.7227 -1.2682 -2.7089 C 0 0 0 0 0 0 0 0 0 16
1.1249 -0.5038 -3.7201 C 0 0 0 0 0 0 0 0 0 17
-0.0264 0.2331 -3.4421 C 0 0 0 0 0 0 0 0 0 18
-0.1566 -0.8549 3.0031 H 0 0 0 0 0 0 0 0 0 19
1.9625 0.4099 3.8762 H 0 0 0 0 0 0 0 0 0 20
0.5579 1.5160 3.8760 H 0 0 0 0 0 0 0 0 0 21
2.8958 1.4577 1.9175 H 0 0 0 0 0 0 0 0 0 22
1.7396 2.7892 2.2167 H 0 0 0 0 0 0 0 0 0 23
-0.5571 -1.6215 0.6187 H 0 0 0 0 0 0 0 0 0 24
-2.7224 0.4488 -2.3829 H 0 0 0 0 0 0 0 0 0 25
-1.8399 1.9691 -2.4624 H 0 0 0 0 0 0 0 0 0 26
-3.2330 1.6099 -0.3298 H 0 0 0 0 0 0 0 0 0 27
-1.5440 2.0235 -0.0299 H 0 0 0 0 0 0 0 0 0 28
-2.6756 -0.8415 -0.0794 H 0 0 0 0 0 0 0 0 0 29
-2.3273 0.0667 1.3974 H 0 0 0 0 0 0 0 0 0 30
1.6183 -1.8738 -0.6418 H 0 0 0 0 0 0 0 0 0 31
2.6200 -1.8543 -2.9148 H 0 0 0 0 0 0 0 0 0 32
1.5568 -0.4841 -4.7225 H 0 0 0 0 0 0 0 0 0 33
-0.4935 0.8253 -4.2332 H 0 0 0 0 0 0 0 0 0 34
1.2259 1.5207 -0.0328 H 0 0 0 0 0 0 0 0 0 35
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
8 4 0 0 0 0
9 4 0 0 0 0
6 5 0 0 0 0
19 5 0 0 0 0
7 6 0 0 0 0
20 6 0 0 0 0
21 6 0 0 0 0
8 7 0 0 0 0
22 7 0 0 0 0
23 7 0 0 0 0
10 9 0 0 0 0
14 9 0 0 0 0
24 9 0 0 0 0
11 10 0 0 0 0
15 10 0 0 0 0
12 11 0 0 0 0
18 11 0 0 0 0
13 12 0 0 0 0
25 12 0 0 0 0
26 12 0 0 0 0
14 13 0 0 0 0
27 13 0 0 0 0
28 13 0 0 0 0
29 14 0 0 0 0
30 14 0 0 0 0
16 15 0 0 0 0
31 15 0 0 0 0
17 16 0 0 0 0
32 16 0 0 0 0
18 17 0 0 0 0
33 17 0 0 0 0
34 18 0 0 0 0
8 35 0 0 0 0
M END
$$$$
tetrahydrozoline_t_p2.sdf
COSMOTHERM 3D 0
35 36 0 0 0 0 0 0 0 0 0 V2000
-2.9312 -0.9333 0.3366 O 0 0 0 0 0 0 0 0 0 1
```

```
1
2
3 -2.8392 -1.5552 -0.4069 H 0 0 0 0 0 0 0 0 0 0 2
4 -3.4982 -0.2196 -0.0059 H 0 0 0 0 0 0 0 0 0 0 3
5 -0.5322 1.7807 -2.2695 C 0 0 0 0 0 0 0 0 0 0 4
6 0.0469 2.7670 -1.2521 C 0 0 0 0 0 0 0 0 0 0 5
7 -0.0904 2.2015 0.1621 C 0 0 0 0 0 0 0 0 0 0 6
8 0.7476 0.9039 0.3010 C 0 0 0 0 0 0 0 0 0 0 7
9 0.5786 -0.0570 -0.8801 C 0 0 0 0 0 0 0 0 0 0 8
10 0.0002 0.3723 -2.0918 C 0 0 0 0 0 0 0 0 0 0 9
11 -0.0816 -0.5400 -3.1597 C 0 0 0 0 0 0 0 0 0 0 10
12 0.3967 -1.8458 -3.0446 C 0 0 0 0 0 0 0 0 0 0 11
13 0.9831 -2.2641 -1.8436 C 0 0 0 0 0 0 0 0 0 0 12
14 1.0740 -1.3693 -0.7769 C 0 0 0 0 0 0 0 0 0 0 13
15 0.4396 0.2525 1.6202 C 0 0 0 0 0 0 0 0 0 0 14
16 1.2520 0.3140 2.6708 N 0 0 0 0 0 0 0 0 0 0 15
17 -0.6781 -0.3959 1.9092 N 0 0 0 0 0 0 0 0 0 0 16
18 0.6916 -0.3834 3.8448 C 0 0 0 0 0 0 0 0 0 0 17
19 -0.7032 -0.8310 3.3217 C 0 0 0 0 0 0 0 0 0 0 18
20 -0.3299 2.1175 -3.2976 H 0 0 0 0 0 0 0 0 0 0 19
21 -1.6321 1.7616 -2.1671 H 0 0 0 0 0 0 0 0 0 0 20
22 -0.4776 3.7312 -1.3190 H 0 0 0 0 0 0 0 0 0 0 21
23 1.1096 2.9619 -1.4738 H 0 0 0 0 0 0 0 0 0 0 22
24 -1.1510 1.9827 0.3663 H 0 0 0 0 0 0 0 0 0 0 23
25 0.2439 2.9261 0.9180 H 0 0 0 0 0 0 0 0 0 0 24
26 1.8096 1.1981 0.3444 H 0 0 0 0 0 0 0 0 0 0 25
27 -0.5268 -0.2077 -4.1011 H 0 0 0 0 0 0 0 0 0 0 26
28 0.3214 -2.5324 -3.8899 H 0 0 0 0 0 0 0 0 0 0 27
29 1.3720 -3.2786 -1.7405 H 0 0 0 0 0 0 0 0 0 0 28
30 1.5419 -1.6975 0.1549 H 0 0 0 0 0 0 0 0 0 0 29
31 -1.4679 -0.5486 1.2494 H 0 0 0 0 0 0 0 0 0 0 30
32 0.6217 0.3017 4.6979 H 0 0 0 0 0 0 0 0 0 0 31
33 1.3323 -1.2314 4.1181 H 0 0 0 0 0 0 0 0 0 0 32
34 -0.8458 -1.9166 3.3828 H 0 0 0 0 0 0 0 0 0 0 33
35 -1.5255 -0.3335 3.8514 H 0 0 0 0 0 0 0 0 0 0 34
36 2.1796 0.7269 2.6435 H 0 0 0 0 0 0 0 0 0 0 35
37
38 2 1 0 0 0 0
39 3 1 0 0 0 0
40 5 4 0 0 0 0
41 9 4 0 0 0 0
42 19 4 0 0 0 0
43 20 4 0 0 0 0
44 6 5 0 0 0 0
45 21 5 0 0 0 0
46 22 5 0 0 0 0
47 7 6 0 0 0 0
48 23 6 0 0 0 0
49 24 6 0 0 0 0
50 8 7 0 0 0 0
51 14 7 0 0 0 0
52 25 7 0 0 0 0
53 9 8 0 0 0 0
54 13 8 0 0 0 0
55 10 9 0 0 0 0
56 11 10 0 0 0 0
57 26 10 0 0 0 0
58 12 11 0 0 0 0
59 27 11 0 0 0 0
60 13 12 0 0 0 0
28 12 0 0 0 0
29 13 0 0 0 0
15 14 0 0 0 0
16 14 0 0 0 0
17 15 0 0 0 0
18 16 0 0 0 0
30 16 0 0 0 0
18 17 0 0 0 0
31 17 0 0 0 0
32 17 0 0 0 0
33 18 0 0 0 0
34 18 0 0 0 0
15 35 0 0 0 0
M END
$$$$
thiazole.sdf
COSMOtherm 3D 0
11 10 0 0 0 0 0 0 0 0 V2000
-3.5655 -0.0614 -0.1825 O 0 0 0 0 0 0 0 0 0 0 1
-2.5737 -0.0184 -0.0789 H 0 0 0 0 0 0 0 0 0 0 2
-3.8407 0.8696 -0.2439 H 0 0 0 0 0 0 0 0 0 0 3
-0.0354 0.0036 1.2692 C 0 0 0 0 0 0 0 0 0 0 4
-0.7453 0.0064 0.0831 N 0 0 0 0 0 0 0 0 0 0 5
0.0611 0.0037 -0.9530 C 0 0 0 0 0 0 0 0 0 0 6
1.7603 -0.0016 -0.5473 S 0 0 0 0 0 0 0 0 0 0 7
1.3273 -0.0008 1.1386 C 0 0 0 0 0 0 0 0 0 0 8
-0.5736 0.0055 2.2153 H 0 0 0 0 0 0 0 0 0 0 9
-0.2670 0.0053 -1.9903 H 0 0 0 0 0 0 0 0 0 0 10
2.0883 -0.0037 1.9131 H 0 0 0 0 0 0 0 0 0 0 11
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
8 4 0 0 0 0
9 4 0 0 0 0
6 5 0 0 0 0
7 6 0 0 0 0
10 6 0 0 0 0
8 7 0 0 0 0
8 11 0 0 0 0
M END
$$$$
thiazole-cation.sdf
COSMOtherm 3D 0
12 11 0 0 0 0 0 0 0 0 V2000
-3.3773 -0.0042 -0.1255 O 0 0 0 0 0 0 0 0 0 0 1
-3.7591 -0.7346 -0.6463 H 0 0 0 0 0 0 0 0 0 0 2
```


[illegible]

[illegible]

[illegible]

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1
2
3      -1.3366      0.8714      2.4441 H      0      0      0      0      0      0      0      0      0      0      13
4      -1.7676      -1.2405      1.0871 H      0      0      0      0      0      0      0      0      0      0      14
5      -0.0542      -1.6561      1.2412 H      0      0      0      0      0      0      0      0      0      0      15
6      -1.7343      -1.2605      -1.1135 H      0      0      0      0      0      0      0      0      0      0      16
7      -0.0127      -1.6473      -1.2507 H      0      0      0      0      0      0      0      0      0      0      17
8      0.3354      0.3500      -2.7215 H      0      0      0      0      0      0      0      0      0      0      18
9      -1.1028      -0.9029      -3.7318 C      0      0      0      0      0      0      0      0      0      0      19
10     -1.3462      0.8450      -2.4716 H      0      0      0      0      0      0      0      0      0      0      20
11      0.7696      1.4042      0.8828 H      0      0      0      0      0      0      0      0      0      0      21
12      0.7930      1.3983      -0.8736 H      0      0      0      0      0      0      0      0      0      0      22
13      2.0771      -0.7789      -0.8571 H      0      0      0      0      0      0      0      0      0      0      23
14      2.0500      -0.7777      0.9112 H      0      0      0      0      0      0      0      0      0      0      24
15      3.3162      0.7482      0.0452 C      0      0      0      0      0      0      0      0      0      0      25
16     -1.0944      -0.1531      5.0492 C      0      0      0      0      0      0      0      0      0      0      26
17     -2.2225      -1.2088      3.5288 H      0      0      0      0      0      0      0      0      0      0      27
18     -0.5782      -1.8100      3.7523 H      0      0      0      0      0      0      0      0      0      0      28
19     -1.0311      -0.1564      -5.0689 C      0      0      0      0      0      0      0      0      0      0      29
20     -2.1302      -1.2706      -3.5691 H      0      0      0      0      0      0      0      0      0      0      30
21     -0.4581      -1.7970      -3.7747 H      0      0      0      0      0      0      0      0      0      0      31
22      4.6095      -0.0738      0.0625 C      0      0      0      0      0      0      0      0      0      0      32
23      3.2889      1.4098      0.9283 H      0      0      0      0      0      0      0      0      0      0      33
24      3.3143      1.4124      -0.8365 H      0      0      0      0      0      0      0      0      0      0      34
25     -1.4374      -0.7907      5.8775 H      0      0      0      0      0      0      0      0      0      0      35
26     -0.0590      0.1515      5.2679 H      0      0      0      0      0      0      0      0      0      0      36
27     -1.7156      0.7560      5.0455 H      0      0      0      0      0      0      0      0      0      0      37
28     -1.3406      -0.8013      -5.9046 H      0      0      0      0      0      0      0      0      0      0      38
29     -0.0066      0.1909      -5.2753 H      0      0      0      0      0      0      0      0      0      0      39
30     -1.6880      0.7273      -5.0651 H      0      0      0      0      0      0      0      0      0      0      40
31      5.4975      0.5755      0.0824 H      0      0      0      0      0      0      0      0      0      0      41
32      4.6839      -0.7154      -0.8294 H      0      0      0      0      0      0      0      0      0      0      42
33      4.6527      -0.7268      0.9482 H      0      0      0      0      0      0      0      0      0      0      43
34
35      2      1      0      0      0      0
36      3      1      0      0      0      0
37      5      4      0      0      0      0
38      11     4      0      0      0      0
39      12     4      0      0      0      0
40      13     4      0      0      0      0
41      6      5      0      0      0      0
42      14     5      0      0      0      0
43      15     5      0      0      0      0
44      7      6      0      0      0      0
45      9      6      0      0      0      0
46      8      7      0      0      0      0
47      16     7      0      0      0      0
48      17     7      0      0      0      0
49      18     8      0      0      0      0
50      19     8      0      0      0      0
51      20     8      0      0      0      0
52      10     9      0      0      0      0
53      21     9      0      0      0      0
54      22     9      0      0      0      0
55      23    10      0      0      0      0
56      24    10      0      0      0      0
57      25    10      0      0      0      0
58      26    11      0      0      0      0
59      27    11      0      0      0      0
60      28    11      0      0      0      0
61      29    19      0      0      0      0
62      30    19      0      0      0      0
63      31    19      0      0      0      0
64      32    25      0      0      0      0
65      33    25      0      0      0      0
66      34    25      0      0      0      0
67      35    26      0      0      0      0
68      36    26      0      0      0      0
69      37    26      0      0      0      0
70      38    29      0      0      0      0
71      39    29      0      0      0      0
72      40    29      0      0      0      0
73      41    32      0      0      0      0
74      42    32      0      0      0      0
75      32    43      0      0      0      0
76
77 M      END
78 $$$$
79 tri-n-propylamine-cation.sdf
80 COSMOTHERM      3D      0
81
82 35 33      0      0      0      0      0      0      0      0      0      0 V2000
83     -2.2688     -1.9643      0.0832 O      0      0      0      0      0      0      0      0      0      0      1
84     -2.0645     -2.8283     -0.3187 H      0      0      0      0      0      0      0      0      0      0      2
85     -3.1503     -1.7345     -0.2629 H      0      0      0      0      0      0      0      0      0      0      3
86     -0.4455      0.0681     -2.5505 C      0      0      0      0      0      0      0      0      0      0      4
87     -0.5291      0.8510     -1.2431 C      0      0      0      0      0      0      0      0      0      0      5
88     -0.2922      0.0103     -0.0031 N      0      0      0      0      0      0      0      0      0      0      6
89     -0.5193      0.8544      1.2366 C      0      0      0      0      0      0      0      0      0      0      7
90     -0.4274      0.0760      2.5460 C      0      0      0      0      0      0      0      0      0      0      8
91      1.0291     -0.7325     -0.0071 C      0      0      0      0      0      0      0      0      0      0      9
92      2.2673      0.1567     -0.0118 C      0      0      0      0      0      0      0      0      0      0      10
93     -0.8908      0.9424     -3.7299 C      0      0      0      0      0      0      0      0      0      0      11
94      0.5826     -0.2812     -2.7262 H      0      0      0      0      0      0      0      0      0      0      12
95     -1.0864     -0.8256     -2.4882 H      0      0      0      0      0      0      0      0      0      0      13
96     -1.5331      1.2784     -1.1175 H      0      0      0      0      0      0      0      0      0      0      14
97      0.1915      1.6793     -1.2194 H      0      0      0      0      0      0      0      0      0      0      15
98     -1.5233      1.2833      1.1168 H      0      0      0      0      0      0      0      0      0      0      16
99      0.2026      1.6813      1.2048 H      0      0      0      0      0      0      0      0      0      0      17
100     0.6014     -0.2751      2.7149 H      0      0      0      0      0      0      0      0      0      0      18
101     -0.8596      0.9574      3.7251 C      0      0      0      0      0      0      0      0      0      0      19
102     -1.0714     -0.8156      2.4916 H      0      0      0      0      0      0      0      0      0      0      20
103      1.0110     -1.3847     -0.8894 H      0      0      0      0      0      0      0      0      0      0      21
104      1.0164     -1.3834      0.8762 H      0      0      0      0      0      0      0      0      0      0      22
105      2.2710      0.8129      0.8721 H      0      0      0      0      0      0      0      0      0      0      23
106      2.2663      0.8106     -0.8975 H      0      0      0      0      0      0      0      0      0      0      24
107      3.5401     -0.7000     -0.0138 C      0      0      0      0      0      0      0      0      0      0      25
108     -0.8191      0.3808     -4.6713 H      0      0      0      0      0      0      0      0      0      0      26
109     -1.9332      1.2725     -3.6100 H      0      0      0      0      0      0      0      0      0      0      27
```



```
1
2
3      27 11  0  0  0  0
4      28 11  0  0  0  0
5      29 19  0  0  0  0
6      30 19  0  0  0  0
7      31 19  0  0  0  0
8      32 25  0  0  0  0
9      33 25  0  0  0  0
10     25 34  0  0  0  0
11 M  END
12 $$$$
13 triethylamine-cation.sdf
14 COSMOtherm      3D      0
15
16 26 24  0  0  0  0  0  0  0  0  0  0 V2000
17 0.0593 -0.7412 -2.6475 O  0  0  0  0  0  0  0  0  0  0  0  0  1
18 0.2544 -1.6840 -2.7985 H  0  0  0  0  0  0  0  0  0  0  0  0  2
19 0.6327 -0.2681 -3.2778 H  0  0  0  0  0  0  0  0  0  0  0  0  3
20 2.5361  0.2823 -0.0242 C  0  0  0  0  0  0  0  0  0  0  0  0  4
21 1.2300  1.0338  0.1831 C  0  0  0  0  0  0  0  0  0  0  0  0  5
22 -0.0041  0.1712 -0.0018 N  0  0  0  0  0  0  0  0  0  0  0  0  6
23 -1.2504  1.0290  0.1025 C  0  0  0  0  0  0  0  0  0  0  0  0  7
24 -2.5357  0.2755 -0.2036 C  0  0  0  0  0  0  0  0  0  0  0  0  8
25 -0.0303 -1.0579  0.8877 C  0  0  0  0  0  0  0  0  0  0  0  0  9
26 -0.0723 -0.7540  2.3762 C  0  0  0  0  0  0  0  0  0  0  0  0 10
27 3.3567  1.0123 -0.0033 H  0  0  0  0  0  0  0  0  0  0  0  0 11
28 2.7304 -0.4555  0.7645 H  0  0  0  0  0  0  0  0  0  0  0  0 12
29 2.5628 -0.2237 -0.9997 H  0  0  0  0  0  0  0  0  0  0  0  0 13
30 1.1282  1.8459 -0.5480 H  0  0  0  0  0  0  0  0  0  0  0  0 14
31 1.1684  1.4769  1.1849 H  0  0  0  0  0  0  0  0  0  0  0  0 15
32 -1.1002  1.8467 -0.6137 H  0  0  0  0  0  0  0  0  0  0  0  0 16
33 -1.2608  1.4641  1.1096 H  0  0  0  0  0  0  0  0  0  0  0  0 17
34 -3.3582  1.0031 -0.2341 H  0  0  0  0  0  0  0  0  0  0  0  0 18
35 -2.7826 -0.4699  0.5629 H  0  0  0  0  0  0  0  0  0  0  0  0 19
36 -2.4910 -0.2201 -1.1838 H  0  0  0  0  0  0  0  0  0  0  0  0 20
37 0.8591 -1.6422  0.6249 H  0  0  0  0  0  0  0  0  0  0  0  0 21
38 -0.9043 -1.6410  0.5752 H  0  0  0  0  0  0  0  0  0  0  0  0 22
39 -0.0854 -1.7098  2.9168 H  0  0  0  0  0  0  0  0  0  0  0  0 23
40 -0.9740 -0.1980  2.6658 H  0  0  0  0  0  0  0  0  0  0  0  0 24
41 0.8100 -0.1948  2.7150 H  0  0  0  0  0  0  0  0  0  0  0  0 25
42 0.0303 -0.1919 -0.9940 H  0  0  0  0  0  0  0  0  0  0  0  0 26
43
44 2  1  0  0  0  0
45 3  1  0  0  0  0
46 5  4  0  0  0  0
47 11 4  0  0  0  0
48 12 4  0  0  0  0
49 13 4  0  0  0  0
50 6  5  0  0  0  0
51 14 5  0  0  0  0
52 15 5  0  0  0  0
53 7  6  0  0  0  0
54 9  6  0  0  0  0
55 8  7  0  0  0  0
56 16 7  0  0  0  0
57 17 7  0  0  0  0
58 18 8  0  0  0  0
59 19 8  0  0  0  0
60 20 8  0  0  0  0
10 10 9  0  0  0  0
11 21 9  0  0  0  0
12 22 9  0  0  0  0
13 23 10 0  0  0  0
14 24 10 0  0  0  0
15 25 10 0  0  0  0
16 6 26 0  0  0  0
17 M  END
18 $$$$
19 triethylamine.sdf
20 COSMOtherm      3D      0
21
22 25 23  0  0  0  0  0  0  0  0  0  0 V2000
23 0.0434 -0.8594 -2.6092 O  0  0  0  0  0  0  0  0  0  0  0  0  1
24 0.0260 -0.4827 -1.6640 H  0  0  0  0  0  0  0  0  0  0  0  0  2
25 0.1234 -0.0755 -3.1794 H  0  0  0  0  0  0  0  0  0  0  0  0  3
26 2.5205  0.2663 -0.1288 C  0  0  0  0  0  0  0  0  0  0  0  0  4
27 1.2068  1.0075  0.1135 C  0  0  0  0  0  0  0  0  0  0  0  0  5
28 -0.0015  0.1583 -0.0261 N  0  0  0  0  0  0  0  0  0  0  0  0  6
29 -1.2148  1.0053  0.0772 C  0  0  0  0  0  0  0  0  0  0  0  0  7
30 -2.5190  0.2631 -0.2088 C  0  0  0  0  0  0  0  0  0  0  0  0  8
31 -0.0142 -1.0061  0.8956 C  0  0  0  0  0  0  0  0  0  0  0  0  9
32 -0.0348 -0.6978  2.3996 C  0  0  0  0  0  0  0  0  0  0  0  0 10
33 3.3473  0.9908 -0.1564 H  0  0  0  0  0  0  0  0  0  0  0  0 11
34 2.7462 -0.4595  0.6646 H  0  0  0  0  0  0  0  0  0  0  0  0 12
35 2.4995 -0.2660 -1.0912 H  0  0  0  0  0  0  0  0  0  0  0  0 13
36 1.1042  1.8132 -0.6303 H  0  0  0  0  0  0  0  0  0  0  0  0 14
37 1.2306  1.5022  1.1054 H  0  0  0  0  0  0  0  0  0  0  0  0 15
38 -1.0899  1.8131 -0.6608 H  0  0  0  0  0  0  0  0  0  0  0  0 16
39 -1.2709  1.4972  1.0692 H  0  0  0  0  0  0  0  0  0  0  0  0 17
40 -3.3458  0.9863 -0.2580 H  0  0  0  0  0  0  0  0  0  0  0  0 18
41 -2.7674 -0.4673  0.5736 H  0  0  0  0  0  0  0  0  0  0  0  0 19
42 -2.4680 -0.2639 -1.1731 H  0  0  0  0  0  0  0  0  0  0  0  0 20
43 0.8663 -1.6186  0.6565 H  0  0  0  0  0  0  0  0  0  0  0  0 21
44 -0.8879 -1.6186  0.6325 H  0  0  0  0  0  0  0  0  0  0  0  0 22
45 -0.0435 -1.6419  2.9635 H  0  0  0  0  0  0  0  0  0  0  0  0 23
46 -0.9281 -0.1273  2.6925 H  0  0  0  0  0  0  0  0  0  0  0  0 24
47 0.8513 -0.1293  2.7170 H  0  0  0  0  0  0  0  0  0  0  0  0 25
48
49 2  1  0  0  0  0
50 3  1  0  0  0  0
51 5  4  0  0  0  0
52 11 4  0  0  0  0
53 12 4  0  0  0  0
54 13 4  0  0  0  0
55 6  5  0  0  0  0
56 14 5  0  0  0  0
57 15 5  0  0  0  0
58 7  6  0  0  0  0
```