Comparison between alpha- and beta-carbonic anhydrases: can $\text{Zn}(\text{His})_3(\text{H}_2\text{O})$ and $\text{Zn}(\text{His})(\text{Cys})_2(\text{H}_2\text{O})$ sites lead to equivalent enzymes?

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Supporting Information

Comparison between α - and β -carbonic anhydrases : could $\text{Zn}(\text{His})_3(\text{H}_2\text{O})$ and $\text{Zn}(\text{His})(\text{Cys})_2(\text{H}_2\text{O})$ enzymes sites be equivalents ?

Florent Pannetier, Gilles Ohanessian and Gilles Frison*

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A) Computational methods

1- DFT level

We use a well established methodology,¹ the GGA density functional BP86,² to optimize all of our geometries. These geometry optimizations were accelerated using the Resolution of Identity (RI) approximation method,³ as implemented in Turbomole.⁴ The geometry optimizations for models **5** were further accelerated using the Multipole Accelerated Resolution of Identity for J (MARI-J) approximation method.⁵ Basis sets of split-valence quality, def2-SVP (and abbreviated SVP),⁶ and the associated auxiliary basis sets to fit Coulomb potentials,⁷ were employed for all atoms in the geometry optimization. In order to hold the structures sufficiently close to the X-ray structure, α -carbons have been fixed at their position in the X-ray analysis (see below).

Improved energies were obtained by single-point calculations at the B3LYP level,⁸ with the extended basis set of valence triple zeta quality, labeled def2-TZVPP (and abbreviated TZVPP).^{7,9} For models **5**, full B3LYP/TZVPP calculations were not possible due to computational limitations as the number of Atomic Orbitals exceed 10000. Thus, a mixed TZVPP (for all atoms included in models **4**) and SVP basis set (for all others atoms) has been used, leading to 7022 and 6531 AOs for **α -5H** and **β -5H** respectively. For an additional gain in speed, the resolution of identity (RI) approximation was used.

We have used these levels of calculations in our former studies.¹⁰ They have been shown to give reliable geometries and relative energetic data for zinc complexes as compared with other density functionals or post-HF calculations.^{1d,11}

Solvation free energy corrections were determined using the conductor-like screening model (COSMO)¹² which is a polarizable continuum solvation model. The COSMO calculations were carried out on the gas-phase BP86/SVP geometries, at the B3LYP/TZVPP level, with dielectric constants ϵ of 78.4.

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¹⁰ (a) D. Picot, G. Ohanessian, G. Frison, Chem. Asian J. 2010, 5, 1445; (b) G. Ohanessian, D. Picot, G. Frison, Int. J. Quantum Chem. In press. DOI : 10.1002/qua.22866

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Binding energies of the zinc-bound water molecule and of the zinc dication have been computed at the gas-phase BP86/SVP geometries of the whole system, without re-optimisation of the fragments. They have been corrected to basis set superposition error (BSSE) by the well established counterpoise method.

Accurate absolute pK_a values could not be obtained from our calculations. However, high level DFT calculations with polarized continuum model solvent corrections have been shown to provide a balanced treatment for the calculation of relative pK_a values for metal-bound water ligands.¹³ This has been achieved through the use of the following equation which gives the expected relative pK_a values from relative PA values :

$$\Delta pK_a = \frac{\Delta PA_{\text{solv}} \text{ (kJ/mol)}}{5.71}$$

The constant $5.71 = RT\log_e(10)$, in kJ/mol

2- Computed models

Our computational models **1-5** have been built from X-ray structures of representatives members of the α -CA and β -CA classes (PDB 2CBA and 1G5C respectively). For 1G5C, we select the zinc site of chain B as it includes a zinc-bound water molecule and no hepes group. For models **1-4**, we have selected molecular groups step-by-step, based on their location and chemical influence. These groups included amino-acid side chain, backbone amide group, amino-acid, peptide or water molecules located in the neighbouring of zinc. For models **5**, we have included all chemical groups located at a distance lower than 9 Å of the zinc atom. In all cases, model **n** includes model **n-1**. When an amino-acid side chain is selected, all the side chain from the C $_{\alpha}$ atom is included in the model, thus allowing fixing this atom in its position in the X-ray structure. When an amino-acid or a peptide is selected, the side-chains have been either conserved, simplified (for example Thr to Ser) or replaced by an H atom, depending on their position and chemical influence. Furthermore, C- and N-termination of amino-acids and peptides have been capped by -N(H)-C $_{\alpha}$ H₃ and -C(O)-C $_{\alpha}$ H₃ groups. Thus, in all cases, backbone amide group, amino-acids and peptides have C $_{\alpha}$ atoms at their two extremities, which are fixed.

Models **1** include the zinc dication, the coordinated water molecule (W263 and W2 for α and β respectively) and the first coordination shell of the metal (side chains of His94, His96 and His119 for α , side chains of Cys32, His87 and Cys90 for β). Models **α -1H** and **β -1H** include thus 49 and 35 atoms respectively.

Models **2** include models **1** and the second coordination shell around protein Zn-ligands. For **α -2**, this corresponds (i) to the side chain of Gln92, hydrogen bonded to His94; (ii) to the backbone amide group between Asn244 and Trp245, hydrogen bonded to His96; (iii) to the side chain of Glu117 and the peptide Glu106-His107, forming a hydrogen bond network around His119. For **β -2**, this corresponds (i) to the backbone amide group between Ala58 and Gly59, and the simplified peptide Cys32-Met33Gly, both hydrogen bonded to Cys32; (ii) to the simplified peptide His87-Thr88Gly-Asp89Gly-Cys90-Gly91 and the water molecule W33, forming a hydrogen bond network around His87 and Cys90. Models **α -2H** and **β -2H** include thus 118 and 101 atoms respectively.

¹³ R. Gilson, M. C. Durrant, Dalton Trans., 2009, 10223-10230.

It should be noted that, through the $-N(H)-C_{\alpha}H_3$ capped group of Gly91, the NH amide group of Met92 is included in **β -2** as it is hydrogen bonded to the S-thiolate of Cys90. Model **β -2** thus also includes the amide group located between Cys90 and Gly91 to “close” the protein backbone and to be chemically pertinent. However, this second NH amide group is hydrogen bonded to the zinc-bound water molecule, and thus should only be part of model **β -3** and larger. In order to evaluate the influence of this interaction, we also built a modified model, noted **β -2'**, in which this amide group located between Cys90 and Gly91 has been replaced by two hydrogen atoms. The obtained structural parameters and energetic properties are presented in Table S1.

Table S1. structural parameters and energetic properties of model **β -2'**
Mains structural parameters for compounds **β -2'H**

	$Zn-O$	$Zn-L_1$	$Zn-L_2$	$Zn-L_3$	$\Sigma(X-O-X)$
β-2'H	2.188	2.283	2.058	2.293	326.3

Energetic properties for compounds β-2'				
	PA_{gaz}^b	PA_{solv}^b	$BE(H_2O_{(Zn)})^c$	$BE(Zn)^c$
β-2'	1315	1240	50	2807

These data show that this hydrogen bond induces a noticeable increase of the Zn-O bond length (2.188 and 2.274 Å in **β -2'H** and **β -2H** respectively) but does not modify significantly any of the energetic data.

Models **3** include models **2**, the “gatekeeper” and its surrounding. For **α -3**, the “gatekeeper” corresponds to the Thr199Ser amino-acid and the side chain of Glu106. Its surroundings include the amide group between Trp245 and Arg246 and W265. For **β -3**, the “gatekeeper” corresponds to the side chain of Asp34 and the peptide Ser35Gly-Arg36. Its surroundings include W17 and the side chain of Asp89. It should be noted that we decided to protonate the side chain of Asp89 to take into account the electronic surroundings of the carboxylate group as it is hydrogen bonded to the side chain of Arg16 (from chain A) and close to the side chain of Arg94. This protonated Asp89 is conserved in **β -4** but not in **β -5** which includes both arginines. Models **α -3H** and **β -3H** include thus 152 and 146 atoms respectively.

Models **4** include models **3** and the remaining chemical groups directly located around the zinc-bound water molecule. For **α -4**, this includes W318 and W338 (called “deep water”), both hydrogen bonded to $H_2O_{(Zn)}$, the amide group between Leu198 and Thr199, and the side chain of Thr200Ser. For **β -4**, this includes W167, hydrogen bonded to $H_2O_{(Zn)}$, W117 and W22. Models **α -4H** and **β -4H** include thus 169 and 155 atoms respectively.

Models **5** include models **4** and all the remaining chemical groups located in a sphere with a radius of 9 Å and centered on zinc.

Models **α -5**, depicted in figure S1, is built with the zinc Zn262, the side chain of Tyr7 and Trp209, the peptides Ser29-Pro30, Ala65-Phe66Gly-Asn67, Gln92-Phe93Gly-His94-Phe95-His96, Ser105-Glu106-His107, Glu117-Leu118-His119-Leu120Gly-Val121, Val143-Leu144Gly-Gly145, Ser197-Leu198Gly-Thr199-Thr200-Pro201 and Asn244-Trp245Gly, and the water molecules W263, W264, W265, W292, W295, W318, W319, W338, W359, W369, W381, W389, W393 and W461. Besides α -carbons, all atoms except H from the side chain of

Tyr7 and Trp209 have been fixed in their position in the X-ray structure, which lead to 60 frozen atoms (58 C, 1 O and 1 N) during the optimisation process. Model **α -5H** includes thus 530 atoms.

Figure S1. Optimized structure of **α -5H** at the BP86/SVP level. The **α -4H** part is depicted in “Tube” whereas the remaining atoms are depicted in “Ball & Stick”. The H atoms have been omitted for clarity.

Models **β -5**, depicted in figure S2, is built with the zinc Zn1002 of chain B, the side chain of Ser19 (chain A), Lys53 (chain A), Leu77 (chain A), Asn131 (chain B), Ile158 (chain B), the amino-acid Glu128 (chain B), the peptides Arg16-Asp17 (chain A), Thr31-Cys32-Met33-Asp34-Ser35-Arg36-Leu37 (chain B), Asn57-Ala58-Gly59-Asn60-Ile61 (chain B), Val85Gly-Gly86-His87-Thr88Gly-Asp89-Cys90-Gly91-Met92-Ala93-Arg94 (chain B), and the water molecules W2, W17, W19, W22, W33, W35, W114, W117, W167, W181, W194, W234 and W295. Besides α -carbons, all atoms except H from the side chain of Leu77 and Ile158 have been fixed in their position in the X-ray structure, which lead to 45 frozen atoms (all C) during the optimisation process. Model **β -5H** includes thus 494 atoms.

Figure S2. Optimized structure of β -5H at the BP86/SVP level. The β -4H part is depicted in “Tube” whereas the remaining atoms are depicted in “Ball & Stick”. The H atoms have been omitted for clarity.

B) Comparison between optimized and crystal structures of α - and β -CA.

The comparison between BP86/SVP optimized structures of all our models and corresponding part of crystal structures (PDB 2CBA and 1G5C) of α - and β -CA enzymes is presented in Table S2.

Table S2. Structural parameters for deprotonated compounds **1-5** as determined by geometry optimisation at the BP86/def2-SVP level of calculation.

	<i>Full model^a</i>	<i>Zn core^b</i>
α -1H	0.354	0.354
α -2H	0.468	0.215
α -3H	0.545	0.205
α -4H	0.420	0.149
α -5H	0.395	0.123
β -5H	0.459	0.125
β -4H	0.353	0.190
β -3H	0.251	0.182
β -2H	0.231	0.229
β -1H	0.639	0.639

^a RMSD values computed for all atoms, except H, in models α/β -XH.

RMSD values computed only for atoms included in models α/β -1H.

RMSD values have been used to estimate the quality of our optimized structures compare to experiment. As shown in Table S3, the optimized structures are close to the

experimental one. There are some minor discrepancies between the experimental and the optimized for the whole systems, due mainly to the residues and water molecules located at the outside part of each model. On the opposite, the zinc active site of the protein is well reproduced, and the larger the used models (from **1** to **5**), the better the quality of our optimized structures to reproduce the zinc core.

C) Structural parameters for $\alpha\text{-X}^-$ and $\beta\text{-X}^-$ (X=1-5)

Table S3. Structural parameters for deprotonated compounds **1-5** as determined by geometry optimisation at the BP86/def2-SVP level of calculation.

	Zn-O^a	$\text{Zn-L}_1^{a,b}$	$\text{Zn-L}_2^{a,c}$	$\text{Zn-L}_3^{a,d}$
$\alpha\text{-1}^-$	1.887	2.051	2.060	2.059
$\alpha\text{-2}^-$	1.872	2.075	2.073	2.070
$\alpha\text{-3}^-$	1.858	2.115	2.043	2.103
$\alpha\text{-4}^-$	1.910	2.069	2.036	2.083
$\alpha\text{-5}^-$	1.933	2.023	2.027	2.035
$\beta\text{-5}^-$	1.993	2.394	2.117	2.361
$\beta\text{-4}^-$	1.933	2.364	2.160	2.368
$\beta\text{-3}^-$	1.918	2.375	2.151	2.382
$\beta\text{-2}^-$	1.931	2.373	2.137	2.368
$\beta\text{-2}^-$	1.920	2.377	2.130	2.394
$\beta\text{-1}^-$	1.960	2.355	2.228	2.349

^a bond lengths (Å). ^b $\text{L}_1 = \text{N}(\text{His94}) / \text{S}(\text{Cys32})$ for $\alpha\text{-}$ / $\beta\text{-CA}$ respectively. ^c $\text{L}_2 = \text{N}(\text{His96}) / \text{N}(\text{His87})$ for $\alpha\text{-}$ / $\beta\text{-CA}$ respectively. ^d $\text{L}_3 = \text{N}(\text{His119}) / \text{S}(\text{Cys90})$ for $\alpha\text{-}$ / $\beta\text{-CA}$ respectively. ^e Sum of the Zn-O-H and H-O-H angles (°).

D) Absolute energies for all models

Table S4. Absolute electronic energies and solvation free energies corrections for all models in u.a.

Structure	E ^a	E ^b	G ^{78.4} _{corr} ^c	E(system-H ₂ O) ^d	E(H ₂ O) ^e	E(system-Zn) ^f	E(Zn) ^g
α-1H	-2769.387080	-2769.731578	-0.226972	-2693.260735	-76.431118	-990.730392	-1778.320502
α-1⁻	-2769.078391	-2769.425377	-0.073610				
β-1H	-3115.105891	-3115.344175	-0.031955	-3038.899728	-76.429999	-1335.839914	-1778.320089
β-1⁻	-3114.538810	-3114.787653	-0.106823				
α-2H	-4333.054027	-4334.157484	-0.120879	-4257.695165	-76.431236	-2554.927206	-1778.320536
α-2⁻	-4332.640262	-4333.751908	-0.079465				
β-2⁺H	-4895.024853	-4896.185526	-0.096816	-4819.735368	-76.431222	-3116.796143	-1778.320317
β-2⁺	-4894.523835	-4895.684670	-0.125544				
β-2H	-5062.418676	-5063.665230	-0.105675	-4987.215471	-76.431404	-3284.291656	-1778.320315
β-2⁻	-5061.934776	-5063.180757	-0.130286				
α-3H	-5246.796173	-5248.380837	-0.095701	-5171.880861	-76.411636	-3468.957255	-1778.320554
α-3⁻	-5246.266926	-5247.872373	-0.140147				
β-3H	-6332.027584	-6333.923778	-0.134192	-6257.447220	-76.423157	-4554.533381	-1778.320487
β-3⁻	-6331.520973	-6333.417167	-0.167121				
α-4H	-5721.916048	-5723.781086	-0.109217	-5647.268050	-76.417556	-3944.367056	-1778.320615
α-4⁻	-5721.415414	-5723.291508	-0.141292				
β-4H	-6561.197070	-6563.252218	-0.134714	-6486.766764	-76.424781	-4783.847649	-1778.320546
β-4⁻	-6560.675411	-6562.743026	-0.181203				
α-5H	-14909.226064	-14905.276937	-0.174177	-14828.764150	-76.417374	-13125.885433	-1778.320719
α-5⁻	-14908.716770	-14904.773883	-0.196738				
β-5H	-14802.027109	-14799.087751	-0.200345	-14722.611871	-76.427603	-13019.694342	-1778.320547
β-5⁻	-14801.524383	-14798.578144	-0.231158				

^a absolute energy of models **1-5** at the ri-BP86/def2-SVP level (marij-BP86 for models 5).

^b absolute energy of models **1-5** at the ri-B3LYP//def2-TZVPP/ri-BP86/def2-SVP level (mixed TZVPP and SVP basis set for models 5).

^c correction to solvation free energy in water ($\epsilon = 78.4$) at the COSMO-ri-B3LYP//def2-TZVPP/ri-BP86/def2-SVP level (mixed TZVPP and SVP basis set for models 5).

^d Counterpoise absolute energy of models **1H-5H** without the zinc-bound water molecule at the ri-B3LYP//def2-TZVPP level (mixed TZVPP and SVP basis set for models 5).

^e Counterpoise absolute energy of the zinc-bound water molecule at the ri-B3LYP//def2-TZVPP level (mixed TZVPP and SVP basis set for models 5).

^f Counterpoise absolute energy of models **1H-5H** without the zinc dication at the ri-B3LYP//def2-TZVPP level (mixed TZVPP and SVP basis set for models 5).

^g Counterpoise absolute energy of the zinc dication at the ri-B3LYP//def2-TZVPP level (mixed TZVPP and SVP basis set for models 5).

E) Cartesian coordinates

Model **α-1H**

O	-15.1945871	14.9479409	22.0873037
Zn	-14.6689737	13.1145095	22.9480787
N	-16.1502394	11.7570087	22.8960621
C	-17.4475549	11.8578576	23.2189575
N	-17.9906665	10.6192589	23.2989539
C	-17.0228089	9.6624358	23.0212422
C	-15.8759600	10.3986674	22.7681175
C	-17.2576965	8.1850518	23.1156059
C	-17.0132740	7.6225650	24.5317940
N	-14.3411416	13.5712461	24.8681959
C	-14.4503446	12.6274533	25.8821423
C	-14.0207062	13.1761794	27.0805955
N	-13.6561435	14.4752900	26.7519616
C	-13.8567915	14.6884318	25.4284150
C	-13.8596672	12.5751684	28.4459363

C	-12.6593800	11.6110050	28.5452740
N	-13.1644041	12.5711147	21.7362644
C	-13.2710362	12.3928255	20.4070007
N	-12.0929984	11.9564721	19.9136265
C	-11.1881153	11.8402950	20.9525591
C	-11.8575239	12.2263553	22.1017410
C	-11.3633745	12.2963031	23.5180278
C	-9.9693200	11.7002250	23.7325670
H	-12.7669873	10.7579257	27.8463253
H	-9.9347197	10.6287412	23.4511584
H	-15.9662265	7.7873399	24.8544965
H	-11.7034622	12.1240640	28.3192675
H	-17.2047601	6.5320720	24.5465919
H	-9.6762010	11.7745745	24.7968113
H	-18.0101967	12.7814116	23.3946674
H	-18.9731747	10.4209934	23.5131974
H	-18.2921551	7.9548231	22.7841138

H	-16.5883049	7.6824539	22.3887396
H	-17.6829616	8.0893057	25.2819958
H	-12.5860458	11.1991965	29.5704732
H	-13.7631327	13.3889335	29.1943807
H	-14.7952641	12.0377463	28.7052614
H	-14.8290402	11.6163063	25.6982675
H	-13.3060441	15.1744275	27.4145684
H	-13.6546107	15.6379277	24.9207375
H	-11.3706684	13.3612041	23.8432516
H	-12.0986604	11.7793427	24.1739064
H	-9.1987898	12.2372335	23.1437291
H	-10.1607756	11.4990090	20.7955904
H	-11.9044816	11.7406855	18.9298300
H	-14.1676730	12.5527546	19.7972001
H	-14.8808223	10.0271921	22.5011936
H	-14.6671291	15.4022597	21.4011321
H	-16.0139219	15.4697728	22.1948813

Model α -1⁻

O	-15.8449653	14.5526726	22.0674366
Zn	-14.8839780	13.4415327	23.2513721
N	-16.0347618	11.7337312	23.2184923
C	-17.1143075	11.8989218	22.4501171
N	-17.8672810	10.7689694	22.4718772
C	-17.2550628	9.8241137	23.2894902
C	-16.1061112	10.4534050	23.7438167
C	-17.8272533	8.4590412	23.5380217
C	-17.0132740	7.6225650	24.5317940
N	-14.3832273	13.8768808	25.1918195
C	-14.0032845	12.9588798	26.1575564
C	-13.5357301	13.6198884	27.2820777
N	-13.6556076	14.9671437	26.9645610
C	-14.1629602	15.0859284	25.7076346
C	-12.9871828	13.1093756	28.5815109
C	-12.6593800	11.6110050	28.5452740
N	-13.1088521	13.3204195	22.2157221
C	-13.1227960	14.0330331	21.0846775
N	-11.9079003	13.9622936	20.4885692
C	-11.0769662	13.1747028	21.2710913
C	-11.8392470	12.7720928	22.3571352
C	-11.4735935	11.8991015	23.5243617
C	-9.9693200	11.7002250	23.7325670
H	-13.5644391	11.0010122	28.3507453
H	-9.4973717	11.1984640	22.8633268
H	-15.9799788	7.4508495	24.1681100
H	-11.9100818	11.3792583	27.7623709
H	-17.4826683	6.6310959	24.6791826
H	-9.7752977	11.0645375	24.6184431
H	-17.3088024	12.8341786	21.9002757
H	-18.7452005	10.6363908	21.9655181
H	-18.8722161	8.5667063	23.9063590
H	-17.9076417	7.9166340	22.5690838

H	-16.9528168	8.1158741	25.5229980
H	-12.2458916	11.2824848	29.5179492
H	-12.0740791	13.6897013	28.8406456
H	-13.7146949	13.3176027	29.3978909
H	-14.0886134	11.8807414	25.9946994
H	-13.4002377	15.7469400	27.5748360
H	-14.3466760	16.0439469	25.2080938
H	-11.9268736	12.3431889	24.4362207
H	-11.9696479	10.9096132	23.3990986
H	-9.4489767	12.6672609	23.8875306
H	-10.0377020	12.9730051	20.9970510
H	-11.6492911	14.4196899	19.6123438
H	-14.0089330	14.5926740	20.7462234
H	-15.3366204	10.0497224	24.4089077
H	-16.3215938	15.3047688	22.4598402

Model β -1H

C	-16.2419399	45.6328016	25.9798260
C	-16.2357075	44.8416825	27.1181618
N	-17.4409283	45.1277813	27.7483889
C	-18.1221918	46.0452870	27.0073950
N	-17.4114024	46.3663446	25.9285984
C	-15.2324598	43.8623401	27.6475910
C	-14.0881150	43.6052950	26.6631430
Zn	-18.1559139	47.6907461	24.5240806
O	-20.2231508	47.8879632	25.7397500
S	-17.8046916	49.8753283	25.0819882
C	-16.9708526	49.6849726	26.7325760
C	-16.3535300	51.0060380	27.1857050

H	-17.1236030	51.8009825	27.2635114
S	-18.9998901	46.7968867	22.6335405
C	-18.5505121	45.0041131	22.7930590
C	-19.4293610	44.1986560	23.7492410
H	-13.5250344	44.5353657	26.4461217
H	-15.8682005	50.9000310	28.1801709
H	-15.5884961	51.3549836	26.4624874
H	-16.1857549	48.9045777	26.6570316
H	-17.7103602	49.3304731	27.4825205
H	-13.3697749	42.8725060	27.0794168
H	-14.8201785	44.2333792	28.6135283
H	-15.7457304	42.9042743	27.8893282

H	-17.7708350	44.7095644	28.6198249
H	-19.1146958	46.4524320	27.2380901
H	-15.4784857	45.7139030	25.1995201
H	-19.3655069	44.5969762	24.7821645
H	-18.6308607	44.5913369	21.7652931
H	-17.4814150	44.9140910	23.0780966
H	-19.8772502	48.8198243	25.6459876
H	-20.6180130	47.6959769	24.8590890
H	-20.4942430	44.2461357	23.4423163
H	-19.1243907	43.1289599	23.7715713
H	-14.4651832	43.2022008	25.7021472

Model β -1⁻

C	-16.2843493	45.6833098	26.8626262
C	-16.2566771	44.4850415	27.5614689
N	-17.5552502	44.3350490	28.0457033
C	-18.3043642	45.4015727	27.6206250
N	-17.5458976	46.2278230	26.9115304
C	-15.1690246	43.4693704	27.7429312
C	-14.0881150	43.6052950	26.6631430
Zn	-18.8060307	47.4053419	25.5010038
O	-20.3962777	46.4981260	26.1998400
S	-18.5778321	49.6748021	26.0869479
C	-16.7948473	49.6686795	26.5748068
C	-16.3535300	51.0060380	27.1857050
H	-16.9581292	51.2416820	28.0877733
S	-17.8402535	46.5651982	23.5308881
C	-17.9951269	44.7406992	23.7814257
C	-19.4293610	44.1986560	23.7492410
H	-13.5968007	44.5979348	26.7115530
H	-15.2783669	50.9931019	27.4788469
H	-16.5064401	51.8379495	26.4653055
H	-16.1660002	49.4366683	25.6862339
H	-16.6143484	48.8509331	27.3065393
H	-13.2977259	42.8362542	26.7859992
H	-14.7011894	43.5519484	28.7532503
H	-15.6076815	42.4460044	27.7019156

H	-17.9091417	43.5265863	28.5570386
H	-19.4083848	45.5516897	27.6283962
H	-15.4912326	46.1584955	26.2748643
H	-20.0419244	44.7079109	24.5254149
H	-17.3862774	44.2554367	22.9838161
H	-17.5156333	44.4547734	24.7460217
H	-20.9656597	47.2028268	26.5629541
H	-19.9032486	44.4060954	22.7656844
H	-19.4575663	43.0961969	23.9236773
H	-14.5252865	43.5014129	25.6503258

Model α -2H

N	-13.0092172	10.3901736	15.8442035
C	-12.9379817	9.7474757	14.6191235
C	-13.0339554	10.7745038	13.6815866
N	-13.1550409	12.0010590	14.2977121
C	-13.1358803	11.7332222	15.5956913
C	-12.8037480	8.2598191	14.4925083
C	-14.1190300	7.4536750	14.6112320
N	-14.8064978	7.6308097	15.8650059
C	-16.1551423	7.8500191	15.9379662
O	-16.8866478	8.0576572	14.9722944
C	-16.7110760	7.8300350	17.3736580
N	-16.1231814	6.7842762	18.1916871
C	-16.8482759	5.8425913	18.8725578
C	-16.0143640	4.6255130	19.2644660
O	-18.0548710	5.9416249	19.1134337
O	-15.0712728	14.8462838	21.9509723
Zn	-14.6822823	13.0964521	23.0793640
N	-16.1915496	11.7743725	23.0421304
C	-17.5310352	11.8069161	23.1490989
N	-18.0319396	10.5517629	23.1442161
C	-16.9840287	9.6539955	23.0333667
C	-15.8403785	10.4323708	22.9688653
C	-17.1539441	8.1665880	23.0979915
C	-17.0132740	7.6225650	24.5317940
N	-14.2582016	13.7174749	24.9275900
C	-14.2116103	12.8447803	26.0063461

C	-13.6062481	13.4772367	27.0832095
N	-13.2952915	14.7487517	26.6269063
C	-13.6920798	14.8625615	25.3400123
C	-13.2930253	13.0119107	28.4784080
C	-12.6593800	11.6110050	28.5452740
N	-13.2705112	12.3604715	21.9136945
C	-13.5551537	11.7100429	20.7474815
N	-12.5109447	11.0174601	20.2826851
C	-11.4908597	11.2200477	21.1861773
C	-11.9442860	12.0465243	22.2059461
C	-11.2226793	12.5250477	23.4316058
C	-9.9693200	11.7002250	23.7325670
O	-12.7289843	9.2102424	18.5431809
C	-12.8138974	7.9568356	18.9358203
C	-12.4299372	7.6219539	20.3768083
C	-12.9703108	6.2605376	20.8272407
C	-12.5945320	5.8774640	22.2573820
O	-13.1783482	7.0613676	18.1611721
O	-12.0158036	16.3334542	28.4137061
C	-11.6245902	17.4028373	28.9187447
C	-11.2346465	17.4817857	30.3882474
C	-10.0507263	16.5592666	30.7469890
C	-8.7104820	17.0011290	30.1496800
N	-11.5200031	18.5475409	28.1976676
O	-20.5679180	9.7548467	23.3419744
C	-21.5034723	8.9602892	23.1115141
C	-22.4808780	8.5979410	24.2242620

N	-21.7107680	8.3918900	21.8956846
C	-20.9018020	8.6345760	20.7021270
H	-21.5557888	8.8647878	19.8382556
H	-13.3310928	10.8353719	28.1250484
H	-10.2148053	10.6278927	23.8693548
H	-16.0133501	7.8517272	24.9520313
H	-11.7032940	11.5723537	27.9864384
H	-12.9722370	6.6150966	22.9978492
H	-8.7332401	17.0113403	29.0395541
H	-13.8805444	6.3761204	14.4478041
H	-17.1439396	6.5222028	24.5475637
H	-8.4290563	18.0198685	30.4893447
H	-13.0136373	4.8887037	22.5316696
H	-9.4706733	12.0557737	24.6558182
H	-21.9183883	8.1187579	25.0496760
H	-23.2979294	7.9236277	23.9047470
H	-18.1501622	12.7071718	23.2293874
H	-19.0578604	10.2726826	23.1897818
H	-18.1416979	7.8903442	22.6770479
H	-16.3988729	7.6949104	22.4375646
H	-17.7748403	8.0639903	25.2058500
H	-12.4522192	11.3314524	29.5969068
H	-12.6279516	13.7670343	28.9448702
H	-14.2288431	13.0249960	29.0796975
H	-14.6115217	11.8275991	25.9419574
H	-12.8055590	15.4820425	27.2085519
H	-13.5577987	15.7616819	24.7290192
H	-7.8941906	16.3160205	30.4534561
H	-9.9746832	16.5188136	31.8535515
H	-10.2990167	15.5282704	30.4171758
H	-12.1328615	17.1680286	30.9610699
H	-11.0116738	18.5293236	30.6816442
H	-11.1869425	19.4164451	28.6145208
H	-11.7581210	18.5477138	27.2043239
H	-10.9468058	13.5990266	23.3192356
H	-11.9137723	12.4841253	24.3019378
H	-9.2264077	11.7740395	22.9129930
H	-10.5068851	10.7585850	21.0513770
H	-12.5714346	10.0024193	19.3246756
H	-14.5398288	11.7276912	20.2619026
H	-11.4938064	5.8167229	22.3901457

H	-14.0751453	6.2675148	20.7158215
H	-12.6085899	5.4901261	20.1166144
H	-12.7706081	8.4412884	21.0462343
H	-11.3171000	7.6423473	20.4331056
H	-12.9512064	9.9296369	16.7659119
H	-13.1997963	12.4728288	16.4056437
H	-13.0155007	10.6775815	12.5878724
H	-12.0795077	7.8834880	15.2488531
H	-12.3584385	8.0261795	13.5033327
H	-14.8273945	7.7549003	13.8134537
H	-14.2361465	7.4784119	16.7118651
H	-17.8013475	7.6547782	17.3194360
H	-15.1154865	6.6146878	18.1051067
H	-22.9167648	9.5328273	24.6275628
H	-14.7984300	10.1118018	22.8639176
H	-22.4940756	7.7414363	21.8092019
H	-20.2511022	9.5048289	20.9003398
H	-20.2654927	7.7623085	20.4410664
H	-14.5139066	14.8434986	21.1453857
H	-15.9524138	15.1550770	21.6622558
H	-16.3641830	3.7641301	18.6587929
H	-14.9296919	4.7538234	19.0936436
H	-16.2008481	4.3624560	20.3244088
H	-16.5596941	8.8404373	17.8238034

Model α -2⁻

N	-12.8994443	10.3065461	15.9449881
C	-12.8422992	9.6927639	14.7067885
C	-12.8921749	10.7423885	13.7896878
N	-12.9725774	11.9586364	14.4314075
C	-12.9736157	11.6567995	15.7247331
C	-12.7682332	8.2046350	14.5427531
C	-14.1190300	7.4536750	14.6112320
N	-14.8060327	7.5920416	15.8686054
C	-16.1460853	7.8431180	15.9397578
O	-16.8711234	8.0808952	14.9721996
C	-16.7110760	7.8300350	17.3736580
N	-16.1400169	6.7962280	18.2141722
C	-16.8755999	5.7822839	18.7626007
C	-16.0143640	4.6255130	19.2644660
O	-18.1096283	5.7736262	18.8300346
O	-15.1933181	15.1447630	22.6165029
Zn	-14.7112754	13.3633288	22.9308385
N	-16.0735982	11.8011603	22.9404752
C	-17.4082250	11.8213338	23.0202759
N	-17.9011948	10.5568791	23.0734138
C	-16.8373765	9.6690710	23.0223702
C	-15.7062840	10.4672372	22.9442035
C	-16.9909069	8.1782154	23.0951817

C	-17.0132740	7.6225650	24.5317940
N	-14.1647717	13.5575655	24.9229812
C	-13.8421716	12.7373550	25.9864973
C	-13.3052263	13.5027108	27.0117793
N	-13.3193440	14.8070052	26.5377160
C	-13.8414234	14.8020182	25.2827598
C	-12.7839138	13.1259575	28.3654831
C	-12.6593800	11.6110050	28.5452740
N	-13.2307223	12.3926789	21.8583046
C	-13.5249105	11.7515361	20.7115527
N	-12.4730337	11.0383645	20.2623252
C	-11.4463397	11.2189609	21.1615073
C	-11.9111620	12.0678721	22.1572753
C	-11.1822568	12.5634006	23.3719863
C	-9.9693200	11.7002250	23.7325670
O	-12.6178317	9.1425818	18.5139755
C	-12.7979254	7.9290381	18.8960937
C	-12.3765992	7.5610355	20.3298788
C	-13.0023144	6.2585079	20.8352893
C	-12.5945320	5.8774640	22.2573820
O	-13.2775352	7.0199559	18.1695897
O	-12.0145054	16.5561067	28.3279702
C	-11.5401450	17.6524510	28.6604020
C	-11.1191933	17.9317876	30.1030425
C	-10.1459225	16.8835267	30.6758880

C	-8.7104820	17.0011290	30.1496800
N	-11.3896171	18.6780219	27.7783124
O	-20.4898547	9.6448386	23.3716475
C	-21.4746459	8.9284545	23.1215361
C	-22.4808780	8.5979410	24.2242620
N	-21.7283401	8.4122062	21.8864579
C	-20.9018020	8.6345760	20.7021270
H	-21.5299069	8.9565132	19.8479351
H	-13.6425610	11.1075993	28.4461967
H	-10.2627466	10.6451184	23.9076403
H	-16.0782551	7.8724377	25.0727075
H	-11.9766556	11.1686640	27.7917526
H	-12.8770000	6.6614838	22.9926616
H	-8.6640675	16.8790001	29.0470659
H	-13.9232364	6.3762691	14.3907941
H	-17.1197574	6.5189871	24.5248516
H	-8.2661509	17.9884601	30.3963364
H	-13.0766059	4.9319215	22.5800100
H	-9.4763365	12.0731611	24.6525831
H	-21.9446275	8.0977127	25.0542212
H	-23.3194390	7.9551902	23.8937138
H	-18.0287096	12.7245433	23.0320524
H	-18.9080113	10.2746791	23.1370820
H	-17.9167507	7.8786992	22.5611501
H	-16.1539827	7.7195604	22.5304203
H	-17.8609579	8.0427505	25.1104446
H	-12.2614944	11.3627443	29.5489740
H	-11.8006323	13.6194993	28.5237976
H	-13.4485432	13.5498600	29.1516288
H	-14.0132333	11.6566567	25.9537472
H	-12.9227599	15.6127407	27.0640538
H	-14.0122394	15.6598256	24.6149796
H	-8.0572685	16.2235573	30.5938318
H	-10.1455013	16.9795584	31.7820260
H	-10.5592758	15.8773282	30.4525092
H	-12.0615636	17.9145934	30.6919536
H	-10.6976848	18.9546553	30.2050872
H	-10.9977136	19.5764424	28.0565070
H	-11.6868834	18.5554685	26.8084412
H	-10.8633390	13.6190426	23.2151941
H	-11.8911555	12.5949017	24.2243214
H	-9.2042435	11.7059155	22.9288674
H	-10.4768831	10.7300179	21.0288412

H	-12.4914134	10.2629303	19.4740096
H	-14.4981675	11.7768525	20.2079566
H	-11.4961907	5.7335955	22.3434302
H	-14.1078902	6.3503347	20.7747896
H	-12.7376238	5.4465532	20.1277626
H	-12.6175684	8.4102981	21.0053224
H	-11.2645888	7.4882277	20.3356647
H	-12.8531480	9.8178175	16.8667190
H	-13.0200866	12.3804659	16.5501158
H	-12.8700831	10.6672864	12.6937892
H	-12.0802174	7.7772177	15.3053470
H	-12.3121031	7.9781709	13.5561041
H	-14.8073449	7.8240180	13.8242460
H	-14.2399403	7.4096398	16.7208503
H	-17.8005261	7.6528276	17.3082549
H	-15.1118478	6.7192180	18.2570300
H	-22.8863569	9.5480269	24.6242378
H	-14.6573651	10.1593456	22.8767852
H	-22.5493479	7.8135319	21.7853327
H	-20.1784999	9.4360490	20.9353000
H	-20.3396603	7.7238903	20.4045242
H	-14.7741911	15.4643533	21.7966289
H	-16.3085799	3.7148012	18.7038589
H	-14.9301331	4.7929796	19.1311038
H	-16.2352262	4.4234816	20.3321665
H	-16.5616220	8.8431191	17.8157552

Model β -2'H

C	-16.5474101	45.8869423	27.1096220
C	-16.2563067	44.6059710	27.5512834
N	-17.4434914	43.8995617	27.4249918
C	-18.3853767	44.7317700	26.9197077
N	-17.8712771	45.9500629	26.7131934
C	-14.9576414	43.9656822	27.9204014
C	-14.0881150	43.6052950	26.6631430
C	-14.8954573	42.6846669	25.7436512
N	-14.9733971	41.3893816	26.1717638
C	-15.8280850	40.4435160	25.4960100
C	-17.3118567	40.7109769	25.7154548
N	-18.0801525	40.3200491	24.6666599
C	-19.5110720	40.4839330	24.6657580
H	-19.8945950	40.2907287	25.6881730
Zn	-18.6416242	47.3451523	25.4116409
O	-20.7087871	46.9232956	25.9918205
S	-18.4869524	49.5290616	26.0604705
C	-16.7815221	49.5802554	26.8032052
C	-16.3535300	51.0060380	27.1857050
C	-17.2341337	51.6127494	28.2947913
N	-18.4494797	52.1061042	27.8620913

C	-19.4968300	52.4967190	28.7877220
C	-20.3268241	51.3701738	29.4488978
N	-20.1557960	50.1195322	28.9218970
C	-20.8177650	48.9625140	29.4766230
H	-21.3281741	49.2794261	30.4074881
S	-18.3688294	46.7639546	23.2105890
C	-18.1650390	44.9424269	23.3451885
C	-19.4293610	44.1986560	23.7492410
C	-22.7275480	45.5430110	22.4402840
C	-22.5348577	46.1701172	21.0674724
N	-21.3467486	46.8367140	20.8992006
C	-21.0249620	47.4929680	19.6508800
O	-16.8954156	51.6212994	29.4758919
N	-13.6019936	44.7747480	25.9704523
C	-12.2647454	45.1211249	26.0673946
O	-11.4720000	44.4769375	26.7573130
C	-11.8563090	46.3648040	25.2852440
N	-19.0957236	42.8165357	24.0416531
C	-20.0482883	41.8711416	24.2599982
O	-21.2577441	42.0688102	24.1765693
O	-23.3901253	46.0712356	20.1872750
O	-15.5100435	43.0633753	24.7351384
O	-17.7692971	41.2005253	26.7560461

O	-21.0821213	51.6316354	30.3842036
H	-20.0970744	48.1511162	29.7118887
O	-15.1286107	45.9452893	23.8771005
N	-18.2674113	51.2523541	23.0838546
C	-17.3618660	50.3306300	22.4372960
C	-18.7601754	52.3605409	22.4424791
O	-18.4692286	52.6602191	21.2832758
C	-19.6971170	53.2246000	23.2799590
H	-21.6024384	48.5485274	28.7970753
H	-19.5564763	49.9927470	28.0887366
H	-19.0395119	53.0504293	29.6315277
H	-20.2021485	53.1888159	28.2845916
H	-18.6989281	51.9442624	26.8829653
H	-15.3215180	50.9789994	27.5874518
H	-16.3579555	51.6486313	26.2792637
H	-20.6527020	46.8540309	21.6566233
H	-16.0650262	49.1679969	26.0639476
H	-16.7671727	48.9339965	27.7045171
H	-19.2208681	54.2112386	23.4510051
H	-20.6218466	53.4124768	22.7001849
H	-19.9671330	52.7816085	24.2595012
H	-17.7698366	49.2985707	22.4050884
H	-17.2074726	50.6909255	21.4017930
H	-16.3751630	50.2907020	22.9486924
H	-18.5464388	51.0238825	24.0461193
H	-19.9799444	39.7357648	23.9970575
H	-17.6184744	39.9806988	23.8204612
H	-14.4485377	41.0973172	26.9966182
H	-15.5972049	40.4420883	24.4098558
H	-15.6016033	39.4281442	25.8827521
H	-14.2354151	45.3051432	25.3399491
H	-12.6052518	46.6557155	24.5238668
H	-11.7116389	47.2049054	25.9950263
H	-10.8779702	46.1724016	24.8057625
H	-13.1730226	43.0877409	27.0314725
H	-14.3500989	44.6499649	28.5441497
H	-15.1435426	43.0559156	28.5286555

H	-17.5525958	42.8665454	27.4860092
H	-19.4213985	44.4346301	26.7281413
H	-15.8787168	46.7495345	27.0430922
H	-18.1063096	42.5856082	24.1688326
H	-19.9000999	44.6870944	24.6308217
H	-17.8099296	44.5781260	22.3585650
H	-17.3627945	44.7259064	24.0807081
H	-22.5930921	44.4429623	22.3898430
H	-23.7691078	45.7246166	22.7680714
H	-20.8566096	48.5821813	19.7897723
H	-20.1157083	47.0623023	19.1791691
H	-21.8853339	47.3436570	18.9715694
H	-15.3332266	45.0027723	23.6996072
H	-15.9599269	46.4254313	23.6398868
H	-20.9631676	47.5610525	26.6916104
H	-21.3491925	47.0697142	25.2661454
H	-22.0245853	45.9367014	23.2031475
H	-20.1898919	44.2334848	22.9423787

Model β -2⁺

C	-16.4862570	45.9326961	27.1578116
C	-16.2389580	44.6354258	27.5801932
N	-17.4688571	43.9892241	27.5031413
C	-18.3910038	44.8846417	27.0526199
N	-17.8163874	46.0683439	26.8303848
C	-14.9581283	43.9461997	27.9197412
C	-14.0881150	43.6052950	26.6631430
C	-14.8606914	42.6763328	25.7226714
N	-14.9748984	41.3864654	26.1780995
C	-15.8280850	40.4435160	25.4960100
C	-17.3128493	40.6792375	25.7485531
N	-18.0835992	40.3044644	24.6941127
C	-19.5110720	40.4839330	24.6657580
H	-19.8730180	40.4629681	25.7145197
Zn	-18.9879522	47.2939773	25.5419362
O	-20.5773481	46.3713770	26.0976375
S	-18.5566044	49.5847739	26.0048869
C	-16.8808578	49.6003530	26.8129018
C	-16.3535300	51.0060380	27.1857050
C	-17.1898491	51.7525985	28.2494007
N	-18.4679271	52.0887657	27.8448180
C	-19.4968300	52.4967190	28.7877220
C	-20.3113137	51.3666804	29.4619107
N	-20.1302719	50.1208728	28.9455813
C	-20.8177650	48.9625140	29.4766230
H	-20.2579547	48.4938081	30.3175703
S	-18.2406776	46.7603102	23.3310810

C	-18.1193744	44.9244030	23.4430917
C	-19.4293610	44.1986560	23.7492410
C	-22.7275480	45.5430110	22.4402840
C	-22.5410733	46.1912595	21.0776657
N	-21.3364101	46.8250619	20.8960488
C	-21.0249620	47.4929680	19.6508800
O	-16.7411450	52.0284247	29.3633697
N	-13.6011675	44.7828576	25.9812775
C	-12.2650038	45.1140537	26.0613749
O	-11.4566952	44.4601292	26.7301824
C	-11.8563090	46.3648040	25.2852440
N	-19.1395561	42.8227764	24.1188315
C	-20.0199566	41.7976178	24.0280496
O	-21.1499269	41.8552210	23.5428250
O	-23.4111942	46.1362323	20.2027185
O	-15.3879205	43.0269827	24.6607478
O	-17.7511393	41.1278503	26.8144498
O	-21.0693395	51.6296296	30.4009613
H	-20.9354307	48.2062779	28.6739208
O	-15.1088779	45.9817475	23.9275575
N	-18.2484859	51.2696747	23.0863940
C	-17.3618660	50.3306300	22.4372960
C	-18.7357641	52.3760143	22.4503848
O	-18.4450757	52.6883240	21.2900253
C	-19.6971170	53.2246000	23.2799590
H	-21.8111861	49.2626429	29.8671481
H	-19.5754452	49.9854147	28.0788525
H	-19.0066394	53.0515993	29.6116553
H	-20.2153977	53.1887145	28.3001186

H	-18.7834558	51.6321609	26.9736008
H	-15.3349397	50.9150416	27.6120703
H	-16.2891427	51.6243956	26.2634766
H	-20.6343040	46.8308015	21.6489446
H	-16.1597873	49.1239071	26.1173060
H	-16.9324501	48.9707286	27.7250582
H	-19.3417102	54.2740742	23.2736956
H	-20.6924837	53.2184273	22.7911692
H	-19.8093118	52.8836744	24.3281001
H	-17.7495975	49.2928127	22.4998662
H	-17.2720396	50.6309897	21.3755261
H	-16.3464641	50.3376249	22.8921748
H	-18.5284230	51.0262676	24.0502284
H	-20.0007737	39.6508993	24.1238503
H	-17.6120919	40.0856099	23.8143929
H	-14.5899687	41.1422215	27.0904470
H	-15.6129223	40.4911578	24.4086334
H	-15.5753350	39.4197324	25.8435857
H	-14.2412025	45.3215154	25.3525430
H	-12.6162908	46.6633026	24.5372902
H	-11.7034362	47.1986595	26.0007005
H	-10.8842489	46.1709068	24.7932550
H	-13.1707162	43.0875602	27.0269880
H	-14.3334106	44.5911124	28.5695709
H	-15.1653926	43.0209526	28.4990257
H	-17.6232868	42.9730103	27.5942440
H	-19.4676346	44.7197810	26.8901312
H	-15.7771281	46.7605980	27.0640897
H	-18.2358337	42.6630395	24.5696523
H	-19.9636558	44.7386823	24.5696906
H	-17.6869733	44.5503795	22.4898293

H	-17.3861499	44.6756531	24.2412330
H	-22.5260921	44.4528351	22.3806480
H	-23.7847373	45.6639648	22.7437779
H	-20.7964068	48.5687994	19.8084506
H	-20.1527872	47.0308385	19.1382690
H	-21.9152803	47.3983095	19.0005845
H	-15.3185003	45.0482017	23.7151977
H	-15.9817347	46.4502357	23.7877705
H	-21.3639221	46.5917804	25.5687216
H	-22.0653121	45.9670611	23.2215630
H	-20.1041504	44.1907456	22.8702850

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C	-16.6160351	45.8304543	27.0953922
C	-16.2848961	44.5599740	27.5379506
N	-17.4475646	43.8170332	27.4082815
C	-18.4146000	44.6121531	26.8966882
N	-17.9413524	45.8494080	26.6887790
C	-14.9702605	43.9565690	27.9129079
C	-14.0881150	43.6052950	26.6631430
C	-14.8505345	42.6725900	25.7179577
N	-15.0123359	41.4010647	26.2002763
C	-15.8280850	40.4435160	25.4960100
C	-17.3196567	40.6850977	25.6733260
N	-18.0828269	40.2709824	24.6312109
C	-19.5110720	40.4839330	24.6657580
H	-19.9623263	40.0252035	25.5676517
Zn	-18.5502468	47.2787228	25.3412252
O	-20.7974398	47.1325536	25.6569026
S	-18.4215256	49.4524244	26.0594776
C	-16.7272513	49.5612814	26.8202486
C	-16.3535300	51.0060380	27.1857050
C	-17.2450106	51.5917297	28.2942940
N	-18.4547885	52.0965877	27.8601002
C	-19.4968300	52.4967190	28.7877220
C	-20.3485587	51.3747020	29.4277177
N	-20.1603818	50.1195821	28.9157840
C	-20.8177650	48.9625140	29.4766230
H	-21.4047669	49.3012629	30.3527547
S	-18.2421472	46.7230809	23.1364147
C	-18.1818008	44.8855789	23.1807314
C	-19.4293610	44.1986560	23.7492410
C	-20.6626959	44.3058001	22.8344990
N	-21.5218745	45.3029770	23.1937774
C	-22.7275480	45.5430110	22.4402840
C	-22.5852614	46.3365010	21.1319172

N	-21.3478122	46.8585486	20.9043477
C	-21.0249620	47.4929680	19.6508800
O	-16.9188997	51.5769715	29.4787884
N	-13.6052707	44.7815320	25.9797789
C	-12.2719184	45.1368418	26.0896792
O	-11.4860669	44.5114445	26.8049200
C	-11.8563090	46.3648040	25.2852440
N	-19.1045710	42.7988005	23.9754700
C	-19.9141458	41.9773989	24.7012131
O	-20.8954307	42.3714668	25.3284198
O	-20.8223033	43.5626254	21.8687221
O	-23.5521944	46.4563009	20.3807769
O	-15.3410717	43.0166329	24.6353669
O	-17.8054630	41.1957894	26.6910904
O	-21.1308328	51.6424099	30.3384714
H	-20.0879381	48.1913809	29.8032909
O	-15.0690753	45.8738062	23.8307820
N	-18.2509846	51.2540347	23.1085400
C	-17.3618660	50.3306300	22.4372960
C	-18.7609644	52.3450400	22.4567434
O	-18.4857357	52.6040572	21.2843026
C	-19.6971170	53.2246000	23.2799590
H	-21.5281240	48.4888693	28.7578640
H	-19.5309880	49.9848722	28.1082016
H	-19.0286092	53.0260308	29.6411662
H	-20.1868923	53.2111466	28.2952371
H	-18.6955772	51.9662004	26.8747595
H	-15.3184355	51.0193444	27.5808332
H	-16.3842764	51.6370885	26.2718732
H	-20.6035153	46.7046258	21.5942301
H	-15.9891312	49.1631746	26.0951765
H	-16.7030889	48.9299015	27.7317085
H	-19.2789635	54.2499737	23.3254194
H	-20.6706395	53.2995191	22.7558015
H	-19.8723033	52.8614282	24.3127030

H	-17.2779366	49.4070497	23.0394876
H	-17.7499517	50.0757274	21.4304032
H	-16.3437368	50.7563273	22.2935665
H	-18.4988663	51.0310157	24.0801678
H	-19.9711926	40.0156879	23.7731069
H	-17.6413901	39.8376793	23.8183544
H	-14.5843016	41.1390049	27.0884847
H	-15.5663877	40.4653085	24.4175224
H	-15.5915298	39.4271172	25.8750943
H	-14.2275533	45.2854451	25.3154982
H	-12.6010509	46.6413913	24.5145083
H	-11.7110460	47.2182850	25.9786182
H	-10.8765735	46.1590116	24.8139888
H	-13.1709724	43.0991800	27.0449025
H	-14.3802822	44.6617333	28.5300110
H	-15.1356502	43.0526161	28.5355656
H	-17.5295671	42.7777822	27.4494688
H	-19.4274294	44.2474833	26.6846534
H	-15.9752282	46.7146915	27.0335068
H	-18.3421768	42.3926750	23.4304437
H	-19.6790719	44.6563741	24.7254361
H	-18.0195255	44.5439851	22.1358912
H	-17.3114102	44.5589612	23.7850123
H	-21.3355679	45.8412460	24.0458969
H	-23.1760591	44.5725831	22.1434481
H	-23.4707250	46.0631995	23.0774569
H	-20.6373638	48.5233418	19.7969064

H	-20.2646508	46.9150282	19.0824112
H	-21.9553218	47.5423828	19.0537859
H	-15.2205535	44.9220992	23.6453065
H	-15.9132254	46.3219303	23.5723721
H	-21.0185857	47.0787892	26.6101911
H	-21.1293620	48.0146791	25.3884389

Model β -2⁻

C	-16.6079786	45.8831144	27.0976311
C	-16.3147713	44.5873615	27.4967862
N	-17.5166442	43.8978810	27.3906549
C	-18.4645396	44.7634793	26.9436806
N	-17.9402797	45.9764615	26.7513625
C	-15.0179898	43.9442561	27.8766685
C	-14.0881150	43.6052950	26.6631430
C	-14.7704436	42.6441425	25.6830729
N	-15.0231479	41.3992276	26.2137114
C	-15.8280850	40.4435160	25.4960100
C	-17.3224261	40.6472690	25.7016692
N	-18.0867540	40.2313939	24.6599060
C	-19.5110720	40.4839330	24.6657580
H	-19.9902360	39.9920887	25.5347994
Zn	-18.9101295	47.2839205	25.3673138
O	-20.6940540	46.5474646	25.4381526
S	-18.5276488	49.5339420	26.0186930
C	-16.8450219	49.5871774	26.8117902
C	-16.3535300	51.0060380	27.1857050
C	-17.2000307	51.7282119	28.2549147
N	-18.4715084	52.0838387	27.8433009
C	-19.4968300	52.4967190	28.7877220
C	-20.3090389	51.3680396	29.4663649
N	-20.1385349	50.1205436	28.9403565
C	-20.8177650	48.9625140	29.4766230
H	-21.3967416	49.2890473	30.3622989
S	-18.0911797	46.7058556	23.2218425
C	-18.1354800	44.8613753	23.2463602
C	-19.4293610	44.1986560	23.7492410
C	-20.6412313	44.3573923	22.8046486
N	-21.5106987	45.3257508	23.1889038
C	-22.7275480	45.5430110	22.4402840
C	-22.5770791	46.2774442	21.0975791
N	-21.3633806	46.8649065	20.9020993
C	-21.0249620	47.4929680	19.6508800
O	-16.7680616	51.9730805	29.3820498
N	-13.6002756	44.7880548	25.9917983

C	-12.2699465	45.1333684	26.0910938
O	-11.4692259	44.5077117	26.7955465
C	-11.8563090	46.3648040	25.2852440
N	-19.1646711	42.7743470	23.9183054
C	-19.8615006	41.9908827	24.7881468
O	-20.6653510	42.3993197	25.6232044
O	-20.7738770	43.6236736	21.8138412
O	-23.5138151	46.3188519	20.2949088
O	-15.0808779	42.9290563	24.5240817
O	-17.7912952	41.1223154	26.7427332
O	-21.0507760	51.6329982	30.4168154
H	-20.0974546	48.1727414	29.7796468
O	-15.0200806	45.9084753	23.8659693
N	-18.2474827	51.2633290	23.1001128
C	-17.3618660	50.3306300	22.4372960
C	-18.7128530	52.3808856	22.4707785
O	-18.3851220	52.6935924	21.3211822
C	-19.6971170	53.2246000	23.2799590
H	-21.5182846	48.5180487	28.7358358
H	-19.5834088	49.9857655	28.0732813
H	-19.0050325	53.0525030	29.6097788
H	-20.2164010	53.1859750	28.2982464
H	-18.7830185	51.6588141	26.9567331
H	-15.3304759	50.9380268	27.6052856
H	-16.3105201	51.6261529	26.2636964
H	-20.6434623	46.7610758	21.6288346
H	-16.1166816	49.1357405	26.1074463
H	-16.8697765	48.9538873	27.7224811
H	-19.3678438	54.2819346	23.2519417
H	-20.6916137	53.1819422	22.7907658
H	-19.8051151	52.9029327	24.3346707
H	-17.3835439	49.3650618	22.9759206
H	-17.6828878	50.1723099	21.3881177
H	-16.3104739	50.6967973	22.4051917
H	-18.5357111	51.0069802	24.0573048
H	-19.9537257	40.0670596	23.7388642
H	-17.6236744	39.9407702	23.7977963
H	-14.8482561	41.2403362	27.2060604
H	-15.5745569	40.5323767	24.4200518

H	-15.5604088	39.4157899	25.8239392
H	-14.2233247	45.2900152	25.3146824
H	-12.6071542	46.6363588	24.5181455
H	-11.7165452	47.2199514	25.9779665
H	-10.8762906	46.1609889	24.8130892
H	-13.1762128	43.1140297	27.0759684
H	-14.4375367	44.6222771	28.5335171
H	-15.2154681	43.0301145	28.4771840
H	-17.6418397	42.8704045	27.4399217
H	-19.5053855	44.4781000	26.7461058
H	-15.9305273	46.7395231	27.0301749
H	-18.7446378	42.3179833	23.1044440
H	-19.7149554	44.6211945	24.7295590
H	-17.9391236	44.5225828	22.2044544
H	-17.3061613	44.4795299	23.8778526
H	-21.3080525	45.8591910	24.0955678
H	-23.2140039	44.5767478	22.1884035
H	-23.4376495	46.1240267	23.0638905
H	-20.7321837	48.5565250	19.7862350
H	-20.1861227	46.9698095	19.1421290
H	-21.9233694	47.4471451	19.0052912
H	-15.1474901	44.9768841	23.5900424

H	-15.9137147	46.3337261	23.7009741
H	-21.1645158	46.5980440	26.2885844

Model α -3H

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C	-16.0143595	4.6255117	19.2644606
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H -15.1139851 6.7613666 18.3233212
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H -15.6837313 15.2298324 21.7777763
H -16.7907906 13.2415953 20.1423561
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Model β -4H

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H	-23.3655225	48.9998367	33.2274444
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H	-21.8563243	48.9627164	29.0682182
H	-19.7019863	47.7663611	28.0469770
H	-19.2601997	47.4688872	29.7626078
H	-19.4599935	49.9101972	28.1168991
H	-19.0543596	52.8440318	29.7481450
H	-20.1055753	53.3160083	28.3573228
H	-18.6984552	51.8398453	26.9250963
H	-15.3213420	50.9643398	27.5865980
H	-16.3523892	51.6691113	26.2935466
H	-20.6521750	46.7742972	21.6317255
H	-16.0507692	49.2087331	26.0091385
H	-16.7588721	48.9112169	27.6299390
H	-19.3540134	54.2775054	23.3073551
H	-20.6680804	53.2129575	22.7443926
H	-19.8624829	52.8641427	24.3145044
H	-17.2240281	49.4473240	23.0878579
H	-17.7687316	49.9927988	21.4614684
H	-16.3709742	50.7936017	22.2348137
H	-18.5831413	50.9750309	24.0363355
H	-19.9902697	38.6191559	25.6665253
H	-19.9626767	40.0402613	26.7643497
H	-19.8846975	40.1349846	23.6803734
H	-17.6312670	39.8608478	23.8584798
H	-14.6939180	41.1641017	27.1559028
H	-15.5869315	40.5066418	24.4151339

H	-15.5910924	39.4129114	25.8367690	H	-21.2741052	45.8490115	24.0336534
H	-14.2151272	45.2677636	25.2825415	H	-23.3060016	44.6108295	22.2739619
H	-12.5869452	46.6134719	24.4913209	H	-23.3218611	46.2412547	23.0746253
H	-11.7617772	47.2289630	25.9745187	H	-20.7699014	48.5618333	19.8185094
H	-10.8560324	46.1815566	24.8491313	H	-20.1664999	47.0152920	19.1281738
H	-13.1779459	43.1044062	27.0682201	H	-21.9176269	47.4338153	18.9980352
H	-14.3874067	44.6542102	28.5258420	H	-15.1621406	44.9327996	23.5763123
H	-15.2168936	43.0842149	28.4918136	H	-15.8882055	46.3107827	23.6166019
H	-17.6137857	42.9641406	27.5151452	H	-20.9123481	46.4813320	26.2671047
H	-19.4577724	44.5718037	26.7498087	H	-22.3226496	47.5143009	24.9886522
H	-15.8374175	46.7603511	26.8654566	H	-23.2312338	46.6228770	30.0762935
H	-18.9455094	51.2112487	31.7932118	H	-23.6982963	47.1860605	25.5994448
H	-17.7643626	51.8611847	31.0684205	H	-23.1205367	45.9789633	27.3186799
H	-18.3511550	42.3848371	23.4967764	H	-24.2012979	46.7891182	28.0075191
H	-19.6892905	44.7131662	24.6950622	H	-24.7588435	46.7839692	30.3741416
H	-18.0106909	44.4585492	22.1267284	H	-23.1693186	39.7804892	24.3862778
H	-17.2994160	44.4638813	23.7740914				

Cartesian coordinates for models **5** could be obtained upon request to the authors.