Tuning the hydrogen bonding strength in 2,6-bis(cycloalkylcarbonylamino)pyridine assemblies by variable flexibility. Association constants measured by hydrogen bonded vs. non-hydrogen bonded protons

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Tuning the hydrogen bonding strength in 2,6-bis(cycloalkylcarbonylamino)pyridine assemblies by variable flexibility. Association constants measured by hydrogen bonded vs. non-hydrogen bonded protons

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Abstract

The association of 2,6-bis(cycloalkylcarbonylamino)pyridines with rigid and non-rigid counterparts was studied in chloroform solution by ^1H NMR and computational methods. The angles within the cycloalkyl ring and rotation of these substituents determine the strength of the association via triple hydrogen-bonding. The dimerization and methyl-methyl repulsion have been addressed as mechanisms restricting heterocomplexation of diacetamide. The association constants obtained by the shift changes of hydrogen-bonded protons are in agreement with those of methine protons. This “dual shift” method was proposed as an additional verification of association constants obtained generally by amino protons.

Keywords

Hydrogen bonding, association, steric effect, multi-probing

1. Introduction

The non-covalent assemblies of small molecules stabilized by weak and directional interactions such as hydrogen bonds [1-3] are under regular studies, so the number of publications on supramolecular chemistry is increasing fast [4]. Various methods have been developed for understanding the stability of associates based on molecular properties [5]. One of the most frequently used methods is the ^1H NMR titration. This is due to the very high sensitivity of chemical shifts of hydrogen-bonded nuclei (usually protons of OH and/or NH groups) to concentration, water content [6] and quite often to many coexisting hydrogen-bonding processes [7-9]. Thus monitoring several nuclei is the method of choice to improve the reliability of obtained results. Moreover, this is especially useful if others overlap NH or OH signals or if the fast proton transfer in NMR time scale restricts direct observation of NH/OH signal. The experimentally obtained association constants and geometry of associates are compared to the results from theoretical calculations [10-13].

Triple hydrogen-bonded associates are met in many structures as in DNA [14,15], amides [16,17], artificial sensors [18-22], materials [23], non-covalent

polymers [4,24-28] and in recently observed associates of orotic acid [29,30]. Triple hydrogen-bonded assemblies carrying 2,6-diaminopyridine DAD-hydrogen bonding moiety were studied by some groups with the use of various methods [4,6,31-47] and also by us [48,49]. We noticed that the use of NH and CH proton shifts as probes in NMR titration gave the similar results of K_{assoc} in case of compounds containing *i*-Pr group [48]. This finding prompted us to enlarge the number of compounds carrying the CH methine proton. We synthesized symmetrical 2,6-bis(cycloalkylcarbonylamino)-pyridines (cycloalkyl = -propyl, -butyl, -pentyl, and -hexyl) and studied their association with some ADA-hydrogen bonding motifs. The goal of this paper is (a) to test if the monitoring of several nuclei in the single titration experiment is useful for determination of association constants, (b) to tune the association of cycloalkylcarbonyl derivatives of 2,6-diaminopyridines with dipyridin-2-ylamine (**5**), 2-acetylaminopyrimidine (**6**), diacetamide (**7**), 2*H*-pyrido[3,2-*b*]-1,4-oxazin-3(4*H*)-one (**8**), and 4,4-dimethylpiperidine-2,6-dione (**9**) (Figure 1), (c) to find out if the size of the rotational cone determined by the β - α - β' angle in cycloalkyl group (Figure 2) might be a parameter crucial for the steric hindrance in non-covalent assemblies.

Figure 1. Formulas of components of the complexes studied and atom labelling

The cycloalkyl rotation about C8/C11- α bonds form cones of different radius depending on the β - α - β' angle. Both, the overall size of the cycloalkyl and mentioned cone should influence the steric hindrance (Scheme 1).

Scheme 1. Rotamerism in 2,6-bis(cycloalkylcarbonylamino)pyridine associates and the steric effect on intermolecular distances

Previously [48] we confirmed results from other group [50] reporting that the 2,6-bis(acylamino)pyridine do not dimerize. Since the cycloalkyl moieties are larger than methyl, it is reasonable to assume that compounds studied here behave similarly (Scheme 2) and do not form quadruply hydrogen-bonded dimers.

Scheme 2. Dimerization of 2,6-bis(cycloalkylcarbonylamino)pyridines

However, the related pyrimidines can behave differently from that of pyridines. The *conditio sine qua non* allowing the formation dimeric structure is N3 in heterocyclic ring (Scheme 3) [51]. This allows free rotation of alkylcarbonyl moiety about N-C bond [51,52].

Scheme 3. Dimerization of 2,4-bis(alkylcarbonylamino)pyrimidine

2. Experimental

2.1 Instrumentation

The compounds **1-4** and **6** were synthesized as previously described for similar derivatives [48,53]. Liquid state NMR acquisition and processing parameters are the same as those in our other publications [54]. The IR spectra were recorded for solid samples on a Bruker Alpha-P equipment. The melting points were determined with the use of Buchi melting point apparatus (K-565) with the 2°C/min. gradient. Remaining substances (**5**, **7-9**) were commercially available from Aldrich and were used after drying for 20 days in a desiccator.

2.2 Materials

The data below collects the physicochemical properties of compounds obtained for this study.

2.2.1 2,6-bis(cyclopropylcarbonylamino)pyridine (**1**) (R=-(CH₂)₂, n=0) δ [ppm]:¹H

NMR (CDCl₃) δ: 7.99 (bs, 2H, H7/H10), 7.84 (d, ³J_{H,H}=7.8Hz, 2H, H3/H5), 7.66 (t, ³J_{H,H}=7.8Hz, 1H, H4), 1.53 (tt, ³J_{H,H}=7.9Hz, ³J_{H,H}=4.2Hz, 2H, α-H), 1.11 (m, 4H, cycloalkyl), 0.92 (m, 4H, cycloalkyl), ¹³C NMR 172.2, 149.5, 140.8, 109.3, 15.8, 8.4, ¹⁵N NMR -240.1, mp 171-173 °C (lit. 171-173°C [55]), IR (cm⁻¹) 1658.2 (amide I band), 1499.9 (amide II band).

2.2.2 2,6-bis(cyclobutylcarbonylamino)pyridine (**2**) ($R=-(CH_2)_3-$, $n=1$) 1H NMR ($CDCl_3$) δ [ppm]: 7.91 (d, $^3J_{H,H}=8Hz$, 2H, H3/H5), 7.68 (t, $^3J_{H,H}=8Hz$, 1H, H4), 7.43 (bs, 2H, H7/H10), 3.15 (quintet, $^3J_{H,H}=8.3Hz$, 2H, α -H), 2.48-1.88 (four multiplets, 12H, cycloalkyl), ^{13}C NMR 173.3, 149.5, 140.8, 109.3, 40.9, 25.2, 18.0, mp 147.6-148.7 $^{\circ}C$, IR (cm^{-1}) 1679.0 (amide I band), 1503.3 (amide II band), elemental analysis: calcd: C, 65.91; H, 7.01; N, 15.37; found: C, 65.87; H, 7.03; N, 15.34.

2.2.3 2,6-bis(cyclopentanecarbonylamino)pyridine (**3**) ($R=-(CH_2)_4-$, $n=2$) 1H NMR ($CDCl_3$) δ [ppm]: 7.89 (d, $^3J_{H,H}=8Hz$, 2H, H3/H5), 7.69 (t, $^3J_{H,H}=8Hz$, 1H, H4), 2.69 (tt, $^3J_{H,H}=8Hz$, 2H, α -H), 7.60 (bs, 2H, H7/H10), 1.98-1.59 (3 multiplets, 16H, cycloalkyl), ^{13}C NMR 174.6, 149.6, 140.7, 109.2, 46.9, 30.3, 25.9, mp 143.2-145.0 $^{\circ}C$, IR (cm^{-1}) 1663.0 (amide I band), 1506.9 (amide II band), elemental analysis: calcd: C, 67.76; H, 7.69; N, 13.94; found: C, 67.72; H, 7.72; N, 13.90.

2.2.4 2,6-bis(cyclohexylcarbonylamino)pyridine (**4**) ($R=-(CH_2)_5-$, $n=3$) 1H NMR ($CDCl_3$) δ [ppm]: 7.90 (d, $^3J_{H,H}=8Hz$, 2H, H3/H5), 7.67 (t, $^3J_{H,H}=8Hz$, 1H, H4), 7.57 (bs, 2H, H7/H10), 2.23 (tt, $^3J_{H,H}=3.5Hz$, 2H, α -H), 1.97-1.23 (multiplets, 20H, cycloalkyl), ^{13}C NMR 174.3, 149.6, 140.8, 109.3, 46.5, 29.5, 25.7, 25.6, mp 77.2-78.5 $^{\circ}C$, IR (cm^{-1}) 1672.1 (amide I band), 1523.1 (amide II band), elemental analysis: calcd: C, 69.27; H, 8.26; N, 12.76; found: C, 69.31; H, 8.23; N, 12.71.

2.2.5 2-acetylaminopyrimidine (**6**) 1H NMR ($CDCl_3$) δ [ppm]: 9.52 (bs, 1H, H1'), 8.63 (d, $^3J_{H,H}=5Hz$, 2H, H4''/H6''), 6.99 (t, $^3J_{H,H}=5Hz$, 1H, H5''), 2.51 (s, 3H, CH_3),

^{13}C NMR 171.4, 158.3, 157.8, 116.0, 25.2, ^{15}N NMR -231.5, -119.7, mp 146.3-148.0 °C (lit. 144-145 °C [56]) IR (cm^{-1}) 1669.5 (amide I band), 1516.8 (amide II band)

2.3 ^1H NMR titrations

The ^1H NMR titrations were performed by adding solid aliquots of **5-9** to the solution containing **1-4** at constant (0.0445 mol/dm^3) concentration. The 1:[titrant] ratios were as follows: 1:1, 1:2, 1:3, 1:5, 1:10, 1:20, 1:30 and in some cases 1:40 (see Supporting Information). Due to the limited solubility of **7** and **8**, titration with these compounds were ran starting from 1:0.1 up to 1:3 or 1:4 ratio with the same relative steps. In all cases the titration was finished when the next portion of the titrant did not made larger change to the H7/H10 chemical shift than ca. 0.1 ppm.

2.4 Calculations

The calculations were carried out with Gaussian 03 [57]. For all monomers and complexes the optimizations were performed at M05/6-311+G(d,p) level using PCM model of solvation (chloroform) with M05 functionals developed by Truhlar *et al.*. These are efficient in describing non-covalent interactions [58]. The energy minimum was confirmed by the frequency calculation (only positive frequencies were obtained). To compare the experimental chemical shifts with those obtained by theoretical methods the GIAO-based [59,60] calculations were carried out at the same level of theory. The calculated chemical shifts (with respect to TMS [61]) were obtained by subtraction of the magnetic shielding tensor values of TMS protons and protons in the complex.

3. Results and Discussion

3.1 Heterocomplexation

Table 1 shows the K_{assoc} values obtained based on H7/H10 (NH) and H α (CH) chemical shift changes during titrations. The H7/H10 chemical shift did not change more than 0.1 ppm during titration of **1** with **7**. Moreover, the chemical shift of H1' during titration vs. the H1' chemical shift in dilution experiment of **7** do not differ much. The difference of $\Delta\text{H1}' = \text{ca. } 0.16$ ppm is observed for 10:1 **1:7** ratio (see chart in SI file). This suggests that **7** prefer to dimerize rather than to form a triply-hydrogen-bonded heterocomplex.

--Table 1 here--

In all complexes, the association constants are low. However, the larger the cycloalkyl ring is, the lower the association constant is. Also, the compounds **5** – **7** with larger degree of freedom (rotation about N1'–C2' or/and N1'–C2'' bonds) associate poorly with **1-4**. It is worth to mention that the association of **5** with **1** is comparable to that with 2,6-bis(pivaloylamino)pyridine or 2-pivaloylamino-6-*iso*-butyroamino-pyridine [48]. The use of both NH and CH protons as probes in NMR titration affords, except K_{assoc} , also other information. Table 1 shows that in the case of **1-4+5**, the K_{assoc} obtained by H α proton are higher than those by H7/H10 proton suggesting that the aromatic ring current of pyridine influences the H α chemical shift significantly yielding deshielding and thus higher K_{assoc} values. In the case of other complexes, the H α -based K_{assoc} values are always lower than H7/H10-based. The extrapolated values of H7/H10 chemical shift in the complex (**1-4** molecules are fully bound) are the highest for complexes of **1-4** with **5** (Table 2), while the K_{assoc} for **1-4+5** are lower than, for example, that with **8** or **9**. On the other hand, the K_{assoc} of **1-**

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3 **4+5** are comparable to **1-4+6**. That suggests the stronger influence of ring current on
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6 H7/H10 chemical shift in complexes with **5** than with **6**.
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10 experimental data (Table 2). The experimental values were obtained from the titration
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12 data when the shifts do not change any more upon additions (see Experimental)
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14 assuming that all **1-4** are associated. Moreover, it is worth to remember that in the
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16 solution the complex–monomer equilibrium is fast in NMR timescale giving the
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18 averaged signal. Thus, the extrapolated values in Table 2 are only estimates.
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29 -- Table 2 here --
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38 The comparison of the calculated and extrapolated chemical shifts is, in
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40 general, in agreement within ± 1.4 ppm for H7/H10 (sensitive NH protons) and 0.5 ppm
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42 for H α (CH protons).
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50 3.2 Dimerization

51 In studied mixtures the self-association may be a competitive process. Thus,
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53 the dimerization constants were determined for **6**, **7** and **8**. Table 3 shows the
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55 dimerization constants for **5-9**.
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-- Table 3--

54 The data collected in Table 3 shows that due to the methyl-methyl interactions
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56 in **7** this compound favours dimerization rather than triple hydrogen-bonding with **1-4**.
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58 Although compound **8** has relatively high dimerization constant (forming doubly
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60 hydrogen-bonded dimer) it still forms triply hydrogen-bonded heterocomplexes with

1-4. However, the dilution experiment is not able to answer the question which dimer of **8** is more stable (Scheme 4). The calculations performed now suggest that **D3** dimer is the most stable. This is necessary to keep in mind that the relative difference between energies of individual dimers is less than 8 kJ/mol. Thus all presented dimers of **8** can coexist in solution. All dimers of **8** are stabilized by two hydrogen bonds. Also, four repulsive secondary interactions [39] are present in each of them. The reason why **D3** is the most stable might be the weak interaction of *ortho*-CH proton with C=O group of the counterpart. This type of interaction is present in associates of pyridine and carboxylic acids [62]. The energies given in Scheme 4 are corrected for the zero point energy and basis set superposition error.

Scheme 4. Calculated interaction energies [kJ/mol] of 2H-pyrido[3,2-b]-1,4-oxazin-3(4H)-one (**8**)

2-Acetylaminopyrimidine (**6**) should be able to form similar dimers as 2*H*-pyrido[3,2-*b*]-1,4-oxazin-3(4*H*)-one (**8**) but the rotation around single bonds in **6** restricts its dimerization. Moreover, the rigid structure of **8** and explains why it dimerizes more readily than **6**. Also, the electron donating properties of sp^3 oxygen atom add the basicity of heterocyclic nitrogen atom yielding stronger hydrogen bonding than in **6**. Diacetamide is also able to form doubly-hydrogen-bonded dimers in the solid state [63], similar to that of 2-[1*H*]pyridone, which, in turn, is considered as the most stable doubly-hydrogen-bonded dimer known [64].

The optimized geometry allowed us to study the structural effects on properties of complexes. Table 4 shows the chosen geometrical data for optimized complexes of **1** with **5-9**. The Cartesian coordinates of all complexes and monomers can be found in SI file.

-- Table 4 here --

The Figure 2 shows structures of optimized complexes. It is seen that the heterocyclic ring in **5** and **6** needs more space to bind effectively with **1**. The molecules in **1+7** are almost coplanar.

Figure 2. Optimized structures for complexes of **1+5-7**

The Figure 3 shows the association constants determined experimentally as a function of $\beta-\alpha-\beta'$ angle optimized with computational methods. It is worth to point out here that the mentioned angle influences the cone volume obtained by rotation of the cycloalkyl group. Also the conformational flexibility of the cycloalkyl (especially cyclohexyl) group contributes to steric hindrance.

Figure 3. The $K_{\text{assoc}}=f(\beta-\alpha-\beta'$ angle) for **1-4** complexes with **9**

4. Conclusions

The use of changes of chemical shifts of several protons obtained by NMR titrations is helpful in estimation of association constants for hydrogen bonded assemblies even when the proton-probe is not involved in hydrogen bonding. The restricted rotation around a single bond in the assembly joined with an anisotropic effect of aromatic ring or polar groups may influence association constants. In spite of the existence of methine group in the closest neighbourhood of hydrogen-bonded atoms in 2,6-bis(cycloalkylcarbonylamino)pyridines, the overall size of cycloalkyl and the $\beta-\alpha-\beta'$ angle is the main driving force that hinder association. The major reason for steric effect in this series comes, most probably, from variable volume of the cone obtained by rotation of cycloalkyl around CO–cycloalkyl bond. Another may be the conformational flexibility of cycloalkyls. The chemical shifts obtained by extrapolation of titration data are in agreement with calculated values. For the purpose

of the current research only the pyridine derivatives were included, although studies with pyrimidines is under progress.

Supporting information available

The supporting information file contains ^1H , ^{13}C and ^{15}N NMR spectra, titration curves based on H7/H10 (NH) and H α (CH) protons, dilution experiments results and Cartesian coordinates of optimized structures.

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Table 1. K_{assoc}^a determined for complexes of **1-4** with **5, 6, 8** and **9**^b.

Complex	K_{assoc}	Complex	K_{assoc}	Complex	K_{assoc}	Complex	K_{assoc}
1+5	14, 24	1+6	15, 10	1+8	30, 27	1+9	70, 60
2+5	5, 10	2+6	6, 5	2+8	24, 20	2+9	30, 27
3+5	6, 8	3+6	6, 4	3+8	29, 23	3+9	27, 25
4+5	6, 7	4+6	5, 3 ^c	4+8	24, 22	4+9	13, ^d

a – values in bold refer to the K_{assoc} found by $H\alpha$ (CH) proton chemical shift change,

b – since **1** does not form a complex with **7** other complexes with **7** were not studied,

c – due to the low quality of the fit the value is uncertain, d – not determined due to signals overlap

Table 2. Calculated and extrapolated (in bold) chemical shifts of H7/H10 (first row) and H α (second row) protons in the complexes studied.

Complex	shift	Complex	shift	Complex	shift	Complex	shift
1+5	11.5, 11.3	1+6	10.8, 10.30	1+8	10.6, 10.0	1+9	10.2, 10.1
	2.1, 1.8		2.0, 1.8		2.1, 1.8		2.5, 2.0
2+5	11.2, 10.2	2+6	10.2, 9.3	2+8	9.9, 9.3	2+9	9.6, 9.5
	3.3, 3.2		3.0, 3.3		3.2, 3.3		3.5, 3.4
3+5	11.2, 10.3	3+6	10.5, 9.7	3+8	10.8, 9.3	3+9	9.7, 9.7
	2.9, 2.8		2.6, 2.9		3.2, 2.8		3.1, 3.0
4+5	11.1, 10.3	4+6	10.1, 9.5	4+8	9.9, 9.2	4+9	9.5, 9.5
	2.7, 2.3		2.8, ^a		2.9, 2.4		2.5, ^a

a – value missing due to signal overlap

Table 3. The dimerization constants (K_{dim}) for compounds **5–9**

Compound	K_{dim}	Compound	K_{dim}
5 ^a	1.8	8	45.0
6	8.0	9 ^a	2.3
7	18.0		

a – from ref. ⁴⁸

Table 4. The geometry (distance [Å], angles [°] and dihedrals [°]) of optimized complexes of **1** with **5-9**

Distance, Angle, Dihedral angle	Complex				
	1+5^a	1+6	1+7^b	1+8	1+9
N1...H1'	2.112	2.198	2.298	2.038	2.129
H7...N3'/O3'	2.076	2.118	1.973	2.160	2.013
H10...N3''/O3''	2.076	1.945 ^c	1.973	2.016 ^c	2.013
H α -N3'/O3'	2.731	2.791	2.360	2.687	2.348
H α -N3''/O3''	2.731	2.425 ^d	2.360	2.393 ^d	2.348
N7H7N3''/O3''	170.0	163.8	169.5	167.5	169.1
N10H10N3'/O3'	170.0	172.5 ^e	169.5	170.4 ^e	169.1
C2N10N3'(or O3')C2'	49.6	43.9	25.4	35.3	17.3
C6N7N3'' (or O3'') C2''	49.6	48.3	25.4	37.7	17.3

a – two heterocyclic rings in **5** are twisted by 41.1° (C7'C2'C2''C7'' dihedral), b – the methyl-methyl repulsion is observed, *i.e.* the C2'-C2'' distance is equal to 2.579 Å, while distance between methyl carbon atoms is equal to 3.068 Å. The C2'N1'C2'' angle is equal to 136.1°, c – the NH...O hydrogen bond, d – H α -O3'' distance, e – N10H10O3' angle.

Scheme 1. Rotamerism in 2,6-bis(cycloalkylcarbonylamino)pyridine associates and the steric effect on intermolecular distances

Scheme 2. Dimerization of 2,6-bis(cycloalkylcarbonylamino)pyridines

Scheme 3. Dimerization of 2,4-bis(alkylcarbonylamino)pyrimidine

Scheme 4. Calculated dimerization energies [kJ/mol] of 2*H*-pyrido[3,2-*b*]-1,4-oxazin-3(4*H*)-one (**8**)

Figure 1. Formulas of components of the complexes studied and atom labelling

Figure 2. Optimized structures for complexes of **1+5-7**

Figure 3. The $K_{\text{assoc}}=f(\beta-\alpha-\beta'$ angle) for **1-4** complexes with **9**

Graphical Abstract

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Graphical Abstract

Tuning the hydrogen bonding strength in 2,6-bis(cycloalkylcarbonylamino)pyridine assemblies by variable flexibility. Association constants measured by hydrogen bonded vs. non-hydrogen bonded protons

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Supporting Information

¹ H, ¹³ C and ¹⁵ N NMR spectra	S2
¹ H titration curves (H7/H10 as a probe)	S13
¹ H titration curves (Hα as a probe)	S22
¹ H dilution experiment results	S30
Cartesian coordinates of compound 1-4 and complexes	S32

¹H NMR spectrum of **1** -CH(CH₂)₂ proton signal in **1**

^{13}C NMR spectrum of **1** ^1H , ^{15}N HMBC NMR spectrum of **1**

^{13}C NMR spectrum of **2**

¹H NMR spectrum of 3

¹³C NMR spectrum of **3**

¹H NMR spectrum of **4**

^{13}C NMR spectrum of 4

¹H NMR spectrum of **6**

^1H titration curves (probe H7/H10)

Titration of **1** with the use of **6** Titration of **2** with the use of **6**

Titration of **3** with the use of **6**

Titration of **4** with the use of **6**

Titration of 1 with the use of 7

Comparison of H1' chemical shift coming from dilution experiment of 7 and its use in titration of 1

Titration of **3** with the use of **8** Titration of **4** with the use of **8**

¹H titration curves (probe H α)

Titration of **1** with the use of **5**

Titration of **2** with the use of **5**

Titration of 3 with the use of 6

Titration of 4 with the use of 6

Titration of 1 with the use of 8

Titration of 2 with the use of 8

Titration of 3 with the use of 8

Titration of 4 with the use of 8

Titration of **3** with the use of **9**

¹H dilution experiment results

Dilution curve ($\delta(\text{NH})=f([\mathbf{6}])$) for compound **6**

Dilution curve ($\delta(\text{NH})=f([\mathbf{7}])$) for compound **7**

Dilution curve ($\delta(\text{NH})=f([\mathbf{8}])$) for compound **8**

Cartesian coordinates of 1-4 and complexes

1

N	-0.06169	0.00019	-0.03183
C	0.01791	-0.10103	1.29387
C	1.22931	-0.10375	1.98813
C	2.38441	0.00583	1.22762
C	2.33206	0.11263	-0.15458
C	1.06326	0.10419	-0.73734
N	-1.23414	-0.20336	1.90773
C	-1.55443	-0.32165	3.24161
O	-0.72416	-0.35592	4.13252
N	0.83522	0.20291	-2.11327
C	1.73438	0.32366	-3.149
O	2.9417	0.36375	-2.99074
C	-3.01826	-0.4043	3.49329
C	-3.54636	0.21703	4.7666
C	-3.48285	-1.26142	4.6491
C	1.08857	0.40098	-4.48688
C	1.82002	-0.22149	-5.65475
C	1.75683	1.2571	-5.53887
H	1.24695	-0.18778	3.06313
H	3.34872	0.00804	1.72412
H	3.21702	0.19878	-0.76485
H	-1.99425	-0.18394	1.24612
H	-0.14477	0.179	-2.34761
H	-3.66928	-0.36353	2.6284
H	-4.5101	0.70613	4.70135
H	-2.81059	0.69922	5.39814
H	-4.40188	-1.81434	4.50095
H	-2.70448	-1.77273	5.2017
H	0.00652	0.35675	-4.51419
H	1.20848	-0.7145	-6.39989
H	2.76294	-0.70024	-5.42149
H	1.1007	1.80619	-6.20239
H	2.65727	1.77196	-5.22776

2

N	0.0002	-0.00479	0.
C	1.14522	0.67278	-0.06009
C	1.20797	2.06759	-0.06508
C	0.00003	2.74689	-0.00253
C	-1.20783	2.06756	0.06129
C	-1.1449	0.67275	0.05886
N	2.26893	-0.15798	-0.12059
C	3.60588	0.16581	-0.1702
O	4.01888	1.31063	-0.19186
N	-2.2685	-0.15803	0.1209
C	-3.60553	0.16569	0.16919
O	-4.01867	1.31049	0.18824
C	4.52115	-1.03286	-0.14388
C	5.17763	-1.37097	1.2189
C	-4.52063	-1.03315	0.14493
C	-5.93506	-0.88731	0.72355
H	2.15796	2.57548	-0.11603
H	-0.00004	3.83149	-0.00354
H	-2.15789	2.57541	0.11126
H	2.03023	-1.13757	-0.11039
H	-2.02968	-1.13761	0.11261
H	4.02221	-1.91738	-0.54778
H	4.70224	-2.14573	1.82322
H	5.29947	-0.46822	1.82175
H	-4.02172	-1.9168	0.55075
H	-6.25936	0.15305	0.66278
H	-6.09947	-1.25882	1.73682

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2				
3	C	5.93533	-0.88798	-0.72332
4	C	6.46664	-1.71592	0.45771
5	C	-6.46581	-1.71764	-0.45604
6	C	-5.17656	-1.37402	-1.21743
7	H	6.2595	0.15255	-0.6647
8	H	6.09943	-1.26144	-1.73592
9	H	7.41483	-1.41353	0.90572
10	H	6.5148	-2.78045	0.21579
11	H	-7.41388	-1.41626	-0.905
12	H	-6.51393	-2.7817	-0.21204
13	H	-5.29828	-0.47248	-1.8221
14		-4.70085	-2.14991	-1.82003
15	3			
16	N	0.67865	-0.16559	0.48749
17	C	0.67989	-0.37062	1.8037
18	C	1.8489	-0.48533	2.55802
19	C	3.04848	-0.37505	1.86986
20	C	3.0778	-0.16114	0.4996
21	C	1.84466	-0.06204	-0.148
22	N	-0.60839	-0.45673	2.34295
23	C	-1.01042	-0.63767	3.64622
24	O	-0.23367	-0.76995	4.57409
25	N	1.70002	0.15241	-1.52251
26	C	2.65758	0.35643	-2.49039
27	O	3.85231	0.33679	-2.26018
28	C	-2.51316	-0.65411	3.83467
29	C	-3.00833	0.46007	4.76693
30	C	2.08277	0.66689	-3.85963
31	C	2.02073	2.20874	-4.0849
32	H	1.80257	-0.65106	3.62252
33	H	3.98291	-0.45832	2.41429
34	H	3.99909	-0.07371	-0.05389
35	H	-1.33007	-0.35491	1.64667
36	H	0.7348	0.18793	-1.81156
37	H	-3.01471	-0.55821	2.8651
38	H	-3.06311	1.42803	4.26302
39	H	-2.29932	0.55981	5.59279
40	H	1.07181	0.25641	-3.92171
41	H	2.27124	2.77506	-3.18441
42	H	1.00059	2.48758	-4.36163
43	C	-3.02463	-1.91928	4.52659
44	C	2.94225	0.11938	-5.00965
45	H	-2.39115	-2.12229	5.39537
46	H	-2.99685	-2.79931	3.87886
47	H	2.57314	-0.84169	-5.37483
48	H	3.96179	-0.03162	-4.64564
49	C	-4.37303	-0.02858	5.2827
50	C	-4.43691	-1.53581	4.96314
51	C	2.98044	2.4924	-5.24042
52	C	2.93455	1.21591	-6.07017
53	H	-5.19313	0.50596	4.79711
54	H	-4.4688	0.16039	6.35446
55	H	-5.13886	-1.71822	4.14379
56	H	-4.77977	-2.13235	5.81151
57	H	3.99484	2.64436	-4.8573
58	H	2.7034	3.38838	-5.80145
59	H	3.76602	1.12722	-6.77377
60	H	2.00604	1.18048	-6.65231
	4			
	N	0.708	0.00045	0.39857
	C	0.73729	-0.07923	1.72775
	C	1.922	-0.08352	2.46652
	C	3.10584	-0.00021	1.74814
	C	3.10574	0.08341	0.36341
	C	1.85949	0.07979	-0.26603

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3	N	-0.53797	-0.15668	2.29812
4	C	-0.90923	-0.27101	3.61864
5	O	-0.1111	-0.29335	4.53724
6	N	1.68542	0.15752	-1.65213
7	C	2.62168	0.27166	-2.65466
8	O	3.82108	0.29351	-2.44901
9	C	-2.4065	-0.40553	3.83089
10	C	-2.88921	0.49787	4.96729
11	C	2.0263	0.40652	-4.04473
12	H	2.08962	1.87711	-4.4865
13	H	1.89874	-0.14887	3.54268
14	H	4.05103	-0.00048	2.28012
15	H	4.01366	0.14849	-0.21484
16	H	-1.27403	-0.13963	1.6096
17	H	0.71491	0.1409	-1.92411
18	H	-2.9269	-0.10821	2.91177
19	H	-2.67863	1.54447	4.72358
20	H	-2.31212	0.26357	5.8677
21	H	0.9704	0.10978	-4.01269
22	H	3.13333	2.20901	-4.44285
23	H	1.52898	2.50329	-3.78425
24	C	-2.7517	-1.87616	4.11353
25	C	2.7468	-0.4973	-5.047
26	H	-2.17294	-2.20863	4.98295
27	H	-2.44245	-2.50203	3.26959
28	H	2.64715	-1.54384	-4.74051
29	H	3.81608	-0.26358	-5.02088
30	C	-4.37705	0.3083	5.24023
31	C	1.55193	2.05989	-5.9013
32	H	-4.95449	0.66157	4.37572
33	H	-4.67715	0.93449	6.08638
34	H	1.65538	3.10793	-6.19946
35	H	0.47653	1.83943	-5.91214
36	C	2.20823	-0.30745	-6.46051
37	C	2.26321	1.15188	-6.89808
38	C	-4.72299	-1.15106	5.51356
39	C	-4.24019	-2.05865	4.38787
40	H	1.16938	-0.66013	-6.50557
41	H	2.7755	-0.93396	-7.15609
42	H	1.8222	1.26526	-7.89361
43	H	3.3121	1.46382	-6.98477
44	H	-5.80288	-1.26421	5.65305
45	H	-4.25295	-1.46359	6.45503
46	H	-4.80738	-1.83759	3.47429
47	H	-4.4417	-3.10676	4.63051
48				
49	1+5			
50				
51	C	1.20361	-3.70006	-0.23601
52	C	1.14295	-2.30487	-0.21983
53	C	0.02382	-4.3876	0.00069
54	C	-1.16321	-3.71254	0.23712
55	C	-1.11738	-2.31678	0.22042
56	N	0.00918	-1.63124	0.00016
57	N	-2.24731	-1.5133	0.40067
58	C	-3.46141	-1.86424	0.94167
59	O	-3.73549	-2.98599	1.33594
60	N	2.26429	-1.48952	-0.40038
	C	3.48205	-1.82786	-0.94119
	O	3.76799	-2.94688	-1.33478
	H	2.13736	-4.20453	-0.42672
	H	0.02958	-5.47234	0.00089
	H	-2.09155	-4.22683	0.42804
	H	-2.14505	-0.55234	0.07305
	H	2.15179	-0.52956	-0.07321
	C	-4.42452	-0.73072	1.01679
	H	-4.06034	0.2373	0.69846
	C	-5.88539	-1.0283	0.7601
	C	-5.42932	-0.73895	2.14413

1				
2				
3	C	4.4331	-0.68424	-1.01694
4	H	4.05868	0.28004	-0.69918
5	C	5.89704	-0.96618	-0.76011
6	C	5.43792	-0.68247	-2.14431
7	H	-6.12786	-2.05603	0.51946
8	H	-6.44728	-0.27207	0.22579
9	H	-5.67079	0.22051	2.58416
10	H	-5.36263	-1.57411	2.83015
11	H	6.15039	-1.99114	-0.5189
12	H	6.4509	-0.20374	-0.22624
13	H	5.66921	0.27925	-2.58486
14	H	5.38009	-1.51867	-2.82987
15	C	3.13609	3.04819	2.17373
16	C	3.10659	1.77949	1.61861
17	N	2.0918	1.30807	0.89194
18	C	1.02481	2.09372	0.70308
19	C	0.94825	3.38796	1.24196
20	C	2.02112	3.85933	1.97459
21	N	-0.00745	1.50174	-0.00109
22	C	-1.04587	2.08193	-0.70599
23	C	-0.98298	3.37623	-1.24645
24	C	-2.06076	3.83537	-1.97965
25	C	-3.1671	3.01227	-2.17778
26	C	-3.12422	1.74463	-1.62109
27	N	-2.10452	1.28483	-0.89387
28	H	3.99107	3.38286	2.74754
29	H	3.94486	1.09971	1.756
30	H	0.05764	3.98969	1.12144
31	H	1.97958	4.85321	2.40715
32	H	-0.00202	0.48109	-0.00054
33	H	-0.09877	3.98747	-1.12667
34	H	-2.0297	4.82911	-2.41343
35	H	-4.02557	3.33721	-2.75198
36	H	-3.95528	1.05588	-1.75764
37				
38	1+6			
39				
40	N	-0.18507	0.32005	0.03902
41	C	-0.09501	0.19186	1.36777
42	C	1.11195	0.28782	2.06223
43	C	2.25362	0.52975	1.31514
44	C	2.19178	0.6614	-0.06196
45	C	0.93502	0.53942	-0.66096
46	N	-1.32014	-0.02976	2.00524
47	C	-1.54917	-0.47754	3.28537
48	O	-0.66849	-0.71392	4.0952
49	N	0.74247	0.59989	-2.04228
50	C	1.63689	0.97871	-3.01877
51	O	2.76777	1.3755	-2.78994
52	C	-2.99452	-0.65762	3.59917
53	C	-3.47638	-0.22176	4.96705
54	C	-3.36506	-1.66997	4.65463
55	C	1.08873	0.86411	-4.39762
56	C	2.05591	0.50623	-5.50304
57	C	1.53093	1.89289	-5.41416
58	H	1.13598	0.17446	3.13377
59	H	3.21153	0.61539	1.81692
60	H	3.06587	0.84742	-0.66451
	H	-2.13686	0.19344	1.4426
	H	-0.17571	0.29727	-2.35944
	H	-3.68897	-0.53899	2.77757
	H	-4.45996	0.22931	5.01578
	H	-2.72796	0.20678	5.62218
	H	-4.2713	-2.23746	4.48374
	H	-2.5403	-2.21201	5.09974
	H	0.07858	0.48696	-4.4898
	H	1.68021	-0.14718	-6.28053
	H	3.08278	0.34352	-5.20012
	H	2.2063	2.65889	-5.05414

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2				
3	H	0.78455	2.21629	-6.12915
4	N	-3.01496	0.54149	-1.47381
5	C	-2.93322	0.1248	-2.78746
6	C	-4.04619	1.1091	-0.74056
7	O	-1.84274	-0.24278	-3.20266
8	N	-3.80379	1.17111	0.57543
9	N	-5.13371	1.55151	-1.36332
10	C	-4.15181	0.10532	-3.65322
11	H	-2.14306	0.42295	-0.95448
12	C	-6.05636	2.12132	-0.59175
13	C	-4.73499	1.76605	1.31523
14	C	-5.90816	2.27496	0.77819
15	H	-4.53398	1.82779	2.3821
16	H	-6.65982	2.75488	1.3896
17	H	-6.94973	2.47668	-1.09887
18	H	-4.99298	-0.37175	-3.15044
19	H	-4.46353	1.12533	-3.88148
20	H	-3.90297	-0.4229	-4.57123
21	1+7			
22	N	-0.08368	0.03924	-0.04808
23	C	0.00421	-0.05361	1.28565
24	C	1.22321	-0.1253	1.96511
25	C	2.37737	-0.10823	1.20058
26	C	2.31781	-0.01934	-0.17976
27	C	1.0499	0.05744	-0.76197
28	N	-1.22797	-0.09257	1.94368
29	C	-1.48213	-0.06849	3.29821
30	O	-0.61656	0.01962	4.15338
31	N	0.8619	0.18106	-2.14118
32	C	1.79767	0.08973	-3.14901
33	O	2.97978	-0.14768	-2.96304
34	C	-2.92915	-0.15875	3.63419
35	C	-3.40865	0.59075	4.85684
36	C	-3.30082	-0.88978	4.90473
37	C	1.23103	0.30677	-4.508
38	C	1.84045	-0.4742	-5.65047
39	C	2.11918	0.9797	-5.53025
40	H	1.24299	-0.19104	3.04051
41	H	3.34333	-0.16547	1.69077
42	H	3.20099	-0.00804	-0.7971
43	H	-2.03749	-0.1632	1.33473
44	H	-0.09258	0.37416	-2.42884
45	H	-3.62066	-0.23816	2.80662
46	H	-4.39106	1.04201	4.79222
47	H	-2.65793	1.16092	5.38969
48	H	-4.20658	-1.48243	4.87332
49	H	-2.47675	-1.30943	5.4681
50	H	0.17213	0.51749	-4.56926
51	H	1.15923	-0.81457	-6.42053
52	H	2.63912	-1.15642	-5.38719
53	H	1.63428	1.66457	-6.21466
54	H	3.10377	1.26939	-5.18509
55	N	-3.03914	0.26474	-1.54532
56	C	-2.92058	0.66899	-2.87035
57	C	-4.08259	-0.06479	-0.68763
58	O	-1.79596	0.84797	-3.30203
59	O	-3.79236	-0.36607	0.45614
60	C	-5.50545	-0.04929	-1.1512
	C	-4.12677	0.87557	-3.73172
	H	-2.12866	0.18926	-1.08583
	H	-6.12337	-0.40921	-0.33251
	H	-5.65495	-0.68634	-2.02258
	H	-3.78622	1.25892	-4.6902
	H	-4.82569	1.58406	-3.28779
	H	-5.81899	0.96324	-1.41145
	H	-4.65364	-0.06621	-3.8954

1+8

N	-0.16238	0.11058	-0.05897
C	-0.08111	0.01103	1.27408
C	1.13539	-0.03143	1.95721
C	2.29224	0.03044	1.19801
C	2.23716	0.12296	-0.1825
C	0.97144	0.15482	-0.77224
N	-1.31505	-0.03077	1.93202
C	-1.57673	-0.44346	3.22043
O	-0.71917	-0.79933	4.01038
N	0.78294	0.20392	-2.15566
C	1.72184	0.41147	-3.14512
O	2.90223	0.6266	-2.92824
C	-3.02472	-0.42509	3.56492
C	-3.40938	0.03031	4.95628
C	-3.51287	-1.40831	4.60134
C	1.15467	0.35025	-4.5189
C	2.03404	-0.2201	-5.60939
C	1.7738	1.24153	-5.57171
H	1.1556	-0.11225	3.03146
H	3.25721	0.00367	1.69274
H	3.12329	0.16872	-0.79396
H	-2.11518	0.28305	1.38888
H	-0.16738	0.03859	-2.47336
H	-3.71125	-0.18197	2.76523
H	-4.31675	0.61573	5.04135
H	-2.59273	0.32689	5.60288
H	-4.49395	-1.83607	4.43712
H	-2.76479	-2.07602	5.01005
H	0.0926	0.16152	-4.5999
H	1.53914	-0.82097	-6.36213
H	3.01486	-0.55924	-5.29994
H	1.09595	1.67093	-6.299
H	2.5807	1.88208	-5.23817
N	-2.81793	0.67996	-1.47655
C	-2.88399	0.3463	-2.78761
C	-3.89	1.23758	-0.78403
O	-1.95059	-0.15313	-3.39486
N	-3.81123	1.31151	0.53335
C	-4.9788	1.7179	-1.52473
O	-4.97505	1.6455	-2.87643
C	-4.22657	0.58118	-3.44612
H	-1.95067	0.47461	-0.96549
C	-6.01313	2.33014	-0.84378
H	-4.79877	-0.35445	-3.3907
H	-4.06805	0.83193	-4.49209
C	-4.81775	1.90704	1.1841
C	-5.92896	2.43082	0.54302
H	-4.72099	1.96747	2.26421
H	-6.71735	2.90691	1.11272
H	-6.85683	2.72562	-1.39717

1+9

N	-0.1574	0.05671	-0.06123
C	-0.07443	-0.09337	1.26857
C	1.14269	-0.20524	1.94485
C	2.29828	-0.15506	1.1847
C	2.24345	-0.00194	-0.18996
C	0.978	0.09952	-0.7735
N	-1.30414	-0.11223	1.93275
C	-1.55997	-0.4011	3.25778
O	-0.70018	-0.70627	4.06692
N	0.79596	0.23894	-2.15216
C	1.75122	0.40416	-3.1345
O	2.94903	0.47068	-2.91597
C	-3.00059	-0.30949	3.61838
C	-3.33932	0.17128	5.01195

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2				
3	C	-3.51646	-1.2635	4.67216
4	C	1.18412	0.49788	-4.50683
5	C	2.00253	-0.08509	-5.63745
6	C	1.90088	1.38968	-5.49559
7	H	1.16067	-0.32789	3.01505
8	H	3.26282	-0.23716	1.67415
9	H	3.12866	0.04156	-0.80234
10	H	-2.11439	0.11388	1.36446
11	H	-0.16687	0.20441	-2.47237
12	H	-3.68682	-0.03533	2.82913
13	H	-4.21643	0.79949	5.10458
14	H	-2.49894	0.43282	5.64298
15	H	-4.51867	-1.64705	4.52672
16	H	-2.79379	-1.96213	5.07515
17	H	0.10908	0.43054	-4.59907
18	H	1.4496	-0.57401	-6.42989
19	H	2.94015	-0.54848	-5.35654
20	H	1.27731	1.94058	-6.18871
21	N	2.77056	1.91343	-5.11861
22	C	-2.96484	0.36255	-1.46888
23	C	-2.96933	0.33118	-2.84975
24	O	-4.05387	0.55598	-0.64194
25	O	-1.92451	0.17587	-3.45377
26	C	-3.90041	0.57199	0.56515
27	C	-5.38959	0.70354	-1.30939
28	C	-5.33671	1.27641	-2.73003
29	C	-4.30429	0.46547	-3.52134
30	C	-4.93609	2.75498	-2.69299
31	C	-6.7083	1.13813	-3.38663
32	H	-2.05313	0.25448	-1.01061
33	H	-6.01906	1.30459	-0.65103
34	H	-5.82672	-0.30309	-1.32505
35	H	-4.66719	-0.55878	-3.67447
36	H	-4.13039	0.88531	-4.51355
37	H	-3.95838	2.91477	-2.22919
38	H	-4.89242	3.16598	-3.70483
39	H	-5.66754	3.33768	-2.12719
40	H	-7.46385	1.69723	-2.82783
41	H	-6.69248	1.53029	-4.40716
42	H	-7.02703	0.09297	-3.43152
43				
44	2+5			
45				
46	C	1.0243	-3.57708	-0.10073
47	C	1.03687	-2.18133	-0.09391
48	C	-0.20542	-4.20066	0.04088
49	C	-1.36903	-3.46097	0.17735
50	C	-1.24858	-2.07	0.15963
51	N	-0.07326	-1.44664	0.02993
52	N	-2.35074	-1.2116	0.23722
53	C	-3.59763	-1.48617	0.74811
54	O	-3.90597	-2.56017	1.23562
55	N	2.21498	-1.4305	-0.17899
56	C	3.44704	-1.83689	-0.63059
57	O	3.68225	-2.95911	-1.04633
58	H	1.9421	-4.13168	-0.21321
59	H	-0.25755	-5.28422	0.04464
60	H	-2.33496	-3.92584	0.29426
61	H	-2.18601	-0.26953	-0.12128
62	H	2.13207	-0.46767	0.14991
63	C	-4.56924	-0.33513	0.61712
64	H	-4.03266	0.61447	0.63959
65	C	-5.52282	-0.51983	-0.59843
66	C	-5.80157	-0.44004	1.53356
67	C	4.51741	-0.77474	-0.55829
68	H	4.08788	0.21114	-0.37271
69	C	5.69789	-1.03711	0.407
70	C	5.54946	-0.71248	-1.69871
71	C	-6.61922	-1.0072	0.36202

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3	C	6.64017	-0.44305	-0.65059
4	H	-5.1958	-1.20164	-1.38751
5	H	-5.76537	0.44531	-1.04866
6	H	-6.14382	0.55064	1.84005
7	H	-5.69235	-1.07308	2.41487
8	H	5.86068	-2.11041	0.52741
9	H	5.65453	-0.56751	1.39245
10	H	5.38251	0.0315	-2.48037
11	H	5.66643	-1.69775	-2.15374
12	H	-7.62339	-0.60631	0.2096
13	H	-6.67521	-2.09624	0.39823
14	H	7.61181	-0.92089	-0.7908
15	C	6.7936	0.62779	-0.49428
16	C	3.08403	3.05204	2.47398
17	C	3.03068	1.78562	1.91547
18	N	2.05796	1.37033	1.10313
19	C	1.05747	2.21455	0.82303
20	C	1.00658	3.51147	1.35804
21	C	2.03725	3.92335	2.18226
22	N	0.06262	1.67631	0.02781
23	C	-0.88051	2.30005	-0.76737
24	C	-0.72848	3.59814	-1.28039
25	C	-1.7175	4.09793	-2.10698
26	C	-2.8229	3.31138	-2.42249
27	C	-2.8692	2.03586	-1.88448
28	N	-1.93804	1.53708	-1.07046
29	H	3.90376	3.33957	3.12022
30	H	3.81365	1.05986	2.12505
31	H	0.16424	4.16163	1.16474
32	H	2.01355	4.91857	2.61302
33	H	0.02068	0.65609	0.0239
34	H	0.15708	4.18154	-1.06812
35	H	-1.61594	5.09544	-2.52085
36	H	-3.6122	3.66908	-3.07161
37	H	-3.70048	1.37278	-2.11328
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39	2+6			
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41	N	0.00198	0.1335	0.10773
42	C	0.05556	-0.00594	1.43687
43	C	1.25114	0.00628	2.15628
44	C	2.4217	0.18086	1.43505
45	C	2.39655	0.32435	0.05783
46	C	1.14777	0.2842	-0.56775
47	N	-1.19616	-0.13801	2.0508
48	C	-1.48169	-0.63521	3.29976
49	O	-0.63504	-1.0283	4.08362
50	N	0.99073	0.36164	-1.95247
51	C	1.90779	0.74236	-2.90616
52	O	3.04923	1.08665	-2.65419
53	C	-2.95146	-0.65159	3.64555
54	C	-3.40555	0.24072	4.82523
55	C	-3.48556	-1.85794	4.43955
56	C	1.34038	0.75085	-4.30399
57	C	2.29776	0.93437	-5.48636
58	C	0.61814	2.046	-4.75247
59	H	1.24715	-0.11851	3.22717
60	H	3.37242	0.20256	1.95685
	H	3.29383	0.45757	-0.52481
	H	-1.98103	0.16767	1.48075
	H	0.07149	0.0884	-2.29434
	H	-3.57127	-0.46643	2.76645
	H	-3.83652	1.21493	4.58263
	H	-2.58771	0.37821	5.53568
	H	-3.98397	-2.64598	3.87166
	H	-2.68494	-2.29297	5.04031
	H	0.6776	-0.10433	-4.45097
	H	2.60336	0.03639	-6.02714
	H	3.18717	1.48297	-5.17112

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3	H	1.02521	2.92096	-4.23846
4	H	-0.47089	2.05783	-4.6751
5	C	-4.3469	-0.89052	5.26551
6	C	1.25623	1.85908	-6.13811
7	H	-4.44466	-1.08171	6.33572
8	H	-5.34509	-0.77198	4.8365
9	H	0.59268	1.3103	-6.81119
10	H	1.61903	2.75157	-6.65207
11	N	-2.75891	0.41453	-1.48801
12	C	-2.6591	-0.06679	-2.77903
13	C	-3.78781	1.04812	-0.80818
14	O	-1.56671	-0.46664	-3.15662
15	N	-3.55573	1.20038	0.5027
16	N	-4.86279	1.46182	-1.47135
17	C	-3.86161	-0.11329	-3.66623
18	H	-1.90126	0.30327	-0.94317
19	C	-5.78363	2.09815	-0.75172
20	C	-4.48434	1.86042	1.18791
21	C	-5.64514	2.34684	0.60524
22	H	-4.29141	1.99949	2.24892
23	H	-6.3943	2.88023	1.17396
24	H	-6.66698	2.42929	-1.29171
25	H	-4.7267	-0.53106	-3.15193
26	H	-4.13837	0.89695	-3.9717
27	H	-3.60864	-0.7075	-4.5419
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N	0.02566	-0.29737	0.03075
C	0.09518	-0.49963	1.35361
C	1.30307	-0.68202	2.03252
C	2.46415	-0.65997	1.27865
C	2.4228	-0.46012	-0.09088
C	1.16572	-0.27634	-0.67264
N	-1.1434	-0.53167	1.9982
C	-1.4164	-0.59845	3.34824
O	-0.55908	-0.64471	4.21222
N	0.99632	-0.03934	-2.03926
C	1.93692	-0.06075	-3.04617
O	3.11035	-0.34248	-2.8772
C	-2.89804	-0.5702	3.65262
C	-3.46446	0.87585	3.71196
C	-3.24453	-0.72026	5.14161
C	1.38401	0.34622	-4.3897
C	2.25676	0.15637	-5.63482
C	1.35652	1.86349	-4.70062
H	1.3102	-0.83477	3.09916
H	3.4214	-0.80229	1.76867
H	3.31163	-0.44369	-0.69997
H	-1.94978	-0.50239	1.38051
H	0.05245	0.21337	-2.31753
H	-3.42129	-1.23257	2.96221
H	-4.48525	0.90612	3.32583
H	-2.88278	1.65889	3.21907
H	-4.18886	-1.25272	5.27196
H	-2.47907	-1.18043	5.76698
H	0.38528	-0.07027	-4.53424
H	2.06725	-0.7257	-6.24994
H	3.31416	0.18358	-5.36577
H	0.41246	2.3828	-4.52858
H	2.15904	2.38616	-4.17334
C	1.76118	1.52016	-6.1432
C	-3.4124	0.80504	5.2469
H	2.48526	2.17319	-6.63446
H	0.88508	1.41763	-6.78839
H	-4.28244	1.17884	5.79041
H	-2.51671	1.28386	5.64748
N	-2.88873	0.1962	-1.45077
C	-2.74133	0.72809	-2.72748

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2				
3	C	-3.95422	-0.18325	-0.64123
4	O	-1.60803	0.86425	-3.15156
5	O	-3.69436	-0.56784	0.48444
6	C	-5.36406	-0.13924	-1.1425
7	C	-3.93039	1.13774	-3.53954
8	H	-1.98675	0.0393	-0.99467
9	H	-6.00194	-0.56083	-0.36977
10	H	-5.4814	-0.71576	-2.06054
11	H	-3.56281	1.60368	-4.45035
12	H	-4.55926	1.8467	-3.00025
13	H	-5.68062	0.88593	-1.33997
14	H	-4.54147	0.27464	-3.80766
15	2+8			
16	N	-0.12411	0.00138	-0.01241
17	C	-0.09015	-0.16663	1.31469
18	C	1.10162	-0.29224	2.02953
19	C	2.28435	-0.23968	1.31054
20	C	2.27587	-0.07643	-0.06497
21	C	1.0319	0.03717	-0.68881
22	N	-1.34236	-0.17509	1.94151
23	C	-1.66282	-0.74142	3.15662
24	O	-0.86096	-1.33936	3.85111
25	N	0.89051	0.16197	-2.07347
26	C	1.84897	0.48504	-3.01048
27	O	3.01421	0.71107	-2.73821
28	C	-3.09987	-0.51812	3.5696
29	C	-3.23116	0.67999	4.55412
30	C	-3.5758	-1.43748	4.70827
31	C	1.30122	0.59258	-4.41182
32	C	2.28776	0.69002	-5.58066
33	C	0.74307	1.97479	-4.83442
34	H	1.08742	-0.42857	3.0987
35	H	3.23129	-0.32977	1.83178
36	H	3.18277	-0.03643	-0.64625
37	H	-2.1023	0.25858	1.42105
38	H	-0.04503	-0.00357	-2.4348
39	H	-3.74175	-0.46762	2.68918
40	H	-4.18047	1.19955	4.4057
41	H	-2.42505	1.41765	4.55172
42	H	-4.64233	-1.65182	4.61311
43	H	-3.02858	-2.3723	4.8337
44	H	0.54489	-0.17491	-4.58774
45	H	2.49236	-0.22499	-6.14017
46	H	3.23121	1.12358	-5.24421
47	H	1.24583	2.78217	-4.29525
48	C	-3.29234	-0.31721	5.72181
49	C	1.36971	1.74564	-6.21876
50	H	-0.33762	2.11448	-4.7656
51	H	-4.04377	-0.13246	6.4919
52	H	-2.31938	-0.44388	6.19883
53	H	1.84062	2.60034	-6.7082
54	H	0.65358	1.29417	-6.90974
55	N	-2.69256	0.63201	-1.49644
56	C	-2.73446	0.27841	-2.8038
57	C	-3.7716	1.21128	-0.83506
58	O	-1.79262	-0.23587	-3.38505
59	N	-3.71584	1.30992	0.48235
60	C	-4.84269	1.68696	-1.60467
	O	-4.81324	1.59133	-2.95485
	C	-4.06267	0.51148	-3.49168
	H	-1.84248	0.41603	-0.95972
	C	-5.88479	2.31903	-0.95471
	H	-4.64272	-0.41895	-3.4295
	H	-3.88402	0.74185	-4.5391
	C	-4.73115	1.92282	1.10281
	C	-5.82628	2.44262	0.43182
	H	-4.65428	2.0016	2.18292

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3	H	-6.62203	2.93339	0.97805
4	H	-6.71487	2.71085	-1.53087
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6	2+9			
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8	N	-0.40916	-0.13116	-0.25354
9	C	-0.41456	-0.11275	1.12768
10	C	0.69783	-0.08279	-1.07865
11	O	-1.47193	-0.14222	1.72861
12	O	0.55265	-0.09024	-2.28643
13	C	2.03871	-0.05525	-0.40485
14	C	2.04055	0.57627	0.99168
15	C	0.92485	-0.08983	1.80489
16	C	1.79743	2.08595	0.89233
17	C	3.38655	0.32152	1.66613
18	H	-1.32408	-0.16398	-0.71611
19	H	2.73327	0.44776	-1.08001
20	H	2.36425	-1.10145	-0.34445
21	H	1.17827	-1.13947	2.00113
22	H	0.79089	0.38508	2.77815
23	H	0.84467	2.32675	0.41201
24	H	1.78934	2.54092	1.8863
25	H	2.58974	2.56526	0.31166
26	H	4.19974	0.77568	1.09333
27	H	3.40563	0.754	2.67029
28	H	3.59379	-0.74854	1.756
29	N	-3.23323	-0.23502	-1.68183
30	C	-3.32405	-0.24958	-3.01988
31	C	-4.54606	-0.27633	-3.69715
32	C	-5.69755	-0.2865	-2.92914
33	C	-5.63466	-0.2719	-1.54652
34	C	-4.36532	-0.2474	-0.96279
35	N	-2.09767	-0.23784	-3.68921
36	C	-1.85044	-0.25913	-5.04714
37	O	-2.72088	-0.30603	-5.89771
38	N	-4.17886	-0.23336	0.42213
39	C	-5.12747	-0.25927	1.42474
40	O	-6.3289	-0.278	1.22579
41	C	-0.38357	-0.17355	-5.38871
42	C	0.24622	1.24136	-5.42761
43	C	-4.53217	-0.31068	2.80983
44	C	-5.46722	-0.18803	4.01746
45	H	-4.56913	-0.28792	-4.77415
46	H	-6.66523	-0.30627	-3.41893
47	H	-6.51694	-0.27909	-0.92838
48	H	-1.27347	-0.19594	-3.09676
49	H	-3.21283	-0.21533	0.73587
50	H	0.19952	-0.81027	-4.72056
51	H	0.78006	1.56596	-4.53291
52	H	-0.4979	1.995	-5.69925
53	H	-3.68793	0.37681	2.88599
54	H	-6.46967	-0.53535	3.76096
55	H	-5.54048	0.79028	4.49674
56	C	0.04414	-0.35203	-6.84917
57	C	1.05942	0.78566	-6.64954
58	C	-4.64354	-1.2821	4.71691
59	C	-4.10986	-1.70389	3.33871
60	H	-0.76462	-0.06073	-7.5215
	H	0.41871	-1.33397	-7.14532
	H	1.18997	1.49939	-7.46532
	H	2.04032	0.40475	-6.35421
	H	-5.18404	-2.03026	5.30017
	H	-3.85071	-0.85717	5.33744
	H	-4.72332	-2.49346	2.8965
	H	-3.05567	-1.96821	3.24261
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	C	1.2164	-3.83031	-0.14871

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4	C	1.1574	-2.43532	-0.14534
5	C	0.05202	-4.51478	0.16186
6	C	-1.1194	-3.83497	0.45519
7	C	-1.07494	-2.43999	0.4168
8	N	0.0375	-1.75818	0.12692
9	N	-2.19884	-1.63665	0.6421
10	C	-3.36217	-1.97517	1.29002
11	O	-3.56847	-3.07173	1.78115
12	N	2.2727	-1.62515	-0.38926
13	C	3.4473	-1.96908	-1.01341
14	O	3.67706	-3.08087	-1.45829
15	H	2.1377	-4.33835	-0.38507
16	H	0.05775	-5.59937	0.17551
17	H	-2.03513	-4.34682	0.70488
18	H	-2.12886	-0.6883	0.27183
19	H	2.18846	-0.66776	-0.04623
20	C	-4.39631	-0.86741	1.33135
21	H	-3.9384	0.07274	1.01398
22	C	-5.58782	-1.15571	0.40724
23	C	-5.03901	-0.67596	2.71851
24	C	4.45597	-0.84218	-1.11483
25	H	4.01391	0.08274	-0.7367
26	C	5.75603	-1.13971	-0.33465
27	C	4.93382	-0.59236	-2.54789
28	C	-6.52258	-0.33615	2.46103
29	C	-6.66376	-0.22041	0.9411
30	C	6.90357	-0.53718	-1.17265
31	C	6.22939	0.18136	-2.3446
32	H	-5.89932	-2.19842	0.53082
33	H	-5.35287	-1.00074	-0.6496
34	H	-4.52435	0.11048	3.27539
35	H	-4.94711	-1.59673	3.29715
36	H	5.88612	-2.21816	-0.22456
37	H	5.71039	-0.7176	0.67238
38	H	4.19405	-0.05802	-3.14976
39	H	5.13468	-1.55255	-3.03313
40	H	-6.83628	0.5752	2.97531
41	H	-7.1599	-1.144	2.83167
42	H	-6.45319	0.80494	0.61551
43	H	-7.665	-0.4753	0.58455
44	H	7.54828	-1.33666	-1.54803
45	H	7.53819	0.13211	-0.58725
46	H	6.85341	0.21094	-3.24116
47	H	6.00004	1.21837	-2.07434
48	C	3.2204	2.93029	2.15216
49	C	3.17454	1.65423	1.61527
50	N	2.14032	1.17351	0.92328
51	C	1.06956	1.95855	0.75202
52	C	1.0085	3.25953	1.27626
53	C	2.10084	3.73965	1.97333
54	N	0.0187	1.35924	0.08245
55	C	-1.04238	1.93253	-0.59399
56	C	-0.99369	3.21866	-1.15508
57	C	-2.09503	3.67309	-1.85514
58	C	-3.21156	2.85302	-1.99979
59	C	-3.15329	1.59274	-1.42815
60	N	-2.10959	1.13659	-0.73365
	H	4.09101	3.27145	2.69792
	H	4.01594	0.97609	1.74047
	H	0.11502	3.8602	1.17267
	H	2.07141	4.73906	2.39411
	H	0.02263	0.33839	0.09722
	H	-0.10238	3.8264	-1.07645
	H	-2.07514	4.66026	-2.3044
	H	-4.08961	3.17401	-2.54595
	H	-3.99264	0.90768	-1.52639

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3	N	-0.02549	0.50835	0.09327
4	C	0.10188	0.28437	1.40547
5	C	1.32088	0.37341	2.07869
6	C	2.43428	0.71648	1.32846
7	C	2.33271	0.95042	-0.03259
8	C	1.06767	0.82424	-0.61222
9	N	-1.09935	-0.02262	2.05702
10	C	-1.26967	-0.63788	3.27459
11	O	-0.34783	-0.99574	3.98642
12	N	0.83974	0.9833	-1.98065
13	C	1.68799	1.48403	-2.94213
14	O	2.7936	1.93478	-2.69854
15	C	-2.71783	-0.82923	3.6796
16	C	-3.11791	0.05227	4.8679
17	C	-3.03164	-2.24343	4.18318
18	C	1.13446	1.37938	-4.35024
19	C	1.48352	0.00358	-4.96583
20	C	1.70711	2.42579	-5.32795
21	H	1.37667	0.17745	3.13736
22	H	3.40041	0.80163	1.81425
23	H	3.18396	1.21804	-0.63738
24	H	-1.9389	0.24051	1.54723
25	H	-0.05834	0.63194	-2.30599
26	H	-3.37255	-0.59557	2.8354
27	H	-3.20565	1.1114	4.60836
28	H	-2.35418	-0.03515	5.64731
29	H	-3.22831	-2.93244	3.35838
30	H	-2.16215	-2.62269	4.72426
31	H	0.0465	1.46331	-4.30847
32	H	0.73538	-0.75383	-4.7216
33	H	2.44924	-0.34288	-4.58106
34	H	2.43826	3.06697	-4.83441
35	H	0.89894	3.06689	-5.68955
36	C	-4.23627	-2.08652	5.13337
37	C	-4.42966	-0.57246	5.33135
38	C	1.60921	0.29234	-6.45683
39	C	2.32995	1.63504	-6.48551
40	H	-4.03557	-2.58278	6.08593
41	H	-5.13769	-2.54893	4.7244
42	H	-4.67763	-0.30722	6.36168
43	H	-5.2503	-0.21106	4.70202
44	H	0.61287	0.3869	-6.90463
45	H	2.13939	-0.49666	-6.9971
46	H	2.24222	2.15197	-7.44454
47	H	3.3977	1.47772	-6.29871
48	N	-2.87742	0.55432	-1.35903
49	C	-2.77983	0.14804	-2.67575
50	C	-3.94587	1.01564	-0.60583
51	O	-1.66454	-0.08483	-3.12054
52	N	-3.67481	1.1389	0.70073
53	N	-5.09534	1.31297	-1.20352
54	C	-4.009	-0.02118	-3.50999
55	H	-1.98668	0.52981	-0.85815
56	C	-6.05713	1.78928	-0.41675
57	C	-4.64938	1.63864	1.45456
58	C	-5.88958	1.99236	0.94435
59	H	-4.42836	1.75427	2.51299
60	H	-6.67442	2.39589	1.56918
	H	-6.99988	2.02484	-0.90386
	H	-4.78225	-0.57615	-2.9794
	H	-4.43494	0.95443	-3.74805
	H	-3.72416	-0.53464	-4.42594
57	3+7			
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59	N	-0.01471	-1.03977	-0.0577
60	C	-1.15204	-1.74377	0.0224
	C	-1.17792	-3.13622	0.13742
	C	0.04051	-3.79393	0.1513

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4	C	1.23136	-3.09373	0.05827
5	C	1.1491	-1.70269	-0.0413
6	N	-2.31346	-0.96855	-0.03388
7	C	-3.62915	-1.36963	0.05965
8	O	-3.97212	-2.5184	0.27572
9	N	2.28062	-0.88546	-0.11566
10	C	3.59611	-1.24875	-0.30307
11	O	3.96363	-2.3991	-0.46356
12	C	-4.62068	-0.24879	-0.18223
13	C	-5.98168	-0.46793	0.4766
14	C	-4.92259	-0.08307	-1.70191
15	C	4.56419	-0.08228	-0.24549
16	C	5.85631	-0.30197	-1.05991
17	C	5.03111	0.1659	1.20677
18	H	-2.11791	-3.65843	0.20776
19	H	0.06219	-4.87518	0.23594
20	H	2.19133	-3.58352	0.0592
21	H	-2.16002	0.01521	-0.23484
22	H	2.10156	0.1066	0.00785
23	H	-4.18976	0.68562	0.18263
24	H	-5.99385	-0.1408	1.51955
25	H	-6.22477	-1.53416	0.4611
26	H	-4.4567	0.83532	-2.06577
27	H	-4.50473	-0.90387	-2.29042
28	H	4.05572	0.81867	-0.59338
29	H	5.90238	0.42561	-1.87418
30	H	5.87349	-1.29614	-1.50768
31	H	4.34205	0.81575	1.75067
32	H	5.0924	-0.78563	1.74662
33	C	6.43029	0.7457	1.04304
34	C	7.02095	-0.09797	-0.08094
35	C	-6.94603	0.30238	-0.4161
36	C	-6.45358	-0.03224	-1.82095
37	H	7.01498	0.70853	1.96605
38	H	6.3653	1.79623	0.73579
39	H	7.34331	-1.06392	0.32232
40	H	7.89278	0.36209	-0.55284
41	H	-6.85525	1.37904	-0.22909
42	H	-7.99166	0.02937	-0.25186
43	H	-6.7888	0.68347	-2.57589
44	H	-6.83742	-1.01428	-2.11469
45	N	-0.0686	2.25105	-0.14583
46	C	1.15641	2.801	0.21617
47	C	-1.31219	2.74363	-0.527
48	O	2.07643	2.03173	0.42829
49	O	-2.20205	1.9345	-0.71758
50	C	-1.54033	4.2111	-0.71534
51	C	1.3304	4.28091	0.35923
52	H	-0.05051	1.22823	-0.12826
53	H	-2.55905	4.34386	-1.07064
54	H	-0.84741	4.63099	-1.44526
55	H	2.34373	4.46176	0.70864
56	H	0.62283	4.69722	1.07705
57	H	-1.41858	4.755	0.22229
58	H	1.18839	4.79095	-0.59445
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53	N	-0.24447	-1.48052	0.08195
54	C	0.88664	-2.18023	-0.06787
55	C	0.89914	-3.54772	-0.34542
56	C	-0.3258	-4.18245	-0.46975
57	C	-1.51065	-3.48283	-0.314
58	C	-1.41701	-2.11921	-0.02901
59	N	2.06222	-1.42749	0.04677
60	C	3.33514	-1.88814	0.30095
61	O	3.60405	-3.06252	0.47815
62	N	-2.5397	-1.31905	0.20143
63	C	-3.85968	-1.58596	-0.09568

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3	O	-4.23442	-2.61365	-0.63066
4	C	4.39635	-0.80658	0.30564
5	C	5.17832	-0.78597	-1.0187
6	C	5.4768	-0.99583	1.38808
7	C	-4.79929	-0.4503	0.25407
8	C	-6.21963	-0.89871	0.59097
9	C	-4.96137	0.5387	-0.93635
10	H	1.83263	-4.07587	-0.45177
11	H	-0.35741	-5.24419	-0.68946
12	H	-2.47519	-3.95548	-0.40349
13	H	1.95526	-0.42169	-0.06093
14	H	-2.35427	-0.41994	0.63699
15	H	3.92009	0.16752	0.43668
16	H	4.62268	-0.30888	-1.83088
17	H	5.39935	-1.81346	-1.32734
18	H	5.27802	-0.33923	2.23843
19	H	5.46052	-2.02157	1.75934
20	H	-4.38789	0.10092	1.10243
21	H	-6.31205	-1.24108	1.62501
22	H	-6.50295	-1.72938	-0.06202
23	H	-4.58101	0.10987	-1.86707
24	C	6.46851	-0.06969	-0.64431
25	C	6.82521	-0.67258	0.71425
26	C	-6.46888	0.83115	-1.03754
27	C	-7.06364	0.32892	0.27608
28	H	-4.38207	1.44509	-0.74435
29	H	6.28087	1.00647	-0.54705
30	H	7.25734	-0.19647	-1.39017
31	H	7.44568	-0.00621	1.31799
32	H	7.39773	-1.59315	0.56617
33	H	-6.90093	0.26864	-1.87093
34	H	-6.67599	1.88801	-1.2228
35	H	-8.13157	0.10736	0.20412
36	H	-6.93807	1.08225	1.06266
37	N	-0.25742	1.5615	0.35841
38	C	-1.32778	2.09231	0.9975
39	C	0.80466	2.33357	-0.10612
40	O	-2.25344	1.41829	1.41937
41	N	1.9028	1.71274	-0.50207
42	C	0.6385	3.72482	-0.15606
43	O	-0.53008	4.2912	0.22581
44	C	-1.27594	3.58971	1.21001
45	H	-0.20725	0.53955	0.26155
46	C	1.66668	4.48867	-0.67318
47	H	-0.85409	3.7752	2.20686
48	H	-2.28791	3.98652	1.18058
49	C	2.89344	2.46242	-1.00004
50	C	2.82076	3.84167	-1.1084
51	H	3.78089	1.92966	-1.32845
52	H	3.64896	4.40359	-1.52182
53	H	1.55286	5.56456	-0.73781
54	3+9			
55	N	-0.61123	0.37056	-0.28955
56	C	-0.52695	0.63124	1.0642
57	C	0.42601	0.01809	-1.13201
58	O	-1.52516	0.95336	1.68136
59	O	0.21129	-0.15424	-2.31688
60	C	1.77478	-0.16067	-0.49853
	C	2.00792	0.68868	0.75601
	C	0.82216	0.46009	1.69979
	C	2.11132	2.17088	0.38151
	C	3.29904	0.24592	1.44045
	H	-1.5363	0.47546	-0.72016
	H	2.52535	0.03365	-1.26665
	H	1.8501	-1.22672	-0.24982
	H	0.84088	-0.56761	2.08481
	H	0.86019	1.11841	2.5692

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4	H	1.21056	2.54127	-0.11638
5	H	2.27011	2.78318	1.27309
6	H	2.95422	2.33851	-0.29383
7	H	4.15754	0.38677	0.77807
8	H	3.47868	0.83148	2.34631
9	H	3.26114	-0.80974	1.72361
10	N	-3.46085	0.68205	-1.61537
11	C	-4.54885	0.85971	-0.85253
12	C	-5.82644	1.04657	-1.38579
13	C	-5.9446	1.04953	-2.765
14	C	-4.8389	0.8672	-3.57781
15	C	-3.60551	0.67989	-2.94863
16	N	-4.30427	0.85505	0.52399
17	C	-5.21339	0.86994	1.56174
18	O	-6.42073	0.86038	1.40246
19	N	-2.4223	0.46704	-3.66169
20	C	-2.23039	0.41403	-5.02766
21	O	-3.11543	0.60357	-5.84231
22	C	-4.57002	0.94962	2.93244
23	C	-5.44103	0.36525	4.06388
24	C	-0.81505	0.04568	-5.42373
25	C	-0.63006	-1.50065	-5.47721
26	H	-6.67367	1.17986	-0.73378
27	H	-6.91996	1.19648	-3.21633
28	H	-4.90552	0.86356	-4.65308
29	H	-3.32581	0.85562	0.79581
30	H	-1.60158	0.27438	-3.09573
31	H	-3.6071	0.43812	2.9019
32	H	-4.89829	-0.44767	4.55371
33	H	-6.37236	-0.04901	3.67656
34	H	-0.1267	0.44351	-4.67625
35	H	-1.58389	-2.02733	-5.38955
36	H	-0.0132	-1.82014	-4.63408
37	C	-4.3192	2.42668	3.32219
38	C	-0.40498	0.54808	-6.80693
39	H	-5.07406	3.07032	2.85685
40	H	-3.33768	2.77212	2.99081
41	H	-0.03985	1.57785	-6.78103
42	H	-1.27043	0.52026	-7.47485
43	C	-5.68789	1.51238	5.04906
44	C	-4.50334	2.44741	4.83499
45	C	0.04859	-1.79401	-6.82389
46	C	0.64244	-0.45926	-7.26366
47	H	-5.78585	1.16828	6.08163
48	H	-6.61535	2.03478	4.79088
49	H	-3.61023	2.04388	5.32642
50	H	-4.66797	3.45487	5.2265
51	H	-0.69911	-2.11595	-7.55542
52	H	0.79148	-2.59221	-6.75036
53	H	0.84181	-0.41176	-8.33726
54	H	1.59177	-0.27766	-6.74594

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49	C	1.2759	-3.85362	-0.20029
50	C	1.1889	-2.46048	-0.18316
51	C	0.13157	-4.5641	0.12589
52	C	-1.04672	-3.91077	0.44984
53	C	-1.03016	-2.51494	0.42807
54	N	0.06238	-1.80827	0.1218
55	N	-2.1637	-1.73609	0.68956
56	C	-3.30446	-2.10586	1.36031
57	O	-3.47622	-3.21312	1.84061
58	N	2.27958	-1.62525	-0.45205
59	C	3.44507	-1.93893	-1.10912
60	O	3.69393	-3.04628	-1.55459
	H	2.202	-4.34072	-0.46034
	H	0.15869	-5.6486	0.12747
	H	-1.94691	-4.44357	0.71133

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3	H	-2.11775	-0.78208	0.3298
4	H	2.18163	-0.67169	-0.10281
5	C	-4.36552	-1.02096	1.43798
6	H	-3.91798	-0.07105	1.13262
7	C	-5.50099	-1.34234	0.45698
8	C	-4.91325	-0.87975	2.86996
9	C	4.42044	-0.78229	-1.23834
10	H	3.92559	0.13945	-0.91462
11	C	5.63495	-1.01633	-0.32907
12	C	4.85776	-0.60058	-2.69463
13	C	-6.35707	-0.36244	2.90505
14	C	-6.52792	-0.20201	0.398
15	C	6.6634	0.10022	-0.47165
16	C	5.88663	0.51563	-2.83375
17	C	-6.64816	0.55652	1.72667
18	H	7.08917	0.29526	-1.92265
19	H	-5.98051	-2.27045	0.78364
20	H	-5.09999	-1.54125	-0.54232
21	H	-4.26016	-0.19976	3.42717
22	H	-4.85738	-1.85068	3.36794
23	H	6.0924	-1.97599	-0.59548
24	H	5.3103	-1.10377	0.71407
25	H	3.98377	-0.38945	-3.32011
26	H	5.28123	-1.5441	-3.05473
27	H	-6.54135	0.1522	3.85243
28	H	-7.05606	-1.20668	2.87705
29	H	-6.26323	0.50027	-0.39963
30	H	-7.50056	-0.62214	0.1217
31	H	7.5344	-0.11976	0.15411
32	H	6.23734	1.03819	-0.09064
33	H	6.21019	0.59024	-3.87692
34	H	5.4166	1.47691	-2.58699
35	H	-5.93979	1.39393	1.7451
36	H	-7.64401	0.99993	1.81688
37	H	7.63841	-0.59372	-2.259
38	H	7.78402	1.13764	-2.00205
39	C	3.23619	2.88924	2.1445
40	C	3.18703	1.62489	1.581
41	N	2.13476	1.1462	0.916
42	C	1.04826	1.91964	0.80135
43	C	0.98877	3.2072	1.35758
44	C	2.10041	3.68657	2.02534
45	N	-0.01575	1.31718	0.15522
46	C	-1.10091	1.87753	-0.49204
47	C	-1.11142	3.18565	-1.00241
48	C	-2.23705	3.61812	-1.6785
49	C	-3.31808	2.7568	-1.8511
50	C	-3.20139	1.47941	-1.32872
51	N	-2.13556	1.04383	-0.65617
52	H	4.12168	3.23031	2.66595
53	H	4.04127	0.95575	1.66118
54	H	0.0839	3.79697	1.30111
55	H	2.07342	4.6757	2.46974
56	H	0.01203	0.29658	0.14071
57	H	-0.24778	3.82926	-0.90517
58	H	-2.26298	4.62229	-2.08788
59	H	-4.21199	3.06041	-2.38127
60	H	-4.0092	0.76091	-1.45053
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3	O	-0.62537	-0.60654	4.19454
4	N	0.93205	0.24673	-1.97431
5	C	1.83744	0.57128	-2.96029
6	O	2.97322	0.95008	-2.73271
7	C	-2.96678	-0.46908	3.68339
8	C	-3.32381	0.31712	4.95405
9	C	-3.35184	-1.96713	3.81192
10	C	1.26865	0.47099	-4.36739
11	C	2.33279	-0.00777	-5.36474
12	H	0.67948	1.84721	-4.78098
13	H	1.24451	0.1659	3.22556
14	H	3.3558	0.38778	1.91112
15	H	3.25064	0.45198	-0.58088
16	H	-2.00274	0.28359	1.49116
17	H	0.01071	-0.05578	-2.28291
18	H	-3.53775	-0.05537	2.84919
19	H	-3.4062	1.38242	4.71478
20	H	-2.50792	0.22207	5.67688
21	H	-4.33674	-2.11044	3.35435
22	H	-2.65864	-2.58776	3.23685
23	H	0.44582	-0.24712	-4.35357
24	H	2.40689	-1.09849	-5.32253
25	H	3.3084	0.38339	-5.0613
26	H	0.33226	2.39366	-3.8988
27	H	-0.21008	1.67129	-5.39572
28	C	-3.40298	-2.42674	5.26224
29	C	-4.6151	-0.20197	5.57227
30	C	2.0147	0.45826	-6.7792
31	C	1.68153	2.67806	-5.5697
32	C	-4.45885	-1.651	6.06076
33	C	2.06255	1.9897	-6.88782
34	H	-2.41456	-2.28913	5.71062
35	H	-3.61104	-3.49967	5.30587
36	H	-4.92499	0.44483	6.39772
37	H	-5.41594	-0.14194	4.82493
38	H	1.01972	0.09338	-7.06143
39	H	2.7128	0.00779	-7.49046
40	H	1.27093	3.67248	-5.76729
41	H	2.57386	2.83331	-4.95468
42	H	-5.42537	-2.16138	5.99424
43	H	-4.18293	-1.65716	7.12002
44	H	1.39013	2.31721	-7.68785
45	H	3.0672	2.30952	-7.1832
46	N	-2.81249	0.39886	-1.45802
47	C	-2.74447	-0.18602	-2.70719
48	C	-3.81805	1.10353	-0.81405
49	O	-1.66988	-0.65026	-3.06206
50	N	-3.57663	1.32454	0.48518
51	N	-4.88164	1.51143	-1.4989
52	C	-3.95952	-0.26329	-3.57503
53	H	-1.95086	0.30304	-0.91666
54	C	-5.77981	2.21697	-0.81578
55	C	-4.48184	2.05203	1.1326
56	C	-5.62886	2.53972	0.524
57	H	-4.28258	2.24504	2.18429
58	H	-6.35922	3.12836	1.06176
59	H	-6.65446	2.54358	-1.37248
60	H	-4.8274	-0.62019	-3.02089
	H	-4.21499	0.7298	-3.94725
	H	-3.73475	-0.92548	-4.40845
55	4+7			
56				
57	N	-0.17567	-0.42478	-0.03871
58	C	-0.10446	-0.68732	1.2739
59	C	1.10336	-0.92186	1.93657
60	C	2.26109	-0.88706	1.17751
	C	2.2167	-0.62631	-0.18153
	C	0.96059	-0.39406	-0.74719

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3	N	-1.34193	-0.72477	1.9205
4	C	-1.61402	-0.8448	3.26887
5	O	-0.74859	-0.9534	4.11853
6	N	0.79089	-0.08298	-2.09922
7	C	1.70996	-0.15718	-3.12405
8	O	2.8421	-0.58496	-2.98517
9	C	-3.10609	-0.81815	3.58446
10	C	-3.68232	0.60572	3.45516
11	C	-3.43238	-1.41175	4.95839
12	C	1.1932	0.38725	-4.44567
13	C	1.90364	-0.24542	-5.65723
14	C	1.33812	1.92607	-4.43481
15	H	1.11303	-1.12348	2.99492
16	H	3.21797	-1.06755	1.65559
17	H	3.103	-0.60061	-0.7941
18	H	-2.14452	-0.69274	1.29904
19	H	-0.13257	0.26028	-2.3459
20	H	-3.59342	-1.43307	2.82235
21	H	-4.77466	0.51436	3.42232
22	H	-3.38599	1.0528	2.50184
23	H	-4.50666	-1.6336	4.96449
24	H	-2.91806	-2.36943	5.07933
25	H	0.12453	0.16614	-4.51116
26	H	1.15869	-0.43445	-6.43813
27	H	2.3162	-1.21682	-5.37647
28	H	0.55533	2.36198	-3.80925
29	H	2.29708	2.20606	-3.98292
30	C	1.26871	2.47917	-5.85157
31	C	3.00107	0.64497	-6.22493
32	C	-3.2955	1.51015	4.61967
33	C	-3.11136	-0.49259	6.13496
34	C	-3.70626	0.89932	5.95494
35	C	2.44559	1.98945	-6.71086
36	H	1.24559	3.57243	-5.82584
37	H	0.31832	2.1668	-6.30023
38	H	3.75679	0.80848	-5.4502
39	H	3.51369	0.13223	-7.04418
40	H	-3.76339	2.4916	4.48946
41	H	-2.21181	1.68153	4.61458
42	H	-3.48693	-0.94519	7.05879
43	H	-2.02635	-0.41121	6.24125
44	H	-4.80246	0.83977	5.9981
45	H	-3.39894	1.55009	6.78024
46	H	3.24811	2.73423	-6.70284
47	H	2.12078	1.90291	-7.75317
48	N	-3.05786	0.13414	-1.49501
49	C	-2.91595	0.80862	-2.70296
50	C	-4.11829	-0.37388	-0.75125
51	O	-1.78374	1.05056	-3.08118
52	O	-3.85958	-0.85548	0.33668
53	C	-5.51865	-0.34673	-1.27929
54	C	-4.11041	1.23822	-3.49604
55	H	-2.15654	-0.03078	-1.03876
56	H	-6.15356	-0.85697	-0.55928
57	H	-5.59049	-0.85097	-2.24366
58	H	-3.75206	1.7963	-4.35743
59	H	-4.77288	1.87257	-2.90628
60	H	-5.87501	0.67689	-1.40245
	H	-4.68375	0.3783	-3.84453
54	4+8			
55				
56	N	-0.22462	0.24349	0.01265
57	C	-0.20542	0.17927	1.34984
58	C	0.97799	0.13019	2.08722
59	C	2.16895	0.14617	1.37976
60	C	2.17663	0.20067	-0.00415
	C	0.93952	0.24333	-0.65075
	N	-1.4674	0.18978	1.9569

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4	C	-1.80312	-0.28237	3.21001
5	O	-0.98775	-0.74514	3.98782
6	N	0.81355	0.24884	-2.04303
7	C	1.78759	0.46875	-2.9954
8	O	2.94958	0.71097	-2.7231
9	C	-3.2884	-0.19431	3.51967
10	C	-3.56573	0.65159	4.77484
11	C	-3.91392	-1.59578	3.64905
12	C	1.26335	0.43421	-4.42206
13	C	2.3019	-0.16211	-5.38092
14	C	0.84499	1.867	-4.85213
15	H	0.95054	0.07726	3.16329
16	H	3.11039	0.1129	1.91743
17	H	3.09035	0.20927	-0.57556
18	H	-2.22481	0.55947	1.38822
19	H	-0.12109	0.06663	-2.39639
20	H	-3.77492	0.29797	2.67585
21	H	-4.63031	0.91709	4.75179
22	H	-3.01423	1.59652	4.71716
23	H	-5.00043	-1.47001	3.56204
24	H	-3.60955	-2.21927	2.80154
25	H	0.36619	-0.18755	-4.44179
26	H	2.266	-1.25405	-5.32278
27	H	3.30314	0.13475	-5.0556
28	H	0.55197	2.4573	-3.97871
29	C	-3.26703	-0.06267	6.0893
30	C	1.9481	2.57046	-5.63053
31	C	-3.60362	-2.29473	4.9679
32	C	-3.96241	-1.41782	6.16308
33	C	2.06765	0.31173	-6.80878
34	C	2.27085	1.82927	-6.93526
35	H	-0.05064	1.79152	-5.47835
36	H	-3.58545	0.57226	6.92295
37	H	-2.18728	-0.20446	6.19212
38	H	2.84225	2.63126	-5.00117
39	H	1.65567	3.60258	-5.8443
40	H	-2.53983	-2.5467	5.00908
41	H	-4.15547	-3.23965	5.01246
42	H	-3.69823	-1.92556	7.09645
43	H	-5.05067	-1.26743	6.18864
44	H	1.04852	0.043	-7.11198
45	H	2.73457	-0.217	-7.4957
46	H	1.6428	2.21279	-7.74623
47	H	3.30541	2.04296	-7.22316
48	N	-2.78173	0.852	-1.53041
49	C	-2.81918	0.45348	-2.82495
50	C	-3.84399	1.50329	-0.9087
51	O	-1.89456	-0.12679	-3.36998
52	N	-3.8063	1.64535	0.40501
53	C	-4.87952	1.99928	-1.71278
54	O	-4.83334	1.85519	-3.05781
55	C	-4.12212	0.72633	-3.5464
56	H	-1.94595	0.62788	-0.97565
57	C	-5.90217	2.70032	-1.1035
58	H	-4.74565	-0.1744	-3.47042
59	H	-3.91188	0.91723	-4.59589
60	C	-4.80128	2.32611	0.98601
	C	-5.86045	2.8711	0.2783
	H	-4.73967	2.4388	2.06468
	H	-6.64116	3.417	0.79298
	H	-6.70414	3.10819	-1.70771
56	4+9			
57				
58	N	-0.55921	0.08037	-0.33107
59	C	-0.56364	0.24428	1.04052
	C	0.54821	-0.05491	-1.14552
	O	-1.62047	0.35811	1.63233
	O	0.40405	-0.17568	-2.34744

1				
2				
3				
4	C	1.8855	-0.07408	-0.46425
5	C	1.94242	0.70825	0.85259
6	C	0.77283	0.23729	1.72418
7	C	1.83247	2.21262	0.58224
8	C	3.26102	0.41511	1.5645
9	H	-1.47343	0.07864	-0.79626
10	H	2.62347	0.28523	-1.18358
11	H	2.11434	-1.13192	-0.28302
12	H	0.93732	-0.799	2.04555
13	H	0.67677	0.83269	2.6337
14	H	0.90318	2.48074	0.0714
15	H	1.86712	2.77543	1.51875
16	H	2.66223	2.55227	-0.04296
17	H	4.11079	0.731	0.95315
18	H	3.31711	0.95332	2.51472
19	N	3.37448	-0.65218	1.77442
20	C	-3.37767	0.10726	-1.77111
21	C	-4.51022	0.15196	-1.05397
22	C	-5.77644	0.23089	-1.63958
23	C	-5.83629	0.2546	-3.02222
24	C	-4.68477	0.20288	-3.78822
25	N	-3.46541	0.13016	-3.10932
26	C	-4.32751	0.10587	0.3312
27	O	-5.28129	0.05637	1.32796
28	N	-6.48067	0.06678	1.11641
29	C	-2.23852	0.07592	-3.7773
30	O	-1.99377	0.04899	-5.13611
31	C	-2.86904	0.10467	-5.98106
32	C	-4.70423	0.01445	2.7326
33	C	-5.59521	-0.79476	3.6735
34	C	-0.52408	-0.09682	-5.49285
35	C	-0.13883	-1.58636	-5.49021
36	H	-6.65818	0.26771	-1.02196
37	H	-6.80164	0.31414	-3.51349
38	H	-4.70591	0.21688	-4.86508
39	H	-3.36283	0.12639	0.64695
40	H	-1.41919	0.00272	-3.18195
41	H	-3.71732	-0.45743	2.69247
42	H	-5.68713	-1.82181	3.30498
43	H	-6.60372	-0.36931	3.65906
44	H	0.07256	0.39656	-4.71908
45	H	-0.78788	-2.12016	-6.19591
46	H	-0.31995	-2.01787	-4.50121
47	C	-4.50805	1.44596	3.2585
48	C	-0.20843	0.54517	-6.84209
49	H	-5.47175	1.96936	3.22595
50	H	-3.82329	1.99253	2.6029
51	H	-0.44435	1.61379	-6.80797
52	H	-0.86296	0.1089	-7.60348
53	C	-5.05358	-0.79227	5.09817
54	C	1.3198	-1.78537	-5.88626
55	H	-4.09517	-1.32742	5.12596
56	H	-5.73467	-1.34642	5.75193
57	H	1.54843	-2.85566	-5.91831
58	H	1.9634	-1.35219	-5.10969
59	C	1.25053	0.34005	-7.23359
60	C	1.63795	-1.13443	-7.22704
	C	-4.85262	0.62445	5.62365
	C	-3.97353	1.4447	4.68664
	H	1.89689	0.88614	-6.53375
	H	1.43096	0.77482	-8.22194
	H	2.70152	-1.24854	-7.46039
	H	1.08734	-1.65587	-8.02079
	H	-4.41518	0.59925	6.62694
	H	-5.83015	1.11443	5.72237
	H	-2.95677	1.03117	4.68692
	H	-3.88958	2.47497	5.04769

For Peer Review Only

The $K_{assoc}=f(\beta-\alpha-\beta'$ angle) for 1-4 complexes with 9
210x161mm (72 x 72 DPI)

Optimized structures for complexes of 1+5-7
850x656mm (72 x 72 DPI)

Optimized structures for complexes of 1+5-7
908x659mm (72 x 72 DPI)

Optimized structures for complexes of 1+5-7
912x877mm (72 x 72 DPI)

Optimized structures for complexes of 1+5-7
850x656mm (72 x 72 DPI)

Optimized structures for complexes of 1+5-7
908x659mm (72 x 72 DPI)

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