

Dinuclear Zn^{II} and mixed Cu^{II}-Zn^{II} complexes of artificial patellamides as phosphatase models

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Supporting Information

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A) Synthesis of H₄pat⁵

General procedure for the formation of the oxazol monomer (GP 1)

A flame-dried Schlenk flask under an atmosphere of argon was charged with a solution of amide (1 eq) in dry DCM before being cooled to 0 °C. Then the given amount of triethylamine (4 eq), triphenylphosphine (2 eq) and carbon tetrachloride (2 eq) were added. After 30 min the reaction mixture was allowed to warm up to rt. Stirring was continued for additional five days. The reaction mixture was concentrated, the residue was dissolved in ethyl acetate, and then washed with saturated sodium hydrogen carbonate solution and brine. The combined organic layers were dried over Na₂SO₄. The solvent was concentrated under reduced pressure. The reaction mixture was purified by column chromatography over silica gel (PE : EE; 3: 1).

General procedure 2 (GP 2) – Cleavage of the Methyl group

The given amount of the protected compound (1 eq) is dissolved in a mixture consisting of methanol/dioxane (10:7; resulting in a 0.08 M solution). Then the quoted amount of 2 M NaOH solution (10 eq) was added dropwise at 0 °C. Afterwards the reaction mixture was allowed to warm up to rt. Stirring was continued until TLC showed the consumption of all starting material. Then brine, 1M HCl and DCM were added. The combined aqueous layers were repeatedly extracted with DCM. The combined organic layers were dried over Na₂SO₄. The solvent was concentrated under reduced pressure to yield the acid compound. Remaining dioxane was removed through repetitive stripping with ethyl acetate.

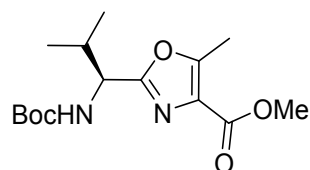
General procedure 3 (GP 3) – Cleavage of the Boc group

The given amount of the protected compound (1 eq) was dissolved in ethyl acetate (resulting in a 0.1 M solution). The solution was cooled to 0 °C. Afterwards TFA (3 ml/mmol starting material) was added dropwise. After 30 min the reaction mixture was allowed to warm up to rt. Stirring was continued for additional three hours. The reaction mixture was concentrated under reduced pressure to provide a quantitative yield of the trifluoroacid salt. Remaining solvent and TFA was removed through repetitive stripping with ethyl acetate.

General procedure 4 (GP 4) – Peptide bond formation

The given amount of acid monomer building block (1 eq) was dissolved in dry DMF at rt. Afterwards EDIPA (3 eq) was added dropwise. The solution was cooled to 0 °C. Then the quoted amount of COMU (0.98 eq) were added. The ice bath was removed, allowing the reaction solution to warm up again to rt and stirring was continued for additional one hour. The given amount of basic monomer building block (1 eq) was added and the reaction mixture was stirred for at least 4 days. Consumption of the starting material was controlled by TLC. After complete conversion, the reaction mixture was diluted with ethyl acetate and washed with 1 M HCl, saturated NaHCO₃ solution and brine. The combined organic layers were dried over MgSO₄. The solvent was removed under reduced pressure.

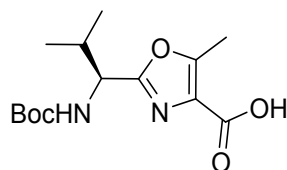
Methyl 2-((S)-1-(tert-butoxycarbonylamino)-2-methylpropyl)-5-methyl-oxazole-4-carboxylate (1):



According to **GP 1** 2.0 g (6.05 mmol; 1 eq) of Methyl-2-((S)-1-(tert-butoxycarbonylamino)-3-methylbutanamido)-3-oxobutanoate, 3.4 ml (24.22 mmol; 4 eq) of triethylamine, 3.2 ml (12.11 mmol; 2 eq) of triphenylphosphine and 1.2 ml (12.11 mmol; 2 eq) of carbon tetrachloride were dissolved in 125 ml dry DCM. Purification by column chromatography (petrol ether and ethyl acetate (3:1)) afforded 1.27 g (4.07 mmol; 67 %) of **1** as yellowish oil.

¹H NMR (200 MHz, CDCl₃): δ = 0.91 (d, J = 6.8 Hz, 3H, CHCH₃); 0.94 (d, J = 6.9 Hz, 3H, CHCH₃); 1.45 (s, 9H, C(CH₃)₃); 2.15 – 2.24 (m, 1H, CH(CH₃)₂); 2.63 (s, 3H, C_{het}CH₃); 3.88 (s, 1H, CO₂CH₃); 4.72 (t, J = 9.2 Hz, 1H, C_αH); 5.25 (d, J = 9.1 Hz, 1H, NH) ppm.

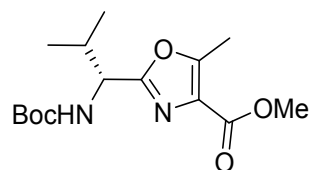
(S)-2-(1-(tert-butoxycarbonylamino)-2-methylpropyl)-5-methyl-oxazole-4-carboxylic acid (2):



According to **GP 2** 1270 mg (4.07 mmol; 1 eq) of **1** and 20 ml (10 eq) of NaOH were dissolved in dioxane/MeOH mixture (51 ml). This gave 863 mg (2.89 mmol; 71%) of **2** as yellowish oil.

¹H NMR (200 MHz, CDCl₃): δ = 0.92 (d, J = 6.9 Hz, 3H, CHCH₃); 0.94 (d, J = 6.9 Hz, 3H, CHCH₃); 1.41 (s, 9H, C(CH₃)₃); 2.11 – 2.26 (m, 1H, CH(CH₃)₂); 2.64 (s, 3H, C_{het}CH₃); 4.74 (t, J = 9.2 Hz, 1H, C_αH); 5.94 (d, J = 9.1 Hz, 1H, NH) ppm.

Methyl 2-((R)-1-(tert-butoxycarbonylamino)-2-methylpropyl)-5-methyl-oxazole-4-carboxylate (3):



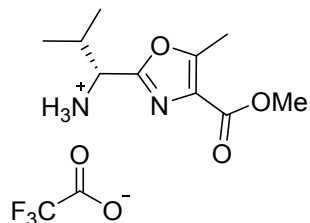
According to **GP 1** 2.0 g (6.05 mmol; 1 eq) of Methyl-2-((R)-1-(tert-butoxycarbonylamino)-3-methylbutanamido)-3-oxobutanoate, 3.4 ml (24.22 mmol; 4 eq) of triethylamine, 3.2 ml (12.11 mmol; 2 eq) of triphenylphosphine and 1.2 ml (12.11 mmol; 2 eq) of carbon tetrachloride were dissolved in 125 ml dry DCM. This afforded 1.57 g (5.03 mmol; 83 %) of **3** as yellowish oil.

¹H NMR (200 MHz, CDCl₃): δ = 0.88 (d, J = 6.8 Hz, 3H, CHCH₃); 0.91 (d, J = 6.9 Hz, 3H, CHCH₃); 1.42 (s, 9H, C(CH₃)₃); 2.10 – 2.20 (m, 1H, CH(CH₃)₂); 2.61 (s, 3H, C_{het}CH₃); 3.90 (s, 1H, CO₂CH₃); 4.72 (t, J = 9.2 Hz, 1H, C_αH); 5.25 (d, J = 9.1 Hz, 1H, NH) ppm.

¹³C NMR (150 MHz, CDCl₃): δ = 12.06, 17.95, 18.80, 28.31, 30.97, 32.91, 52.06, 54.09, 79.95, 127.25, 155.42, 156.53, 162.17, 162.74, 162.77 ppm.

ESI MS: m/z calcd. for [MH⁺] 313.18, found 313.02, calcd. for [MNa⁺] 335.16, found 335.09

(R)-1-(4-carboxylate-5-methyl-oxazol-2-yl)-2-methylpropan-1-ammonium trifluoro acetate (4):



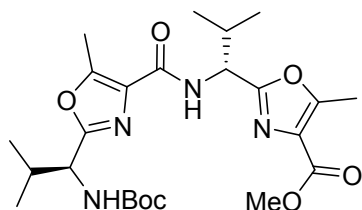
According to **GP 3**. 1.57 g (5.03 mmol; 1 eq) of **3** and 15.1 ml TFA were dissolved in 50 ml ethyl acetate. This yielded 1.64 g (5.04 mmol; 100 %) of **4** as yellowish oil.

¹H NMR (200 MHz, CDCl₃): δ = 1.02 (d, J = 6.9 Hz, 3H, CHCH₃); 1.14 (d, J = 6.9 Hz, 3H, CHCH₃); 2.38 – 2.52 (m, 1H, CH(CH₃)₂); 2.59 (s, 3H, C_{het}CH₃); 3.90 (s, 1H, CO₂CH₃); 4.46-4.52 (m, J = 6.4 Hz, 1H, C_αH); 8.97 (m, 1H, COOH) ppm.

¹³C NMR (150 MHz, MeOD-d₄): δ = 17.26, 19.47, 29.31, 51.15, 53.77, 115.81, 117.75, 127.40, 157.37, 157.69, 161.40, 161.63, 162.25 ppm.

ESI MS m/z calcd. for [MH⁺] 213.12, found 213.01

Methyl 2-((R)-1-((S)-1-(1-(tert-butoxycarbonylamino)-2-methylpropyl)-5-methyloxazole-4-carboxamido)-2-methylpropyl)-oxazole-4-carboxylate (5):

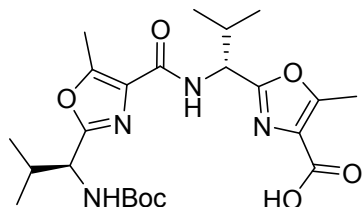


According to **GP 4** 0.75 g (2.51 mmol; 1 eq) of **2**, 1.09 g (3.27 mmol; 1.3 eq) of **4**, 1.06 g (2.46 mmol; 0.98 eq) of COMU and 1.31 ml (7.54 mmol; 3 eq) of EDIPA were dissolved in 150 ml dry DMF and stirred for 17 days. This gained 1.08 g (2.19 mmol; 87%) of **5** as yellowish oil.

¹H NMR (200 MHz, CDCl₃): δ = 0.94 (d, J = 6.9 Hz, 3H, CHCH₃); 0.95 (d, J = 6.9 Hz, 3H, CHCH₃); 0.96 (d, J = 6.8 Hz, 3H, CHCH₃); 1.00 (d, J = 6.9 Hz, 3H, CHCH₃); 1.46 (s, 9H, C(CH₃)₃); 2.08 – 2.21 (m, 1H, CH(CH₃)₂); 2.23 – 2.37 (m, 1H, CH(CH₃)₂); 2.59 (s, 3H, C_{het}CH₃); 2.61 (s, 3H, C_{het}CH₃); 3.90 (s, 1H, CO₂CH₃); 4.68 (t, J = 9.1 Hz, 1H, C_αH); 5.13 (t, J = 9.4 Hz, 1H, C_αH); 7.41 (d, J = 9.5 Hz, 1H, NH) ppm.

ESI MS m/z calcd. for [MNa⁺] 515.25, found 515.13

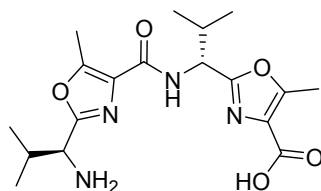
Methyl 2-((*R*)-1-(1-((*S*)-1-(*tert*-butoxycarbonylamino)-2-methylpropyl)-5-methyloxazole-4-carboxamido)-2-methylpropyl)-oxazole-4-carboxylic acid (6**):**



According to **GP 2** 1.08 g (2.19 mmol; 1 eq) of **5** and 30 ml (30 Äq) of NaOH were dissolved in dioxane/MeOH mixture (51 ml). This afforded 0.66 g (1.37 mmol; 63 %) of **6** as yellowish oil.

¹H NMR (200 MHz, CDCl₃): δ = 0.88 (d, J = 6.9 Hz, 3H, CHCH₃); 0.92 (d, J = 6.9 Hz, 3H, CHCH₃); 0.96 (d, J = 6.8 Hz, 3H, CHCH₃); 1.00 (d, J = 6.9 Hz, 3H, CHCH₃); 1.46 (s, 9H, C(CH₃)₃); 2.08 – 2.21 (m, 1H, CH(CH₃)₂); 2.23 – 2.37 (m, 1H, CH(CH₃)₂); 2.59 (s, 3H, C_{het}CH₃); 2.61 (s, 3H, C_{het}CH₃); 4.69 (t, J = 9.1 Hz, 1H, C_αH); 5.14 (t, J = 9.1 Hz, 1H, C_αH); 7.43 (d, J = 9.7 Hz, 1H, NH) ppm.

Methyl 2-((*R*)-1-(1-((*S*)-2-methylpropyl-1-ammonium fluoro acetate)-5-methyl-oxazol-2-yl-4-carboxamido)-2-methylpropyl)-oxazole-4-carboxylic acid (7**):**

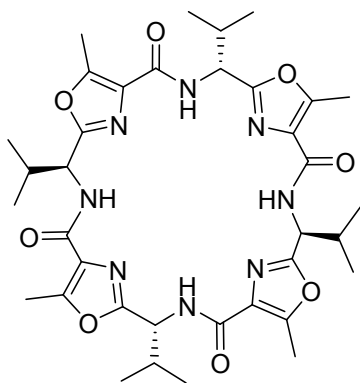


According to **GP 3** 0.66 g (1.37 mmol; 1 eq) of **6** and 4.1 ml TFA were dissolved in ethyl acetate (20 ml). A quantitative yield was obtained 0.68 g (1.37 mmol; 100%) of **7** as yellowish solid.

¹H NMR (200 MHz, CDCl₃): δ = 0.89 (d, J = 6.9 Hz, 3H, CHCH₃); 0.92 (d, J = 6.9 Hz, 3H, CHCH₃); 0.95 (d, J = 6.8 Hz, 3H, CHCH₃); 1.01 (d, J = 6.9 Hz, 3H, CHCH₃); 2.09 – 2.20 (m, 1H, CH(CH₃)₂); 2.24 – 2.36 (m, 1H, CH(CH₃)₂); 2.59 (s, 3H, C_{het}CH₃); 2.61 (s, 3H, C_{het}CH₃); 4.67 (t, J = 9.1 Hz, 1H, C_αH); 5.12 (t, J = 9.1 Hz, 1H, C_αH); 7.46 (d, J = 9.7 Hz, 1H, NH) ppm.

ESI MS m/z calcd. for [M]⁺ 377.18, found 377.49

Cyclic *pseudo*-octapeptide H₄pat⁵ (8):

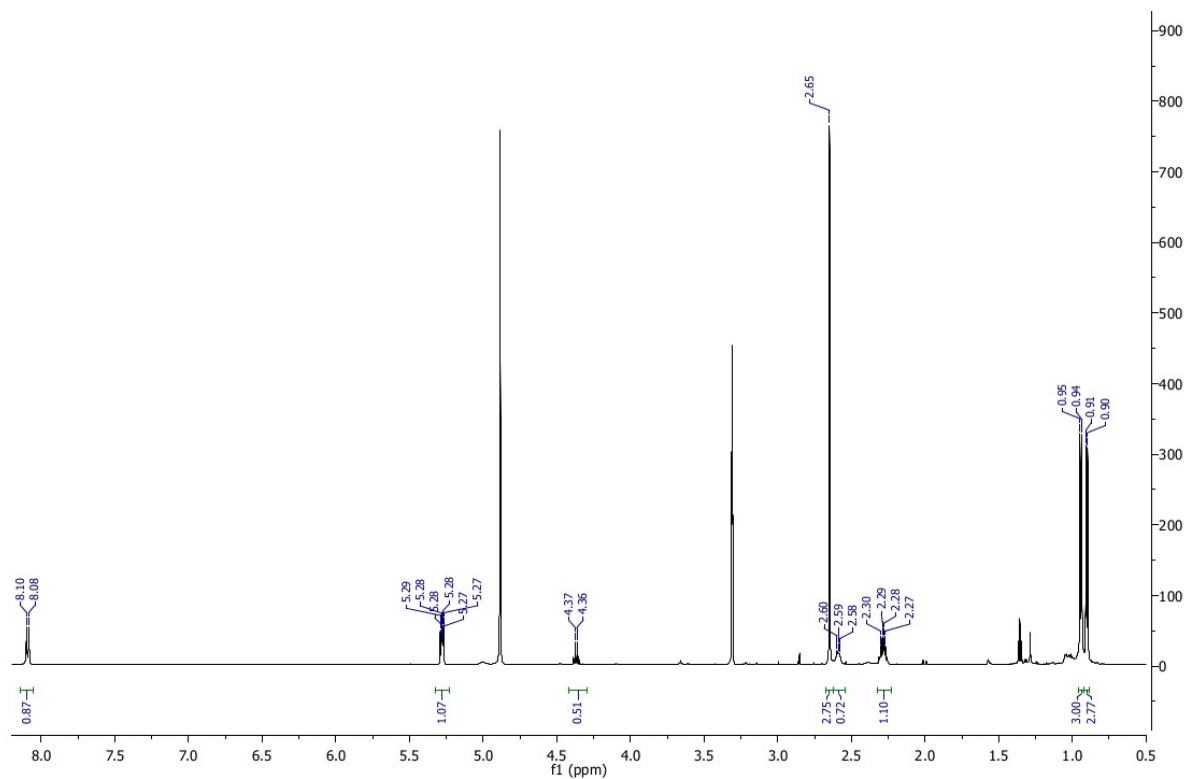


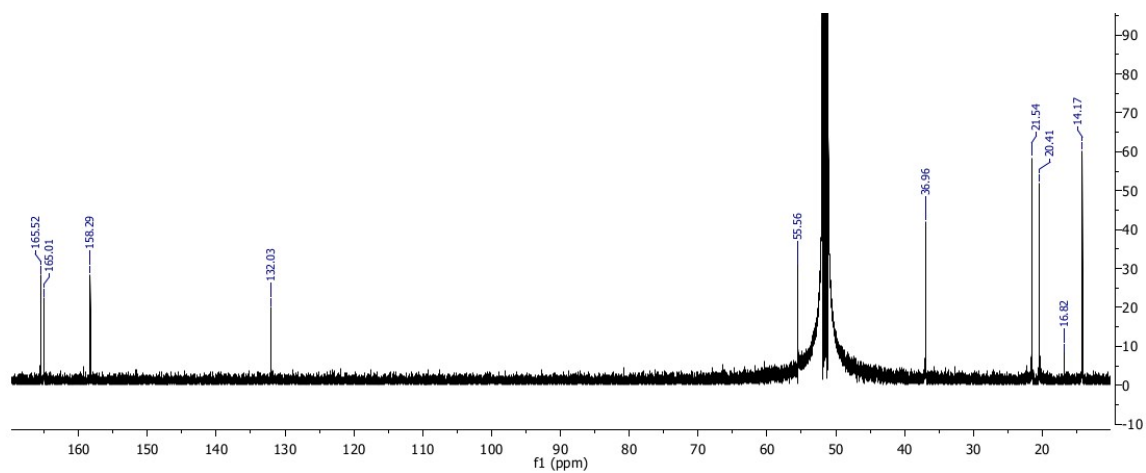
According to **GP 4** 0.68 g (2.26 mmol; 1 eq) of **7**, 0.95 g (2.22 mmol; 0.98 eq) of COMU and 1.18 ml (6.78 mmol; 3 eq) of EDIPA were dissolved in 150 ml dry DMF. Work up and subsequent column chromatography (PE:EE 2:1) yielded 0.582g (37%) of the desired product as a white powder.

¹H NMR (600 MHz, MeOD-d₄): δ = 0.91 (d, J = 6.9 Hz, 3H, CHCH₃); 0.95 (d, J = 6.9 Hz, 3H, CHCH₃), 2.25-2.32 (m, 1H, CH(CH₃)₂); 2.56-2.62 (m, 1H, CH(CH₃)₂); 2.65 (s, 3H, C_{het}CH₃); 5.28 (t, J = 9.2 Hz, 1H, C $_{\alpha}$ H); 8.09 (d, J = 9.6 Hz, 1H, NH) ppm.

¹³C NMR (150 MHz, MeOD-d₄): δ = 14.17, 16.82, 20.40, 21.53, 55.56, 132.03, 158.29, 165.01, 165.52 ppm.

HR-ESI MS m/z calcd. for [MNa⁺] 743.35, found 743.35





B) DFT optimized structures of dinuclear complexes

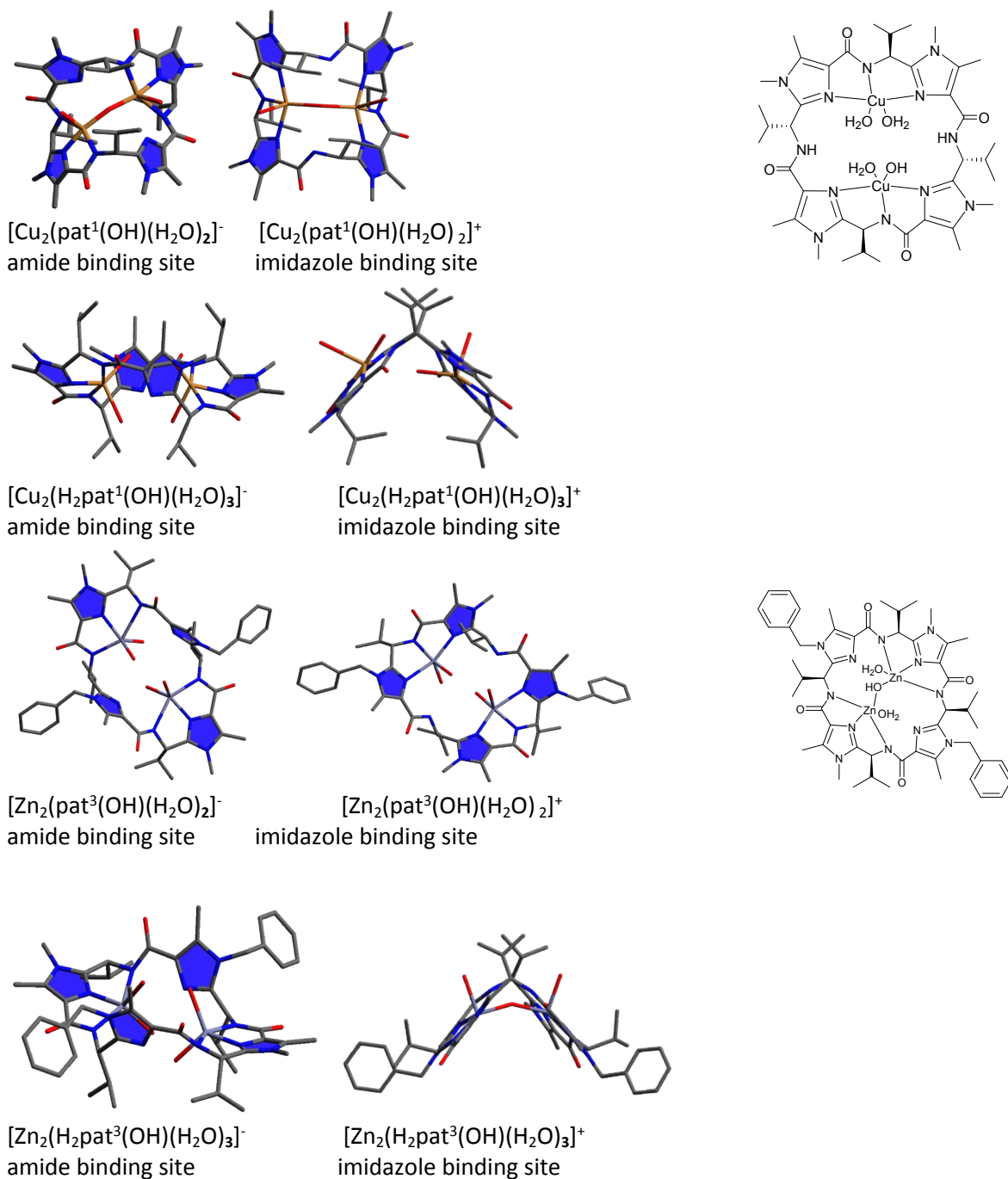


Figure S1. Calculated structures of a) $[\text{Cu}_2(\text{H}_2\text{pat}^1)(\text{OH})(\text{H}_2\text{O})_3]^+$ (top) and b) $[\text{Zn}(\text{H}_3\text{pat}^3)]^+$ (bottom) .

C) ITC measurements

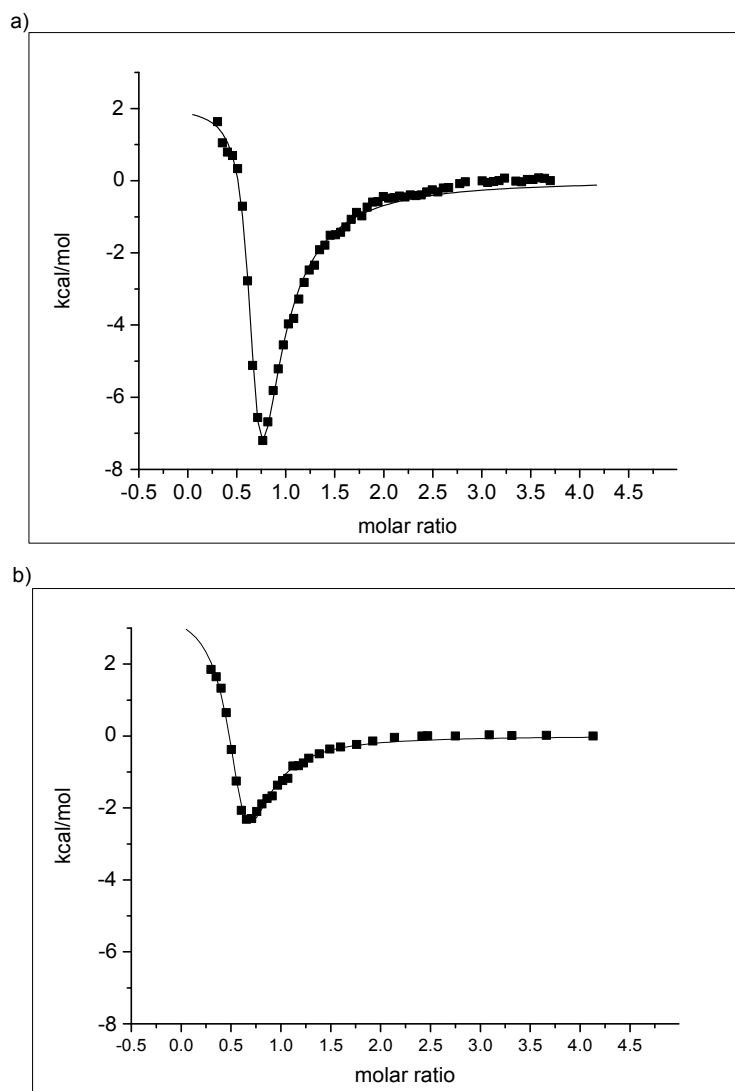
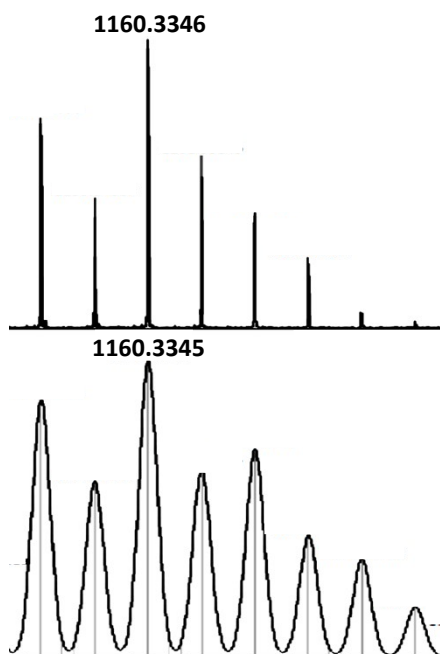


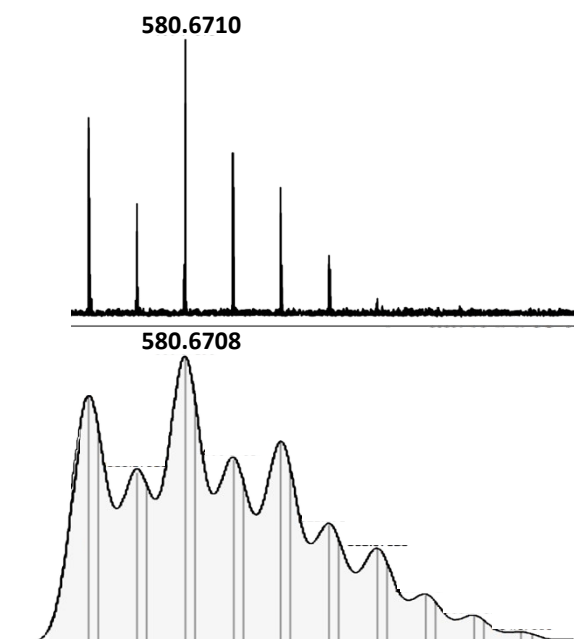
Figure S2. Isothermal titration calorimetry plots of the Zn^{II} titration to the ligands (a) H₄pat¹ and (b) H₄pat² (1 mM ligand in MeOH, 0.1 M (nBu₄)N(ClO₄), 200 μ L, 2mM (nBu₄)N(OMe), 25°C; addition of Zn(OTf)₂ (20 mM in MeOH), in 38 steps of 1 μ L or 76 steps of 0.5 μ L by an injection syringe; spectra and fitted curves analyzed by the Origin 7® with the Plug-in MicroCal LLC – VPViewer 2000 ITC®.¹

D) Mass spectra

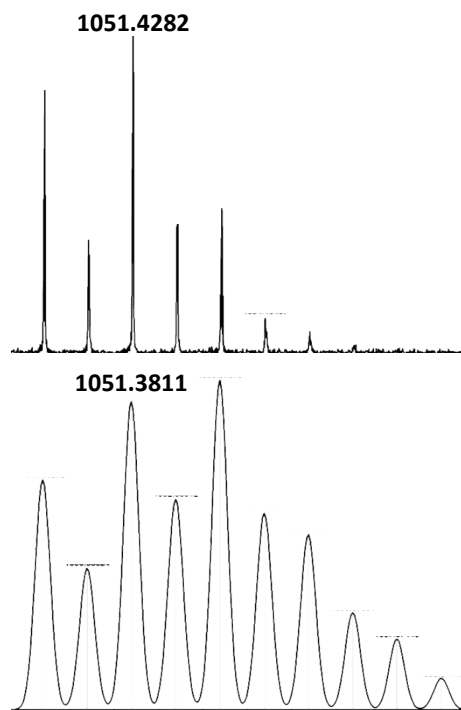
a)



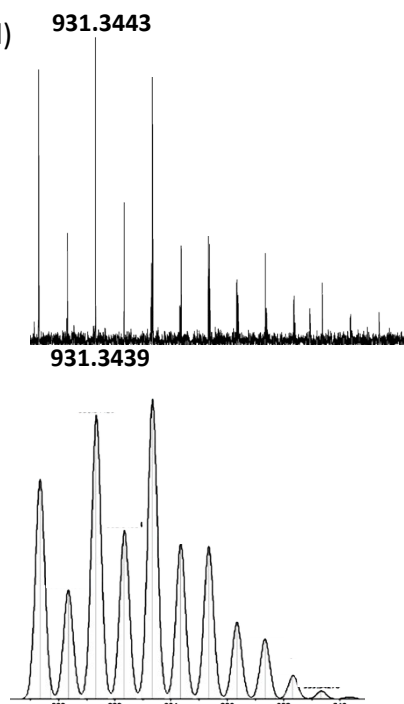
b)



c)



d)



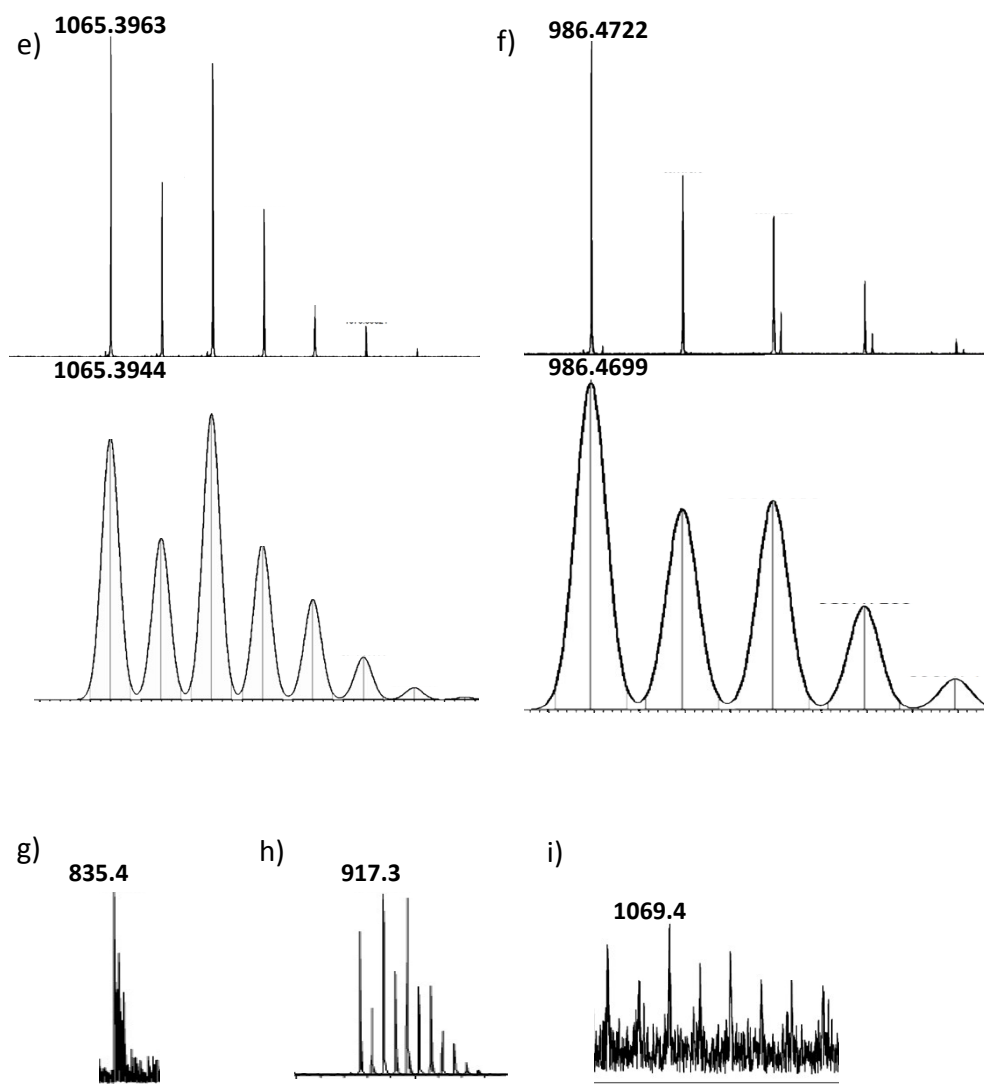


Figure S3. ESI and HR-ESI⁺ mass spectra of: a) $[[\text{Cu}^{\text{II}}\text{Zn}^{\text{II}}(\text{H}_2\text{pat}^3)(\text{OH})(\text{OMe})]+\text{Zn}]^+$ (odd), b) $[\text{Cu}^{\text{II}}\text{Zn}^{\text{II}}(\text{H}_2\text{pat}^3)(\text{OH})(\text{OMe})]+\text{Zn}]^{2+}$ (even), c) $[\text{Zn}^{\text{II}}_2(\text{Hpat}^3)]^+$, d) $[\text{Zn}^{\text{II}}_2(\text{H}_2\text{pat}^1)(\text{OMe})]^+$, e) $[\text{Cu}^{\text{II}}_2(\text{H}_2\text{pat}^3)(\text{OH})]^+$, f) $[\text{Cu}^{\text{II}}(\text{H}_3\text{pat}^3)(\text{OH})]^+$, g) $[\text{Zn}^{\text{II}}(\text{H}_3\text{pat}^1)]^+$, h) $[\text{Zn}^{\text{II}}_2(\text{H}_2\text{pat}^2)(\text{OH})]^+$ and i) $[\text{Zn}^{\text{II}}_2(\text{H}_2\text{pat}^3)(\text{OH})]^+$.

E) NMR spectra

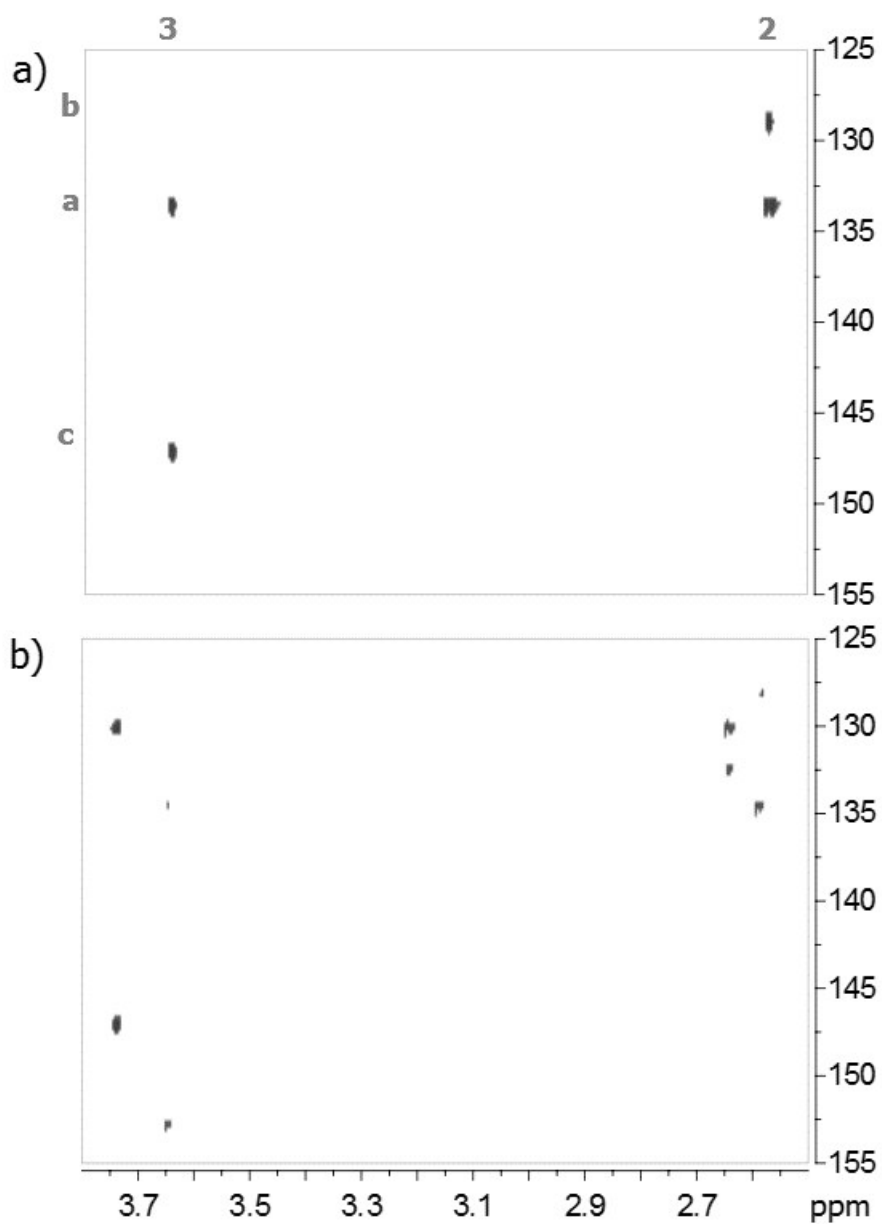


Figure S4. ^{13}C - ^1H HMBC spectra of a) H_4pat^1 and b) $[\text{Zn}^{\text{II}}_2(\text{H}_2\text{pat}^1)(\text{OH})]^+$ in CD_3OD (10 mM); 600 MHz, 25°C.

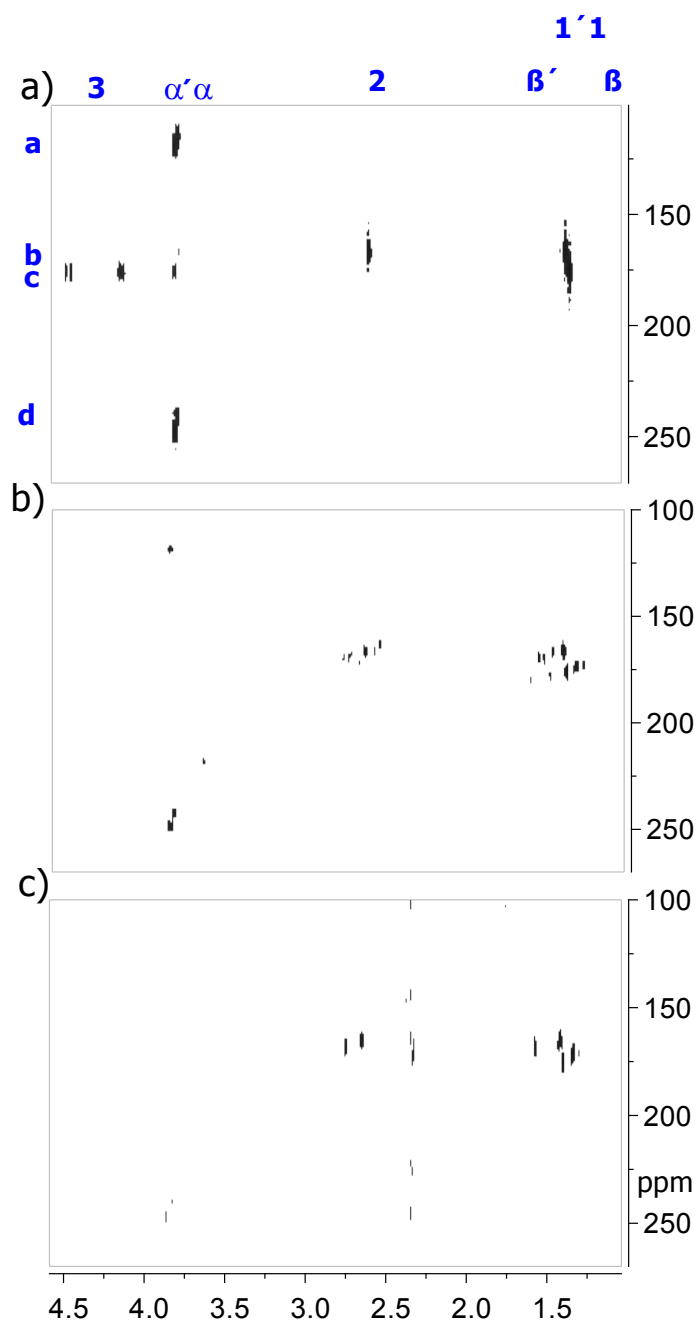


Figure S5. ^{15}N - ^1H HMBC NMR spectra of a) H_4pat^4 , b) $\text{H}_4\text{pat}^4 + 2\text{eq ZnOTf}_2$ and c) H_4pat^4 together with $[\text{Zn}^{\text{II}}_2(\text{H}_2\text{pat}^4)(\text{OH})]^+$ (measured with a smaller number of scans) in a $\text{CD}_3\text{OD}/\text{CDCl}_3$ mixture of 3:1 (10 mM), $\nu = 600\text{ MHz}$, 25°C .

F) EPR spectra

Figure S6 shows EPR spectra of the complexation of H_4pat^3 with Cu^{II} in MeOH at 140K (different $H_4pat^3 : Cu^{II} : MeO^-$ ratios). In contrast to similar experiments with other patellamide derivatives,² at low $[Cu^{II}]$ and with $[MeO^-] < 1$ eq., a mononuclear complex is observed (Figure 6a, see also Figure S7, simulation with XSophe,³ parameters, see Table S2; the hyperfinecoupling was simulated with two different types of N atoms – an amide and to imidazoles), indicating less cooperativity in Cu^{II} complexation. With $[Cu^{II}] > 0.5$ eq. dinuclear complexes are formed (see Figure 6b,c).

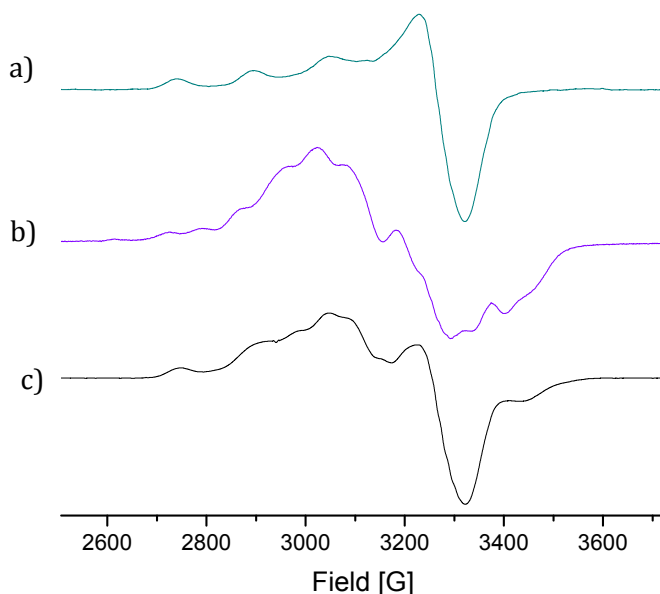


Figure S6. EPR spectroscopy with H_4pat^3 : traces of selected EPR spectra (140 K, 1 mM in MeOH) at distinct $H_4pat^3 : Cu^{II} : OMe^-$ ratios; a) 1 : 0.5 : 0.5, $\nu = 9.445927$ GHz, b) 1 : 2 : 2, $\nu = 9.440451$ GHz, c) 1 : 2 : 4, $\nu = 9.452096$ GHz.

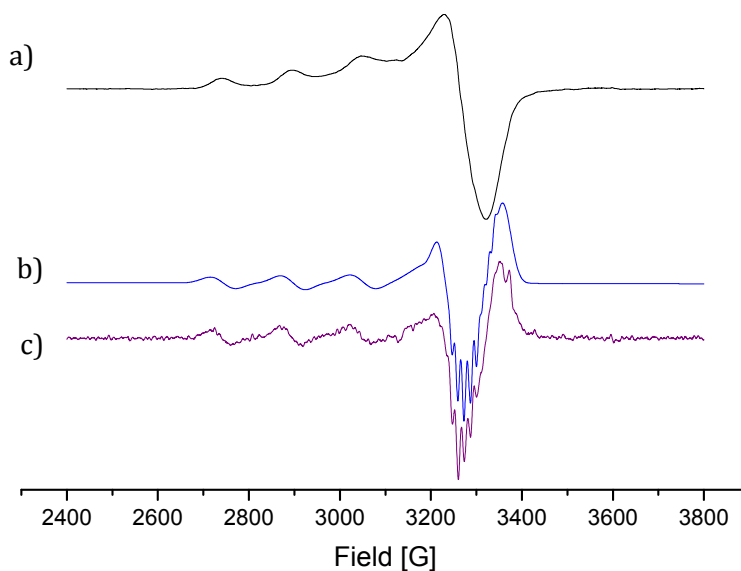


Figure S7. EPR spectra of $[\text{Cu}(\text{H}_3\text{pat}^3)(\text{OH})]$ (see Figure S6a); a) first derivative spectrum, b) second derivative spectrum, c) second derivative simulated spectrum; 140 K, 1 mM in MeOH, $\nu = 9.445927$ GHz.

At $\text{H}_4\text{pat}^3 : \text{Cu}^{\text{II}} : \text{MeO}^- = 1 : 2 : 2$, the EPR spectrum shows a single dinuclear Cu^{II} complex (Figure S8). The stoichiometry $[\text{Cu}^{\text{II}}_2(\text{H}_2\text{pat}^3)(\text{OH})]^+$ also emerges from ESI-MS (Figure S3e). The formally forbidden $\Delta m_s = 2$ transitions that are typical for dicopper(II) complexes are detected but not well resolved. The simulated spin hamiltonian parameters are given in Table S1 (simulation with Molecular Sophe⁴). The $\text{Cu}^{\text{II}} \cdots \text{Cu}^{\text{II}}$ distance is longer than in a structurally related, well characterized analogue,⁵ i.e. the hydroxide probably is terminal.²

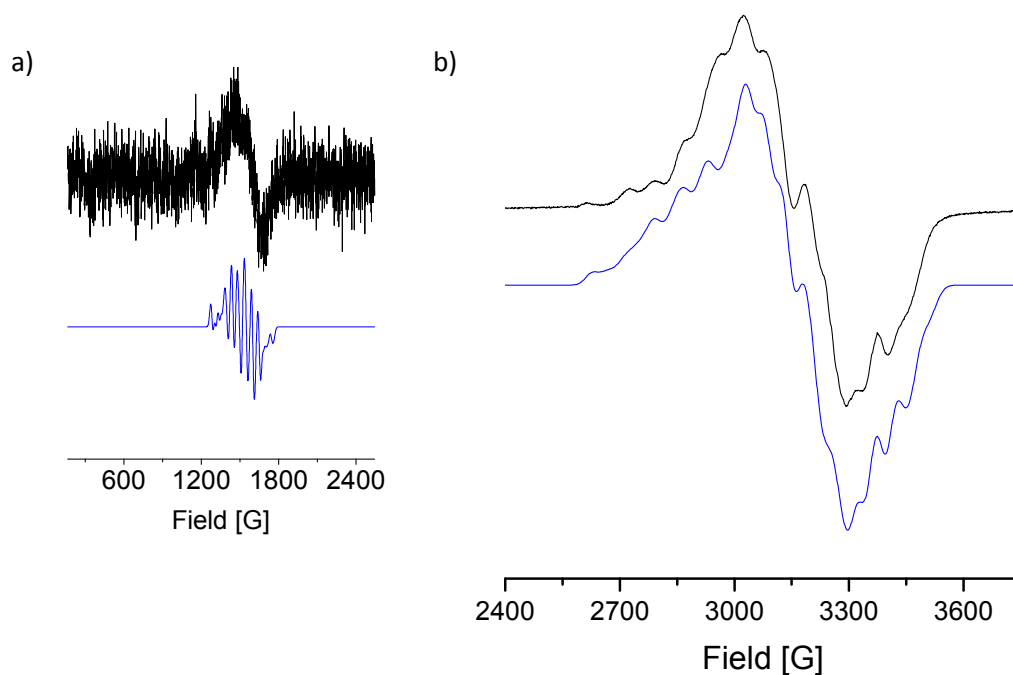


Figure S8. EPR spectra of $[\text{Cu}^{\text{II}}_2(\text{H}_2\text{pat}^3)(\text{OH})]^+$; a) $\Delta m_s = 2$ region and b) $\Delta m_s = 1$ region; measured (black) and simulated (blue; 140 K, 1 mM in MeOH, $\nu = 9.440451$ GHz).

Table S1. Spin Hamiltonian and structural parameters for $[\text{Cu}^{\text{II}}_2(\text{H}_2\text{pat}^3)(\text{OH})]^+$ from the simulation of the EPR spectra in Figure S8.

	Cu_a	Cu_b		
g_x	2.035	2.055	r [Å]	5.210
g_y	2.150	2.155	χ [°]	17
g_z	2.286	2.215		
A_x [10^{-4}cm^{-1}]	125	25	τ [°]	47
A_y [10^{-4}cm^{-1}]	65	110		
A_z [10^{-4}cm^{-1}]	212	120	ρ [°]	17

Table S2. Spin Hamiltonian parameters for $[\text{Cu}^{\text{II}}(\text{H}_3\text{pat}^3)(\text{OH})]$ and $[\text{Cu}^{\text{II}}\text{Zn}^{\text{II}}(\text{H}_2\text{pat}^3)(\text{OH})]^+$ from the simulation of the EPR spectra in Figure S7 and S10.

	$[\text{Cu}^{\text{II}}\text{Zn}^{\text{II}}(\text{H}_2\text{pat}^3)(\text{OH})]^+$	$[\text{Cu}^{\text{II}}(\text{H}_3\text{pat}^3)(\text{OH})]$	superhyperfine coupling [10^{-4}cm^{-1}]		
g_x	2.046	2.048	$A_x(N_{\text{im}})$	12.1	7.2
g_y	2.078	2.076	$A_y(N_{\text{im}})$	7.0	11.6
g_z	2.280	2.269	$A_z(N_{\text{im}})$	12.9	13.0
A_x [10^{-4}cm^{-1}]	13.4	6.3	$A_x(N_{\text{am}})$	6.7	12.1
A_y [10^{-4}cm^{-1}]	11.5	6.8	$A_y(N_{\text{am}})$	11.0	7.9
A_z [10^{-4}cm^{-1}]	155.0	159.0	$A_z(N_{\text{am}})$	13.2	13.1

In order to compare the solution chemistry with that used for the phosphoester hydrolysis, EPR spectra of H_4pat^3 and Cu^{II} were also recorded in methanol-aqueous buffer mixtures (buffer : $\text{MeOH} = 1 : 3$, $[\text{Cu}^{\text{II}}] = 5 \text{ mM}$). The spectra in Figure S9 suggest that at $\text{pH} = 6.5$ (Figure S9a), a mononuclear Cu^{II} complex forms, and at the higher $\text{pH} = 9.5$, a more complex spectrum of a dinuclear complex is observed (Figure 9b).

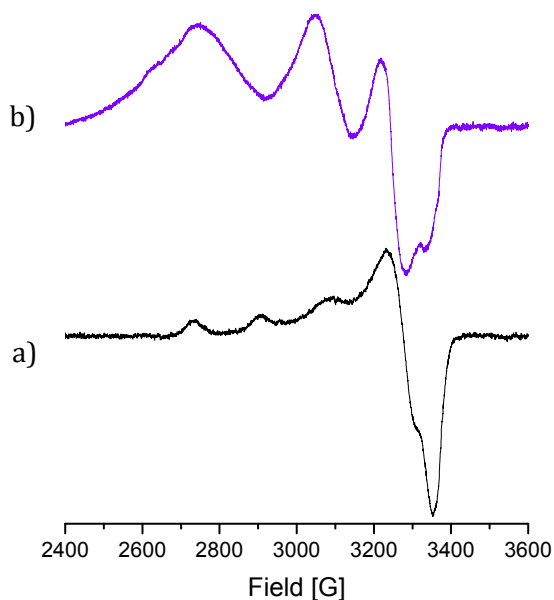


Figure S9. EPR spectra of 5 mM frozen solutions of H_4pat^3 + 0.5 eq. of copper(II) triflate and 1.5 eq. of $\text{Zn}(\text{OTf})_2$ in methanol/ buffer mixtures; a) $\text{pH} 6.5$, $\nu = 9.444516 \text{ GHz}$, b) $\text{pH} 9.5$, $\nu = 9.445288 \text{ GHz}$, (140 K, 5 mM in buffer / $\text{MeOH} 1 : 3$)

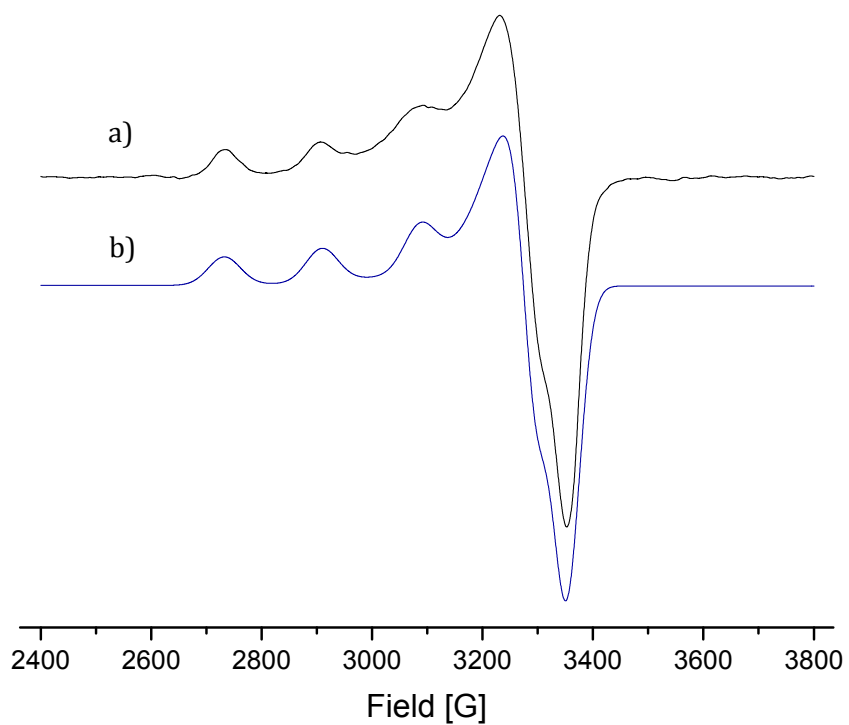


Figure S10. EPR spectrum of H_4pat^3 + 0.5 eq. of $\text{Cu}(\text{OTf})_2$ and 1.5 eq. $\text{Zn}(\text{OTf})_2$ at pH 6.5: a) measured and b) simulated (140 K, 5 mM in aqueous buffer : MeOH = 1 : 3, ν = 9.444516 GHz).

Table S3. Spin Hamiltonian parameters for $[\text{Cu}^{\text{II}}\text{Zn}^{\text{II}}(\text{H}_2\text{pat}^3)(\text{OH})]^+$ from the simulation of the EPR spectra in Figure S10.

	pH 6.5	$[\text{Cu}^{\text{II}}\text{Zn}^{\text{II}}(\text{H}_2\text{pat}^3)(\text{OH})]^+$
g_x	2.054	2.046
g_y	2.077	2.078
g_z	2.250	2.280
A_x [10^{-4}cm^{-1}]	4.7	13.4
A_y [10^{-4}cm^{-1}]	17.1	11.5
A_z [10^{-4}cm^{-1}]	185.7	155.0

For the formation of heterodinuclear $\text{Cu}^{\text{II}}\text{-Zn}^{\text{II}}$ complexes with the all-*S* configured ligand H_4pat^2 a single mononuclear species was not expected due to cooperativity,² and $\text{Zn}(\text{OTrif})_2$ was therefore titrated to a solution that already contained a mixture of mono- and dinuclear Cu^{II} complexes (Figure S11). The blue spectrum shows a mixture of a dicopper(II) species and a mononuclear complex². Upon addition of 4 equivalents of Zn^{II} and one equivalent of OMe^- , the black spectrum in Figure S11 obtains, and this is assigned to a single monocopper(II) complex. Based on the simulation of this spectrum (Figure S12, parameters listed in Table S4), and in comparison with the genuine monocopper(II) complex, also listed in Table S4, this spectrum is assigned to a heterodinuclear $[\text{Cu}^{\text{II}}\text{Zn}^{\text{II}}(\text{H}_2\text{pat}^2)(\text{OH})]^+$ complex (see main text).

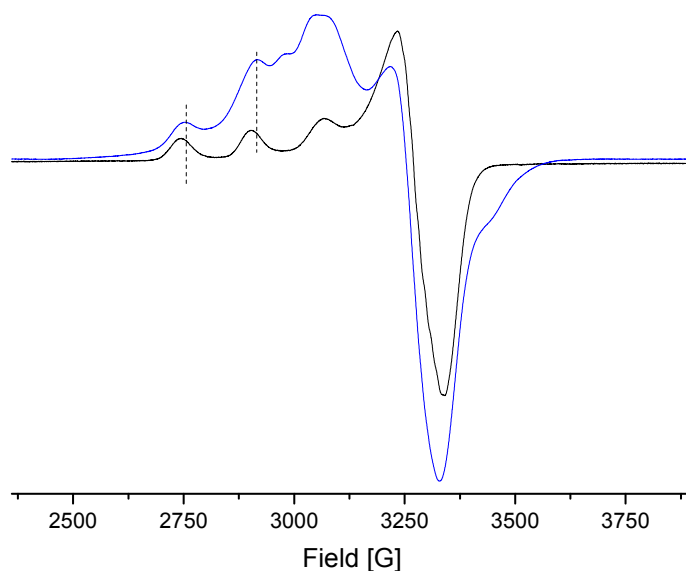


Figure S11. Overlay of selected EPR spectra at distinct $\text{H}_4\text{pat}^2 : \text{Cu}^{\text{II}} : \text{Zn}^{\text{II}} : \text{OMe}^-$ ratios; blue, 1 : 1 : 0 : 1 ($\nu = 9.447735$ GHz); black, 1 : 1 : 4 : 2 ($\nu = 9.446188$ GHz, 140 K, 1 mM in MeOH).

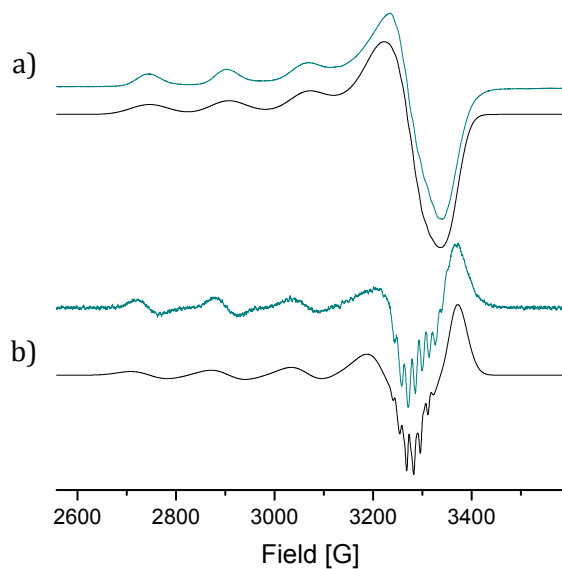


Figure S12. EPR spectra of $[\text{Cu}^{\text{II}}\text{Zn}^{\text{II}}(\text{H}_2\text{pat}^2)(\text{OH})]^+$; a) first derivative, b) second derivative spectra (exp.: turquoise, sim.: black); $\nu = 9.446188$ GHz, 140 K, 1 mM in MeOH, simulation with XSophe,³⁾.

Table S4. Spin Hamiltonian parameters for $[\text{Cu}^{\text{II}}\text{Zn}^{\text{II}}(\text{H}_2\text{pat}^2)(\text{OH})]^+$ and $[\text{Cu}^{\text{II}}\text{Zn}^{\text{II}}(\text{H}_2\text{pat}^2)(\text{OH})]$ from the simulation of the EPR spectra in Figure S12.

	$[\text{Cu}^{\text{II}}\text{Zn}^{\text{II}}(\text{H}_2\text{pat}^2)(\text{OH})]$	$[\text{Cu}(\text{H}_3\text{pat}^2)(\text{OH})]$	Superhyperfine [10^{-4}cm^{-1}]	
g_x	2.082	2.074	$A_x(N_{\text{im}})$	11.8
g_y	2.045	2.051	$A_y(N_{\text{im}})$	12.6
g_z	2.260	2.259	$A_z(N_{\text{im}})$	10.8
$A_x [10^{-4}\text{cm}^{-1}]$	13.8	14.2	$A_x(N_{\text{am}})$	11.3
$A_y [10^{-4}\text{cm}^{-1}]$	15.2	14.7	$A_y(N_{\text{am}})$	7.2
$A_z [10^{-4}\text{cm}^{-1}]$	168.6	150.0	$A_z(N_{\text{am}})$	15.4

G) UV-vis-NIR spectra

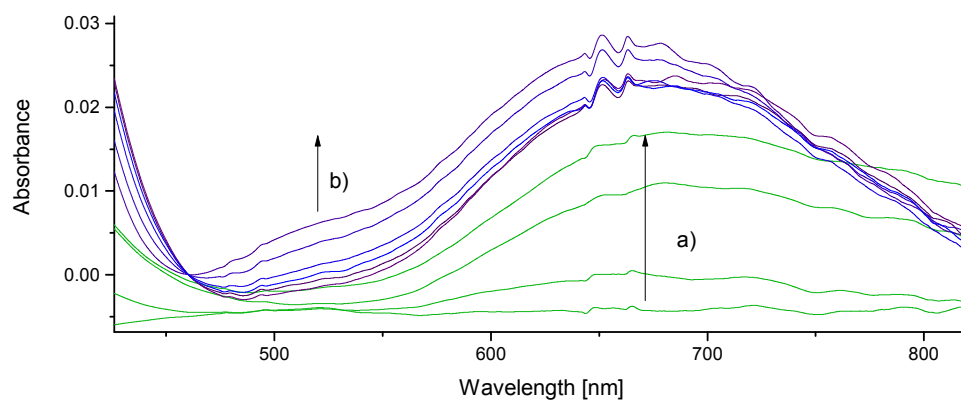


Figure S13. UV-vis titration of a) 0-0.5 eq. $\text{Cu}(\text{OTf})_2$ to H_4pat^3 and one equivalent. $\text{Zn}(\text{OTf})_2$ and b) 0-1.5 equivalents $(n\text{-Bu})_4\text{OMe}$.

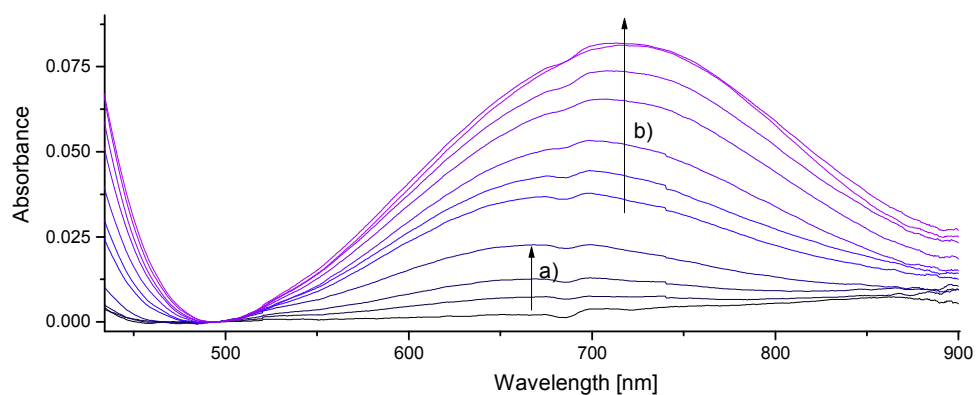


Figure S14. UV-vis titration of a) 0-0.5 equivalents $\text{Cu}(\text{OTf})_2$ to H_4pat^2 and one equivalent $\text{Zn}(\text{OTf})_2$ and b) 0-1.5 equivalents $(n\text{-Bu})_4\text{OMe}$.

H) pH profiles and Michaelis Menten plots of phosphatase models

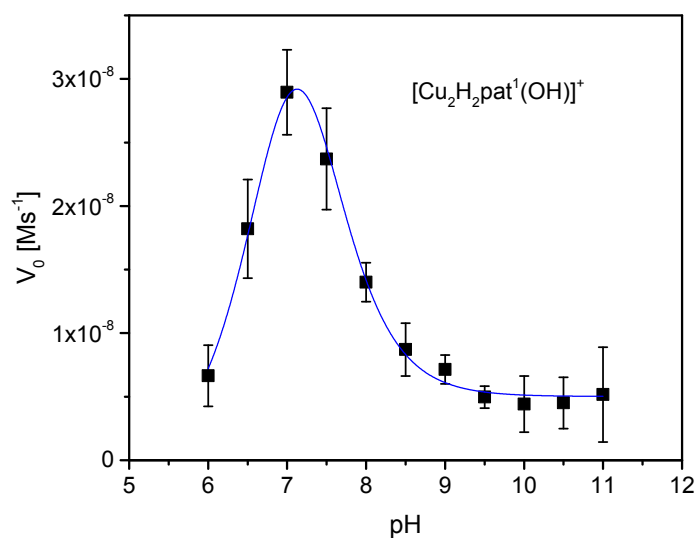


Figure S15. pH profile of BDNPP hydrolysis with $[\text{Cu}_2(\text{H}_2\text{pat}^1)(\text{OH})]^+$ ([BDNPP] 6.25 mM and [cat.] 40 μM , 25°C.). Reprinted with permission from Ref: [1]

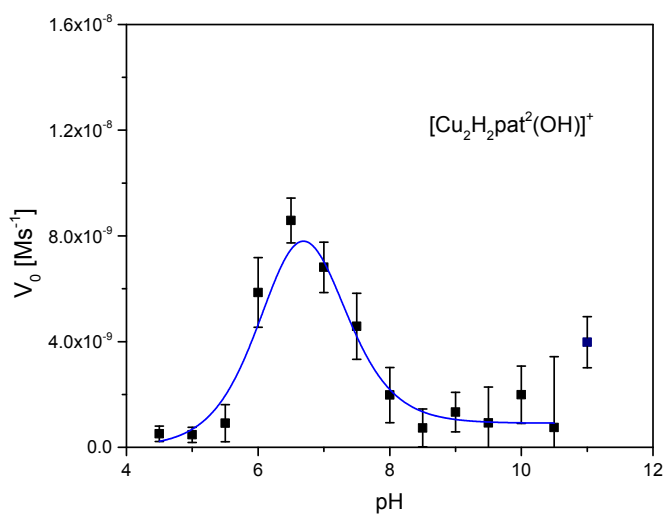


Figure S16. pH profile of BDNPP hydrolysis with $[\text{Cu}_2(\text{H}_2\text{pat}^2)(\text{OH})]^+$ ([BDNPP] = 6.25 mM and [cat] = 40 μM , 25°C.).

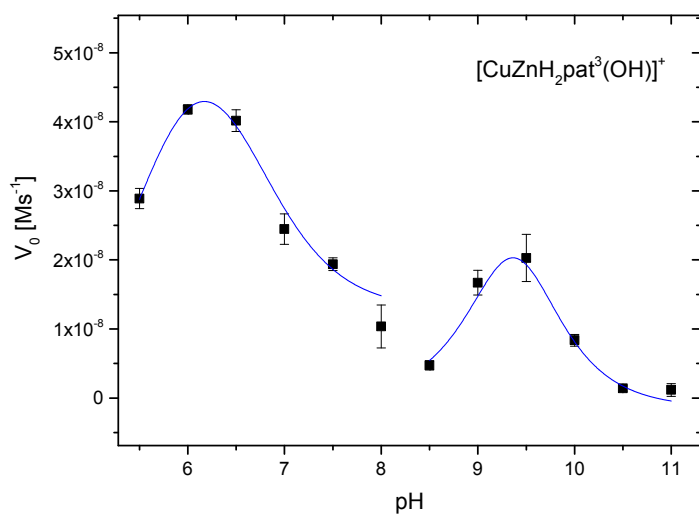


Figure S17. pH profile of the BDNPP hydrolysis with $[\text{CuZn}(\text{H}_3\text{pat}^3)(\text{OH})]^+$ (generated with $\text{Zn}(\text{OAc})_2$ instead of $\text{Zn}(\text{OTf})_2$), $[\text{BDNPP}] = 8 \text{ mM}$ and $[\text{cat}] = 15 \text{ }\mu\text{M}$, 25°C .

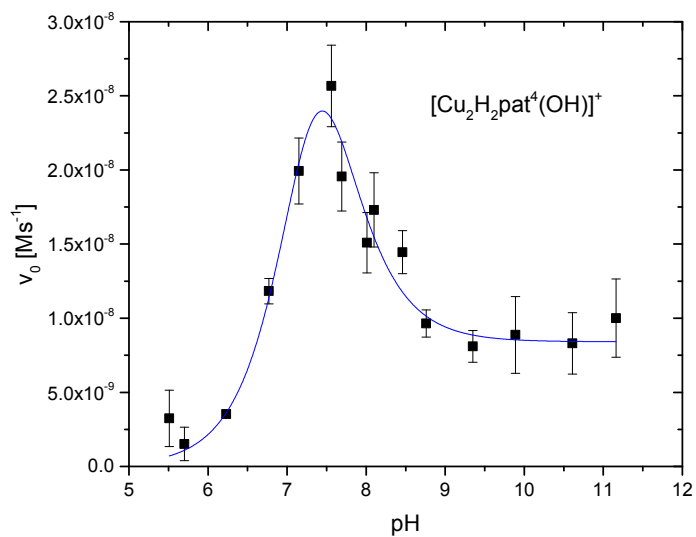


Figure S18. pH profile of the BDNPP hydrolysis with $[\text{Cu}_2(\text{H}_3\text{pat}^4)(\text{OH})]^+$, $[\text{BDNPP}] = 7 \text{ mM}$ and $[\text{cat}] = 30 \text{ }\mu\text{M}$, 25°C .

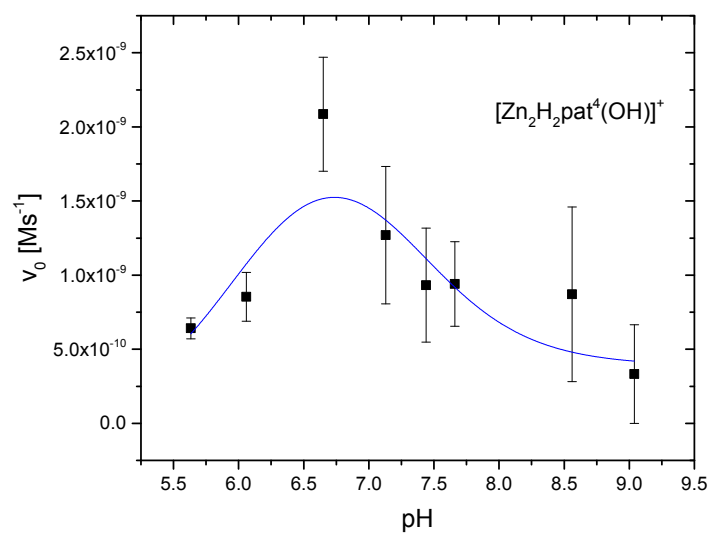


Figure S19. pH profile of the BDNPP hydrolysis with $[\text{Zn}_2(\text{H}_3\text{pat}^4)(\text{OH})]^+$, $[\text{BDNPP}] = 7 \text{ mM}$ and $[\text{cat}] = 30 \text{ }\mu\text{M}$, 25°C .

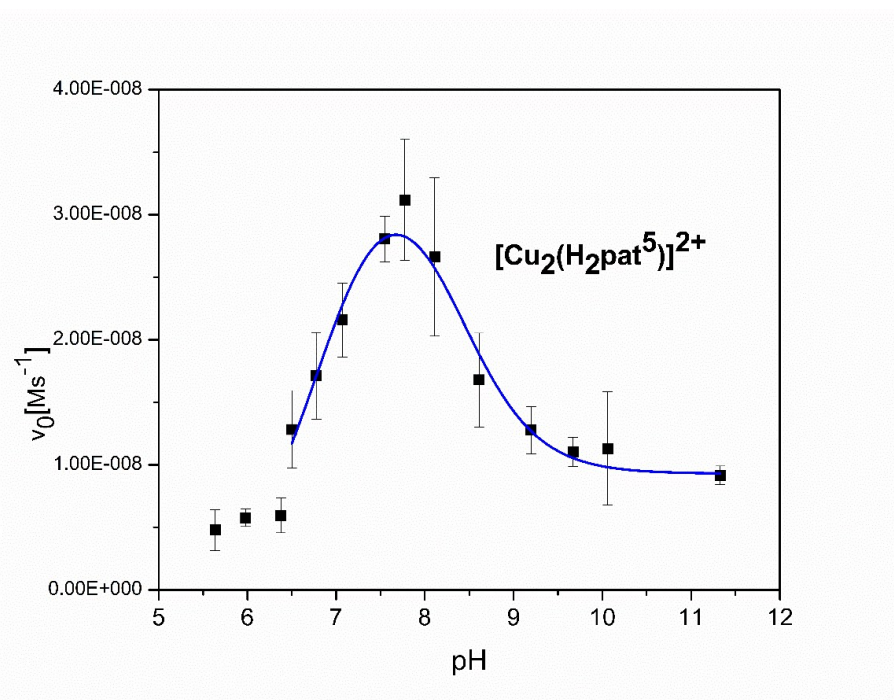


Figure S20. pH profile of the BDNPP hydrolysis with $[\text{Cu}_2(\text{H}_3\text{pat}^5)(\text{OH})]^+$, $[\text{BDNPP}] = 5 \text{ mM}$ and $[\text{cat}] = 40 \text{ }\mu\text{M}$, 25°C .

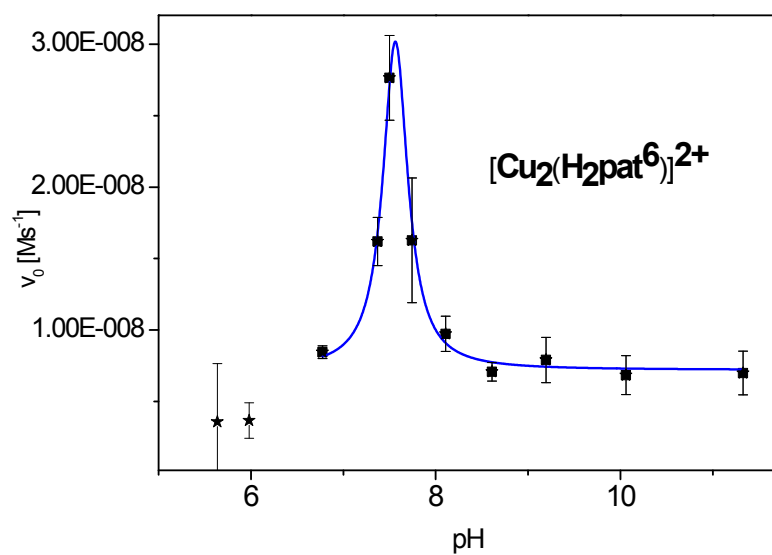


Figure S21. pH profile of the BDNPP hydrolysis with $[\text{Cu}_2(\text{H}_3\text{pat}^6)(\text{OH})]^+$, $[\text{BDNPP}] = 5 \text{ mM}$ and $[\text{cat}] = 40 \text{ }\mu\text{M}$, 25°C .

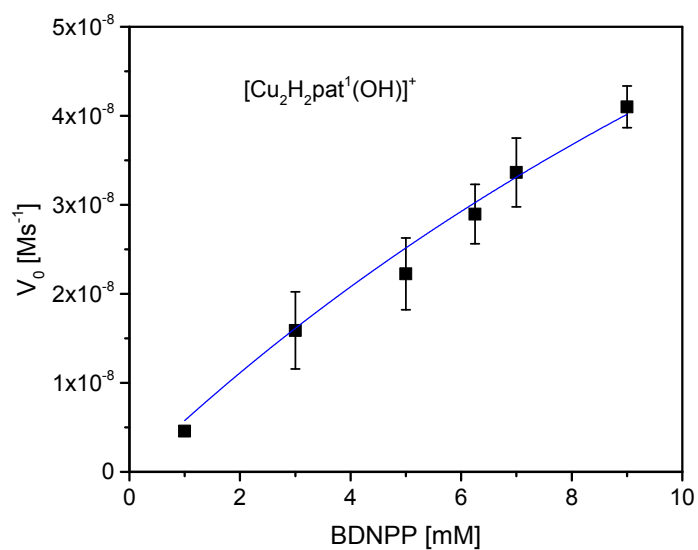


Figure S22. Michaelis-Menten measurement of $[\text{Cu}_2(\text{H}_3\text{pat}^1)(\text{OH})]^+$, $[\text{cat}] = 40 \text{ }\mu\text{M}$, 25°C . Reprinted with permission from Ref: [1].

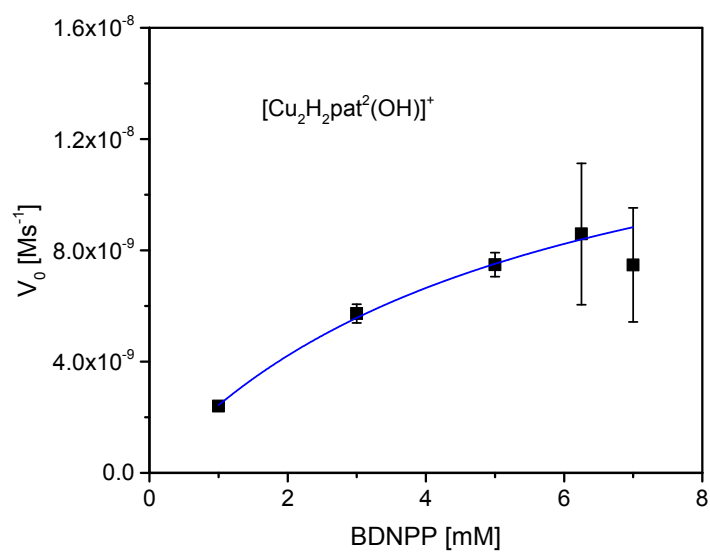


Figure S23. Michaelis-Menten measurement of $[\text{Cu}_2(\text{H}_3\text{pat}^2)(\text{OH})]^+$, $[\text{cat}] = 40 \mu\text{M}$, 25°C .

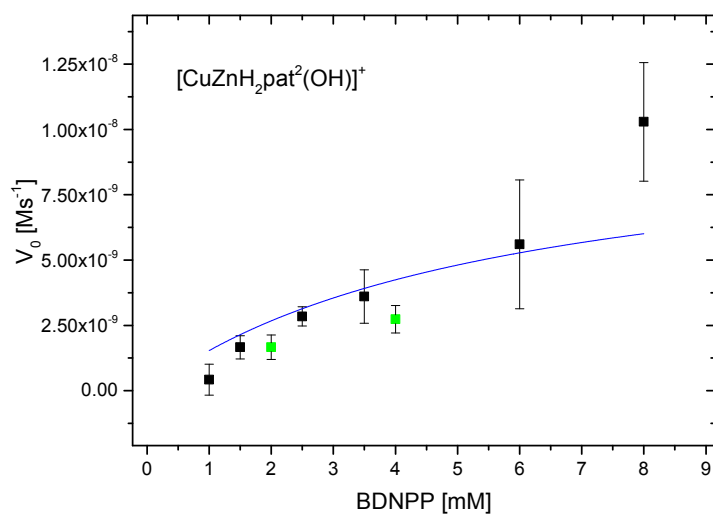


Figure S24. Michaelis-Menten measurement of $[\text{Cu}_2(\text{H}_3\text{pat}^2)(\text{OH})]^+$, $[\text{cat}] = 30 \mu\text{M}$, 25°C ; green points are masked data, not considered for fitting.

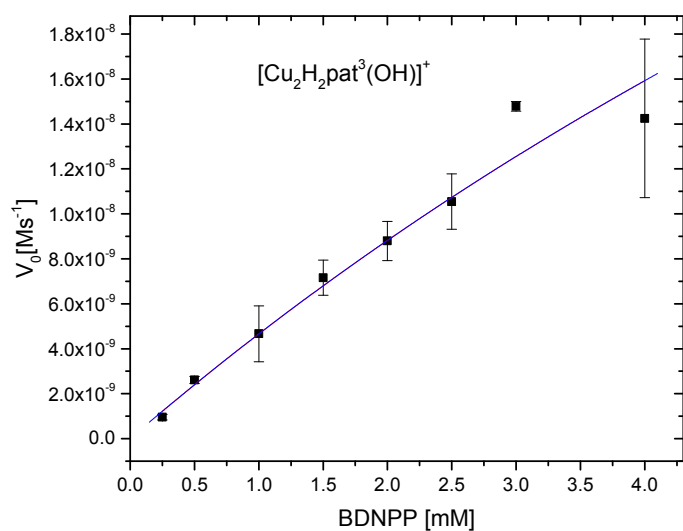


Figure S25. Michaelis-Menten measurement of $[\text{Cu}_2(\text{H}_3\text{pat}^3)(\text{OH})]^+$, $[\text{cat}] = 40 \mu\text{M}$, 25°C .

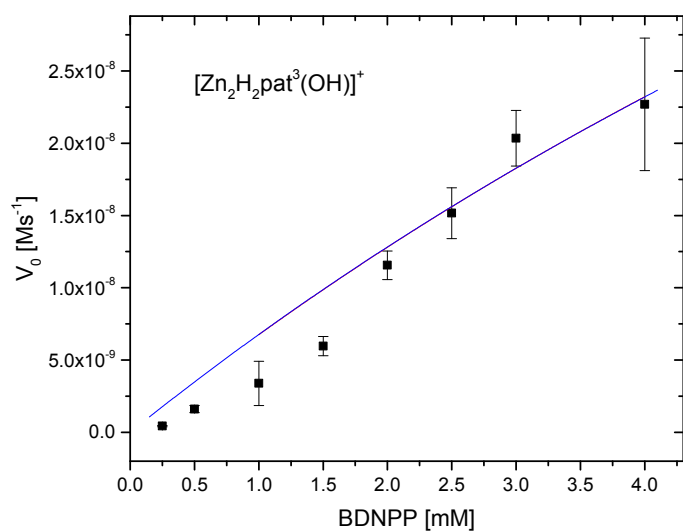


Figure S26. Michaelis-Menten measurement of $[\text{Zn}_2(\text{H}_3\text{pat}^3)(\text{OH})]^+$, $[\text{cat}] = 40 \mu\text{M}$, 25°C .

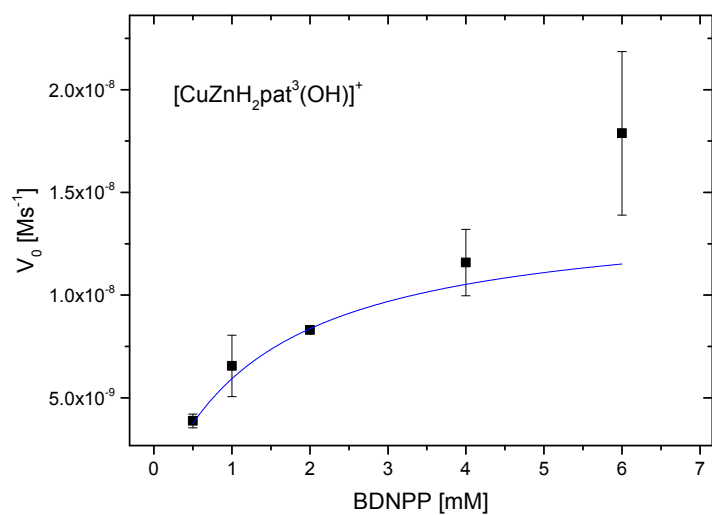


Figure S27. Michaelis-Menten measurement of $[\text{CuZn}(\text{H}_3\text{pat}^3)(\text{OH})]^+$, $[\text{cat}] = 15 \mu\text{M}$, 25°C .

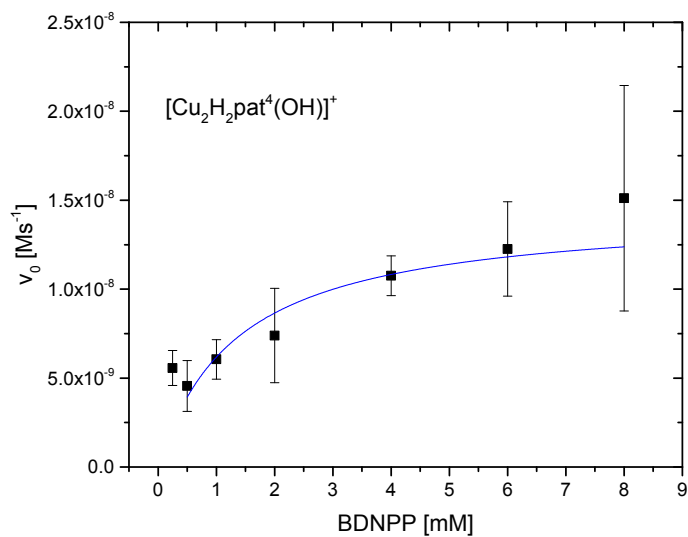


Figure S28. Michaelis-Menten measurement of $[\text{Cu}_2(\text{H}_3\text{pat}^4)(\text{OH})]^+$, $[\text{cat}] = 30 \mu\text{M}$, 25°C .

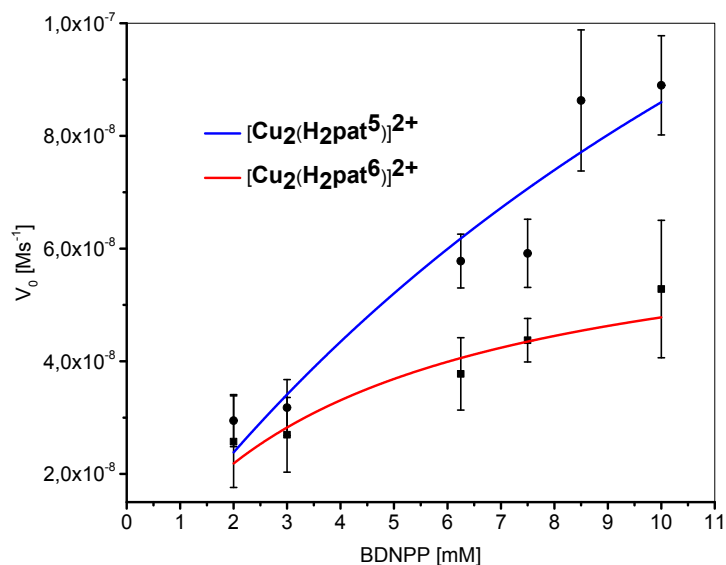


Figure S29. Overlay of Michaelis-Menten measurements of $[\text{Cu}_2(\text{H}_3\text{pat}^5)(\text{OH})]^+$ (blue) and $[\text{Cu}_2(\text{H}_3\text{pat}^6)(\text{OH})]^+$ (red), $[\text{cat}] = 30 \mu\text{M}$, 25°C .

References

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- (3) Hanson, G. R.; Gates, K. E.; Noble, C. J.; Griffin, M.; Mitchell, A.; Benson, S. J. *Inorg. Biochem.* **2004**, *98*, 903.
- (4) Hanson, G.; Bruker Biospin: Germany, Switzerland, France, U.S., 2007.
- (5) Comba, P.; Dovalil, N.; Hanson, G. R.; Linti, G. *Inorg. Chem.* **2011**, *50*, 5165.

I) MOMEc force field parameters

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STR CI	NT 6.700	1.317	Dirk Kuppert		
STR CI	CT 5.000	1.500	Dirk Kuppert		

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 STR CU1 NP 0.700 2.000 test PC
 STR CU1 NT 0.100 2.220

STR CU2	ND	0.600 1.920	
STR CU2	NP	0.600 1.940	
STR CU2	OC	0.800 1.900	
STR CU2	ONO	0.100 2.500	
STR CU2	OP	0.100 2.150	
STR CU2	OCO	0.100 2.500	pentanone
STR CU2	OW	0.100 2.500	
STR CU2	SW	0.600 2.290	
STR CU2C	ND	0.600 1.920	
STR CU2C	NP	0.600 1.940	
STR CU2C	NT	0.600 1.970	
STR CU2C	OC	0.800 1.900	
STR CU2C	OW	0.100 2.500	
STR CU2C	SW	0.600 2.290	
STR CU2P	NAX	0.34001752535970 1.93455385468332	pat ae
STR CU2P	ND	0.70808990485520 1.91211234352184	
STR CU2P	NAH	0.900 1.940	bisp energy
STR CU2P	NP	0.600 1.940	
STR CU2P	NPOA	0.200 2.400	bisp N7
STR CU2P	NT	0.600 1.970	bisp energy (1.94!)
STR CU2P	NTA	0.200 2.000	bisp N7
STR CU2P	NTOA	0.200 2.400	bisp N7
STR CU2P	OC	0.800 1.900	
STR CU2P	ONO	0.100 2.500	
STR CU2P	OP	0.100 2.150	
STR CU2P	OW	0.100 2.500	bisp energy, 0.6;1.89; Cuperoxo, 0.1;2.5
STR CU2P	OXCU	0.600 1.830	
STR CU2B	NAH	0.900 1.940	bisp energy
STR CU2B	NP	0.800 1.970	bisp
STR CU2B	NPOA	0.200 2.400	bisp N7
STR CU2B	NT	0.800 2.000	bisp energy (1.94!)

STR CU2B NTA 0.300 2.150 bisp N7
 STR CU2B NTOA 0.200 2.400 bisp N7
 STR CU2T ND 0.600 1.890
 STR CU2T NP 0.600 1.940
 STR DY3 O2 0.072 2.195
 STR DY3 OH 0.072 2.195
 STR DY3 OW 0.072 2.195
 STR ER3 O2 0.074 2.150
 STR ER3 OH 0.074 2.150
 STR EU3 O2 0.067 2.245
 STR EU3 OH 0.067 2.245
 STR FE3H OC 1.000 1.990
 STR FE3H OW 0.500 1.900
 STR FE3L NP 1.700 1.925
 STR FE3L NT 1.700 1.950
 STR FE3L C3 1.700 1.923
 STR GD3 O2 0.069 2.226
 STR GD3 OH 0.069 2.226
 STR GD3 OW 0.069 2.226
 STR H NA 6.030 0.910
 STR H NT 5.640 0.910
 STR H NTA 5.640 0.910 bisp N7
 STR H NTOA 5.640 0.910 bisp N7
 STR H OP 5.000 0.910
 STR H OW 5.000 0.910
 STR HO3 O2 0.073 2.178
 STR HO3 OH 0.073 2.178
 STR HO3 OW 0.073 2.178
 STR LA3 O2 0.049 2.409
 STR LA3 OH 0.049 2.409
 STR LA3 OW 0.049 2.409

STR LU3	O2	0.076 2.038
STR LU3	OH	0.076 2.038
STR LU3	OW	0.076 2.038
STR MN3	OC	0.300 1.950
STR NAH	H	5.000 0.910
STR NAH	NAH	1.500 1.360
STR NAH	NAX	1.500 1.360
STR ND	H	6.97300856958640 0.87801647821748
STR ND3	O2	0.058 2.320
STR ND3	OH	0.058 2.320
STR ND3	OW	0.058 2.320
STR NI2	NT	0.600 2.090
STR NI2C	NP	0.600 2.025
STR NI2C	NT	0.600 2.035
STR NI2C	OC	0.650 2.040
STR NI2P	NP	0.600 2.025
STR NI2P	NT	0.600 2.050
STR NI2T	ND	0.600 1.760
STR NI2T	NP	0.600 1.855
STR NI2T	NT	0.600 1.830 Slava/Alex
STR NOO	ONO	6.500 1.213
STR OXCO	OXCO	3.250 1.470
STR OXCU	OXCU	3.250 1.430
STR P	O2	7.297 1.448
STR P	OH	3.197 1.665
STR P	OS	3.197 1.686
STR PM3	O2	0.062 2.285
STR PM3	OH	0.062 2.285
STR PR3	O2	0.056 2.345
STR PR3	OH	0.056 2.345
STR PR3	OW	0.056 2.345

STR PT2	NB	2.540	2.010	
STR PT2	NT	2.540	2.030	
STR RH3	NT	1.750	2.050	
STR SM3	O2	0.064	2.258	
STR SM3	OH	0.064	2.258	
STR SM3	OW	0.064	2.258	
STR TB3	O2	0.071	2.213	
STR TB3	OH	0.071	2.213	
STR TI3	OC	0.800	2.080	
STR TI3	OW	0.500	2.035	
STR TI4	OCC	1.500	1.980	
STR TI4	OCCT	1.500	2.040	
STR TI4	OW	0.500	1.722	
STR TM3	O2	0.075	2.215	
STR TM3	OH	0.075	2.215	
STR V3	OC	0.500	1.920	
STR V3	OW	0.500	1.980	
STR Y3	O2	0.074	2.160	
STR Y3	OH	0.074	2.160	
STR YB3	O2	0.076	2.095	
STR YB3	OH	0.076	2.095	
STR YB3	OW	0.076	2.095	
STR ZN2	ND	0.350	2.000	
STR ZN2	NP	0.350	2.100	
STR ZN2	NT	0.350	2.220	
STR ZN2	NAX	0.300	2.003	pat ae
STR ZN2	OW	0.300	1.900	pat ae
BEN CCO	OC	OCO	00.0	2.0 dummy (bm)
BEN CCO	CT	OCO	00.0	2.0 dummy (bm)
BEN CT	CT	OC	00.0	2.0 dummy (bm)
BEN H	CT	OC	00.0	2.0 dummy (bm)

BEN CU2P CT NT 00.0 2.0 dummy (bm)
 BEN CU2P CU2P NT 00.0 2.0 dummy (bm)
 BEN CU2P NT NT 00.0 2.0 dummy (bm)
 BEN CU2P NP NT 00.0 2.0 dummy (bm)
 BEN CU2P OW NT 00.0 2.0 dummy (bm)
 BEN CU2P CA NP 00.0 2.0 dummy (bm)
 BEN CA CT NP 00.0 2.0 dummy (bm)
 BEN CU2P CU2P NP 00.0 2.0 dummy (bm)
 BEN CU2P NP NP 00.0 2.0 dummy (bm)
 BEN CU2P OW NP 00.0 2.0 dummy (bm)
 BEN CA OW OW 00.0 2.0 dummy (bm)
 BEN H CA CT 00.0 2.0 dummy (bm)
 BEN H H CT 00.0 2.0 dummy (bm)
 BEN CCO CCO CT 00.0 2.0 dummy (bm)
 BEN H H CA 00.0 2.0 dummy (bm)
 BEN CU2P CU2P OW 00.0 2.0 dummy (bm)
 BEN CU2P NT OW 00.0 2.0 dummy (bm)
 BEN CU2P NP OW 00.0 2.0 dummy (bm)
 BEN H CI H 00.000 2.045 Dirk Kuppert
 BEN CI NT CT 0.450 1.911 Dirk Kuppert
 BEN NT CI H 0.450 2.094 Dirk Kuppert
 BEN NT CI CT 0.450 2.094 Dirk Kuppert
 BEN CI NT H 0.450 2.050 Dirk Kuppert
 BEN NI CI NT 0.150 2.094 Dirk Kuppert
 BEN NT CT CI 0.450 1.911 Dirk Kuppert
 BEN CT CI H 0.450 2.094 Dirk Kuppert
 BEN CT CI NI 0.450 2.094 Dirk Kuppert
 BEN NI CO3 NI 0.050 1.571 Dirk Kuppert
 BEN NT CO3 NI 0.050 1.571 Dirk Kuppert
 BEN CI CT H 0.360 1.909 Dirk Kuppert
 BEN CI CT CT 0.450 1.911 Dirk Kuppert

BEN NI	CI	CT	0.450	2.094	Dirk Kuppert
BEN CO3	NI	CT	0.200	1.920	Dirk Kuppert
BEN CO3	NI	CI	0.400	2.150	Dirk Kuppert
BEN OR	CT	H	0.360	1.909	Dirk Kuppert
BEN CT	OW	H	0.360	1.909	Dirk Kuppert
BEN NI	CT	CT	0.450	1.911	Dirk Kuppert
BEN NI	CT	H	0.450	1.911	Dirk Kuppert
BEN C3	FE3L	C3	0.942	1.571	
BEN CB	C	NA	0.970	1.943	
BEN CB	C	O	1.110	2.248	
BEN NA	C	O	1.110	2.105	
BEN CA	CA	CA	0.970	2.094	
BEN CA	CA	CFC	0.970	2.094	
BEN CA	CA	CON	0.970	2.094	
BEN CA	CA	CT	0.450	2.094	
BEN CA	CA	H	0.450	2.094	
BEN CA	CA	NP	0.970	2.094	
BEN CA	CA	NPA	0.970	2.094	bisp N2py33
BEN CA	CA	NPOA	0.970	2.094	bisp N2py33
BEN CA	CA	NT	0.450	2.094	
BEN CA	CA	OW	0.450	2.094	bisp energy
BEN CAH	CA	CA	0.450	2.024	
BEN CAH	CA	H	0.450	2.122	
BEN CFC	CA	H	0.450	2.094	
BEN CFC	CA	NP	0.970	2.094	
BEN CI	CA	CA	0.250	2.094	
BEN CON	CA	NP	0.970	2.094	
BEN CT	CA	NP	0.450	2.094	
BEN CT	CA	NPA	0.450	2.094	bisp N2py33
BEN CT	CA	NPOA	0.450	2.094	bisp N2py33
BEN H	CA	NP	0.450	2.094	

BEN H CA NPA 0.450 2.094 bisp N2py33
 BEN H CA NPOA 0.450 2.094 bisp N2py33
 BEN NA CA NA 0.970 2.152
 BEN NA CA NT 0.970 2.025
 BEN NA CA NT 0.970 2.091
 BEN CA CA CCO 0.970 2.094 PC Demi
 BEN NP CA CCO 0.450 2.094 PC Demi
 BEN CAH CAH CA 0.150 2.122
 BEN CAH CAH CAH 0.100 1.850
 BEN CAH CAH CI 0.650 2.304
 BEN CAH CAH CT 0.65802389624957 2.27751282596100
 BEN CAH CAH H 0.450 2.215
 BEN CAH CAH NAH 0.14674105487646 1.87788908603260
 BEN CAH CAH NAX 0.12789258258110 1.90525462186666
 BEN CI CAH NAH 0.650 2.112
 BEN CT CAH NAH 0.64837303405349 2.12123504565852
 BEN CT CAH NAX 0.64556190446008 2.07369167428063
 BEN NAH CAH CA 0.150 2.292
 BEN NAH CAH H 0.350 2.094
 BEN NAH CAH NAH 0.150 1.955
 BEN SAH CAH H 0.350 2.094 thiazole
 BEN CAH SAH CAH 0.300 1.570 thiazole
 BEN SAH CAH CAH 0.120 1.955 thiazole
 BEN C CB CB 1.180 2.080
 BEN C CB NB 0.970 2.269
 BEN CB CB N* 0.970 1.854
 BEN CB CB NA 0.970 2.229
 BEN CB CB NB 0.970 1.911
 BEN NA CB N* 0.970 2.199
 BEN COC CCC COC 0.970 2.094
 BEN COC CCC H 0.970 2.094

BEN CT	CCO	OC	0.250	2.067	
BEN CT	CCO	OCO	0.250	2.067	
BEN CT	CCO	CT	0.250	2.094	pentanone
BEN OC	CCO	CCO	0.800	1.993	
BEN OC	CCO	OC	0.250	2.094	
BEN OC	CCO	OCO	0.250	2.149	
BEN OCO	CCO	CCO	0.950	2.115	
BEN OCO	CCO	CA	0.250	2.067	PC Demi
BEN OC	CCO	CA	0.250	2.067	PC Demi
BEN CA	CFC	CA	0.970	2.094	
BEN CA	CFC	CFC	0.450	2.094	
BEN CA	CFC	COC	0.350	2.094	
BEN CA	CFC	NP	0.970	2.094	
BEN CFC	CFC	NP	0.450	2.094	
BEN CA	CI	H	0.450	2.094	
BEN CAH	CI	H	0.450	2.094	
BEN CAH	CI	NI	0.150	2.094	
BEN NI	CI	CA	0.150	2.094	
BEN NI	CI	H	0.450	2.094	
BEN H	CK	N*	0.490	2.148	
BEN H	CK	NB	0.490	2.148	
BEN NAX	CU2P	ND	0.050	1.571	analog NAH CU2P NAH pat ae
BEN NAX	CU2P	NAX	0.050	1.571	analog NAH CU2P NAH pat ae
BEN NAX	CU2P	OW	0.050	1.571	analog NAH CU2P NAH pat ae
BEN NB	CK	N*	0.970	1.960	
BEN NP	CO2	NP	0.023	1.571	
BEN NP	CO2	NT	0.020	1.571	bisp N2py4
BEN NT	CO2	NT	0.017	1.571	
BEN NP	CO3	NP	0.050	1.571	
BEN NP	CO3	NT	0.050	1.571	
BEN NT	CO3	NT	0.050	1.571	

BEN NP	CO3C	NP	0.050	1.571	
BEN NP	CO3C	NT	0.050	1.571	
BEN OC	CO3C	NP	0.050	1.571	PC Demi
BEN NT	CO3C	NT	0.050	1.571	
BEN NT	CO3C	OC	0.045	1.571	
BEN NT	CO3C	OCC	0.045	1.571	
BEN OC	CO3C	OC	0.040	1.571	
BEN OCC	CO3C	OCC	0.040	1.571	
BEN CCC	COC	CFC	0.350	2.094	
BEN CCC	COC	CT	0.350	2.094	
BEN CCC	COC	OCC	0.970	2.094	
BEN CCC	COC	OCCT	0.970	2.094	
BEN CFC	COC	OCC	0.350	2.094	
BEN CFC	COC	OCCT	0.350	2.094	
BEN CT	COC	OCC	0.350	2.094	
BEN CT	COC	OCCT	0.350	2.094	
BEN CA	CON	ND	0.250	2.067	
BEN CA	CON	OCO	0.250	2.067	
BEN CT	CON	ND	0.250	2.067	
BEN CT	CON	OCO	0.250	2.067	
BEN ND	CON	OCO	0.24733301373645	2.07864999382910	
BEN NP	CR3	NP	0.025	1.571	
BEN NP	CR3	NT	0.025	1.571	
BEN NT	CR3	NT	0.025	1.571	
BEN CA	CT	CA	0.450	1.911	
BEN CA	CT	CT	0.450	1.911	
BEN CA	CT	H	0.360	1.909	
BEN CA	CT	ND	0.450	1.911	
BEN CA	CT	NTOA	0.450	1.911	bispidine
BEN CA	CT	NT	0.450	1.911	
BEN CA	CT	OP	0.450	1.911	

BEN CA	CT	OW	0.450	1.911	
BEN CAH	CT	CA	0.450	1.911	
BEN CAH	CT	CAH	0.450	1.960	
BEN CAH	CT	CT	0.45249176067951	1.89567506884792	
BEN CAH	CT	H	0.34332745636862	1.88571950759416	
BEN CAH	CT	NT	0.450	1.911	
BEN CAH	CT	OP	0.450	1.911	
BEN CAH	CT	OW	0.450	1.911	
BEN CCO	CT	CCO	0.450	1.911	
BEN CCO	CT	CT	0.450	1.911	
BEN CCO	CT	H	0.360	1.909	
BEN CCO	CT	ND	0.450	1.911	
BEN CCO	CT	NT	0.450	1.911	
BEN COC	CT	H	0.350	1.909	
BEN CON	CT	CON	0.450	1.911	
BEN CON	CT	CT	0.450	1.911	
BEN CON	CT	H	0.360	1.909	
BEN CON	CT	NT	0.450	1.911	
BEN CT	CT	CT	0.44733334760329	1.90848409823545	
BEN CT	CT	H	0.36495015069721	1.91063562623086	
BEN CT	CT	N*	0.500	1.909	
BEN CT	CT	NAH	0.450	1.911	
BEN CT	CT	ND	0.43912703535736	1.90180720658024	
BEN CT	CT	NOO	0.450	1.911	
BEN CT	CT	NT	0.450	1.911	
BEN CT	CT	NTA	0.450	1.911	bisp N7
BEN CT	CT	NTOA	0.450	1.911	bisp N7
BEN CT	CT	OR	0.450	1.909	Dirk Kuppert
BEN CT	CT	OW	0.450	1.911	
BEN CT	CT	SW	0.690	1.911	
BEN H	CT	H	0.32165986422603	1.90219619773278	

BEN H	CT	N*	0.360 1.909
BEN H	CT	ND	0.35550697047991 1.85862611774370
BEN H	CT	NT	0.360 1.909
BEN H	CT	NTA	0.360 1.909 bisp N7
BEN H	CT	NTOA	0.360 1.909 bisp N7
BEN H	CT	OW	0.360 1.909
BEN H	CT	SW	0.450 1.911
BEN NAH	CT	H	0.35211480254925 1.90257250532312
BEN NAH	CT	OP	0.450 1.885
BEN NAH	CT	OW	0.450 1.885
BEN NI	CT	CT	0.450 1.911
BEN NI	CT	H	0.450 1.911
BEN NT	CT	NT	0.450 1.911
BEN OS	CT	H	0.485 1.911
BEN CT	CTO	CTO	0.450 1.920
BEN H	CTO	H	0.320 1.911
BEN ND	CU2	ND	0.013 1.571
BEN ND	CU2	NP	0.013 1.571
BEN ND	CU2	NT	0.013 1.571
BEN ND	CU2	OW	0.007 1.571
BEN NP	CU2	NP	0.013 1.571
BEN NP	CU2	NT	0.013 1.571
BEN NP	CU2	ONO	0.007 1.571
BEN NP	CU2	OW	0.007 1.571
BEN NP	CU2	SW	0.013 1.571
BEN NT	CU2	NT	0.013 1.571
BEN NT	CU2	ONO	0.007 1.571
BEN NT	CU2	OW	0.007 1.571
BEN OW	CU2	OCO	0.002 3.141 pentanone
BEN NT	CU2	OCO	0.007 1.571 pentanone
BEN CU2	OCO	CU2	0.050 2.094

BEN NT	CU2	SW	0.013	1.571	
BEN ONO	CU2	ONO	0.002	3.141	
BEN ONO	CU2	OW	0.002	1.571	
BEN ONO	CU2	SW	0.007	1.571	
BEN OW	CU2	OW	0.002	3.141	
BEN OW	CU2	SW	0.007	1.571	
BEN SW	CU2	SW	0.013	1.571	
BEN CU2P	OP	CU2P	0.050	2.094	pat ae
BEN ZN2	OP	ZN2	0.050	2.094	pat ae
BEN ND	CU2C	ND	0.013	1.571	
BEN ND	CU2C	NP	0.013	1.571	
BEN ND	CU2C	NT	0.013	1.571	
BEN ND	CU2C	OC	0.015	1.571	
BEN ND	CU2C	OW	0.007	1.571	
BEN NP	CU2C	NP	0.013	1.571	
BEN NP	CU2C	NT	0.013	1.571	
BEN NP	CU2C	ONO	0.007	1.571	
BEN NP	CU2C	OW	0.007	1.571	
BEN NP	CU2C	SW	0.013	1.571	
BEN NT	CU2C	NT	0.013	1.571	
BEN NT	CU2C	OC	0.015	1.571	
BEN NT	CU2C	ONO	0.007	1.571	
BEN NT	CU2C	OW	0.007	1.571	
BEN NT	CU2C	SW	0.013	1.571	
BEN OC	CU2C	OC	0.017	1.571	
BEN OC	CU2C	OW	0.009	1.571	
BEN ONO	CU2C	ONO	0.002	3.141	
BEN ONO	CU2C	OW	0.002	1.571	
BEN ONO	CU2C	SW	0.007	1.571	
BEN OW	CU2C	OW	0.002	3.141	
BEN OW	CU2C	SW	0.007	1.571	

BEN SW	CU2C	SW	0.013	1.571	
BEN ND	CU2P	ND	0.013	1.571	
BEN ND	CU2P	NP	0.013	1.571	
BEN ND	CU2P	NT	0.013	1.571	
BEN ND	CU2P	OW	0.007	1.571	
BEN NP	CU2P	NP	0.013	1.571	
BEN NP	CU2P	NT	0.013	1.571	
BEN NP	CU2P	NTA	0.013	1.571	bisp N7
BEN NP	CU2P	NTOA	0.013	1.571	bisp N7
BEN NPOA	CU2P	NTOA	0.013	1.571	bisp N7
BEN NAH	CU2P	NAH	0.013	1.571	bisp energy
BEN NT	CU2P	NAH	0.013	1.571	bisp energy
BEN NTA	CU2P	NAH	0.013	1.571	bisp N7
BEN NP	CU2P	ONO	0.007	1.571	
BEN NP	CU2P	OW	0.007	1.571	
BEN NP	CU2P	SW	0.013	1.571	
BEN NT	CU2P	OXCU	0.007	1.571	Cuperoxo
BEN NP	CU2P	OXCU	0.007	1.571	Cuperoxo
BEN NT	CU2P	NT	0.013	1.571	
BEN NTA	CU2P	NT	0.013	1.571	bisp N7
BEN NTOA	CU2P	NT	0.013	1.571	bisp N7
BEN NPOA	CU2P	NT	0.013	1.571	bisp N2py33
BEN NPOA	CU2P	NP	0.013	1.571	bisp N2py33
BEN NT	CU2P	OC	0.015	1.571	
BEN NT	CU2P	ONO	0.007	1.571	
BEN NT	CU2P	OW	0.007	1.571	
BEN NT	CU2P	SW	0.013	1.571	
BEN OC	CU2P	OC	0.017	1.571	
BEN OC	CU2P	OW	0.009	1.571	
BEN ONO	CU2P	ONO	0.002	3.141	
BEN ONO	CU2P	OW	0.002	1.571	

BEN ONO CU2P SW 0.007 1.571
 BEN OW CU2P OW 0.002 3.141
 BEN OW CU2P SW 0.007 1.571
 BEN SW CU2P SW 0.013 1.571
 BEN NP CU2B NP 0.013 1.571
 BEN NP CU2B NT 0.013 1.571
 BEN NP CU2B NTA 0.013 1.571 bisp N7
 BEN NP CU2B NTOA 0.013 1.571 bisp N7
 BEN NPOA CU2B NTOA 0.013 1.571 bisp N7
 BEN NAH CU2B NAH 0.013 1.571 bisp energy
 BEN NT CU2B NAH 0.013 1.571 bisp energy
 BEN NTA CU2B NAH 0.013 1.571 bisp N7
 BEN NT CU2B NT 0.013 1.571
 BEN NTA CU2B NT 0.013 1.571 bisp N7
 BEN NTOA CU2B NT 0.013 1.571 bisp N7
 BEN NPOA CU2B NT 0.013 1.571 bisp N2py33
 BEN NPOA CU2B NP 0.013 1.571 bisp N2py33
 BEN NP FE3L NP 0.042 1.571
 BEN NP FE3L NT 0.042 1.571
 BEN NT FE3L NT 0.042 1.571
 BEN NT CU1 NT 0.000 1.571 test PC
 BEN NP CU1 NT 0.000 1.571 test PC
 BEN NP CU1 NP 0.000 1.571 test PC
 BEN CB N* CK 0.970 1.859
 BEN CB N* CT 0.970 2.196
 BEN CK N* CT 0.970 2.248
 BEN C NA CA 0.970 2.206
 BEN C NA H 0.490 2.039
 BEN CA NA CB 0.970 1.958
 BEN CA NA H 0.490 2.059
 BEN CAH NAH CAH 0.16210787602085 1.91418712029035

BEN CAH NAH CT 0.61164298134150 2.18562238963547
 BEN CAH NAH CU2P 0.050 2.147 bisp (0.2)
 BEN CAH NAH CU2B 0.050 2.147 bisp
 BEN CAH NAH H 0.350 2.094
 BEN CAH NAH NAH 0.200 1.885
 BEN CU2P NAH NAH 0.200 2.269
 BEN NAH NAH CT 0.650 2.094
 BEN NAH NAH H 0.350 2.094
 BEN NAX NAH CAH 0.200 1.885
 BEN NAX NAH CT 0.650 2.094
 BEN CAH NAX CU2P 0.100 2.147
 BEN CAH NAX NAH 0.200 1.823
 BEN CU2P NAX NAH 0.100 2.304
 BEN CB NB CK 0.970 1.841
 BEN PT2 NB CB 0.300 2.221
 BEN PT2 NB CK 0.300 2.221
 BEN CT ND CON 0.26792463786882 2.03348589213472
 BEN CU2 ND CON 0.200 2.094
 BEN CU2 ND CT 0.200 2.094
 BEN CU2C ND CON 0.200 2.094
 BEN CU2C ND CT 0.200 2.094
 BEN CU2P ND CON 0.200 2.094
 BEN CU2P ND CT 0.200 2.094
 BEN CU2P OW CA 0.200 2.094 bisp energy
 BEN CU2B OW CA 0.200 2.094 bisp energy
 BEN CI NI CT 0.450 2.094
 BEN CI NI CU2P 0.100 2.356
 BEN CT NI CI 0.450 2.007
 BEN CT NI CU2P 0.200 1.920
 BEN CU1 NI CI 0.100 2.356
 BEN CU1 NI CT 0.100 1.912

BEN NP	NI2	NT	0.025	1.571	
BEN NT	NI2	NT	0.025	1.571	
BEN NP	NI2C	NP	0.025	1.571	
BEN NP	NI2C	NT	0.025	1.571	
BEN NP	NI2C	OC	0.026	1.571	
BEN NT	NI2C	NT	0.025	1.571	
BEN NT	NI2C	OC	0.026	1.571	
BEN OC	NI2C	OC	0.027	1.571	
BEN NP	NI2P	NP	0.025	1.571	
BEN NP	NI2P	NT	0.025	1.571	
BEN NT	NI2P	NT	0.025	1.571	
BEN ND	NI2T	ND	0.025	1.571	Slava/Alex
BEN NT	NI2T	ND	0.025	1.571	Slava/Alex
BEN NT	NI2T	NT	0.025	1.571	Slava/Alex
BEN CT	NOO	ONO	0.450	2.059	
BEN ONO	NOO	ONO	0.650	2.164	
BEN CA	NP	CA	0.970	2.094	
BEN CA	NPOA	CA	0.970	2.094	bisp N2py33
BEN CA	NP	CFC	0.970	2.094	
BEN CFC	NP	CFC	0.970	2.094	
BEN CO2	NP	CA	0.200	2.094	
BEN CO2	NP	CFC	0.200	2.094	
BEN CO3	NP	CA	0.200	2.094	
BEN CO3	NP	CFC	0.200	2.094	
BEN CO3	NP	CT	0.200	2.094	
BEN CO3C	NP	CA	0.200	2.094	
BEN CO3C	NP	CFC	0.200	2.094	
BEN CO3C	NP	CT	0.200	2.094	
BEN CR3	NP	CA	0.200	2.094	
BEN CR3	NP	CFC	0.200	2.094	
BEN CU2	NP	CA	0.200	2.094	

BEN CU2 NP CFC 0.200 2.094
 BEN CU2C NP CA 0.200 2.094
 BEN CU2C NP CFC 0.200 2.094
 BEN CU2P NP CA 0.050 2.094 bisp (0.2)
 BEN CU2P NOAP CA 0.050 2.094 bisp (0.2)
 BEN CU2B NP CA 0.050 2.094 bisp (0.2)
 BEN CU2B NOAP CA 0.050 2.094 bisp (0.2)
 BEN CU2P NP CFC 0.200 2.094
 BEN CU1 NP CA 0.200 2.094 test PC
 BEN FE3L NP CA 0.200 2.094
 BEN FE3L NP CFC 0.200 2.094
 BEN NI2C NP CA 0.200 2.094
 BEN NI2C NP CFC 0.200 2.094
 BEN NI2P NP CA 0.200 2.094
 BEN NI2P NP CFC 0.200 2.094
 BEN CA NT CT 0.450 1.911
 BEN CA NT H 0.450 1.909
 BEN CO2 NT CT 0.200 1.920
 BEN CO2 NT H 0.100 1.915
 BEN CO3 NT CA 0.200 1.920
 BEN CO3 NT CT 0.200 1.920
 BEN CO3 NT H 0.100 1.915
 BEN CO3C NT CA 0.200 1.920
 BEN CO3C NT CT 0.200 1.920
 BEN CO3C NT H 0.100 1.915
 BEN CR3 NT CT 0.200 1.920
 BEN CR3 NT H 0.100 1.915
 BEN CT NT CT 0.450 1.911
 BEN CT NTA CT 0.450 1.911 bisp N7
 BEN CT NTOA CT 0.450 1.911 bisp N7
 BEN CT NT H 0.450 1.909

BEN CT NTA H 0.450 1.909 bisp N7
 BEN CT NTOA H 0.450 1.909 bisp N7
 BEN CU1 NT CT 0.200 1.920
 BEN CU1 NT H 0.100 1.915
 BEN CU2 NT CA 0.200 1.920
 BEN CU2 NT CT 0.200 1.920
 BEN CU2 NT H 0.100 1.915
 BEN CU2C NT CA 0.200 1.920
 BEN CU2C NT CT 0.200 1.920
 BEN CU2C NT H 0.100 1.915
 BEN CU2P NT CA 0.200 1.920
 BEN CU2P NT CT 0.200 1.920
 BEN CU2P NTA CT 0.200 1.920 bisp N7
 BEN CU2P NTOA CT 0.200 1.920 bisp N7
 BEN CU2P NT H 0.100 1.915
 BEN CU2P NTA H 0.100 1.915 bisp N7
 BEN CU2P NTOA H 0.100 1.915 bisp N7
 BEN CU2P NPOA CA 0.050 2.094 bisp N2py33
 BEN CU2P OXCU OXCU 0.500 1.911 Cuperoxo
 BEN CU2B NT CA 0.200 1.920
 BEN CU2B NT CT 0.200 1.920
 BEN CU2B NTA CT 0.200 1.920 bisp N7
 BEN CU2B NTOA CT 0.200 1.920 bisp N7
 BEN CU2B NT H 0.100 1.915
 BEN CU2B NTA H 0.100 1.915 bisp N7
 BEN CU2B NTOA H 0.100 1.915 bisp N7
 BEN CU2B NPOA CA 0.050 2.094 bisp N2py33
 BEN FE3L C3 N3 0.450 3.141
 BEN FE3L NT CT 0.200 1.920
 BEN FE3L NT H 0.100 1.915
 BEN H NT H 0.330 1.902

BEN NI2	NT	CT	0.200	1.920	
BEN NI2	NT	H	0.100	1.915	
BEN NI2C	NT	CT	0.200	1.920	
BEN NI2C	NT	H	0.100	1.915	
BEN NI2P	NT	CT	0.200	1.920	
BEN NI2P	NT	H	0.100	1.915	
BEN NI2T	ND	CON	0.200	2.094	Slava/Alex
BEN NI2T	ND	CT	0.200	2.094	Slava/Alex
BEN NI2T	NT	H	0.100	1.915	Slava/Alex
BEN NI2T	NT	CT	0.200	1.920	Slava/Alex
BEN PT2	NT	CT	0.200	1.920	
BEN PT2	NT	H	0.100	1.915	
BEN RH3	NT	CT	0.200	1.920	
BEN RH3	NT	H	0.100	1.915	
BEN ZN2	NT	CT	0.200	1.920	
BEN ZN2	NT	H	0.100	1.915	
BEN CO3	OC	CCO	0.050	2.094	
BEN CO3C	OC	CCO	0.050	2.094	
BEN CR3	OC	CCO	0.400	1.998	
BEN CU2C	OC	CCO	0.050	2.094	
BEN CU2P	OC	CCO	0.050	2.094	
BEN CU2P	OC	CU2P	0.100	1.830	
BEN FE3H	OC	CCO	0.750	2.030	
BEN MN3	OC	CCO	0.300	2.028	
BEN NI2C	OC	CCO	0.050	2.094	
BEN TI3	OC	CCO	0.450	2.062	
BEN V3	OC	CCO	0.500	2.030	
BEN CO3C	OCC	COC	0.600	2.094	
BEN TI4	OCC	COC	0.600	2.094	
BEN TI4	OCCT	COC	0.600	2.094	
BEN P	OH	H	0.624	2.039	

BEN CU2 ONO NOO 0.320 2.094
 BEN CU2C ONO NOO 0.320 2.094
 BEN CU2P ONO NOO 0.320 2.094
 BEN CAH NAX ZN2 0.200 2.094 pat ae
 BEN CT OP CU2P 0.200 2.094
 BEN CU2 OP H 0.100 1.915
 BEN CU2C OP H 0.100 1.915
 BEN CU2P OP CU2P 0.100 1.745
 BEN CU2P OP H 0.100 1.915
 BEN H OP H 0.320 1.902
 BEN CT OR CT 0.750 1.911
 BEN P OS CT 1.386 2.065
 BEN CU2 OCO CCO 0.100 2.094 pentanone
 BEN CU2 OW H 0.100 1.915
 BEN CU2C OW H 0.100 1.915
 BEN CU2P OW CU2P 0.100 1.745
 BEN CU2P OW H 0.100 1.915
 BEN H OW H 0.320 1.902
 BEN TI4 OW CT 0.050 1.915
 BEN CO3 OX OX 0.500 1.911
 BEN CU2P OX OX 0.500 1.911
 BEN O2 P OS 1.386 2.003
 BEN OH P O2 0.624 2.011
 BEN OH P OS 0.624 1.764
 BEN OS P OS 0.624 1.716
 BEN CT SW CT 0.500 1.740
 BEN CU2 SW CT 0.100 1.920
 BEN CU2C SW CT 0.100 1.920
 BEN CU2P SW CT 0.100 1.920 test
 BEN OCO CON ND 0.45104876072051 2.09622876745753 pat ae
 BEN OCO CON CAH 0.450 2.094 pat ae

BEN ND CON CAH 0.450 2.094 pat ae
 BEN NAX CAH SAH 0.450 2.094 pat ae
 BEN SAH CAH CT 0.450 2.094 pat ae
 BEN CT ND H 0.09619468293472 2.06021165621619
 BEN CAH CON OCO 0.11305146759259 2.19875574038820
 BEN CAH CON ND 0.11260495850541 2.03457788576222
 BEN CON ND H 0.11865015015240 2.06124909711061
 BEN CAH CAH CON 0.10691732257450 2.23953597759928
 BEN CAH CT ND 0.12107982496755 1.98414567683231
 BEN CAH NAX CAH 0.31469205022982 1.87283223270942
 BEN CON CAH NAX 0.12348383240567 2.14780916789294
 BEN CON CAH NAX 0.12243213544806 2.14997199763844
 BEN CON CT NAX 0.100 1.999 pat ae
 BEN CT CT NAX 0.100 2.251 pat ae
 BEN CT CT OOX 0.100 2.129 pat ae
 BEN NAX CT H 0.100 1.868 pat ae
 BEN CT NAX CT 0.100 2.094 pat ae
 BEN OOX CT H 0.100 1.860 pat ae
 BEN CT OOX CT 0.100 1.860 pat ae
 BEN NAX CT OOX 0.100 1.860 pat ae
 BEN NAH CAH NAX 0.10000000000000 1.94318000000000
 BEN NAH CAH NAX 0.10000000000000 1.94318000000000
 BEN OP CU2P OW 0.10000000000000 1.62913000000000
 BEN NAX CU2P OP 0.10000000000000 1.74226250000000
 BEN ND CU2P OP 0.10000000000000 2.84078500000000
 BEN OP CU2P OW 0.10000000000000 1.62913000000000
 BEN NAX CU2P OP 0.10000000000000 1.74226250000000
 BEN ND CU2P OP 0.10000000000000 2.84078500000000
 BEN CON CAH NAH 0.10000000000000 2.09559000000000
 BEN H ND H 0.10000000000000 2.12655000000000
 BEN CON CAH NAH 0.10000000000000 2.09559000000000

BEN H	ND	H		0.100000000000000	2.12655000000000		
TOR **	CI	NT	**	0.001	6.0000	0.524	Dirk Kuppert
TOR **	CI	CT	**	0.0005	6.000	0.524	Dirk Kuppert
TOR **	OR	CT	**	0.0080	3.000	0.000	Dirk Kuppert
TOR **	NI	CI	**	0.0250	2.000	1.571	Dirk Kuppert
TOR **	C	CB	**	0.0074	2.000	1.571	
TOR **	C	NA	**	0.0092	2.000	1.571	
TOR **	CA	CA	**	0.0500	2.000	1.571	
TOR **	CA	CFC	**	0.0500	2.000	1.571	
TOR **	CA	CON	**	0.0030	2.000	1.571	
TOR **	CA	CT	**	0.0050	6.000	0.524	
TOR **	CA	NA	**	0.0102	2.000	1.571	
TOR **	CA	NP	**	0.0500	2.000	1.571	
TOR **	CA	NPOA	**	0.0500	2.000	1.571	bisp N7
TOR **	CA	NT	**	0.0005	6.000	0.524	
TOR **	CA	OW	**	0.1500	3.000	4.680	
TOR **	CA	CCO	**	0.0050	2.000	1.571	PC Demi
TOR **	CAH	CA	**	0.0650	2.000	1.571	
TOR **	SAH	CAH	**	0.0150	2.000	1.571	thiazole
TOR **	CAH	CAH	**	0.00976826286139	2.000	1.55136829333741	
TOR **	CAH	CI	**	0.0250	2.000	1.571	
TOR **	CAH	CT	**	0.00168033157555	6.000	0.80228966291567	
TOR **	CAH	NAH	**	0.01691774985961	2.000	1.56971832803358	
TOR **	CAH	NAX	**	0.04877988534146	2.000	1.56879587016893	
TOR **	CAH	NI	**	0.0030	2.000	1.571	
TOR **	CB	CB	**	0.0280	2.000	1.571	
TOR **	CB	N*	**	0.0112	2.000	1.571	
TOR **	CB	NA	**	0.0142	2.000	1.571	
TOR **	CB	NB	**	0.0086	2.000	1.571	
TOR **	CCC	COC	**	0.0300	2.000	1.571	
TOR **	CCO	CCO	**	0.0000	2.000	3.097	

TOR **	CCO	CT	**	0.0010	6.000	0.524	
TOR **	CCO	OC	**	0.0045	2.000	1.571	
TOR **	CFC	CFC	**	0.0300	2.000	1.571	
TOR **	CFC	COC	**	0.0300	2.000	1.571	
TOR **	CFC	NP	**	0.0030	2.000	1.571	
TOR **	CI	CA	**	0.0100	6.000	1.571	
TOR **	CK	N*	**	0.0114	2.000	1.571	
TOR **	CK	N*	**	0.0114	2.000	1.571	
TOR **	CK	NB	**	0.0340	2.000	1.571	
TOR **	CK	NB	**	0.0340	2.000	1.571	
TOR **	COC	CT	**	0.0050	6.000	0.524	
TOR **	COC	OCC	**	0.0300	2.000	1.571	
TOR **	COC	OCCT	**	0.0300	2.000	1.571	
TOR **	CON	CT	**	0.0010	6.000	0.524	
TOR **	CON	ND	**	0.01506895186255	2.000	1.58012579094675	
TOR **	CT	CT	**	0.00166411294957	3.000	0.00240573130340	
TOR **	CT	NAH	**	0.00253131359632	6.000	0.52467414069507	
TOR **	CT	ND	**	0.00021673758629	6.000	0.52249849391110	
TOR **	CT	NOO	**	0.0025	6.000	0.524	
TOR **	CT	NT	**	0.0010	3.000	0.000	
TOR **	CT	NTA	**	0.0010	3.000	0.000	bisp N7
TOR **	CT	NTOA	**	0.0010	3.000	0.000	bisp N2py33
TOR **	CT	OP	**	0.0010	3.000	0.000	
TOR **	CT	OW	**	0.0080	3.000	0.000	
TOR **	CT	SW	**	0.0008	3.000	0.000	
TOR **	CTO	CTO	**	0.0110	3.000	0.000	
TOR **	CTO	CTOC	**	0.0110	3.000	0.000	
TOR **	CTOC	CTOC	**	0.0110	3.000	0.000	
TOR **	NAH	NAH	**	0.0200	2.000	1.571	
TOR **	NAH	NAX	**	0.0650	2.000	1.571	
TOR **	NI	CI	**	0.0250	2.000	1.571	

TOR ** NI CT ** 0.0001 2.000 0.524
 TOR ** O2 P ** 0.0520 3.000 0.390
 TOR ** OH P ** 0.0520 3.000 0.635
 TOR ** OS CT ** 0.0800 3.000 0.050
 TOR ** OS P ** 0.0520 3.000 0.390
 TOR ** OXCO OXCO ** 0.9000 2.000 0.000
 TOR ** OXCU OXCU ** 0.9000 2.000 0.000
 TOR ** PT2 NB ** 0.0000 2.000 2.094
 TOR ** PT2 NT ** 0.0000 2.000 2.094
 TOR ** CU2P NAH ** 0.0050 2.000 0.262 bispidine
 TOR ** CU2P NP ** 0.0050 2.000 0.262 bispidine
 TOR ** CU2P NPOA ** 0.0050 2.000 0.262 bispidine
 TOR ** CU2B NAH ** 0.0050 2.000 0.262 bispidine
 TOR ** CU2B NP ** 0.0050 2.000 0.262 bispidine
 TOR ** CU2B NPOA ** 0.0010 2.000 0.262 bispidine
 #TOR ** NAX CU2P ** 0.0000 2.000 0.001 pat ae
 #TOR ** OP CU2P ** 0.0000 2.000 0.001 pat ae
 TOR ** CON CAH ** 0.00624834555850 2.000 0.34922245621946 pat ae
 TOR CT CT NAX CT 0.0010 2.000 2.443 pat ae
 TOR CON CT NAX CT 0.0010 2.000 1.641 pat ae
 TOR H CT OOX CT 0.0010 2.000 0.698 pat ae
 TOR CT CT OOX CT 0.0010 2.000 1.798 pat ae
 #TOR ** ND ZN2 ** 0.0000 2.000 0.001 pat ae
 #TOR ** NAX ZN2 ** 0.0000 2.000 0.001 pat ae
 #TOR ** OW ZN2 ** 0.0000 2.000 0.001 pat ae
 #TOR ** CU2P NAX ** 0.0000 2.000 0.001 pat ae
 #TOR ** CU2P ND ** 0.0000 2.000 0.001 pat ae
 #TOR ** CU2P OW ** 0.0000 2.000 0.001 pat ae
 #TOR NAX CU2P OP CU2P 0.0100 2.000 2.049 pat ae
 #TOR ND CU2P OP CU2P 0.0100 2.000 0.11954279695406 pat ae
 #TOR NAX CU2P ND CT 0.0500 2.000 0.001 pat ae

#TOR NAX CU2P ND CON 0.0500 2.000 0.001 pat ae
 #TOR CON CAH NAX CU2P 0.0500 2.000 0.001 pat ae
 JT1 CU2 NT 0 2.16
 JT1 CU2 NP 1 2.14
 HBD H NC 316.0 86.0 taken from 'green booklet'
 NBD OR 1.700 0.055 Dirk Kuppert
 NBD NI 1.800 0.050 Dirk Kuppert
 NBD CI 1.900 0.044 Dirk Kuppert
 NBD SAH 2.000 0.185 thiazole
 NBD SW 2.000 0.185
 NBD C 1.900 0.044
 NBD C3 1.900 0.044
 NBD CA 1.900 0.044
 NBD CB 1.900 0.044
 NBD CCC 1.900 0.044
 NBD CCO 1.900 0.044
 NBD CFC 1.900 0.044
 NBD CK 1.900 0.044
 NBD COC 1.900 0.044
 NBD CON 1.900 0.044
 NBD CT 1.900 0.044
 NBD CAH 1.900 0.044 bisp energy
 NBD N3 1.800 0.052
 NBD NA 1.800 0.052
 NBD NB 1.800 0.052
 NBD ND 1.800 0.050
 NBD NOO 1.800 0.050
 NBD NP 1.800 0.050
 NBD NPOA 1.800 0.050 bisp N7
 NBD NT 1.800 0.050
 NBD NTA 1.800 0.050 bisp N7

NBD NTOA 1.800 0.050 bisp N7
 NBD N* 1.800 0.052
 NBD NAH 1.800 0.052 bisp energy
 NBD NAX 1.800 0.052 pat ae
 NBD O 1.700 0.055
 NBD OC 1.700 0.055
 NBD OCC 1.700 0.055
 NBD OCCT 1.700 0.055
 NBD OCO 1.700 0.055
 NBD ONO 1.700 0.055
 NBD OP 1.700 0.055
 NBD OXCU 1.700 0.055 Cuperoxo
 NBD OW 1.700 0.055
 NBD OOX 1.700 0.055 pat ae
 NBD PT2 1.650 0.300
 NBD H 1.440 0.024
 NBD TI4 0.000 0.000
 NBD CR2 0.000 0.000
 NBD CR3 0.000 0.000
 NBD FE3L 0.000 0.000
 NBD CO2 0.000 0.000
 NBD CO3 0.000 0.000
 NBD CO3C 0.000 0.000
 NBD NI2 0.000 0.000
 NBD NI2C 0.000 0.000
 NBD NI2P 0.000 0.000
 NBD CU2 0.000 0.000
 NBD CU2C 0.000 0.000
 NBD CU2P 0.000 0.000
 NBD CU2B 0.000 0.000
 NBD ZN2 0.000 0.000

NBD RH3	0.000	0.000		
NBD PT4	0.000	0.000		
OOP CA	CAH	CA	H	2.000
OOP CA	NP	CA	H	2.000
OOP CA	NP	CA	CU2P	2.000 bispidine
OOP CAH	NAH	CAH	CU2P	2.000 bispidine
OOP CA	NPOA	CA	CU2P	1.000 bispidine N7
OOP CA	NP	CA	CU2B	2.000 bispidine
OOP CAH	NAH	CAH	CU2B	2.000 bispidine
OOP CA	NPOA	CA	CU2B	0.100 bispidine N7
OOP CA	NP	CT	H	2.000
OOP CA	NP	CA	CCO	2.000 PC Demi
OOP CAH	CAH	CA	NAH	2.000
OOP CAH	CAH	CAH	H	2.000
OOP CAH	CAH	NAH	CT	2.000
OOP CAH	CAH	NAH	CI	2.000
OOP CAH	CAH	NAH	H	2.000
OOP CAH	CAH	NAX	CT	2.000
OOP CAH	CAH	SAH	H	2.000 thiazole
OOP CAH	NAH	NAH	CI	2.000
OOP CAH	NAH	NAH	H	2.000
OOP CAH	NAH	NAH	CT	2.000
OOP CCC	COC	COC	H	0.500
OOP CCO	CT	OCO	OC	0.120
OOP CCO	OC	OC	OC	0.500
OOP CI	NI	CAH	H	1.500
OOP CO2T	ND	NI	NA	0.070
OOP COC	CCC	OCC	CFC	0.500
OOP COC	CCC	OCC	CT	0.500
OOP COC	CCC	OCCT	CFC	0.500
OOP COC	CCC	OCCT	CT	0.500

OOP CCO CA OCO OC 0.120 PC Demi
 OOP CON CT OCO ND 0.120
 OOP CU2T ND NI NA 0.050
 OOP NI2T ND NI NA 0.070
 OOP NOO CT ONO ONO 0.120
 OOP OW CT CU2P CU2P 0.500
 OOP PT2 NB NB NT 1.000
 OOP PT2 NB NT NB 1.000
 OOP PT2 NB NT NT 1.000
 OOP PT2 NT NB NB 1.000
 OOP PT2 NT NT NB 1.000
 #OOP CAH NAX NAH CT 5.000 pat ae
 #OOP CAH NAX CAH CON 5.000 pat ae
 #OOP CAH NAX CAH ND 5.000 pat ae
 #OOP CON ND OCO CAH 2.000 pat ae
 #OOP CT ND CAH CT 2.000 pat ae
 #OOP NAH CAH CAH CT 5.000 pat ae
 #OOP ND CON CAH CT 5.000 pat ae
 #OOP ND CON CAH NAH 5.000 pat ae
 #OOP CU2P NAX CAH CAH 2.000 pat ae
 #OOP ZN2 NAX CAH ND 2.000 pat ae
 #OOP ZN2 NAX CAH CAH 2.000 pat ae
 #OOP ND CT CAH NAH 2.000 pat ae
 #OOP ND CT CAH NAX 2.000 pat ae
 #OOP NAX CU2P CAH CAH 2.000 pat ae
 #OOP CU2P ND CON CAH 2.000 pat ae
 #OOP CU2P NAX CAH CT 2.000 pat ae
 #OOP CU2P NAX CAH CON 2.000 pat ae
 #OOP ZN2 NAX CAH CT 2.000 pat ae
 #OOP ZN2 NAX CAH CON 2.000 pat ae
 TWT CU2 NT NT NT NT 0.200 0.00

LF CO3 F 4000.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 2000.0 0.0 0.0 0.0 0.0 0.0 0.0 2000.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0
 0.0 0.0 0.0 0.0 0.0 0.0 0.0

LF CO3 NT 6000.0 -1000.0 0.0 0.0 0.0 0.0 0.0 0.0 2500.0 -1000.0 0.0 0.0 0.0 0.0 0.0 2500.0 -1000.0 0.0 0.0 0.0 0.0 0.0
 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0

LF FE2 CL 18000.0 -1200.0
 0.0 0.0 0.0 0.0 0.0 0.0 0.0

LF CU2 NP 6000.0
 0.0 0.0 0.0 0.0 0.0 0.0 0.0

LF CU2 I 4000.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 1000.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 1000.0 0.0 0.0 0.0 0.0 0.0 0.0
 0.0 0.0 0.0 0.0 0.0 0.0 0.0

LF CU2 BR 6000.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 2000.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 2000.0 0.0 0.0 0.0 0.0 0.0 0.0
 0.0 0.0 0.0 0.0 0.0 0.0 0.0

LF CU2 OW 6000.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 2000.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 2000.0 0.0 0.0 0.0 0.0 0.0 0.0
 0.0 0.0 0.0 0.0 0.0 0.0 0.0

LF CU2 NT 0.0
 0.0 0.0 0.0 0.0 0.0

CHG CO3 0.0 0.0

CHG CO3C 0.0 0.0

CHG CR3 0.0 0.0

CHG CU2 0.0 0.0

CHG CU2C 0.0 0.0

CHG CU2P 0.0 0.0

CHG CU2B 0.0 0.0

CHG CU2T 0.0 0.0

CHG FE2H 0.0 0.0

CHG FE2L 0.0 0.0

CHG FE3H 0.0 0.0

CHG FE3L 0.0 0.0

CHG H 0.0 0.0

CHG C 0.0 0.0

CHG C3 0.0 0.0

CHG CA 0.0 0.0

CHG CAH 0.0 0.0

CHG CB 0.0 0.0

CHG CCC	0.0	0.0
CHG CCO	0.0	0.0
CHG CFC	0.0	0.0
CHG CI	0.0	0.0
CHG CK	0.0	0.0
CHG CMC	0.0	0.0
CHG COC	0.0	0.0
CHG CON	0.0	0.0
CHG CT	0.0	0.0
CHG N	0.0	0.0
CHG N*	0.0	0.0
CHG N3	0.0	0.0
CHG NA	0.0	0.0
CHG NAH	0.0	0.0
CHG NAX	0.0	0.0
CHG NB	0.0	0.0
CHG ND	0.0	0.0
CHG NI	0.0	0.0
CHG NOO	0.0	0.0
CHG NP	0.0	0.0
CHG NPA	0.0	0.0
CHG NPOA	0.0	0.0
CHG NT	0.0	0.0
CHG NTA	0.0	0.0
CHG NTOA	0.0	0.0
CHG O	0.0	0.0
CHG O2	0.0	0.0
CHG OC	0.0	0.0
CHG OCC	0.0	0.0
CHG OCCT	0.0	0.0
CHG OCO	0.0	0.0

CHG OH	0.0	0.0
CHG ONO	0.0	0.0
CHG OP	0.0	0.0
CHG OR	0.0	0.0
CHG OS	0.0	0.0
CHG OW	0.0	0.0
CHG OXCO	0.0	0.0
CHG OXCU	0.0	0.0
CHG P	0.0	0.0
CHG SAH	0.0	0.0
CHG SW	0.0	0.0
CHG CL	0.0	0.0
CHG BR	0.0	0.0
CHG OOX	0.0	0.0

J) MOME C final cartesian coordinates of dinuclear Cu^{II} and Zn^{II} complexes with H₄pat¹, H₄pat² and H₄pat⁴

		[H ₄ pat ¹]		[H ₄ pat ²]		[H ₄ pat ⁴]	
		Amide	Imidazole	Amide	Imidazole	Amide	Imidazole
Cu ²⁺	μ-OH	A	C	E	G	I	K
	OH	B	D	F	H	J	L
Zn ²⁺	μ-OH	M	O	Q	S	U	W
	OH	N	P	R	T	V	X

A:
121

Cu	-2.59770	1.57390	-0.85890
N	-1.66080	2.24050	1.69020
N	-1.93610	3.51060	-0.88590
N	-2.91470	2.09730	-2.64630
N	-3.69240	0.04530	-1.63920
N	-2.24820	2.97820	3.70140
N	-2.95300	3.44120	-4.38090
O	-1.95540	5.45060	0.27620
O	-4.64160	-0.63440	-3.61510
O	-0.53770	0.80070	-0.41550
O	-4.77260	2.90850	-0.36620
C	-1.72320	1.93760	2.99160
C	-2.50620	3.96370	2.78640
C	-2.09720	3.50680	1.55680
C	-1.98110	4.20580	0.27410
C	-1.81520	4.18310	-2.18020
H	-2.32710	5.02210	-2.15790
C	-2.51650	3.25820	-3.11030
C	-3.59180	2.25020	-4.71270
C	-3.58650	1.45160	-3.58740
C	-4.01580	0.20950	-2.94740
C	-4.03780	-1.16970	-0.91230

H	-4.76680	-1.59850	-1.41020
C	-2.48420	3.05630	5.15100
H	-2.21460	2.23180	5.60860
H	-3.44000	3.20420	5.32100
H	-1.96950	3.80330	5.52720
C	-3.06090	5.29250	3.17830
H	-3.56350	5.67040	2.42420
H	-2.31860	5.89070	3.41400
H	-3.66590	5.19650	3.94540
C	-0.36590	4.41760	-2.62200
H	-0.38400	4.74740	-3.54830
C	0.46360	3.13620	-2.60520
H	1.36390	3.30860	-2.95890
H	0.04700	2.44080	-3.16000
H	0.55300	2.79850	-1.68770
C	0.31980	5.49280	-1.78210
H	1.21160	5.69000	-2.14430
H	0.42590	5.19670	-0.85170
H	-0.20470	6.32350	-1.79370
C	-2.80280	4.63510	-5.22060
H	-2.32800	5.34540	-4.73740
H	-3.68990	4.96930	-5.47690
H	-2.29520	4.40850	-6.03010
C	-4.23300	2.02400	-6.03800
H	-4.25910	1.05980	-6.22250
H	-3.71800	2.47420	-6.74230
H	-5.14720	2.38170	-6.01490
C	-4.54540	-0.84330	0.49400
H	-3.89140	-0.24830	0.92370
C	-5.88700	-0.11600	0.42640
H	-6.16930	0.16530	1.32450
H	-6.57960	-0.70270	0.05010
H	-5.82380	0.68240	-0.13980
C	-4.70600	-2.09410	1.35830
H	-5.03690	-1.85000	2.25060
H	-3.84640	-2.55430	1.47640
H	-5.34490	-2.71920	0.95090
H	-4.82950	3.10510	0.52040
H	-4.79800	3.68110	-0.84600
Cu	0.18490	-0.65360	1.13040
C	-1.22930	0.64520	3.56320
C	-2.88940	-2.12940	-0.88970

N	-1.61950	-1.75680	-0.69660
N	1.23210	-1.71620	-0.26990
N	1.97600	-0.40840	1.67650
O	0.47940	-2.97380	2.27730
C	-0.85840	-2.85900	-0.83310
C	0.60310	-2.75590	-0.86520
C	2.98540	-0.84860	0.96330
H	1.31100	-3.31040	2.12560
C	2.68900	-1.57860	-0.29800
C	2.42890	0.13590	2.79550
H	-0.14250	-3.56160	1.96810
C	-1.68180	-3.94000	-1.04000
O	1.25070	-3.65870	-1.42700
N	4.15660	-0.64490	1.61480
N	-2.96860	-3.47590	-1.09570
H	3.09940	-2.46900	-0.22600
C	3.21600	-0.81030	-1.51560
C	3.80580	0.04780	2.76960
C	1.22660	0.54490	3.51910
C	-1.34060	-5.37600	-1.26000
C	5.49920	-1.07320	1.20640
C	-4.17260	-4.28340	-1.34380
H	4.17550	-0.64660	-1.37510
C	2.53830	0.54690	-1.68780
C	3.09070	-1.62300	-2.80220
C	4.80610	0.46780	3.79010
N	0.03120	0.25000	2.94750
O	1.34350	1.14090	4.60580
H	-0.51230	-5.59140	-0.77890
H	-1.21380	-5.52930	-2.22170
H	-2.06070	-5.95270	-0.92450
H	5.46710	-1.56500	0.35770
H	5.87890	-1.66140	1.89500
H	6.07780	-0.28750	1.09590
H	-4.98510	-3.73410	-1.34710
H	-4.26330	-4.96260	-0.64040
H	-4.09470	-4.72900	-2.21550
H	2.94800	1.04000	-2.43230
H	2.63090	1.09100	-0.87520
H	1.58350	0.43040	-1.88450
H	3.52130	-1.14870	-3.54720
H	2.14790	-1.76790	-3.03570

H	3.53090	-2.49560	-2.70090
H	4.45780	1.24290	4.28230
H	5.64970	0.71470	3.35270
H	4.95960	-0.27730	4.41110
H	-1.04200	0.79820	4.51440
C	-2.27120	-0.47060	3.45470
H	-2.32570	-0.74650	2.51280
C	-1.85220	-1.68150	4.28630
C	-3.65790	-0.01520	3.91000
H	-2.48300	-2.42300	4.15330
H	-1.83300	-1.45450	5.24210
H	-0.95770	-1.99000	4.02780
H	-4.29870	-0.75730	3.85080
H	-3.99270	0.71420	3.34380
H	-3.63260	0.29520	4.84160

B:
126

Cu	-2.73640	1.51440	-0.80760
N	-1.53380	2.15810	1.72560
N	-2.02690	3.41090	-0.94040
N	-3.42070	2.06490	-2.46290
N	-3.97680	0.00790	-1.32880
N	-2.03220	3.03660	3.70750
N	-3.77380	3.42340	-4.14100
O	-1.78400	5.34000	0.19290
O	-5.37840	-0.62700	-3.02950
O	-4.84640	2.88450	-0.02190
C	-1.52950	1.94910	3.05400
C	-2.29600	3.97200	2.74560
C	-1.95200	3.43070	1.52370
C	-1.88790	4.09970	0.21680
C	-2.16610	4.10240	-2.22430
H	-2.64360	4.94940	-2.07890
C	-3.08240	3.21540	-2.99340
C	-4.53070	2.26530	-4.31740
C	-4.29980	1.44210	-3.23290
C	-4.59930	0.19870	-2.51970
C	-4.06180	-1.23340	-0.57220
H	-4.86700	-1.71250	-0.86320
C	-2.24480	3.20270	5.15440

H	-1.98720	2.40100	5.65690
H	-3.19480	3.38260	5.32660
H	-1.70840	3.95710	5.48210
C	-2.92160	5.28800	3.07610
H	-2.65490	5.96340	2.41650
H	-2.63370	5.58910	3.96490
H	-3.89820	5.18550	3.06330
C	-0.84140	4.33930	-2.96030
H	-1.05020	4.75800	-3.82520
C	-0.08450	3.04710	-3.25400
H	0.73890	3.23960	-3.75420
H	-0.63340	2.44270	-3.79940
H	0.16120	2.59380	-2.41890
C	0.06400	5.31090	-2.20700
H	0.86370	5.51440	-2.74030
H	0.35590	4.92580	-1.35180
H	-0.40780	6.15480	-2.03270
C	-3.74350	4.60720	-5.00710
H	-3.13580	5.28920	-4.64830
H	-4.64420	4.99370	-5.06720
H	-3.43980	4.35070	-5.90510
C	-5.38960	2.04160	-5.51390
H	-6.12460	1.43620	-5.27370
H	-4.84610	1.63540	-6.22360
H	-5.76260	2.89400	-5.82720
C	-4.21970	-0.96270	0.92470
H	-3.48000	-0.38470	1.21610
C	-5.53730	-0.24160	1.20440
H	-5.62420	-0.04080	2.16190
H	-6.30100	-0.79720	0.93330
H	-5.58240	0.60470	0.71110
C	-4.18790	-2.26180	1.73060
H	-3.32790	-2.72350	1.62420
H	-4.30730	-2.07210	2.68720
H	-4.90480	-2.86780	1.44040
H	-4.66890	3.77500	0.03210
H	-5.53190	2.75790	-0.60670
Cu	0.38410	-0.71260	1.32290
C	-0.96860	0.72520	3.71430
C	-2.86740	-2.08410	-0.88290
N	-1.63840	-1.88820	-0.35730
N	1.33670	-1.91750	-0.03630

N	2.15750	-0.72470	1.96590
O	0.01870	-3.10990	2.20230
C	-0.80730	-2.77950	-0.94870
C	0.64530	-2.85410	-0.73050
C	3.13050	-1.30190	1.30400
H	0.54950	-3.27330	2.92280
C	2.79990	-1.97410	0.02010
C	2.63160	-0.21750	3.09310
H	-0.85210	-3.24560	2.42720
C	-1.55090	-3.53070	-1.84420
O	1.25960	-3.82140	-1.21730
N	4.29140	-1.24190	2.00310
N	-2.84810	-3.10720	-1.77950
H	3.08240	-2.91150	0.10960
C	3.50500	-1.29460	-1.16190
C	3.97840	-0.51200	3.14580
C	1.46990	0.38460	3.74340
C	-1.13950	-4.65840	-2.73530
C	5.59090	-1.82180	1.64530
C	-3.97680	-3.66190	-2.54440
H	4.47160	-1.31010	-0.98220
C	3.10110	0.16740	-1.33310
C	3.29530	-2.04500	-2.47510
C	4.99580	-0.14110	4.16910
N	0.27430	0.25880	3.11200
O	1.61520	0.93940	4.84830
H	-0.21620	-4.52410	-3.03930
H	-1.71960	-4.70060	-3.52580
H	-1.20390	-5.50000	-2.23350
H	5.53820	-2.30250	0.79130
H	5.87090	-2.45530	2.34140
H	6.26050	-1.10760	1.56830
H	-4.82200	-3.21280	-2.33280
H	-4.07580	-4.61620	-2.33450
H	-3.80670	-3.55840	-3.50600
H	3.60170	0.57570	-2.07330
H	3.29980	0.67800	-0.51810
H	2.14260	0.23950	-1.53310
H	3.84080	-1.64340	-3.18680
H	2.35460	-2.00790	-2.75480
H	3.56480	-2.98500	-2.38030
H	4.55260	-0.03130	5.03850

H	5.67660	-0.84480	4.24020
H	5.41840	0.70500	3.90480
H	-0.74560	0.99190	4.63170
C	-1.97920	-0.42110	3.79940
H	-2.06380	-0.81530	2.90370
C	-1.48290	-1.50550	4.75490
C	-3.36140	0.04300	4.25840
H	-2.09440	-2.27460	4.74630
H	-1.42920	-1.15920	5.67280
H	-0.59050	-1.82090	4.49540
H	-3.98380	-0.71660	4.28600
H	-3.73110	0.71110	3.64090
H	-3.31620	0.43610	5.15730
O	-1.13290	0.11000	-2.26490
H	-0.26060	0.27530	-2.06900
H	-1.27700	0.23510	-3.15430
O	1.04160	1.58670	0.40670
H	1.22560	2.17540	1.07550
H	0.38560	1.92550	-0.12360

C:
123

Cu	1.01280	2.54750	13.43920
N	0.39840	3.32040	11.68290
N	-0.65710	1.52410	13.20030
N	0.83570	1.66760	15.22580
N	2.79870	3.71250	15.93230
H	2.42220	3.74770	15.13930
N	-0.07260	4.29770	9.72580
N	-0.26670	0.22910	16.51960
O	-2.40770	1.23750	11.77250
O	2.96520	2.67490	17.91610
O	3.03920	1.69250	13.46460
O	-0.10380	4.28080	14.42060
C	0.81350	4.20220	10.75410
C	-1.12040	3.46690	10.05180
C	-0.78850	2.86490	11.23560
C	-1.37450	1.84690	12.10470
C	-0.84060	0.33830	14.02040
H	-1.79680	0.25290	14.23170
C	-0.08150	0.69330	15.26080

C	0.68200	0.88250	17.28500
C	1.35610	1.78150	16.46740
C	2.40980	2.75210	16.80450
C	3.85450	4.66430	16.25160
H	3.66360	4.98880	17.15930
C	0.08170	5.11800	8.51610
H	0.15850	6.06420	8.76700
H	0.89300	4.84490	8.03490
H	-0.68460	5.01520	7.91230
C	-2.31520	3.27120	9.18110
H	-3.07230	2.97560	9.73210
H	-2.11020	2.58740	8.50690
H	-2.55680	4.11400	8.73990
C	-0.30190	-0.88370	13.26430
H	-0.82180	-0.96350	12.43270
C	1.16700	-0.73620	12.87120
H	1.46240	-1.51680	12.35290
H	1.73430	-0.66500	13.66990
H	1.29950	0.06120	12.31340
C	-0.49920	-2.18860	14.02910
H	0.06890	-2.21010	14.82960
H	-0.25500	-2.95390	13.46330
H	-1.43980	-2.29320	14.29250
C	-1.30160	-0.71250	16.97470
H	-1.25390	-0.86120	17.94280
H	-2.18860	-0.34990	16.76000
H	-1.19610	-1.58120	16.53450
C	0.86920	0.59830	18.73970
H	1.49220	-0.15420	18.83890
H	0.01210	0.38040	19.16430
H	1.23730	1.39070	19.18640
C	3.85550	5.87080	15.30820
H	3.94170	5.54130	14.38590
C	2.54610	6.64990	15.43050
H	1.77740	6.08130	15.20840
H	2.54220	7.41640	14.81640
H	2.42830	6.98620	16.34610
C	5.02650	6.81260	15.58420
H	5.88500	6.35230	15.45840
H	4.98580	7.15550	16.50390
H	5.00250	7.57510	14.96500
H	-0.28960	4.93530	13.81700

H	-0.88310	3.98600	14.78600
Cu	4.99930	2.57070	13.45660
C	2.13650	4.89670	10.83990
C	5.18660	3.98210	16.27200
N	5.60580	3.18820	15.26980
N	6.57730	1.41540	13.67880
N	5.19450	1.87470	11.59240
O	6.15500	4.35220	12.63870
C	6.79030	2.69240	15.67670
C	7.36030	1.73650	14.72960
C	6.10550	0.90370	11.46810
H	7.00520	4.10120	12.43390
C	6.83870	0.40340	12.66840
C	4.67640	2.08790	10.36170
H	6.18510	5.02750	13.24710
C	7.12590	3.19750	16.90420
O	8.45870	1.19490	14.95080
N	6.23590	0.48770	10.19330
N	6.07420	3.99150	17.30350
H	7.80120	0.39780	12.46850
C	6.33540	-0.98560	13.07870
C	5.32620	1.23180	9.48000
C	3.62160	3.08020	10.10660
C	8.32260	2.93150	17.75330
C	7.14810	-0.53940	9.67350
C	5.91770	4.70110	18.58090
H	6.46480	-1.59080	12.31430
C	4.84690	-0.99090	13.42350
C	7.14280	-1.55860	14.24110
C	5.12160	1.02850	8.01550
N	3.20430	3.93360	11.07160
O	3.09060	3.11610	8.98110
H	9.07970	2.68670	17.17820
H	8.12050	2.19190	18.36680
H	8.56200	3.73410	18.26490
H	7.69930	-0.91900	10.39130
H	7.74440	-0.14190	9.00210
H	6.62820	-1.26210	9.25880
H	5.83550	5.66530	18.41450
H	6.68570	4.54960	19.17220
H	5.10880	4.38220	19.03730
H	4.55250	-1.90000	13.65170

H	4.31210	-0.68580	12.65820
H	4.66410	-0.40560	14.19090
H	8.10160	-1.55640	14.02670
H	6.99920	-1.03570	15.05980
H	6.87140	-2.48600	14.41890
H	4.83740	1.87200	7.60190
H	4.42840	0.34550	7.88370
H	5.95780	0.73750	7.59170
H	3.56440	3.88570	11.87170
H	2.32350	5.30710	9.96680
C	2.12060	6.00980	11.89170
H	2.03560	5.59540	12.77930
C	3.42250	6.80940	11.84580
C	0.94050	6.96120	11.70030
H	3.41810	7.51510	12.52890
H	3.53820	7.23110	10.96600
H	4.19630	6.22970	12.01520
H	0.95500	7.66300	12.38780
H	0.08670	6.48250	11.77950
H	0.98010	7.38860	10.81660

D:
127

Cu	1.16056722	2.65189676	13.70126014
N	1.29393195	2.56256851	11.75723864
N	0.14426348	0.98343940	13.45302145
N	0.81477365	2.26209656	15.52739439
N	3.04984868	4.16491654	15.84205636
H	2.89677304	3.81915882	15.04830423
N	1.52062238	2.75957030	9.55083643
N	-0.11164407	1.01758833	17.10934674
O	-0.82872913	-0.19253508	11.74820954
O	2.44043726	4.28240997	18.00632270
O	-1.25869902	3.52922628	12.98998253
C	1.85717285	3.27885682	10.77195145
C	0.76411624	1.63198174	9.82027562
C	0.62397441	1.55691505	11.17595120
C	-0.06278266	0.70454757	12.14465540
C	-0.42522686	0.22237709	14.61291624
H	-1.38397521	0.65432828	14.52167520
C	0.03598440	1.19669021	15.76809497

C	0.61368652	2.03704214	17.71565041
C	1.22203808	2.76479196	16.71347503
C	2.22222807	3.83550068	16.86469424
C	4.35624251	4.78207118	16.03949530
H	4.37898443	5.11406555	16.96254145
C	1.85073984	3.27834465	8.21578422
H	2.37402329	4.10545205	8.26576751
H	1.02164563	3.47141233	7.72602497
H	2.36827567	2.60678483	7.72022324
C	0.24047715	0.71562969	8.76366235
H	1.16284720	0.40813228	8.62159135
H	0.41930183	0.82498798	7.80427984
H	-0.35084083	1.44042594	8.46344008
C	0.08652739	-1.65429445	14.82653594
H	-0.15149054	-2.18757245	15.67883655
C	-0.36781864	-0.62017714	14.64709578
H	-1.17677626	-1.10718327	15.13298844
H	0.73761114	-0.57855852	14.80106422
H	0.55883308	-1.06286496	14.87990889
C	-0.19502297	-2.58115988	13.62047830
H	0.18266135	-3.46990596	13.80192705
H	0.23314246	-2.24336180	12.80291231
H	-1.15921678	-2.68814278	13.45808459
C	-0.91527365	-0.02248077	17.76913511
H	-1.84574798	0.03885790	17.46033294
H	-0.90627923	0.08003203	18.74497906
H	-0.55857346	-0.91037894	17.55196708
C	0.79666393	2.16015589	19.19846455
H	0.21140860	1.80114546	19.90056675
H	1.04146625	1.20812233	19.20763451
H	-0.03698931	2.68152589	19.14396905
C	4.58859920	5.96840191	15.09620469
H	4.39782024	5.64322511	14.18696248
C	3.60524263	7.10356341	15.39840418
H	3.72048539	7.83980010	14.75793727
H	3.74457937	7.45568205	16.30519861
H	2.67859953	6.78590925	15.33333123
C	6.05004158	6.44291941	15.09470381
H	5.94882126	7.13332317	14.40247432
H	6.64213848	7.06962500	15.56463257
H	5.84653883	6.59088791	16.04321187
H	-1.28992377	3.71048696	12.09870970

H	-1.90046172	2.91696235	13.19284744
Cu	4.50503583	2.50452791	13.17281592
C	2.59466924	4.54603400	11.07554108
C	5.44322782	3.75886891	15.90260092
N	5.49109137	2.89426290	14.87076423
N	5.63210734	0.90635545	13.22062417
N	4.88309387	2.22023278	11.18402764
O	6.28832513	4.34070306	12.61376660
C	6.49196319	2.03539171	15.14358229
C	6.59427583	0.94942983	14.16767783
C	5.37831607	0.99550078	10.93504066
H	5.89735232	5.05173591	12.20253144
C	5.61942881	0.03988788	12.05420453
C	4.92159942	2.86645135	9.98892312
H	6.93735034	4.00157855	12.07385995
C	7.10679248	2.39542751	16.31012543
O	7.47642985	0.07776987	14.27381219
N	5.69596890	0.79986758	9.64570942
N	6.42698828	3.48178404	16.80836821
H	6.51515623	-0.35165143	11.94964996
C	4.55069704	-1.05522861	12.12376891
C	5.35123972	1.96871998	9.01860910
C	4.67396449	4.28720364	9.69819840
C	8.23481218	1.74650380	17.03700315
C	6.29595032	-0.40869395	9.06255057
C	6.71520399	4.18331343	18.06791328
H	4.67175497	-1.64213754	11.34348436
C	3.12985627	-0.49891144	12.05288767
C	4.73232852	-1.91855287	13.37063557
C	5.51554853	2.16112341	7.54717817
N	3.64632918	5.01894199	10.18805223
O	5.42951836	4.86085520	8.89095329
H	7.87046493	1.08021098	17.65986234
H	8.75007529	2.41848026	17.53405686
H	8.82643848	1.30459040	16.38962142
H	7.15764896	-0.59012774	9.49768030
H	6.45200585	-0.30406088	8.09945416
H	5.69767615	-1.17502635	9.20083114
H	6.09837778	4.93144943	18.21666327
H	7.62997674	4.54002757	18.04301253
H	6.63327513	3.55597975	18.81929737
H	2.47189219	-1.22289312	12.14285002

H	2.97196410	0.15657488	12.76538453
H	2.97646533	-0.05991859	11.18765992
H	5.63842265	-2.29822154	13.39409204
H	4.59313816	-1.39136615	14.18746614
H	4.08852588	-2.66100356	13.36899131
H	4.88696933	2.84724646	7.23371980
H	5.32347485	1.32425433	7.07131044
H	6.43684201	2.44681508	7.36216435
H	3.60308455	5.84460010	9.89076119
H	3.06916276	4.36748849	11.91883145
C	1.55542594	5.64049949	11.35949966
H	0.91893351	5.28496419	12.01968403
C	2.18728707	6.88291372	11.98574513
C	0.74910548	6.02401019	10.11908658
H	1.48990608	7.51543303	12.26734349
H	2.78160376	7.34271726	11.35341922
H	2.70968826	6.63219247	12.77746320
H	0.08440300	6.71143429	10.34540279
H	0.26582436	5.24606308	9.76423537
H	1.33355293	6.37911617	9.41391945
O	3.60268992	0.88014190	15.18734463
H	2.78180922	0.53291815	15.01450945
H	3.59351393	1.28412107	16.00210006
O	0.31715841	4.96324342	14.64023518
H	0.88024222	5.63308079	14.39488184

E:
122

N	-0.77360	3.04900	-1.07310
N	-0.28180	4.92270	-0.04330
N	-2.31420	1.23430	-1.40130
N	-1.97060	-1.08690	0.28190
N	-4.17740	-1.14370	0.35780
N	0.03830	-2.03960	1.91130
C	-1.80950	3.30750	-0.29190
C	-1.55590	4.50310	0.34750
C	0.09820	4.02560	-0.99330
C	0.50790	6.03710	0.49860
H	1.34640	5.68840	0.87220

H	0.01920	6.50100	1.21190
H	0.71740	6.68710	-0.20470
C	-2.37490	5.22540	1.36110
H	-3.32260	5.00950	1.22160
H	-2.25050	6.19460	1.26650
H	-2.09810	4.93920	2.25880
C	-2.71610	2.18340	-0.51800
C	-3.10280	0.03010	-1.62150
H	-4.02570	0.32080	-1.79280
C	-2.60770	-0.75490	-2.83780
H	-1.64020	-0.90670	-2.74170
C	-3.29610	-2.11400	-2.95750
H	-3.09870	-2.67660	-2.17690
H	-2.97790	-2.58810	-3.75710
H	-4.27000	-2.00430	-3.02660
C	-2.85360	0.04710	-4.11440
H	-2.44700	0.93790	-4.04760
H	-3.81680	0.16210	-4.27090
H	-2.46420	-0.41390	-4.88980
C	-3.08820	-0.79860	-0.37650
C	-2.31600	-1.61400	1.46420
C	-3.68940	-1.64540	1.54500
C	-5.58250	-0.99330	-0.04700
H	-6.19390	-1.32350	0.64540
H	-5.74130	-1.50460	-0.87030
H	-5.78120	-0.04590	-0.21220
C	-4.57100	-2.15270	2.63700
H	-5.38660	-1.61010	2.69710
H	-4.09530	-2.09810	3.49390
H	-4.80490	-3.08770	2.44920
C	-1.22030	-1.91510	2.38910
C	1.15840	-2.55980	2.69740
H	0.81160	-3.04510	3.47880
C	2.07150	-1.40520	3.12240
H	1.54020	-0.81650	3.70510
C	3.26800	-1.89250	3.93520
H	3.74020	-1.12820	4.33320
H	3.90290	-2.37390	3.36140
H	2.97540	-2.48560	4.66180
C	2.55600	-0.57130	1.93660
H	3.10430	0.18070	2.25160
H	1.79600	-0.20210	1.43580

H	3.09960	-1.11520	1.32520
O	-3.80640	2.14530	0.08170
O	-1.46650	-2.08260	3.59780
C	1.31510	3.94900	-1.85000
C	1.82280	-3.54780	1.78750
N	1.34660	2.51600	-2.14260
H	2.10420	4.21780	-1.32930
C	1.14280	4.75520	-3.14550
C	2.49900	1.86190	-2.41820
H	0.36590	4.39770	-3.63220
C	2.36120	4.63710	-4.06020
C	0.87220	6.23520	-2.88580
C	2.47280	0.48310	-2.91520
H	2.49870	3.70840	-4.34620
H	3.17070	4.95070	-3.60010
H	2.23490	5.17770	-4.87090
H	0.78480	6.72150	-3.73510
H	1.60870	6.63630	-2.37410
H	0.03150	6.35350	-2.39290
N	1.35690	-0.25270	-2.79200
C	3.43360	-0.28060	-3.53900
C	1.62900	-1.47660	-3.24980
N	2.90750	-1.54000	-3.70830
C	4.83070	0.07360	-3.92840
C	0.69260	-2.63700	-3.11750
C	3.57780	-2.72230	-4.26850
H	5.43750	-0.16530	-3.19430
H	4.88650	1.03800	-4.10310
H	5.08980	-0.40490	-4.74520
N	0.90510	-3.19800	-1.79090
H	0.93460	-3.30710	-3.79410
C	-0.77020	-2.23320	-3.32420
H	4.50060	-2.52200	-4.53410
H	3.08590	-3.03680	-5.05810
H	3.60310	-3.43640	-3.59630
C	1.65330	-4.31420	-1.58520
H	-1.02560	-1.58750	-2.62690
C	-0.97630	-1.57810	-4.68970
C	-1.68960	-3.44770	-3.20950
C	2.11880	-4.56590	-0.21960
H	-0.44120	-0.75880	-4.77240
H	-1.92000	-1.33340	-4.81200

H	-0.71740	-2.19310	-5.41090
H	-2.62710	-3.18070	-3.33260
H	-1.46370	-4.11950	-3.89010
H	-1.60790	-3.86270	-2.32440
N	1.57770	-3.53310	0.48100
C	2.77910	-5.30670	0.73630
N	2.55430	-4.69260	1.99010
C	3.58690	-6.54780	0.56810
C	2.98930	-5.18770	3.30300
H	3.32370	-6.98930	-0.26860
H	3.42820	-7.16410	1.31530
H	4.53770	-6.30620	0.52590
H	3.56850	-4.52600	3.73770
H	3.48910	-6.02790	3.22250
H	2.20220	-5.34380	3.86920
Cu	0.37990	-2.15540	-0.11560
Cu	-0.43970	1.51620	-2.13590
H	1.45100	-3.17670	0.97630
O	3.59700	2.43820	-2.30680
O	1.98130	-5.10020	-2.49270
O	0.39000	0.19330	-0.30560
O	-1.26270	-4.19950	0.30970
O	-0.12900	1.74000	-4.69490
H	-1.18970	-4.49800	1.16620
H	-1.05790	-4.88550	-0.25150
H	0.62630	2.20340	-4.89870
H	-0.07600	0.91410	-5.07280

F:
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N	-1.42180	3.49880	-2.04590
N	-1.42460	5.68300	-2.24890
N	-2.49070	1.52770	-1.18340
N	-1.17190	-0.84150	0.82390
N	-2.55050	0.54710	1.87580
N	0.51310	-2.89400	1.94830
C	-2.61530	3.88640	-1.63240
C	-2.66990	5.25820	-1.76950
C	-0.72960	4.53130	-2.46300
C	-0.94370	7.06090	-2.42240
H	-0.15220	7.20200	-1.85850

H	-1.63130	7.71130	-2.16450
H	-0.70330	7.22880	-3.35750
C	-3.78970	6.19260	-1.46170
H	-4.39370	5.76590	-0.81560
H	-4.28040	6.38560	-2.29010
H	-3.44540	7.02500	-1.07230
C	-3.25660	2.64910	-1.18900
C	-2.93150	0.26190	-0.61530
H	-3.88540	0.35700	-0.40010
C	-2.79420	-0.86820	-1.64060
H	-1.84190	-0.98340	-1.85980
C	-3.33270	-2.19140	-1.09550
H	-2.83630	-2.47670	-0.29790
H	-3.24450	-2.89930	-1.77100
H	-4.28180	-2.10580	-0.85620
C	-3.54150	-0.52520	-2.92910
H	-3.19710	0.30480	-3.32470
H	-4.50100	-0.40840	-2.75230
H	-3.43070	-1.24310	-3.59060
C	-2.23370	-0.02520	0.68290
C	-0.87490	-0.88340	2.14420
C	-1.71680	-0.01430	2.81070
C	-3.59030	1.56130	2.10630
H	-3.64170	1.82180	3.05040
H	-4.46480	1.20830	1.83260
H	-3.38390	2.36510	1.58280
C	-1.77650	0.34770	4.25970
H	-1.21970	1.14200	4.41290
H	-1.44410	-0.39680	4.80520
H	-2.70170	0.53190	4.52960
C	0.06650	-1.86390	2.70160
C	1.00160	-4.15480	2.51810
H	1.73740	-3.93090	3.13070
C	-0.16160	-4.85910	3.23280
H	-0.46930	-4.26670	3.95490
C	-1.35420	-5.10850	2.31140
H	-1.69970	-4.26000	1.95910
H	-2.08230	-5.54580	2.80520
H	-1.10000	-5.68530	1.55790
C	0.25070	-6.16510	3.90380
H	-0.47340	-6.49270	4.48160
H	1.04860	-6.03000	4.46080

H	0.43240	-6.85560	3.23050
O	-4.44010	2.68190	-0.80470
O	0.31280	-1.85300	3.92170
C	0.65020	4.28400	-2.97110
C	1.55980	-4.94090	1.36350
N	0.92030	2.97420	-2.37840
H	1.26560	4.96190	-2.61370
C	0.68260	4.18130	-4.50280
C	2.16680	2.53520	-2.09260
H	0.06220	3.47020	-4.78000
C	2.07060	3.80940	-5.02220
C	0.22970	5.46770	-5.18840
C	2.43600	1.09210	-2.07280
H	2.33750	2.92000	-4.70350
H	2.73810	4.46760	-4.72800
H	2.07320	3.78110	-6.00430
H	0.29490	5.37750	-6.16450
H	0.79010	6.22450	-4.90850
H	-0.70900	5.66000	-4.97500
N	1.44030	0.18690	-2.20000
C	3.64260	0.43900	-2.18100
C	2.01390	-0.95930	-2.60240
N	3.36930	-0.84130	-2.59390
C	5.03300	0.96470	-2.04070
C	1.26760	-2.19840	-2.99900
C	4.33630	-1.88270	-2.97170
H	5.62980	0.26290	-1.70210
H	5.03680	1.70990	-1.40160
H	5.34820	1.27630	-2.91700
N	1.30220	-3.18260	-1.92580
H	1.75770	-2.57560	-3.76230
C	-0.16870	-1.93080	-3.46090
H	5.25980	-1.55810	-2.90810
H	4.17240	-2.16400	-3.89810
H	4.23850	-2.65630	-2.37560
C	1.98810	-4.35010	-2.04140
H	-0.67890	-1.55450	-2.70840
C	-0.21530	-0.94280	-4.62720
C	-0.84440	-3.23030	-3.89870
C	2.19040	-5.12150	-0.81680
H	0.15260	-0.06940	-4.37180
H	-1.14350	-0.80130	-4.91660

H	0.30000	-1.28480	-5.39070
H	-0.85330	-3.88710	-3.16930
H	-0.37020	-3.62640	-4.66280
H	-1.77520	-3.06010	-4.16320
N	1.46740	-4.45860	0.12390
C	2.80940	-6.12490	-0.12370
N	2.52060	-5.93350	1.24360
C	3.75770	-7.16170	-0.61980
C	3.17970	-6.62590	2.36030
H	3.55600	-7.35780	-1.56070
H	3.66110	-7.98560	-0.09480
H	4.67530	-6.82110	-0.54050
H	3.60300	-5.96360	2.94900
H	3.87410	-7.23940	2.03790
H	2.53150	-7.14950	2.87520
Cu	0.49800	-2.82910	-0.09400
Cu	-0.66390	1.77250	-1.99220
H	1.22960	-4.32850	0.69350
O	3.12400	3.33090	-2.11770
O	2.53890	-4.72970	-3.09120
O	-1.75540	-3.65900	-0.74630
O	-0.65780	0.90970	-4.33400
H	-2.38670	-3.37300	-0.15720
H	-1.75150	-4.56870	-0.76190
H	-0.75810	0.00540	-4.32920
H	-1.34620	1.28300	-4.79700
O	0.12100	2.14380	0.40500
H	0.76930	1.53880	0.60880
O	2.62240	-1.58530	0.59980
H	3.32970	-1.87240	0.10510
H	2.51320	-0.69020	0.48020

G:
123

N	2.14770	1.63280	-0.00030
N	2.12900	3.78140	0.62140
N	3.11320	0.22720	-1.92740
N	2.01120	-1.98710	-1.48370
N	2.63740	-3.00400	-3.36550
N	0.25100	-2.82580	0.65390
C	2.75660	2.36960	-0.94970

C	2.74410	3.69570	-0.60850
C	1.74420	2.51280	0.93700
C	1.94520	4.98240	1.44810
H	0.98850	5.14370	1.59430
H	2.33130	5.77560	1.01900
H	2.38790	4.85320	2.31520
C	3.32230	4.87180	-1.32080
H	3.35570	4.68340	-2.28380
H	4.23030	5.03420	-0.98420
H	2.76460	5.66620	-1.17450
C	3.25490	1.56220	-2.06150
C	3.78080	-0.80290	-2.70750
H	3.83430	-0.53160	-3.65070
C	5.15380	-1.11380	-2.09320
H	5.02640	-1.32530	-1.14140
C	5.83380	-2.32100	-2.73380
H	5.29220	-3.13080	-2.61160
H	6.70600	-2.48550	-2.31230
H	5.97950	-2.16640	-3.69280
C	6.10250	0.08140	-2.17460
H	5.76250	0.83600	-1.64700
H	6.21690	0.36950	-3.10700
H	6.98430	-0.15490	-1.81140
C	2.82420	-1.94320	-2.54500
C	1.36750	-3.17370	-1.51960
C	1.73560	-3.81390	-2.69900
C	3.22420	-3.20610	-4.69990
H	2.91030	-4.04010	-5.10930
H	4.20170	-3.24680	-4.64660
H	2.96820	-2.45850	-5.28300
C	1.31490	-5.14590	-3.22890
H	1.27200	-5.13060	-4.20890
H	0.42280	-5.37040	-2.88760
H	1.96090	-5.82400	-2.93380
C	0.44710	-3.58880	-0.44900
C	-0.64110	-3.24230	1.72820
H	-0.34440	-4.14330	1.98220
C	-0.56390	-2.33870	2.96370
H	-0.79600	-1.42080	2.69690
C	0.84700	-2.32070	3.55020
H	1.49310	-1.97440	2.89730
H	1.12380	-3.22560	3.81470

H	0.88040	-1.74020	4.34220
C	-1.54990	-2.78680	4.04230
H	-1.48500	-2.20170	4.82880
H	-1.36070	-3.70950	4.32220
H	-2.47420	-2.74380	3.71330
O	3.85200	2.08830	-3.01860
O	-0.10500	-4.70170	-0.53160
C	0.96110	2.09750	2.14570
C	-2.04420	-3.31510	1.21020
N	-0.40140	1.85310	1.69270
H	0.94410	2.84160	2.78720
C	1.56880	0.87270	2.83600
H	-0.54100	1.09410	1.27250
C	-1.31920	2.83920	1.55880
H	1.60190	0.12570	2.19650
C	0.71450	0.43830	4.02570
C	2.99150	1.16920	3.30850
C	-2.46020	2.69250	0.64260
H	-0.19060	0.19400	3.73270
H	0.64490	1.16300	4.68550
H	1.11220	-0.34610	4.46380
H	3.37290	0.38420	3.75940
H	2.99700	1.92330	3.93830
H	3.57180	1.39360	2.54830
N	-2.76720	1.51790	0.04590
C	-3.39090	3.63290	0.21970
C	-3.85210	1.73250	-0.70890
N	-4.31250	2.99660	-0.57810
C	-3.53200	5.07290	0.58670
C	-4.44540	0.60910	-1.49660
C	-5.54620	3.57080	-1.13140
H	-4.07930	5.14250	1.39900
H	-2.64470	5.45900	0.75140
H	-3.95950	5.56910	-0.14460
N	-3.92030	-0.55440	-0.80330
H	-5.42380	0.61670	-1.40470
C	-4.00390	0.57440	-2.96390
H	-5.32730	4.32030	-1.72710
H	-6.11280	3.89570	-0.39800
H	-6.05230	2.90090	-1.63870
C	-4.55960	-1.72460	-0.60050
H	-4.36390	-0.25310	-3.35640

C	-4.57870	1.73820	-3.76710
C	-2.48380	0.53350	-3.11820
C	-3.82230	-2.72680	0.16500
H	-5.55840	1.75270	-3.69670
H	-4.34380	1.64530	-4.71660
H	-4.22210	2.59480	-3.44530
H	-2.10540	-0.23780	-2.64180
H	-2.07360	1.35330	-2.76520
H	-2.24080	0.45140	-4.06670
N	-2.60890	-2.28660	0.55090
C	-4.02400	-4.00870	0.59840
N	-2.87920	-4.39500	1.25230
C	-5.18180	-4.92370	0.38450
C	-2.62690	-5.70680	1.86510
H	-6.00330	-4.39290	0.29890
H	-5.27500	-5.53670	1.14560
H	-5.03320	-5.43750	-0.43900
H	-1.73760	-5.74900	2.27660
H	-2.68770	-6.40650	1.17850
H	-3.29740	-5.87810	2.56180
Cu	-2.13960	-0.39000	0.03220
Cu	2.06610	-0.35030	-0.35270
H	0.65660	-2.04870	0.71120
O	-1.16770	3.91590	2.16440
O	-5.69720	-1.96250	-1.04580
O	-0.15900	-0.06210	-1.05080
O	-3.32020	-0.04030	2.34920
O	3.70910	-1.64580	1.03880
H	-2.70620	0.15370	2.99170
H	-3.78560	-0.78230	2.59560
H	3.38760	-2.48060	1.20480
H	3.86720	-1.22400	1.82860

H:
128

N	-2.46530	-2.05080	0.32780
N	-4.45680	-1.04800	0.20230
N	-1.48090	-4.14830	1.45790
N	0.97980	-3.67690	1.17760
N	1.72170	-5.27330	2.54590
N	2.46410	-1.16560	0.49300

C	-3.33210	-2.69020	1.13940
C	-4.55320	-2.08100	1.10150
C	-3.16730	-1.05550	-0.25350
C	-5.54230	-0.13770	-0.18710
H	-5.24390	0.51210	-0.85760
H	-5.86080	0.35290	0.60170
H	-6.28460	-0.65640	-0.56710
C	-5.82670	-2.43890	1.79000
H	-5.62190	-2.87560	2.64520
H	-6.33520	-3.05440	1.21830
H	-6.35780	-1.63150	1.96300
C	-2.74700	-3.84790	1.81270
C	-0.72600	-5.34150	1.80130
H	-0.99600	-5.66500	2.68920
C	-0.90330	-6.39650	0.70130
H	-0.65590	-5.99200	-0.16020
C	-0.00890	-7.61690	0.90380
H	0.93860	-7.36000	0.88440
H	-0.15250	-8.26890	0.18290
H	-0.20990	-8.05400	1.76020
C	-2.35580	-6.85840	0.59490
H	-2.94300	-6.11250	0.34430
H	-2.66390	-7.23110	1.45020
H	-2.44600	-7.55000	-0.09720
C	0.66810	-4.79750	1.84510
C	2.30800	-3.47830	1.34220
C	2.79300	-4.50170	2.14910
C	1.70270	-6.33730	3.56160
H	2.58890	-6.46440	3.96260
H	1.41970	-7.18850	3.16640
H	1.07420	-6.09230	4.27530
C	4.17320	-4.73490	2.66990
H	4.27080	-4.27530	3.53230
H	4.83380	-4.38610	2.03380
H	4.33270	-5.69650	2.78570
C	3.04990	-2.36280	0.73580
C	3.18970	-0.00770	-0.01490
H	4.09020	-0.30670	-0.26900
C	2.52530	0.57160	-1.26880
H	1.64630	0.94020	-1.02470
C	2.30270	-0.51160	-2.32330
H	1.70310	-1.20990	-1.98110

H	3.15530	-0.92790	-2.57860
H	1.88880	-0.12730	-3.12720
C	3.37330	1.69180	-1.87110
H	2.93290	2.06270	-2.66730
H	4.25770	1.35350	-2.13360
H	3.49920	2.42340	-1.22840
O	-3.42600	-4.56040	2.57460
O	4.25230	-2.53520	0.46340
C	-2.55950	-0.08450	-1.22290
C	3.36360	1.01770	1.06600
N	-2.09080	1.10360	-0.51960
H	-3.27240	0.19240	-1.83870
C	-1.44870	-0.71820	-2.06770
H	-1.41860	1.00450	0.03800
C	-2.68510	2.31690	-0.62260
H	-0.75080	-1.07090	-1.47040
C	-0.80060	0.31620	-2.98680
C	-1.99590	-1.86820	-2.91310
C	-2.22570	3.47070	0.16310
H	-0.38370	1.03330	-2.46140
H	-1.46890	0.71490	-3.58670
H	-0.09960	-0.10240	-3.53340
H	-1.28020	-2.26270	-3.45820
H	-2.70340	-1.54860	-3.51540
H	-2.36870	-2.57680	-2.34450
N	-0.94420	3.67580	0.54290
C	-2.98280	4.52920	0.64350
C	-0.91370	4.84590	1.19850
N	-2.15200	5.37220	1.34170
C	-4.44070	4.81030	0.48610
C	0.38750	5.40620	1.68290
C	-2.54250	6.56920	2.09910
H	-4.93090	3.96360	0.40490
H	-4.57450	5.34850	-0.32420
H	-4.78160	5.29760	1.26700
N	1.20780	4.20780	1.74050
H	0.28470	5.78070	2.58570
C	0.99040	6.40770	0.68900
H	-3.18370	6.32000	2.79970
H	-2.96020	7.22200	1.49580
H	-1.76500	6.98520	2.52930
C	2.21520	3.94080	2.59710

H	1.09570	5.95880	-0.17960
C	0.09880	7.62740	0.46680
C	2.37280	6.87910	1.13750
C	2.99590	2.74050	2.30030
H	-0.76700	7.36150	0.08800
H	0.52030	8.24720	-0.16840
H	-0.05190	8.10580	1.31140
H	3.00280	6.12710	1.17790
H	2.32400	7.29990	2.02410
H	2.73510	7.53410	0.50100
N	2.50800	2.04140	1.25590
C	4.11940	2.13600	2.79380
N	4.36480	1.04310	1.99100
C	5.00260	2.53910	3.92630
C	5.48400	0.09580	2.08820
H	4.48190	3.06440	4.57190
H	5.74140	3.08360	3.57700
H	5.35820	1.74530	4.38100
H	5.13680	-0.80800	2.24950
H	6.09100	0.33060	2.82220
H	5.99530	0.10290	1.24970
Cu	0.83240	2.78730	0.43690
Cu	-0.60030	-2.82120	0.30630
H	1.62000	-1.04990	0.70830
O	-3.66040	2.47970	-1.37900
O	2.54400	4.71090	3.51800
O	-0.22520	1.61490	2.50790
O	0.31210	-4.03510	-1.69710
O	0.88860	3.83000	-1.84340
O	-0.54280	-1.58940	2.60460
H	-0.82180	2.16680	2.91690
H	0.41960	1.38340	3.10660
H	0.76560	-3.45900	-2.23540
H	-0.37040	-4.40880	-2.16840
H	0.78150	3.19450	-2.48510
H	1.68620	4.24890	-1.97030
H	0.27830	-1.23010	2.75940
H	-1.16810	-0.92890	2.62220

I:

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N	-2.09140	1.29930	0.38540
N	-3.83570	0.06380	-0.22630
N	-1.97290	-1.77260	1.49830
N	-1.54120	-3.33000	-0.25210
N	-2.13270	-5.16450	-1.30570
N	0.40530	-2.64430	-1.53420
O	-3.47380	-3.20280	2.47920
O	2.32120	-3.39040	-2.46340
C	-2.52470	1.75430	-0.80500
C	-3.57370	0.96630	-1.22760
C	-2.90030	0.29300	0.73500
C	-2.68310	-0.57720	1.93210
H	-3.57140	-0.86120	2.23720
C	-2.59170	-2.97590	1.63040
C	-2.43130	-3.91810	0.52640
C	-2.82310	-5.08570	-0.09880
C	-1.36330	-4.05510	-1.32670
C	-0.40680	-3.55200	-2.34270
H	0.12900	-4.31140	-2.66230
C	1.75720	-2.71350	-1.58360
C	-4.38210	1.04460	-2.48090
H	-3.83760	1.43630	-3.19760
H	-5.17000	1.60760	-2.31790
H	-4.66460	0.14920	-2.76560
C	-4.88900	-0.96730	-0.19100
H	-4.41750	-1.82540	-0.11720
H	-5.35190	-0.96300	-1.05570
C	-5.97800	-0.95580	0.85170
C	-6.06210	0.05810	1.78850
H	-5.42150	0.78680	1.78430
C	-7.06320	0.04560	2.73870
H	-7.11690	0.75860	3.39550
C	-7.98840	-0.97810	2.75430
H	-8.69270	-0.98660	3.42250
C	-7.91290	-1.98810	1.81700
H	-8.56410	-2.70820	1.82610
C	-6.91120	-1.97590	0.86720
H	-6.86200	-2.69110	0.21230
C	-2.01000	0.15400	3.09530
H	-1.18160	0.56970	2.77290
C	-2.92020	1.25550	3.63720
H	-3.14710	1.90040	2.93210

H	-2.47210	1.74330	4.36280
H	-3.75500	0.87380	3.98770
C	-1.64800	-0.81050	4.22300
H	-2.45070	-1.26490	4.56140
H	-1.22680	-0.32470	4.96580
H	-1.01180	-1.48930	3.90770
C	-3.84890	-6.08540	0.30840
H	-3.90830	-6.10410	1.28840
H	-3.59910	-6.97690	-0.01840
H	-4.71590	-5.82290	-0.07060
C	-2.23230	-6.20690	-2.33240
H	-1.63880	-6.00700	-3.08860
H	-3.15660	-6.25800	-2.66020
H	-1.97500	-7.07360	-1.94900
C	-1.11740	-2.84440	-3.49940
H	-1.68140	-3.50830	-3.95690
C	-0.10140	-2.32400	-4.51350
H	0.46640	-3.05790	-4.83640
H	0.47310	-1.63650	-4.11040
H	-0.56160	-1.92960	-5.28680
C	-2.02460	-1.70740	-3.03090
H	-2.72610	-2.04430	-2.43160
H	-2.46500	-1.28470	-3.80060
H	-1.50840	-1.02130	-2.55470
C	-1.94310	2.94090	-1.44040
N	-0.76110	3.46630	-1.03760
O	-2.60740	3.51350	-2.32430
C	-0.30300	4.75020	-1.56970
C	1.16650	4.53100	-1.62080
H	-0.63890	4.89480	-2.48180
C	-0.67380	5.89410	-0.61720
N	1.67120	3.58560	-0.86650
N	2.13610	5.12670	-2.36270
H	-0.32400	5.68080	0.27720
C	-2.18850	6.05880	-0.50320
C	-0.06240	7.22800	-1.04090
C	2.98730	3.57390	-1.00800
C	3.32170	4.55160	-1.91950
C	1.97680	6.12860	-3.42300
H	-2.60530	5.24430	-0.14730
H	-2.58170	6.25550	-1.38180
H	-2.40780	6.79560	0.10860

H	0.91820	7.18130	-1.03010
H	-0.33050	7.93950	-0.41870
H	-0.36220	7.47610	-1.94280
C	3.43200	2.52470	-0.09680
C	4.65330	4.92220	-2.47430
H	1.02930	6.34270	-3.56230
H	2.34360	5.77640	-4.26310
H	2.45690	6.94980	-3.17920
N	2.47320	1.89290	0.62590
O	4.64910	2.28710	0.00880
H	5.34470	4.73790	-1.80170
H	4.66910	5.87720	-2.70140
H	4.82310	4.38620	-3.27940
C	2.81320	0.83140	1.56240
C	3.03770	-0.41720	0.77030
H	3.63740	1.08600	2.03090
C	1.70920	0.65510	2.60380
C	2.59560	-1.99220	-0.62280
N	2.04510	-1.07350	0.17410
N	4.24130	-0.98760	0.47680
H	0.86660	0.48070	2.12920
C	1.99780	-0.52090	3.53560
C	1.55820	1.92720	3.43560
C	3.95330	-2.00770	-0.40050
C	5.57080	-0.59470	0.97750
H	2.07210	-1.35970	3.03110
H	1.27070	-0.62480	4.18810
H	2.83800	-0.37680	4.02390
H	1.38920	2.70240	2.85750
H	0.80720	1.83890	4.06300
H	2.37610	2.10290	3.95090
C	5.00940	-2.84730	-1.03790
H	5.48500	0.20280	1.54170
H	6.12060	-0.34890	0.20130
C	6.27840	-1.63490	1.80680
H	4.63030	-3.71970	-1.28030
H	5.75470	-2.99390	-0.41840
H	5.33450	-2.39150	-1.84460
C	5.68460	-2.10220	2.96430
C	7.51420	-2.12540	1.42690
H	4.81790	-1.76220	3.23870
C	6.31880	-3.05660	3.73390

C	8.14830	-3.08000	2.19660
H	7.94050	-1.80260	0.61650
H	5.89780	-3.38360	4.54530
C	7.55070	-3.54630	3.35000
H	9.01510	-3.42370	1.92620
H	7.99670	-4.21780	3.89110
Cu	-0.57870	-1.70320	0.00230
Cu	0.55490	2.44760	0.17570
O	0.72300	-3.23500	1.65460
H	0.28360	-3.29970	2.44860
O	0.11330	0.41380	-0.88210
H	0.51360	0.35490	-1.69710
H	0.81970	-4.06680	1.29910
O	-0.89060	3.67300	1.94240
H	-0.92670	3.20260	2.71920
H	-1.73890	3.79820	1.63960

J:
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N	-1.76710	1.39750	-0.06150
N	-3.53510	0.62560	-1.17320
N	-2.81830	-1.64820	0.94310
N	-1.99570	-3.78280	0.21310
N	-2.42420	-5.86400	-0.32200
N	0.15370	-3.42660	-0.85050
O	-4.89420	-2.52910	1.37410
O	1.44390	-3.65010	-2.67540
C	-1.86890	2.08290	-1.22160
C	-2.89860	1.54720	-1.96280
C	-2.83260	0.57760	-0.00880
C	-3.20040	-0.26300	1.17530
H	-4.18040	-0.23410	1.23810
C	-3.71330	-2.66780	1.00540
C	-3.26260	-3.97650	0.53710
C	-3.56240	-5.28920	0.23970
C	-1.47780	-4.89170	-0.25710
C	-0.05540	-4.86550	-0.69680
H	0.03380	-5.32500	-1.56090
C	0.99460	-2.91430	-1.77700
C	-3.28760	1.78590	-3.38560
H	-3.07710	2.70930	-3.64100

H	-4.24870	1.63660	-3.51330
H	-2.78280	1.16610	-3.95590
C	-4.73150	-0.15870	-1.52800
H	-4.87380	-0.82580	-0.82350
H	-4.50130	-0.64700	-2.34890
C	-6.07100	0.50010	-1.73890
C	-6.23160	1.86360	-1.57200
H	-5.47950	2.42020	-1.31440
C	-7.46780	2.44650	-1.76590
H	-7.57610	3.40410	-1.64820
C	-8.55020	1.66910	-2.12450
H	-9.41960	2.07930	-2.26020
C	-8.39560	0.30750	-2.28710
H	-9.15680	-0.24080	-2.53730
C	-7.15940	-0.27550	-2.09320
H	-7.05750	-1.23420	-2.20840
C	-2.63990	0.27470	2.49550
H	-1.65830	0.30340	2.43660
C	-3.02070	-0.63220	3.66530
H	-2.64530	-0.28370	4.50370
H	-2.67260	-1.54080	3.53540
H	-3.99740	-0.68540	3.75860
C	-3.16320	1.68310	2.78050
H	-2.80700	2.01420	3.63410
H	-4.14430	1.68310	2.83370
H	-2.89270	2.31280	2.07760
C	-4.83020	-6.04460	0.44220
H	-4.79590	-6.49430	1.31450
H	-4.94660	-6.70950	-0.27070
H	-5.58490	-5.41650	0.42450
C	-2.29830	-7.21140	-0.88920
H	-2.94340	-7.32070	-1.62140
H	-2.48000	-7.88130	-0.19450
H	-1.39650	-7.35750	-1.24740
C	0.89090	-5.41740	0.37680
H	0.74150	-4.91750	1.21020
C	2.35690	-5.23400	-0.01370
H	2.94520	-5.61010	0.67750
H	2.58030	-4.28210	-0.10380
H	2.54730	-5.68570	-0.86520
C	0.63300	-6.89260	0.67460
H	-0.27520	-7.02280	1.02400

H	1.26120	-7.21870	1.35600
H	0.74640	-7.43480	-0.13660
C	-1.14880	3.34580	-1.42040
N	-0.23550	3.76660	-0.51620
O	-1.54170	4.12490	-2.30830
C	0.12560	5.17820	-0.38230
C	1.48490	5.12610	0.21730
H	0.20680	5.58090	-1.27540
C	-0.83930	5.96340	0.51410
N	1.95370	3.95720	0.57680
N	2.43150	6.08640	0.34600
H	-0.45950	6.86010	0.64930
C	-1.00990	5.31980	1.88870
C	-2.20450	6.16030	-0.14090
C	3.19930	4.09320	0.99950
C	3.52550	5.43040	0.91360
C	2.31920	7.49500	-0.05110
H	-0.14390	5.23830	2.34470
H	-1.40930	4.42660	1.80460
H	-1.59800	5.86910	2.45210
H	-2.10360	6.57040	-1.02800
H	-2.76180	6.75470	0.40820
H	-2.67600	5.30430	-0.23730
C	3.62160	2.73080	1.31380
C	4.80770	6.11490	1.24000
H	2.12110	7.54890	-1.01150
H	3.15390	7.98020	0.12380
H	1.59540	7.92630	0.45260
N	2.73390	1.73550	1.05950
O	4.76610	2.54030	1.76410
H	5.36240	6.15670	0.43080
H	5.27550	5.60480	1.93670
H	4.63190	7.02200	1.57170
C	3.10440	0.32950	1.12140
C	2.71870	-0.36610	-0.14610
H	4.08230	0.29080	1.17880
C	2.54720	-0.36660	2.36660
C	1.66740	-1.63790	-1.51640
N	1.57040	-1.04380	-0.31050
N	3.47490	-0.40580	-1.27890
H	1.56460	-0.34070	2.33190
C	3.00340	-1.82510	2.42920

C	2.99940	0.34200	3.64290
C	2.73630	-1.11070	-2.19490
C	4.83400	0.13360	-1.46500
H	2.66670	-2.33710	1.66220
H	2.66580	-2.25430	3.24580
H	3.98450	-1.88100	2.43170
H	2.69520	1.27500	3.65470
H	3.97930	0.33430	3.71420
H	2.62530	-0.10610	4.43310
C	3.20340	-1.36760	-3.58850
H	4.81610	1.10330	-1.30830
H	5.12440	-0.01560	-2.39030
C	5.84000	-0.53970	-0.56660
H	2.42970	-1.57400	-4.15670
H	3.82740	-2.12590	-3.58360
H	3.65140	-0.57110	-3.94680
C	6.00610	-1.91050	-0.63690
C	6.59500	0.19400	0.32940
H	5.48120	-2.43420	-1.26380
C	6.90990	-2.54410	0.19190
C	7.49930	-0.43950	1.15780
H	6.49220	1.15740	0.38070
H	7.01970	-3.50750	0.14340
C	7.65560	-1.80910	1.09090
H	8.02530	0.07890	1.78810
H	8.29090	-2.25470	1.67430
Cu	-0.99240	-2.18190	0.26880
Cu	0.93850	2.37870	0.39010
O	-1.86780	-1.65130	-2.07890
H	-1.27720	-1.12130	-2.52390
O	-0.38230	-2.62280	2.65360
H	-0.18880	-1.84090	3.07570
H	0.34000	-3.17230	2.70330
O	0.42370	2.36980	2.84500
H	-0.46180	2.51640	2.98350
H	0.89860	3.02670	3.25800
H	-2.00090	-2.41650	-2.55270
O	1.72690	2.25450	-2.02850
H	2.63570	2.25100	-2.06500
H	1.40580	1.49940	-2.42120

K:

N	0.64780	-1.08650	2.85610
N	1.00650	-3.28580	2.80070
N	2.84480	-0.34640	1.90850
N	2.56620	2.18410	1.81800
N	3.70200	3.96310	1.10200
N	0.49260	4.54710	1.52310
H	0.08640	3.80400	1.28720
O	4.71480	-0.27110	0.60520
O	0.76740	6.76110	1.17530
C	-0.53470	-1.68810	3.10270
C	-0.33110	-3.05740	3.06850
C	1.56330	-2.04820	2.71950
C	2.99290	-1.67700	2.47890
H	3.39800	-2.27740	1.81480
C	3.73910	0.29760	1.12840
C	3.63720	1.75570	1.12770
C	4.34770	2.82920	0.66290
C	2.62630	3.52970	1.82110
C	1.57900	4.38070	2.47730
H	1.96830	5.26080	2.67220
C	0.19610	5.69750	0.87270
C	-1.33280	-4.16280	3.12980
H	-2.06510	-3.90550	3.73060
H	-0.92380	-4.98830	3.46590
H	-1.68800	-4.31670	2.22740
C	1.66040	-4.58680	2.57610
H	2.57640	-4.39520	2.28030
H	1.18480	-4.98490	1.81400
C	1.79030	-5.66340	3.62440
C	1.31000	-5.47390	4.90730
H	0.87980	-4.63940	5.15280
C	1.44300	-6.46980	5.85390
H	1.10470	-6.33210	6.75340
C	2.05780	-7.66020	5.52330
H	2.15160	-8.36040	6.18930
C	2.54100	-7.85300	4.24510
H	2.97500	-8.68950	4.01150
C	2.40840	-6.85670	3.29880
H	2.75150	-6.99880	2.40160
C	3.78780	-1.60940	3.79060

H	3.35790	-0.94910	4.38040
C	3.80180	-2.94380	4.53230
H	2.89190	-3.19790	4.79630
H	4.33700	-2.87520	5.35330
H	4.18530	-3.65190	3.96970
C	5.23050	-1.15940	3.56480
H	5.72790	-1.16420	4.41210
H	5.26150	-0.24330	3.21370
H	5.68550	-1.75890	2.93330
C	5.62010	2.87260	-0.11320
H	5.68810	2.06590	-0.66890
H	6.37440	2.90560	0.51470
H	5.63670	3.66400	-0.69390
C	4.10680	5.35160	0.84310
H	5.00830	5.50300	1.20180
H	4.11140	5.51790	-0.12480
H	3.49220	5.98980	1.26380
C	1.07420	3.77460	3.79110
H	0.69460	2.88500	3.60990
C	-0.02720	4.64010	4.40160
H	-0.79480	4.70730	3.79220
H	0.30590	5.54590	4.58580
H	-0.34430	4.24640	5.24410
C	2.21390	3.61540	4.79670
H	2.91100	3.01940	4.44540
H	1.87850	3.22600	5.63410
H	2.62120	4.48640	4.99860
C	-1.74630	-0.87520	3.27740
N	-1.65240	0.47110	3.38070
O	-2.85500	-1.43820	3.33500
H	-0.84720	0.81950	3.36920
C	-2.79880	1.36200	3.48060
C	-3.65410	1.25360	2.25450
H	-3.30910	1.04310	4.25610
C	-2.39980	2.81860	3.74790
N	-3.27010	1.75200	1.05590
N	-4.92910	0.75700	2.20070
H	-1.83610	3.13530	3.00620
C	-1.59950	2.94730	5.04390
C	-3.63070	3.72150	3.83130
C	-4.32570	1.54350	0.24260
C	-5.33850	0.90900	0.90300

C	-5.72450	0.18150	3.29570
H	-2.12650	2.62780	5.80920
H	-1.35650	3.88590	5.20330
H	-0.76800	2.42680	4.99920
H	-4.12890	3.71690	2.98490
H	-3.36290	4.64860	4.01540
H	-4.23160	3.42180	4.54870
C	-4.15680	2.09290	-1.09880
C	-6.69620	0.51210	0.43020
H	-5.23190	0.17900	4.14360
H	-5.96450	-0.74500	3.07610
H	-6.54500	0.70790	3.41520
N	-3.00100	2.74910	-1.32570
O	-5.09560	2.08140	-1.91610
H	-6.65900	0.30610	-0.52900
H	-7.31720	1.25710	0.58430
H	-7.00560	-0.28330	0.91530
C	-2.77990	3.67440	-2.42520
C	-1.99140	4.76810	-1.77750
H	-3.64720	4.02870	-2.72200
C	-2.04540	2.94430	-3.55570
C	-0.68190	5.65880	-0.30500
N	-1.37270	4.53930	-0.61420
N	-1.85240	6.05860	-2.17010
H	-2.60800	2.18210	-3.82240
C	-1.86270	3.81640	-4.79500
C	-0.69470	2.38500	-3.11220
C	-0.93950	6.60020	-1.28650
C	-2.52670	6.74360	-3.28590
H	-2.73010	4.15650	-5.10610
H	-1.46400	3.29180	-5.52400
H	-1.26930	4.57510	-4.60390
H	-0.80220	1.78340	-2.34320
H	-0.08280	3.11170	-2.86260
H	-0.28250	1.87210	-3.84190
C	-0.42800	7.99630	-1.42410
H	-3.05500	6.07120	-3.76650
H	-1.80980	7.04680	-3.88550
C	-3.46380	7.90600	-3.07570
H	-0.99990	8.60300	-0.90590
H	-0.42400	8.26660	-2.36770
H	0.49010	8.04110	-1.07990

C	-3.76550	8.36210	-1.80560
C	-4.04060	8.51850	-4.17320
H	-3.37950	7.93510	-1.02460
C	-4.62890	9.42590	-1.63560
C	-4.90350	9.58260	-4.00340
H	-3.83870	8.20320	-5.06910
H	-4.83820	9.74250	-0.74200
C	-5.19720	10.03780	-2.73420
H	-5.30430	10.01070	-4.77720
H	-5.80470	10.78550	-2.61430
Cu	-1.68690	2.70790	0.15800
O	0.47770	2.59680	-1.33980
Cu	1.33260	0.77110	2.55120
O	0.15120	-0.02140	0.36760
O	-0.06750	2.62580	1.79880
H	0.40450	1.92680	-1.95080
H	1.22220	2.46260	-0.83350
H	-0.54550	0.52170	0.15060
H	0.74500	-0.04510	-0.32100
H	0.57340	3.19640	1.50010
H	-0.44410	2.99910	2.53810

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N	0.73488209	-1.07064532	2.69474572
N	1.32290811	-3.21536898	2.48347804
N	3.04739914	-0.11378178	2.90320558
N	2.50500579	2.37860136	2.57140126
N	3.62580561	4.26717944	2.13675935
N	0.36354158	4.36183819	1.24651521
H	-0.32415657	3.81632933	1.20377417
O	5.24083004	0.20623686	2.36032180
O	1.64399345	5.86373102	0.17022161
C	-0.38566219	-1.75775895	2.37812501
C	-0.02092832	-3.08722672	2.19783496
C	1.72680795	-1.96393262	2.81261532
C	3.08034807	-1.51855797	3.27144106
H	3.78662318	-1.97886732	2.76615840
C	4.08975183	0.65220417	2.52040343
C	3.80515190	2.07718235	2.37309681
C	4.52457344	3.21684496	2.09179515

C	2.40782156	3.71238518	2.39212505
C	1.11013808	4.45450649	2.49561443
H	1.31819664	5.40583903	2.63163150
C	0.66587063	5.09462094	0.14764569
C	-0.85335021	-4.25027488	1.76597564
H	-1.53804791	-3.94458960	1.13228410
H	-1.28854134	-4.64528097	2.55263334
H	-0.29703804	-4.92570856	1.32100130
C	2.14677874	-4.43304876	2.37401855
H	3.07665750	-4.16246620	2.53478908
H	2.08267872	-4.70266215	1.43112448
C	1.93651234	-5.67825545	3.19848657
C	0.94358059	-5.74125360	4.15880162
H	0.36684133	-4.97791906	4.32006701
C	0.76944705	-6.88951661	4.90510763
H	0.07177978	-6.92867334	5.57918059
C	1.58758367	-7.98099187	4.69572411
H	1.46516804	-8.78837541	5.22095632
C	2.58173815	-7.92200420	3.74044250
H	3.15912337	-8.68855237	3.59313142
C	2.75622630	-6.77319208	2.99493166
H	3.45810432	-6.73836343	2.32490664
C	3.25217538	-1.64886212	4.79080387
H	2.54127767	-1.12930831	5.23090638
C	3.13101067	-3.09335034	5.27085963
H	2.23366345	-3.44274477	5.08240960
H	3.26957068	-3.14468287	6.24247955
H	3.79853065	-3.66465344	4.83104667
C	4.59575851	-1.08494953	5.25234275
H	4.65831406	-0.12454536	5.05690187
H	5.33785712	-1.54821770	4.80461931
H	4.69949158	-1.19597578	6.22327089
C	5.97680318	3.42254316	1.79818127
H	5.57076187	3.14974461	0.94598185
H	6.27586799	2.75893211	2.45732122
H	6.66049453	3.12513067	1.15931097
C	3.90770481	5.70136789	1.94590986
H	4.61375789	6.35329220	2.14728181
H	4.30334578	5.57540432	1.05552516
H	4.37196543	5.49903855	2.78765095
C	0.28000069	3.98740386	3.69773342
H	0.04063481	3.04199093	3.56954146

C	-1.01450751	4.79195702	3.81996213
H	-1.57374802	4.68354440	3.01968451
H	-0.81858689	5.74796915	3.93604533
H	-1.53618432	4.48467745	4.59401964
C	1.07057100	4.11309867	5.00064779
H	1.87920632	3.55593028	4.97859539
H	0.52408760	3.81726825	5.76190948
H	1.33938608	5.04591805	5.15367675
C	-1.71825420	-1.14247909	2.26559316
N	-1.91280716	0.18523002	2.45569989
O	-2.69894840	-1.89519320	2.12548696
H	-1.20214566	0.69479159	2.53921519
C	-3.23325164	0.79529590	2.56314871
C	-3.92948441	0.77825981	1.23437438
H	-3.74351789	0.23828208	3.19104353
C	-3.17437223	2.21164993	3.15079809
N	-3.69665291	1.70870650	0.28638944
N	-4.88887423	-0.10639888	0.81513555
H	-2.63909025	2.78350245	2.55493934
C	-2.51413038	2.21274605	4.53014552
C	-4.57287334	2.81861782	3.27069652
C	-4.46609175	1.36351610	-0.76473296
C	-5.17856864	0.23423580	-0.48251263
C	-5.53040427	-1.18185120	1.58659666
H	-2.48861849	3.12445376	4.89602444
H	-1.58959327	1.88505047	4.48007210
H	-3.01388734	1.64098519	5.15394961
H	-5.00261726	2.89344662	2.39063607
H	-4.52203202	3.72115906	3.65607183
H	-5.14231808	2.26436013	3.84894098
C	-4.34227546	2.28687391	-1.88973952
C	-6.19054152	-0.49161087	-1.30228861
H	-5.19026217	-1.22277202	2.50572901
H	-5.36434645	-2.04672155	1.15168220
H	-6.49882675	-1.02204521	1.62477084
N	-3.55558843	3.36218850	-1.67626247
O	-5.01658741	2.13311896	-2.92472397
H	-5.97191538	-0.38893006	-2.25416002
H	-7.07804897	-0.11048687	-1.12410246
H	-6.18821350	-1.44697091	-1.07541594
C	-3.42935557	4.53743494	-2.52182415
C	-2.00924758	4.91696111	-2.22939840

H	-3.53021158	4.27836737	-3.46452730
C	-4.42975457	5.62777526	-2.09559952
C	-0.22566571	5.14316516	-1.02195868
N	-1.44466973	4.55913663	-1.06592637
N	-1.15462603	5.62812329	-3.00805503
H	-4.30045696	5.81720464	-1.13588117
C	-4.14791097	6.93674690	-2.83389762
C	-5.89172231	5.23434405	-2.36962717
C	-0.01635651	5.77120867	-2.24276141
C	-1.35870609	6.08116357	-4.39621527
H	-3.25183672	7.26973048	-2.61347274
H	-4.78614978	7.63449344	-2.56665359
H	-4.21678317	6.81104918	-3.80594684
H	-5.67032413	4.50259275	-1.75733340
H	-6.65212674	4.80761288	-1.91801120
H	-6.29798572	6.07564629	-2.06516829
C	1.19219511	6.49182112	-2.74444579
H	-2.22597162	5.72417771	-4.68612289
H	-0.66688250	5.62032182	-4.92031250
C	-1.34601713	7.52410460	-4.83454203
H	1.15388993	7.42830127	-2.45176529
H	1.23540006	6.45212217	-3.72436517
H	1.99904192	6.06814154	-2.37916391
C	-1.16317553	8.54755069	-3.92285309
C	-1.52765773	7.82843211	-6.17116603
H	-1.04328354	8.35069115	-2.98046268
C	-1.15843423	9.86204345	-4.34434451
C	-1.52197489	9.14284913	-6.59316317
H	-1.65914801	7.11746590	-6.81926153
H	-1.03090237	10.57722544	-3.70026633
C	-1.33674688	10.16060132	-5.67981535
H	-1.64891418	9.35139738	-7.53285761
H	-1.33359103	11.08521018	-5.97602943
Cu	-2.60118541	3.38373795	0.04217209
O	-1.32662243	3.25874385	2.17997400
O	-4.28834933	4.59728378	1.38679542
Cu	1.31571847	0.80987009	3.02336808
O	0.10339016	0.69192279	5.21274574
O	0.74448545	0.93891957	0.53846531
H	-0.87977754	4.04041646	2.31184729
H	-1.90124361	3.12621381	2.87294926
H	-4.24959350	4.30983947	2.24916137

H	-5.11606215	4.41959515	1.05321031
H	-0.39311187	0.79706230	4.45717989
H	-0.62152580	0.69270214	5.76338259
H	0.34981757	1.73731022	0.35218548
H	1.50793577	0.86295488	0.04940221

M:
121

Zn	-2.64240	1.60360	-0.49900
N	-1.48980	2.42730	2.01650
N	-1.87330	3.67850	-0.55050
N	-3.02230	2.22280	-2.27750
N	-3.82880	-0.01640	-1.39020
N	-2.00950	3.17070	4.04260
N	-3.11110	3.58500	-3.99470
O	-1.71780	5.63560	0.55800
O	-4.82270	-0.46620	-3.39630
O	-0.65900	0.74700	-0.18960
O	-4.16010	2.26150	0.51060
C	-1.58420	2.10180	3.31220
C	-2.13240	4.20960	3.15730
C	-1.83790	3.72600	1.90160
C	-1.79600	4.39380	0.59560
C	-1.81670	4.28830	-1.87710
H	-2.27410	5.15800	-1.84920
C	-2.62400	3.38820	-2.74550
C	-3.78730	2.41160	-4.30690
C	-3.74240	1.59180	-3.19630
C	-4.17980	0.30510	-2.66050
C	-4.15120	-1.30790	-0.79890
H	-4.90270	-1.68220	-1.30740
C	-2.27890	3.22440	5.48750
H	-2.12560	2.35630	5.91760
H	-3.21470	3.48270	5.63590
H	-1.68960	3.88710	5.90910
C	-2.61050	5.55940	3.57990
H	-2.24730	6.24340	2.97710
H	-2.31160	5.75530	4.49420
H	-3.59170	5.57450	3.54240
C	-0.38860	4.42520	-2.41800
H	-0.44770	4.72280	-3.35350

C	0.36840	3.09910	-2.40260
H	1.25560	3.20910	-2.81010
H	-0.11620	2.41250	-2.91120
H	0.48920	2.78340	-1.48070
C	0.40810	5.48870	-1.66570
H	1.28300	5.62310	-2.09210
H	0.56020	5.21970	-0.73350
H	-0.07090	6.34650	-1.67480
C	-2.96840	4.77930	-4.83550
H	-2.45780	5.47670	-4.37040
H	-3.85750	5.13480	-5.05350
H	-2.50010	4.54510	-5.66630
C	-4.49090	2.21450	-5.60540
H	-4.54080	1.25390	-5.80270
H	-4.00140	2.66680	-6.32630
H	-5.39740	2.58560	-5.53580
C	-4.58070	-1.12210	0.65880
H	-3.91630	-0.54650	1.09750
C	-5.94030	-0.42850	0.73280
H	-6.17370	-0.23270	1.66690
H	-6.64060	-1.00100	0.34910
H	-5.93130	0.41780	0.23570
C	-4.64870	-2.43810	1.43260
H	-4.93230	-2.27340	2.35880
H	-3.76860	-2.87230	1.46460
H	-5.29050	-3.05390	1.01570
H	-4.43600	2.30850	1.37620
H	-4.70180	2.78610	0.00140
Zn	0.00800	-0.77620	1.22730
C	-1.26530	0.74170	3.85220
C	-2.99150	-2.24480	-0.93970
N	-1.71440	-1.87270	-0.78220
N	1.13730	-1.88340	-0.31840
N	1.84380	-0.67060	1.78620
O	-0.54800	-2.47910	1.96900
C	-0.95010	-2.96010	-1.01190
C	0.51370	-2.86720	-1.00670
C	2.85340	-1.12430	1.07030
H	0.14030	-2.95550	2.32560
C	2.58990	-1.73930	-0.26020
C	2.29110	-0.17170	2.93180
H	-1.29210	-3.00230	1.95770

C	-1.77700	-4.02740	-1.27280
O	1.17140	-3.72980	-1.61760
N	4.01680	-0.97350	1.74990
N	-3.06910	-3.57280	-1.23880
H	3.00100	-2.63230	-0.25900
C	3.15340	-0.86670	-1.38800
C	3.66220	-0.34000	2.93570
C	1.16140	0.33530	3.70760
C	-1.43790	-5.44210	-1.60570
C	5.36110	-1.38740	1.33100
C	-4.27830	-4.37210	-1.48770
H	4.10940	-0.72130	-1.20910
C	2.48360	0.50400	-1.45370
C	3.05840	-1.55940	-2.74560
C	4.66810	0.08130	3.95130
N	-0.08530	0.20350	3.18950
O	1.38200	0.90260	4.79350
H	-0.59230	-5.68590	-1.17040
H	-1.34460	-5.52610	-2.57960
H	-2.14310	-6.04600	-1.28680
H	5.33650	-1.82350	0.45200
H	5.72800	-2.02310	1.98340
H	5.94680	-0.60080	1.27950
H	-5.09280	-3.83050	-1.41500
H	-4.33270	-5.09970	-0.83040
H	-4.23840	-4.75480	-2.39120
H	2.90740	1.05710	-2.14640
H	2.56560	0.97600	-0.59610
H	1.53120	0.41080	-1.67360
H	3.50910	-1.02210	-3.43380
H	2.12140	-1.67780	-3.01460
H	3.49320	-2.43980	-2.71250
H	4.24370	0.10250	4.83650
H	4.99580	0.97780	3.72080
H	5.41790	-0.55220	3.96860
H	-1.04490	0.84130	4.80360
C	-2.43410	-0.23720	3.71040
H	-2.48820	-0.50640	2.76700
C	-2.19090	-1.48740	4.55470
C	-3.77800	0.37480	4.10380
H	-2.89730	-2.15130	4.39380
H	-2.18610	-1.26190	5.51100

H	-1.32770	-1.89940	4.33430
H	-4.49680	-0.28640	3.99660
H	-3.99440	1.14380	3.53300
H	-3.76500	0.67000	5.04060

N:
126

Zn	-2.82340	1.61860	-1.04470
N	-1.56020	2.55130	1.46840
N	-2.24360	3.75270	-1.18300
N	-3.89630	2.28130	-2.46980
N	-4.05020	-0.11270	-1.61190
N	-0.33540	3.44950	3.08650
N	-4.72230	3.71850	-3.90030
O	-1.60740	5.68540	-0.22970
O	-5.78290	-0.51590	-3.04370
O	-4.18490	2.14460	0.28470
C	-1.10090	2.38600	2.72490
C	-0.37870	4.32550	2.03490
C	-1.19960	3.78960	1.06220
C	-1.67210	4.44370	-0.16790
C	-2.73010	4.40320	-2.40010
H	-3.17730	5.24270	-2.15150
C	-3.77960	3.49870	-2.95000
C	-5.42230	2.51290	-3.99650
C	-4.86760	1.62820	-3.09060
C	-4.94560	0.26740	-2.55900
C	-3.89520	-1.49500	-1.17890
H	-4.57220	-2.03740	-1.63940
C	0.39200	3.64490	4.34960
H	0.27040	2.88660	4.95920
H	0.06450	4.45700	4.79450
H	1.35180	3.74130	4.16600
C	0.32180	5.64390	2.07730
H	0.56430	5.91560	1.16560
H	1.14170	5.57810	2.61290
H	-0.27960	6.31170	2.47320
C	-1.63700	4.65370	-3.44840
H	-2.07740	4.98230	-4.26340
C	-0.87500	3.38440	-3.82220
H	-0.23880	3.57050	-4.54730

H	-1.49130	2.68550	-4.13280
H	-0.37040	3.04660	-3.05060
C	-0.65120	5.74090	-3.02670
H	-0.04350	5.95380	-3.76880
H	-0.10660	5.44640	-2.26450
H	-1.13000	6.56270	-2.78080
C	-4.94640	4.96200	-4.64950
H	-4.14300	5.19190	-5.16410
H	-5.14770	5.69050	-4.02250
H	-5.69590	4.87010	-5.27570
C	-6.53250	2.29400	-4.96700
H	-7.11230	1.57430	-4.63510
H	-6.15140	2.03690	-5.83470
H	-7.06640	3.11170	-5.06480
C	-4.11510	-1.65500	0.32780
H	-3.41960	-1.14570	0.79890
C	-5.47720	-1.11410	0.75930
H	-5.58930	-1.20840	1.73090
H	-6.20210	-1.60270	0.31090
H	-5.56240	-0.16230	0.53850
C	-4.01570	-3.12280	0.74400
H	-4.13050	-3.20970	1.71600
H	-3.14020	-3.49990	0.50850
H	-4.71040	-3.65630	0.29890
H	-4.13240	2.94650	0.71050
H	-5.04920	2.02110	0.03010
Zn	0.20130	-0.64120	1.33070
C	-1.34000	1.16450	3.56180
C	-2.54810	-1.99760	-1.60490
N	-1.41960	-1.86670	-0.88260
N	1.41180	-1.94340	0.00080
N	1.68840	-1.12060	2.42290
O	-0.75190	-2.26560	1.85750
C	-0.42380	-2.45890	-1.57730
C	0.94390	-2.63610	-1.06520
C	2.72260	-1.77920	1.95390
H	-0.38060	-3.09030	1.95630
C	2.77440	-2.11510	0.50440
C	1.83380	-0.89270	3.72170
H	-1.63890	-2.32330	2.04280
C	-0.93870	-2.86220	-2.79650
O	1.67010	-3.48550	-1.61380

N	3.60500	-2.03450	2.94890
N	-2.28760	-2.59960	-2.78970
H	3.02180	-3.06420	0.43900
C	3.80690	-1.22900	-0.20460
C	3.03900	-1.46440	4.08640
C	0.67390	-0.13970	4.19710
C	-0.25600	-3.52310	-3.94890
C	4.88170	-2.75130	2.85230
C	-3.27040	-2.91010	-3.83890
H	4.65520	-1.30750	0.28710
C	3.41010	0.24570	-0.20570
C	4.08540	-1.69080	-1.63320
C	3.72490	-1.46900	5.40900
N	-0.27100	0.21450	3.29060
O	0.62470	0.20510	5.39200
H	0.68940	-3.25940	-3.96520
H	-0.66690	-3.24540	-4.79570
H	-0.32660	-4.49730	-3.84670
H	5.04400	-3.05430	1.93270
H	4.86460	-3.53630	3.44200
H	5.61440	-2.15680	3.12450
H	-3.96460	-3.50140	-3.47440
H	-2.85370	-3.36120	-4.60380
H	-3.68710	-2.07950	-4.15590
H	4.12370	0.78990	-0.60560
H	3.25970	0.56860	0.70960
H	2.59050	0.38070	-0.72960
H	4.82450	-1.17140	-2.01980
H	3.29540	-1.56700	-2.20320
H	4.34150	-2.63930	-1.64380
H	3.05110	-1.42160	6.12170
H	4.31780	-0.68800	5.46230
H	4.24940	-2.29210	5.51530
H	-1.29270	1.42780	4.50650
C	-2.71810	0.54550	3.31430
H	-2.77300	0.27810	2.37030
C	-2.92950	-0.69360	4.18340
C	-3.83870	1.54400	3.60280
H	-3.79560	-1.11010	3.97830
H	-2.91470	-0.45410	5.13620
H	-2.22730	-1.36050	4.02540
H	-4.71310	1.14000	3.40830

H	-3.74850	2.34880	3.04840
H	-3.82330	1.81770	4.54630
O	-1.32990	0.87980	-2.00190
H	-0.44040	0.69130	-2.02910
H	-1.57270	1.06260	-1.14480
O	0.37020	1.18920	0.74630
H	0.70890	1.67440	0.05520
H	0.13190	0.36500	0.44510

O:

127

Zn	0.57697594	2.31389908	12.88303946
N	0.00518994	3.03215788	10.91890556
N	-1.51402987	2.72441686	13.08278661
N	0.07308888	2.13012854	14.94293007
N	3.03000024	2.82562428	16.89693705
H	2.74381265	2.85720413	17.72662874
N	-0.42177925	3.71649269	8.83144174
N	-1.37135548	2.10226114	16.62089069
O	-3.29278124	3.64904314	12.01594789
O	2.73350409	2.19422503	14.76901273
O	1.18359470	4.16668114	13.14278124
C	0.51309440	3.14013010	9.65791547
C	-1.54617715	3.92825093	9.57058462
C	-1.26349928	3.49064240	10.83624779
C	-2.08219990	3.35949372	12.03786450
C	-2.25750938	2.20011237	14.21868981
H	-2.90540452	2.88862701	14.48912916
C	-1.21508098	2.07881481	15.27917809
C	-0.09704461	2.08117205	17.14371720
C	0.80850882	2.13904055	16.07740092
C	2.25832716	2.30203414	15.91481613
C	4.11725769	3.73350966	16.56161802
H	4.04956217	3.87833708	15.59347998
C	-0.25941259	4.02497704	7.40218139
H	0.47734883	4.66340759	7.28179439
H	-1.07733755	4.42171729	7.03125769
H	-0.06064998	3.20116986	6.90534401
C	-2.77984108	4.53927131	8.98869374
H	-2.52915727	5.31825812	9.53254845
H	-3.18665292	3.66232071	9.16379109
H	-3.60834476	4.76760126	9.46365040

C	-2.93344169	0.87154339	13.84067924
H	-3.50299638	1.03730451	13.05200425
C	-1.89169654	-0.16378883	13.41309600
H	-2.32963483	-0.98842544	13.10674001
H	-1.29828269	-0.39194089	14.16217087
H	-1.34764190	0.17594614	12.66892816
C	-3.78973705	0.27964729	14.97020815
H	-4.12591007	-0.49466529	14.46681060
H	-4.69662340	0.34271054	15.34140434
H	-4.20776853	1.16681400	14.92522823
C	-2.63115732	2.18840574	17.37144986
H	-3.18424985	1.39791930	17.19544100
H	-3.12142517	2.99581495	17.10208903
H	-2.46132102	2.23305449	18.33742915
C	0.11722410	2.14198190	18.62266053
H	0.64276139	2.95335551	18.44525497
H	0.25702175	1.17335153	18.51435167
H	0.94795832	1.94993288	19.10993345
C	3.90870731	5.12976365	17.16496182
H	3.89809062	5.06860646	18.14502834
C	5.02170752	6.09573214	16.75774199
H	4.86643261	6.98149719	17.15404256
H	5.05497441	6.19448418	15.78076836
H	5.89685755	5.77779887	17.07010171
C	2.56073808	5.70858742	16.73241808
H	2.51294390	5.78353262	15.75354161
H	1.82029719	5.13932424	17.03773732
H	2.43146847	6.60248884	17.11976443
H	2.09092345	4.22956814	13.14303146
H	0.86024850	4.52202027	13.91551080
Zn	5.62546720	2.33420892	13.74118325
C	1.86752070	2.67485542	9.19455106
C	5.49628028	3.17539691	16.73210581
N	6.17221668	2.68053569	15.68299032
N	7.72085920	1.87851592	13.75305074
N	6.08324506	2.30553023	11.78493903
O	5.45188414	4.27311145	13.39565270
C	7.43937435	2.48218400	16.06245753
C	8.31127371	2.10082981	14.95105348
C	7.34813554	2.05924140	11.44415179
H	5.96880671	4.77032421	13.95532911
C	8.37337422	1.67108579	12.46342781

C	5.34812545	2.50367514	10.66656200
H	4.58831796	4.55464003	13.44555696
C	7.54559834	2.78036287	17.39608684
O	9.54349873	2.18078512	15.10433140
N	7.52258437	2.17484911	10.11861137
N	6.29886117	3.17749053	17.83835938
H	9.05977063	2.36758445	12.35856084
C	8.81199429	0.22914623	12.08868333
C	6.26791194	2.45178548	9.60434774
C	3.87947135	2.66075404	10.74491940
C	8.74350172	2.75614909	18.28295481
C	8.79969263	2.05274580	9.39903184
C	5.93391756	3.49966234	19.22433591
H	9.30207909	-0.60425010	12.22819755
C	7.61911265	-0.61948392	12.56107902
C	10.13755355	0.36185751	12.90248858
C	6.06971227	2.70536806	8.14565996
N	3.17664513	3.10409880	9.67899247
O	3.27342583	2.24423620	11.74813802
H	9.37727272	2.08268623	17.95225077
H	8.48391921	2.52709239	19.20173034
H	9.16686711	3.64226275	18.26878980
H	8.68966163	2.20137140	8.43563996
H	9.43349691	2.71918239	9.74402823
H	9.17345445	1.15474620	9.53407538
H	4.97837851	3.70137821	19.30731380
H	6.45537018	4.27227342	19.53420897
H	6.12649431	2.72735623	19.79975877
H	7.67629640	-1.55668811	12.26247626
H	6.77651040	-0.28314460	12.18595146
H	7.54384049	-0.62650179	13.54188566
H	10.89213168	-0.22170127	12.62884761
H	9.99535744	0.19308889	13.86352572
H	10.56823932	1.24179650	12.81836791
H	6.25986840	3.65061113	7.95892182
H	5.14767995	2.50052067	7.88617811
H	6.66698821	2.13530306	7.61515128
H	3.66177665	3.56617122	9.11020473
H	1.90746871	3.12239180	8.32096908
C	1.78254277	1.18959043	8.80719657
H	0.99395625	1.08642698	8.22641710
C	2.98489474	0.72347827	7.98833236

C	1.57314233	0.25030887	9.99104748
H	3.12078894	1.30945772	7.21138521
H	2.83882477	-0.19039696	7.65789843
H	3.79998178	0.72185047	8.53613420
H	2.35393480	0.25617582	10.58524396
H	1.44113081	-0.67046067	9.67423208
H	0.77350263	0.50859424	10.49849423
O	5.00724728	0.52274395	13.99975196
H	4.74835080	0.37921031	14.86006654
H	4.31646623	0.32846711	13.44068538
O	1.33085097	0.51971763	12.96439376
H	1.16238318	0.08274288	13.74414802

P:
127

Zn	1.08610	2.53430	13.27520
N	0.53950	3.20960	11.40770
N	-0.65320	1.38090	12.85250
N	0.66440	1.60590	15.07060
N	2.84710	3.47920	15.88770
H	2.62820	3.45140	15.03790
N	0.29010	4.18680	9.44010
N	-0.55360	0.24950	16.32540
O	-2.45210	1.41970	11.45900
O	2.65350	2.57160	17.92340
O	-0.03060	4.01920	13.98350
C	1.10540	4.04970	10.52660
C	-0.79830	3.37010	9.67050
C	-0.62410	2.78530	10.89720
C	-1.31710	1.82920	11.76320
C	-1.08520	0.39270	13.82960
H	-2.04200	0.53590	14.00370
C	-0.33400	0.71840	15.08170
C	0.40260	0.85020	17.11530
C	1.16350	1.71480	16.32620
C	2.26130	2.60720	16.74240
C	3.84140	4.45190	16.32460
H	3.54240	4.76170	17.20720
C	0.50510	5.03540	8.25980
H	1.34490	5.53810	8.32490
H	-0.23450	5.67640	8.17960

H	0.53810	4.47630	7.45320
C	-1.94160	3.26700	8.71940
H	-2.36990	2.38940	8.82170
H	-1.62410	3.36240	7.79540
H	-2.58930	3.97640	8.92300
C	-0.80750	-1.05030	13.38880
H	-1.03420	-1.64290	14.13980
C	0.66160	-1.29200	13.04800
H	0.81290	-2.24290	12.85290
H	1.24180	-1.04090	13.79980
H	0.92220	-0.77250	12.25680
C	-1.69020	-1.47210	12.21660
H	-1.57240	-2.42960	12.03010
H	-1.45720	-0.97270	11.40390
H	-2.63730	-1.31570	12.42610
C	-1.59580	-0.69170	16.75770
H	-2.16460	-0.96250	16.00540
H	-2.16500	-0.26460	17.43440
H	-1.17790	-1.49240	17.14320
C	0.52710	0.52120	18.56700
H	0.85460	1.30430	19.05920
H	1.15980	-0.22260	18.67000
H	-0.34560	0.26560	18.93620
C	3.89390	5.66240	15.38600
H	4.05900	5.34040	14.47180
C	2.56330	6.41400	15.39940
H	2.58880	7.16930	14.77180
H	2.37210	6.76230	16.29790
H	1.82480	5.82510	15.13330
C	5.01710	6.63090	15.75400
H	5.01810	7.39880	15.14110
H	5.89420	6.19430	15.68590
H	4.90160	6.96310	16.67130
H	-0.44200	4.78810	13.72400
H	0.86060	4.09750	13.83040
Zn	5.11840	2.36970	13.72320
C	2.44810	4.68150	10.74530
C	5.19150	3.82340	16.48910
N	5.73550	3.01510	15.56700
N	6.94040	1.29210	14.00010
N	5.56640	1.66150	11.83700
O	6.05130	4.03370	13.09620

C	6.93430	2.61740	16.01330
C	7.62320	1.71620	15.08770
C	6.61680	0.84200	11.71850
H	6.36750	4.71480	13.60970
C	7.42560	0.45220	12.91510
C	5.05570	1.88660	10.60010
H	6.34040	4.16660	12.24390
C	7.14900	3.18220	17.24320
O	8.79730	1.37120	15.31350
N	6.84980	0.53210	10.42720
N	6.05150	3.96450	17.53930
H	8.35990	0.70090	12.73770
C	7.29820	-1.04890	13.20470
C	5.84780	1.15360	9.71610
C	3.92580	2.77280	10.26490
C	8.33900	3.09550	18.13690
C	7.94770	-0.27880	9.88280
C	5.86870	4.78660	18.74340
H	7.55590	-1.53540	12.39030
C	5.87110	-1.46870	13.54860
C	8.25360	-1.50130	14.30650
C	5.72640	0.98610	8.23670
N	3.45880	3.70390	11.13060
O	3.42120	2.70270	9.12880
H	8.78640	2.23270	17.99760
H	8.06350	3.16530	19.07660
H	8.95600	3.82700	17.91640
H	8.54570	-0.59320	10.59420
H	8.47620	0.26150	9.25580
H	7.58020	-1.05750	9.41050
H	5.88960	4.21340	19.54040
H	6.59280	5.44760	18.80060
H	5.01250	5.26500	18.72640
H	5.81410	-2.44650	13.62500
H	5.24250	-1.18100	12.85080
H	5.59670	-1.07990	14.40690
H	8.00380	-1.10780	15.17080
H	9.17530	-1.23770	14.09130
H	8.22860	-2.47930	14.39750
H	5.35280	1.80200	7.83940
H	6.60740	0.82190	7.83660
H	5.13310	0.22590	8.05150

H	3.79300	3.72760	11.94240
H	2.75550	5.04140	9.88480
C	2.36710	5.84350	11.74150
H	2.19540	5.47500	12.63590
C	3.68600	6.61440	11.78980
C	1.23150	6.80930	11.40680
H	3.63360	7.34330	12.44620
H	3.89260	7.00150	10.91070
H	4.42730	6.02690	12.05210
H	0.36140	6.35560	11.45000
H	1.21350	7.55000	12.05200
H	1.34810	7.18210	10.50530
O	4.09230	0.97010	14.64740
H	4.31290	0.82430	15.51790
H	3.53650	0.30000	14.38440
O	2.31360	1.32220	12.41930
H	2.33800	2.02030	13.00130

Q:
122

N	-1.24710	2.00620	-1.60660
N	-3.05620	3.30530	-1.51360
N	1.09030	2.36340	-3.38490
N	2.91230	0.70350	-2.81060
N	3.64610	0.27500	-4.83010
N	3.11680	0.09600	-0.37060
C	-1.18390	2.89240	-2.62190
C	-2.27410	3.72860	-2.55180
C	-2.40080	2.24540	-0.96020
C	-4.34650	3.88320	-1.10760
H	-4.73200	3.41060	-0.33970
H	-4.97990	3.82920	-1.85620
H	-4.22100	4.82450	-0.85750
C	-2.67050	4.86380	-3.43660
H	-1.86470	5.28990	-3.80120
H	-3.17800	5.53210	-2.92710
H	-3.22280	4.51740	-4.17100
C	-0.14820	2.83560	-3.65770
C	2.13920	2.33660	-4.40180
H	1.74600	2.24230	-5.29750
C	3.03880	3.57420	-4.29070

H	3.40190	3.61510	-3.37690
C	4.21980	3.51290	-5.25770
H	4.79570	2.74340	-5.05730
H	4.77000	4.32300	-5.17740
H	3.90460	3.44210	-6.18540
C	2.25910	4.86460	-4.53830
H	2.85590	5.64260	-4.47650
H	1.85050	4.85610	-5.43180
H	1.55180	4.97980	-3.86700
C	2.89080	1.09810	-4.06150
C	3.71130	-0.34410	-2.67510
C	4.20130	-0.63530	-3.93530
C	3.83010	0.31840	-6.28550
H	4.77990	0.45250	-6.49590
H	3.31130	1.05130	-6.68170
H	3.52760	-0.52880	-6.67930
C	5.10250	-1.73840	-4.37220
H	4.55600	-2.51170	-4.63200
H	5.69340	-1.98600	-3.62800
H	5.64850	-1.44630	-5.13410
C	3.77540	-0.69200	-1.25810
C	3.34650	-0.04520	1.06090
H	4.32010	0.02590	1.17380
C	2.69650	1.09490	1.85120
H	1.72000	1.02950	1.75890
C	3.12880	2.45600	1.30770
H	2.86150	2.55670	0.36780
H	4.10390	2.55970	1.36910
H	2.70500	3.17930	1.82020
C	3.03220	1.01130	3.33960
H	2.60190	1.74690	3.82850
H	4.00290	1.07100	3.47930
H	2.71040	0.16650	3.72370
O	-0.42420	3.26400	-4.79390
O	4.54410	-1.60340	-0.90010
C	-2.91500	1.39390	0.16030
C	2.90870	-1.38250	1.58220
N	-2.72140	-0.02730	-0.08750
H	-3.88840	1.51390	0.20990
C	-2.30810	1.79320	1.50850
C	-3.38910	-0.66700	-1.08100
H	-1.36580	1.51120	1.52230

C	-3.04480	1.09150	2.64900
C	-2.34920	3.30260	1.74500
C	-3.35880	-2.12830	-1.10230
H	-3.04520	0.11820	2.52040
H	-3.97860	1.39370	2.69490
H	-2.61140	1.28740	3.50880
H	-1.96460	3.52020	2.62250
H	-3.27400	3.63320	1.72130
H	-1.82620	3.77920	1.06380
N	-2.56720	-2.52910	-0.11970
C	-3.86820	-3.27310	-1.69120
C	-2.56240	-3.83490	-0.04150
N	-3.32180	-4.37430	-1.02530
C	-4.78580	-3.40530	-2.85800
C	-1.80730	-4.47140	1.07080
C	-3.48680	-5.80060	-1.33390
H	-4.25080	-3.51420	-3.67430
H	-5.33490	-2.59420	-2.92860
H	-5.37620	-4.18030	-2.73890
N	-0.67860	-3.56530	1.27720
H	-1.49360	-5.35520	0.77680
C	-2.66200	-4.55690	2.34160
H	-4.06620	-5.92950	-2.11530
H	-3.88540	-6.26820	-0.56900
H	-2.60860	-6.19480	-1.52830
C	0.55000	-4.05600	1.57730
H	-2.94680	-3.64750	2.58750
C	-3.91980	-5.39760	2.13220
C	-1.86940	-5.12850	3.51620
C	1.70570	-3.17860	1.81040
H	-4.49290	-5.00080	1.44040
H	-4.44370	-5.44180	2.96210
H	-3.68310	-6.31280	1.86500
H	-1.10370	-4.55350	3.73400
H	-1.53880	-6.02930	3.30500
H	-2.43610	-5.18460	4.31690
N	1.73170	-1.94410	1.28900
C	2.93580	-3.40730	2.40170
N	3.68290	-2.25520	2.27420
C	3.43660	-4.61210	3.12850
C	5.04580	-2.00680	2.76770
H	2.97710	-5.41390	2.79860

H	3.25820	-4.50190	4.08780
H	4.40000	-4.72520	2.97970
H	5.63970	-1.80680	2.01160
H	5.40390	-2.78390	3.24730
H	5.03870	-1.24200	3.38320
Zn	-1.55610	-1.48850	1.04710
Zn	1.90530	1.58190	-1.47710
O	-4.13830	-0.06720	-1.87390
O	0.71930	-5.28410	1.69290
O	-0.87880	-1.18240	2.81960
O	0.27650	-0.15670	0.07590
O	2.04570	3.27220	-0.60640
H	-0.97640	-1.72800	3.54130
H	-0.15630	-0.64510	2.95030
H	0.26280	-0.37800	-0.80650
H	1.48820	2.55710	-0.53310
H	2.87560	2.97910	-0.83720

R:
126

N	-0.92160	1.65500	-2.07460
N	-2.84350	1.25600	-3.11570
N	1.67800	2.26180	-3.18570
N	3.85170	1.60180	-2.07500
N	5.27310	2.55520	-3.44460
N	3.60430	-0.06930	-0.19730
C	-0.67680	1.59950	-3.40050
C	-1.83930	1.25960	-4.05210
C	-2.25160	1.53510	-1.92530
C	-4.27810	1.02570	-3.34030
H	-4.56990	0.24360	-2.82340
H	-4.47350	0.86240	-4.28760
H	-4.78830	1.81360	-3.05190
C	-2.08470	1.03270	-5.50670
H	-1.25860	0.70930	-5.92770
H	-2.35910	1.87960	-5.92130
H	-2.78530	0.35710	-5.63350
C	0.57710	2.11790	-3.95970
C	2.76110	3.17580	-3.54160
H	2.81700	3.27810	-4.51730
C	2.57270	4.52120	-2.82890

H	2.52930	4.35740	-1.85960
C	3.73490	5.47900	-3.08390
H	4.57530	5.10790	-2.73760
H	3.57920	6.33460	-2.62670
H	3.83470	5.65460	-4.04520
C	1.26750	5.19940	-3.24290
H	0.49280	4.65000	-2.99310
H	1.24890	5.35070	-4.21360
H	1.17340	6.06640	-2.79040
C	3.97670	2.47090	-3.05160
C	5.03940	1.11900	-1.74230
C	5.96520	1.72640	-2.56840
C	5.82820	3.32510	-4.56410
H	6.48400	3.97420	-4.22790
H	5.12010	3.80790	-5.04230
H	6.27020	2.71470	-5.19370
C	7.43840	1.52170	-2.65600
H	7.62250	0.80560	-3.30220
H	7.78170	1.26630	-1.77220
H	7.87720	2.35100	-2.94530
C	4.86300	0.17380	-0.64400
C	3.32640	-0.97800	0.90600
H	4.18020	-1.36730	1.19620
C	2.72990	-0.22480	2.10030
H	1.84920	0.13070	1.84450
C	3.61390	0.95510	2.50380
H	3.70010	1.59790	1.76650
H	4.51230	0.64520	2.75340
H	3.22300	1.42930	3.27040
C	2.55050	-1.14420	3.30880
H	2.16960	-0.64430	4.06410
H	3.41430	-1.51990	3.58850
H	1.94130	-1.88660	3.10460
O	0.55120	2.60680	-5.10460
O	5.87610	-0.33560	-0.13060
C	-2.98050	1.68070	-0.62340
C	2.46940	-2.12220	0.45210
N	-3.29820	0.37670	-0.05880
H	-3.82910	2.12970	-0.83110
C	-2.22960	2.55260	0.38870
C	-4.57620	-0.05340	0.09860
H	-1.35650	2.14090	0.57650

C	-2.99890	2.64870	1.70600
C	-1.99470	3.96330	-0.15210
C	-4.79840	-1.37160	0.68480
H	-3.11990	1.76090	2.10770
H	-3.88500	3.04780	1.56110
H	-2.50720	3.20480	2.34970
H	-1.51600	4.50750	0.51130
H	-2.84990	4.40220	-0.35570
H	-1.45270	3.94520	-0.97040
N	-3.62240	-1.90010	0.98860
C	-5.75980	-2.28940	1.06080
C	-3.78770	-3.08700	1.52660
N	-5.10470	-3.41330	1.55230
C	-7.24070	-2.22850	0.90980
C	-2.58720	-3.84080	1.97960
C	-5.71220	-4.68100	1.97430
H	-7.48840	-2.61520	0.04180
H	-7.53060	-1.29110	0.94930
H	-7.67440	-2.73110	1.63320
N	-1.51470	-3.28360	1.15840
H	-2.71070	-4.79510	1.78060
C	-2.29930	-3.59430	3.46590
H	-6.32390	-4.52210	2.72590
H	-5.02460	-5.32270	2.25480
H	-6.21430	-5.06880	1.22470
C	-0.49560	-4.04390	0.69460
H	-2.19540	-2.62630	3.60800
C	-3.43910	-4.07300	4.36300
C	-1.00090	-4.27010	3.90440
C	0.75970	-3.43470	0.23950
H	-3.22050	-3.91400	5.30750
H	-3.59750	-5.03460	4.23880
H	-4.26740	-3.58450	4.16500
H	-1.04460	-5.23890	3.74670
H	-0.84100	-4.11660	4.86150
H	-0.23320	-3.90430	3.41330
N	1.14190	-2.20860	0.65680
C	1.82620	-4.03380	-0.38680
N	2.91180	-3.21550	-0.22940
C	1.92580	-5.37490	-1.03380
C	4.27970	-3.49280	-0.69000
H	1.05410	-5.61660	-1.41560

H	2.18600	-6.03710	-0.35700
H	2.59350	-5.35680	-1.75320
H	4.89330	-2.76650	-0.45100
H	4.28500	-3.59400	-1.66670
H	4.60370	-4.32270	-0.27670
Zn	-1.89390	-1.15150	0.66470
Zn	2.15170	1.11940	-1.34020
O	-5.56650	0.63400	-0.21200
O	-0.53600	-5.28240	0.81710
O	-1.55110	-1.59390	-1.19020
O	1.34930	2.38170	-0.14010
O	-0.98390	-0.49170	2.21690
O	1.64770	-0.51690	-2.25940
H	-1.66510	-1.55510	-2.09190
H	-0.90480	-1.00220	-0.94700
H	2.22070	2.56920	0.04050
H	1.24780	1.48170	-0.22430
H	-0.83360	-0.10370	1.40840
H	-1.81380	-0.26150	2.50930
H	2.39090	-0.90780	-2.60990
H	0.92300	-0.79180	-2.73540

S:
124

N	-2.67750	-2.11600	-0.36040
N	-4.75600	-1.32350	-0.54960
N	-1.54010	-4.29320	0.47590
N	0.79600	-3.41840	0.93150
N	1.43940	-5.07140	2.27340
N	2.46220	-0.97470	0.19800
C	-3.53020	-2.99870	0.19040
C	-4.81470	-2.52700	0.11840
C	-3.44310	-1.10850	-0.83470
C	-5.87300	-0.43570	-0.90330
H	-5.73850	0.44310	-0.48570
H	-6.73210	-0.79940	-0.60010
H	-5.91020	-0.32690	-1.87860
C	-6.08910	-3.14650	0.58480
H	-5.89970	-3.75320	1.33310
H	-6.48860	-3.65140	-0.15660
H	-6.71290	-2.45380	0.89190

C	-2.86810	-4.19750	0.69630
C	-0.67030	-5.38850	0.86940
H	-1.08950	-5.89670	1.59860
C	-0.34580	-6.26810	-0.34310
H	0.06060	-5.70480	-1.03970
C	0.64990	-7.37560	-0.00510
H	1.50510	-6.99560	0.29210
H	0.82940	-7.92680	-0.79830
H	0.29510	-7.95700	0.70280
C	-1.61460	-6.88930	-0.92470
H	-2.23530	-6.19240	-1.23070
H	-2.06910	-7.44200	-0.25130
H	-1.39590	-7.45520	-1.69750
C	0.52940	-4.65370	1.37140
C	1.95840	-3.01780	1.50210
C	2.38200	-4.07250	2.31660
C	1.42600	-6.31230	3.06080
H	2.22370	-6.84680	2.85500
H	0.62860	-6.84880	2.86320
H	1.42230	-6.09230	4.01790
C	3.58760	-4.18330	3.19180
H	3.37730	-3.80510	4.07330
H	4.33520	-3.69090	2.78950
H	3.85210	-5.12350	3.28970
C	2.65770	-1.73830	1.29990
C	3.41560	0.04940	-0.21870
H	4.27140	-0.42800	-0.29360
C	3.10700	0.63240	-1.60350
H	2.22340	1.06170	-1.57650
C	3.07140	-0.45630	-2.67660
H	2.88280	-0.06220	-3.55660
H	2.36880	-1.11630	-2.49040
H	3.93410	-0.92420	-2.72390
C	4.14080	1.68480	-2.00550
H	3.93450	2.04420	-2.89630
H	5.04180	1.29340	-2.02790
H	4.14410	2.43690	-1.37410
O	-3.52460	-5.11070	1.22940
O	3.53340	-1.41630	2.12300
C	-2.89770	0.09680	-1.53620
C	3.60700	1.12880	0.80720
N	-2.58250	1.12360	-0.55240

H	-3.61570	0.44530	-2.10890
C	-1.69960	-0.24530	-2.42890
H	-2.20250	0.86890	0.19710
C	-2.85950	2.43840	-0.70820
H	-0.98470	-0.62380	-1.86950
C	-1.14470	0.99590	-3.12690
C	-2.08820	-1.27570	-3.48940
C	-2.31530	3.45400	0.20410
H	-0.82990	1.65600	-2.47210
H	-1.83400	1.41590	-3.68710
H	-0.38270	0.75460	-3.69820
H	-1.31450	-1.49380	-4.05430
H	-2.80460	-0.92670	-4.06430
H	-2.40200	-2.10860	-3.07480
N	-1.02070	3.62720	0.57610
C	-3.05950	4.45550	0.81010
C	-0.96960	4.74680	1.30470
N	-2.20310	5.24870	1.54940
C	-4.52820	4.71460	0.73280
C	0.35490	5.31180	1.71010
C	-2.54580	6.36260	2.44770
H	-4.86680	5.04290	1.59330
H	-4.99460	3.87880	0.51360
H	-4.69780	5.37920	0.03010
N	1.19780	4.12650	1.72970
H	0.29910	5.69840	2.61200
C	0.88170	6.31090	0.66910
H	-3.51370	6.51880	2.47270
H	-2.11380	7.19160	2.15390
H	-2.24110	6.15070	3.35690
C	2.32770	3.95130	2.44760
H	0.92660	5.85680	-0.20180
C	-0.02890	7.52380	0.49470
C	2.28960	6.80090	1.00460
C	3.20660	2.85640	2.04200
H	-0.91650	7.24970	0.17700
H	0.34480	8.13850	-0.17450
H	-0.12150	8.01080	1.34280
H	2.93300	6.05980	0.98490
H	2.30850	7.21670	1.89460
H	2.58860	7.46450	0.34460
N	2.70640	2.10340	1.04770

C	4.45360	2.40560	2.38380
N	4.72300	1.32080	1.57470
C	5.39890	2.91000	3.42230
C	5.96660	0.53600	1.51820
H	5.21110	3.85720	3.59940
H	6.32620	2.82790	3.11200
H	5.27380	2.39070	4.24630
H	5.78370	-0.40580	1.72360
H	6.63010	0.86560	2.16120
H	6.35000	0.59800	0.61620
Zn	0.84590	2.62080	0.25760
Zn	-0.60370	-2.56290	-0.34760
H	1.79620	-1.19820	-0.32900
O	-3.56500	2.82360	-1.65920
O	2.66700	4.73470	3.35340
O	0.10560	1.20780	0.00390
O	0.27400	-3.07310	-1.96350
O	1.24810	3.48630	-1.41080
H	0.17990	0.78350	0.80550
H	-0.38530	-3.57240	-2.34270
H	0.72540	-2.63000	-2.61740
H	2.02370	3.96170	-1.40110
H	0.64330	3.91380	-1.93930

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N	-2.24830	-2.02600	-0.77840
N	-4.00390	-1.44690	-2.00470
N	-1.57270	-3.99190	0.84200
N	0.94390	-3.53940	1.08700
N	1.53520	-5.43810	2.06810
N	2.60670	-1.20670	0.37520
C	-3.15110	-3.01570	-0.69650
C	-4.23930	-2.69800	-1.46820
C	-2.75990	-1.07830	-1.58600
C	-4.89980	-0.65810	-2.86280
H	-5.74550	-1.12720	-3.02740
H	-5.10220	0.19900	-2.42850
H	-4.46330	-0.48750	-3.72580
C	-5.50460	-3.45670	-1.68850
H	-5.33410	-4.41550	-1.56410

H	-5.83440	-3.31210	-2.60150
H	-6.17580	-3.15370	-1.03880
C	-2.72960	-4.12860	0.15630
C	-0.95400	-4.95770	1.73850
H	-1.10820	-5.85780	1.37490
C	-1.46460	-4.84530	3.18040
H	-0.98550	-5.51180	3.72110
C	-1.19050	-3.47480	3.79680
H	-0.22740	-3.28180	3.80340
H	-1.50990	-3.44810	4.72560
H	-1.64810	-2.76840	3.29030
C	-2.95040	-5.18020	3.28950
H	-3.13320	-6.06210	2.89690
H	-3.49680	-4.50680	2.82860
H	-3.22540	-5.20320	4.23250
C	0.50990	-4.66440	1.65800
C	2.29600	-3.52950	1.13780
C	2.67830	-4.72990	1.73650
C	1.43590	-6.75320	2.71760
H	2.32150	-7.12610	2.91440
H	0.95830	-7.37550	2.12680
H	0.94560	-6.67130	3.56370
C	4.04520	-5.23240	2.06850
H	4.26540	-4.97030	2.98890
H	4.70190	-4.84570	1.45070
H	4.08110	-6.20930	1.98320
C	3.11850	-2.44400	0.57790
C	3.33810	-0.09990	-0.22850
H	4.19750	-0.44520	-0.55580
C	2.57560	0.46790	-1.43040
H	1.72450	0.84820	-1.11590
C	2.25190	-0.62840	-2.44490
H	1.76820	-0.25170	-3.21260
H	1.68320	-1.32060	-2.04200
H	3.07590	-1.05210	-2.77200
C	3.37790	1.57170	-2.11860
H	2.87340	1.93800	-2.87800
H	4.23280	1.22060	-2.45220
H	3.56690	2.30860	-1.49780
O	-3.42920	-5.15480	0.23580
O	4.30810	-2.67670	0.29470
C	-2.05130	0.19900	-1.92870

C	3.64180	0.94940	0.79990
N	-1.69350	1.03250	-0.78630
H	-2.68540	0.74280	-2.44610
C	-0.84970	-0.07100	-2.84330
H	-0.84490	1.18210	-0.61450
C	-2.61690	1.74090	-0.09260
H	-0.14440	-0.50250	-2.31180
C	-0.28230	1.22980	-3.41110
C	-1.20790	-1.00040	-4.00330
C	-2.23710	2.87800	0.76580
H	0.01080	1.82840	-2.69090
H	-0.95880	1.69760	-3.94870
H	0.49540	1.04370	-3.98190
H	-0.42540	-1.14380	-4.57980
H	-1.92920	-0.61350	-4.54680
H	-1.49890	-1.87900	-3.67490
N	-0.96010	3.23580	1.03060
C	-3.03410	3.79710	1.44630
C	-0.95680	4.31770	1.81270
N	-2.21870	4.64510	2.16890
C	-4.52130	3.87650	1.54830
C	0.33370	4.97120	2.20520
C	-2.64440	5.65830	3.14430
H	-4.92720	3.56220	0.71190
H	-4.81990	3.31110	2.29370
H	-4.80180	4.80440	1.70300
N	1.30480	3.90540	2.00610
H	0.31460	5.21670	3.15650
C	0.65430	6.16500	1.29460
H	-3.16190	5.22660	3.85860
H	-3.20420	6.33340	2.70260
H	-1.87050	6.10460	3.55020
C	2.48960	3.71860	2.62910
H	0.65570	5.85360	0.36170
C	-0.38590	7.27840	1.39900
C	2.03430	6.75210	1.58660
C	3.34580	2.63690	2.13630
H	-1.26870	6.95880	1.11220
H	-0.14210	8.03000	0.81490
H	-0.44720	7.61070	2.32130
H	2.74010	6.09500	1.40220
H	2.09880	7.03480	2.52530

H	2.20330	7.53240	1.01400
N	2.77660	1.91500	1.15810
C	4.58640	2.11520	2.40530
N	4.77750	1.04940	1.54320
C	5.61790	2.57140	3.38140
C	5.96310	0.18880	1.43040
H	5.17780	3.04710	4.11900
H	6.24320	3.17600	2.92560
H	6.10410	1.80200	3.74880
H	5.71330	-0.74160	1.61980
H	6.66460	0.45840	2.06090
H	6.32580	0.24750	0.51970
Zn	0.85810	2.39770	0.56680
Zn	-0.46470	-2.25950	0.25810
H	1.77720	-1.05020	0.61830
O	-3.82550	1.50560	-0.27600
O	2.87160	4.45200	3.55930
O	0.38800	1.13720	2.05080
O	0.31110	-2.85910	-1.44560
O	1.25960	3.50050	-0.96210
O	-1.12500	-1.28870	1.78450
H	0.93720	0.49490	2.38780
H	-0.23130	1.33930	2.68620
H	-0.05420	-3.59210	-1.84210
H	1.10260	-2.66910	-1.85200
H	1.93120	4.10980	-0.88810
H	0.53560	3.90380	-1.33760
H	-0.61390	-1.11810	1.05210
H	-1.87310	-0.77180	1.75360

U:
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N	-1.99630	1.91250	0.59290
N	-3.98340	1.24540	-0.11120
N	-2.84290	-1.08410	1.54080
N	-2.22060	-3.23520	0.40170
N	-3.00490	-5.16360	-0.32190
N	-0.02380	-3.22630	-0.83490
O	-4.93500	-1.91480	1.97620
O	1.11450	-3.83330	-2.68240
C	-2.23320	2.49800	-0.59090

C	-3.43800	2.06170	-1.07050
C	-3.06910	1.18350	0.89950
C	-3.12820	0.24450	2.06240
H	-4.04880	0.25730	2.40420
C	-3.80480	-2.03800	1.46920
C	-3.49350	-3.27180	0.76290
C	-4.02790	-4.45950	0.31030
C	-1.91540	-4.36360	-0.19530
C	-0.50370	-4.58540	-0.59800
H	-0.48310	-5.11570	-1.42510
C	0.92160	-3.00090	-1.77690
C	-4.16960	2.45300	-2.31030
H	-4.74490	1.71970	-2.61730
H	-4.71800	3.24460	-2.11860
H	-3.51940	2.66460	-3.01500
C	-5.28820	0.56700	-0.17720
H	-5.48600	0.21300	0.71540
H	-5.95280	1.26720	-0.35940
C	-5.51790	-0.57520	-1.13430
C	-6.75830	-1.18420	-1.17880
H	-7.47560	-0.87060	-0.60460
C	-6.98410	-2.24110	-2.03760
H	-7.85690	-2.66530	-2.06590
C	-5.96890	-2.69680	-2.85370
H	-6.12700	-3.44120	-3.45660
C	-4.72750	-2.09580	-2.80850
H	-4.01130	-2.41860	-3.37890
C	-4.50200	-1.03820	-1.95050
H	-3.62220	-0.62960	-1.92160
C	-2.17740	0.61090	3.20470
H	-1.25470	0.57770	2.86730
C	-2.45310	2.01590	3.73970
H	-2.32420	2.69360	3.04100
H	-1.83800	2.22640	4.47630
H	-3.37470	2.08400	4.07310
C	-2.29440	-0.39690	4.34710
H	-2.08230	-1.30410	4.03660
H	-3.20570	-0.39950	4.71440
H	-1.66690	-0.17000	5.06830
C	-5.41780	-4.98050	0.44360
H	-5.46640	-5.56130	1.23380
H	-5.67250	-5.48380	-0.35950

H	-6.03430	-4.22390	0.55200
C	-3.08370	-6.45610	-1.01650
H	-2.82730	-6.33620	-1.95680
H	-3.99330	-6.82210	-0.98360
H	-2.47770	-7.10520	-0.60070
C	0.30690	-5.23630	0.53100
H	0.24130	-4.66730	1.33050
C	1.78740	-5.35600	0.17190
H	2.19050	-4.46990	0.04450
H	1.90270	-5.87870	-0.65190
H	2.28070	-5.80100	0.89570
C	-0.22660	-6.61600	0.90880
H	-1.14710	-6.55200	1.24470
H	0.32090	-7.01090	1.62260
H	-0.20670	-7.21850	0.13310
C	-1.36990	3.61190	-0.98050
N	-0.20070	3.79760	-0.32690
O	-1.86260	4.52260	-1.67200
C	0.29010	5.14070	-0.03160
C	1.76230	4.93940	-0.04190
H	0.04060	5.76760	-0.74620
C	-0.20730	5.59320	1.34790
N	2.23510	3.74310	0.22970
N	2.76760	5.80330	-0.33510
H	0.06200	4.92100	2.01370
C	-1.73070	5.70360	1.39450
C	0.40030	6.92760	1.77400
C	3.55850	3.78390	0.19920
C	3.93300	5.07470	-0.11050
C	2.64040	7.17750	-0.83920
H	-2.02430	6.02280	2.27610
H	-2.15110	4.82940	1.24470
H	-2.05330	6.33190	0.71160
H	1.37650	6.85580	1.85070
H	0.05410	7.19590	2.65340
H	0.17810	7.63110	1.12530
C	4.06520	2.45340	0.50520
C	5.29700	5.64440	-0.29870
H	2.13220	7.16920	-1.67950
H	3.52120	7.57350	-1.01270
H	2.17090	7.73960	-0.18710
N	3.16620	1.45150	0.67660

O	5.29700	2.29030	0.58400
H	5.93650	5.13470	0.24490
H	5.31330	6.58350	-0.01310
H	5.54230	5.57920	-1.24730
C	3.59860	0.07830	0.88670
C	3.17280	-0.74350	-0.28890
H	4.57950	0.06950	0.90770
C	3.09090	-0.46890	2.22330
C	1.93600	-1.96730	-1.56160
N	2.04630	-1.45350	-0.32680
N	3.79080	-0.76170	-1.50290
H	2.10780	-0.46630	2.21370
C	3.57570	-1.89960	2.45810
C	3.55240	0.41490	3.38100
C	3.01630	-1.56120	-2.30960
C	5.02800	-0.04990	-1.86750
H	3.24780	-2.50460	1.75770
H	3.24560	-2.23380	3.32100
H	4.55750	-1.93510	2.46470
H	4.53350	0.44440	3.42410
H	3.21190	0.06600	4.23400
H	3.21830	1.33240	3.27570
C	3.35960	-1.84870	-3.73390
H	5.16480	-0.15260	-2.83370
H	4.84520	0.90070	-1.70290
C	6.34980	-0.38490	-1.22390
H	3.02910	-1.11400	-4.29540
H	2.93860	-2.68960	-4.01380
H	4.33150	-1.93830	-3.83770
C	6.45800	-1.41050	-0.30230
C	7.47390	0.34320	-1.56700
H	5.68100	-1.93840	-0.05890
C	7.67670	-1.69720	0.27900
C	8.69280	0.05640	-0.98600
H	7.40880	1.06320	-2.21510
H	7.74740	-2.41680	0.92680
C	8.79450	-0.96310	-0.06140
H	9.47890	0.57240	-1.22760
H	9.65170	-1.16500	0.34730
Zn	-0.93740	-1.79300	0.64730
Zn	1.08760	2.18760	0.54290
O	-0.13950	-2.18680	2.34560

H	0.64780	-2.56650	2.59630
O	-0.06150	0.23670	-0.27700
H	-0.68950	-0.31780	-0.63270
H	0.01480	-1.60350	1.66590
O	0.72980	2.39170	2.41430
H	0.75690	2.13320	3.28600
H	0.66930	1.65310	1.88780

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146

N	-1.88600	1.45030	-0.16510
N	-3.56620	0.68500	-1.40210
N	-3.01570	-1.62690	0.77250
N	-2.16350	-4.00720	0.60520
N	-2.75340	-6.10620	0.38010
N	0.28470	-4.19900	0.17810
O	-5.16950	-2.39830	0.71160
O	1.94230	-5.03910	-1.12200
C	-1.90520	2.14010	-1.32540
C	-2.85000	1.58820	-2.15240
C	-2.95630	0.63880	-0.18380
C	-3.38420	-0.23090	0.96220
H	-4.36410	-0.19970	0.98130
C	-3.94400	-2.61260	0.66630
C	-3.48610	-3.99470	0.55690
C	-3.89230	-5.30790	0.42480
C	-1.71750	-5.24350	0.53190
C	-0.25000	-5.48510	0.61090
H	0.00960	-6.19460	-0.01750
C	1.38980	-4.06000	-0.58750
C	-3.20810	1.94850	-3.55530
H	-2.41660	2.31460	-4.00670
H	-3.92400	2.62060	-3.54020
H	-3.50800	1.15380	-4.04670
C	-4.75600	-0.08070	-1.81280
H	-4.51590	-1.02530	-1.69080
H	-4.89500	0.06290	-2.77320
C	-6.10400	0.14250	-1.17500
C	-6.28970	1.12080	-0.21490
H	-5.55160	1.68770	0.06000
C	-7.53130	1.30480	0.35920

H	-7.65630	1.99140	1.03410
C	-8.59530	0.51550	-0.02700
H	-9.46860	0.64530	0.37670
C	-8.41700	-0.45590	-0.99090
H	-9.16530	-1.01040	-1.26510
C	-7.17520	-0.63990	-1.56500
H	-7.05610	-1.32670	-2.24090
C	-2.89040	0.29010	2.31560
H	-1.90800	0.30930	2.30510
C	-3.40150	1.70410	2.59470
H	-3.08970	2.33830	1.91330
H	-3.07380	2.01880	3.46580
H	-4.38390	1.72010	2.60660
C	-3.32880	-0.63090	3.45380
H	-2.96140	-1.53410	3.33600
H	-4.30870	-0.69460	3.48950
H	-3.00610	-0.28660	4.31550
C	-5.26970	-5.87310	0.36960
H	-5.87890	-5.20100	-0.00640
H	-5.55470	-6.10430	1.28040
H	-5.28480	-6.67470	-0.19710
C	-2.69470	-7.55990	0.18820
H	-1.76510	-7.87440	0.17710
H	-3.11250	-7.79550	-0.66870
H	-3.17520	-8.00920	0.91740
C	0.20170	-5.77360	2.04720
H	-0.10170	-5.03670	2.62460
C	1.72480	-5.84360	2.14660
H	2.13140	-4.98490	1.89770
H	2.07810	-6.54370	1.55480
H	1.99900	-6.04550	3.06820
C	-0.40050	-7.06690	2.59170
H	-1.38000	-7.00730	2.62430
H	-0.08280	-7.23300	3.50640
H	-0.14480	-7.83140	2.03030
C	-1.19230	3.41750	-1.44380
N	-0.21060	3.72640	-0.56710
O	-1.65430	4.29280	-2.19900
C	0.18020	5.09150	-0.22740
C	1.63190	4.94490	0.08180
H	0.06310	5.68590	-1.00130
C	-0.61480	5.55290	1.00160

N	2.09010	3.76340	0.42980
N	2.65450	5.83770	0.02300
H	-0.46350	4.90930	1.73020
C	-2.11730	5.58800	0.72510
C	-0.16910	6.92400	1.50330
C	3.38510	3.83010	0.70890
C	3.76620	5.14030	0.50480
C	2.60600	7.20980	-0.50040
H	-2.31640	6.18450	-0.02980
H	-2.45770	4.69040	0.51880
H	-2.60370	5.91150	1.51510
H	0.76770	6.89780	1.79610
H	-0.71110	7.19880	2.27540
H	-0.26950	7.59970	0.79730
C	3.83280	2.50130	1.12130
C	5.11720	5.75590	0.63010
H	2.29940	7.19020	-1.43310
H	3.49250	7.62960	-0.47370
H	1.98830	7.75840	0.02750
N	2.95490	1.48540	0.94070
O	4.95760	2.38080	1.63840
H	5.63690	5.25800	1.29820
H	5.03700	6.69060	0.91930
H	5.56950	5.71280	-0.24050
C	2.97040	0.08450	1.32780
C	2.79100	-0.94370	0.25200
H	2.10970	0.06250	1.80080
C	4.01460	-0.32860	2.37500
C	2.03730	-2.75170	-0.66400
N	2.02360	-2.01630	0.44480
N	3.28800	-0.94750	-1.03750
H	4.13150	0.41940	3.00290
C	3.52540	-1.51420	3.20740
C	5.37590	-0.67100	1.77500
C	2.78400	-2.11030	-1.60550
C	4.14210	0.04840	-1.71760
H	3.42420	-2.31910	2.65360
H	2.65980	-1.30940	3.62470
H	4.16650	-1.71490	3.92440
H	5.74390	0.09460	1.28720
H	5.30540	-1.43460	1.16130
H	6.01260	-0.90480	2.48560

C	3.09380	-2.54370	-2.99960
H	3.64940	0.89690	-1.69540
H	4.18840	-0.22290	-2.65840
C	5.57920	0.32230	-1.36130
H	2.40840	-3.18050	-3.29810
H	3.97440	-2.97810	-3.01070
H	3.08980	-1.77570	-3.61030
C	6.48610	-0.72090	-1.37440
C	6.01110	1.59820	-1.05060
H	6.19250	-1.61840	-1.60040
C	7.80960	-0.49470	-1.05390
C	7.33480	1.82500	-0.73150
H	5.38840	2.34220	-1.06280
H	8.44210	-1.23120	-1.05680
C	8.23380	0.77780	-0.72900
H	7.63340	2.72200	-0.51060
H	9.16460	0.93710	-0.50410
Zn	-1.00610	-2.48560	0.70320
Zn	0.97380	2.19380	0.44110
O	-0.89930	-1.78770	-1.10410
H	-1.18080	-2.49510	-1.60200
O	-0.36360	-2.13340	2.46410
H	-0.20590	-1.42760	1.91210
H	0.42820	-2.43410	2.79590
O	0.99970	1.16430	-1.19340
H	0.83380	0.45960	-1.74350
H	1.41660	1.81450	-1.67400
H	-1.02280	-1.02800	-1.58790
O	0.15560	2.12910	2.16780
H	0.53650	2.79650	2.65460
H	0.22200	1.35210	2.63590

W:
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N	0.65450	-0.27680	2.48950
N	1.41790	-2.29140	1.89820
N	2.90670	0.89030	2.56990
N	2.36320	3.42800	2.88320
N	3.50070	5.34760	2.76340
N	0.34360	5.91160	2.24230
H	0.25610	6.76930	2.07320

O	5.03530	1.37550	1.93470
O	-0.04700	3.79600	1.58650
C	-0.42840	-1.01050	2.13010
C	0.04670	-2.26860	1.75340
C	1.72740	-1.07180	2.41560
C	3.07060	-0.53650	2.79540
H	3.75840	-0.88630	2.18710
C	3.89450	1.75490	2.25730
C	3.62160	3.16990	2.48420
C	4.34150	4.32730	2.39920
C	2.30000	4.77030	3.07380
C	1.05020	5.51050	3.45170
H	1.32640	6.34610	3.88860
C	-0.12010	5.01510	1.34270
C	-0.69540	-3.43560	1.18790
H	-1.61330	-3.44860	1.53380
H	-0.26270	-4.27560	1.44960
H	-0.71030	-3.36100	0.20890
C	2.34400	-3.33490	1.41730
H	3.24730	-3.05890	1.68430
H	2.30270	-3.25060	0.43940
C	2.24470	-4.81040	1.72340
C	2.30580	-5.27420	3.02420
H	2.41250	-4.65570	3.76080
C	2.20830	-6.62540	3.28950
H	2.25080	-6.94400	4.20560
C	2.04860	-7.52360	2.25450
H	1.97930	-8.47390	2.44100
C	1.98550	-7.06770	0.95390
H	1.87160	-7.69780	0.22410
C	2.08300	-5.71630	0.68970
H	2.03510	-5.40740	-0.22940
C	3.40220	-0.79110	4.27140
H	2.73250	-0.33280	4.82700
C	3.34350	-2.27250	4.62730
H	2.42990	-2.60880	4.50280
H	3.58470	-2.41140	5.56950
H	3.96320	-2.78860	4.06660
C	4.77670	-0.24140	4.64970
H	4.80320	0.73480	4.54910
H	5.47580	-0.63840	4.08490
H	4.98130	-0.44590	5.58870

C	5.77520	4.54530	2.04990
H	6.07160	3.83940	1.43540
H	6.31100	4.51320	2.87220
H	5.89050	5.41670	1.61290
C	3.84220	6.77730	2.79880
H	3.08080	7.32510	3.08550
H	4.11310	7.07260	1.90230
H	4.58500	6.92200	3.42490
C	0.16990	4.75480	4.45300
H	-0.09330	3.88970	4.06840
C	-1.10460	5.53900	4.76230
H	-1.63250	5.68190	3.94650
H	-0.88700	6.41520	5.14990
H	-1.66340	5.04460	5.40160
C	0.92950	4.49150	5.75270
H	1.74480	3.97100	5.58400
H	0.36860	3.98360	6.37940
H	1.18700	5.33780	6.18040
C	-1.82630	-0.54750	2.13230
N	-2.19780	0.58170	2.77940
O	-2.70840	-1.28020	1.64720
H	-1.56430	1.10330	3.09200
C	-3.59630	0.86920	3.07400
C	-4.41820	1.04040	1.83150
H	-3.92430	0.07220	3.54560
C	-3.74560	2.08210	4.00190
N	-3.99120	1.74310	0.77000
N	-5.67270	0.55440	1.59380
H	-3.32140	2.85780	3.57070
C	-3.05140	1.84320	5.34310
C	-5.21050	2.43330	4.26130
C	-4.97500	1.74470	-0.14080
C	-6.03230	1.02050	0.34740
C	-6.48930	-0.29210	2.47490
H	-2.09070	1.68100	5.22190
H	-3.44290	1.06700	5.80100
H	-3.15010	2.62950	5.92400
H	-5.66790	2.67450	3.42640
H	-5.27480	3.20370	4.86760
H	-5.68140	1.67510	4.67190
C	-4.65600	2.53290	-1.33060
C	-7.33580	0.68190	-0.29270

H	-6.01970	-0.50000	3.31070
H	-6.69930	-1.13510	2.01690
H	-7.32530	0.17310	2.69620
N	-3.42730	3.09220	-1.39830
O	-5.52570	2.73140	-2.19850
H	-7.24100	-0.16670	-0.77770
H	-7.58440	1.39470	-0.92050
H	-8.03710	0.59790	0.38910
C	-2.97220	4.06730	-2.37990
C	-2.00880	4.91250	-1.61190
H	-3.73410	4.62730	-2.64870
C	-2.30350	3.40430	-3.58900
C	-0.70910	5.40950	0.05910
N	-1.57600	4.50630	-0.42450
N	-1.48070	6.12040	-1.92740
H	-1.98720	4.11840	-4.18570
C	-1.09530	2.55600	-3.19450
C	-3.29370	2.56510	-4.39340
C	-0.67000	6.45460	-0.85000
C	-1.71530	6.90820	-3.14710
H	-0.41960	3.10290	-2.73710
H	-0.67680	2.16790	-3.99420
H	-1.36300	1.82330	-2.59740
H	-4.07050	3.10720	-4.65390
H	-3.60570	1.79390	-3.87140
H	-2.86780	2.22850	-5.21240
C	0.13260	7.71120	-0.82030
H	-2.15030	7.74680	-2.87780
H	-2.34360	6.42320	-3.72490
C	-0.47860	7.21470	-3.95380
H	0.30180	7.97270	0.11010
H	-0.35770	8.43470	-1.26720
H	0.98660	7.55500	-1.27930
C	0.29540	6.18410	-4.45400
C	-0.10650	8.52470	-4.19500
H	0.04770	5.26120	-4.28680
C	1.43080	6.46020	-5.18890
C	1.02880	8.80090	-4.93030
H	-0.64090	9.25700	-3.84790
H	1.97210	5.73320	-5.53690
C	1.79800	7.76880	-5.42790
H	1.28670	9.72200	-5.09690

H	2.59680	7.96310	-5.94450
Zn	-2.26510	2.78060	0.40270
O	-2.88180	3.83520	1.95130
Zn	0.99860	1.76040	3.03150
O	0.51510	1.46780	4.86100
O	-0.13100	2.08400	0.97880
H	-2.76740	3.66670	2.83810
H	-3.30420	4.63540	1.85210
H	1.37610	1.63660	5.10060
H	0.24870	0.68690	5.24430
H	0.63060	2.02470	0.48460
H	-0.83900	1.84710	0.45850

X:
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N	0.47860	-1.45340	2.77980
N	0.58240	-3.60620	2.22260
N	2.93220	-0.83460	2.35800
N	2.65190	1.75610	2.34630
N	3.76860	3.53990	1.65680
N	0.63290	4.30050	1.80060
H	0.23160	3.64340	1.37620
O	4.79690	-0.67650	1.06280
O	1.06020	6.51610	1.88770
C	-0.79140	-1.91960	2.78960
C	-0.73600	-3.26990	2.45870
C	1.27800	-2.47250	2.44940
C	2.75660	-2.27810	2.36960
H	3.07000	-2.63470	1.50890
C	3.87370	-0.12960	1.69340
C	3.76010	1.32780	1.72370
C	4.47410	2.41320	1.29210
C	2.66030	3.10190	2.32510
C	1.54850	3.94520	2.87830
H	1.95670	4.77210	3.21620
C	0.48260	5.56280	1.33300
C	-1.85150	-4.23160	2.20950
H	-2.13750	-4.14620	1.27400
H	-1.56140	-5.15290	2.38110
H	-2.60590	-4.02430	2.80160
C	1.11320	-4.91300	1.79960

H	2.06320	-4.78940	1.58480
H	0.64900	-5.13080	0.96140
C	1.05050	-6.12580	2.69340
C	0.52240	-6.04540	3.96910
H	0.18390	-5.20190	4.30920
C	0.47740	-7.16560	4.77460
H	0.10550	-7.10490	5.66940
C	0.96250	-8.37120	4.31010
H	0.93110	-9.15870	4.87700
C	1.49520	-8.45490	3.03980
H	1.83880	-9.30200	2.71270
C	1.54050	-7.33460	2.23450
H	1.91700	-7.40040	1.34190
C	3.47130	-2.95460	3.54480
H	3.26790	-3.91640	3.50930
C	4.98760	-2.81530	3.43110
H	5.29940	-3.16010	2.56550
H	5.43120	-3.32850	4.14190
H	5.26060	-1.87550	3.51450
C	2.99390	-2.43450	4.89980
H	2.03540	-2.61240	5.02000
H	3.14990	-1.46770	4.97840
H	3.47580	-2.88660	5.62690
C	5.73950	2.47350	0.50540
H	6.28220	1.67960	0.70310
H	6.25000	3.27730	0.74430
H	5.51870	2.49270	-0.45120
C	4.14930	4.92980	1.37240
H	5.02060	5.12370	1.78170
H	4.21110	5.06160	0.40110
H	3.49150	5.56130	1.73260
C	0.81220	3.27300	4.04260
H	0.44780	2.41200	3.73610
C	1.75600	3.01130	5.21610
H	2.13690	3.85390	5.54830
H	2.49380	2.42020	4.95070
H	1.27220	2.57690	5.95270
C	-0.35680	4.13300	4.52130
H	-1.01330	4.26110	3.80200
H	-0.04000	5.01500	4.81660
H	-0.81610	3.69820	5.27320
C	-1.99460	-1.12410	3.06900

N	-2.15350	0.10310	2.51970
O	-2.92950	-1.65950	3.69280
H	-1.48650	0.44440	2.05980
C	-3.43340	0.79680	2.44480
C	-3.81350	0.92400	0.99920
H	-4.11710	0.23350	2.86870
C	-3.39700	2.13400	3.19190
N	-3.53630	2.00450	0.24340
N	-4.39790	-0.03960	0.22610
H	-2.68920	2.69600	2.80310
C	-3.07640	1.91360	4.67010
C	-4.72820	2.87760	3.08210
C	-3.98810	1.75370	-0.99660
C	-4.53350	0.49990	-1.03310
C	-4.80490	-1.39030	0.63810
H	-2.21710	1.45210	4.77940
H	-3.77410	1.36960	5.09770
H	-3.02050	2.77460	5.14020
H	-4.68820	3.72330	3.58070
H	-4.93990	3.09200	2.14790
H	-5.45940	2.33360	3.44940
C	-3.79570	2.87170	-1.91810
C	-5.11310	-0.25930	-2.17820
H	-4.60610	-1.55140	1.58470
H	-4.32370	-2.05660	0.10050
H	-5.77110	-1.50020	0.50130
N	-3.29690	4.01040	-1.39170
O	-4.15820	2.78790	-3.10570
H	-5.50220	0.37140	-2.82230
H	-5.81610	-0.86700	-1.86160
H	-4.39890	-0.77530	-2.61170
C	-3.09360	5.28710	-2.05720
C	-1.81610	5.74500	-1.42600
H	-2.96470	5.13530	-3.01950
C	-4.26930	6.22580	-1.76210
C	-0.27240	5.83260	0.10240
N	-1.44450	5.25550	-0.23890
N	-0.88640	6.60090	-1.92010
H	-4.35610	6.32360	-0.78730
C	-4.05880	7.61990	-2.34700
C	-5.58250	5.65300	-2.29330
C	0.08290	6.68210	-0.93710

C	-0.86860	7.24870	-3.24320
H	-3.27760	8.04800	-1.93620
H	-4.83800	8.18960	-2.16370
H	-3.92870	7.57470	-3.31960
H	-5.79290	4.79890	-1.85670
H	-5.52870	5.50700	-3.26350
H	-6.32460	6.27050	-2.11120
C	1.35510	7.43740	-1.14320
H	-1.62960	6.88660	-3.74650
H	-0.04910	6.92470	-3.67780
C	-0.91940	8.74150	-3.45260
H	1.70640	7.73540	-0.27670
H	1.20710	8.22370	-1.71030
H	2.00770	6.84260	-1.57270
C	-1.01870	9.61040	-2.38130
C	-0.87570	9.24900	-4.73820
H	-1.05840	9.26880	-1.47380
C	-1.06900	10.97340	-2.59360
C	-0.92510	10.61210	-4.95070
H	-0.80890	8.64740	-5.49750
H	-1.13950	11.57960	-1.83850
C	-1.02120	11.47520	-3.87830
H	-0.89300	10.96370	-5.85510
H	-1.05700	12.43390	-4.02740
Zn	-2.65810	3.83460	0.63320
O	-1.49950	3.39100	2.07680
O	-4.09780	4.71590	1.54760
Zn	1.35060	0.37590	3.13610
O	2.10320	0.12930	4.91390
O	0.15940	1.73840	3.77940
H	-1.92810	2.64960	1.76850
H	-1.20480	3.87780	1.36660
H	-3.77290	5.56300	1.61670
H	-4.89930	4.73770	1.11740
H	2.59630	0.81920	5.24380
H	1.48960	-0.12230	5.53690
H	0.52940	1.51620	2.97810
H	-0.01560	2.63120	3.78530

K) DFT final cartesian coordinates of dinuclear Cu^{II} and Zn^{II} complexes with H₄pat¹, H₄pat² and H₄pat⁴

A:

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Cu	-2.61766843256525	1.17409234143857	-0.75122581440589
N	-1.83641826884804	2.50854185770092	1.96313080752254
N	-1.90126941533623	3.44138487492584	-0.72133083542185
N	-3.43047623912222	2.00869303799017	-2.25440860501009
N	-3.76185622943186	-0.47282020339663	-1.72172544715315
N	-0.74135556024558	3.40197606971881	3.64978306690863
N	-3.76574415480025	3.33539698041644	-3.93147246488728
O	-1.72000631265704	5.60486746673852	0.09704552666464
O	-5.22309265317195	-0.82184990945894	-3.51079730364832
O	-1.47613875751948	0.07499677046305	0.31678565619090
O	-4.12215642103634	1.77763978347073	0.80914157009438
C	-1.36601514217468	2.27723146083713	3.17024366141107
C	-0.83149775575009	4.38912252407307	2.67700074748018
C	-1.49822443193038	3.79826927975203	1.61357815243430
C	-1.73242419467826	4.34366567950647	0.24326714592279
C	-2.05059537494583	3.98754230054016	-2.07033177032121
H	-2.30474295101091	5.05934169544728	-2.03418265938321
C	-3.13705159353810	3.19209212002347	-2.73218841204324
C	-4.46750185303280	2.15610668151254	-4.20857667235666
C	-4.22350410040937	1.32277771950035	-3.13417382655268
C	-4.46238073045007	-0.11072247649463	-2.79607722129434
C	-3.87589170305728	-1.84994485599009	-1.26335073914397
H	-4.65023481841463	-2.37669874060616	-1.84602888182988
C	-0.12682774257151	3.58482167136881	4.95735686347199
H	-0.84419067217805	4.02306273174850	5.66987644371870
H	0.73130642127700	4.26343274789656	4.86683694529838
H	0.24000244341538	2.62005999122410	5.32940711647831
C	-0.29311419947141	5.76397524363037	2.88361337394992
H	-0.48334761571843	6.34888817036935	1.97555494221164
H	0.79032429680382	5.76636248639049	3.09661924282161
H	-0.78648351746052	6.26757043730452	3.73310560742093
C	-0.73643505930358	3.83991171577079	-2.91053498363064
H	-0.94304117258305	4.30647973873660	-3.89152880421204
C	-0.36166242238993	2.37250137481961	-3.14727663840788
H	0.60484322085581	2.29849638664730	-3.66866300197110
H	-1.10980794548074	1.84306820024249	-3.75649358335211
H	-0.26748097631880	1.83649373720126	-2.19234878717485
C	0.41966140531053	4.60258291926626	-2.26014567387073

H	1.32808527344520	4.51688622564173	-2.87894693117504
H	0.64207650969846	4.18649935554593	-1.26612891842787
H	0.18052585799715	5.66874906295517	-2.13115796444592
C	-3.69062414058366	4.48495917176602	-4.81616588051845
H	-3.22088845724666	5.31978890778043	-4.28343441661836
H	-4.69813231025589	4.78903913112613	-5.13184760531474
H	-3.09537048538249	4.24493506598013	-5.71000786879985
C	-5.25706880179178	1.98454576736193	-5.45796785889345
H	-5.67685966170250	0.97050914597382	-5.48371691079821
H	-4.63103219625669	2.13374724274450	-6.35387233291736
H	-6.09171851997303	2.70404599412604	-5.51857820767648
C	-4.31274145851785	-1.85705793762714	0.23610489032982
H	-3.58111365588812	-1.22079086310445	0.76126134423296
C	-5.69034243028225	-1.21009569818571	0.38273740600765
H	-5.98393378170431	-1.17144237609137	1.44453793265151
H	-6.45593144313965	-1.79185281514649	-0.15950131823620
H	-5.68090831987177	-0.18436119446292	-0.00708840453205
C	-4.31322087907790	-3.24932001470804	0.87317345029280
H	-4.65241203494481	-3.19066080608588	1.92000377479154
H	-3.31975709093986	-3.72304813438216	0.87777340043727
H	-5.00518826564781	-3.92753496067823	0.34848103077037
H	-3.28434304428936	1.98374757762382	1.33810753588248
H	-4.34709880588233	2.63428379631046	0.41944653454741
Cu	0.15542046786301	-0.52240233150466	1.17340333829510
C	-1.29939083703855	0.90289309434175	3.79567749078628
C	-2.54753328114208	-2.55283827500425	-1.44913643716454
N	-1.40004088616480	-1.92771614463932	-1.31974081083747
N	1.24124009336126	-1.35087588946778	-0.35536329224253
N	1.87743935210409	-0.64543931738311	1.96470201093992
O	-0.74072811347609	-2.51713044671979	1.70300456882643
C	-0.39100134692715	-2.86062862253936	-1.28992908645610
C	1.03410759336979	-2.46198342572392	-1.07615703232583
C	2.92916316740002	-0.73041126467215	1.19510979275411
H	-0.68768641873371	-2.97712906294964	0.84707546434093
C	2.66448128563265	-0.95607421620797	-0.26561282054611
C	2.20525328629526	-0.12240103765535	3.18006498203160
H	-1.67195640057413	-2.26876114832559	1.78531254617009
C	-0.95104046003546	-4.12246000455449	-1.44944558444366
O	1.92277703784720	-3.20216362158374	-1.58320617077918
N	4.01298416733791	-0.31741592748758	1.90649938467462
N	-2.31904135097019	-3.90377306573494	-1.55819478937737
H	3.29924120001966	-1.75671302105824	-0.67012526680483
C	2.95009584481992	0.33844910404356	-1.08506360555138
C	3.57342074066035	0.08303156422579	3.17977055682947
C	1.02117605258348	0.30063182110640	3.99088902308446
C	-0.36464960859327	-5.48998769812233	-1.47445794500647

C	5.38625189605828	-0.26677127259572	1.43072459890188
C	-3.29637219235150	-4.95983846103298	-1.76412823677789
H	4.03601459445221	0.52615247144017	-0.99524727639970
C	2.21068240838821	1.56762044319773	-0.54609377832514
C	2.63285256442857	0.10172459636310	-2.56341407691795
C	4.50347684751076	0.64280586081616	4.19604263024944
N	-0.08969040074527	0.27871926942616	3.24959446388541
O	1.15704362720794	0.65834861901502	5.19451791810189
H	0.69379870369202	-5.43608049927426	-1.19042407452120
H	-0.42720413610840	-5.94562857604487	-2.47791376701919
H	-0.88680908068084	-6.16470489097676	-0.77680844999699
H	5.47259692715848	-0.87474838946387	0.52248933953906
H	6.06457124987757	-0.67694497716654	2.19080324624952
H	5.68757261035651	0.76697878595244	1.20184055107815
H	-4.26432604401995	-4.51493846026266	-2.01853547763896
H	-3.41237627419158	-5.57096802786326	-0.85767243917441
H	-2.97626767913572	-5.60802854408293	-2.59086129919041
H	2.40842612100051	2.43947168114861	-1.18786636954888
H	2.52412299379441	1.82821027394416	0.47710374084939
H	1.12255287605247	1.40778190811324	-0.53316467357140
H	2.90878210642359	0.98156383312284	-3.16618654486738
H	1.55523830372351	-0.07614043725507	-2.69819620683141
H	3.17593436832426	-0.77132836763805	-2.95741928078406
H	3.91822722108865	1.01358904497677	5.04786007849203
H	5.09464479502625	1.47758053350635	3.78369926584005
H	5.21693097963736	-0.11325419448921	4.56660284049003
H	-1.20670331995240	1.00303569819366	4.88980128631219
C	-2.54814670917506	0.05160913086775	3.47458137167858
H	-2.55698902030852	-0.05906831035585	2.37947024189761
C	-2.44353679476696	-1.33434835162975	4.11810000382358
C	-3.85790236544352	0.71514580566523	3.90757935364487
H	-3.20658958951074	-2.01559574398145	3.70583070673454
H	-2.62000557364425	-1.27609124537981	5.20663947859497
H	-1.45365779402079	-1.78351243383712	3.95953819280793
H	-4.71533333258046	0.13291629912382	3.53263637043547
H	-3.93302400347636	0.75764363515700	5.00839540250634
H	-3.96079925513195	1.73563358979157	3.51423805217864
H	-1.42422644241844	-0.62572801406475	-0.38403392544382

B:

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Cu	-3.28327922914242	1.30387741992286	-1.06191089906912
N	-1.89083201481971	2.34939332180360	1.84761689908235
N	-3.02360123525267	3.33202541620653	-0.91465979868141
N	-4.74412451775541	1.96112383294826	-2.12777047781633

N	-3.99094028779786	-0.42856442397760	-1.89878664355167
N	0.18029122527629	2.91802277433294	2.31365425140049
N	-5.46005847539260	3.22991782549920	-3.72551901457120
O	-2.55442233144404	5.32130970270727	0.15379244077410
O	-5.53400612708257	-1.21775003691459	-3.47195228731520
O	-3.77286024957791	0.81376392899969	0.92053687767232
C	-0.85225257601480	2.08279406122074	2.62285379652584
C	-0.22673209050047	3.74863705140679	1.28284223395488
C	-1.53042237762514	3.38539635143121	1.00803372429120
C	-2.44362022730331	4.06887507018078	0.03212044586732
C	-3.70191360614429	4.10635709583927	-1.98058415249172
H	-4.10864384901627	5.04848108225400	-1.58222222917267
C	-4.76739496100473	3.19857864617516	-2.54622934317904
C	-5.79206032881809	1.91437634426382	-4.07678423741334
C	-5.30680929600114	1.12804752704696	-3.04784617922877
C	-4.96586452542166	-0.30495768625463	-2.82064608802798
C	-3.64125881641301	-1.80186646715389	-1.52450496455119
H	-4.12216135199704	-2.46775642088616	-2.26258797760865
C	1.54021590248293	2.80253197047896	2.80578675818447
H	2.06099401041374	3.75878237230676	2.67646270845246
H	2.06695601815975	2.01352155899411	2.25033144324475
H	1.53708441211034	2.54046415318362	3.87052484937130
C	0.67557825092107	4.74375600498969	0.64189162359992
H	0.09254719763307	5.36608976802524	-0.04870948388126
H	1.48146866019984	4.24969341097785	0.07114761281997
H	1.15455459536586	5.41182090788450	1.37788870827934
C	-2.71400292983625	4.44910756241013	-3.14909401003411
H	-3.30023909895871	5.02896894330476	-3.88221358408753
C	-2.18527853158268	3.18687240979991	-3.84365596636056
H	-1.48254225723893	3.46465065764047	-4.64467800176097
H	-2.98718551556608	2.58839443906506	-4.30207013389924
H	-1.65702557011332	2.54292057446971	-3.12406152445773
C	-1.55002841720472	5.33655942593291	-2.70390452062067
H	-0.96172346031189	5.64780814963279	-3.58278197618315
H	-0.87827406176899	4.78794981588396	-2.02800419504487
H	-1.89770641781084	6.23237197001050	-2.17202299174240
C	-5.77943397056798	4.40479094963508	-4.52158258331372
H	-5.66490643204237	5.30082065800415	-3.90089386278950
H	-6.82025235631289	4.34973557867487	-4.86891886150667
H	-5.11722372831424	4.48020853814725	-5.39709992666473
C	-6.45331712451509	1.57557053549183	-5.36588645240786
H	-6.40434472829917	0.48820313964006	-5.51415140937001
H	-5.95243881118527	2.06855640341497	-6.21493505299213
H	-7.51379083789988	1.88219619689632	-5.38576763621541
C	-4.18447254601814	-2.22295543437465	-0.13420717059927
H	-3.58092353581367	-1.71824928099694	0.63430420050157

C	-5.64144308091050	-1.79030428642920	0.04688703637017
H	-6.02580710474164	-2.14444017200465	1.01752158054213
H	-6.28212891518954	-2.21771383731779	-0.74250950468291
H	-5.74663360412652	-0.69829239213921	0.01449922782920
C	-4.07001993762567	-3.74262759709532	0.04077344080345
H	-4.38045089799377	-4.04558260857436	1.05438102966765
H	-3.04311924606909	-4.09843371862038	-0.12306161418029
H	-4.72786372243109	-4.26641117757095	-0.67481857763494
H	-3.09542030447452	1.38655432226886	1.42376964397580
H	-4.63595683109283	1.18929166598731	1.13710423310941
Cu	0.63761991451575	-0.88296973832379	1.74509863339238
C	-0.77516867879516	1.07478257290029	3.73977048547338
C	-2.15331034422642	-2.02170640167026	-1.64659343676543
N	-1.29197093257117	-2.31505226529795	-0.68516730658443
N	1.63452315497058	-2.18457581406038	0.51444615774183
N	1.85747985163652	-1.75536210363675	2.97548842679809
O	-1.16719578240538	-1.94341286121931	1.91273120848471
C	-0.04031943932224	-2.43750181831242	-1.25724879934549
C	1.21198178549609	-2.88005254376329	-0.54371782791377
C	2.89671494489575	-2.41021746232537	2.53817685790167
H	-1.03113072222337	-2.77400921515387	2.38508061060291
C	2.94666160288780	-2.64082580482794	1.04696670831439
C	2.12509969194616	-1.16601876663231	4.17396368360809
H	-1.35364983048850	-2.19287166691233	0.95406315967867
C	-0.14609810280278	-2.20765162427115	-2.61674156837260
O	1.79049335770623	-3.88376070260425	-1.04978333708883
N	3.86440035217186	-2.36575114214976	3.50710851065824
N	-1.48875737738434	-1.93277849259372	-2.84353657297155
H	3.10597281071792	-3.69799286979906	0.78762754687140
C	4.14380258759575	-1.82394483495520	0.45536228853279
C	3.39230025282599	-1.56566643246988	4.55815985237759
C	1.14280243037852	-0.09643628902343	4.52051882440612
C	0.87249290006588	-2.22357746383276	-3.70182947920968
C	5.16233614894739	-3.02149504544279	3.49220855474647
C	-2.06940130652791	-1.57600699049653	-4.12929417691005
H	5.05650249595875	-2.29265577309695	0.86235169365049
C	4.13033948738380	-0.35206027100061	0.88879935167707
C	4.22288077361999	-1.93303586381326	-1.06816008397395
C	4.21777521919841	-1.24983524502625	5.75526082819328
N	0.30768044410078	0.12868471809348	3.49729589216502
O	1.19416007548416	0.49886045611341	5.63093964815946
H	1.83679547953601	-2.53686377361476	-3.28176541992374
H	0.99381863406847	-1.23379200528543	-4.17345919148707
H	0.60597264419160	-2.93590698421655	-4.50043137639467
H	5.22690680236625	-3.68196788595965	2.62055663734820
H	5.29167780857255	-3.62897330503470	4.39948281724480

H	5.97288502706154	-2.27870086300603	3.44398221845542
H	-3.11671604473406	-1.89809490218208	-4.16780759113021
H	-1.51323649855704	-2.07399845265407	-4.93264147885937
H	-2.03449174858796	-0.48686841226260	-4.28389866032997
H	4.96887056988305	0.18953734798049	0.42494965605113
H	4.21452195180303	-0.22771996929299	1.97900502779645
H	3.19883892687165	0.14079162396033	0.57325563868695
H	5.12733430100040	-1.42348027103387	-1.43761576247730
H	3.35390647854186	-1.45048373142996	-1.54096197230018
H	4.24298828954131	-2.97942863830468	-1.40196195957426
H	3.64560526589182	-0.58732270770108	6.41758432767629
H	5.15748214457180	-0.74216107248313	5.47918216171455
H	4.49065953906935	-2.15671769071380	6.32142274096073
H	-0.53022890195115	1.63979044417758	4.65905915338645
C	-2.13131482032724	0.36586423619239	4.00252596998106
H	-2.47884553557588	-0.06436016595785	3.05156942837508
C	-1.95845662978547	-0.78637845816066	4.99514766036345
C	-3.18029357728710	1.35527028472469	4.52498099819674
H	-2.93033149656645	-1.26455502540237	5.20285684862634
H	-1.54458185040225	-0.42528502215822	5.95160232167603
H	-1.27898162721637	-1.55303807163295	4.60020126693038
H	-4.14172292090114	0.84417788158258	4.69963589012877
H	-2.85642219970069	1.79540996306787	5.48528476597590
H	-3.35521925541958	2.17628480450311	3.81687154107142
O	-1.23339061369399	0.86980910435932	-1.20170131047825
H	-0.54350633548155	0.75663878202747	-0.36071146915457
H	-1.19905577723474	0.00267820951149	-1.62026775611802
O	0.48483013961614	0.54513492460400	0.50124480446282
H	1.19160624305765	0.35504356232010	-0.12771569439160

C:

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Cu	1.29101353477437	2.69011924351474	13.43083535173856
N	0.93141940226253	2.83901336559901	11.43019704633165
N	0.13307022102007	1.14057179467747	13.24482766581393
N	0.80401778349297	2.42481662661905	15.47153899126707
N	2.66982303959845	4.48875716493361	16.13811740274457
H	2.61689191273036	4.01125990116185	15.24243472330573
N	0.51649210829227	3.12964963093836	9.29820335301194
N	-0.59374980530295	1.37387483478362	16.81076975508701
O	-1.36991675639566	0.09159768223847	11.82876002391751
O	2.00321667383953	4.39200558653757	18.31293869761638
O	3.08218374366702	3.56707492714688	13.49810245453869
O	-0.04760329268748	4.75848335472019	13.78020178258385
C	1.22332522203330	3.57888189399434	10.37328736485560

C	-0.27029267585398	2.05629127685784	9.70048027933045
C	0.00791985661524	1.88667236409424	11.04037512903147
C	-0.48677947550242	0.93734581718146	12.07226343567885
C	-0.29004546284941	0.45416429019063	14.44878321311300
H	-1.35205860937026	0.17099187239552	14.36491925269896
C	-0.08262127405396	1.44353225954913	15.55625261548439
C	-0.00292725837124	2.35525924712563	17.58176429930079
C	0.87994741153575	3.01029508293948	16.73719737586168
C	1.87595002575376	4.02732105095470	17.13640730653468
C	3.99271913324559	5.03123852885689	16.44133005829755
H	3.91812585790772	5.54742511808661	17.40473679874215
C	0.54567538672529	3.68931508631031	7.95106351115573
H	0.31279702141894	2.90041975197765	7.22725726990942
H	-0.19087057046779	4.49951598284479	7.84852698431489
H	1.54735176150085	4.07768231914926	7.73088956317828
C	-1.16853378840017	1.31250319062836	8.77560170093710
H	-0.59294463786734	0.79198171206915	7.99148103269005
H	-1.72954977028850	0.56380940166836	9.34869005793313
H	-1.88360837679024	1.98456867803433	8.27424873863704
C	0.52616177065149	-0.84355907187074	14.77495786235490
H	-0.00604569681678	-1.32764200440914	15.61225322064140
C	1.95289347184473	-0.53244736499670	15.24370986918836
H	2.54604199190113	-1.45630185105825	15.30586193021535
H	1.97248806649505	-0.05246412673838	16.23389308317660
H	2.46904755306323	0.14107518905738	14.54550358019893
C	0.51914987727927	-1.82154025360320	13.60082369486133
H	1.04376219371010	-2.74681610343557	13.88964178297493
H	1.03584097681345	-1.39387547129900	12.72856322565551
H	-0.50358003852593	-2.07826252555449	13.28955848201672
C	-1.57409415619593	0.41185781326320	17.29749197032704
H	-2.34396582537293	0.93356947367744	17.88004865413036
H	-2.05428743831263	-0.08588496944235	16.44831877704740
H	-1.08490380733352	-0.34039746575736	17.93313337828094
C	-0.34373953788600	2.53762495516806	19.01804273915517
H	0.22933369849352	3.37401609483538	19.42943386467579
H	-0.10680202632602	1.62935003318026	19.59716944437481
H	-1.41970522681856	2.74284655793999	19.14548736541247
C	4.47787317681455	6.04723785131308	15.38559855131604
H	4.56824066733427	5.51728076415947	14.42386016860415
C	3.48676530370281	7.20029671047147	15.22666158343224
H	3.84280738510305	7.90777801387029	14.46215203752514
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H	2.49036837994796	6.84306645429535	14.92478250298049
C	5.87761237496620	6.55250590506128	15.74972297673145
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H	-0.77247469589027	4.79163643865515	13.13888397254509
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Cu	4.83195415049553	2.60904858673262	13.66622163904936
C	2.25271389122883	4.67854170735002	10.36908052919204
C	4.93675943152676	3.86766390769074	16.58084436433941
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N	5.30763039770010	2.07405516525642	11.68310902912541
O	6.32259301354877	4.52561195315683	13.07687436579243
C	6.06896678180268	2.04975282815998	16.14194819505632
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H	7.04041024650011	4.61921748993834	13.71970409923451
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H	6.77275332534721	4.26371400068895	12.26042908550169
C	6.34974401061988	2.37108028737782	17.45222801654135
O	7.40529689081633	0.14275982553169	15.58505945738295
N	6.69839337916984	0.83900777437771	10.50318682866763
N	5.61519000393002	3.52116447188089	17.71037369063324
H	7.36749992526905	-0.10713941823676	13.06838904435421
C	5.46492415074525	-1.11223838710054	12.78807570432315
C	6.18761588089537	1.77301686848876	9.62310790034061
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C	7.21464449924600	1.70681639333031	18.46298878654055
C	7.66012481512823	-0.19649598002665	10.14847946418275
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H	5.97902291089176	-1.71090510014721	12.01558712203786
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H	7.71335062804229	0.85007342413867	17.99282134648005
H	6.62331361727238	1.34309229974388	19.31996327910626
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H	7.17509835278570	-0.97700897380919	9.54487100811675
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H	6.37705973088002	0.84325481230548	7.70028592962412
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H	3.51735811254916	3.65629563657359	11.68285015582234
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H	1.66015060990275	5.45165361628423	12.28852509298724
C	2.96933707683797	6.89510691690611	11.37443217887450
C	0.53591270771455	6.47196308950894	10.79489945372242
H	2.66155795683488	7.72929506685641	12.02291553750024
H	3.21029727915552	7.30898179769019	10.38101347844971
H	3.89282074720679	6.46267322650254	11.78966890838016
H	0.22020312146791	7.28620222316553	11.46356590373036
H	-0.27830033282621	5.72967428491663	10.76662763668276
H	0.64435004593605	6.89093353240852	9.78011673167673
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C	3.50173492450269	-2.64271042349435	-0.23778284274587
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C	2.01622705000183	-3.12076431911224	1.29803115524831
N	2.69981846819616	-4.26802559952676	1.00110670039720
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O	4.77730449741518	-2.24522835983939	-2.22496313402918
Cu	2.55172543615375	-0.06493980782927	0.32437949427343
O	1.55563988346656	0.53471182817999	1.82915511395886
C	0.79390119506203	-3.09560446942578	2.19282203638303
C	0.91875374091617	-2.19857943268638	3.44153296752391
C	-0.20254462794106	-2.48103063232559	4.44477448750489
N	2.20761933836195	1.75533430479532	-0.83820430803502
C	1.84262115374626	3.09822269619566	-0.71028083361040
C	2.53706606361574	3.83674625510044	-1.65264611212460
N	3.31675310493851	2.92701918705658	-2.34273007256229
C	3.07952413903796	1.68585566941377	-1.84028919791561
C	0.77251277258176	3.63461952479482	0.17203052221069
O	0.23966269833168	4.72956043025947	-0.07279675869192
C	3.62173598656523	0.37840196794078	-2.35495046941720
C	2.76564338566049	-0.19553558304442	-3.53641037996396
C	1.31015436341460	-0.43962462299388	-3.13599450394500
N	0.38199835482486	2.86380463309875	1.20302379102199

C	-0.78437108381671	3.21279164283817	2.00021835074393
C	-0.87877616987770	2.29334786993550	3.24229547395017
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C	-2.04930196992089	3.18247577344016	1.17643244221985
N	-2.56732611590360	2.13342016195088	0.54978452427364
C	-3.78932406310862	2.52405673068169	0.01502549799713
C	-4.01029717128477	3.84653914421216	0.32476836932337
N	-2.90117907830026	4.24149822930618	1.05433923392300
C	-4.54308989413624	1.56146612399161	-0.83022753700089
O	-5.58095666327000	1.87762625204934	-1.44777882846662
Cu	-2.24446297794218	0.17274573727480	0.07106356924028
O	-0.25216202049891	0.04692435259971	0.14627296560729
N	-2.42899728591579	-1.75680090251683	-0.61548514295960
C	-1.92807213040696	-3.04386721008182	-0.46375012889866
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N	-3.61621290013330	-3.10529273450773	-1.88594694446982
C	-3.43208586174854	-1.82053064180342	-1.48243339489765
C	-0.78814180973453	-3.48731891127545	0.37264438106688
N	-0.39233301614489	-2.72478999652638	1.41638698407877
C	-4.15421235085225	-0.57859715201337	-1.93126069791354
N	-3.93379651694841	0.37375697177326	-0.85657709928545
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C	-3.60276412354469	0.01002225769776	-3.27727104715193
C	-2.16084215905090	0.50986498760481	-3.14884261910930
C	-3.72472429560991	-0.94775944169064	-4.46252797494635
O	-2.58996183422759	-0.60107426456034	2.24354202530681
O	4.70504455337846	0.72321645041835	1.25664937418633
N	3.60397822381336	-0.52517303845157	-1.21843217416721
C	-2.22644420186176	2.44817305696963	3.95462177857827
C	2.85003797266152	0.64829045351760	-4.80854887351629
C	2.29624273154312	-2.34719098209884	4.09427366150550
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H	-0.79263766631189	1.25509859862612	2.88088500529502
H	0.25587440863098	1.84819239348793	5.04456857632646
H	0.19364243817571	3.57897417624160	4.63656221664092
H	1.25590652120739	2.48490875381780	3.71771588584706
H	-2.27138194565324	1.78820196776121	4.83456284231024
H	-3.07950135813447	2.20625198872919	3.30041576589907
H	-2.37124448197851	3.48115086772220	4.31262947036094
H	4.64884214283700	0.52255330198568	-2.73071023952658
H	3.23242909234995	-1.16814649278807	-3.75155239108028
H	0.77223819124016	0.50996338364606	-2.98674013922823
H	1.22705790832180	-1.02706839392933	-2.20987175677957
H	0.78370805510438	-0.99115550753839	-3.92994561648894
H	2.36988025457842	1.63254024859477	-4.68016050508733
H	3.89152048518591	0.80848439731667	-5.12904617315999

H	0.64690710311473	-4.12686629786207	2.54141950786992
H	0.80910621555003	-1.16238322838573	3.09142839949216
H	-0.10203908523763	-1.81845069206838	5.31832817769186
H	-0.15852873884640	-3.52195321619367	4.80682976006047
H	-1.19799799483144	-2.30936605243558	4.00797058740383
H	2.37415805558518	-1.69276326401343	4.97589133706686
H	3.11066710220081	-2.08031563776526	3.40356337852550
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H	-5.22655403009742	-0.79587760019999	-2.06857562663210
H	-4.25225662613871	0.87729897370995	-3.47505055945374
H	-1.47546405705252	-0.31179662542627	-2.89025220907509
H	-2.05794073337496	1.29780348778188	-2.38860518338690
H	-1.81921270847584	0.93669294490078	-4.10415702355291
H	-4.75780324297187	-1.29449430409422	-4.61637774364503
H	-3.07598578496217	-1.83037697891403	-4.33590939883172
H	0.93362443650227	2.03852271878455	1.48274020452014
H	-0.89392924827273	-1.88332337771234	1.65759205871888
H	-3.40344725999944	-0.43711204788274	-5.38400449520328
H	2.32435026376676	0.13777720680902	-5.63094876300133
H	-2.83894170483339	0.09419750434872	2.87019710360907
H	-3.33761475806330	-1.21815789710697	2.26244163694713
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H	5.07569490574168	0.23551806038930	2.00718989416625
H	1.96735677336724	0.31114688756233	2.66872578090389
H	0.28645504337070	0.15839380968970	0.99315518090974
H	0.17957106398316	0.64500938911383	-0.48460029121188
C	4.50312865894053	-5.02792459874674	-0.59811154612325
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H	5.12622162308553	-4.55453392672649	-1.36633679868079
H	5.15879639019464	-5.50753323660435	0.14776005892554
C	2.43527848341792	-5.61012014521571	1.50391148710545
H	1.69240718813986	-6.11173373361881	0.86896234160012
H	3.37091809653773	-6.18016946863607	1.50777654565759
H	2.06047955658055	-5.56590783303755	2.53205352552707
C	4.26884446361263	3.30341018525663	-3.38133564312431
H	4.80603674753903	2.41931827912182	-3.73383189104594
H	3.74241960915314	3.76431740529158	-4.22804609063736
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C	2.52827207621172	5.28470326027727	-1.99557021609263
H	1.88609824728838	5.47513204577868	-2.87270434380541
H	2.12742115511148	5.86885313319829	-1.16058888474385
H	3.53775528138089	5.64604083496027	-2.24127763394378
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H	-1.84451733086770	-5.58689729852115	-2.29325758512269
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C	-4.67649461143778	-3.61491042156297	-2.74918656392990
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C	-5.11577076602103	4.77528009461178	-0.03106618368788
H	-5.88610473389795	4.22032646395292	-0.57984060414704
H	-5.56817269920306	5.23135601407413	0.86470013613719
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N	-2.04540508747717	-1.41534943068078	0.76792609105805
N	-3.69330345870508	-0.56980559926292	1.95883746872946
N	0.37491149889571	-2.56945944409373	1.58745442580809
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C	-1.97189066419908	4.04444801964110	1.05855902830524
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C	0.10008625537043	5.48825047366659	1.24688712402517
H	0.92455934216487	5.77931245732377	0.58687912808392
H	0.51645068285923	5.03243586754469	2.15813146516432
H	-0.46935437530242	6.38672880201514	1.52082572294523
C	-2.50885656296574	4.43002590327455	2.39128825354724
H	-3.44089281411837	3.87852109062536	2.57215539988544
H	-2.72192403068720	5.50996264109284	2.46479688970876
H	-1.79571888921175	4.17772903401926	3.19490114736152
C	-3.39783681333088	2.02505925255714	0.08534574004801
C	-3.72744493227288	-0.24718860184706	-0.58996128442534
H	-4.80486817233982	-0.01958289818469	-0.52318047858664
C	-3.46677870397859	-1.13921309638641	-1.81744507021933
H	-2.37975414751333	-1.31182779028162	-1.84187215369594
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H	-3.99376075063695	-2.98523151981016	-0.74669528150051
H	-3.80457331404194	-3.17140466406935	-2.49743242009714
H	-5.26422897988731	-2.38241359361437	-1.84870253429016
C	-3.86476208832274	-0.43169343976086	-3.11387013934319
H	-3.29710446762774	0.49574163541852	-3.25415148649563
H	-4.94337135505622	-0.19321545943217	-3.11749114802733
H	-3.66387885439556	-1.08514367517374	-3.97911059313951

C	-3.24140485186251	-0.87405845246874	0.69620165693437
C	-1.64752762515970	-1.38601285525035	2.08417630474562
C	-2.68334232786359	-0.87187917391075	2.85593311991465
C	-5.03753599101572	-0.17975115217527	2.35044123781984
H	-5.47525118360682	-0.95787719097016	2.99435145544824
H	-5.65057568412766	-0.05786946624541	1.45429472169065
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C	-2.85626018433251	-0.68926253840513	4.32328245151336
H	-3.12230239289269	0.35087718962607	4.57959289682359
H	-1.92012238483871	-0.95863977108799	4.82591755979995
H	-3.66318463719573	-1.33076768585437	4.71741198145652
C	-0.31549799224445	-1.88007676456702	2.51141717636277
C	1.40116951514841	-3.45802696603331	2.17176795360356
H	1.90890910727937	-2.99353434848092	3.03361971550599
C	0.76626508795091	-4.81728182335134	2.63872552226585
H	0.35942997980111	-5.28512598590822	1.72221920744190
C	-0.39458431702883	-4.65282624098029	3.62189468874472
H	-1.21950125206217	-4.06932569732037	3.19032073040953
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H	2.56349625628749	-6.07938904016041	2.47783022674796
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C	0.62770328579742	3.93221205044865	-1.59798189977136
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H	-0.75100877703964	4.47626639359005	-3.14138628949275
C	1.18771934430957	4.93419413601042	-3.92986607679618
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O	-0.04255616510223	-0.46743119006027	-1.09570925462600
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H	0.94860788996896	4.89812380360226	-3.48890641955782
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H	0.44213668141890	3.48992424404081	4.00800615526015
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H	-2.89882143011274	2.04456573961329	3.08035097748103
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H	-3.78230852841625	-3.91361897110925	0.75154094847115
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H	5.23503477030691	3.98735716306588	2.25531692690767
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H	7.08700017902084	2.43989027775841	2.50643895007122
H	7.52114803475460	2.38963316703977	0.78732230166588
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H	6.75885573706957	-4.08384887776148	0.14205759404126
H	8.05723399551384	-2.91835455378102	0.53218285654982
H	7.66197517227628	-3.26548286956560	-1.16378193155435
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H	1.75644835507423	-4.28594089274482	1.09842500707827
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H	-2.21997214993654	3.50564028555038	-2.32002122860941
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H	0.17341005024774	-3.96868778832645	4.01873813179769
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C	-2.08375903818280	-5.50549347634014	-0.82565303840258
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H	5.95222557417042	-4.03204545376668	-2.44026318571465
H	6.74732366195221	-2.80919405006284	-1.45595057102986
C	-6.12087405005289	3.73515461611664	-1.45859596698375
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H	-6.74302973146596	2.83367018655974	-1.51846085567384
H	1.70236573273735	0.62718159102073	-2.29917236879021
C	6.87407091755579	-4.80546585546721	-0.65737780151034
C	6.45582449363563	-5.31303052086775	0.57739612819893
C	8.04004741568435	-5.31991981544451	-1.24600113766687
C	7.18574962891189	-6.32496190040462	1.21202837086186
H	5.55505988909086	-4.92475098465905	1.05583276045971
C	8.77292879378342	-6.32482939031479	-0.61104875643565

H	8.37826731313049	-4.92477922847489	-2.20855110967144
C	8.34406542029967	-6.83516410676995	0.62035363952447
H	6.83831442441366	-6.71927743392696	2.17035501388601
H	9.67655477007022	-6.71849620768332	-1.08357764327088
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C	-6.86163982529387	4.82805562556369	-0.71231676057554
C	-6.44971290298194	5.32026527731261	0.53090795256719
C	-8.01570410691713	5.36145385070404	-1.30755337702993
C	-7.17340410347587	6.33577459458159	1.16684057579143
H	-5.55784721468963	4.91807655570686	1.01449898416440
C	-8.74293339125817	6.36958677902187	-0.67105189507328
H	-8.34888415445495	4.97902340923074	-2.27695910106086
C	-8.31991651610026	6.86471428472200	0.56851763842638
H	-6.82979227016531	6.71875292057896	2.13117721470545
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H	-8.88456844926548	7.65754150343030	1.06533816482830

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N	-2.29673825372208	3.29618377480372	-0.79047486442032
N	-4.11672272682397	2.26938348234811	-2.17620981451793
N	-3.93475804211476	-0.18467575242634	-1.58273642234443
N	-0.22169600088715	3.06876625519527	3.15035426103690
N	-3.96762565372157	3.23541580327183	-4.11706922343488
O	-1.82792969813493	5.43666206209357	-0.01785561568352
O	-5.50991828397745	-0.80769499133419	-3.20763969253286
O	-1.43177213239968	0.49861294006358	0.33700262583250
O	-4.26522389799486	1.68047991034218	1.01454514168983
C	-1.28691948844702	2.20409425817894	3.09056958162490
C	-0.34735459973892	3.98426319135249	2.11870245211270
C	-1.51536712198004	3.63937575814983	1.46369684500561
C	-1.93754891256375	4.18443428755078	0.14079851396656
C	-2.37595577467970	3.88611175632795	-2.14003086307030
H	-2.41713058509973	4.98193217070404	-2.07810214472769
C	-3.58717893775666	3.28341042323618	-2.80189435684411
C	-4.70528833474234	2.06219927392802	-4.30893693518794
C	-4.74211751399230	1.45104271348686	-3.06492492916340
C	-4.79321102753317	0.03400008659941	-2.60263824555858
C	-3.87112383742088	-1.59491899054429	-1.18499871925738
H	-4.62181869061947	-2.16105687727624	-1.75682417479969
C	0.92311499752063	2.99423463704841	4.03841650946508
H	1.26402330214900	4.00624743880042	4.29257535382165
H	1.75035087861540	2.44868005023542	3.55955462476544

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C	0.67524032019727	5.02659894892820	1.82819349858533
H	0.36462125603469	5.58567522639243	0.93700428954608
H	1.66713923469931	4.58201610656217	1.64082909378660
H	0.78600483616692	5.74333952203235	2.66026230441182
C	-1.10636769607544	3.49313903135428	-2.96771600303472
H	-1.20202916459732	3.99967439004305	-3.94347368984591
C	-1.00659785243690	1.98229459252963	-3.21609880269124
H	-0.13293023292946	1.75767546293574	-3.84763284659729
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H	1.04184025719419	3.81301202988930	-2.95279705046833
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H	0.12432428526839	5.08500925624621	-2.09275276396813
C	-3.60827099781401	4.16542734243966	-5.17350608901434
H	-3.13060515255326	5.04812973607437	-4.73335528486082
H	-4.50666150908453	4.48935640579924	-5.71768928441867
H	-2.91329630032980	3.69398886902105	-5.88514253258287
C	-5.23166386158600	1.67533944595472	-5.64591293979819
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H	-6.01661978784941	2.37031417826199	-5.99125134162865
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H	-3.54280838302111	-1.10520375715937	0.87892514437432
C	-5.66346426740605	-1.28659524003140	0.57504332179919
H	-5.92306555905299	-1.40504388368191	1.63983774539268
H	-6.37889728691452	-1.88387319068640	-0.01571037054604
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H	-4.32990660369952	-3.26737492570963	1.89226673800256
H	-3.06223155849644	-3.60387304665996	0.69325102149113
H	-4.76088553264674	-3.88163499544657	0.28659758193095
H	-3.46643255386180	2.01079139781173	1.57765942225307
H	-4.78799368244843	2.47221030431166	0.82805117374012
Zn	0.02616859638440	-0.45977152468048	1.34989359301081
C	-1.31859224927983	0.87511011612226	3.81572455818056
C	-2.50886535811493	-2.17300735201833	-1.49142819320900
N	-1.38529276214065	-1.51447648108222	-1.32548772378188
N	1.23420067806221	-1.03187767885440	-0.20440789164695
N	1.86065438775492	-0.91683312122682	2.21278984837126
O	-0.81062542139332	-2.37118364383631	1.58712655828563
C	-0.34004597021705	-2.40157160986264	-1.40632596709474
C	1.07097313121116	-1.98735493262300	-1.12881874733826
C	2.91468664149292	-0.73987825401589	1.46849813400687
H	-0.69041522189025	-2.80860247204933	0.72390931233549

C	2.64618226587811	-0.63224774276380	-0.01499868921264
C	2.09836050410189	-0.48923152075918	3.48234311706625
H	-1.76764551003490	-2.35285332287923	1.72782324281349
C	-0.84830557603768	-3.66361316714143	-1.68834122842038
O	1.97565409033451	-2.60118895089116	-1.76465576569764
N	3.93783057330600	-0.29018353050712	2.26000247295102
N	-2.22570191505741	-3.49527136953700	-1.75216985903232
H	3.30292138572737	-1.28500573975181	-0.60532586632783
C	2.88278798076319	0.83558422567420	-0.48762899620774
C	3.43202960397366	-0.11810374606245	3.55784299631043
C	0.84326042003545	-0.07117287834617	4.18839537001602
C	-0.20181609686746	-4.99248755852889	-1.86806068190976
C	5.30262276825260	-0.00391831967075	1.84821854740423
C	-3.15714544807384	-4.56188567170165	-2.08070426122838
H	3.95969728247226	1.03622077620463	-0.34642533436322
C	2.10198529564123	1.87143473442936	0.32894034625650
C	2.57462058519803	0.96439223475401	-1.98015713076720
C	4.26463125572048	0.40298456577583	4.67436112435925
N	-0.14714633877697	0.14717173063207	3.30029915293475
O	0.83177984271077	0.14241356061014	5.42855536034003
H	0.86027312920549	-4.91508923390026	-1.60292268164684
H	-0.26752565586280	-5.34415435032001	-2.91258826652385
H	-0.67312926683008	-5.76108321025660	-1.23425779678152
H	5.47580603001037	-0.43297106344640	0.85436392340092
H	6.01382386532094	-0.45812664231451	2.55186472737513
H	5.48553597398764	1.08110280481598	1.80873966391832
H	-4.13525752032975	-4.13191992108376	-2.32265017255402
H	-3.27342292573216	-5.26304124732170	-1.24153976815924
H	-2.78963132509648	-5.11428701212306	-2.95594325344371
H	2.34759932606719	2.88543086987364	-0.02193465526568
H	2.34919187281987	1.82959737580778	1.40090083341280
H	1.01281090176493	1.74350005792481	0.22147840579831
H	2.81984410991662	1.97572787581086	-2.34154273690898
H	1.50561312586482	0.78882877155225	-2.16737275056305
H	3.15140503941954	0.23782457254753	-2.57323747370714
H	3.61996707306160	0.58591338918599	5.54452731235722
H	4.77195534951924	1.34442499928765	4.40487062487487
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H	-1.19572618838354	1.03234843972822	4.90037386114253
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H	-2.74547198596652	0.03370498723016	2.47775252228398
C	-2.56358208008360	-1.31760151444169	4.14273243237310
C	-3.86214751760576	0.81699396300534	4.14256929138865
H	-3.41938414875565	-1.91647544369121	3.79004564673387
H	-2.60695711906656	-1.30445671894785	5.24520361339793
H	-1.63706381471599	-1.83194281997390	3.85504455181388

H	-4.78046523807656	0.31568399574334	3.79705158060693
H	-3.85218332886492	0.78946808612253	5.24597792728271
H	-3.92113021002240	1.86724972987502	3.82647015441731
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C	2.405420	-3.009526	-0.835638
C	4.550142	-1.997815	-0.921129
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C	5.271867	-1.036509	0.009998
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C	5.139239	0.891373	1.046740
C	4.194235	1.988121	1.423683
C	1.933860	2.677836	1.518123
H	2.457078	3.639538	1.670599
C	-2.591779	-3.517168	-1.095710
H	-2.568905	-4.292369	-1.871786
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H	-3.245852	-3.851472	-0.282737
C	-0.094866	-3.755678	-2.791271
H	0.924242	-3.662229	-3.188105
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C	4.838796	-1.511243	-2.382578
H	5.932904	-1.581205	-2.510395
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H	4.690680	0.274906	-3.616632
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C	4.213832	-2.399029	-3.458960
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H	3.115439	-2.364955	-3.413396

H	4.517006	-3.449657	-3.349222
C	7.728246	-0.998070	-0.640353
H	7.540906	-2.018813	-0.992399
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H	8.040866	-0.378083	-1.493995
C	7.635635	1.665574	0.756708
H	7.325631	2.600150	1.242912
H	8.080744	1.907780	-0.223120
H	8.429470	1.204428	1.369304
C	1.250286	2.306149	2.860935
H	0.573335	1.462440	2.662783
C	2.257157	1.830313	3.908966
H	1.724153	1.544526	4.830649
H	2.984233	2.619109	4.158528
H	2.808720	0.951231	3.553287
C	0.436130	3.481848	3.413723
H	-0.138229	3.168430	4.300566
H	-0.275946	3.880344	2.677820
H	1.103986	4.305997	3.718764
H	1.242719	-1.763158	1.743233
H	2.608999	-1.493789	2.502560
Zn	-2.508086	0.176623	0.282936
C	-1.934623	-2.533316	1.720152
C	0.921030	2.890498	0.420484
N	-0.383542	2.676215	0.472939
N	-3.076271	1.819405	-0.803771
N	-4.494692	0.273292	0.579995
O	-1.788136	1.158995	2.025597
C	-0.916596	2.953017	-0.773021
C	-2.391136	2.930820	-1.094854
C	-5.255332	1.003502	-0.179173
H	-2.551155	1.617411	2.402050
C	-4.518954	1.888797	-1.169718
C	-5.149497	-0.827932	1.026917
H	-1.225934	1.871554	1.559189
C	0.107038	3.347021	-1.614573
O	-2.852291	3.976343	-1.626471
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N	1.262255	3.308236	-0.838732
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C	-4.810616	1.333178	-2.604049
C	-6.463826	-0.721441	0.602814
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C	0.117414	3.678275	-3.065696
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H	-5.896387	1.462258	-2.754007
C	-4.496468	-0.163277	-2.734906
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O	-4.657582	-2.925832	2.083450
H	-0.891736	3.538406	-3.474170
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H	0.420689	4.721548	-3.258104
H	-7.515985	1.941816	-1.240398
H	-8.536133	1.022357	-0.104483
H	-8.011131	0.271094	-1.640851
H	3.217672	3.976058	-0.483647
H	2.569991	4.347760	-2.105487
H	3.090188	2.680804	-1.696480
H	-4.802208	-0.529445	-3.727917
H	-5.020091	-0.774585	-1.985374
H	-3.418820	-0.355798	-2.624700
H	-4.422977	1.726811	-4.694805
H	-3.020245	2.034010	-3.639804
H	-4.364234	3.192648	-3.668941
H	-7.368138	-2.468898	1.385914
H	-8.129013	-1.888394	-0.124522
H	-8.436651	-1.040460	1.404973
H	-2.436918	-3.489206	1.958363
C	-1.271666	-2.018541	3.027130
H	-0.602027	-1.190852	2.752882
C	-2.302413	-1.457019	4.008858
C	-0.447469	-3.112614	3.714576
H	-1.791880	-1.085125	4.912560
H	-3.028634	-2.227633	4.313320
H	-2.856649	-0.619875	3.567921
H	0.117759	-2.686316	4.559314
H	-1.106158	-3.904077	4.113020
H	0.272555	-3.582238	3.030382
O	1.147012	0.219961	-1.087451
H	-0.079324	-0.160467	-1.087376
H	1.063801	1.172228	-1.195293
O	-1.196631	-0.388501	-1.186972
H	-1.477020	0.238830	-1.866992

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Zn	1.24497438635554	2.86330692113903	13.48423378162701
N	0.87529416856425	2.87457298348302	11.38950718516503
N	0.17250681481696	1.18670955793004	13.35492973519339

N	0.73557416756195	2.56926224239753	15.61666672660232
N	2.78133184386749	4.29629303503715	16.36672555509631
H	2.76962147749140	3.70550007838811	15.54487962792238
N	0.55673034403739	2.86401466883656	9.22058907156713
N	-0.75694922382879	1.57565734775900	16.88790811678158
O	-1.34413021036579	0.08144775570471	11.99295817463578
O	1.73342647919354	4.78357571420063	18.33222606350055
O	3.13372922932382	3.47508657623325	13.48807895497758
O	0.26078261608266	4.80062996742162	13.81360355995642
C	1.18751441637517	3.48019701776902	10.25921609086552
C	-0.20075486713964	1.81307434733374	9.72724844334949
C	0.02175173486549	1.82656048175130	11.09181072878784
C	-0.45260752317890	0.93416132020608	12.19773487516952
C	-0.28471782021756	0.56012648719399	14.58020042224929
H	-1.33489879548334	0.24450167653624	14.46838508740146
C	-0.15684542986944	1.59699781132739	15.66676136226311
C	-0.21094313517204	2.58304702638085	17.66435965934265
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C	1.76537069992678	4.17415480704688	17.25634189196578
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H	-0.09865596661601	4.03202206481326	7.58230358524033
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H	-0.00746412945445	-1.13296894079096	15.87013322069791
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H	-0.45725050904221	-2.03463165865356	13.58351792259509
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C	5.87489627948708	6.54199120704219	16.07460611890457
H	6.18338842396083	7.31146132258105	15.35099310112536
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C	2.20436814533311	4.58866682885302	10.15686974416622
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C	-2.84281429678888	-0.94221483683197	2.88522093450442
C	-5.14886070808658	-0.12176365539136	2.35518944713695
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H	-5.73617421565625	0.06732883934407	1.45380590018231
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H	-3.29597055205420	0.24494757054069	4.62840920775598
H	-2.12693457004882	-1.09591635802132	4.86729088238331
H	-3.87540779104979	-1.42765343068824	4.71209433161647
C	-0.49589468910611	-2.01356304908782	2.57450236217596
C	1.29169071913341	-3.49656232196177	2.22465302511117
H	1.71333561171919	-3.04787754558882	3.13939127898632
C	0.74044539867160	-4.92025673196258	2.58033931826313
H	0.36870996256136	-5.34017585839375	1.62650283231270
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H	-0.79061102749813	-5.90540812907921	3.75696912420660
C	1.83825135212994	-5.84932391842899	3.11112701928392
H	1.40651225426204	-6.81481685574732	3.41907428383387
H	2.33255750714688	-5.41233296868219	3.99530937476073
H	2.60753568822989	-6.06244975039424	2.35458647009646
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C	2.33425351799361	-3.63315842150548	1.15401942597929
N	0.79166287270218	2.52811319555325	-2.21591394868295
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C	0.19539495242821	4.91044179582497	-2.79177103072298
C	2.01735156835156	2.25423257043962	-2.68858951105411
H	-0.76333952402886	4.49549136321886	-3.15353634772252
C	1.14403370974852	5.01065572408944	-3.98698602155296
C	-0.08244172195007	6.30729365300695	-2.21670857916185
C	2.19392149793281	0.96217707226125	-3.41693451072681

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H	-0.48161047593777	6.97315009659069	-2.99841815514652
H	0.84351816800594	6.76766354079476	-1.82994760940941
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C	4.68048331464908	1.02849674338372	-4.30355403203279
C	1.10219380264107	-2.45198899760324	-3.88555058549127
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H	5.46605183688025	0.41213291472021	-3.83425742185188
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H	4.90363428499199	1.06573928320461	-5.38373032192149
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H	1.59269983495612	-3.14450350519081	-4.58848596411681
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H	4.23502004746778	-1.11355807577426	-6.11418016964404
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H	-0.91569318890601	-1.83899738157193	-3.43924543456059
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C	-0.93147648890476	-3.92551384972861	-3.95379408547432
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H	-0.48270281813090	-0.95480009615094	-5.72711082957932
H	-1.80574392825077	-2.14442880413029	-5.79707277716149
H	-0.17186541007374	-2.60223812436861	-6.33050874811588
H	-0.78204039397366	-4.25082086814873	-2.91690335782668
H	-0.41106297296524	-4.63095620229453	-4.62438813052626
H	-2.00939905177610	-3.98373403634196	-4.17838264450586
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C	4.53835699488974	-4.12036522021090	2.28333722761219
H	5.57101023972673	-4.22033061407784	-1.68162688258765
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H	6.18675213336320	-3.58454577834212	-0.12983326837411
H	5.43828308924119	-3.50505206689393	2.14894140626131
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H	4.01607574531457	-3.79045082621160	3.18811601748186
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Zn	-0.93636760666770	1.22653505851434	-1.59760574372387

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H	-1.83879576846174	-2.69710882903128	-0.15673106927276
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C	3.77410000	2.36140000	-3.13950000
C	4.88560000	0.85650000	-1.99230000

C	5.79380000	1.43670000	-2.85470000
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C	4.93920000	-0.19300000	-0.92950000
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H	4.63440000	-1.67310000	1.00900000
C	3.16160000	-0.45900000	2.02240000
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C	-3.13350000	1.75710000	-0.69760000
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C	-2.97290000	2.93930000	1.53450000
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H	-4.64270000	-5.45700000	1.88230000
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C	-0.87660000	-3.71780000	4.17380000
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H	-3.32770000	-3.51940000	5.49320000
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O	-0.32741699	-1.28720360	-0.66383576
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O	-0.61575584	0.17499417	2.05030188
O	1.63051513	-0.68590171	-2.83191032
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N	1.03895512071934	-3.95725576429631	3.13485048978039
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C	-3.50646757566113	-2.30069723172898	-0.27130543468158
C	-4.73586714123148	-2.02136035386637	-0.83347998819711
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C	-5.46520616044762	-0.45114112736420	-2.68858155390093
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C	-0.20125813012622	-6.68789243105225	1.91260772028988
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H	-0.12583909565714	-7.64265120415125	1.36925351524810
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H	3.08117118802167	-2.96877695593690	4.81838187779158

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C	3.26462475419601	-2.20079629318974	0.84847495169001
C	3.75978477609612	-0.51150167529957	-0.83716518681200
H	4.70418500316838	-1.02222563753446	-1.05987177461684
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H	2.57529427847126	-0.68459362693214	-4.11490148147090
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H	3.42425475009272	1.67422925302436	-3.55069193293400
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V:
145

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C	-3.38489688088092	-4.11517574209722	0.01728351487695
C	-3.71832611292270	-5.41084394967531	-0.32153554466447
C	-1.48512484210462	-5.18477663722984	-0.26533231594329
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H	0.31876477426662	-5.91482291831127	-1.16409992672771
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H	-0.55324728151881	5.70116254890191	-1.01646747837196
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C	-2.52076342021032	5.71681860454424	0.95568597793050
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H	-1.02474224253381	7.46863630471373	2.34919883539669
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C	4.71340438065090	5.90915191440769	0.23300959502275
H	1.12217411894149	7.43276319590450	-0.94595175263627
H	2.85870760621014	7.40764171255106	-1.34353735324556
H	2.32214801548609	7.95062664649065	0.27269404875604
N	2.89582915081679	1.58079629139595	0.79479963153651
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H	5.15563130895505	-1.59093460339046	2.73036933280411
H	5.11724683017866	-1.91738910953850	4.48585840057878
H	4.86762267501507	-0.26384185230955	3.87776957388539
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H	2.98176558502875	-1.73459178764775	5.78436393802501
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H	6.55211516941139	3.93476300915883	2.19522588965807
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H	3.74006614199547	6.83097040918510	2.73476841771145
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H	5.28956900258306	6.05956494878450	3.20256290235707
C	0.71879033672740	5.01711756319732	4.52489086144908
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H	-1.82195188749697	1.10324655845218	2.97508867882057
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C	-6.31483477378464	-0.25397750461562	1.88157698928357

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H	-5.38051217133450	4.04008107020181	4.52822550902738
H	-6.13869007837158	2.45213775533805	4.27564391875357
C	-3.54824907524586	2.26138155756939	-1.49064573116236
C	-6.13143215617363	0.16490236833297	-1.09075310435138
H	-6.41167986781421	0.01941990777240	2.93738404235109
H	-6.05939685067447	-1.32038145607022	1.80540031719892
H	-7.27718910032081	-0.06624637772787	1.38915348764258
N	-2.61903161867768	3.17297850674892	-1.19466172345731
O	-3.97007810972321	1.96410823930081	-2.62897276349711
H	-5.79427874733816	0.40591690351434	-2.10570480196228
H	-7.15314687932134	0.56014470841581	-0.95739590547471
H	-6.17974753004623	-0.93052345491228	-0.97839814230566
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