

Supporting Information

Confined Metal Centers in a Symmetric Cage: Mono- and Heterodinuclear Complexes for Photocatalytic Hydrogen Evolution

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1. Materials and Methods

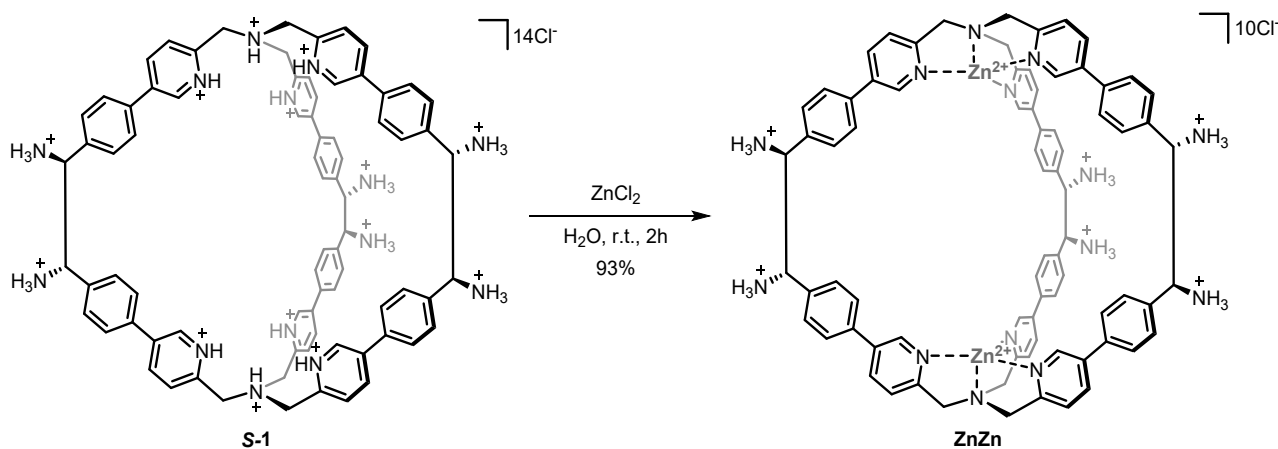
All reagents were obtained from standard suppliers and utilized without additional purification. $[\text{Ru}(\text{bpy})_3]\text{Cl}_2 \cdot 6\text{H}_2\text{O}$, **ZnZn** and **CoCo** were synthesized following literature procedures.^[S1,S2,S3] Chemicals were purchased from Merck, TCI, or Apollo Scientific and used without further purification. NMR spectra were recorded at 301 K on Bruker Avance-300 MHz and Bruker 400 Avance III BBI-z grad 5 mm. The following abbreviations are used in reporting the multiplicity for NMR resonances; s=single, d=doublet, t= triplet, and m=multiplet. The NMR data were processed using Bruker Topspin 3.5 pl2 and MestReNova 12.0.0. High resolution electrospray ionization mass spectrometry HRMS (ESI-TOF) analyses were performed in positive mode with Waters Xevo G2-S QToF. The analysis was performed with Fast Flow Injection: 10 μL of sample injected, ACN/ H_2O (50:50) + 0.1% FA at 30 $\mu\text{L}/\text{min}$., Capillary: 1.5 kV, Sample cone: 40 V, Source temperature: 100 $^\circ\text{C}$, Desolvation temperature: 350 $^\circ\text{C}$. UV-Vis spectra were recorded between 700 and 200 nm, with a Varian UV-Vis-NIR Cary 50 instrument, using 1 cm path length quartz cells, and a scan rate of 600 nm/min. Fourier-transform infrared (FT-IR) spectra were collected in absorption mode with a FT-IR Jasco 4100 spectrophotometer using a KBr pellet. Elemental analysis were performed with a varioMICRO CHNS Elementar v 4.0.10 Analysensysteme GmbH, and the weightings were carried out with an Ultra Analytical Balance Sartorius Cubis MSA 6.6S-000-DM.

2. Photochemistry

Light-driven hydrogen evolution experiments were performed upon continuous visible light irradiation using a 460-nm LED of a reactor containing the solution. In a typical photochemical experiment, samples were prepared in 20 mL scintillation vials by mixing stock solutions of $[\text{Ru}(\text{bpy})_3]\text{Cl}_2 \cdot 6\text{H}_2\text{O}$ and the cages. Sodium ascorbate was added as a solid. The solution was then placed in the reactor and purged with argon for 20 minutes, continuously stirred. Experiments were run in duplicate and the results are reported as the average of two independent experiments. H_2 was detected and quantified using a GC. The photoreactor cell was sealed during the reaction, with the headspace comprising four ports closed with Swagelok[®] connections. Two ports were part of a closed loop involving GC gas inlet and sample vent to analyze the headspace content without significant gas consumption, while the other two were for the degassing procedure (input and output). The gas phase of the reaction vessel was analyzed using an Agilent Technologies 490 microGC equipped with a 5 $\text{\AA}$ molecular sieve column (10 m), a thermal conductivity detector, and argon as the carrier gas. The portion of gas not injected into the column was reintroduced into the headspace, ensuring minimal gas consumption throughout the catalytic experiment. Calibration of the system to quantify the exact amount of H_2 was performed using the external calibration method, conducting galvanostatic electrolysis (current of 1 mA) of a 1 M H_2SO_4 solution (assuming 100% faradaic efficiency).

3. Synthesis and characterization

3.1 Synthesis of Complex ZnZn

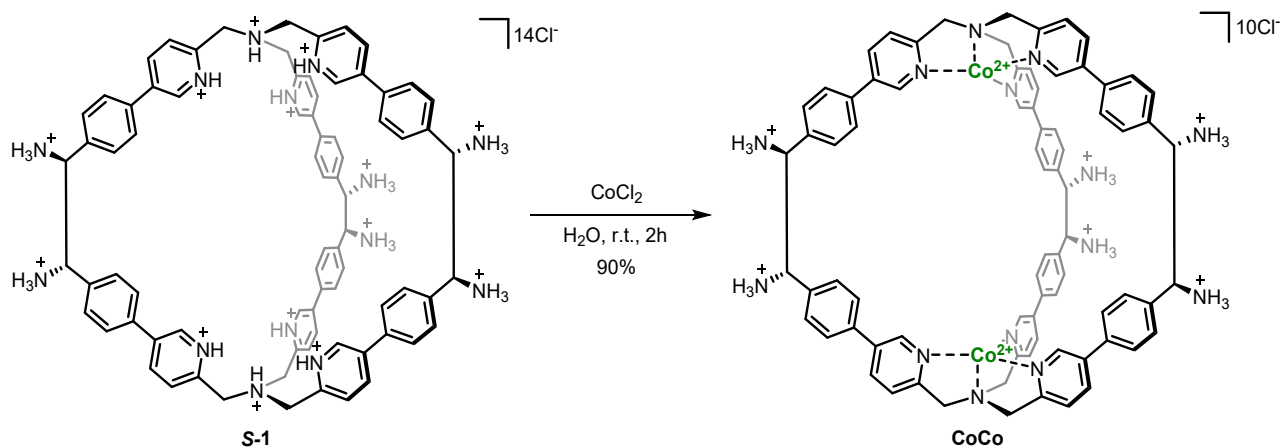


Complex **ZnZn** was synthesized according to a published procedure.^[S2]

HRMS (m/z): [M+2Cl]²⁺ calcd. for [C₇₈H₇₂Zn₂N₁₄+2Cl]²⁺, 702.1991; found 702.1958.

Elemental Analysis: [C₇₈H₇₈Cl₁₀Zn₂N₁₄]*5H₂O calcd. C: 55.21%; N: 11.56%; H: 4.63%; found C: 55.70%; N: 10.81%; H: 4.34%.

3.2 Synthesis of Complex CoCo

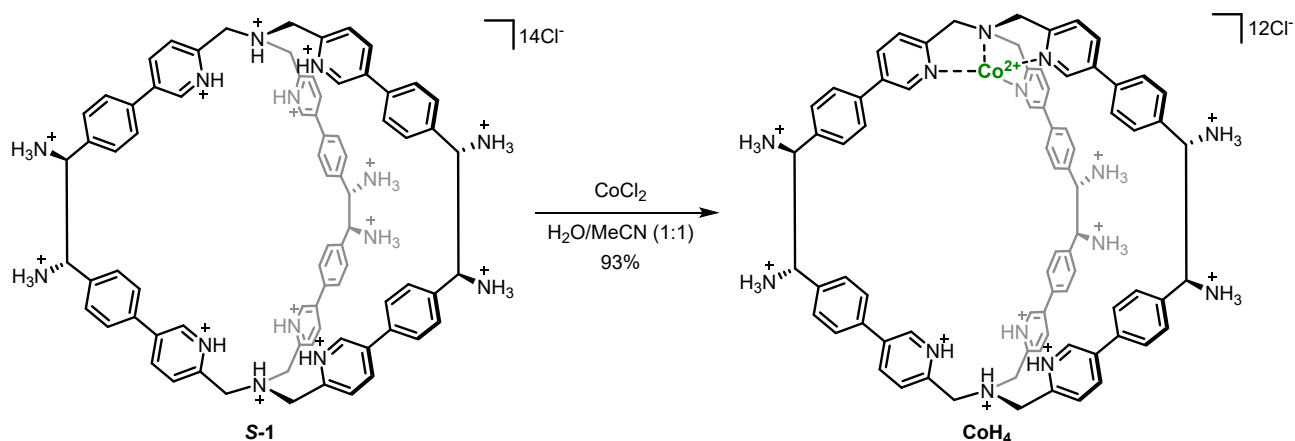


Complex **CoCo** was synthesized according to a published procedure.^[S3]

HRMS (m/z): [M+2Cl]²⁺ calcd. for [C₇₈H₇₂Co₂N₁₄+2Cl]²⁺, 696.2047; found 696.2047.

Elemental Analysis: [C₇₈H₇₈Cl₁₀Co₂N₁₄]*5H₂O calcd. C: 52.81%; N: 11.05%; H: 5.00%; found C: 52.98%; N: 11.15%; H: 4.93%.

3.3 Synthesis of Complex CoH₄

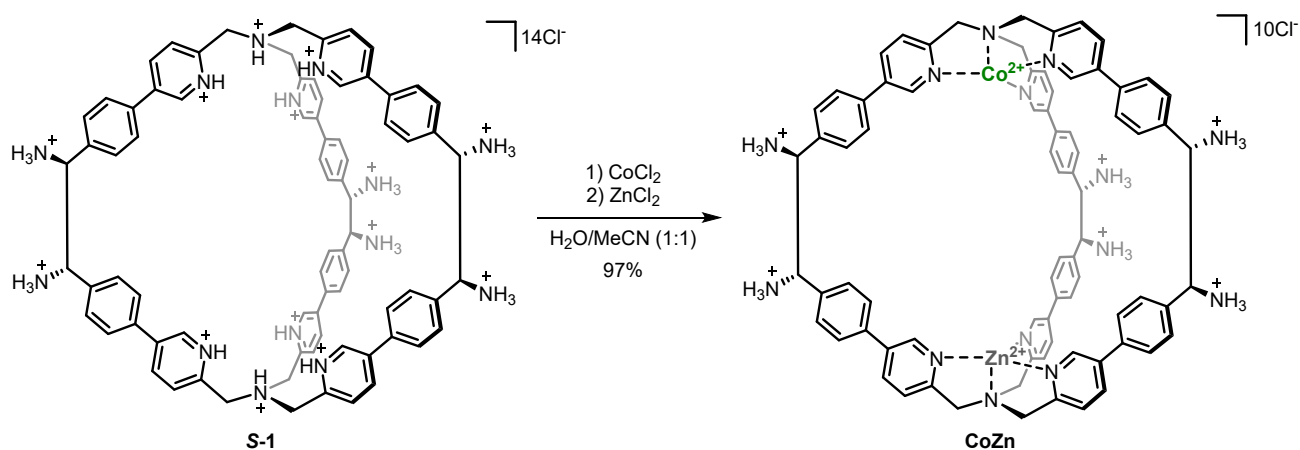


757 μL of a 77 mM solution of CoCl_2 in $\text{CD}_3\text{CN}/\text{D}_2\text{O}$ (1:1) (58.3 μmol , 1.0 equiv.) was added dropwise to a 3 mL $\text{CD}_3\text{CN}/\text{D}_2\text{O}$ (1:1) solution of ligand **S-1** (100 mg, 58.3 μmol). The green solution mixture was stirred at room temperature for 1 hour. ESI-MS monitoring result showed an ion peak at $m/z = 650$, confirming the formation of the monometallic **CoH₄** complex. Then acetone (15 mL) was added, obtaining a green solid. After centrifugation and removal of the solvent, the precipitate was washed with 15 mL of acetone and dried under vacuum at 100 $^\circ\text{C}$. Complex **CoH₄** resulted as a green solid (92 mg, 93 %).

HRMS (m/z): $[\text{M}+4\text{H}^++2\text{Cl}^-+2\text{HCO}_2^-]^{2+}$ calcd. for $[\text{C}_{78}\text{H}_{72}\text{CoN}_{14}+4\text{H}^++2\text{Cl}^-+2\text{HCO}_2^-]^{2+}$, 713.7514; found 714.2032.

Elemental Analysis: $[\text{C}_{78}\text{H}_{82}\text{Cl}_{12}\text{CoN}_{14}\cdot 5\text{H}_2\text{O}]$ calcd. C: 52.34%; N: 10.96%; H: 5.18%; found C: 52.65%; N: 10.32%; H: 4.71%.

3.4 Synthesis of Complex CoZn



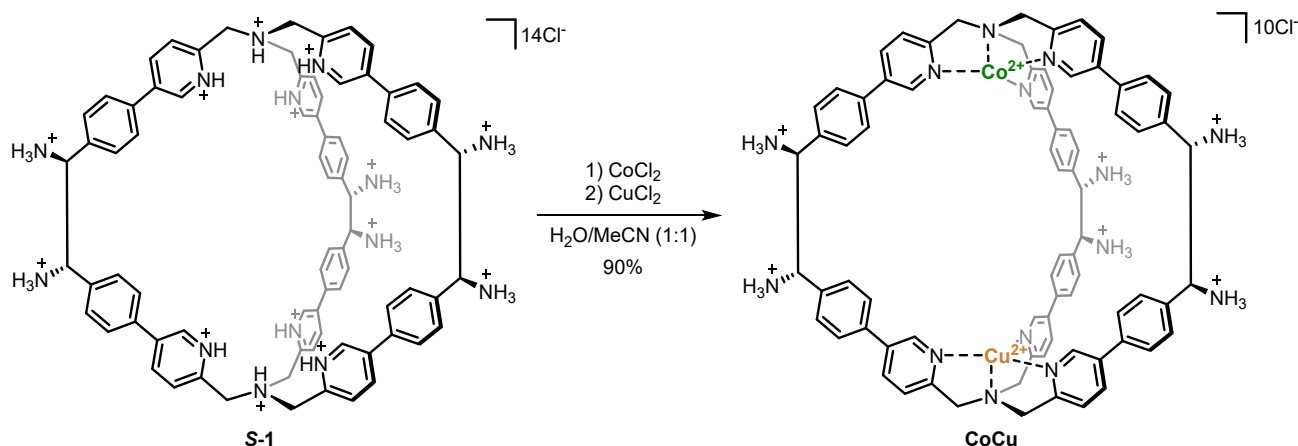
227 μL of a 77 mM solution of CoCl_2 in $\text{CD}_3\text{CN}/\text{D}_2\text{O}$ (1:1) (17.48 μmol , 1.0 equiv.) was added dropwise to a 3 mL $\text{CD}_3\text{CN}/\text{D}_2\text{O}$ (1:1) solution of ligand **S-1** (30 mg, 17.48 μmol). The green solution mixture was stirred at room temperature for 1 hour. ^1H NMR spectra and ESI-MS monitoring result shows an ion peak at $m/z = 650$, confirming the formation of the monometallic **CoH₄** complex. Subsequently, 238 μL of a 73.4 mM solution of ZnCl_2 (17.48

μmol , 1.0 equiv.) was added to the mixture, resulting in a light green solution. Further stirring for additional 2 h, the solution was precipitated under stirring with acetone to get a light green powder (28.8 mg, 97 %).

HRMS (m/z): $[\text{M}+2\text{Cl}]^{2+}$ calcd. for $[\text{C}_{78}\text{H}_{72}\text{CoN}_{14}\text{Zn}+2\text{Cl}]^{2+}$, 698.7027; found 698.6993.

Elemental Analysis: $[\text{C}_{78}\text{H}_{78}\text{Cl}_{10}\text{CoN}_{14}\text{Zn}]\cdot 5\text{H}_2\text{O}$ calcd. C: 52.62%; N: 11.01%; H: 4.98%; found C: 52.48%; N: 10.85%; H: 4.48%.

3.5 Synthesis of Complex CoCu



227 μL of a 77 mM solution of CoCl_2 in $\text{CD}_3\text{CN}/\text{D}_2\text{O}$ (1:1) (17.48 μmol , 1.0 equiv.) was slowly added to a 3 mL $\text{CD}_3\text{CN}/\text{D}_2\text{O}$ (1:1) solution of ligand **S-1** (30 mg, 17.48 μmol). The green solution mixture was stirred at room temperature for 1 hour. ^1H NMR spectra and ESI-MS monitoring result shows an ion peak at $m/z = 650$, confirming the formation of the monometallic **CoH₄** complex. Subsequently, 298 μL of a 58.66 mM solution of CuCl_2 (17.48 μmol , 1.0 equiv.) was added to the mixture, resulting in a light green solution. Further stirring for additional 2 h, the solution was precipitated under stirring with acetone to get a green powder (26.6 mg, 90 %).

HRMS (m/z): $[\text{M}+2\text{Cl}]^{2+}$ calcd. for $[\text{C}_{78}\text{H}_{72}\text{CoCuN}_{14}+2\text{Cl}]^{2+}$, 698.2029; found 698.2015.

Elemental Analysis: $[\text{C}_{78}\text{H}_{78}\text{Cl}_{10}\text{CoCuN}_{14}]\cdot 5\text{H}_2\text{O}$ calcd. C: 52.67%; N: 11.03%; H: 4.99%; found C: 51.99%; N: 10.64%; H: 4.61%.

4. Light-driven hydrogen production

The photocatalytic activity was assessed by analyzing several key performance indicators derived from the kinetics of hydrogen evolution.^[S3,S4] The results are collected in Table S1.

- 1) The total amount of H₂ produced ($n_{\max}$, mol) estimated at the plateau of the kinetics.
- 2) The maximum turnover number (TON) per cobalt center, associated with eq. S1 where n_{Co} are the moles of cobalt present according to the nature of the catalyst.

$$TON = \frac{n_{\max}}{n_{Co}} \quad (S1)$$

- 3) The initial rate of hydrogen production (r , mol·s⁻¹) calculated from the slope in the linear portion of the kinetic trace.
- 4) The turnover frequencies (TOF, s⁻¹) defined according to eq. S2.

$$TOF = \frac{r}{n_{Co}} = \frac{TON}{t} \quad (S2)$$

- 5) The quantum efficiency (QE) calculated according to eq. S3 where Φ is the quantum yield defined according to eq. S4 where φ is the absorbed photon flux (Einstein·s⁻¹). Since photochemical HER using ascorbate as the sacrificial electron donor is a two-photon process, a theoretical maximum value of 0.5 is expected for the quantum yield.

$$QE = \frac{\Phi}{0.5} \times 100 \quad (S3)$$

$$\Phi = \frac{r}{\varphi} \quad (S4)$$

The quantification of the absorbed photon flux (φ) was obtained employing the photoreaction between [Ru(bpy)₃]Cl₂·6H₂O and 9,10-diphenylanthracene (DPA) in aerated acetonitrile solution as an actinometer, following established protocols.^[S5] A 6 mL solution consisting of

0.5 mM [Ru(bpy)₃]Cl₂·6H₂O and 0.1 mM DPA in acetonitrile was prepared and its UV-Vis spectrum recorded. Subsequently, the solution was subjected to one minute of irradiation using the same light source and setup employed in the photochemical experiments. A new UV-Vis spectrum of the irradiated sample was then acquired. Both samples were diluted for the UV-Vis spectra measurements by combining 1 mL of the sample with 2 mL of acetonitrile. The moles of DPA consumed were computed following eq. S5 where A_i is the absorbance at 372 nm before the irradiation, A_f is the absorbance at 372 nm after the irradiation, V is the volume of the sample (considering dilution) and $\epsilon_{372\text{nm}} = 11,100 \text{ M}^{-1}\text{cm}^{-1}$ is the attenuation coefficient of DPA at 372 nm in acetonitrile. A cuvette with a 1 cm path length was employed.

$$nDPA_{consumed} = \frac{A_i - A_f}{\epsilon_{372\text{ nm}}} \times V \quad (\text{S5})$$

The absorbed photon flux (ϕ) was calculated using eq. S6 where $\Phi_{\text{ref}} = 0.019$ is the quantum yield of the actinometer and $t = 60 \text{ s}$ is the irradiation time.

$$\phi = \frac{nDPA_{consumed}}{\Phi_{\text{ref}} t} \quad (\text{S6})$$

Table S1. Photochemical hydrogen evolution experiments.^[a]

Entry	Compound	[Co] / μM	TON	TOF / h^{-1}	QE / %
1	CoCo	100	63	50	3.7
2	CoH₄	100	95	83	6.0
3	CoZn	100	68	36	2.6
4	CoCu	100	51	23	1.7
5	CoCo	50	76	50	1.8
6	CoH₄	50	131	82	3.0
7	CoZn	50	86	52	1.9
8	CoCu	50	67	38	1.4

^[a] Upon continuous irradiation (460-nm LED) of 1 M acetate buffer solution (pH 5) containing 0.5 mM $[\text{Ru}(\text{bpy})_3]\text{Cl}_2 \cdot 6\text{H}_2\text{O}$ and 0.1 M sodium ascorbate.

Table S2. Control experiments.^[a]

Entry	Compound (concentration)	n (H ₂) / μmol ^[b]
1	-	0.7
2	S-1 (100 μM)	1.9
3	ZnZn (100 μM)	0.6

^[a] Continuous irradiation (460-nm LED) of 1 M acetate buffer solution (pH 5) containing 0.5 mM $[\text{Ru}(\text{bpy})_3]\text{Cl}_2 \cdot 6\text{H}_2\text{O}$ and 0.1 M sodium ascorbate; ^[b] obtained after 3 h of irradiation.

5. NMR and ESI Characterization

5.1 Compound ZnZn

Raulin- Eluents: H₂O/ACN (50:50) + 0.1 %FA
2025-02-19-ZONTA-ZnZn 67 (1.269) Cm (67.78-19.27)

1: TOF MS ES+
2.12e5

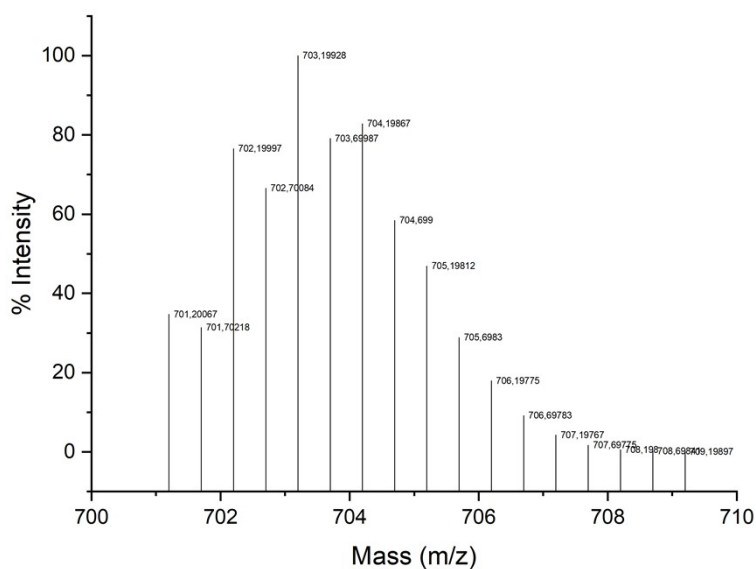
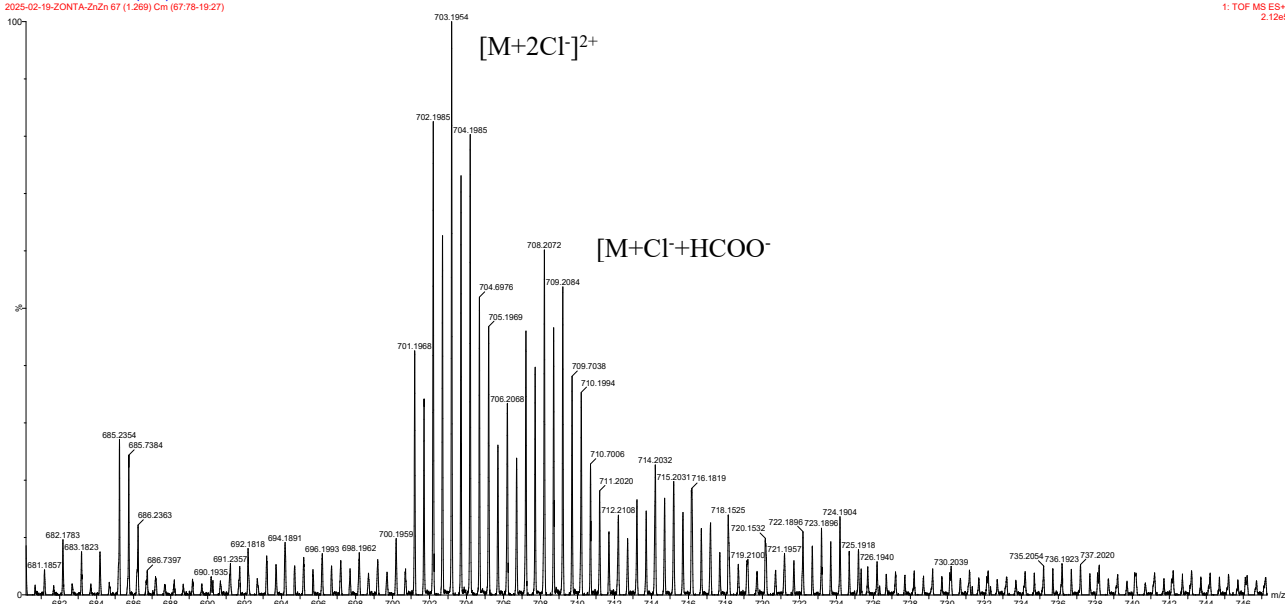


Figure S1. Experimental and calculated HRMS pattern of **ZnZn** for $[C_{78}H_{72}N_{14}Zn_2+2Cl]^{2+}$ adduct in CH₃CN/H₂O (50:50)/0.1% HCOOH.

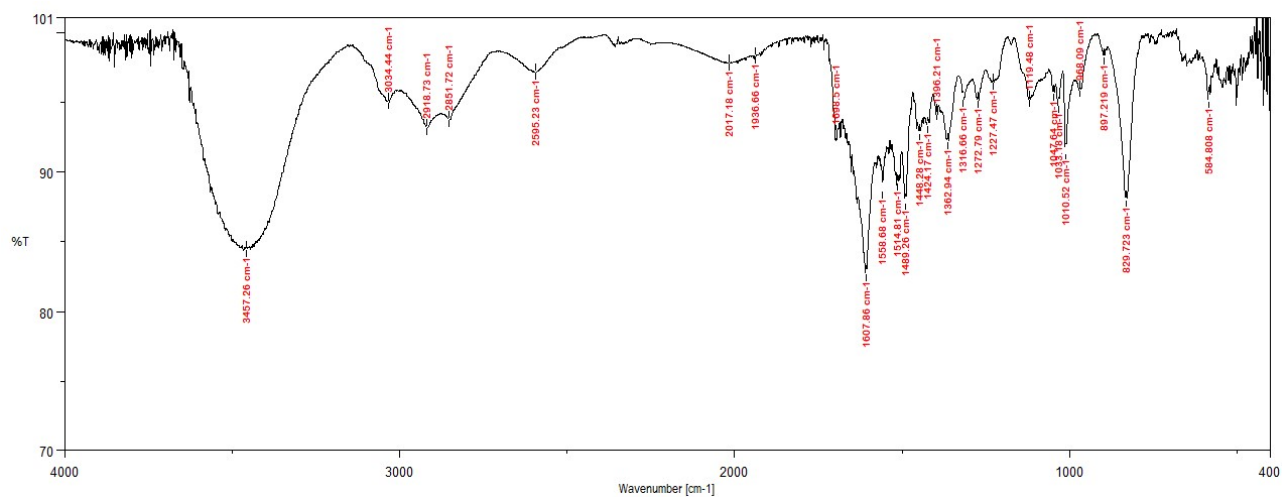


Figure S2. FT-IR spectrum of compound **ZnZn** (KBr pellets).

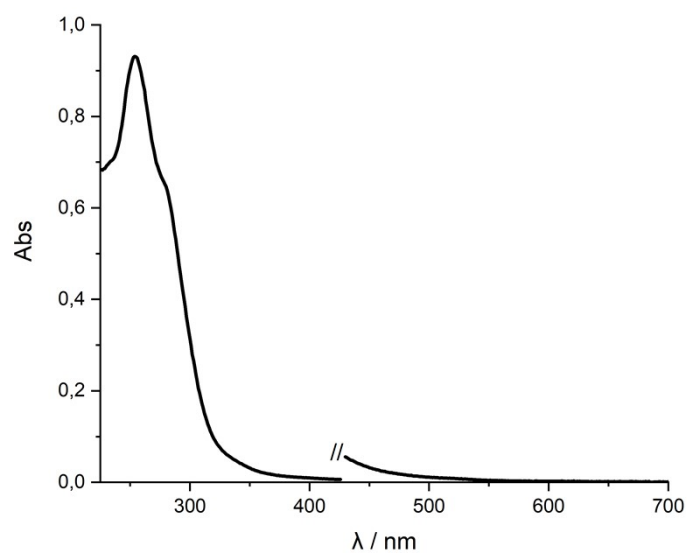


Figure S3. Absorption spectrum of **ZnZn** in H₂O (Recorded at 1 mM for the bands in the visible, and at 0.01 mM for the bands in the UV).

5.2 Compound CoCo

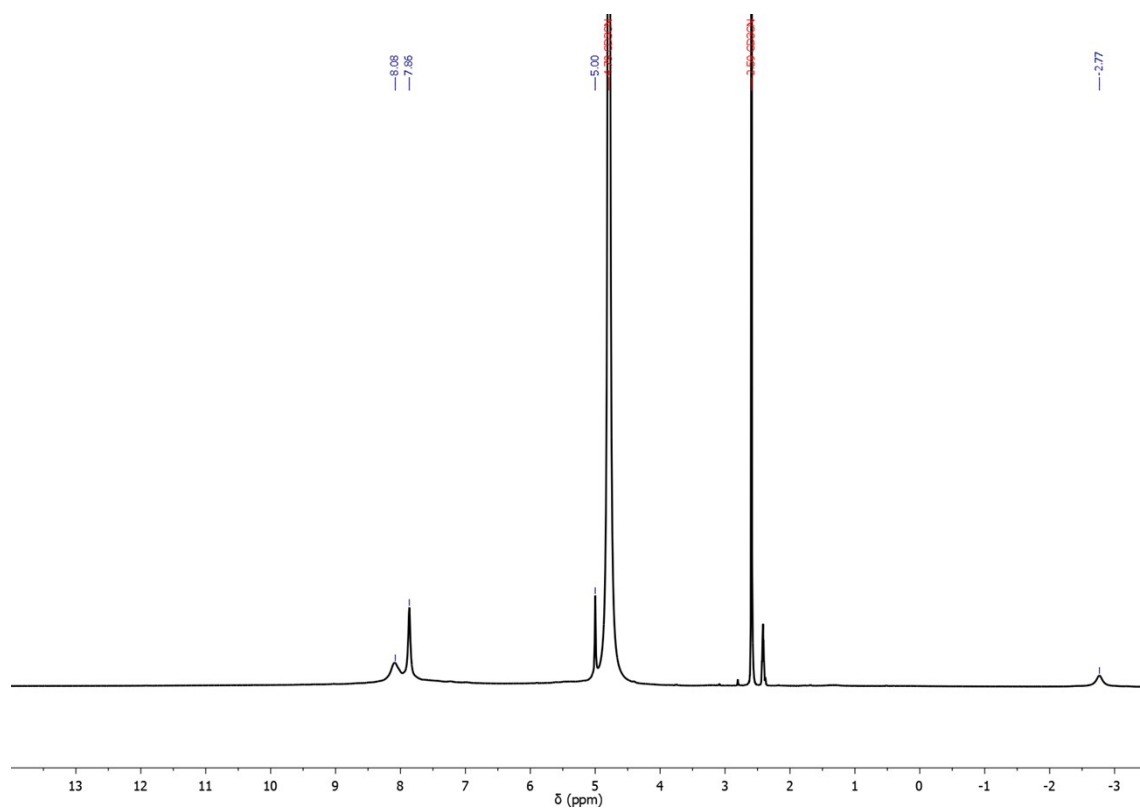


Figure S4. ^1H -NMR spectrum (300 MHz, 301 K, $\text{D}_2\text{O}/\text{CD}_3\text{CN}$) of compound **CoCo**.

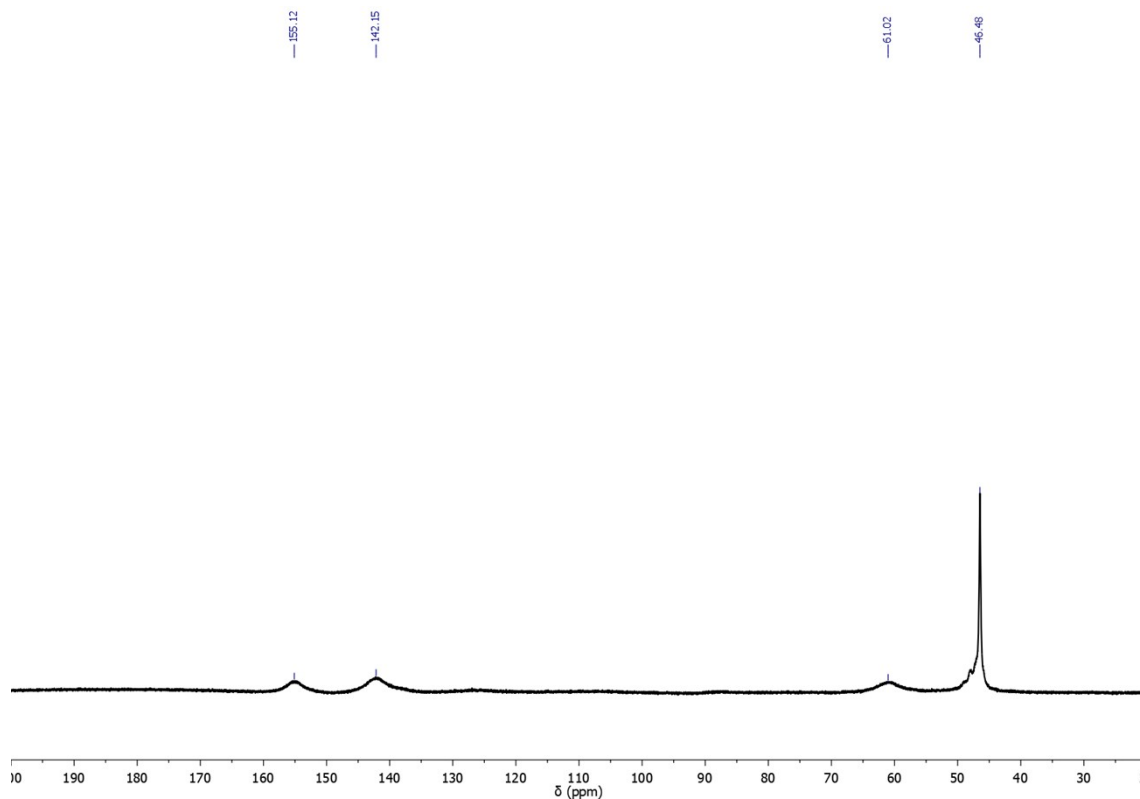


Figure S5. ^1H -NMR spectrum (300 MHz, 301 K, $\text{D}_2\text{O}/\text{CD}_3\text{CN}$) highlight of the paramagnetic region of compound **CoCo**.

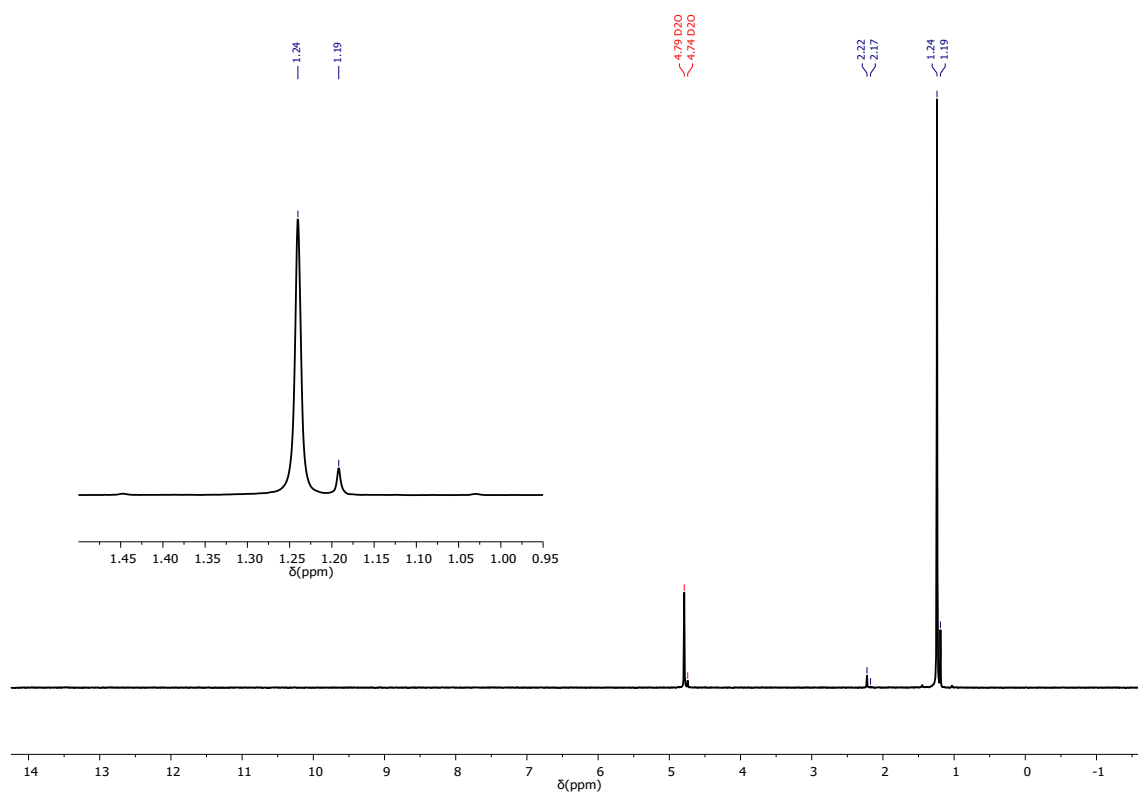
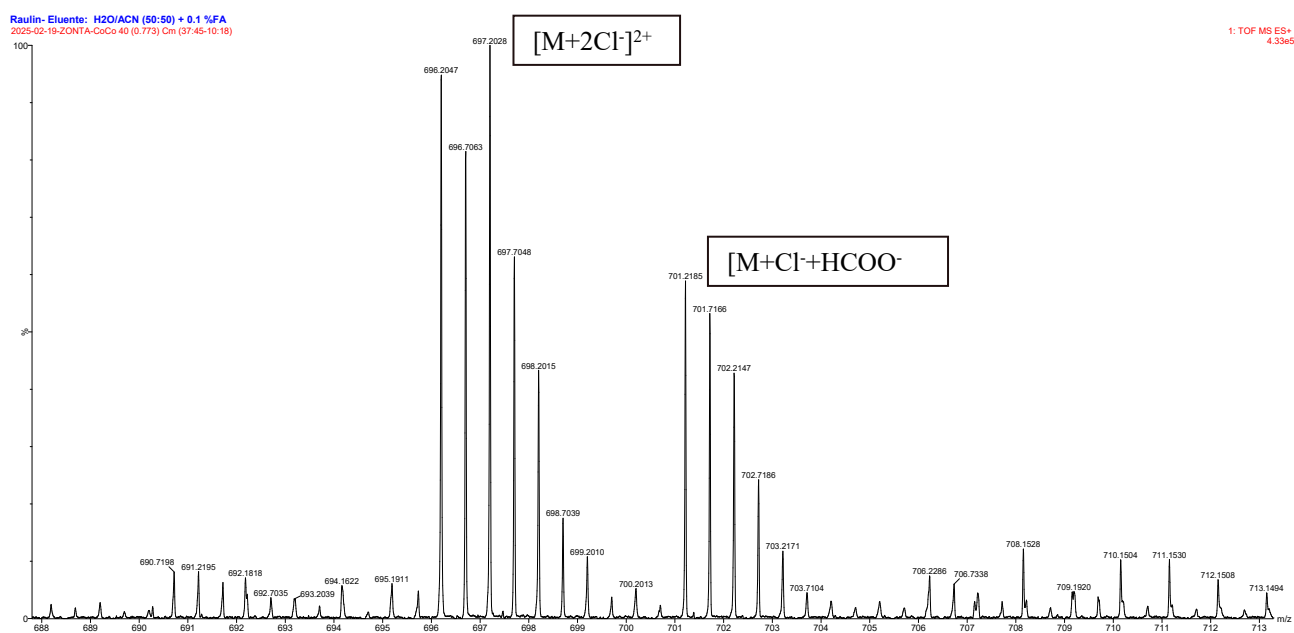


Figure S6. ^1H -NMR spectrum (300 MHz, 301 K, $\text{D}_2\text{O}/\text{CD}_3\text{CN}$) Evans method applied to complex **CoCo**.



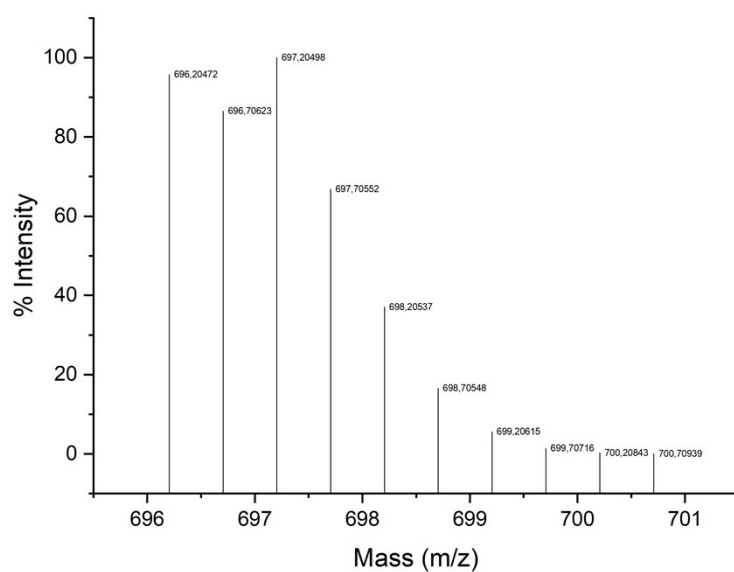


Figure S7. Experimental and calculated HRMS pattern of **CoCo** for $[C_{78}H_{72}Co_2N_{14}+2Cl^-]^{2+}$ adduct in CH_3CN/H_2O (50:50)/0.1% $HCOOH$.

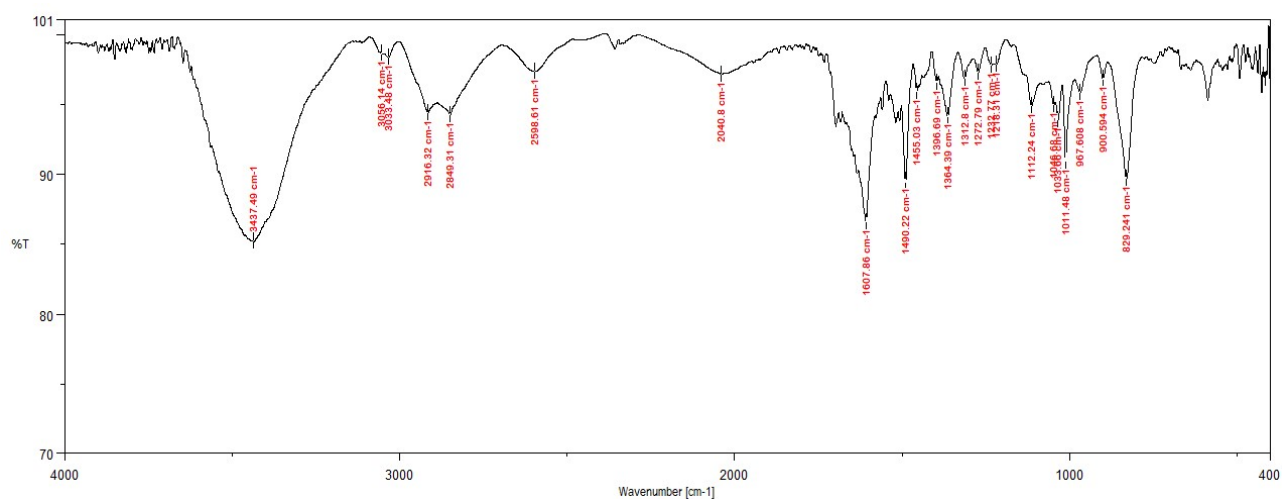


Figure S8. FT-IR spectrum of compound **CoCo** (KBr pellets).

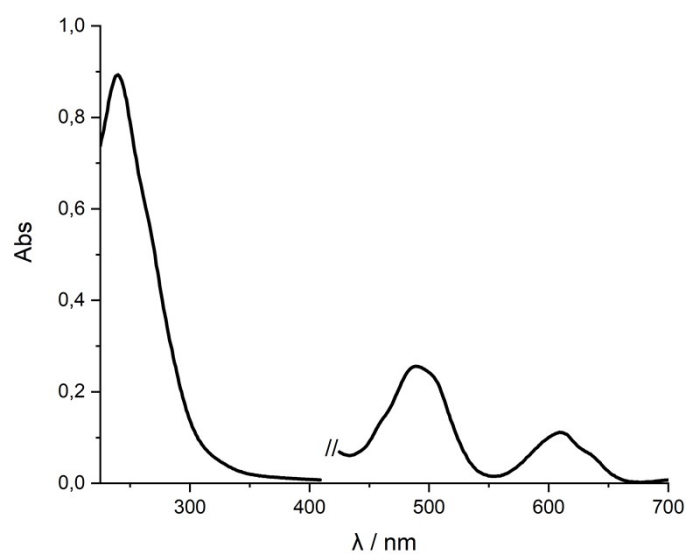


Figure S9. Absorption spectrum of **CoCo** in H_2O (Recorded at 1 mM for the bands in the visible, and at 0.01 mM for the bands in the UV).

5.3 Compound **CoH₄**

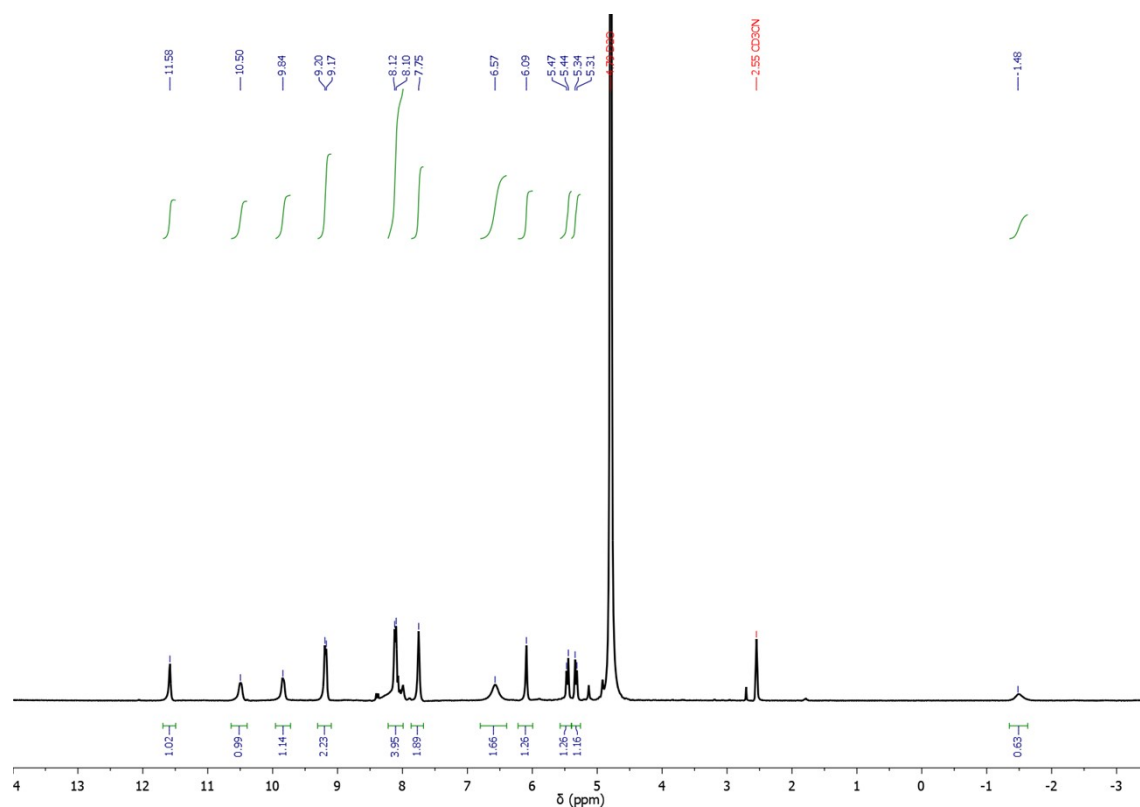


Figure S10. ^1H -NMR spectrum (300 MHz, 301 K, $\text{D}_2\text{O}/\text{CD}_3\text{CN}$) of compound **CoH₄**.

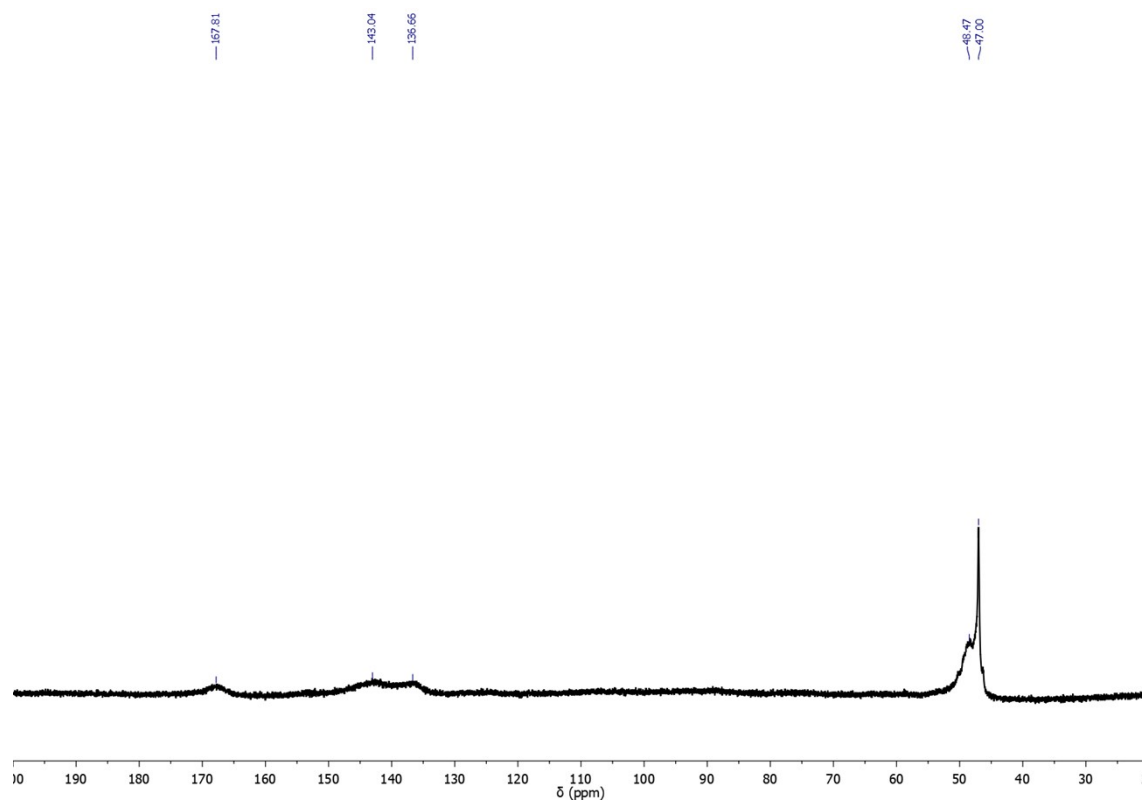


Figure S11. ^1H -NMR spectrum (300 MHz, 301 K, $\text{D}_2\text{O}/\text{CD}_3\text{CN}$) highlight of the paramagnetic region of compound **CoH_4** .

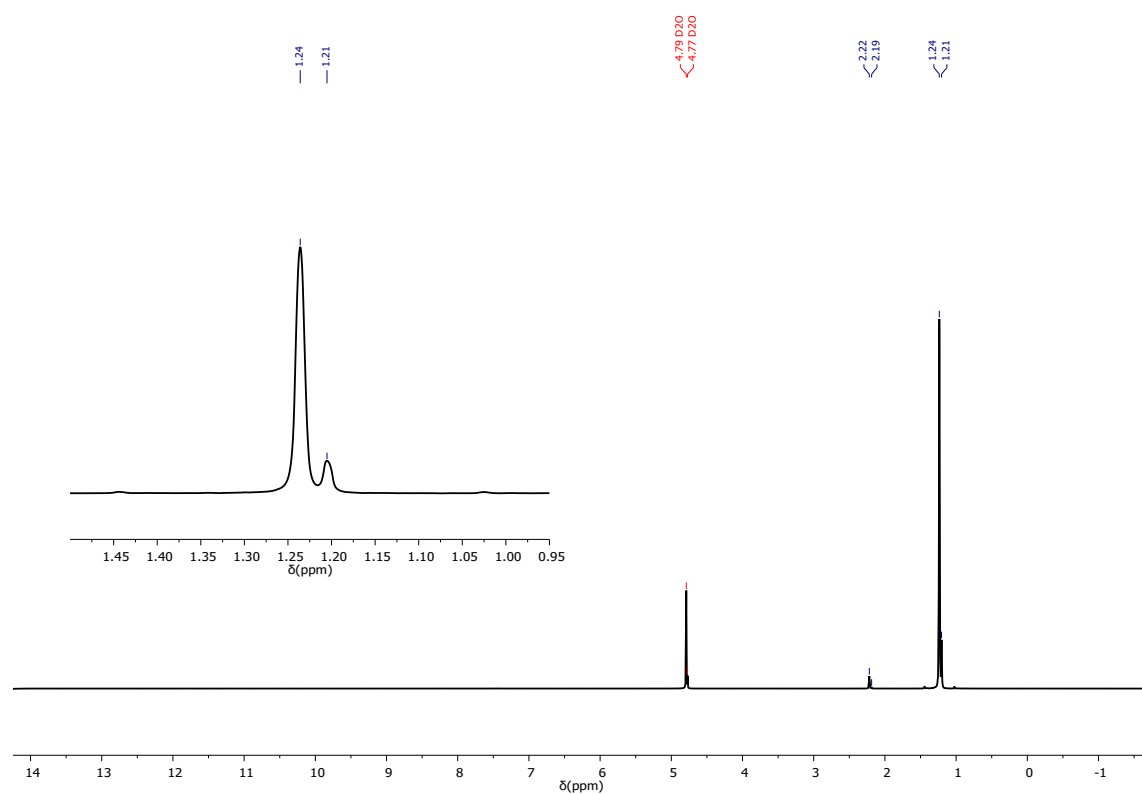


Figure S12. ^1H -NMR spectrum (300 MHz, 301 K, $\text{D}_2\text{O}/\text{CD}_3\text{CN}$) Evans method applied to complex **CoH_4** .

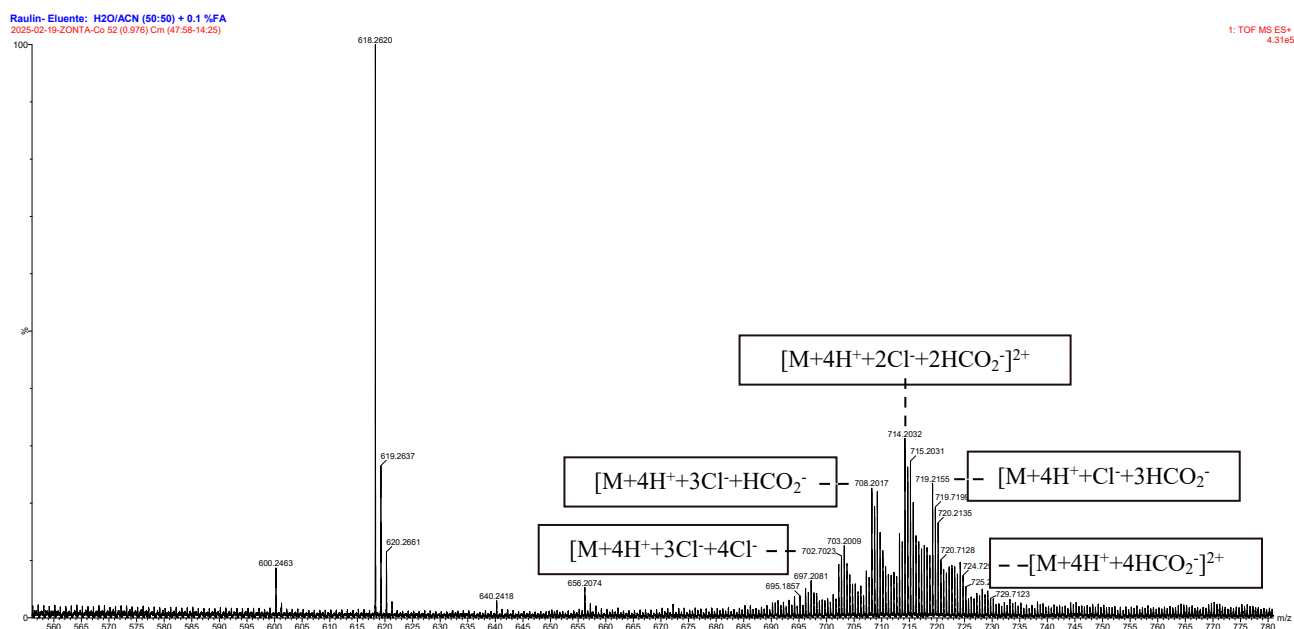
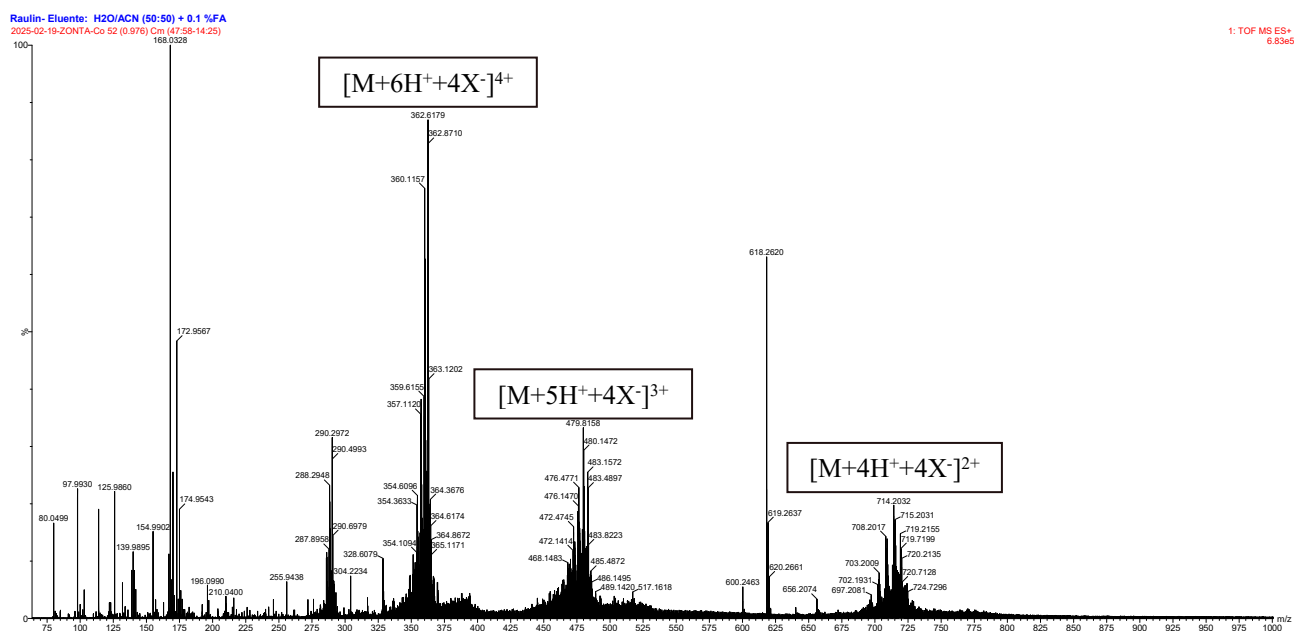


Figure S13. Experimental HRMS pattern of **CoH₄** for $[C_{78}H_{72}CoN_{14}+4H^++4X^-]^{2+}$ adduct in CH₃CN/H₂O (50:50)/0.1% HCOOH.

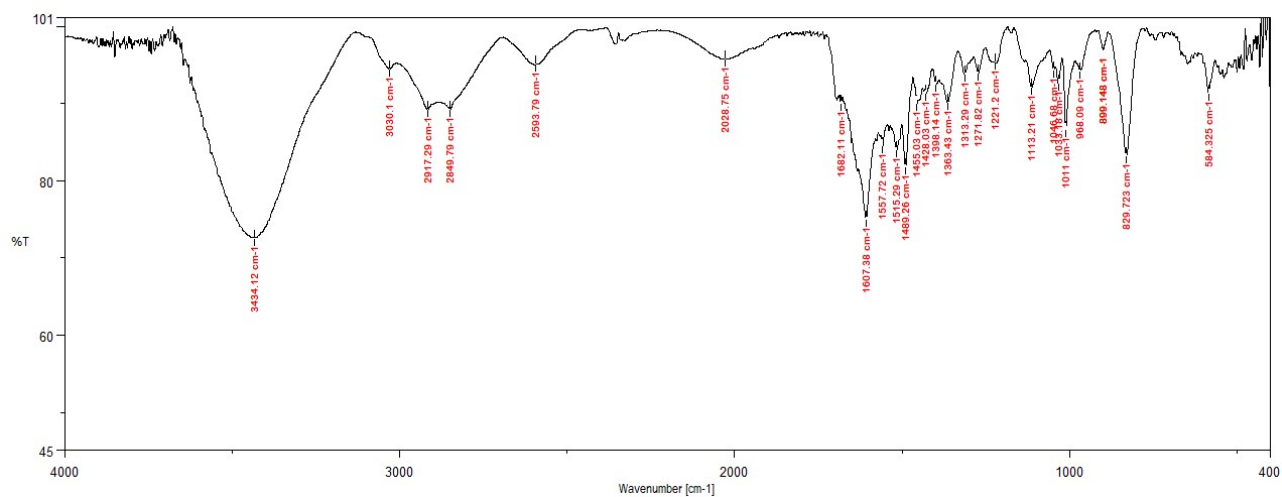


Figure S14. FT-IR spectrum of compound CoH_4 (KBr pellets).

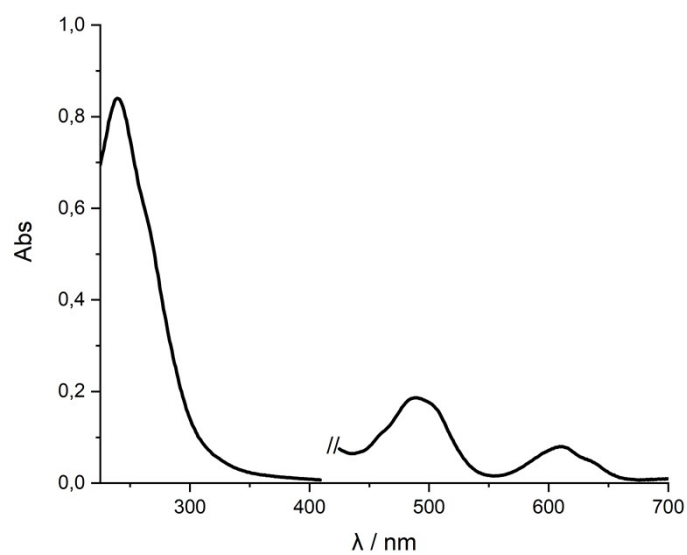


Figure S15. Absorption spectrum of CoH_4 in H_2O (Recorded at 1 mM for the bands in the visible, and at 0.01 mM for the bands in the UV).

5.4 Compound CoZn

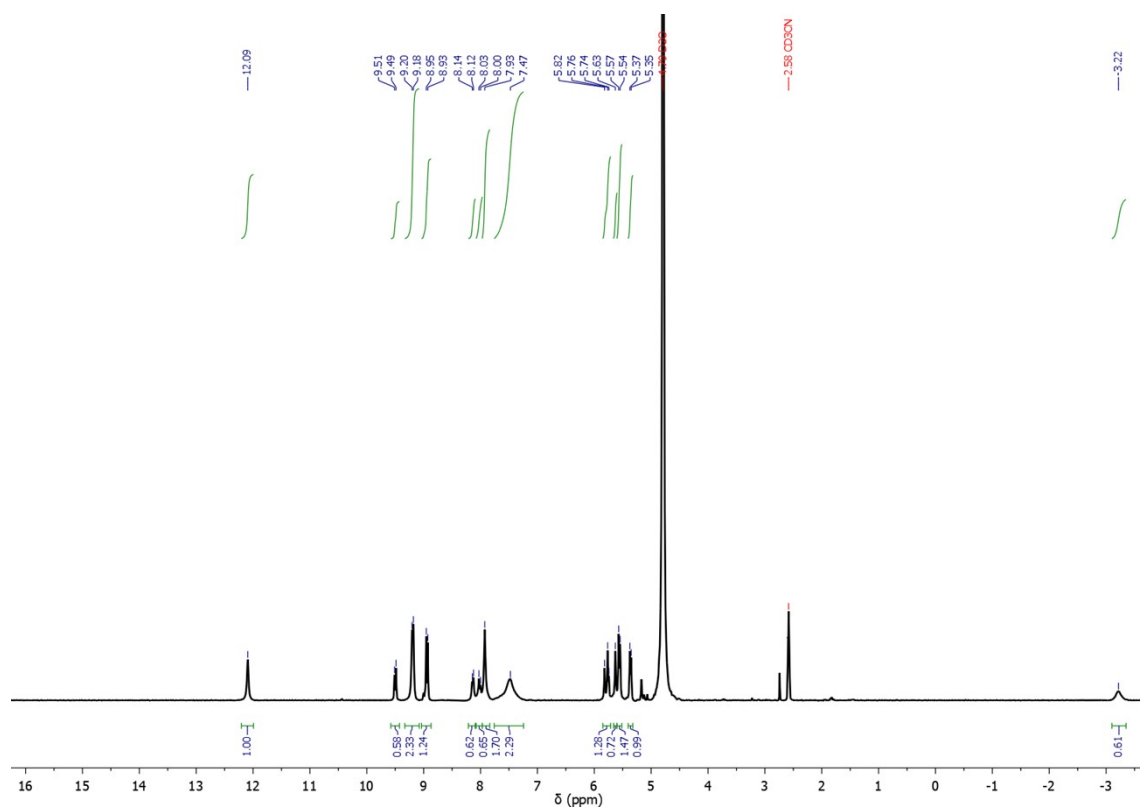


Figure S16. ^1H -NMR spectrum (300 MHz, 301 K, $\text{D}_2\text{O}/\text{CD}_3\text{CN}$) of compound **CoZn**.

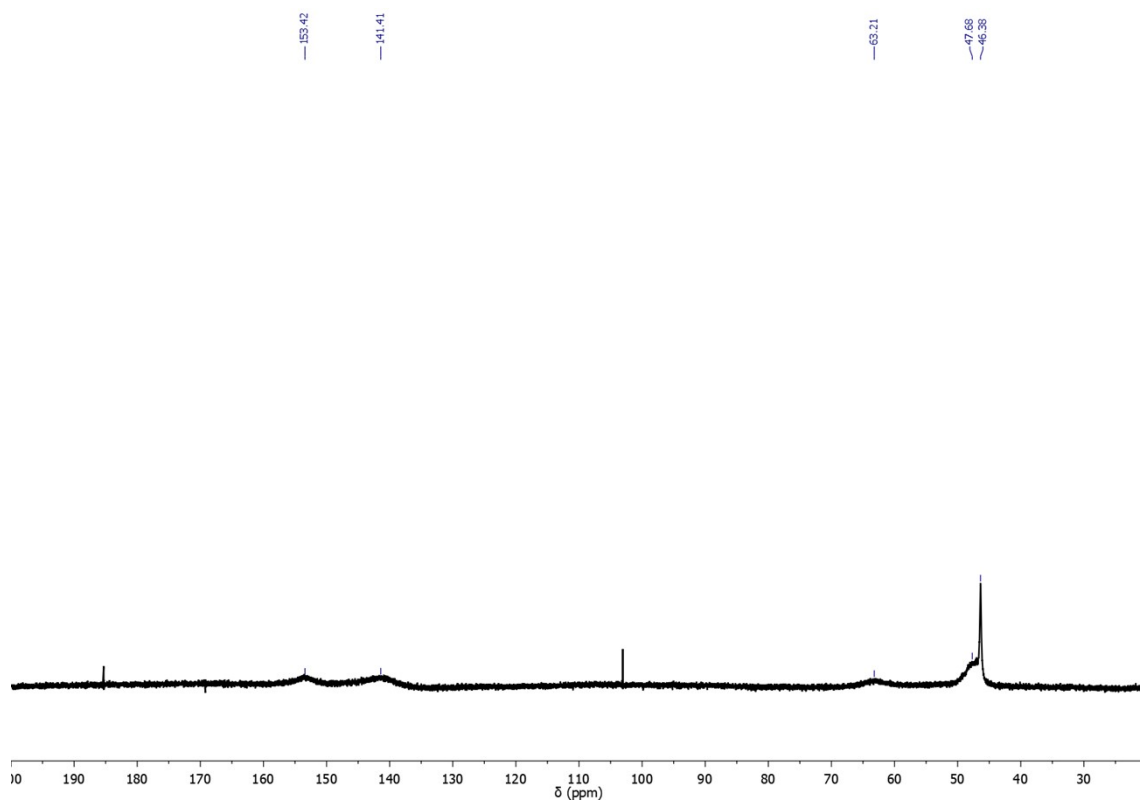


Figure S17. ^1H -NMR spectrum (300 MHz, 301 K, $\text{D}_2\text{O}/\text{CD}_3\text{CN}$) highlight of the paramagnetic region of compound **CoZn**.

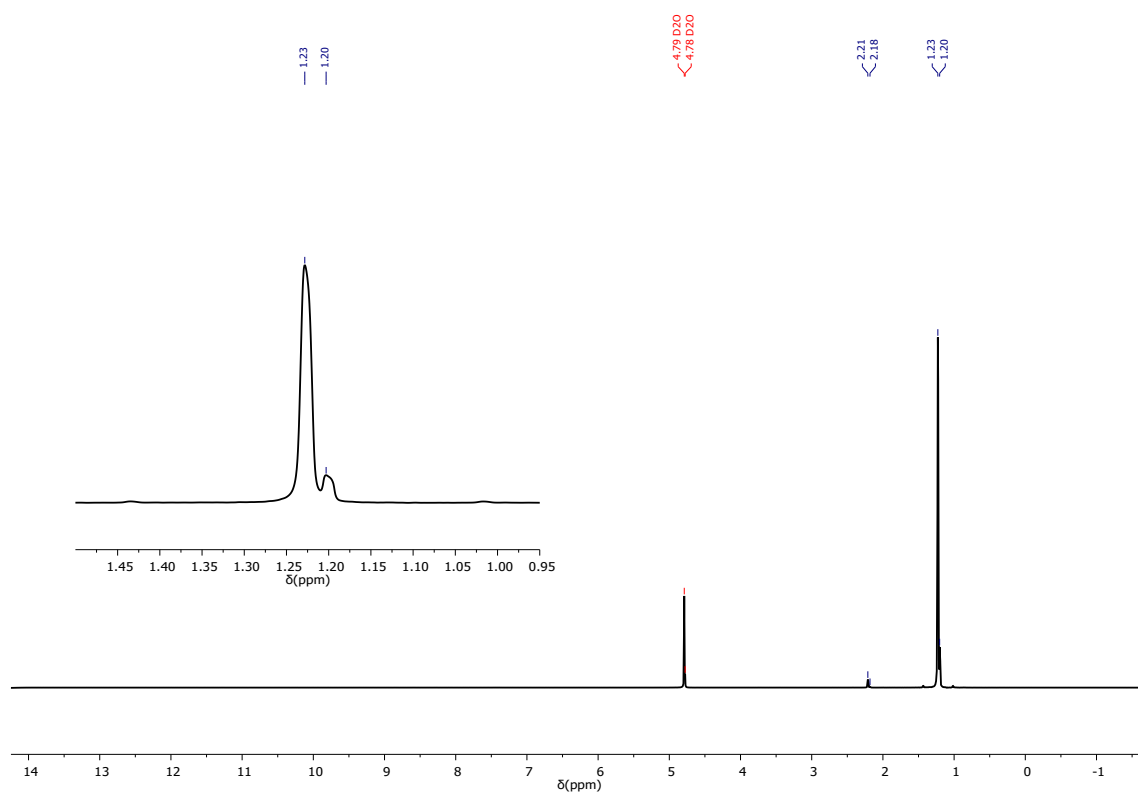
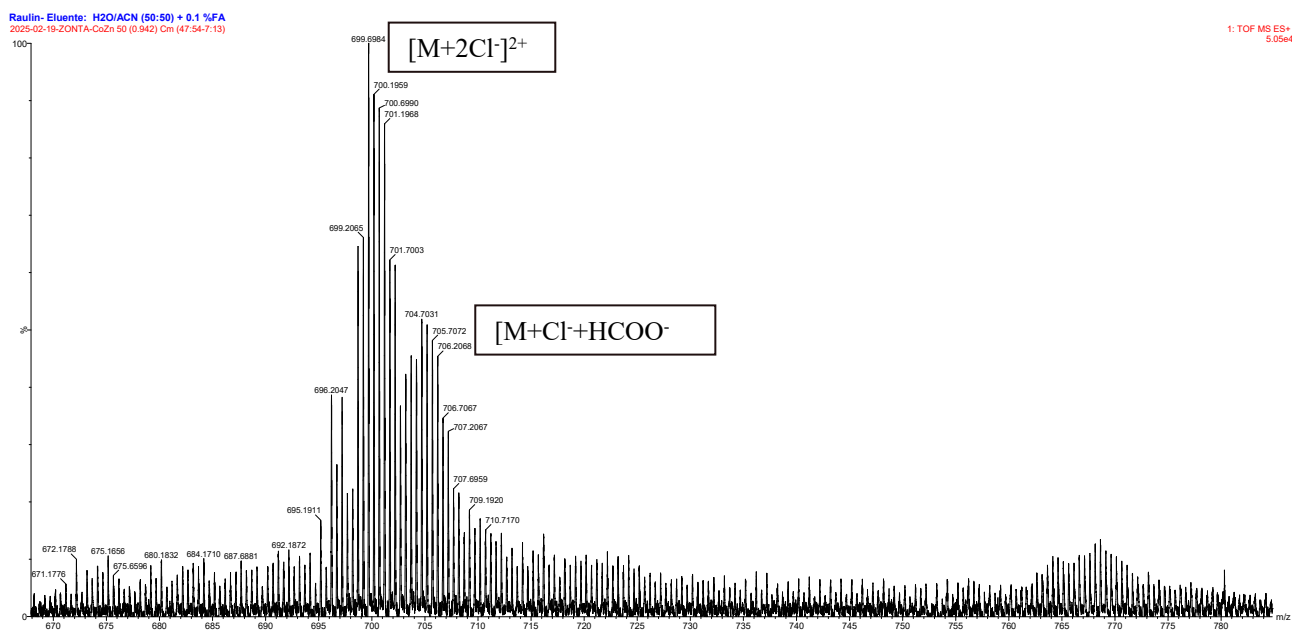


Figure S18. ^1H -NMR spectrum (300 MHz, 301 K, $\text{D}_2\text{O}/\text{CD}_3\text{CN}$) Evans method applied to complex **CoZn**.



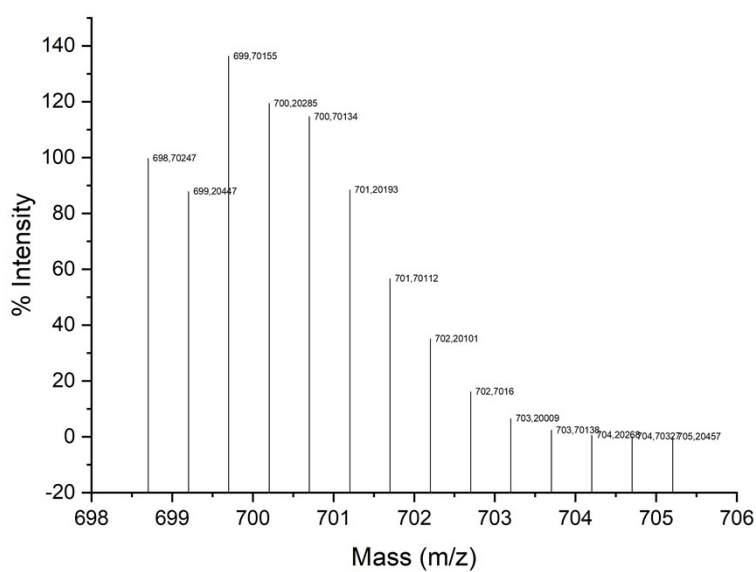


Figure S19. a) Experimental and b) calculated HRMS pattern of **CoZn** for $[C_{78}H_{72}CoN_{14}Zn+2Cl]^{2+}$ adduct in CH_3CN/H_2O (50:50)/0.1% $HCOOH$.

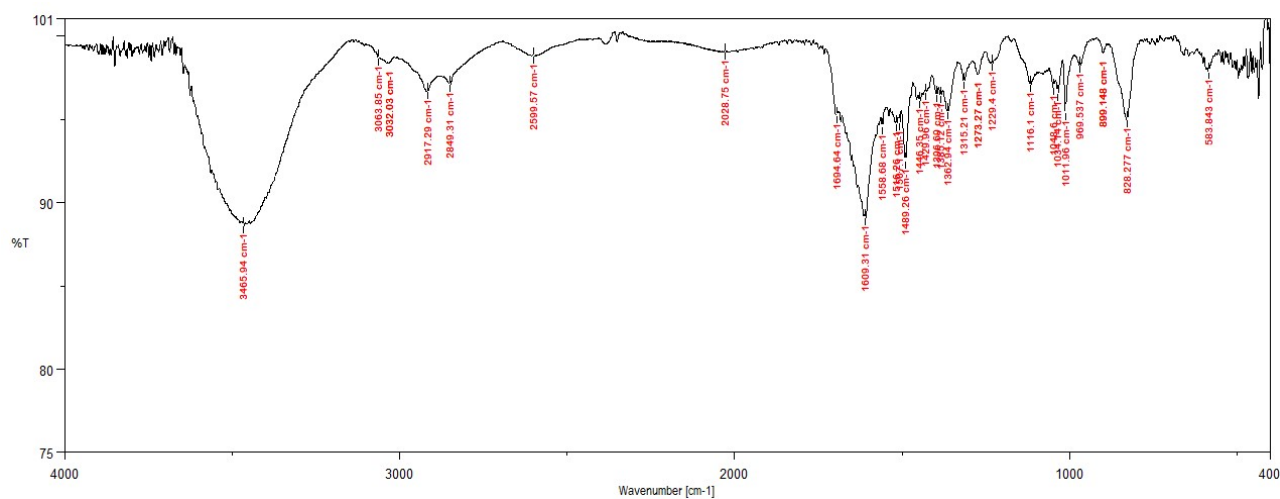


Figure S20. FT-IR spectrum of compound **CoZn** (KBr pellets).

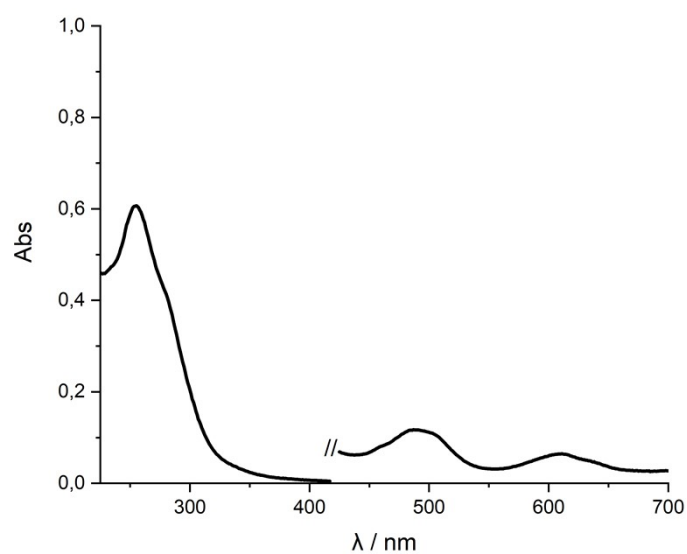


Figure S21. Absorption spectrum of **CoZn** in H₂O (Recorded at 1 mM for the bands in the visible, and at 0.01 mM for the bands in the UV).

5.5 Compound CoCu

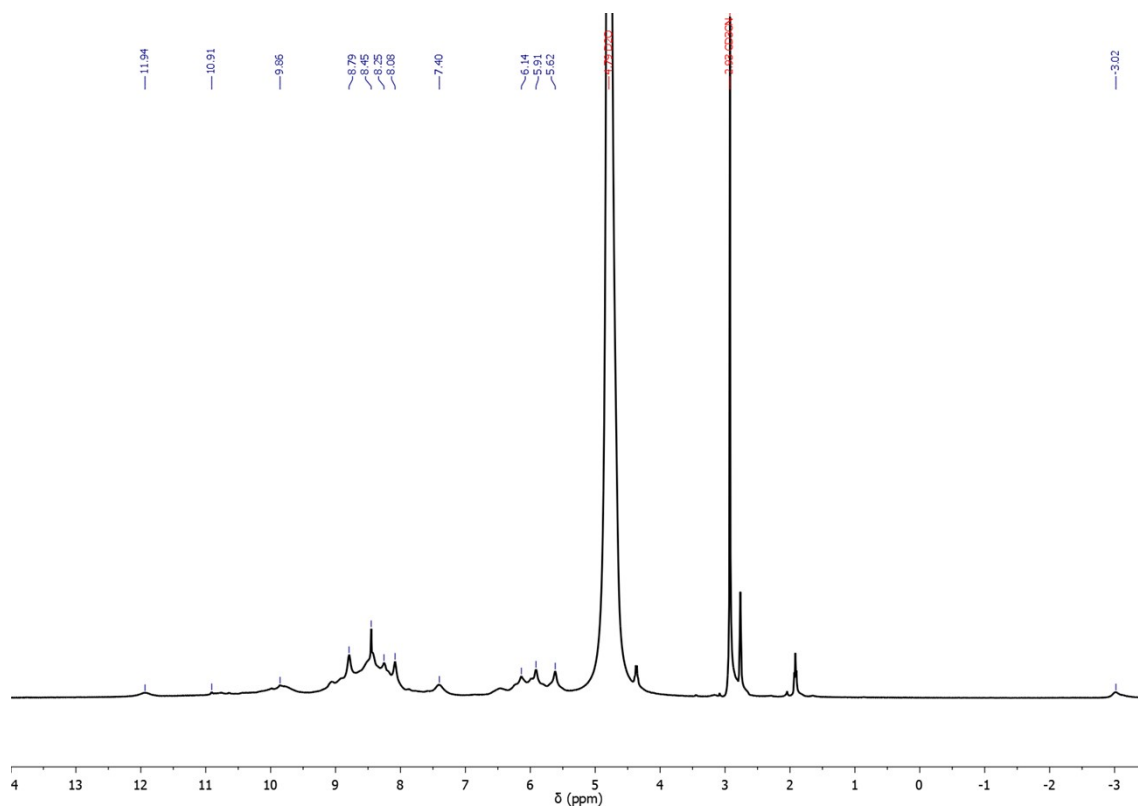


Figure S22. ¹H-NMR spectrum (300 MHz, 301 K, D₂O/CD₃CN) of compound **CoCu**.

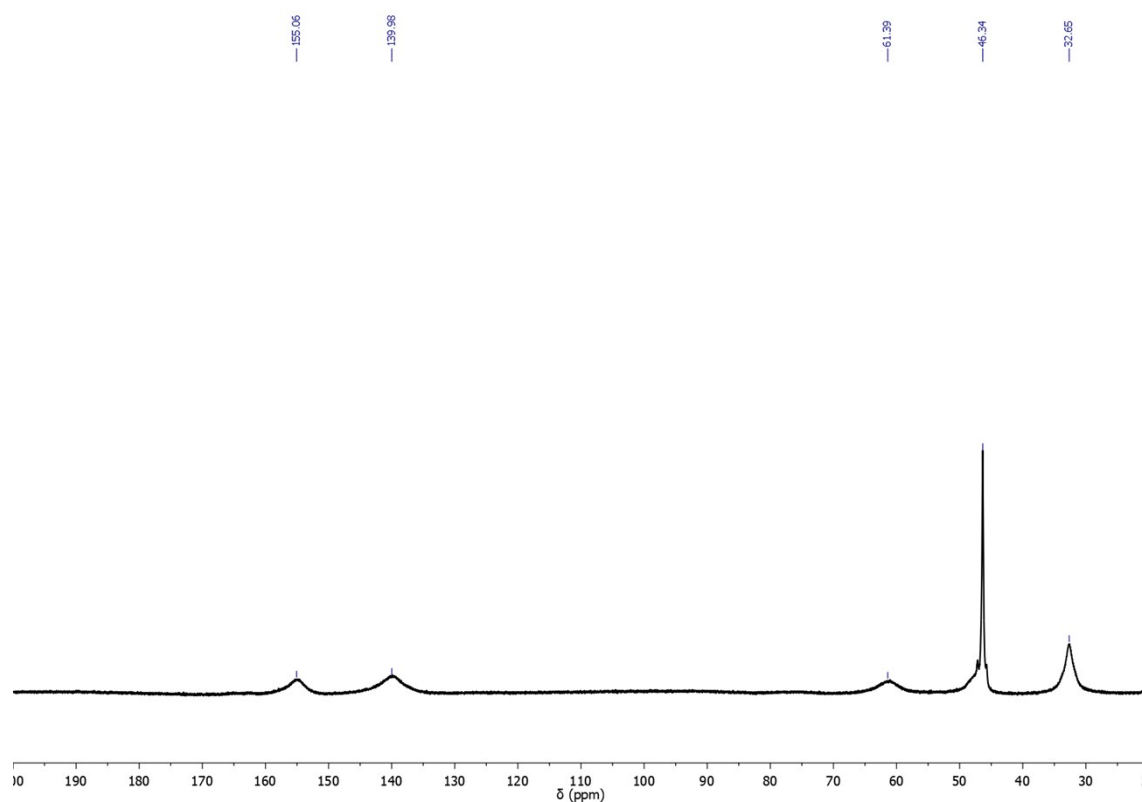


Figure S23. ^1H -NMR spectrum (300 MHz, 301 K, $\text{D}_2\text{O}/\text{CD}_3\text{CN}$) highlight of the paramagnetic region of compound **CoCu**.

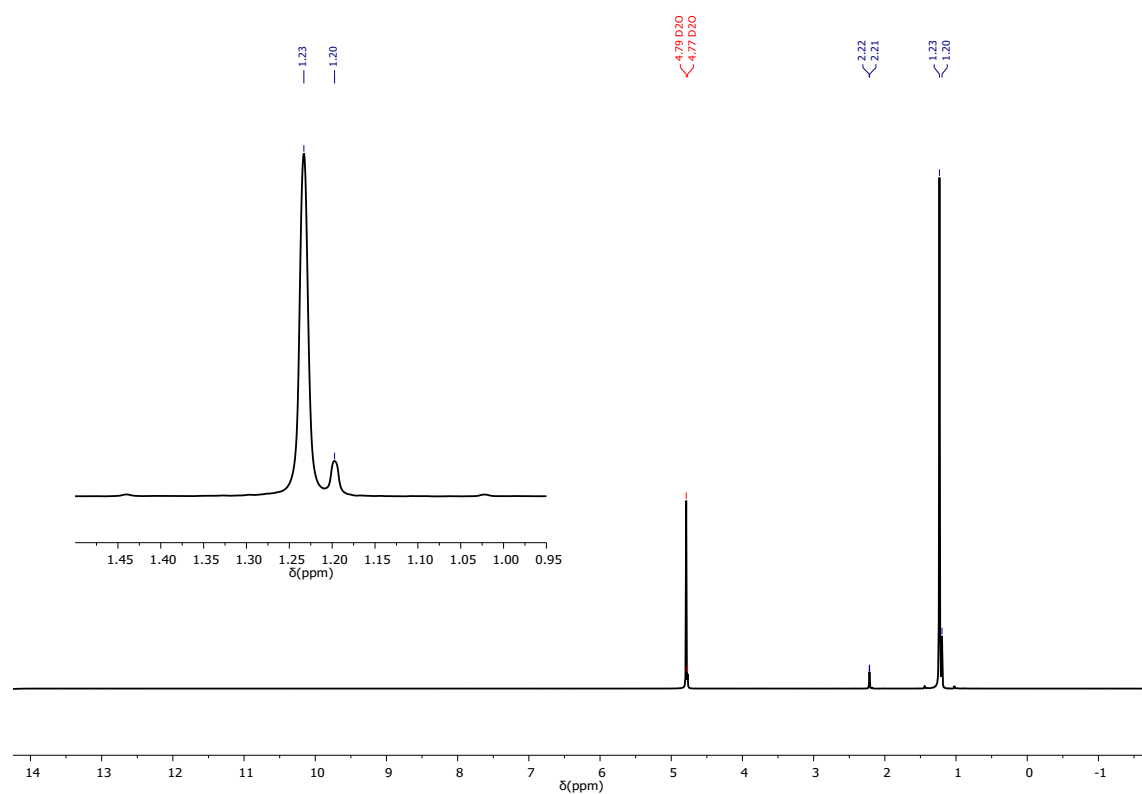


Figure S24. ^1H -NMR spectrum (300 MHz, 301 K, $\text{D}_2\text{O}/\text{CD}_3\text{CN}$) Evans method applied to complex **CoCu**.

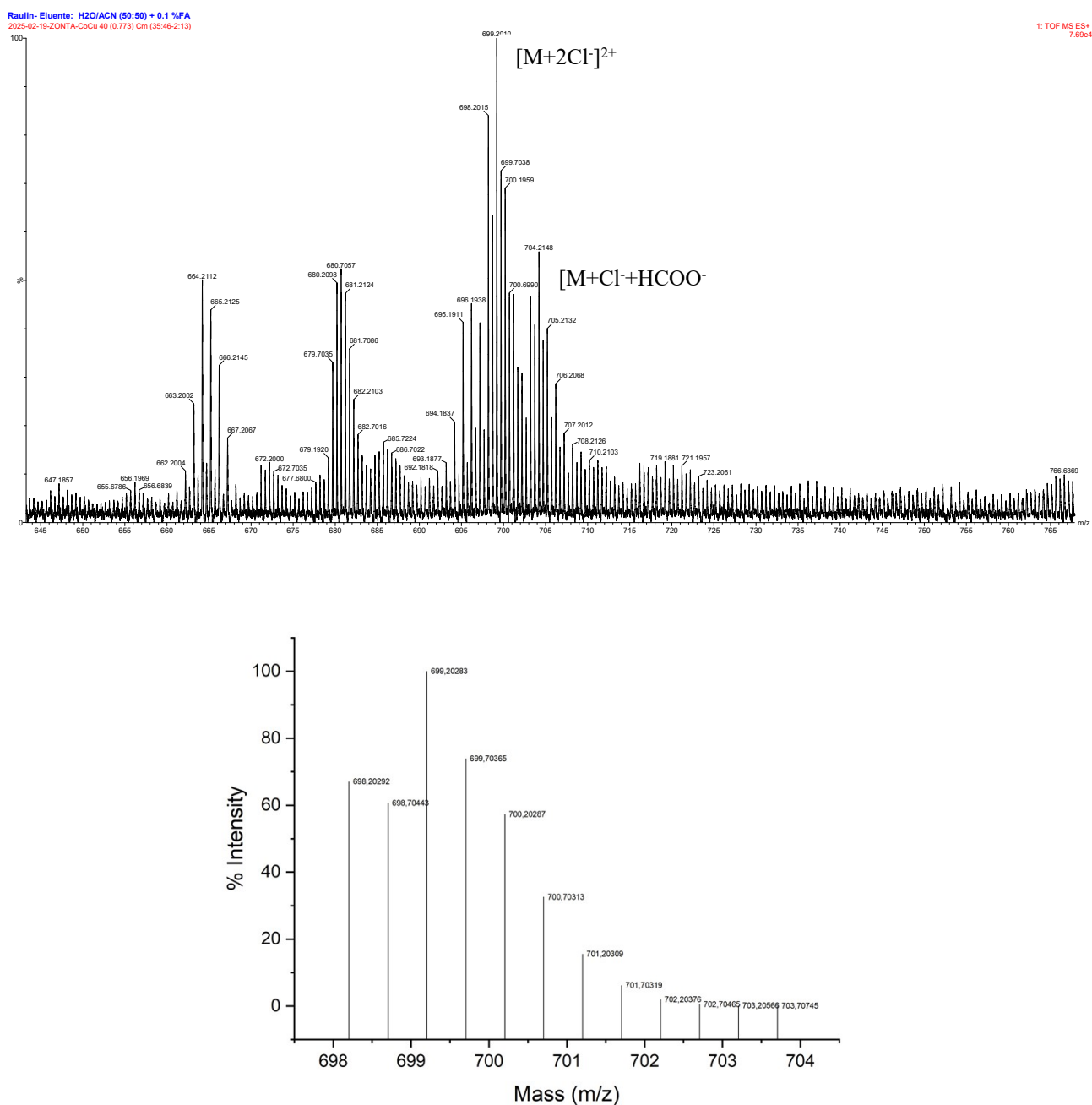


Figure S25. a) Experimental and b) calculated HRMS pattern of **CoCu** for $[C_{78}H_{72}CoCuN_{14}+2Cl]^{2+}$ adduct in CH_3CN/H_2O (50:50)/0.1% $HCOOH$.

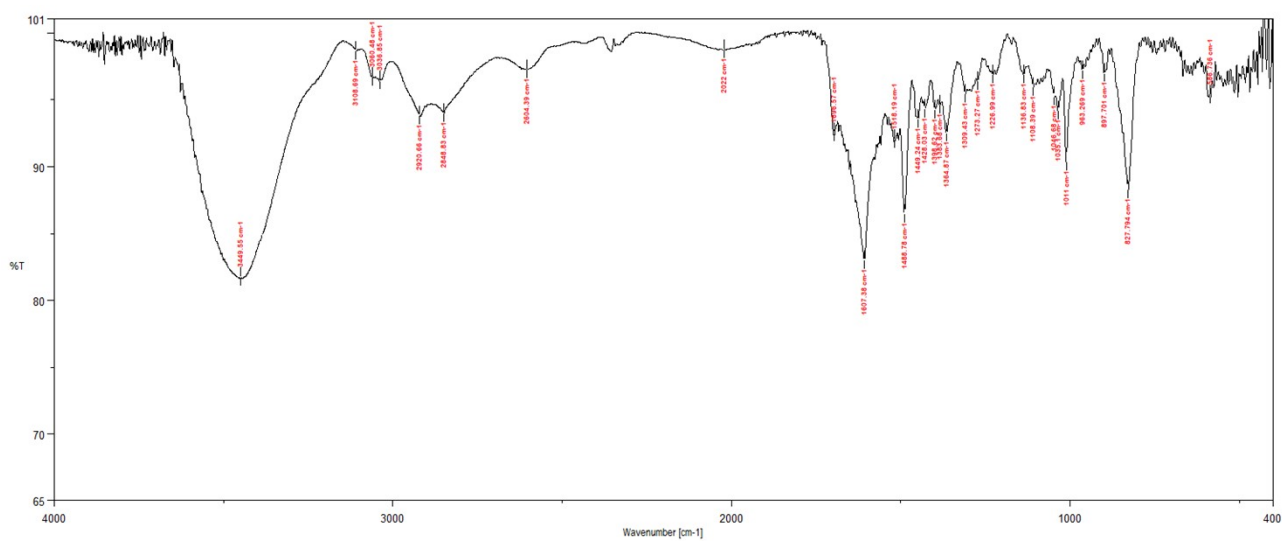


Figure S26. FT-IR spectrum of compound **CoCu** (KBr pellets).

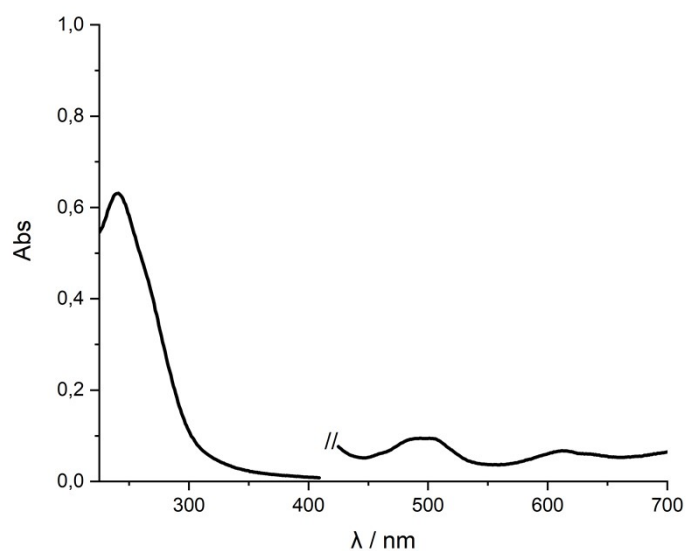


Figure S27. Absorption spectrum of **CoCu** in H_2O (Recorded at 1 mM for the bands in the visible, and at 0.01 mM for the bands in the UV).

5.6 Additional NMR Experiments

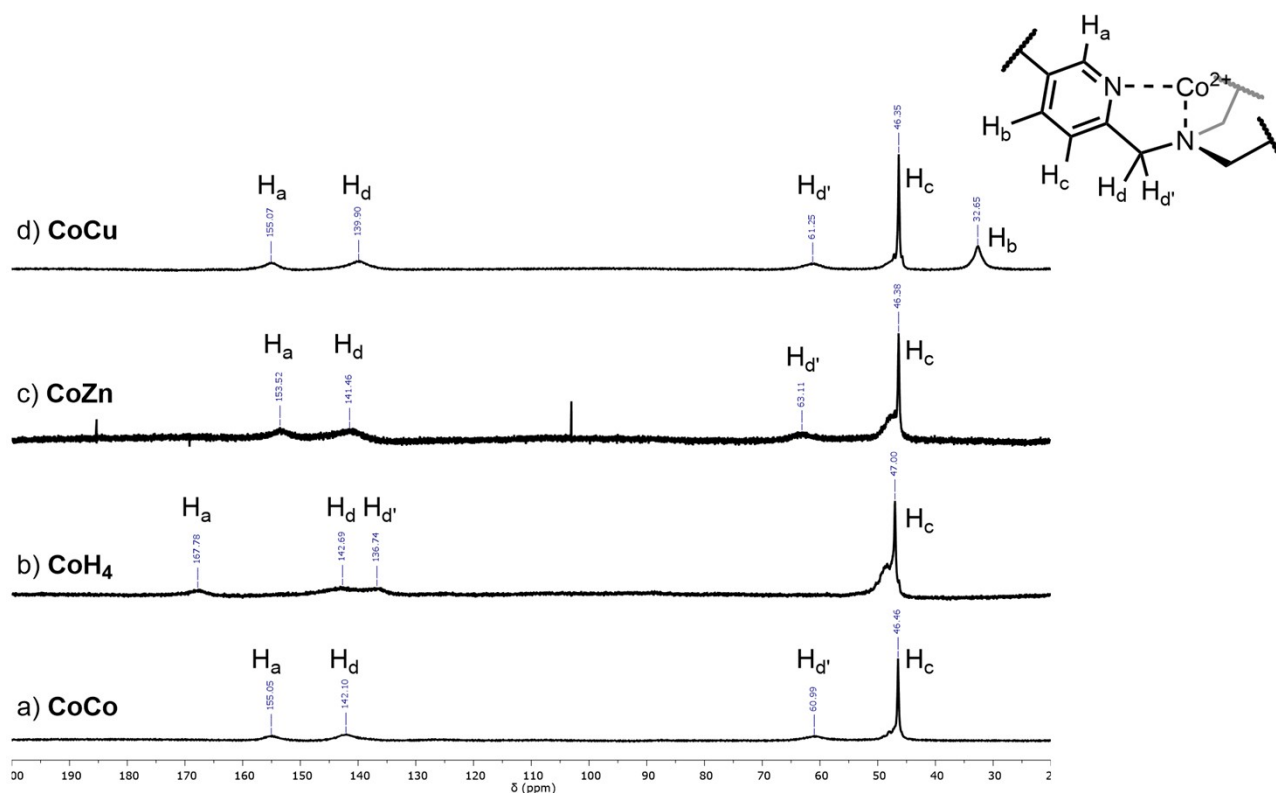


Figure S28. ^1H -NMR (400 MHz, 301 K, $\text{CD}_3\text{CN}/\text{D}_2\text{O}$) highlight of the paramagnetic region of a) complex **CoCo**, b) complex **Co**, c) complex **CoZn**, d) complex **CoCu**. The assignment of the paramagnetic peaks of the complexes was based on the report of Karlin.^[S6]

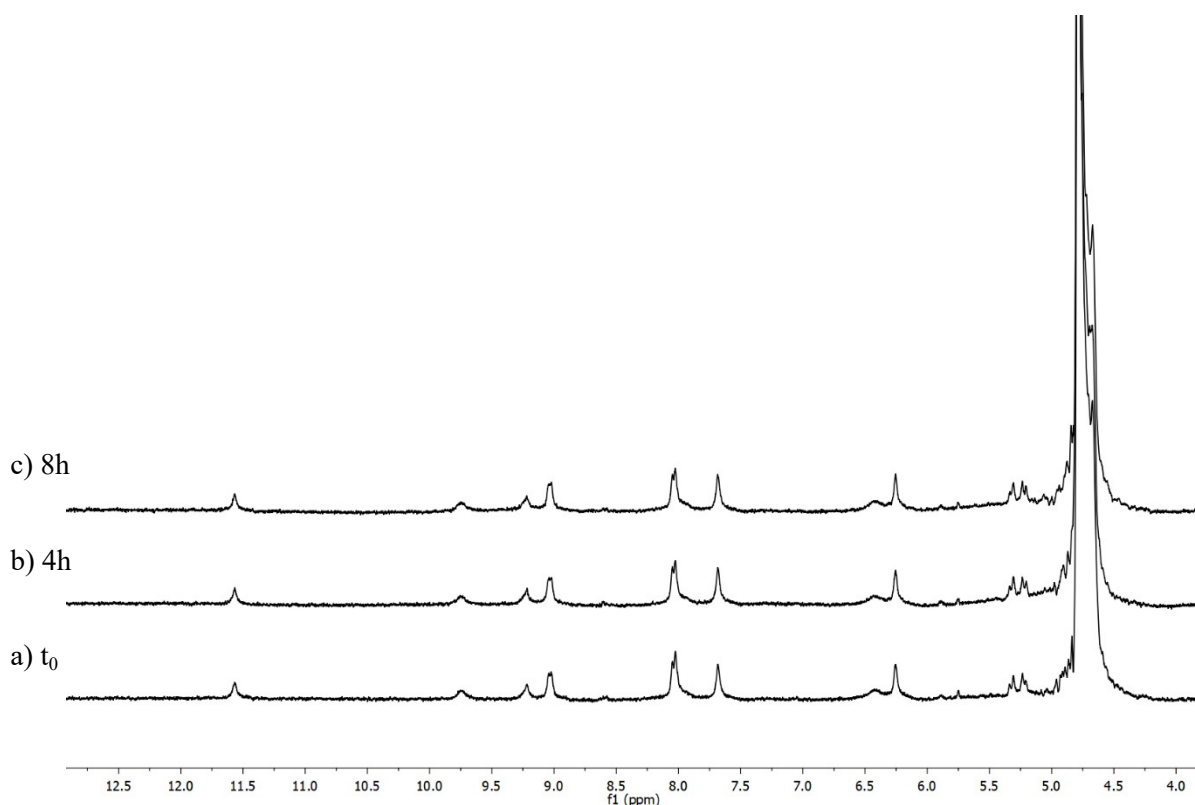


Figure S29. ^1H -NMR (300 MHz, 298 K, $\text{CD}_3\text{CN}/\text{D}_2\text{O}$) spectra of the mononuclear complex CoH_4 recorded at t_0 , 4 h and 8 h, showing no significant changes and confirming its stability in solution over this time period.

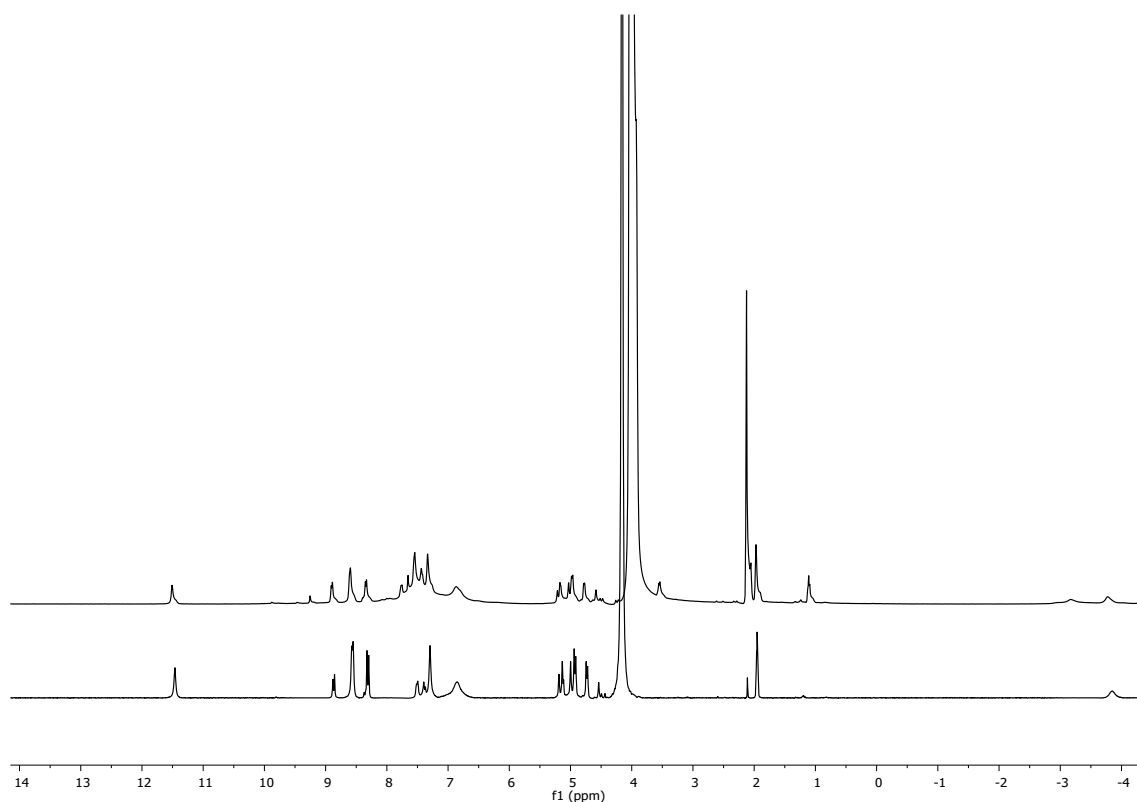


Figure S30. ^1H -NMR (300 MHz, 298 K, $\text{CD}_3\text{CN}/\text{D}_2\text{O}$) spectra of the heterodinuclear complex CoZn a) freshly prepared and b) after two weeks, showing that the characteristic CoZn signals remain dominant, with minor additional peaks appearing over time, attributed to CoCo and ZnZn .

6. Magnetic moment calculation – Evans method

The cage complexes were dissolved in 970 μL of D_2O and 30 μL of *tert*-butanol ($[c] = 0,5 \times 10^{-6} \text{ M}$) and placed in a NMR tube. A solution of 970 μL of D_2O and 30 μL of *tert*-butanol was prepared and placed in a coaxial capillary tube. Once the coaxial set was mounted, the ^1H NMR spectrum was recorded and the frequency difference Δf (in Hz) between the two methyl peaks of *tert*-butanol was measured.

The molar magnetic susceptibility can be calculated according to the following equation:

$$\chi_M = \frac{3\Delta f}{4\pi Fc} \quad (\text{S7})$$

χ_M Molar magnetic susceptibility ($\text{cm}^3 \text{mol}^{-1}$)
 Δf Frequency shift difference of the two *tert*-butanol peaks (Hz)
 F Frequency of the spectrometer ($300 \times 10^6 \text{ Hz}$)
 c Concentration of the sample (mol/mL)

The magnetic moment of the complexes μ is calculated from the χ_M value, according to Equation (S8).

$$\mu = \sqrt{8(\chi_M T)} \quad (\text{S8})$$

T Temperature (K)

The magnetic moment can be correlated to the number of unpaired electrons N by Equation (S9).

$$N = -1 + \sqrt{\mu^2 + 1} \quad (\text{S9})$$

This method however is valid under the Spin-Only approximation, which implies the magnetic moment of a substance to be determined only by the spin component, while the orbital angular momentum component is negligible.

Table S3. Magnetic susceptibility, magnetic moment and number of unpaired electrons estimated using the Evans method (^1H NMR, 300 MHz, $\text{D}_2\text{O}/\text{CD}_3\text{CN}$ 1:1).

Complex	c (mol/mL)	Δf (Hz)	χ_M	μ	N
CoCo	5.71×10^{-7}	14.642	2.04×10^{-2}	6.98	5.9
CoH₄	9.15×10^{-7}	9.32	8.10×10^{-3}	4.39	3.4
CoZn	8.97×10^{-7}	7.725	6.85×10^{-3}	4.04	3.1
CoCu	8.86×10^{-7}	10.689	9.60×10^{-3}	4.78	3.8

7. Titration Experiments of Cage S-1 with Metal Salts

To a solution of cage **S-1** (500 μL , 0.5 μmol , 0.001 M) in $\text{D}_2\text{O}/\text{CD}_3\text{CN}$ in an NMR tube, were added successive small aliquots of a stock solution (15 mM) of the corresponding metal salt (CoCl_2 , ZnCl_2 or $\text{Zn}(\text{OTf})_2$). After each addition, the solution was allowed to equilibrate at room temperature during 30 seconds before acquisition of the ^1H NMR spectrum.

7.1 With CoCl_2

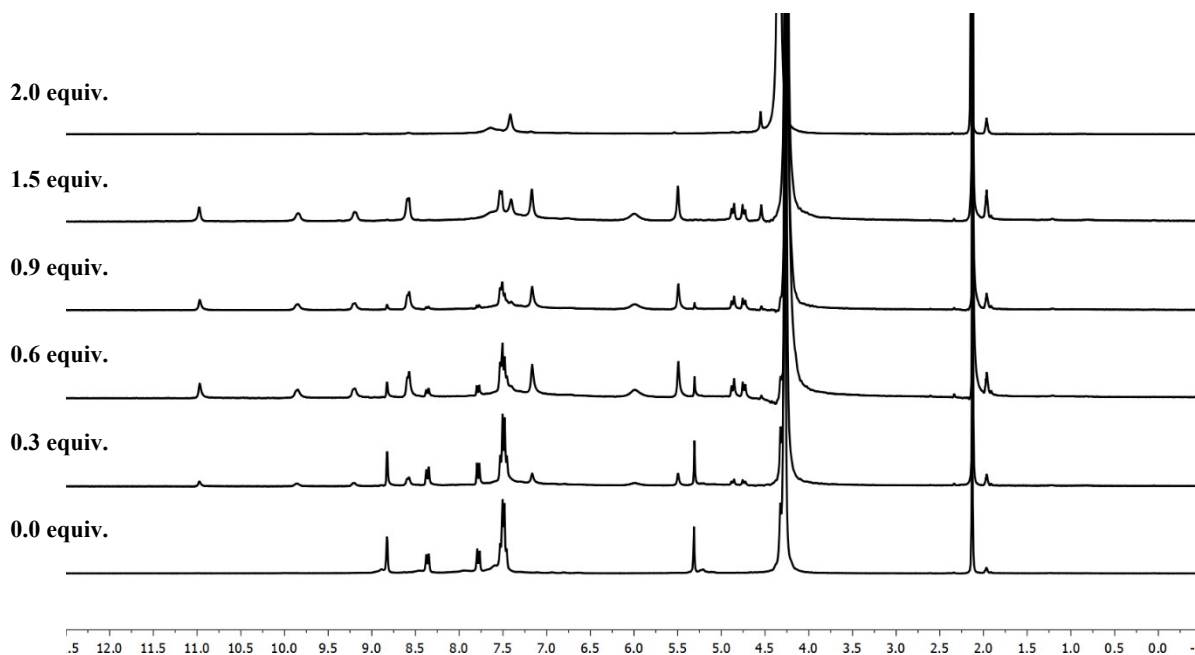


Figure S31. ^1H -NMR titration study of Cage **S-1** (1 μmol) upon incremental addition of CoCl_2 in $\text{D}_2\text{O}/\text{CD}_3\text{CN}$ (1:1, 0.5 mL) (300 MHz, 298 K). Spectra recorded from 0.0 (bottom) to 2.0 equivalents (top) of CoCl_2 .

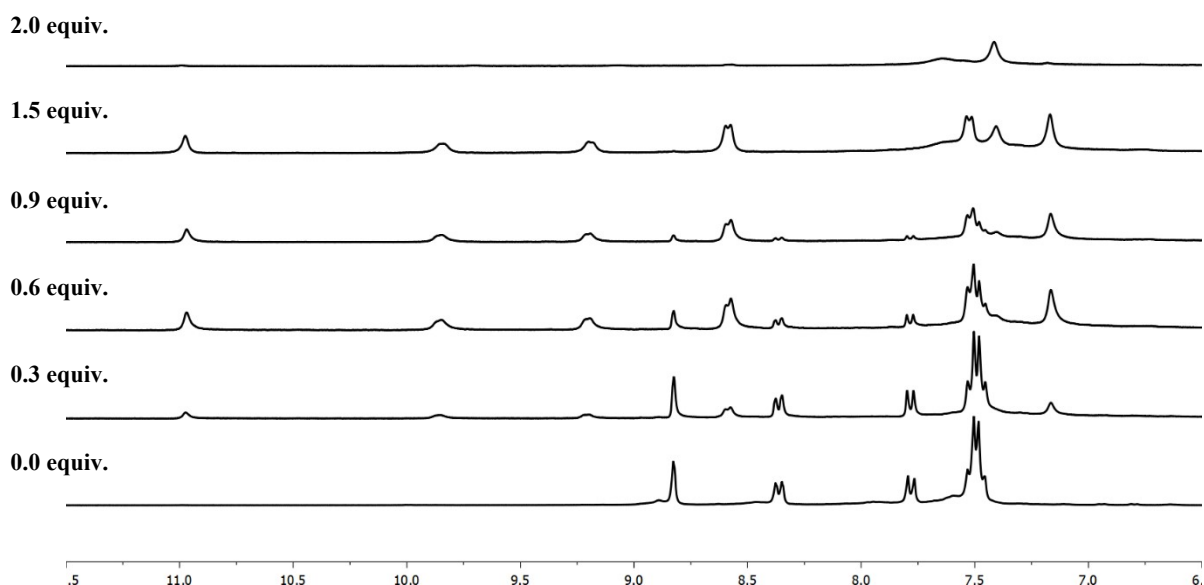
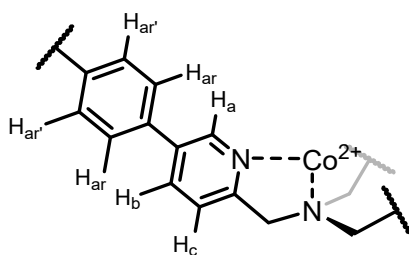


Figure S32. Partial ^1H -NMR titration study of Cage **S-1** (1 μmol) upon incremental addition of CoCl_2 in $\text{D}_2\text{O}/\text{CD}_3\text{CN}$ (1:1, 0.5 mL) (300 MHz, 298 K). Spectra recorded from 0.0 (bottom) to 2.0 equivalents (top) of CoCl_2 .

Table S4. Selected ^1H NMR chemical shifts (300 MHz, 298 K, $\text{D}_2\text{O}/\text{CD}_3\text{CN}$ 1:1) for **S-1**, **CoH₄** and **CoCo**. H_a - H_c correspond to the pyridyl resonances, Har/Har' to the aromatic envelope. Multiplicities are indicated as observed. For the paramagnetic attribution of Co complexes, see Figure S28.

	S-1	CoH₄	CoCo
Ha	8.83 (s, 6H)	10.97 (m, 6H)	-
Hb	8.37 (d, 6H)	9.85 (m, 6H)	-
Hc	7.78 (d, 6H)	9.20 (m, 6H)	-
Har	7.50 (m, 24H)	8.59 (m, 12H)	-
Har'	-	7.52 (m, 12H)	-



7.2 With ZnCl₂

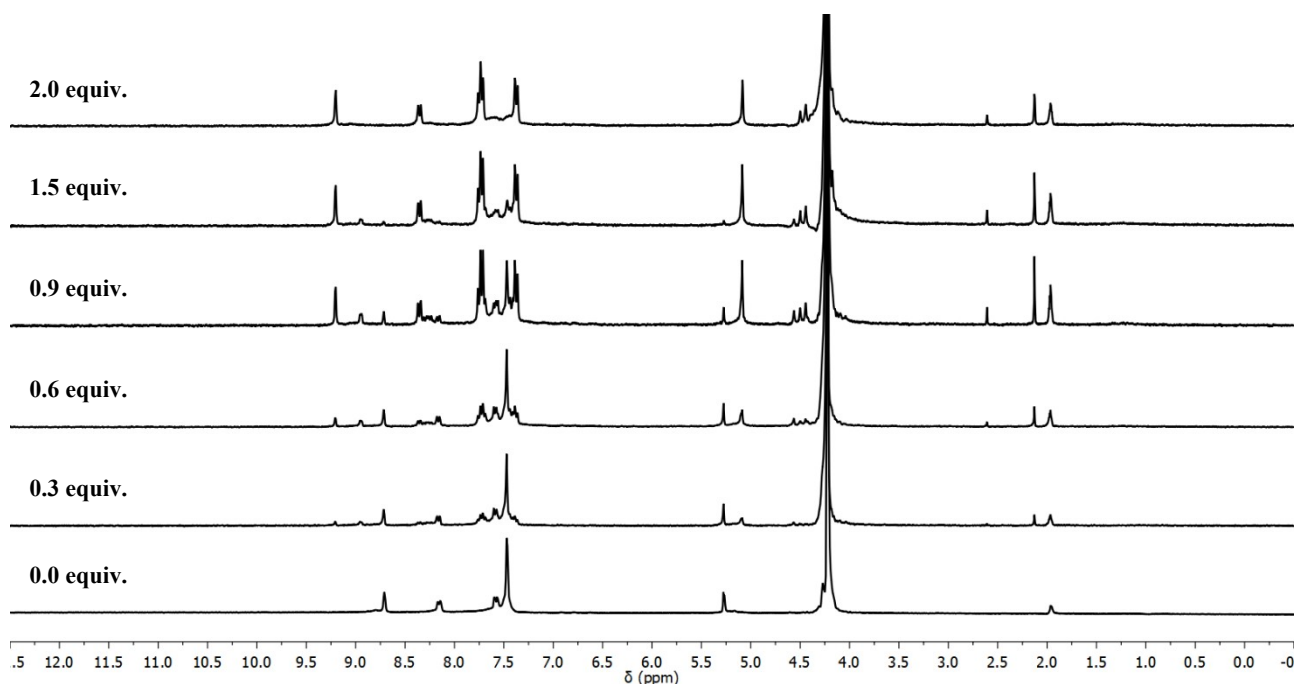


Figure S33. ¹H-NMR titration study of Cage **S-1** (1 μmol) upon incremental addition of ZnCl₂ in D₂O/CD₃CN (1:1, 0.5 mL) (300 MHz, 298 K). Spectra recorded from 0.0 (bottom) to 2.0 equivalents (top) of ZnCl₂.

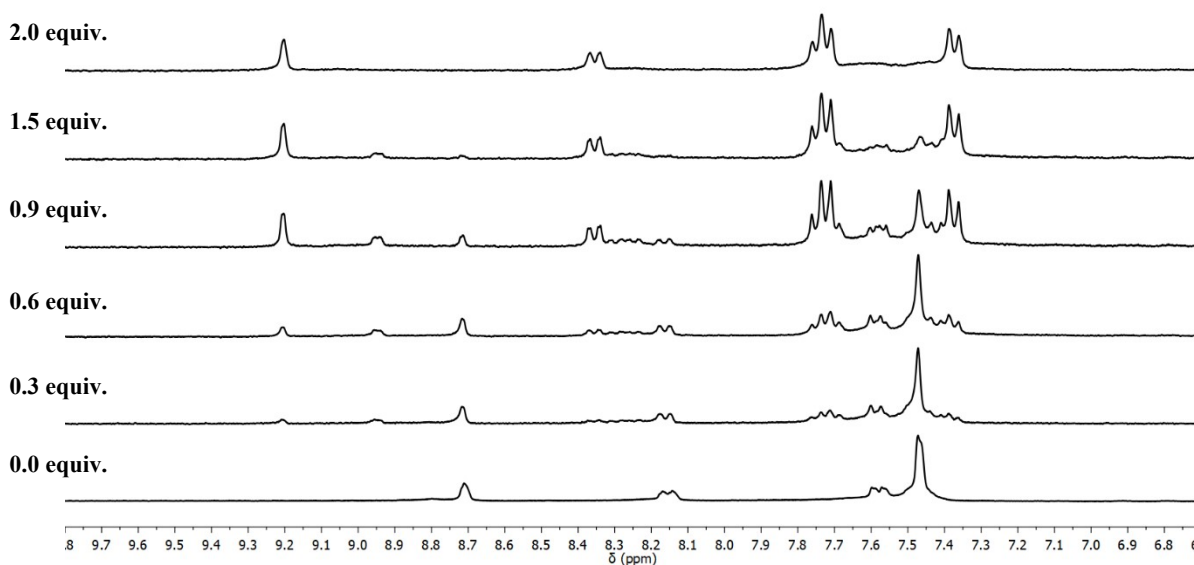
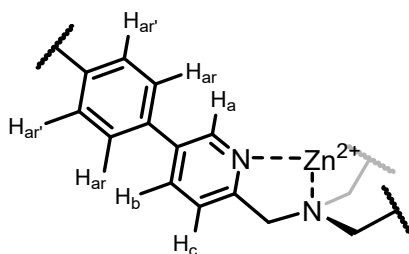


Figure S34. Partial ¹H-NMR titration study of Cage **S-1** (1 μmol) upon incremental addition of ZnCl₂ in D₂O/CD₃CN (1:1, 0.5 mL) (300 MHz, 298 K). Spectra recorded from 0.0 (bottom) to 2.0 equivalents (top) of ZnCl₂.

Table S5. Selected ¹H NMR chemical shifts (300 MHz, 298 K, D₂O/CD₃CN 1:1) for **S-1**, **ZnH₄** and **ZnZn**. H_a-H_c correspond to the pyridyl resonances, Har/Har' to the aromatic envelope. Multiplicities are indicated as observed.

	S-1	ZnH₄	ZnZn
--	------------	------------------------	-------------

Ha	8.72 (s, 6H)	8.95 (d, 6H)	9.20 (s, 6H)
Hb	8.16 (d, 6H)	8.27 (dd, 6H)	8.36 (d, 6H)
Hc	7.58 (d, 6H)	7.58 (m, 6H)	7.75 (d, 6H)
Har	7.47 (m, 24H)	7.70 (d, 12H)	7.72 (d, 12H)
Har'	-	7.43 (d, 12H)	7.38 (d, 12H)



7.3 With Zn(OTf)₂

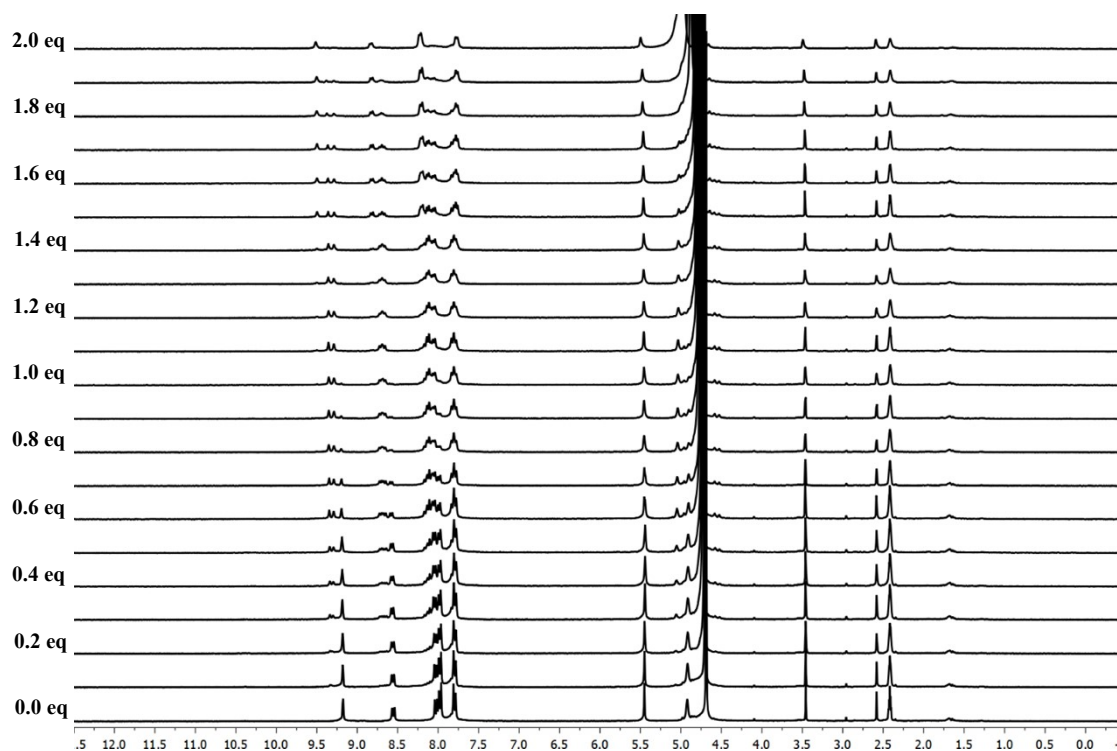


Figure S35. ¹H-NMR titration study of Cage **S-1** (1 μmol, with OTf⁻ as counterions) upon incremental addition of Zn(OTf)₂ in D₂O/CD₃CN (1:1, 0.5 mL) (300 MHz, 298 K). Spectra recorded from 0.0 (bottom) to 2.0 equivalents (top) of Zn(OTf)₂, increasing by 0.1 equiv. per addition.

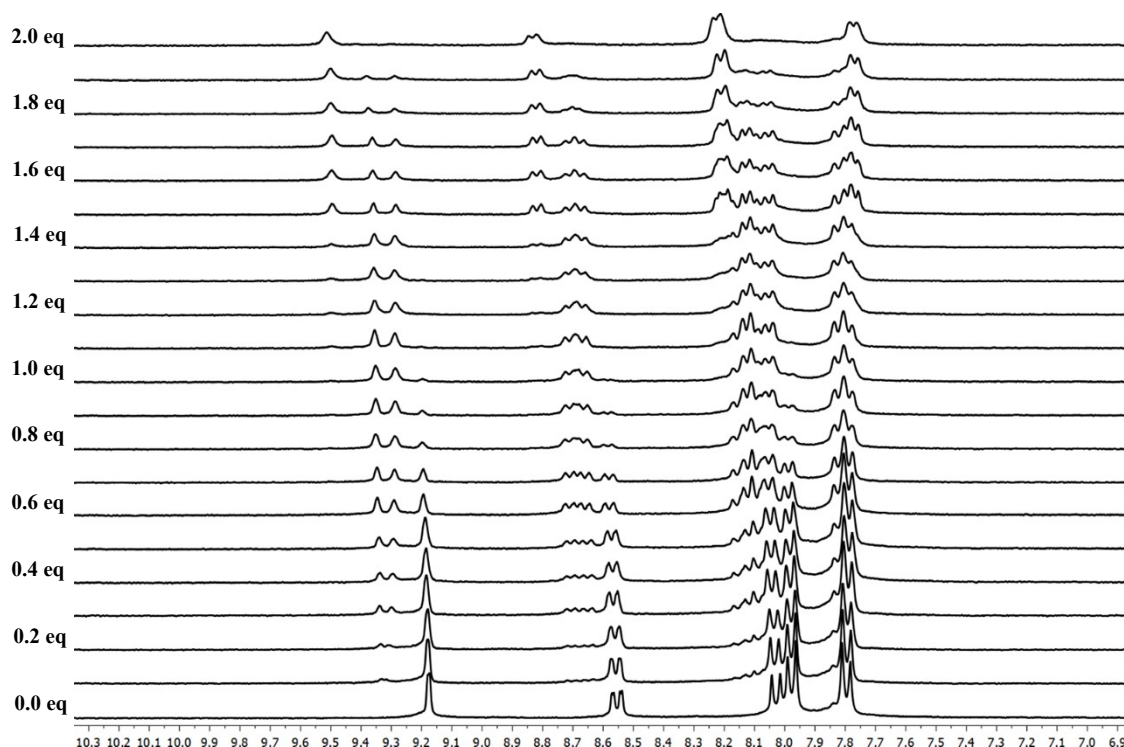


Figure S36. Partial ^1H -NMR titration study of Cage **S-1** (1 μmol , with OTf^- as counterions) upon incremental addition of $\text{Zn}(\text{OTf})_2$ in $\text{D}_2\text{O}/\text{CD}_3\text{CN}$ (1:1, 0.5 mL) (300 MHz, 298 K). Spectra recorded from 0.0 (bottom) to 2.0 equivalents (top) of $\text{Zn}(\text{OTf})_2$, increasing by 0.1 equiv. per addition.

8. Single Crystal X-Ray Analysis

CoCo and **ZnZn** single crystals were grown by slow evaporation of saturated water-DMSO solutions.

Data collections were performed at the X-ray diffraction beamline (XRD2) of the Elettra Synchrotron (Trieste, Italy).^[S7] The crystals were dipped in NHV oil (Jena Bioscience, Jena, Germany) and mounted on the goniometer head with nylon loops (MiTeGen, Ithaca, USA). Complete datasets were collected at 100 K (nitrogen stream supplied through an Oxford Cryostream 700). Data were acquired using a monochromatic wavelength of 0.6198 Å through the rotating crystal method on a Pilatus 6M hybrid-pixel area detector (DECTRIS Ltd., Baden-Daettwil, Switzerland). The diffraction data was indexed and integrated using XDS.^[S8]

Both the structures were solved in the $P6_3$ space group with Olex2^[S9] by using ShelXT^[S10] structure solution program by Intrinsic Phasing and refined with the ShelXL^[S11] refinement package using least-squares minimization. In the last cycles of refinement, non-hydrogen atoms were refined anisotropically. Hydrogen atoms were included in calculated positions, and a riding model was used for their refinement. Deposition Numbers 2455177 and 2455178 contain the supplementary crystallographic data for this paper. These data are provided free of charge by the joint Cambridge Crystallographic Data Centre and Fachinformationszentrum Karlsruhe Access Structures service <http://www.ccdc.cam.ac.uk/structures>.

8.1 CoCo refinement details

One chloride anion and one DMSO molecule were disordered, Figure S34. These atoms were split in two parts and modelled with the help of SADI, SIMU and RIGU restraints for DMSO molecule, and ISOR restraints was applied to the disordered Cl anion. The structure was refined a racemic twin (BASF 0.21(3)). The final Fourier map revealed the presence of non-negligible residual electron density located in a large array of voids. The contribution of these peaks was removed using the mask routine of OLEX2. The solvent mask calculated 1156 electrons found in a volume of 2658 Å³ in 1 void per unit cell (probe radius: 1.2 Å). This is consistent with the presence of 27.5 DMSO molecules per unit cell which account for 1150 electrons or 115 water molecules per unit cell which account for 1150 electrons. Combinations of the two crystallization solvents cannot be excluded.

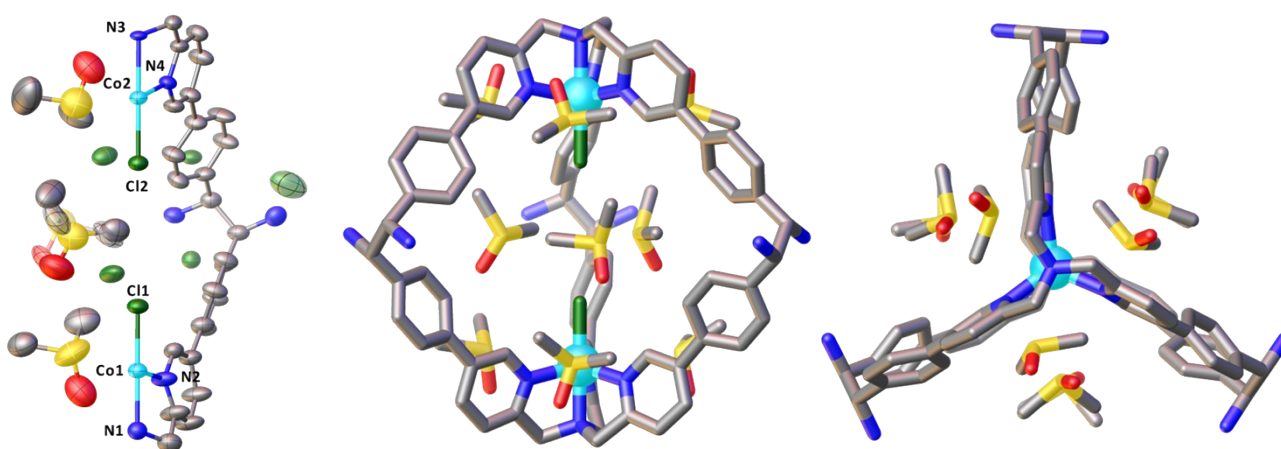


Figure S37. Asymmetric unit of the **CoCo** cage with thermal ellipsoids shown at the 50% probability level, disordered regions are shown as translucent. Side and top views illustrate the DMSO molecules occupying the cage windows. Color code: Co, cyan; N, blue; Cl, green; O, red; S, yellow; C, grey. H atoms are omitted for clarity.

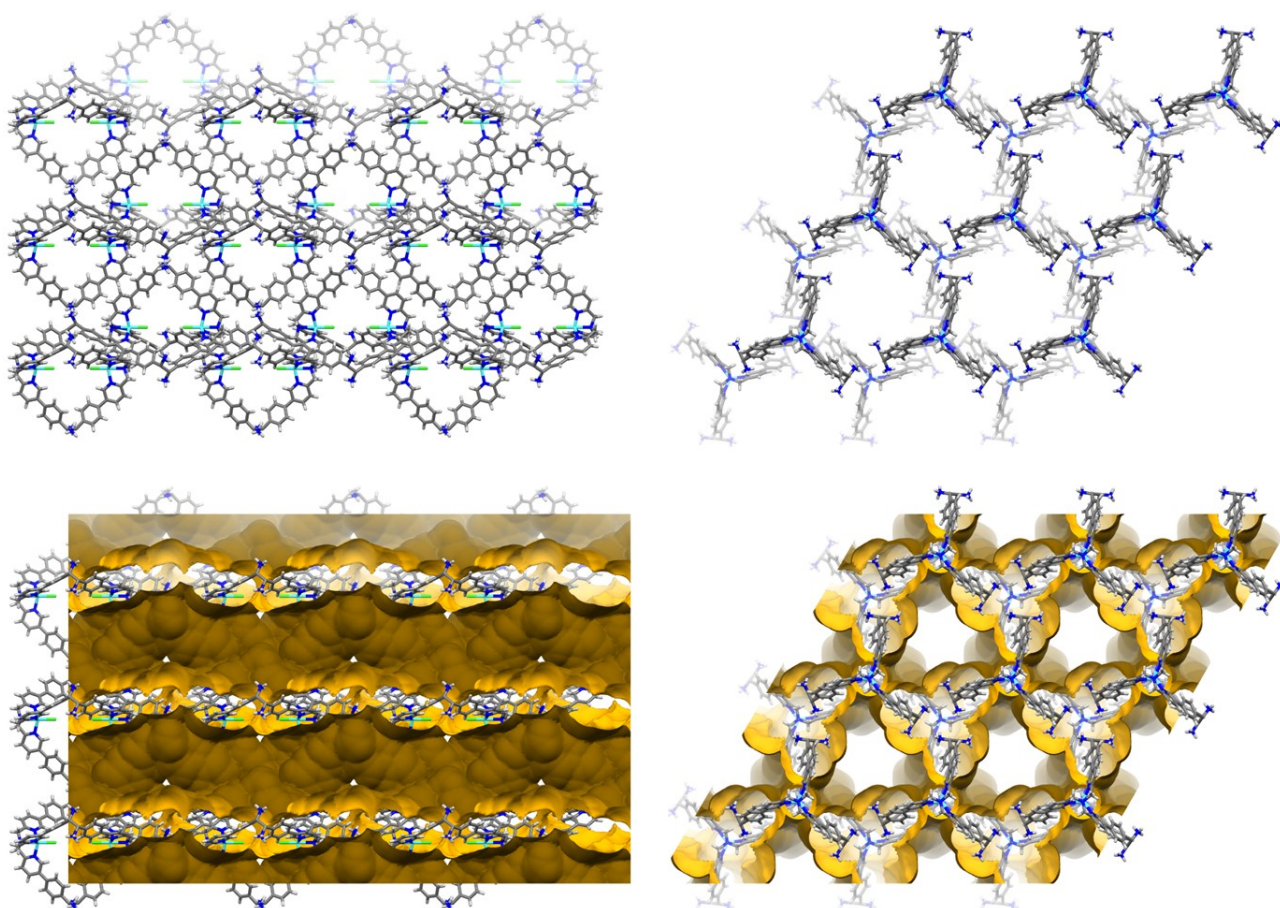


Figure S38. Top: packing of **CoCo** cage viewed along the *b* and *c* axes, disordered regions, uncoordinated Cl⁻ anions and solvent molecules are omitted for clarity. Bottom: voids calculated after removing solvent molecules and anions (probe radius 1.2 Å). Color code: Co, cyan; N, blue; Cl, green; voids outside, yellow; voids inside, dark yellow.

8.2 ZnZn refinement details

One chloride anion, two DMSO molecules and same atoms of the TPMA fragment near Zn1 were disordered, Figure S36. These atoms were split in two parts and modelled with the help of SADI, SIMU and RIGU restrains for DMSO molecules and TPMA fragment, and EADP constrain was applied to the disordered Cl anion and to the C atoms of the disordered DMSO molecule. The final Fourier map revealed the presence of non-negligible residual electron density located in a large array of voids. The contribution of these peaks was removed using the mask routine of OLEX2. The solvent mask calculated 1149 electrons found in a volume of 2553 Å³ in 1 void per unit cell (probe radius: 1.2 Å). This is consistent with the presence of 27.5 DMSO molecules per unit cell which account for 1155 electrons or 115 water molecules per unit cell which account for 1150 electrons. Combinations of the two crystallization solvents cannot be excluded. Since **CoCo** and **ZnZn** are isostructural, the packing of the **ZnZn** cage results in a similar array of voids, as shown in Figure S38.

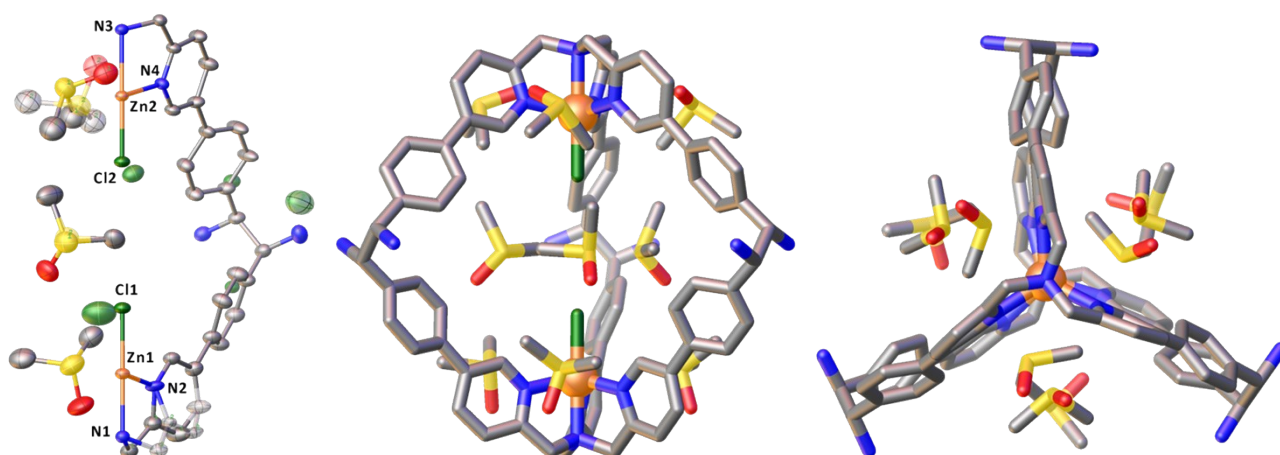


Figure S39. Asymmetric unit of the **ZnZn** cage with thermal ellipsoids shown at the 50% probability level, disordered regions are shown as translucent. Side and top views illustrate the DMSO molecules occupying the cage windows. Color code: Zn, orange; N, blue; Cl, green; O, red; S, yellow; C, grey. H atoms are omitted for clarity.

Table S6. Selected bond lengths (Å) and angle (°) for **CoCo** and **ZnZn**.

CoCo		ZnZn	
Co1-Cl1	2.2818(5)	Zn1-Cl1	2.3003(14)
Co1-N1	2.1338(4)	Zn1-N1	2.228(5)
Co1-N2	2.0732(2)	Zn1-N2	2.054(3)
Co2-Cl2	2.3200(9)	Zn2-Cl2	2.2927(14)
Co2-N3	2.209(4)	Zn2-N3	2.312(5)
Co2-N4	2.018(4)	Zn2-N4	2.048(2)
Co1...Co2	9.682(2)	Zn1...Zn2	9.700(2)
Co1-Cl1...Cl2-Co2	5.080(1)	Zn1-Cl1...Cl2-Zn2	5.1065(18)
Cl1-Co1-N1	180.0	Cl1-Zn1-N1	180
Cl1-Co1-N2	102.316(3)	Cl1-Zn1-N2	101.42(7)
N1-Co1-N2	77.684(3)	N1-Zn1-N2	78.58(7)
Cl2-Co2-N3	180	Cl2-Zn2-N3	180

Cl2-Co2-N4	101.65(9)	Cl2-Zn2-N4	102.56(7)
N3-Co2-N4	78.35(9)	N3-Zn2-N4	77.44(7)

Table S7. Crystal data and structure refinement for **CoCo** and **ZnZn**.

Compound	CoCo	ZnZn
Empirical formula	C ₉₆ H ₁₃₂ Cl ₁₀ Co ₂ N ₁₄ O ₉ S ₉	C ₉₆ H ₁₃₂ Cl ₁₀ N ₁₄ O ₉ S ₉ Zn ₂
Formula weight	2387.05	2399.93
Temperature/K	100.00	100.00
Crystal system	hexagonal	hexagonal
Space group	<i>P</i> 6 ₃	<i>P</i> 6 ₃
<i>a</i> /Å	19.164(3)	19.113(3)
<i>b</i> /Å	19.164(3)	19.113(3)
<i>c</i> /Å	25.006(5)	25.150(5)
α /°	90	90
β /°	90	90
γ /°	120	120
Volume/Å ³	7953(3)	7957(3)
<i>Z</i>	2	2
ρ_{calc} /g/cm ³	0.997	1.002
μ /mm ⁻¹	0.363	0.428
<i>F</i> (000)	2492.0	2504.0
Crystal size/mm ³	0.1 × 0.05 × 0.02	0.1 × 0.05 × 0.02
Radiation	Synchrotron (λ = 0.6198)	Synchrotron (λ = 0.6198)
2 θ range for data collection/°	3.556 to 52.548	2.146 to 55.356
Index ranges	-27 ≤ <i>h</i> ≤ 27, -27 ≤ <i>k</i> ≤ 27, -35 ≤ <i>l</i> ≤ 35	-28 ≤ <i>h</i> ≤ 28, -28 ≤ <i>k</i> ≤ 28, -37 ≤ <i>l</i> ≤ 37
Reflections collected	152666	160741
Independent reflections	16134 [<i>R</i> _{int} = 0.0546, <i>R</i> _{sigma} = 0.0254]	18741 [<i>R</i> _{int} = 0.0546, <i>R</i> _{sigma} = 0.0266]
Data/restraints/parameters	16134/208/456	18741/519/479
Goodness-of-fit on <i>F</i> ²	1.075	1.046
Final <i>R</i> indexes [<i>I</i> > 2 σ (<i>I</i>)]	<i>R</i> ₁ = 0.0862, <i>wR</i> ₂ = 0.2400	<i>R</i> ₁ = 0.0639, <i>wR</i> ₂ = 0.1953
Final <i>R</i> indexes [all data]	<i>R</i> ₁ = 0.0966, <i>wR</i> ₂ = 0.2589	<i>R</i> ₁ = 0.0653, <i>wR</i> ₂ = 0.1992
Largest diff. peak/hole / e Å ⁻³	2.54/-1.00	2.48/-0.65
Flack parameter	0.21(3)	0.099(15)
CCDC number	2455177	2455178

9. Computational Methods

All Density Functional Theory (DFT) calculations were carried out using Gaussian16.^[S12] Geometry optimizations were conducted using PBE1PBE functional,^[S13-15] with the inclusion of Grimme D3 dispersion correction combined to the Becke-Johnson damping function.^[S16,17] 6-31G(d) basis set was employed for all atoms, except for metals, which are described with the SDD basis set,^[S18] including the effective core potential. Solvation effects (water) were included in the optimization procedure using SMD.^[S19] Frequency calculations were performed for all optimized structures to assess the nature of the stationary states; real frequencies are associated to minima, while one imaginary frequency is associated to transition states. Fully optimized molecular cages were computed including a network of three water molecules to obtain the initial structure for each system. Afterwards, minimal models of the cages were used, considering only the tetradentate tripodal ligands, the metals and the water molecules. Constrained optimizations of minimal models were

performed maintaining every atom frozen but the metals, the water molecules and the hydrogens involved in the reaction. Then, to obtain more accurate estimates of energies, single-point calculations were carried out using the same functional combined with the larger 6-311+G(d,p) and def2-TZVP (for metals) basis sets. This level of theory is denoted as SMD-PBE1PBE-D3(BJ)/6-311+G(d,p),def2-TZVP // SMD-PBE1PBE-D3(BJ)/6-31G(d),SDD. All metallic species were described as high spin systems with ferromagnetic coupling in bimetallic models, consistently to a similar Co(II)Co(II) cage.^[S3] Lastly, spin contamination was checked for all species and Co(III)H systems resulted to be highly contaminated due to presence of a partial radical character on the hydrogen. Thus, energy values were corrected by means of the Yamaguchi correction.^[S20,21]

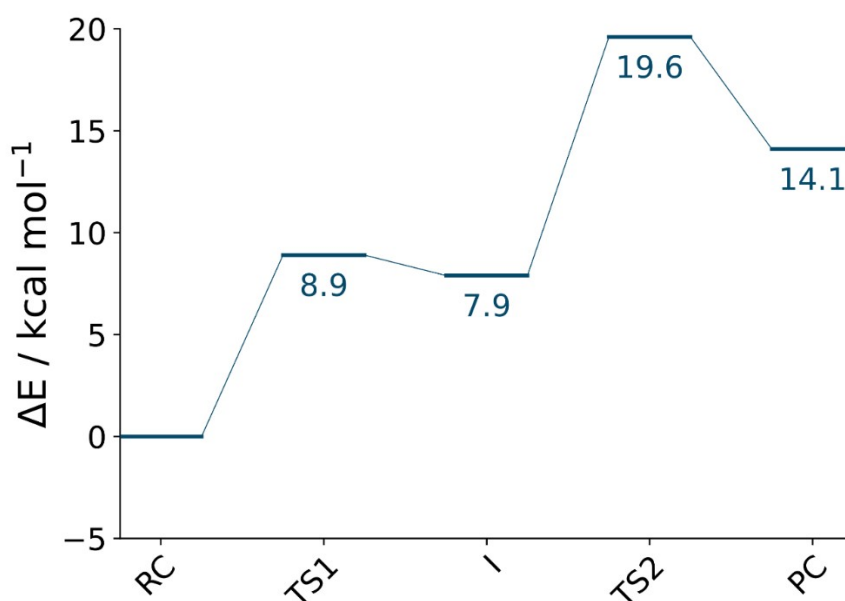


Figure S40. Electronic energy profile (kcal mol⁻¹) for the protonation and oxidation of Co(I) to Co(III)H in the mononuclear **CoH₄** system. Level of theory: SMD-PBE1PBE-D3(BJ)/6-311+G(d,p),def2-TZVP // SMD-PBE1PBE-D3(BJ)/6-31G(d),SDD.

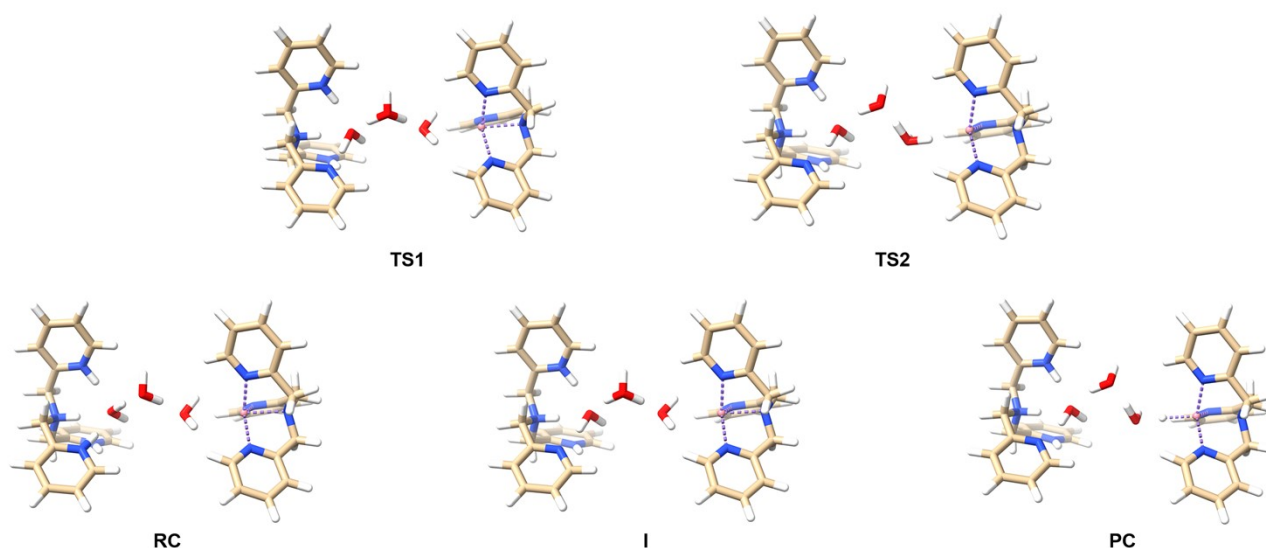


Figure S41. Optimized geometries of the reactant complex (RC), transition state 1 (TS1), key intermediates (I), transition state 2 (TS2) and product complex (PC) involved in the proposed proton-transfer pathway for the **CoH₄** cage, visualized using ChimeraX.

Table 8. Electronic reaction energies (kcal mol⁻¹) for the protonation and oxidation of Co(I) to Co(III)H in the dinuclear metal systems and mononuclear **CoH₄** system with full cage relaxation according to Scheme 1a and 1b. Level of theory: SMD-PBE1PBE-D3(BJ)/6-311+G(d,p),def2-TZVP // SMD-PBE1PBE-D3(BJ)/6-31G(d),SDD.

	CoCo	CoZn	CoCu	CoH ₄ full
PC (a)	29.0	28.0	-	9.6 (1.3)*
PC (b)	7.8	6.5	8.6	-

*no water molecule included in the overall system.

Table S9. Coordinates (Å) and energies (E, Hartree) of stationary points and imaginary frequencies (Nimag, cm⁻¹) of transition states. Level of theory: SMD-PBE1PBE-D3(BJ)/6-31G(d),SDD.

CoH₄				C	3.333304000	-0.834656000	-3.136462000
full RC				C	5.743609000	-1.192395000	-2.478572000
E= -4157.45864715				C	6.694796000	-2.219552000	-2.406020000
N	0.451866000	-0.357982000	-5.934294000	H	6.547029000	-3.134346000	-2.972371000
N	2.315971000	-0.878052000	-4.011993000	C	7.825870000	-2.086075000	-1.614402000
C	1.383390000	-1.442818000	-6.203987000	H	8.543194000	-2.902721000	-1.574502000
H	0.840374000	-2.388337000	-6.071862000	C	8.037122000	-0.915061000	-0.881322000
H	1.760390000	-1.429878000	-7.237344000	C	7.078387000	0.097391000	-0.919089000
C	2.537761000	-1.404976000	-5.236035000	H	7.234151000	1.005868000	-0.343800000
C	3.778737000	-1.911291000	-5.599300000	C	5.938814000	-0.041493000	-1.705386000
H	3.922399000	-2.313914000	-6.597016000	H	5.219681000	0.771426000	-1.756272000
C	4.822369000	-1.867697000	-4.690481000	C	9.286761000	-0.745292000	-0.053199000
H	5.806496000	-2.230315000	-4.971440000	C	9.319799000	-1.753209000	1.106837000
C	4.615166000	-1.307086000	-3.424190000				

N	0.014705000	1.683950000	-4.169439000	N	2.290608000	-0.002694000	4.094666000
C	0.974015000	0.958269000	-6.285064000	C	0.965996000	0.846250000	5.994776000
H	2.050836000	0.960115000	-6.075857000	H	0.808295000	1.867991000	5.634007000
H	0.851959000	1.184262000	-7.353643000	H	1.041718000	0.870417000	7.082772000
C	0.317495000	2.019076000	-5.446459000	C	2.233499000	0.304955000	5.406929000
C	0.050769000	3.276736000	-5.963564000	C	3.394112000	0.206100000	6.154149000
C	-0.556030000	4.230087000	-5.159640000	H	3.364955000	0.440512000	7.212068000
H	-0.808341000	5.206062000	-5.562243000	C	4.579563000	-0.180894000	5.537858000
C	-0.887238000	3.902780000	-3.839468000	H	5.490518000	-0.252075000	6.123753000
C	-0.568634000	2.617273000	-3.393996000	C	4.602852000	-0.503024000	4.177335000
C	-1.594327000	4.894651000	-3.002789000	C	3.404950000	-0.409587000	3.480705000
C	-1.280620000	6.255117000	-3.133038000	C	5.832566000	-0.887719000	3.465426000
H	-0.452217000	6.559352000	-3.765721000	C	7.011938000	-0.170909000	3.684175000
C	-2.014702000	7.223598000	-2.464668000	H	7.026577000	0.646773000	4.398744000
H	-1.743642000	8.269744000	-2.587597000	C	8.152934000	-0.458972000	2.947122000
C	-3.088610000	6.855046000	-1.649391000	H	9.037959000	0.150652000	3.107306000
C	-3.381396000	5.501739000	-1.478775000	C	8.139229000	-1.493107000	2.008615000
H	-4.207788000	5.208202000	-0.837183000	C	6.975119000	-2.240546000	1.822866000
C	-2.638774000	4.530136000	-2.143914000	H	6.966747000	-3.054027000	1.103391000
H	-2.904140000	3.482493000	-2.031209000	C	5.824155000	-1.931456000	2.533740000
C	-3.925305000	7.911553000	-0.968848000	H	4.919214000	-2.511012000	2.374486000
C	-3.107852000	8.660971000	0.102006000	N	-1.043114000	-2.579371000	4.339300000
N	-1.437308000	-1.403381000	-4.209046000	C	-0.230493000	-1.320863000	6.251390000
C	-0.895056000	-0.592428000	-6.441058000	H	0.774600000	-1.721207000	6.092114000
H	-1.416018000	0.372806000	-6.459767000	H	-0.410738000	-1.213227000	7.322005000
H	-0.892240000	-0.976515000	-7.470333000	C	-1.253367000	-2.210714000	5.620540000
C	-1.657691000	-1.523084000	-5.538134000	C	-2.407881000	-2.651554000	6.238766000
C	-2.567310000	-2.435639000	-6.050904000	H	-2.589697000	-2.382804000	7.272829000
H	-2.716498000	-2.498576000	-7.124190000	C	-3.334380000	-3.402532000	5.515599000
C	-3.257187000	-3.270280000	-5.183078000	H	-4.246752000	-3.739701000	5.997416000
H	-3.958450000	-4.005015000	-5.567373000	C	-3.125162000	-3.674833000	4.161717000
C	-3.006305000	-3.192235000	-3.809606000	C	-1.926635000	-3.253894000	3.599777000
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C	-5.065591000	-4.356046000	-3.046541000	H	-4.209128000	-6.144390000	4.513947000
H	-5.625294000	-3.794764000	-3.789109000	C	-5.396588000	-6.321085000	2.731344000
C	-5.720235000	-5.294614000	-2.261920000	H	-5.690775000	-7.337580000	2.974162000
H	-6.789821000	-5.437234000	-2.398625000	C	-5.838923000	-5.697607000	1.562731000
C	-5.010227000	-6.039950000	-1.316269000	C	-5.433642000	-4.390774000	1.284250000
C	-3.649675000	-5.790463000	-1.132648000	H	-5.791550000	-3.890726000	0.389421000
H	-3.094764000	-6.357773000	-0.390566000	C	-4.552223000	-3.738249000	2.134529000
C	-2.999482000	-4.829413000	-1.901327000	H	-4.221775000	-2.729819000	1.902843000
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C	-5.710490000	-7.089664000	-0.486780000	C	-1.506243000	0.801418000	6.060952000
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N	-0.263406000	0.061901000	5.646995000	H	-1.442646000	0.964941000	7.137847000

C	-1.685752000	2.106186000	5.348363000	H	-2.194283000	9.064049000	-0.341345000
C	-1.979629000	3.289116000	6.002763000	H	-4.813674000	9.628952000	0.904001000
C	-2.193269000	4.452181000	5.265762000	H	-3.871702000	10.621632000	-0.031413000
H	-2.425356000	5.379334000	5.780653000	H	-3.369729000	10.202246000	1.481724000
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C	-1.774731000	3.229900000	3.267447000	H	10.384198000	-0.255258000	-1.753258000
C	-2.269117000	5.621767000	3.014274000	H	10.514727000	-2.158576000	2.768034000
C	-3.404949000	6.419738000	3.163105000	H	-8.001039000	-7.029940000	2.020476000
H	-4.114798000	6.210521000	3.957877000	H	-5.789568000	-8.351044000	-2.141955000
C	-3.667729000	7.433129000	2.249636000	H	1.427506000	0.059416000	3.505301000
H	-4.591432000	7.995044000	2.354698000	H	-0.168474000	-2.307274000	3.887237000
C	-2.776045000	7.687476000	1.205488000	H	-1.360880000	1.269079000	3.481470000
C	-1.604485000	6.935412000	1.099779000	H	-0.285318000	-0.030192000	4.611544000
H	-0.898501000	7.143351000	0.301389000	O	0.062477000	-0.096981000	-0.875205000
C	-1.360722000	5.896520000	1.985882000	H	0.881281000	0.005789000	-1.390434000
H	-0.462671000	5.294442000	1.879250000	H	-0.636089000	0.165474000	-1.498525000
N	-3.844186000	9.847210000	0.642366000	O	0.246279000	1.947021000	0.896868000
N	-4.468124000	8.839609000	-2.016572000	H	0.187065000	1.280818000	0.165414000
N	10.485765000	-0.883040000	-0.946902000	H	1.177899000	2.216786000	0.903842000
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N	-7.538238000	-7.451241000	1.205045000	H	-0.386032000	-0.586959000	2.263683000
N	-6.430133000	-8.036124000	-1.403660000	H	0.091589000	0.901794000	2.068734000
H	0.297593000	3.492390000	-6.998480000				
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H	3.103863000	-0.404849000	-2.164986000	N	0.451837000	-0.357891000	-5.934154000
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H	-0.778846000	2.319945000	-2.369801000	C	1.383386000	-1.442834000	-6.204026000
H	-2.036300000	3.296332000	7.085066000	H	0.840377000	-2.388337000	-6.071851000
H	-1.879546000	-2.106069000	-2.316843000	H	1.760367000	-1.429896000	-7.237353000
H	-1.642683000	-3.456868000	2.574466000	C	2.537811000	-1.404724000	-5.236136000
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H	9.335402000	0.268880000	0.352174000	H	3.922399000	-2.313914000	-6.597016000
H	10.587482000	-1.837608000	-1.312266000	C	4.822369000	-1.867697000	-4.690481000
H	11.364174000	-0.627663000	-0.481064000	H	5.806496000	-2.230315000	-4.971440000
H	9.281795000	-2.773370000	0.718076000	C	4.615182000	-1.307016000	-3.424221000
H	10.856868000	-0.685914000	2.091460000	C	3.333266000	-0.834878000	-3.136464000
H	11.388144000	-2.083663000	1.372215000	N	0.014732000	1.683943000	-4.169167000
H	-7.237141000	-7.599176000	-1.865665000	C	0.974043000	0.958231000	-6.285105000
H	-6.763391000	-8.880132000	-0.922952000	H	2.050839000	0.960109000	-6.075874000
H	-4.979483000	-7.701352000	0.048194000	H	0.851959000	1.184261000	-7.353643000
H	-7.012219000	-8.269274000	1.537623000	C	0.317630000	2.019055000	-5.446433000
H	-8.284048000	-7.787657000	0.584459000	C	0.050769000	3.276736000	-5.963564000
H	-7.344083000	-5.752368000	0.023752000	C	-0.556031000	4.230087000	-5.159640000
H	-4.800007000	7.458088000	-0.496250000	H	-0.808341000	5.206062000	-5.562243000
H	-3.740980000	9.448573000	-2.411573000	C	-0.887250000	3.902776000	-3.839472000
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N	-1.437335000	-1.403486000	-4.208965000
C	-0.895042000	-0.592426000	-6.441093000
H	-1.416016000	0.372807000	-6.459772000
H	-0.892239000	-0.976540000	-7.470323000
C	-1.657710000	-1.523011000	-5.538131000
C	-2.567330000	-2.435620000	-6.050902000
H	-2.716498000	-2.498576000	-7.124190000
C	-3.257188000	-3.270280000	-5.183078000
H	-3.958450000	-4.005015000	-5.567373000
C	-3.006320000	-3.192221000	-3.809604000
C	-2.088598000	-2.233404000	-3.375623000
N	-0.263404000	0.061910000	5.646990000
N	2.290828000	-0.002270000	4.094033000
C	0.966008000	0.846253000	5.994809000
H	0.808298000	1.867989000	5.633998000
H	1.041721000	0.870412000	7.082772000
C	2.233239000	0.304926000	5.406903000
C	3.394095000	0.206029000	6.154165000
H	3.364955000	0.440512000	7.212068000
C	4.579563000	-0.180894000	5.537858000
H	5.490518000	-0.252075000	6.123753000
C	4.602850000	-0.503029000	4.177337000
C	3.405018000	-0.409937000	3.481060000
N	-1.043100000	-2.579367000	4.339293000
C	-0.230495000	-1.320862000	6.251398000
H	0.774603000	-1.721203000	6.092122000
H	-0.410746000	-1.213228000	7.322004000
C	-1.253373000	-2.210717000	5.620536000
C	-2.407882000	-2.651552000	6.238765000
H	-2.589697000	-2.382804000	7.272829000
C	-3.334380000	-3.402532000	5.515599000
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C	-1.926640000	-3.253896000	3.599785000
N	-1.623161000	2.126293000	4.001821000
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H	-2.357477000	0.148652000	5.847157000
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C	-2.193269000	4.452181000	5.265762000
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C	-2.073147000	4.442416000	3.873564000
C	-1.774620000	3.229975000	3.267536000
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H	-2.036300000	3.296332000	7.085066000
H	-1.879557000	-2.106060000	-2.316842000
H	-1.642684000	-3.456866000	2.574465000
Co	0.302714000	-0.340154000	-3.823829000
H	1.425662000	0.050965000	3.511959000
H	-0.171696000	-2.301491000	3.885023000
H	-1.344161000	1.273489000	3.477788000
H	-0.282715000	-0.030604000	4.611484000
O	0.036317000	-0.271426000	-0.823335000
H	0.851594000	-0.425388000	-1.330588000
H	-0.565528000	0.137621000	-1.468495000
O	0.688529000	1.749759000	0.862333000
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O	-0.129070000	0.202497000	2.775442000
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H	5.806496000	-2.230315000	-4.971440000
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C	-0.887230000	3.902783000	-3.839466000	H	0.297593000	3.492390000	-6.998480000
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N	-1.437333000	-1.403482000	-4.208968000	H	3.103876000	-0.404802000	-2.165004000
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C	-3.257188000	-3.270280000	-5.183078000	H	1.195835000	0.124504000	3.356713000
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C	-3.006320000	-3.192221000	-3.809604000	H	-1.318985000	1.286085000	3.485575000
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N	-0.263404000	0.061909000	5.646993000	O	0.077928000	-0.208570000	-0.811363000
N	2.290853000	-0.002394000	4.094150000	H	0.886035000	-0.383632000	-1.324723000
C	0.966005000	0.846249000	5.994806000	H	-0.543865000	0.159721000	-1.463677000
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H	3.364955000	0.440512000	7.212068000	H	-0.057163000	-0.550652000	2.377364000
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C	4.602850000	-0.503031000	4.177337000	H	-3.867776000	-4.193472000	3.573552000
C	3.405031000	-0.409827000	3.481010000	H	5.413881000	-1.242815000	-2.700088000
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C	-3.334380000	-3.402532000	5.515599000	C	1.383383000	-1.442838000	-6.204024000
H	-4.246752000	-3.739701000	5.997416000	H	0.840376000	-2.388337000	-6.071853000
C	-3.125162000	-3.674833000	4.161717000	H	1.760366000	-1.429896000	-7.237353000
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N	-1.623163000	2.126297000	4.001823000	C	3.778735000	-1.911296000	-5.599299000
C	-1.506314000	0.801400000	6.060938000	H	3.922399000	-2.313914000	-6.597016000
H	-2.357477000	0.148652000	5.847157000	C	4.822369000	-1.867697000	-4.690481000
H	-1.442642000	0.964949000	7.137845000	H	5.806496000	-2.230315000	-4.971440000
C	-1.685464000	2.106231000	5.348379000	C	4.615194000	-1.306975000	-3.424237000
C	-1.979678000	3.289105000	6.002761000	C	3.333032000	-0.834806000	-3.136536000
C	-2.193269000	4.452181000	5.265762000	N	0.014703000	1.683939000	-4.169203000

C	0.974047000	0.958229000	-6.285103000	H	-1.442641000	0.964950000	7.137845000
H	2.050839000	0.960110000	-6.075872000	C	-1.685464000	2.106230000	5.348377000
H	0.851962000	1.184260000	-7.353644000	C	-1.979678000	3.289105000	6.002761000
C	0.317628000	2.019053000	-5.446436000	C	-2.193269000	4.452181000	5.265762000
C	0.050777000	3.276738000	-5.963562000	H	-2.425356000	5.379334000	5.780653000
C	-0.556030000	4.230087000	-5.159640000	C	-2.073150000	4.442415000	3.873564000
H	-0.808341000	5.206062000	-5.562243000	C	-1.774623000	3.229973000	3.267534000
C	-0.887424000	3.902714000	-3.839527000	H	0.297593000	3.492390000	-6.998480000
C	-0.568838000	2.617157000	-3.394169000	H	-1.661639000	3.106943000	2.197193000
N	-1.437327000	-1.403486000	-4.208971000	H	3.104014000	-0.405037000	-2.164677000
C	-0.895041000	-0.592429000	-6.441094000	H	3.309496000	-0.625151000	2.423007000
H	-1.416015000	0.372807000	-6.459774000	H	-0.778478000	2.320126000	-2.369460000
H	-0.892239000	-0.976539000	-7.470323000	H	-2.036300000	3.296332000	7.085066000
C	-1.657712000	-1.523014000	-5.538130000	H	-1.879558000	-2.106059000	-2.316842000
C	-2.567330000	-2.435620000	-6.050902000	H	-1.642682000	-3.456870000	2.574467000
H	-2.716498000	-2.498576000	-7.124190000	Co	0.303670000	-0.343725000	-3.831021000
C	-3.257186000	-3.270281000	-5.183078000	H	0.978527000	0.116310000	3.182743000
H	-3.958450000	-4.005015000	-5.567373000	H	-0.175003000	-2.295864000	3.882048000
C	-3.006320000	-3.192221000	-3.809604000	H	-1.332681000	1.283398000	3.484653000
C	-2.088602000	-2.233406000	-3.375629000	H	-0.273309000	-0.041714000	4.613915000
N	-0.263401000	0.061907000	5.647001000	O	0.028545000	-0.206917000	-0.831112000
N	2.290772000	-0.002321000	4.093389000	H	0.838131000	-0.416410000	-1.331266000
C	0.966004000	0.846294000	5.994799000	H	-0.609435000	0.088861000	-1.505824000
H	0.808299000	1.867988000	5.633996000	O	0.528100000	1.700553000	0.719176000
H	1.041734000	0.870392000	7.082772000	H	0.332560000	0.964816000	-0.004931000
C	2.233115000	0.305006000	5.406877000	H	-0.136016000	2.406324000	0.602064000
C	3.394090000	0.206006000	6.154170000	O	0.041779000	0.259061000	2.762489000
H	3.364955000	0.440512000	7.212068000	H	-0.184856000	-0.562658000	2.294048000
C	4.579563000	-0.180894000	5.537858000	H	0.316254000	1.216753000	1.610555000
H	5.490518000	-0.252075000	6.123753000	H	-3.503464000	-3.848792000	-3.110918000
C	4.602849000	-0.503037000	4.177339000	H	-3.867776000	-4.193472000	3.573552000
C	3.405203000	-0.409909000	3.481378000	H	5.413881000	-1.242815000	-2.700088000
N	-1.043109000	-2.579370000	4.339298000	H	5.514930000	-0.811815000	3.688294000
C	-0.230499000	-1.320859000	6.251399000	H	-1.370883000	4.617071000	-3.189640000
H	0.774605000	-1.721200000	6.092129000	H	-2.207123000	5.342684000	3.292215000
H	-0.410754000	-1.213229000	7.322003000				
C	-1.253364000	-2.210718000	5.620534000	TS2	E= -2206.05569999		
C	-2.407880000	-2.651555000	6.238766000	Nimag=	-2218.71		
H	-2.589697000	-2.382804000	7.272829000	N	0.451841000	-0.357885000	-5.934138000
C	-3.334380000	-3.402532000	5.515599000	N	2.315886000	-0.877980000	-4.011806000
H	-4.246752000	-3.739701000	5.997416000	C	1.383384000	-1.442828000	-6.204030000
C	-3.125162000	-3.674832000	4.161717000	H	0.840376000	-2.388337000	-6.071856000
C	-1.926638000	-3.253892000	3.599778000	H	1.760366000	-1.429896000	-7.237353000
N	-1.623163000	2.126297000	4.001823000	C	2.537795000	-1.404770000	-5.236117000
C	-1.506315000	0.801400000	6.060937000	C	3.778734000	-1.911297000	-5.599299000
H	-2.357477000	0.148653000	5.847155000	H	3.922399000	-2.313914000	-6.597016000

C	4.822369000	-1.867697000	-4.690481000	C	-3.125163000	-3.674832000	4.161717000
H	5.806496000	-2.230315000	-4.971440000	C	-1.926640000	-3.253890000	3.599780000
C	4.615191000	-1.306986000	-3.424233000	N	-1.623163000	2.126296000	4.001823000
C	3.333128000	-0.834766000	-3.136535000	C	-1.506314000	0.801401000	6.060935000
N	0.014695000	1.683956000	-4.169202000	H	-2.357477000	0.148652000	5.847156000
C	0.974065000	0.958228000	-6.285101000	H	-1.442641000	0.964951000	7.137845000
H	2.050839000	0.960111000	-6.075869000	C	-1.685464000	2.106230000	5.348377000
H	0.851964000	1.184258000	-7.353644000	C	-1.979678000	3.289105000	6.002761000
C	0.317590000	2.019039000	-5.446450000	C	-2.193269000	4.452181000	5.265762000
C	0.050785000	3.276741000	-5.963559000	H	-2.425356000	5.379334000	5.780653000
C	-0.556030000	4.230087000	-5.159640000	C	-2.073150000	4.442415000	3.873564000
H	-0.808341000	5.206062000	-5.562243000	C	-1.774623000	3.229973000	3.267534000
C	-0.887406000	3.902721000	-3.839521000	H	0.297593000	3.492390000	-6.998480000
C	-0.568928000	2.617171000	-3.394178000	H	-1.661640000	3.106943000	2.197193000
N	-1.437313000	-1.403488000	-4.208964000	H	3.103953000	-0.405059000	-2.164751000
C	-0.895042000	-0.592427000	-6.441095000	H	3.309513000	-0.625084000	2.422992000
H	-1.416014000	0.372807000	-6.459776000	H	-0.778382000	2.320088000	-2.369440000
H	-0.892239000	-0.976537000	-7.470324000	H	-2.036300000	3.296332000	7.085066000
C	-1.657697000	-1.523025000	-5.538131000	H	-1.879557000	-2.106060000	-2.316842000
C	-2.567334000	-2.435616000	-6.050902000	H	-1.642682000	-3.456871000	2.574467000
H	-2.716498000	-2.498576000	-7.124190000	Co	0.300455000	-0.309804000	-3.675749000
C	-3.257186000	-3.270281000	-5.183078000	H	0.896156000	0.107350000	3.123682000
H	-3.958450000	-4.005015000	-5.567373000	H	-0.168456000	-2.306435000	3.888929000
C	-3.006320000	-3.192221000	-3.809604000	H	-1.324875000	1.283221000	3.484383000
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N	-0.263402000	0.061910000	5.646995000	O	0.297839000	-0.687319000	-0.625634000
N	2.290693000	-0.002294000	4.093427000	H	0.449924000	-0.555721000	-1.662138000
C	0.965984000	0.846206000	5.994831000	H	-0.569834000	-1.133290000	-0.558565000
H	0.808300000	1.867987000	5.633993000	O	0.110036000	1.519035000	0.430200000
H	1.041732000	0.870396000	7.082772000	H	0.181166000	0.323457000	-0.191444000
C	2.233214000	0.305158000	5.406839000	H	-0.766724000	1.894723000	0.241346000
C	3.394086000	0.205988000	6.154174000	O	-0.055578000	0.214338000	2.781766000
H	3.364955000	0.440512000	7.212068000	H	-0.272147000	-0.598482000	2.295832000
C	4.579563000	-0.180894000	5.537858000	H	0.065829000	1.228576000	1.380029000
H	5.490518000	-0.252075000	6.123753000	H	-3.503464000	-3.848792000	-3.110918000
C	4.602852000	-0.503019000	4.177334000	H	-3.867776000	-4.193472000	3.573552000
C	3.405158000	-0.410067000	3.481400000	H	5.413881000	-1.242815000	-2.700088000
N	-1.043105000	-2.579369000	4.339296000	H	5.514930000	-0.811815000	3.688294000
C	-0.230500000	-1.320857000	6.251401000	H	-1.370883000	4.617071000	-3.189640000
H	0.774606000	-1.721200000	6.092129000	H	-2.207123000	5.342684000	3.292215000
H	-0.410754000	-1.213229000	7.322003000				
C	-1.253365000	-2.210721000	5.620534000	PC	E= -2206.05885376		
C	-2.407880000	-2.651556000	6.238767000	N	0.451841000	-0.357885000	-5.934138000
H	-2.589697000	-2.382804000	7.272829000	N	2.315848000	-0.877962000	-4.011725000
C	-3.334380000	-3.402532000	5.515599000	C	1.383388000	-1.442815000	-6.204035000
H	-4.246752000	-3.739701000	5.997416000	H	0.840376000	-2.388337000	-6.071856000

H	1.760366000	-1.429896000	-7.237353000	C	-2.407880000	-2.651556000	6.238767000
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H	3.922399000	-2.313914000	-6.597016000	H	-4.246752000	-3.739701000	5.997416000
C	4.822369000	-1.867697000	-4.690481000	C	-3.125163000	-3.674832000	4.161717000
H	5.806496000	-2.230315000	-4.971440000	C	-1.926641000	-3.253889000	3.599781000
C	4.615188000	-1.306995000	-3.424231000	N	-1.623127000	2.126226000	4.001728000
C	3.333164000	-0.834721000	-3.136579000	C	-1.506304000	0.801411000	6.060944000
N	0.014702000	1.683992000	-4.169150000	H	-2.357477000	0.148651000	5.847157000
C	0.974060000	0.958226000	-6.285103000	H	-1.442645000	0.964943000	7.137846000
H	2.050839000	0.960111000	-6.075869000	C	-1.685463000	2.106253000	5.348375000
H	0.851964000	1.184258000	-7.353644000	C	-1.979673000	3.289106000	6.002761000
C	0.317590000	2.019024000	-5.446454000	C	-2.193269000	4.452181000	5.265762000
C	0.050784000	3.276741000	-5.963559000	H	-2.425356000	5.379334000	5.780653000
C	-0.556030000	4.230087000	-5.159640000	C	-2.073141000	4.442417000	3.873565000
H	-0.808341000	5.206062000	-5.562243000	C	-1.774667000	3.229975000	3.267546000
C	-0.887406000	3.902721000	-3.839521000	H	0.297593000	3.492390000	-6.998480000
C	-0.568931000	2.617176000	-3.394187000	H	-1.661632000	3.106945000	2.197194000
N	-1.437288000	-1.403374000	-4.208885000	H	3.103951000	-0.405066000	-2.164748000
C	-0.895057000	-0.592414000	-6.441094000	H	3.309507000	-0.625109000	2.422998000
H	-1.416014000	0.372807000	-6.459776000	H	-0.778375000	2.320091000	-2.369438000
H	-0.892239000	-0.976537000	-7.470324000	H	-2.036300000	3.296332000	7.085066000
C	-1.657638000	-1.523106000	-5.538133000	H	-1.879547000	-2.106069000	-2.316843000
C	-2.567338000	-2.435612000	-6.050902000	H	-1.642682000	-3.456872000	2.574467000
H	-2.716498000	-2.498576000	-7.124190000	Co	0.308037000	-0.311964000	-3.704269000
C	-3.257186000	-3.270281000	-5.183078000	H	0.879110000	0.113126000	3.109699000
H	-3.958450000	-4.005015000	-5.567373000	H	-0.174627000	-2.295112000	3.883412000
C	-3.006303000	-3.192236000	-3.809606000	H	-1.325583000	1.282344000	3.484202000
C	-2.088666000	-2.233374000	-3.375648000	H	-0.272450000	-0.045443000	4.608837000
N	-0.263340000	0.061919000	5.646946000	O	0.053564000	-0.641283000	-0.533984000
N	2.290575000	-0.002431000	4.093362000	H	0.269403000	-0.364740000	-1.971255000
C	0.965964000	0.846191000	5.994853000	H	-0.886021000	-0.894311000	-0.574569000
H	0.808300000	1.867987000	5.633993000	O	0.004923000	1.774147000	0.505381000
H	1.041735000	0.870392000	7.082772000	H	0.043576000	0.308071000	-0.186416000
C	2.233225000	0.305223000	5.406822000	H	-0.904299000	2.051777000	0.312633000
C	3.394092000	0.206016000	6.154168000	O	-0.078475000	0.200089000	2.792444000
H	3.364955000	0.440512000	7.212068000	H	-0.266210000	-0.585635000	2.252896000
C	4.579563000	-0.180894000	5.537858000	H	-0.041049000	1.407242000	1.417857000
H	5.490518000	-0.252075000	6.123753000	H	-3.503464000	-3.848792000	-3.110918000
C	4.602859000	-0.502986000	4.177326000	H	-3.867776000	-4.193472000	3.573552000
C	3.405173000	-0.410057000	3.481421000	H	5.413881000	-1.242815000	-2.700088000
N	-1.043103000	-2.579368000	4.339295000	H	5.514930000	-0.811815000	3.688294000
C	-0.230499000	-1.320850000	6.251414000	H	-1.370883000	4.617071000	-3.189640000
H	0.774605000	-1.721201000	6.092126000	H	-2.207123000	5.342684000	3.292215000
H	-0.410754000	-1.213229000	7.322003000				
C	-1.253362000	-2.210725000	5.620532000				

full PC E= -4157.44015991

N	0.321053000	-0.369746000	-5.738264000	N	-1.409461000	-1.637686000	-4.111241000
N	2.168308000	-1.000963000	-3.900073000	C	-1.029767000	-0.577708000	-6.255855000
C	1.213485000	-1.479161000	-6.073365000	H	-1.568134000	0.376571000	-6.206660000
H	0.656132000	-2.416282000	-5.953448000	H	-1.019383000	-0.890551000	-7.307722000
H	1.550666000	-1.430805000	-7.116774000	C	-1.752247000	-1.582090000	-5.410383000
C	2.384818000	-1.481273000	-5.138124000	C	-2.744212000	-2.400817000	-5.931586000
C	3.631447000	-1.954267000	-5.521816000	H	-2.991140000	-2.343177000	-6.986414000
H	3.778190000	-2.330925000	-6.528562000	C	-3.384761000	-3.296393000	-5.092433000
C	4.676430000	-1.901640000	-4.615420000	H	-4.143799000	-3.963549000	-5.489615000
H	5.666714000	-2.236953000	-4.908541000	C	-3.026204000	-3.371139000	-3.741002000
C	4.471179000	-1.367294000	-3.337608000	C	-2.025072000	-2.506354000	-3.298173000
C	3.181040000	-0.938150000	-3.024068000	C	-3.686363000	-4.348813000	-2.853693000
C	5.609616000	-1.237820000	-2.406361000	C	-5.060580000	-4.582167000	-2.993973000
C	6.570368000	-2.255706000	-2.343584000	H	-5.640375000	-3.991841000	-3.697317000
H	6.420996000	-3.175706000	-2.901149000	C	-5.696642000	-5.550068000	-2.231442000
C	7.713595000	-2.104114000	-1.572753000	H	-6.768312000	-5.691959000	-2.350442000
H	8.437430000	-2.915104000	-1.537520000	C	-4.967528000	-6.319178000	-1.320891000
C	7.927532000	-0.922667000	-0.857922000	C	-3.602824000	-6.079051000	-1.160082000
C	6.957781000	0.079418000	-0.884557000	H	-3.034427000	-6.666762000	-0.444650000
H	7.115752000	0.994948000	-0.321311000	C	-2.967736000	-5.097068000	-1.913674000
C	5.803890000	-0.078994000	-1.645613000	H	-1.899116000	-4.938486000	-1.797385000
H	5.073970000	0.724646000	-1.688557000	C	-5.659245000	-7.366832000	-0.483453000
C	9.194976000	-0.731170000	-0.062152000	C	-6.605060000	-6.697486000	0.531724000
C	9.240879000	-1.695141000	1.135368000	N	-0.199531000	0.105224000	5.558861000
N	-0.118477000	1.706931000	-4.072050000	N	2.237646000	0.152450000	4.191271000
C	0.871531000	0.922950000	-6.142977000	C	0.956993000	0.878708000	6.116246000
H	1.953436000	0.908537000	-5.962844000	H	0.777334000	1.932844000	5.882923000
H	0.723843000	1.111324000	-7.214035000	H	0.946155000	0.751767000	7.199956000
C	0.261754000	2.020446000	-5.323426000	C	2.250747000	0.422974000	5.503105000
C	0.115409000	3.306988000	-5.822883000	C	3.410282000	0.337342000	6.264404000
C	-0.445312000	4.280047000	-5.014405000	H	3.381580000	0.553235000	7.327326000
H	-0.595408000	5.283740000	-5.400298000	C	4.594247000	-0.030633000	5.637286000
C	-0.862905000	3.961669000	-3.715684000	H	5.515203000	-0.105030000	6.208029000
C	-0.669759000	2.646594000	-3.289147000	C	4.586214000	-0.340337000	4.275208000
C	-1.514995000	4.999433000	-2.889684000	C	3.367100000	-0.234681000	3.602220000
C	-1.050015000	6.320025000	-2.957352000	C	5.800232000	-0.736069000	3.540810000
H	-0.150054000	6.548351000	-3.520568000	C	6.995616000	-0.035057000	3.725093000
C	-1.727688000	7.346706000	-2.316835000	H	7.035107000	0.789721000	4.430808000
H	-1.341128000	8.360560000	-2.392695000	C	8.120922000	-0.349310000	2.973622000
C	-2.896871000	7.078596000	-1.599413000	H	9.018126000	0.247776000	3.113322000
C	-3.335597000	5.759419000	-1.481200000	C	8.078429000	-1.395995000	2.049271000
H	-4.233652000	5.540959000	-0.910098000	C	6.898873000	-2.126102000	1.893127000
C	-2.647810000	4.727033000	-2.113490000	H	6.865282000	-2.949297000	1.185156000
H	-3.028050000	3.711498000	-2.046172000	C	5.765802000	-1.791054000	2.621228000
C	-3.684485000	8.205729000	-0.972389000	H	4.851318000	-2.361883000	2.487442000
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H	0.844124000	-1.694271000	5.853132000	H	-1.385492000	3.271325000	2.114887000
H	-0.352388000	-1.305353000	7.113011000	H	2.942091000	-0.537159000	-2.043862000
C	-1.182814000	-2.172023000	5.350287000	H	3.304661000	-0.444752000	2.537282000
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C	-3.126017000	-3.578676000	5.297446000	H	-1.710237000	-2.492899000	-2.259424000
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C	-4.008560000	-4.426564000	3.093548000	H	10.470238000	-1.886196000	-1.294868000
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H	-3.863562000	-6.212763000	4.290821000	H	9.187252000	-2.728226000	0.783609000
C	-5.181721000	-6.481411000	2.616609000	H	10.803921000	-0.610150000	2.058295000
H	-5.368263000	-7.521667000	2.868531000	H	11.311503000	-2.033890000	1.374388000
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C	-5.494202000	-4.555937000	1.194697000	H	-6.722770000	-9.156241000	-0.888588000
H	-5.960427000	-4.088433000	0.332673000	H	-4.924225000	-7.969842000	0.056010000
C	-4.602241000	-3.833633000	1.974645000	H	-6.875546000	-8.493288000	1.616314000
H	-4.379797000	-2.799458000	1.727560000	H	-8.185506000	-8.085278000	0.680707000
N	-1.465140000	2.191230000	3.860667000	H	-7.316988000	-6.053174000	0.009267000
C	-1.517349000	0.756743000	5.852983000	H	-4.634177000	7.832610000	-0.580387000
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C	-1.692079000	2.085785000	5.185101000	H	-1.935784000	9.239498000	-0.215121000
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C	-1.619122000	3.324952000	3.172514000	H	10.247416000	-0.329814000	-1.814050000
C	-2.252171000	5.686949000	2.979293000	H	10.461980000	-2.057261000	2.787686000
C	-3.450712000	6.403122000	3.012250000	H	-7.883428000	-7.262110000	2.077581000
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C	-3.657173000	7.455485000	2.128662000	H	0.960163000	0.331575000	2.948168000
H	-4.622208000	7.954590000	2.132025000	H	-0.317769000	-1.903336000	3.507948000
C	-2.649313000	7.830249000	1.236973000	H	-1.089558000	1.387888000	3.318140000
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H	-0.642200000	7.450542000	0.560015000	O	-0.281815000	-0.574646000	-0.378007000
C	-1.236965000	6.076724000	2.098972000	H	0.144605000	-0.374270000	-1.860218000
H	-0.293731000	5.538112000	2.086352000	H	-1.156405000	-0.971415000	-0.538797000
N	-3.591807000	10.059593000	0.729350000	O	-0.480963000	1.981757000	0.310159000
N	-4.048392000	9.191917000	-2.044929000	H	-0.458356000	0.400800000	-0.218514000
N	10.371121000	-0.913991000	-0.978563000	H	0.252798000	2.422915000	-0.146651000
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H	-7.495039000	1.076687000	1.503791000
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H	-3.587376000	-6.497752000	-1.217325000
C	-2.188825000	-7.011592000	-2.753544000
H	-2.226151000	-8.070261000	-2.507783000
C	-1.375743000	-6.548984000	-3.792631000
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C	4.083650000	-0.085161000	4.825802000
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H	4.394943000	-1.170251000	7.279186000
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C	1.544667000	0.426799000	8.218230000
C	1.280118000	1.112865000	7.030378000
H	0.418715000	1.770342000	6.965582000
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H	5.883543000	1.829621000	1.374993000
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C	5.452608000	2.481262000	-0.618653000
C	6.092674000	3.222265000	-1.593768000
H	7.171260000	3.160364000	-1.681210000
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C	3.398616000	6.187246000	-3.517064000
H	4.247395000	6.653716000	-3.026023000
C	2.577316000	6.943583000	-4.344004000
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C	1.483869000	6.352840000	-4.981172000
C	1.214126000	4.998736000	-4.771602000
H	0.374752000	4.529700000	-5.276164000
C	2.006983000	4.252359000	-3.911535000
H	1.787979000	3.200614000	-3.749793000
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C	6.272547000	-0.364972000	-1.217896000
H	6.050492000	0.414634000	-1.951100000
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H	-6.939711000	1.898436000	3.586103000	C	-5.351767000	3.543499000	-3.458580000
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H	-1.983507000	1.403360000	8.295530000	C	-1.532061000	6.757307000	-4.374541000
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C	-1.423264000	-1.285767000	6.286163000	H	-0.910925000	6.975521000	-2.326829000
H	-0.897278000	-2.236303000	6.272572000	C	-2.295999000	5.346980000	-2.566128000
C	-2.166549000	-0.886879000	5.179930000	H	-2.303487000	5.102610000	-1.507527000
H	-2.231788000	-1.540800000	4.314817000	C	-0.692570000	7.908900000	-4.870779000
C	-0.620443000	-0.948082000	8.650001000	C	0.497459000	7.391712000	-5.700387000
C	0.575245000	-0.023608000	8.916273000	N	6.106774000	0.416069000	0.027632000
N	-4.528480000	-1.684005000	-0.567301000	N	4.685665000	0.040433000	2.135724000
C	-6.660707000	-1.021330000	0.342145000	C	6.789498000	-0.416085000	1.065544000
H	-6.581958000	-1.086631000	1.433531000	H	6.885412000	-1.434653000	0.679624000
H	-7.713789000	-1.173138000	0.081054000	H	7.791892000	-0.019306000	1.238908000
C	-5.784973000	-2.067629000	-0.267391000	C	5.931472000	-0.405680000	2.304798000
C	-6.204462000	-3.370760000	-0.484471000	C	6.406387000	-0.868038000	3.526711000
C	-5.310375000	-4.281457000	-1.023088000	H	7.427268000	-1.223486000	3.622785000
H	-5.630395000	-5.300463000	-1.217595000	C	5.543124000	-0.849780000	4.611735000
C	-4.008221000	-3.883757000	-1.352899000	H	5.883925000	-1.190143000	5.585179000
C	-3.661960000	-2.558048000	-1.102213000	C	4.241346000	-0.356649000	4.458108000
C	-3.061637000	-4.843404000	-1.954997000	C	3.865045000	0.073786000	3.185493000
C	-3.046579000	-6.169322000	-1.504146000	C	3.299694000	-0.279769000	5.589232000
H	-3.675805000	-6.464644000	-0.669701000	C	3.208326000	-1.330748000	6.508976000
C	-2.223892000	-7.110543000	-2.104353000	H	3.815059000	-2.221224000	6.372539000
H	-2.224507000	-8.128658000	-1.722494000	C	2.326852000	-1.257269000	7.578858000
C	-1.410216000	-6.750422000	-3.181944000	H	2.257194000	-2.100504000	8.261917000
C	-1.398764000	-5.425544000	-3.617696000	C	1.541853000	-0.116190000	7.763813000
H	-0.760902000	-5.138355000	-4.448823000	C	1.624435000	0.932644000	6.848871000
C	-2.211639000	-4.476965000	-3.004935000	H	1.011152000	1.818234000	6.988776000
H	-2.214444000	-3.455171000	-3.373697000	C	2.489318000	0.848292000	5.765233000
C	-0.547958000	-7.784697000	-3.864100000	H	2.559913000	1.678125000	5.067918000
C	0.580738000	-8.253395000	-2.928837000	N	4.355160000	2.809089000	-0.528469000
N	-4.533599000	1.713115000	-1.572459000	C	6.514171000	1.852460000	0.154714000
C	-6.693923000	0.652472000	-1.423977000	H	6.405152000	2.116329000	1.210907000
H	-6.656937000	-0.250678000	-2.044415000	H	7.565048000	1.927754000	-0.126483000
H	-7.737164000	0.985824000	-1.385277000	C	5.693335000	2.758843000	-0.706096000
C	-5.806042000	1.698834000	-2.016046000	C	6.246889000	3.562200000	-1.684884000

H	7.318757000	3.537678000	-1.842792000
C	5.424676000	4.369033000	-2.464693000
H	5.861175000	4.993897000	-3.237516000
C	4.037314000	4.345671000	-2.295971000
C	3.528670000	3.540971000	-1.285570000
C	3.130121000	5.131470000	-3.151276000
C	3.370886000	6.489709000	-3.367357000
H	4.210621000	6.976852000	-2.880873000
C	2.519306000	7.229655000	-4.177724000
H	2.718183000	8.290826000	-4.298090000
C	1.444633000	6.611158000	-4.820297000
C	1.214103000	5.248686000	-4.617450000
H	0.388675000	4.757566000	-5.123942000
C	2.037730000	4.517435000	-3.772519000
H	1.854858000	3.457058000	-3.623893000
N	4.183286000	-1.381569000	-1.543186000
C	6.265789000	-0.107129000	-1.366362000
H	5.880191000	0.649352000	-2.055487000
H	7.332785000	-0.240524000	-1.549824000
C	5.534157000	-1.395572000	-1.575872000
C	6.160975000	-2.597871000	-1.842807000
C	5.399112000	-3.742352000	-2.061942000
H	5.895902000	-4.684477000	-2.271902000
C	4.003931000	-3.695828000	-1.986149000
C	3.419004000	-2.464432000	-1.718536000
C	3.155258000	-4.880338000	-2.204859000
C	3.396772000	-5.715225000	-3.298555000
H	4.208068000	-5.489560000	-3.984170000
C	2.574808000	-6.808263000	-3.540773000
H	2.766986000	-7.408669000	-4.425346000
C	1.525744000	-7.105344000	-2.667667000
C	1.300046000	-6.286212000	-1.559503000
H	0.491096000	-6.519012000	-0.873249000
C	2.096639000	-5.170877000	-1.337719000
H	1.912868000	-4.539568000	-0.473042000
N	1.323136000	-9.425291000	-3.494470000
N	-1.417269000	-8.927185000	-4.305413000
N	-1.570340000	-1.002347000	9.811781000
N	1.283602000	-0.360604000	10.194077000
N	1.228478000	8.509944000	-6.373158000
N	-1.560801000	8.839298000	-5.671552000
H	-7.223663000	-3.655203000	-0.246599000
H	2.348689000	-2.307420000	-1.665773000
H	-2.548202000	0.019769000	2.458148000
H	2.859796000	0.443698000	3.001834000
H	-2.669301000	-2.179093000	-1.318057000

H	7.243717000	-2.632090000	-1.876630000
H	-2.664159000	2.591489000	-1.624229000
H	2.474615000	3.477213000	-1.044087000
Co	-4.144241000	0.257572000	-0.190709000
H	-0.268480000	-1.973413000	8.513313000
H	-1.865374000	-0.066307000	10.116272000
H	-1.173291000	-1.490129000	10.623312000
H	0.231071000	1.006182000	9.037486000
H	1.503640000	-1.361569000	10.268110000
H	0.743430000	-0.091889000	11.024495000
H	-1.821027000	8.445230000	-6.584285000
H	-1.113879000	9.748746000	-5.836980000
H	-0.319296000	8.500950000	-4.031431000
H	1.452732000	9.282097000	-5.733495000
H	0.695171000	8.899674000	-7.158971000
H	0.125536000	6.757451000	-6.509142000
H	-0.112662000	-7.373697000	-4.778307000
H	-1.741378000	-9.500292000	-3.516341000
H	-0.946154000	-9.546646000	-4.975025000
H	0.153496000	-8.609033000	-1.988211000
H	1.580381000	-9.296726000	-4.481026000
H	0.780215000	-10.294047000	-3.422926000
H	2.191716000	-9.576505000	-2.968880000
H	-2.250750000	-8.558870000	-4.779609000
H	-2.415018000	-1.518599000	9.539395000
H	2.172710000	0.151854000	10.239180000
H	2.114114000	8.162459000	-6.762888000
H	-2.430478000	9.026437000	-5.158231000
H	3.929436000	2.270854000	0.226357000
H	3.701396000	-0.495872000	-1.388282000
H	5.109558000	0.368550000	0.343938000
H	-2.632004000	0.170603000	-0.274867000

CoCo

full RC E= -4301.32586022

N	-6.410830000	-0.004525000	0.134781000
N	-4.632992000	0.379897000	2.146456000
C	-6.796394000	0.951979000	1.162689000
H	-6.693478000	1.958455000	0.735118000
H	-7.845295000	0.840118000	1.474718000
C	-5.885310000	0.839184000	2.360490000
C	-6.310801000	1.220557000	3.626644000
H	-7.328729000	1.570251000	3.767735000
C	-5.432074000	1.134814000	4.695687000
H	-5.757454000	1.411511000	5.694210000
C	-4.134988000	0.650482000	4.486921000

C	-3.789448000	0.289706000	3.185325000	C	-3.125177000	4.231262000	-3.288160000
C	-3.184308000	0.511432000	5.606473000	C	-3.140017000	4.643218000	-4.625677000
C	-3.141312000	1.485431000	6.612087000	H	-3.807944000	4.158143000	-5.331585000
H	-3.770189000	2.367591000	6.536278000	C	-2.302649000	5.660400000	-5.061110000
C	-2.291366000	1.344603000	7.699699000	H	-2.323121000	5.943717000	-6.110613000
H	-2.273606000	2.124466000	8.457677000	C	-1.458300000	6.311374000	-4.158104000
C	-1.479108000	0.213338000	7.815253000	C	-1.416367000	5.886638000	-2.830078000
C	-1.499914000	-0.751193000	6.807981000	H	-0.752405000	6.382026000	-2.127047000
H	-0.865531000	-1.629216000	6.891534000	C	-2.233076000	4.845593000	-2.401400000
C	-2.339617000	-0.600732000	5.709936000	H	-2.214193000	4.539540000	-1.359110000
H	-2.367582000	-1.373397000	4.946710000	C	-0.581591000	7.450532000	-4.615536000
C	-0.572460000	0.039159000	9.007698000	C	0.597688000	6.900741000	-5.429646000
C	0.592390000	1.035640000	8.929194000	N	6.301314000	-0.024207000	0.098820000
N	-4.516245000	-1.888922000	-0.392335000	N	4.593514000	-0.219836000	2.151517000
C	-6.728660000	-1.386357000	0.480920000	C	6.718503000	-0.878552000	1.209307000
H	-6.610263000	-1.496899000	1.565842000	H	6.607760000	-1.924725000	0.898427000
H	-7.769370000	-1.647620000	0.243025000	H	7.775264000	-0.726831000	1.465808000
C	-5.780959000	-2.331710000	-0.205256000	C	5.843970000	-0.635174000	2.404143000
C	-6.185045000	-3.595245000	-0.607455000	C	6.284950000	-0.848960000	3.704281000
C	-5.276423000	-4.431538000	-1.240497000	H	7.304601000	-1.175231000	3.881026000
H	-5.583647000	-5.411870000	-1.591839000	C	5.411729000	-0.623615000	4.756612000
C	-3.974346000	-3.974858000	-1.473579000	H	5.744775000	-0.769843000	5.779955000
C	-3.643855000	-2.698613000	-1.016644000	C	4.112911000	-0.167763000	4.500554000
C	-3.024298000	-4.816578000	-2.226083000	C	3.754433000	0.015541000	3.166382000
C	-2.981178000	-6.196118000	-1.988339000	C	3.169726000	0.116695000	5.598092000
H	-3.575758000	-6.622984000	-1.186113000	C	3.121310000	-0.728941000	6.712931000
C	-2.184242000	-7.024261000	-2.764291000	H	3.739677000	-1.621215000	6.741363000
H	-2.160482000	-8.088875000	-2.544681000	C	2.277455000	-0.447281000	7.777451000
C	-1.431144000	-6.492794000	-3.814229000	H	2.250928000	-1.131144000	8.622341000
C	-1.435886000	-5.115043000	-4.031947000	C	1.480591000	0.700591000	7.757746000
H	-0.837829000	-4.695465000	-4.836170000	C	1.505028000	1.534579000	6.640419000
C	-2.217614000	-4.281995000	-3.237961000	H	0.879911000	2.423063000	6.618524000
H	-2.239122000	-3.214136000	-3.436978000	C	2.336701000	1.241336000	5.565340000
C	-0.604020000	-7.398581000	-4.691201000	H	2.368247000	1.913670000	4.712565000
C	0.572936000	-7.968908000	-3.889280000	N	4.588908000	1.841780000	-0.743575000
N	-4.567233000	1.250603000	-1.508415000	C	6.712354000	1.366225000	0.295431000
C	-6.817559000	0.361215000	-1.218502000	H	6.585535000	1.618635000	1.355232000
H	-6.771749000	-0.546054000	-1.833403000	H	7.771813000	1.516070000	0.050565000
H	-7.853115000	0.725107000	-1.259854000	C	5.841967000	2.270094000	-0.526108000
C	-5.880686000	1.380720000	-1.811787000	C	6.283862000	3.487690000	-1.026716000
C	-6.339278000	2.384215000	-2.651350000	H	7.304060000	3.808592000	-0.843660000
H	-7.399062000	2.452238000	-2.876277000	C	5.413304000	4.261452000	-1.778374000
C	-5.438846000	3.305862000	-3.170724000	H	5.750074000	5.204130000	-2.199624000
H	-5.783770000	4.113584000	-3.809532000	C	4.113189000	3.807404000	-2.030688000
C	-4.088873000	3.216599000	-2.819105000	C	3.748662000	2.581988000	-1.475011000
C	-3.704615000	2.159560000	-1.993951000	C	3.179093000	4.584981000	-2.865804000

C	3.148466000	5.981310000	-2.768832000	H	-1.627784000	1.185897000	10.441264000
H	3.773657000	6.487179000	-2.038978000	H	-0.871421000	-0.141451000	11.096865000
C	2.311304000	6.728379000	-3.585142000	H	0.202427000	2.051556000	8.831949000
H	2.298757000	7.809455000	-3.471311000	H	1.690310000	0.093629000	10.477378000
C	1.502055000	6.093903000	-4.531391000	H	0.921418000	1.480182000	10.973920000
C	1.512595000	4.701986000	-4.620172000	H	-1.668528000	8.069424000	-6.327218000
H	0.878625000	4.205028000	-5.349257000	H	-0.917697000	9.324953000	-5.543332000
C	2.338180000	3.952904000	-3.789750000	H	-0.204830000	8.009853000	-3.755722000
H	2.357530000	2.871043000	-3.886884000	H	1.676119000	8.724984000	-5.424446000
N	4.596948000	-1.630909000	-1.229586000	H	0.876473000	8.440764000	-6.851777000
C	6.756897000	-0.541757000	-1.190758000	H	0.219916000	6.283200000	-6.248178000
H	6.698987000	0.269047000	-1.927462000	H	-0.223295000	-6.847778000	-5.554765000
H	7.804971000	-0.865445000	-1.151959000	H	-1.802712000	-9.140484000	-4.548677000
C	5.872133000	-1.662708000	-1.648109000	H	-1.006092000	-9.010986000	-6.001573000
C	6.331156000	-2.667115000	-2.490176000	H	0.202171000	-8.470347000	-2.992377000
C	5.453326000	-3.660663000	-2.891744000	H	1.552605000	-8.719761000	-5.611212000
H	5.799806000	-4.467418000	-3.531003000	H	0.799167000	-9.900022000	-4.720320000
C	4.129426000	-3.647258000	-2.437344000	H	2.205025000	-9.231017000	-4.177574000
C	3.749192000	-2.595758000	-1.605320000	H	-2.311077000	-8.051962000	-5.688118000
C	3.187890000	-4.717797000	-2.810894000	H	-2.241268000	-0.331634000	10.199733000
C	3.190748000	-5.225350000	-4.115052000	H	2.273023000	1.579321000	10.035440000
H	3.846642000	-4.789970000	-4.863145000	H	2.246260000	7.594985000	-6.493447000
C	2.347232000	-6.268538000	-4.468724000	H	-2.270658000	8.640986000	-4.894301000
H	2.357476000	-6.624846000	-5.495823000	O	-1.282111000	-0.108615000	0.350122000
C	1.503100000	-6.842732000	-3.515025000	H	-1.932257000	-0.790119000	0.588356000
C	1.483533000	-6.331501000	-2.217325000	H	-1.813604000	0.580188000	-0.082322000
H	0.820921000	-6.770146000	-1.476487000	O	0.372973000	-1.192632000	-1.512592000
C	2.311880000	-5.271154000	-1.869770000	H	-0.340576000	-0.835685000	-0.926950000
H	2.306180000	-4.895245000	-0.850663000	H	0.348568000	-0.619957000	-2.294570000
N	1.321426000	-9.017923000	-4.655591000	O	2.011055000	-0.008211000	0.216085000
N	-1.478465000	-8.476851000	-5.262402000	H	1.523157000	-0.477843000	-0.522161000
N	-1.369149000	0.206600000	10.268802000	H	1.736653000	-0.477672000	1.020230000
N	1.412807000	1.039451000	10.187144000				
N	1.391278000	7.992028000	-6.085031000	RC (a)	E= -2349.93574520		
N	-1.403494000	8.431299000	-5.402943000	N	-6.410830000	-0.004525000	0.134779000
H	-7.211921000	-3.907225000	-0.443744000	N	-4.632993000	0.379897000	2.146453000
H	2.730297000	-2.507056000	-1.240953000	C	-6.796394000	0.951980000	1.162689000
H	-2.793063000	-0.076639000	2.955354000	H	-6.693478000	1.958455000	0.735118000
H	2.757296000	0.352251000	2.899286000	H	-7.845295000	0.840118000	1.474718000
H	-2.638543000	-2.305653000	-1.148453000	C	-5.885310000	0.839184000	2.360490000
H	7.368439000	-2.671797000	-2.808242000	C	-6.310801000	1.220557000	3.626644000
H	-2.660735000	2.020908000	-1.725598000	H	-7.328729000	1.570251000	3.767735000
H	2.748109000	2.180618000	-1.606401000	C	-5.432074000	1.134814000	4.695687000
Co	4.073500000	-0.040714000	0.073403000	H	-5.757454000	1.411511000	5.694210000
Co	-4.291939000	0.086921000	0.144908000	C	-4.134988000	0.650482000	4.486921000
H	-0.182984000	-0.980907000	9.041428000	C	-3.789448000	0.289706000	3.185325000

N	-4.516244000	-1.888922000	-0.392334000
C	-6.728660000	-1.386357000	0.480920000
H	-6.610263000	-1.496899000	1.565842000
H	-7.769370000	-1.647620000	0.243025000
C	-5.780959000	-2.331710000	-0.205255000
C	-6.185045000	-3.595245000	-0.607454000
C	-5.276423000	-4.431537000	-1.240496000
H	-5.583648000	-5.411868000	-1.591842000
C	-3.974339000	-3.974868000	-1.473556000
C	-3.643855000	-2.698613000	-1.016632000
N	-4.567231000	1.250600000	-1.508422000
C	-6.817559000	0.361215000	-1.218502000
H	-6.771749000	-0.546054000	-1.833403000
H	-7.853115000	0.725107000	-1.259854000
C	-5.880686000	1.380718000	-1.811789000
C	-6.339278000	2.384214000	-2.651351000
H	-7.399062000	2.452238000	-2.876277000
C	-5.438846000	3.305862000	-3.170725000
H	-5.783770000	4.113585000	-3.809531000
C	-4.088874000	3.216600000	-2.819103000
C	-3.704620000	2.159540000	-1.993943000
N	6.301314000	-0.024207000	0.098820000
N	4.593522000	-0.219858000	2.151545000
C	6.718503000	-0.878551000	1.209307000
H	6.607760000	-1.924725000	0.898427000
H	7.775264000	-0.726831000	1.465808000
C	5.843983000	-0.635136000	2.404141000
C	6.284954000	-0.848946000	3.704282000
H	7.304601000	-1.175231000	3.881026000
C	5.411730000	-0.623613000	4.756612000
H	5.744775000	-0.769843000	5.779955000
C	4.112913000	-0.167758000	4.500554000
C	3.754432000	0.015519000	3.166387000
N	4.588841000	1.841728000	-0.743558000
C	6.712355000	1.366223000	0.295428000
H	6.585535000	1.618635000	1.355232000
H	7.771813000	1.516070000	0.050565000
C	5.841973000	2.270084000	-0.526123000
C	6.283863000	3.487688000	-1.026719000
H	7.304060000	3.808592000	-0.843660000
C	5.413304000	4.261452000	-1.778374000
H	5.750074000	5.204130000	-2.199625000
C	4.113188000	3.807406000	-2.030686000
C	3.748648000	2.581988000	-1.474995000
N	4.596925000	-1.630935000	-1.229582000
C	6.756896000	-0.541754000	-1.190762000

H	6.698987000	0.269047000	-1.927462000
H	7.804971000	-0.865445000	-1.151959000
C	5.872119000	-1.662671000	-1.648153000
C	6.331152000	-2.667106000	-2.490189000
C	5.453326000	-3.660662000	-2.891745000
H	5.799806000	-4.467418000	-3.531003000
C	4.129426000	-3.647258000	-2.437344000
C	3.749207000	-2.595780000	-1.605297000
H	-7.211921000	-3.907225000	-0.443744000
H	2.730304000	-2.507071000	-1.240930000
H	-2.793063000	-0.076639000	2.955354000
H	2.757289000	0.352231000	2.899285000
H	-2.638479000	-2.305620000	-1.148485000
H	7.368439000	-2.671797000	-2.808242000
H	-2.660724000	2.020985000	-1.725636000
H	2.748106000	2.180623000	-1.606393000
Co	4.080423000	-0.038792000	0.077742000
Co	-4.291926000	0.088951000	0.144850000
O	-1.272791000	-0.104652000	0.339510000
H	-1.924861000	-0.793709000	0.548422000
H	-1.804232000	0.607155000	-0.053685000
O	0.421263000	-0.911664000	-1.625815000
H	-0.310439000	-0.680357000	-1.000871000
H	0.372350000	-0.225204000	-2.309068000
O	2.025471000	0.033230000	0.258213000
H	1.526543000	-0.324193000	-0.535395000
H	1.756945000	-0.544916000	0.990608000
H	-3.351870000	3.924832000	-3.181139000
H	3.408001000	4.376249000	-2.625241000
H	-3.417944000	0.554192000	5.294375000
H	3.405273000	0.036051000	5.295551000
H	-3.233554000	-4.583194000	-1.980704000
H	3.416435000	-4.413805000	-2.717478000

PC (a) E= -2349.89079147

N	-6.410830000	-0.004525000	0.134779000
N	-4.633025000	0.379944000	2.146386000
C	-6.796408000	0.951939000	1.162696000
H	-6.693478000	1.958455000	0.735118000
H	-7.845295000	0.840118000	1.474718000
C	-5.885239000	0.839377000	2.360492000
C	-6.310818000	1.220507000	3.626653000
H	-7.328729000	1.570251000	3.767735000
C	-5.432074000	1.134814000	4.695687000
H	-5.757454000	1.411511000	5.694210000
C	-4.134989000	0.650478000	4.486922000

C	-3.789472000	0.289543000	3.185330000
N	-4.516234000	-1.888913000	-0.392205000
C	-6.728645000	-1.386379000	0.480971000
H	-6.610263000	-1.496899000	1.565842000
H	-7.769370000	-1.647620000	0.243025000
C	-5.781013000	-2.331645000	-0.205464000
C	-6.185041000	-3.595251000	-0.607441000
C	-5.276423000	-4.431537000	-1.240496000
H	-5.583648000	-5.411868000	-1.591842000
C	-3.974351000	-3.974851000	-1.473595000
C	-3.643767000	-2.698654000	-1.016456000
N	-4.567243000	1.250387000	-1.508499000
C	-6.817556000	0.361203000	-1.218519000
H	-6.771749000	-0.546054000	-1.833403000
H	-7.853115000	0.725107000	-1.259854000
C	-5.880689000	1.380801000	-1.811740000
C	-6.339280000	2.384224000	-2.651338000
H	-7.399062000	2.452238000	-2.876277000
C	-5.438846000	3.305862000	-3.170725000
H	-5.783770000	4.113585000	-3.809531000
C	-4.088879000	3.216618000	-2.819078000
C	-3.704640000	2.159557000	-1.993947000
N	6.301314000	-0.024207000	0.098820000
N	4.593578000	-0.219915000	2.151548000
C	6.718518000	-0.878505000	1.209309000
H	6.607760000	-1.924725000	0.898427000
H	7.775264000	-0.726831000	1.465808000
C	5.843911000	-0.635342000	2.404157000
C	6.284972000	-0.848889000	3.704285000
H	7.304601000	-1.175231000	3.881026000
C	5.411730000	-0.623613000	4.756612000
H	5.744775000	-0.769843000	5.779955000
C	4.112915000	-0.167753000	4.500554000
C	3.754435000	0.015669000	3.166355000
N	4.588847000	1.841812000	-0.743447000
C	6.712336000	1.366252000	0.295480000
H	6.585535000	1.618635000	1.355232000
H	7.771813000	1.516070000	0.050565000
C	5.842042000	2.269982000	-0.526318000
C	6.283854000	3.487702000	-1.026694000
H	7.304060000	3.808592000	-0.843660000
C	5.413304000	4.261452000	-1.778374000
H	5.750074000	5.204130000	-2.199625000
C	4.113201000	3.807387000	-2.030720000
C	3.748564000	2.582031000	-1.474856000
N	4.596877000	-1.630786000	-1.229709000

C	6.756894000	-0.541749000	-1.190770000
H	6.698987000	0.269047000	-1.927462000
H	7.804971000	-0.865445000	-1.151959000
C	5.872128000	-1.662707000	-1.648122000
C	6.331159000	-2.667122000	-2.490165000
C	5.453326000	-3.660662000	-2.891745000
H	5.799806000	-4.467418000	-3.531003000
C	4.129435000	-3.647276000	-2.437317000
C	3.749237000	-2.595814000	-1.605277000
H	-7.211921000	-3.907225000	-0.443744000
H	2.730303000	-2.507069000	-1.240933000
H	-2.793047000	-0.076589000	2.955345000
H	2.757272000	0.352180000	2.899283000
H	-2.638497000	-2.305594000	-1.148545000
H	7.368439000	-2.671797000	-2.808242000
H	-2.660726000	2.020992000	-1.725626000
H	2.748128000	2.180588000	-1.606453000
Co	4.047370000	-0.040488000	0.076928000
Co	-4.175293000	0.038520000	0.162030000
O	-1.093645000	-0.219301000	0.745361000
H	-2.488504000	-0.000283000	0.326784000
H	-0.822063000	0.697714000	0.927678000
O	0.343135000	-0.735864000	-1.373966000
H	-0.629896000	-0.447188000	-0.130406000
H	0.141005000	-0.021238000	-1.997536000
O	2.111802000	0.179616000	0.266593000
H	1.122419000	-0.374329000	-0.823206000
H	1.834557000	-0.406685000	0.986390000
H	-3.351870000	3.924832000	-3.181139000
H	3.408001000	4.376249000	-2.625241000
H	-3.417944000	0.554192000	5.294375000
H	3.405273000	0.036051000	5.295551000
H	-3.233554000	-4.583194000	-1.980704000
H	3.416435000	-4.413805000	-2.717478000

RC (b) E= -2350.36520021

N	-6.410826000	-0.004523000	0.134785000
N	-4.632987000	0.379895000	2.146456000
C	-6.796394000	0.951979000	1.162689000
H	-6.693478000	1.958455000	0.735118000
H	-7.845295000	0.840119000	1.474717000
C	-5.885308000	0.839189000	2.360492000
C	-6.310801000	1.220558000	3.626644000
H	-7.328729000	1.570251000	3.767735000
C	-5.432074000	1.134814000	4.695687000
H	-5.757454000	1.411511000	5.694210000

C	-4.134987000	0.650484000	4.486921000
C	-3.789448000	0.289703000	3.185325000
N	-4.516271000	-1.888897000	-0.392385000
C	-6.728658000	-1.386356000	0.480929000
H	-6.610263000	-1.496899000	1.565842000
H	-7.769370000	-1.647620000	0.243026000
C	-5.780963000	-2.331708000	-0.205263000
C	-6.185043000	-3.595248000	-0.607447000
C	-5.276423000	-4.431537000	-1.240496000
H	-5.583648000	-5.411868000	-1.591842000
C	-3.974329000	-3.974882000	-1.473523000
C	-3.643861000	-2.698616000	-1.016677000
N	-4.567206000	1.250549000	-1.508469000
C	-6.817560000	0.361218000	-1.218499000
H	-6.771750000	-0.546054000	-1.833403000
H	-7.853115000	0.725107000	-1.259854000
C	-5.880683000	1.380709000	-1.811797000
C	-6.339278000	2.384215000	-2.651350000
H	-7.399062000	2.452238000	-2.876277000
C	-5.438846000	3.305862000	-3.170725000
H	-5.783770000	4.113585000	-3.809531000
C	-4.088869000	3.216580000	-2.819132000
C	-3.704647000	2.159559000	-1.993904000
N	6.301314000	-0.024207000	0.098820000
N	4.593526000	-0.219799000	2.151554000
C	6.718499000	-0.878563000	1.209307000
H	6.607760000	-1.924725000	0.898427000
H	7.775264000	-0.726831000	1.465808000
C	5.844000000	-0.635085000	2.404140000
C	6.284947000	-0.848967000	3.704281000
H	7.304601000	-1.175231000	3.881026000
C	5.411730000	-0.623613000	4.756612000
H	5.744775000	-0.769843000	5.779955000
C	4.112910000	-0.167766000	4.500554000
C	3.754410000	0.015487000	3.166377000
N	4.588777000	1.841687000	-0.743586000
C	6.712350000	1.366230000	0.295440000
H	6.585535000	1.618635000	1.355232000
H	7.771813000	1.516070000	0.050565000
C	5.841993000	2.270050000	-0.526170000
C	6.283858000	3.487696000	-1.026704000
H	7.304060000	3.808592000	-0.843660000
C	5.413304000	4.261452000	-1.778374000
H	5.750074000	5.204130000	-2.199625000
C	4.113188000	3.807406000	-2.030686000
C	3.748661000	2.582025000	-1.474973000

N	4.596925000	-1.630945000	-1.229549000
C	6.756902000	-0.541767000	-1.190742000
H	6.698987000	0.269047000	-1.927462000
H	7.804971000	-0.865445000	-1.151959000
C	5.872093000	-1.662617000	-1.648236000
C	6.331157000	-2.667117000	-2.490173000
C	5.453326000	-3.660662000	-2.891745000
H	5.799806000	-4.467418000	-3.531003000
C	4.129423000	-3.647252000	-2.437353000
C	3.749225000	-2.595819000	-1.605237000
H	-7.211921000	-3.907225000	-0.443744000
H	2.730296000	-2.507055000	-1.240955000
H	-2.793063000	-0.076639000	2.955354000
H	2.757291000	0.352236000	2.899285000
H	-2.638502000	-2.305623000	-1.148475000
H	7.368439000	-2.671797000	-2.808242000
H	-2.660640000	2.021020000	-1.725531000
H	2.748110000	2.180617000	-1.606403000
Co	4.097554000	-0.045040000	0.074116000
Co	-4.299553000	0.090213000	0.145050000
O	-1.287296000	-0.125307000	0.275306000
H	-1.935010000	-0.793802000	0.561958000
H	-1.824548000	0.610333000	-0.068287000
O	0.231239000	-1.014658000	-1.460414000
H	-0.531146000	-0.657286000	-0.799240000
H	0.149395000	-0.537186000	-2.308754000
O	1.981647000	0.046894000	0.161274000
H	1.061500000	-0.668548000	-1.004047000
H	1.668530000	-0.359163000	0.989135000
H	-3.351870000	3.924832000	-3.181139000
H	3.408001000	4.376249000	-2.625241000
H	-3.417944000	0.554192000	5.294375000
H	3.405273000	0.036051000	5.295551000
H	-3.233554000	-4.583194000	-1.980704000
H	3.416435000	-4.413805000	-2.717478000
H	1.726428000	0.984945000	0.224384000

PC (b) E= -2350.35191654

N	-6.410830000	-0.004525000	0.134779000
N	-4.632912000	0.379957000	2.146317000
C	-6.796411000	0.951930000	1.162697000
H	-6.693478000	1.958455000	0.735118000
H	-7.845295000	0.840118000	1.474718000
C	-5.885236000	0.839390000	2.360484000
C	-6.310822000	1.220491000	3.626658000
H	-7.328729000	1.570251000	3.767735000

C	-5.432074000	1.134814000	4.695687000
H	-5.757454000	1.411511000	5.694210000
C	-4.134990000	0.650478000	4.486922000
C	-3.789481000	0.289507000	3.185334000
N	-4.516184000	-1.888960000	-0.392203000
C	-6.728643000	-1.386382000	0.480979000
H	-6.610263000	-1.496899000	1.565842000
H	-7.769370000	-1.647620000	0.243025000
C	-5.781009000	-2.331646000	-0.205443000
C	-6.185037000	-3.595258000	-0.607428000
C	-5.276423000	-4.431537000	-1.240496000
H	-5.583648000	-5.411868000	-1.591842000
C	-3.974352000	-3.974850000	-1.473597000
C	-3.643779000	-2.698642000	-1.016489000
N	-4.567184000	1.250334000	-1.508575000
C	-6.817554000	0.361192000	-1.218534000
H	-6.771749000	-0.546054000	-1.833403000
H	-7.853115000	0.725107000	-1.259854000
C	-5.880696000	1.380857000	-1.811684000
C	-6.339281000	2.384229000	-2.651331000
H	-7.399062000	2.452238000	-2.876277000
C	-5.438846000	3.305862000	-3.170725000
H	-5.783770000	4.113585000	-3.809531000
C	-4.088883000	3.216633000	-2.819057000
C	-3.704666000	2.159583000	-1.993945000
N	6.301314000	-0.024207000	0.098820000
N	4.593560000	-0.219932000	2.151527000
C	6.718518000	-0.878505000	1.209309000
H	6.607760000	-1.924725000	0.898427000
H	7.775264000	-0.726831000	1.465808000
C	5.843895000	-0.635395000	2.404150000
C	6.284975000	-0.848881000	3.704285000
H	7.304601000	-1.175231000	3.881026000
C	5.411730000	-0.623613000	4.756612000
H	5.744775000	-0.769843000	5.779955000
C	4.112915000	-0.167753000	4.500554000
C	3.754465000	0.015733000	3.166365000
N	4.588779000	1.841825000	-0.743363000
C	6.712330000	1.366261000	0.295496000
H	6.585535000	1.618635000	1.355232000
H	7.771813000	1.516070000	0.050565000
C	5.842091000	2.269905000	-0.526452000
C	6.283855000	3.487701000	-1.026696000
H	7.304060000	3.808592000	-0.843660000
C	5.413304000	4.261452000	-1.778374000
H	5.750074000	5.204130000	-2.199625000

C	4.113205000	3.807381000	-2.030730000
C	3.748538000	2.582068000	-1.474788000
N	4.596731000	-1.630701000	-1.229669000
C	6.756892000	-0.541745000	-1.190776000
H	6.698987000	0.269047000	-1.927462000
H	7.804971000	-0.865445000	-1.151959000
C	5.872127000	-1.662706000	-1.648126000
C	6.331161000	-2.667126000	-2.490159000
C	5.453326000	-3.660662000	-2.891745000
H	5.799806000	-4.467418000	-3.531003000
C	4.129438000	-3.647281000	-2.437309000
C	3.749260000	-2.595853000	-1.605230000
H	-7.211921000	-3.907225000	-0.443744000
H	2.730301000	-2.507065000	-1.240939000
H	-2.793040000	-0.076567000	2.955341000
H	2.757271000	0.352176000	2.899283000
H	-2.638501000	-2.305588000	-1.148559000
H	7.368439000	-2.671797000	-2.808242000
H	-2.660724000	2.020984000	-1.725638000
H	2.748126000	2.180591000	-1.606448000
Co	4.080263000	-0.040701000	0.077043000
Co	-4.187013000	0.041374000	0.166674000
O	-1.062916000	-0.115904000	0.771139000
H	-2.519053000	0.032883000	0.356008000
H	-0.720274000	0.755751000	0.506434000
O	0.035529000	-1.661220000	-1.098965000
H	-0.744838000	-0.736162000	0.048585000
H	-0.239206000	-1.285508000	-1.949971000
O	1.957904000	-0.035765000	0.079974000
H	0.865621000	-1.185000000	-0.885216000
H	1.613327000	-0.241706000	0.966434000
H	-3.351870000	3.924832000	-3.181139000
H	3.408001000	4.376249000	-2.625241000
H	-3.417944000	0.554192000	5.294375000
H	3.405273000	0.036051000	5.295551000
H	-3.233554000	-4.583194000	-1.980704000
H	3.416435000	-4.413805000	-2.717478000
H	1.620499000	0.856369000	-0.111203000

CoZn

full RC **E= -4382.58456020**

N	-0.621665000	6.363914000	-1.010413000
N	-2.498094000	4.444377000	-0.586339000
C	-1.791791000	6.762764000	-0.242598000
H	-1.485459000	6.854686000	0.808253000
H	-2.186507000	7.743029000	-0.548858000

C	-2.875948000	5.717976000	-0.339579000	C	1.888425000	6.954232000	1.616190000
C	-4.209207000	6.056283000	-0.146960000	H	2.007805000	8.030261000	1.536948000
H	-4.479559000	7.092160000	0.032721000	C	2.408583000	6.255023000	2.697541000
C	-5.176484000	5.065410000	-0.199273000	H	2.940736000	6.777670000	3.486840000
H	-6.224669000	5.316552000	-0.067714000	C	2.199969000	4.875007000	2.786181000
C	-4.797677000	3.743404000	-0.462126000	C	1.500569000	4.258904000	1.749073000
C	-3.439302000	3.490859000	-0.646634000	C	2.694167000	4.120478000	3.953056000
C	-5.810276000	2.676013000	-0.558938000	C	3.980437000	4.370043000	4.444856000
C	-6.905200000	2.677894000	0.314523000	H	4.633978000	5.059234000	3.917997000
H	-6.966435000	3.423079000	1.102221000	C	4.432706000	3.739803000	5.595120000
C	-7.911349000	1.731828000	0.190082000	H	5.443196000	3.943523000	5.939528000
H	-8.746833000	1.755189000	0.885901000	C	3.592810000	2.869766000	6.295121000
C	-7.851822000	0.773077000	-0.824573000	C	2.321447000	2.590544000	5.792801000
C	-6.749366000	0.743509000	-1.677958000	H	1.670630000	1.904852000	6.328516000
H	-6.696616000	-0.007320000	-2.461760000	C	1.879805000	3.200798000	4.623914000
C	-5.732714000	1.682377000	-1.542381000	H	0.877271000	3.000578000	4.256058000
H	-4.895250000	1.669991000	-2.234468000	C	4.054144000	2.221039000	7.576333000
C	-8.968672000	-0.223699000	-0.998351000	C	5.026238000	1.073951000	7.263435000
C	-8.981420000	-1.212226000	0.176280000	N	0.374399000	-6.200638000	1.127679000
N	0.279642000	4.275165000	-2.506904000	N	-1.787470000	-4.679796000	0.430936000
C	-0.822537000	6.441377000	-2.453875000	C	-0.659799000	-6.836114000	0.320118000
H	-1.874849000	6.210720000	-2.660558000	H	-0.283526000	-6.923326000	-0.706838000
H	-0.633256000	7.449979000	-2.846954000	H	-0.884069000	-7.852977000	0.668194000
C	0.034365000	5.430177000	-3.165666000	C	-1.915412000	-6.008568000	0.295464000
C	0.518162000	5.663907000	-4.444275000	C	-3.159214000	-6.594968000	0.096963000
C	1.284353000	4.691619000	-5.071926000	H	-3.237432000	-7.673122000	0.002230000
H	1.694603000	4.868763000	-6.061513000	C	-4.281716000	-5.786884000	0.035394000
C	1.564039000	3.499128000	-4.395010000	H	-5.264016000	-6.229129000	-0.102268000
C	1.028844000	3.341638000	-3.116080000	C	-4.154795000	-4.400837000	0.188326000
C	2.433022000	2.478366000	-5.012062000	C	-2.870923000	-3.895924000	0.385057000
C	2.326107000	2.205988000	-6.382155000	C	-5.345660000	-3.531334000	0.153032000
H	1.546421000	2.684061000	-6.967968000	C	-6.354821000	-3.781832000	-0.784353000
C	3.204820000	1.329004000	-7.001140000	H	-6.223939000	-4.566663000	-1.523539000
H	3.093255000	1.134062000	-8.065602000	C	-7.517991000	-3.026240000	-0.790244000
C	4.223059000	0.717031000	-6.264502000	H	-8.272342000	-3.231650000	-1.545644000
C	4.312052000	0.951184000	-4.892658000	C	-7.708968000	-2.022751000	0.162829000
H	5.095669000	0.468652000	-4.315046000	C	-6.695243000	-1.747581000	1.081299000
C	3.420413000	1.818528000	-4.270273000	H	-6.832785000	-0.957557000	1.814322000
H	3.523538000	2.022972000	-3.208205000	C	-5.517547000	-2.487493000	1.069698000
C	5.227759000	-0.175397000	-6.950199000	H	-4.743928000	-2.280248000	1.803996000
C	4.562749000	-1.485681000	-7.398583000	N	0.978432000	-4.067023000	2.694353000
N	1.015502000	4.927745000	0.689343000	C	0.130609000	-6.335643000	2.560555000
C	0.626615000	6.976736000	-0.569251000	H	-0.947586000	-6.237912000	2.736119000
H	1.349666000	6.881512000	-1.388909000	H	0.431998000	-7.321693000	2.937087000
H	0.515288000	8.050160000	-0.363332000	C	0.843151000	-5.248223000	3.315537000
C	1.189333000	6.269005000	0.634468000	C	1.327334000	-5.442120000	4.602632000

H	1.214223000	-6.408964000	5.081867000
C	1.970985000	-4.395684000	5.242733000
H	2.378297000	-4.537151000	6.239228000
C	2.134617000	-3.167842000	4.589914000
C	1.606852000	-3.056009000	3.304091000
C	2.848838000	-2.056460000	5.245715000
C	2.667828000	-1.832797000	6.616146000
H	1.960598000	-2.438977000	7.174433000
C	3.365996000	-0.826936000	7.267292000
H	3.185123000	-0.666925000	8.327511000
C	4.278864000	-0.035251000	6.564989000
C	4.454000000	-0.242779000	5.196709000
H	5.156159000	0.375718000	4.644610000
C	3.739958000	-1.239481000	4.539977000
H	3.904419000	-1.406985000	3.479313000
N	1.708447000	-4.687576000	-0.703124000
C	1.718322000	-6.630702000	0.750931000
H	2.401168000	-6.377038000	1.571009000
H	1.774586000	-7.717935000	0.612573000
C	2.187802000	-5.920625000	-0.489140000
C	3.110898000	-6.493112000	-1.356702000
C	3.530775000	-5.773544000	-2.464542000
H	4.237421000	-6.212199000	-3.162999000
C	3.012098000	-4.495390000	-2.704045000
C	2.097909000	-3.996014000	-1.778546000
C	3.404994000	-3.711161000	-3.889514000
C	4.739731000	-3.697108000	-4.310016000
H	5.492599000	-4.233744000	-3.740117000
C	5.118595000	-2.979307000	-5.435649000
H	6.168120000	-2.966716000	-5.717793000
C	4.163732000	-2.282666000	-6.180967000
C	2.832646000	-2.287011000	-5.763738000
H	2.086898000	-1.742601000	-6.336163000
C	2.457363000	-2.986965000	-4.623032000
H	1.414505000	-2.998720000	-4.319155000
N	5.463145000	-2.308837000	-8.273482000
N	5.832516000	0.577793000	-8.098677000
N	-10.267850000	0.515149000	-1.134805000
N	-10.167140000	-2.132936000	0.126079000
N	5.686904000	0.542039000	8.502070000
N	4.671485000	3.255745000	8.469716000
H	0.306331000	6.609948000	-4.932993000
H	1.670461000	-3.004424000	-1.890270000
H	-3.081828000	2.482361000	-0.836529000
H	-2.696728000	-2.829594000	0.492988000
H	1.194207000	2.426748000	-2.553863000

H	3.479685000	-7.495861000	-1.166481000
H	1.337576000	3.184181000	1.747137000
H	1.674744000	-2.127774000	2.743399000
Zn	0.232881000	-4.015979000	0.701124000
Co	-0.439902000	4.291515000	-0.571868000
H	-8.845366000	-0.770994000	-1.935879000
H	-10.567029000	0.947961000	-0.252226000
H	-11.030212000	-0.087301000	-1.464858000
H	-9.076558000	-0.666542000	1.117875000
H	-10.274799000	-2.583818000	-0.790349000
H	-11.046028000	-1.650228000	0.346288000
H	5.602945000	3.551172000	8.151392000
H	4.756807000	2.930929000	9.439985000
H	3.197994000	1.832335000	8.133360000
H	5.010535000	0.313253000	9.241219000
H	6.370687000	1.200793000	8.893792000
H	5.840438000	1.442875000	6.634770000
H	6.059370000	-0.398106000	-6.277526000
H	5.163768000	0.722580000	-8.864736000
H	6.660425000	0.112288000	-8.488935000
H	3.685151000	-1.264183000	-8.010517000
H	6.407329000	-2.414450000	-7.883169000
H	5.554371000	-1.913335000	-9.216839000
H	5.069530000	-3.250880000	-8.383237000
H	6.136146000	1.505116000	-7.777923000
H	-10.162806000	1.267395000	-1.825801000
H	-10.054281000	-2.877537000	0.824264000
H	6.200125000	-0.318684000	8.278085000
H	4.076269000	4.092791000	8.489676000
O	-0.201971000	1.284808000	-0.533866000
H	0.391966000	1.909311000	-0.084742000
H	-0.810951000	1.858099000	-1.029651000
O	-1.394504000	-0.390912000	1.250874000
H	-1.066417000	0.320511000	0.646671000
H	-2.272564000	-0.612534000	0.903901000
O	0.323851000	-2.048294000	0.093288000
H	-0.367302000	-1.500957000	0.573430000
H	1.171781000	-1.736551000	0.450433000

RC (a) E= -2431.19500423

N	-0.621665000	6.363914000	-1.010413000
N	-2.498094000	4.444377000	-0.586339000
C	-1.791791000	6.762764000	-0.242598000
H	-1.485459000	6.854686000	0.808253000
H	-2.186507000	7.743029000	-0.548858000
C	-2.875948000	5.717976000	-0.339579000

C	-4.209207000	6.056283000	-0.146960000
H	-4.479559000	7.092160000	0.032721000
C	-5.176484000	5.065410000	-0.199273000
H	-6.224669000	5.316552000	-0.067714000
C	-4.797677000	3.743404000	-0.462126000
C	-3.439302000	3.490859000	-0.646634000
N	0.279642000	4.275165000	-2.506904000
C	-0.822537000	6.441377000	-2.453875000
H	-1.874849000	6.210720000	-2.660558000
H	-0.633256000	7.449979000	-2.846954000
C	0.034365000	5.430177000	-3.165666000
C	0.518162000	5.663907000	-4.444275000
C	1.284353000	4.691619000	-5.071926000
H	1.694603000	4.868763000	-6.061513000
C	1.564039000	3.499128000	-4.395010000
C	1.028844000	3.341638000	-3.116080000
N	1.015502000	4.927745000	0.689343000
C	0.626615000	6.976736000	-0.569251000
H	1.349666000	6.881512000	-1.388909000
H	0.515288000	8.050160000	-0.363332000
C	1.189333000	6.269005000	0.634468000
C	1.888425000	6.954232000	1.616190000
H	2.007805000	8.030261000	1.536948000
C	2.408583000	6.255023000	2.697541000
H	2.940736000	6.777670000	3.486840000
C	2.199969000	4.875007000	2.786181000
C	1.500569000	4.258904000	1.749073000
N	0.374399000	-6.200638000	1.127679000
N	-1.787470000	-4.679796000	0.430936000
C	-0.659799000	-6.836114000	0.320118000
H	-0.283526000	-6.923326000	-0.706838000
H	-0.884069000	-7.852977000	0.668194000
C	-1.915412000	-6.008568000	0.295464000
C	-3.159214000	-6.594968000	0.096963000
H	-3.237432000	-7.673122000	0.002230000
C	-4.281716000	-5.786884000	0.035394000
H	-5.264016000	-6.229129000	-0.102268000
C	-4.154795000	-4.400837000	0.188326000
C	-2.870923000	-3.895924000	0.385057000
N	0.978432000	-4.067023000	2.694353000
C	0.130609000	-6.335643000	2.560555000
H	-0.947586000	-6.237912000	2.736119000
H	0.431998000	-7.321693000	2.937087000
C	0.843151000	-5.248223000	3.315537000
C	1.327334000	-5.442120000	4.602632000
H	1.214223000	-6.408964000	5.081867000

C	1.970985000	-4.395684000	5.242733000
H	2.378297000	-4.537151000	6.239228000
C	2.134617000	-3.167842000	4.589914000
C	1.606852000	-3.056009000	3.304091000
N	1.708447000	-4.687576000	-0.703124000
C	1.718322000	-6.630702000	0.750931000
H	2.401168000	-6.377038000	1.571009000
H	1.774586000	-7.717935000	0.612573000
C	2.187802000	-5.920625000	-0.489140000
C	3.110898000	-6.493112000	-1.356702000
C	3.530775000	-5.773544000	-2.464542000
H	4.237421000	-6.212199000	-3.162999000
C	3.012098000	-4.495390000	-2.704045000
C	2.097909000	-3.996014000	-1.778546000
H	0.306331000	6.609948000	-4.932993000
H	1.670461000	-3.004424000	-1.890270000
H	-3.081828000	2.482361000	-0.836529000
H	-2.696728000	-2.829594000	0.492988000
H	1.194207000	2.426748000	-2.553863000
H	3.479685000	-7.495861000	-1.166481000
H	1.337576000	3.184181000	1.747137000
H	1.674744000	-2.127774000	2.743399000
Zn	0.234752000	-4.018520000	0.700694000
Co	-0.441723000	4.293094000	-0.570598000
O	-0.176200000	1.286784000	-0.539167000
H	0.416791000	1.916460000	-0.096181000
H	-0.795140000	1.855437000	-1.028027000
O	-1.335359000	-0.373505000	1.270519000
H	-1.009836000	0.334138000	0.659706000
H	-2.212396000	-0.599403000	0.923780000
O	0.326030000	-2.055055000	0.080507000
H	-0.337064000	-1.491748000	0.582443000
H	1.193369000	-1.749429000	0.392886000
H	2.572241000	4.290073000	3.620068000
H	2.645044000	-2.331669000	5.053329000
H	-5.521123000	2.938084000	-0.523955000
H	-5.010612000	-3.736471000	0.158588000
H	2.168498000	2.714536000	-4.836813000
H	3.302587000	-3.907362000	-3.566935000

PC (a) E= -2431.14930531

N	-0.621693000	6.363887000	-1.010385000
N	-2.497987000	4.444421000	-0.586350000
C	-1.791789000	6.762758000	-0.242583000
H	-1.485461000	6.854680000	0.808254000
H	-2.186500000	7.743034000	-0.548850000

C	-2.875970000	5.717972000	-0.339570000	H	1.214223000	-6.408964000	5.081867000
C	-4.209205000	6.056280000	-0.146941000	C	1.970985000	-4.395684000	5.242733000
H	-4.479559000	7.092160000	0.032721000	H	2.378297000	-4.537151000	6.239228000
C	-5.176484000	5.065410000	-0.199273000	C	2.134623000	-3.167844000	4.589911000
H	-6.224669000	5.316552000	-0.067714000	C	1.606791000	-3.055985000	3.304114000
C	-4.797677000	3.743404000	-0.462124000	N	1.708389000	-4.687585000	-0.703130000
C	-3.439312000	3.490870000	-0.646665000	C	1.718318000	-6.630698000	0.750933000
N	0.279712000	4.275173000	-2.506848000	H	2.401168000	-6.377039000	1.571010000
C	-0.822509000	6.441397000	-2.453864000	H	1.774586000	-7.717935000	0.612573000
H	-1.874851000	6.210727000	-2.660557000	C	2.187865000	-5.920593000	-0.489094000
H	-0.633246000	7.449977000	-2.846956000	C	3.110895000	-6.493113000	-1.356704000
C	0.034239000	5.430115000	-3.165716000	C	3.530775000	-5.773544000	-2.464542000
C	0.518179000	5.663915000	-4.444268000	H	4.237421000	-6.212199000	-3.162999000
C	1.284353000	4.691619000	-5.071926000	C	3.012102000	-4.495388000	-2.704043000
H	1.694603000	4.868763000	-6.061513000	C	2.097900000	-3.996026000	-1.778557000
C	1.564028000	3.499123000	-4.395015000	H	0.306331000	6.609948000	-4.932993000
C	1.028909000	3.341680000	-3.116065000	H	1.670462000	-3.004423000	-1.890269000
N	1.015463000	4.927870000	0.689229000	H	-3.081830000	2.482364000	-0.836549000
C	0.626636000	6.976730000	-0.569265000	H	-2.696727000	-2.829594000	0.492983000
H	1.349667000	6.881510000	-1.388908000	H	1.194179000	2.426734000	-2.553877000
H	0.515287000	8.050160000	-0.363330000	H	3.479685000	-7.495861000	-1.166481000
C	1.189226000	6.269025000	0.634594000	H	1.337558000	3.184184000	1.747147000
C	1.888428000	6.954231000	1.616188000	H	1.674755000	-2.127778000	2.743394000
H	2.007805000	8.030261000	1.536948000	Zn	0.224977000	-3.963192000	0.692495000
C	2.408583000	6.255023000	2.697541000	Co	-0.418450000	4.162824000	-0.586002000
H	2.940736000	6.777670000	3.486840000	O	0.328038000	1.193933000	0.158889000
C	2.199969000	4.875007000	2.786181000	H	-0.119512000	2.515284000	-0.146844000
C	1.500675000	4.258816000	1.748969000	H	0.713114000	0.948341000	-0.701518000
N	0.374381000	-6.200675000	1.127683000	O	-1.767258000	-0.326864000	0.325731000
N	-1.787505000	-4.679856000	0.430967000	H	-0.548743000	0.670931000	0.211393000
C	-0.659795000	-6.836115000	0.320120000	H	-2.174252000	-0.282518000	-0.553556000
H	-0.283527000	-6.923323000	-0.706839000	O	0.044690000	-2.121600000	0.104537000
H	-0.884070000	-7.852977000	0.668194000	H	-1.122638000	-1.121927000	0.258515000
C	-1.915406000	-6.008565000	0.295428000	H	0.753563000	-1.641811000	0.558085000
C	-3.159214000	-6.594968000	0.096960000	H	2.567459000	4.306754000	3.627870000
H	-3.237432000	-7.673122000	0.002230000	H	2.647515000	-2.342910000	5.061956000
C	-4.281716000	-5.786884000	0.035394000	H	-5.528953000	2.950734000	-0.519648000
H	-5.264016000	-6.229129000	-0.102268000	H	-5.016113000	-3.750119000	0.155193000
C	-4.154794000	-4.400836000	0.188317000	H	2.171967000	2.728833000	-4.846085000
C	-2.870915000	-3.895911000	0.385080000	H	3.307967000	-3.920856000	-3.569361000
N	0.978385000	-4.067035000	2.694373000				
C	0.130608000	-6.335627000	2.560564000	RC (b)	E= -2431.62486273		
H	-0.947586000	-6.237914000	2.736119000	N	-0.621593000	6.363930000	-1.010440000
H	0.431996000	-7.321694000	2.937086000	N	-2.498140000	4.444368000	-0.586199000
C	0.843249000	-5.248252000	3.315508000	C	-1.791774000	6.762792000	-0.242577000
C	1.327327000	-5.442118000	4.602635000	H	-1.485462000	6.854675000	0.808255000

H	-2.186510000	7.743026000	-0.548862000	C	1.327372000	-5.442133000	4.602616000
C	-2.875935000	5.717994000	-0.339664000	H	1.214223000	-6.408964000	5.081867000
C	-4.209207000	6.056283000	-0.146961000	C	1.970985000	-4.395684000	5.242733000
H	-4.479559000	7.092160000	0.032721000	H	2.378297000	-4.537151000	6.239228000
C	-5.176484000	5.065410000	-0.199273000	C	2.134643000	-3.167851000	4.589903000
H	-6.224670000	5.316551000	-0.067715000	C	1.606952000	-3.056070000	3.304090000
C	-4.797682000	3.743411000	-0.462169000	N	1.708507000	-4.687666000	-0.703010000
C	-3.439318000	3.490845000	-0.646608000	C	1.718300000	-6.630785000	0.750952000
N	0.279519000	4.275135000	-2.506895000	H	2.401171000	-6.377023000	1.571002000
C	-0.822541000	6.441392000	-2.453874000	H	1.774582000	-7.717933000	0.612556000
H	-1.874848000	6.210716000	-2.660558000	C	2.187816000	-5.920615000	-0.489153000
H	-0.633257000	7.449979000	-2.846954000	C	3.110899000	-6.493112000	-1.356702000
C	0.034392000	5.430181000	-3.165665000	C	3.530775000	-5.773544000	-2.464542000
C	0.518163000	5.663908000	-4.444274000	H	4.237421000	-6.212199000	-3.162999000
C	1.284353000	4.691619000	-5.071926000	C	3.012106000	-4.495386000	-2.704039000
H	1.694603000	4.868763000	-6.061513000	C	2.097829000	-3.996037000	-1.778590000
C	1.564042000	3.499130000	-4.395008000	H	0.306331000	6.609948000	-4.932993000
C	1.028895000	3.341672000	-3.116069000	H	1.670477000	-3.004416000	-1.890259000
N	1.015372000	4.927778000	0.689451000	H	-3.081699000	2.482377000	-0.836482000
C	0.626619000	6.976746000	-0.569293000	H	-2.696728000	-2.829594000	0.492984000
H	1.349668000	6.881505000	-1.388906000	H	1.194199000	2.426744000	-2.553867000
H	0.515286000	8.050159000	-0.363326000	H	3.479685000	-7.495861000	-1.166481000
C	1.189385000	6.268999000	0.634417000	H	1.337610000	3.184126000	1.747035000
C	1.888438000	6.954230000	1.616182000	H	1.674729000	-2.127769000	2.743406000
H	2.007805000	8.030261000	1.536948000	Zn	0.242977000	-4.048806000	0.704564000
C	2.408583000	6.255023000	2.697541000	Co	-0.442027000	4.301122000	-0.575366000
H	2.940736000	6.777670000	3.486840000	O	-0.255382000	1.299787000	-0.568940000
C	2.199984000	4.875004000	2.786172000	H	0.333257000	1.904971000	-0.082645000
C	1.500455000	4.258914000	1.749080000	H	-0.804859000	1.882552000	-1.124330000
N	0.374668000	-6.200508000	1.127567000	O	-1.615907000	-0.062541000	0.983932000
N	-1.787349000	-4.679693000	0.430940000	H	-1.099258000	0.619337000	0.340026000
C	-0.659837000	-6.836134000	0.320173000	H	-2.514335000	-0.189651000	0.620779000
H	-0.283523000	-6.923333000	-0.706836000	O	0.049512000	-1.943193000	0.285778000
H	-0.884084000	-7.852969000	0.668207000	H	-1.111813000	-0.923965000	0.824353000
C	-1.915413000	-6.008564000	0.295513000	H	0.883519000	-1.546910000	0.597372000
C	-3.159211000	-6.594966000	0.096938000	H	2.572241000	4.290073000	3.620068000
H	-3.237432000	-7.673122000	0.002230000	H	2.645044000	-2.331669000	5.053329000
C	-4.281716000	-5.786884000	0.035394000	H	-5.521123000	2.938084000	-0.523955000
H	-5.264016000	-6.229129000	-0.102268000	H	-5.010612000	-3.736471000	0.158588000
C	-4.154793000	-4.400836000	0.188312000	H	2.168498000	2.714536000	-4.836813000
C	-2.870961000	-3.895974000	0.385108000	H	3.302587000	-3.907362000	-3.566935000
N	0.978063000	-4.066984000	2.694254000	H	0.066906000	-1.827454000	-0.680963000
C	0.130569000	-6.335720000	2.560537000				
H	-0.947582000	-6.237872000	2.736123000	PC (b)	E= -2431.61110627		
H	0.431985000	-7.321698000	2.937084000	N	-0.621693000	6.363887000	-1.010385000
C	0.843139000	-5.248199000	3.315578000	N	-2.497975000	4.444416000	-0.586321000

C	-1.791790000	6.762761000	-0.242601000
H	-1.485461000	6.854680000	0.808254000
H	-2.186500000	7.743034000	-0.548850000
C	-2.875963000	5.717966000	-0.339526000
C	-4.209207000	6.056283000	-0.146960000
H	-4.479559000	7.092160000	0.032721000
C	-5.176484000	5.065410000	-0.199273000
H	-6.224669000	5.316552000	-0.067714000
C	-4.797677000	3.743404000	-0.462123000
C	-3.439305000	3.490865000	-0.646692000
N	0.279675000	4.275173000	-2.506890000
C	-0.822533000	6.441385000	-2.453876000
H	-1.874851000	6.210727000	-2.660557000
H	-0.633246000	7.449977000	-2.846956000
C	0.034320000	5.430156000	-3.165673000
C	0.518146000	5.663899000	-4.444283000
C	1.284353000	4.691619000	-5.071925000
H	1.694603000	4.868763000	-6.061513000
C	1.564024000	3.499121000	-4.395017000
C	1.028898000	3.341677000	-3.116073000
N	1.015464000	4.927844000	0.689207000
C	0.626627000	6.976731000	-0.569260000
H	1.349667000	6.881510000	-1.388908000
H	0.515287000	8.050160000	-0.363330000
C	1.189255000	6.269020000	0.634573000
C	1.888422000	6.954232000	1.616192000
H	2.007805000	8.030261000	1.536948000
C	2.408583000	6.255023000	2.697541000
H	2.940736000	6.777670000	3.486840000
C	2.199960000	4.875009000	2.786186000
C	1.500672000	4.258859000	1.748998000
N	0.374381000	-6.200675000	1.127683000
N	-1.787438000	-4.679868000	0.430962000
C	-0.659794000	-6.836114000	0.320113000
H	-0.283527000	-6.923323000	-0.706839000
H	-0.884070000	-7.852977000	0.668194000
C	-1.915419000	-6.008566000	0.295454000
C	-3.159212000	-6.594966000	0.096942000
H	-3.237432000	-7.673122000	0.002230000
C	-4.281716000	-5.786884000	0.035394000
H	-5.264016000	-6.229129000	-0.102268000
C	-4.154793000	-4.400835000	0.188308000
C	-2.870942000	-3.895949000	0.385069000
N	0.978347000	-4.067027000	2.694337000
C	0.130633000	-6.335636000	2.560553000
H	-0.947586000	-6.237914000	2.736119000

H	0.431996000	-7.321694000	2.937086000
C	0.843169000	-5.248219000	3.315553000
C	1.327356000	-5.442128000	4.602623000
H	1.214223000	-6.408964000	5.081867000
C	1.970985000	-4.395684000	5.242733000
H	2.378297000	-4.537151000	6.239228000
C	2.134629000	-3.167846000	4.589908000
C	1.606856000	-3.056016000	3.304098000
N	1.708377000	-4.687563000	-0.703081000
C	1.718336000	-6.630689000	0.750945000
H	2.401168000	-6.377039000	1.571010000
H	1.774586000	-7.717935000	0.612573000
C	2.187802000	-5.920627000	-0.489151000
C	3.110913000	-6.493104000	-1.356691000
C	3.530775000	-5.773544000	-2.464542000
H	4.237421000	-6.212199000	-3.162999000
C	3.012100000	-4.495389000	-2.704044000
C	2.097923000	-3.995995000	-1.778529000
H	0.306331000	6.609948000	-4.932993000
H	1.670441000	-3.004434000	-1.890283000
H	-3.081828000	2.482361000	-0.836532000
H	-2.696728000	-2.829595000	0.492997000
H	1.194204000	2.426746000	-2.553865000
H	3.479685000	-7.495861000	-1.166481000
H	1.337569000	3.184182000	1.747141000
H	1.674721000	-2.127766000	2.743409000
Zn	0.236920000	-4.034386000	0.704111000
Co	-0.411434000	4.184906000	-0.590819000
O	0.351109000	1.167660000	0.097925000
H	-0.055429000	2.595623000	-0.180966000
H	0.544964000	0.897162000	-0.817064000
O	-1.965453000	-0.034480000	0.603528000
H	-0.560230000	0.785305000	0.285307000
H	-2.458462000	0.035174000	-0.229066000
O	0.002788000	-1.957542000	0.254849000
H	-1.475933000	-0.880261000	0.520535000
H	0.701191000	-1.445515000	0.698812000
H	2.567459000	4.306754000	3.627870000
H	2.647515000	-2.342910000	5.061956000
H	-5.528953000	2.950734000	-0.519648000
H	-5.016113000	-3.750119000	0.155193000
H	2.171967000	2.728833000	-4.846085000
H	3.307967000	-3.920856000	-3.569361000
H	0.164340000	-1.819941000	-0.693847000

CoCu

full RC E= -4352.89106578

N	-0.586116000	6.387194000	-1.000714000	C	4.448348000	-1.516091000	-7.454757000
N	-2.463330000	4.466544000	-0.582711000	N	1.039452000	4.942126000	0.704222000
C	-1.757783000	6.783623000	-0.233452000	C	0.662305000	6.994220000	-0.551546000
H	-1.453468000	6.870819000	0.818405000	H	1.390443000	6.893606000	-1.366048000
H	-2.151010000	7.765487000	-0.536305000	H	0.555167000	8.068422000	-0.347303000
C	-2.842407000	5.739812000	-0.336788000	C	1.210888000	6.284191000	0.657200000
C	-4.176790000	6.077425000	-0.150127000	C	1.892494000	6.967279000	1.652336000
H	-4.448407000	7.112950000	0.029684000	H	2.010533000	8.043877000	1.579135000
C	-5.143733000	5.086314000	-0.208809000	C	2.396718000	6.265101000	2.739451000
H	-6.192720000	5.336905000	-0.082501000	H	2.914893000	6.786323000	3.538918000
C	-4.762833000	3.764812000	-0.470794000	C	2.190167000	4.884273000	2.820008000
C	-3.403548000	3.512771000	-0.647421000	C	1.508927000	4.270311000	1.769288000
C	-5.771304000	2.694600000	-0.575113000	C	2.670363000	4.127562000	3.991602000
C	-6.871625000	2.690316000	0.291270000	C	3.946259000	4.386056000	4.505487000
H	-6.942378000	3.435371000	1.078311000	H	4.602446000	5.083093000	3.992482000
C	-7.870087000	1.736884000	0.161388000	C	4.385742000	3.754402000	5.659825000
H	-8.709341000	1.754000000	0.852869000	H	5.389173000	3.965195000	6.020164000
C	-7.797772000	0.777841000	-0.852216000	C	3.543393000	2.872996000	6.342399000
C	-6.690433000	0.755509000	-1.699356000	C	2.283010000	2.584675000	5.818043000
H	-6.627398000	0.004246000	-2.481997000	H	1.630216000	1.889656000	6.339124000
C	-5.681204000	1.701357000	-1.557922000	C	1.854185000	3.197023000	4.645195000
H	-4.838971000	1.694097000	-2.244258000	H	0.859826000	2.988275000	4.260295000
C	-8.905691000	-0.228013000	-1.029888000	C	3.992410000	2.222600000	7.627492000
C	-8.912967000	-1.216077000	0.145186000	C	4.978273000	1.084878000	7.321950000
N	0.302736000	4.300610000	-2.508888000	N	0.431522000	-6.283373000	1.164485000
C	-0.783222000	6.475277000	-2.444095000	N	-1.701901000	-4.674452000	0.394997000
H	-1.837757000	6.257711000	-2.653844000	C	-0.602048000	-6.860918000	0.335634000
H	-0.582741000	7.484330000	-2.830388000	H	-0.211336000	-6.932815000	-0.688070000
C	0.061632000	5.458907000	-3.163370000	H	-0.872014000	-7.884771000	0.639660000
C	0.534192000	5.689461000	-4.446792000	C	-1.845135000	-6.007745000	0.296727000
C	1.281704000	4.709400000	-5.084995000	C	-3.093194000	-6.595550000	0.118415000
H	1.681964000	4.883076000	-6.079278000	H	-3.173061000	-7.676346000	0.053254000
C	1.554823000	3.512307000	-4.413450000	C	-4.218616000	-5.792416000	0.040620000
C	1.034171000	3.359475000	-3.128112000	H	-5.202632000	-6.236079000	-0.080615000
C	2.401676000	2.480179000	-5.042173000	C	-4.083773000	-4.404976000	0.160787000
C	2.273814000	2.209330000	-6.410809000	C	-2.794155000	-3.901891000	0.335593000
H	1.494142000	2.699062000	-6.986927000	C	-5.272208000	-3.532079000	0.119389000
C	3.131251000	1.318776000	-7.040337000	C	-6.288354000	-3.791383000	-0.808477000
H	3.003226000	1.124760000	-8.103175000	H	-6.162049000	-4.585066000	-1.539019000
C	4.149479000	0.692014000	-6.315857000	C	-7.452235000	-3.036654000	-0.815148000
C	4.259116000	0.925521000	-4.945396000	H	-8.211056000	-3.251208000	-1.563565000
H	5.042833000	0.432179000	-4.377149000	C	-7.638762000	-2.023875000	0.129161000
C	3.388094000	1.805840000	-4.312321000	C	-6.617834000	-1.737696000	1.036405000
H	3.507010000	2.008334000	-3.251586000	H	-6.750911000	-0.940244000	1.762304000
C	5.133859000	-0.214472000	-7.012545000	C	-5.439336000	-2.476696000	1.024270000
				H	-4.661181000	-2.260924000	1.751454000

N	0.952855000	-4.063106000	2.742802000
C	0.181217000	-6.372375000	2.586957000
H	-0.899740000	-6.265888000	2.746398000
H	0.469661000	-7.346360000	3.012809000
C	0.880489000	-5.266930000	3.337423000
C	1.408600000	-5.485713000	4.605203000
H	1.337959000	-6.471786000	5.053796000
C	2.039351000	-4.444794000	5.268460000
H	2.478682000	-4.605007000	6.248808000
C	2.144893000	-3.196329000	4.646990000
C	1.571979000	-3.064171000	3.380750000
C	2.843475000	-2.077865000	5.307106000
C	2.676326000	-1.869175000	6.681644000
H	1.992143000	-2.498832000	7.242899000
C	3.358242000	-0.851294000	7.332110000
H	3.185542000	-0.702915000	8.395509000
C	4.244715000	-0.034144000	6.625036000
C	4.406410000	-0.226646000	5.252885000
H	5.087616000	0.411796000	4.697083000
C	3.705615000	-1.233261000	4.597319000
H	3.858041000	-1.387638000	3.532773000
N	1.718551000	-4.683831000	-0.683863000
C	1.776290000	-6.641467000	0.770094000
H	2.456789000	-6.340580000	1.577445000
H	1.908537000	-7.726684000	0.635870000
C	2.197983000	-5.922552000	-0.487312000
C	3.081579000	-6.512737000	-1.385919000
C	3.476495000	-5.809178000	-2.513377000
H	4.152907000	-6.261128000	-3.233286000
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C	2.089827000	-4.013882000	-1.778565000
C	3.339297000	-3.743925000	-3.929760000
C	4.662600000	-3.750466000	-4.386507000
H	5.420367000	-4.303388000	-3.839064000
C	5.025486000	-3.033749000	-5.517977000
H	6.067497000	-3.039764000	-5.827115000
C	4.064817000	-2.314940000	-6.234086000
C	2.745338000	-2.297320000	-5.781523000
H	1.995521000	-1.735118000	-6.331200000
C	2.387163000	-2.997589000	-4.635338000
H	1.352613000	-2.991552000	-4.304032000
N	5.327412000	-2.341813000	-8.348232000
N	5.738332000	0.530252000	-8.166746000
N	-10.210462000	0.500353000	-1.170185000
N	-10.097425000	-2.138817000	0.098908000
N	5.645263000	0.561638000	8.561418000

N	4.588399000	3.259581000	8.531938000
H	0.326838000	6.638312000	-4.932028000
H	1.680306000	-3.013024000	-1.885061000
H	-3.045597000	2.503739000	-0.833047000
H	-2.625327000	-2.830867000	0.414043000
H	1.195838000	2.441949000	-2.569159000
H	3.442911000	-7.519986000	-1.201864000
H	1.348334000	3.195283000	1.760640000
H	1.596551000	-2.109395000	2.861445000
Cu	0.257914000	-4.000744000	0.742606000
Co	-0.405943000	4.312589000	-0.573131000
H	-8.775439000	-0.774663000	-1.966860000
H	-10.515497000	0.931477000	-0.288749000
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H	5.517827000	3.570509000	8.222733000
H	4.671820000	2.928769000	9.500343000
H	3.132324000	1.824310000	8.171439000
H	4.973450000	0.329680000	9.303516000
H	6.325290000	1.226080000	8.949508000
H	5.789489000	1.460804000	6.693617000
H	5.969237000	-0.449437000	-6.348832000
H	5.063834000	0.688266000	-8.925142000
H	6.553725000	0.050832000	-8.566198000
H	3.562461000	-1.284633000	-8.050896000
H	6.277350000	-2.456428000	-7.974964000
H	5.405673000	-1.944521000	-9.291968000
H	4.925086000	-3.280685000	-8.454110000
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H	-10.109760000	1.252814000	-1.861570000
H	-9.981230000	-2.882586000	0.797454000
H	6.163596000	-0.296041000	8.337628000
H	3.981415000	4.088000000	8.553861000
O	-0.224175000	1.305358000	-0.542840000
H	0.380440000	1.918867000	-0.093113000
H	-0.797048000	1.887361000	-1.069707000
O	-1.498050000	-0.273714000	1.295716000
H	-1.152874000	0.399955000	0.661734000
H	-2.323178000	-0.580896000	0.889685000
O	0.411754000	-1.849031000	0.155570000
H	-0.305261000	-1.364969000	0.637568000
H	1.219857000	-1.615731000	0.636454000

RC (b)

E= -2401.93415504

N	-0.586113000	6.387195000	-1.000718000	C	0.181218000	-6.372375000	2.586956000
N	-2.463321000	4.466540000	-0.582694000	H	-0.899740000	-6.265888000	2.746398000
C	-1.757784000	6.783623000	-0.233453000	H	0.469661000	-7.346360000	3.012809000
H	-1.453468000	6.870818000	0.818405000	C	0.880482000	-5.266927000	3.337428000
H	-2.151009000	7.765487000	-0.536304000	C	1.408590000	-5.485710000	4.605207000
C	-2.842406000	5.739813000	-0.336793000	H	1.337959000	-6.471786000	5.053796000
C	-4.176790000	6.077425000	-0.150127000	C	2.039347000	-4.444790000	5.268467000
H	-4.448407000	7.112950000	0.029684000	H	2.478689000	-4.605009000	6.248804000
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H	-6.192721000	5.336907000	-0.082510000	C	1.572118000	-3.064168000	3.380746000
C	-4.762834000	3.764813000	-0.470800000	N	1.718572000	-4.683822000	-0.683841000
C	-3.403547000	3.512777000	-0.647467000	C	1.776291000	-6.641467000	0.770095000
N	0.302739000	4.300613000	-2.508903000	H	2.456789000	-6.340580000	1.577445000
C	-0.783221000	6.475278000	-2.444095000	H	1.908537000	-7.726684000	0.635870000
H	-1.837757000	6.257710000	-2.653844000	C	2.197983000	-5.922552000	-0.487316000
H	-0.582742000	7.484330000	-2.830388000	C	3.081585000	-6.512734000	-1.385915000
C	0.061634000	5.458907000	-3.163371000	C	3.476497000	-5.809178000	-2.513378000
C	0.534192000	5.689461000	-4.446792000	H	4.152903000	-6.261130000	-3.233289000
C	1.281704000	4.709400000	-5.084995000	C	2.967228000	-4.525488000	-2.736002000
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C	1.554823000	3.512307000	-4.413450000	H	0.326838000	6.638312000	-4.932028000
C	1.034172000	3.359477000	-3.128113000	H	1.680422000	-3.012965000	-1.884915000
N	1.039453000	4.942131000	0.704214000	H	-3.045657000	2.503747000	-0.832999000
C	0.662306000	6.994220000	-0.551548000	H	-2.625255000	-2.830863000	0.413955000
H	1.390442000	6.893608000	-1.366049000	H	1.195838000	2.441949000	-2.569159000
H	0.555166000	8.068422000	-0.347301000	H	3.442911000	-7.519986000	-1.201864000
C	1.210892000	6.284190000	0.657197000	H	1.348369000	3.195255000	1.760619000
C	1.892494000	6.967279000	1.652336000	H	1.596348000	-2.109405000	2.861369000
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C	2.396709000	6.265103000	2.739453000	Co	-0.408317000	4.313130000	-0.573293000
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H	-0.211336000	-6.932815000	-0.688070000	O	0.251178000	-1.752885000	0.368576000
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C	-3.093192000	-6.595549000	0.118400000	H	3.235005000	-3.940918000	-3.609005000
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C	-4.218619000	-5.792415000	0.040616000	H	-5.485321000	2.959092000	-0.536765000
H	-5.202632000	-6.236079000	-0.080610000	H	2.549815000	4.297235000	3.657787000
C	-4.083766000	-4.404978000	0.160765000	H	-4.936397000	-3.736352000	0.120971000
C	-2.794194000	-3.901885000	0.335637000	H	2.642370000	-2.356520000	5.118918000
N	0.952828000	-4.063100000	2.742839000	H	0.450738000	-1.604854000	-0.571627000

PC (b) E= -2401.91770429

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H	-1.453458000	6.870859000	0.818399000
H	-2.151028000	7.765474000	-0.536325000
C	-2.842411000	5.739790000	-0.336737000
C	-4.176791000	6.077426000	-0.150135000
H	-4.448407000	7.112950000	0.029684000
C	-5.143733000	5.086314000	-0.208811000
H	-6.192720000	5.336905000	-0.082500000
C	-4.762835000	3.764816000	-0.470818000
C	-3.403537000	3.512762000	-0.647441000
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C	-0.783273000	6.475265000	-2.444085000
H	-1.837751000	6.257685000	-2.653846000
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C	0.061728000	5.458959000	-3.163334000
C	0.534172000	5.689452000	-4.446801000
C	1.281702000	4.709399000	-5.084996000
H	1.681965000	4.883077000	-6.079277000
C	1.554783000	3.512288000	-4.413468000
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N	1.039607000	4.942139000	0.704351000
C	0.662295000	6.994243000	-0.551559000
H	1.390448000	6.893592000	-1.366042000
H	0.555171000	8.068425000	-0.347318000
C	1.210921000	6.284190000	0.657176000
C	1.892487000	6.967280000	1.652340000
H	2.010533000	8.043877000	1.579135000
C	2.396719000	6.265101000	2.739451000
H	2.914894000	6.786323000	3.538918000
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C	1.508932000	4.270318000	1.769290000
N	0.431522000	-6.283373000	1.164485000
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C	-4.083787000	-4.404964000	0.160824000

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C	0.880459000	-5.266921000	3.337437000
C	1.408604000	-5.485714000	4.605201000
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N	1.718599000	-4.683802000	-0.683802000
C	1.776279000	-6.641472000	0.770087000
H	2.456789000	-6.340580000	1.577445000
H	1.908537000	-7.726684000	0.635870000
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C	3.081575000	-6.512739000	-1.385921000
C	3.476504000	-5.809173000	-2.513369000
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C	2.967282000	-4.525459000	-2.735973000
C	2.089717000	-4.013947000	-1.778633000
H	0.326838000	6.638312000	-4.932028000
H	1.680277000	-3.013054000	-1.885132000
H	-3.045598000	2.503740000	-0.833051000
H	-2.625428000	-2.830947000	0.414035000
H	1.195822000	2.441942000	-2.569166000
H	3.442911000	-7.519986000	-1.201864000
H	1.348322000	3.195285000	1.760647000
H	1.596500000	-2.109334000	2.861408000
Cu	0.293032000	-4.042730000	0.732421000
Co	-0.379537000	4.193874000	-0.600523000
O	0.229560000	1.147472000	-0.153443000
H	0.628725000	1.196747000	0.733855000
H	-0.138511000	2.530753000	-0.352700000
O	-2.070060000	-0.103678000	0.239958000
H	-0.689181000	0.760653000	-0.002845000
H	-2.454267000	-0.155135000	-0.649509000
O	0.032862000	-1.827618000	0.341163000
H	-1.484415000	-0.895510000	0.292218000
H	0.560587000	-1.328972000	0.985642000
H	3.235045000	-3.940880000	-3.608994000
H	2.142993000	2.719547000	-4.860562000
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H 2.642269000 -2.356480000 5.119038000 H 0.458928000 -1.631471000 -0.508852000

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