

Electronic supplementary information for

Structural snapshots of the rearrangement of the bis(*di-tert*-butyl-aniline)amine pincer ligand in the presence of transition metal ions

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1. Experimental section

1.1 Materials and Instruments

Unless otherwise noted, all operations were performed under anaerobic conditions under a pure argon atmosphere using standard Schlenk techniques. Anhydrous triethylamine was distilled over CaH_2 under an argon atmosphere prior to use. Anhydrous acetonitrile and methanol were purchased from Acros. Synthetic procedures for the preparation of $\text{H}_3\text{L}^{\text{N,N,N}}$ and **1** were reported elsewhere.¹ All other chemicals were purchased from Acros, Alfa-Aesar, Sigma-Aldrich or TCI and were used as received. NMR spectra were recorded on a Bruker Avance 400 or 500 (^1H at 400 or 500 MHz, ^{13}C at 100 or 125 MHz). The EPR spectra were recorded on an EMX plus spectrometer equipped with an Oxford Helium cryostat and a dual-mode resonant cavity. The spectra were treated using the Easyspin software.² Chemical shifts are given relative to solvent residual peaks. Mass spectra were recorded on a Bruker Esquire 3000 (ESI/Ion Trap) apparatus. Microanalysis were performed by using an apparatus designed by the Service Central d'Analyse du CNRS (Lyon, France). UV/Vis spectra were recorded on a Perkin-Elmer Lambda 1050 spectrophotometer in quartz cells (Hellma) of 1.00 mm path length.

1.2 Crystal structure analysis

A single crystal was coated with a parafin mixture, picked up with nylon loops and mounted in the nitrogen cold stream of a Nonius 4 circles diffractometer at 200 K. The Mo-K α radiation ($\lambda = 0.71073\text{\AA}$) from an Incoatec micro Mo-target X-ray source equipped with Montel optics was used. The data were collected with a Bruker APEXII detector. Final cell parameters were obtained from refinement using all data. Intensities were corrected for absorption using a multiscan method implemented with the program SADABS and then for Lorentz and polarisation effects using XPREP. The structures were solved and refined by charge flipping methods and subsequent difference Fourier techniques. The OLEX software was used for the refinement.³ All non-hydrogen atoms were anisotropically refined and hydrogen atoms were placed at calculated positions and refined as riding atoms with isotropic displacement parameters. CCDC-1578912-1578916 contain the crystallographic data for the compounds described in this article; these data can be obtained free of charge via <http://www.ccdc.cam.ac.uk/conts/retrieving.html>

1.3 Computational details

Full geometric optimizations were performed with the Gaussian 9.0 program,⁴ by using the B3LYP functional^{5, 6} in combination with the 6-31g* basis set⁷ for all atoms. Numerical frequency calculations were systematically performed in order to ensure that the optimized structures correspond to a real energy minimum and not a saddle point. The relative energies are given in the gas phase. They were calculated at the same level of theory.

1.4 Synthesis

Compound **2**. Under argon and at rt, $\text{Co}(\text{OAc})_2 \cdot 4\text{H}_2\text{O}$ (29 mg, 0.12 mmol, 0.5 eq.) and Et_3N (66 μL , 0.47 mmol, 2.0 eq.) were added to a degassed solution of $\text{H}_3\text{L}^{\text{N,N,N}}$ (100 mg, 0.24 mmol, 1.0 eq.) in CH_3CN (5 mL). The resulting mixture was stirred at 80°C during 1 hour and turned rapidly from colorless to dark blue. The reaction was then cooled to r.t. and exposed to air during 1 hour. The deep dark blue precipitate that formed was filtrated through a frit and washed with CH_3CN . Yield: 78

% (When the reaction was carried out in MeOH, a lower yield of 54 % was obtained). Suitable crystals for X-ray analysis were obtained under argon by slow diffusion of MeOH in a benzene solution. MS (ESI): $m/z = 900$ $[M-H]^+$. IR: $\nu(\text{cm}^{-1})$ 3489, 3387, 2953, 2903, 2864, 1575, 1539, 1476, 1443, 1306, 1144. Anal. Calcd for $\text{C}_{56}\text{H}_{86}\text{N}_6\text{Co}$, 1.5 H_2O : C, 72.38; H, 9.65; N, 9.04. Found: C, 72.39; H, 9.43; N, 9.00.

Compound **3⁺** • SbF_6^- . Under argon and at rt, $\text{CoCl}_2 \cdot 6\text{H}_2\text{O}$ (29 mg, 0.12 mmol, 0.5 eq.) and Et_3N (100 μL , 0.72 mmol, 3.0 eq.) were added to a degassed solution of $\text{H}_3\text{L}^{\text{N,N,N}}$ (102 mg, 0.24 mmol, 1.0 eq.) in MeOH (25 mL). The resulting mixture was stirred at 80°C under argon during 30 min and was then allowed to cool to rt. Upon cooling, the reaction vessel was opened to air and the mixture was stirred at rt for an additional hour. After filtration through a frit, KSbF_6 (33 mg, 0.12 mmol, 1.0 eq.) was added to the filtrate. The methanolic solution was then concentrated under reduced pressure. The remaining residue was dissolved in a toluene/acetone mixture. Slow evaporation of the resulting solution over 1 week afforded dark purple crystals. The material was filtrated through a frit and dried under vacuum. Yield: 81 %. IR: $\nu(\text{cm}^{-1})$ 3351, 2950, 2909, 2873, 1596, 1479, 1461, 1392, 1363, 1042, 726. HRMS (ESI, $[M - \text{SbF}_6]^+$): m/z calcd for $\text{C}_{56}\text{H}_{82}\text{N}_6\text{Co}$: 897.5933, found: 897.5924.

Compound **4⁺** • SbF_6^- . Under air, a black suspension of **1** (20 mg, 0.022 mmol, 1.0 eq.) in MeOH (4 mL) was vigorously stirred at rt. The mixture progressively turns into a clear red solution over several hours. After 22h, KSbF_6 (20 mg, 0.073 mmol, 3.3 eq.) was added in one portion and the solution was stirred for 2 additional hours. The volatiles were then removed under reduced pressure. The remaining orange solid residue was triturated in CH_2Cl_2 and filtrated through a pad of celite. The filtrate was concentrated under reduced pressure to afford a red solid. Yield: 100%. An analytical sample was obtained by recrystallization from MeOH. ^1H NMR (500 MHz, CDCl_3): δ (ppm) = 11.12 (br s, 1H), 7.70 (s, 1H), 7.49 (d, $J = 2.0\text{Hz}$, 1H), 7.45 (d, $J = 2.5\text{ Hz}$, 1H), 7.22 (s, 1H), 6.98 (d, $J = 2.5\text{ Hz}$, 1H), 6.89 (d, $J = 2.0\text{ Hz}$, 1H), 6.60 (s, 1H), 6.16 (s, 1H), 4.72 (s, 2H), 1.50 (s, 9H), 1.43 (s, 9H), 1.32 (s, 9H), 1.28 (s, 9H), 1.242 (s, 9H), 1.235 (s, 9H), 1.13 (s, 9H), 1.04 (s, 9H). ^{13}C NMR (125 MHz, CDCl_3): δ (ppm) = 164.1, 163.2, 161.4, 157.3, 150.7, 148.5, 147.8, 144.9, 140.7, 140.6, 140.3, 138.2, 136.7, 128.7, 126.9, 126.1, 123.9, 123.71, 123.65, 117.6, 115.4, 112.2, 105.1, 37, 4, 37.2, 36.5, 36.29, 36.27, 35.8, 35.2, 34.6, 31.8, 31.4, 31.1, 30.7, 30.3, 30.2, 29.5, 28.5. IR: $\nu(\text{cm}^{-1})$ 3500, 3379, 2962, 2906, 2867, 1629, 1608, 1479, 1464, 1366, 654. HRMS (ESI, $[M - \text{SbF}_6]^+$): m/z calcd for $\text{C}_{56}\text{H}_{83}\text{N}_6$: 839.6679, found: 839.6680.

Compound **5**. The filtrate obtained from the synthesis of **2** was allowed to stand at rt for several weeks and afforded light blue crystals. Yield: 2%. IR $\nu(\text{cm}^{-1})$ 3433, 2952, 1714, 1616, 1606, 1480, 1363, 1264, 1049. HRMS (ESI, $[M + H]^+$): m/z calcd for $\text{C}_{56}\text{H}_{81}\text{N}_6\text{O}$ 853.6472, found: 853.6447.

1,3,7,9-Tetra-tert-butylphenazine (6). *Method (A)*: Under argon and at rt, FeCl_3 (19 mg, 0.12 mmol, 0.5 eq.) and Et_3N (100 mL, 0.72 mmol, 3.0 eq.) were added to a degassed solution of $\text{H}_3\text{L}^{\text{N,N,N}}$ (100 mg, 0.24 mmol, 1.0 eq.) in MeOH (10 mL). The resulting mixture was stirred at 80°C during 1 hour. Upon cooling to rt, the reaction vessel was opened to air and allowed to stir for an additional hour (when exposed to air, a color change from dark purple to dark blue was observed). KSbF_6 was then added in small portions (265 mg, 0.96 mmol, 4.0 eq.), followed by water. The black insoluble solids that formed were filtrated through a frit, abundantly washed with H_2O and dried under vacuum in the presence of P_2O_5 . In these conditions, 98mg of a black impure powder were recovered. A sample was dissolved in a 1:1 mixture of CH_2Cl_2 and CH_3CN and the slow evaporation of the resulting solution afforded yellow crystals of the title compound.

Method (B): Under air and at rt, H₃L^{N,N,N} (50 mg, 0.12 mmol, 1.0 eq.) was added to a solution of Cu(BF₄)₂ • H₂O (28 mg, 0.12 mmol, 1.0 eq.) in CH₃CN (12 mL). A color change to brown, then yellow occurred within 15 min. The mixture was stirred at 85°C during 1 hour, then cooled to rt and concentrated under reduced pressure. The remaining residue was dissolved in CH₂Cl₂. The resulting solution was filtrated through a pad of celite and concentrated under reduced pressure to afford **6** quantitatively.

¹H NMR (400 MHz, CDCl₃): δ (ppm)= 7.95 (d, *J* = 2.3 Hz, 2H), 7.84 (d, *J* = 2.3 Hz, 2H), 1.77 (s, 18H), 1.48 (s, 18H). ¹³C NMR (100 MHz, CDCl₃): δ (ppm) = 152.2, 147.6, 143.4, 139.7, 125.9, 122.9, 36.9, 35.6, 31.6, 31.0. MS (ESI): *m/z*= 405 [M + H]⁺. IR: ν(cm⁻¹) 2955, 2908, 2867, 1616, 1458, 1391, 1359, 1344, 1261, 1033, 998, 878. HRMS (ESI, [M + H]⁺): *m/z* calcd for C₂₈H₄₀N₂: 405.3270, found: 405.3272.

2. Figures

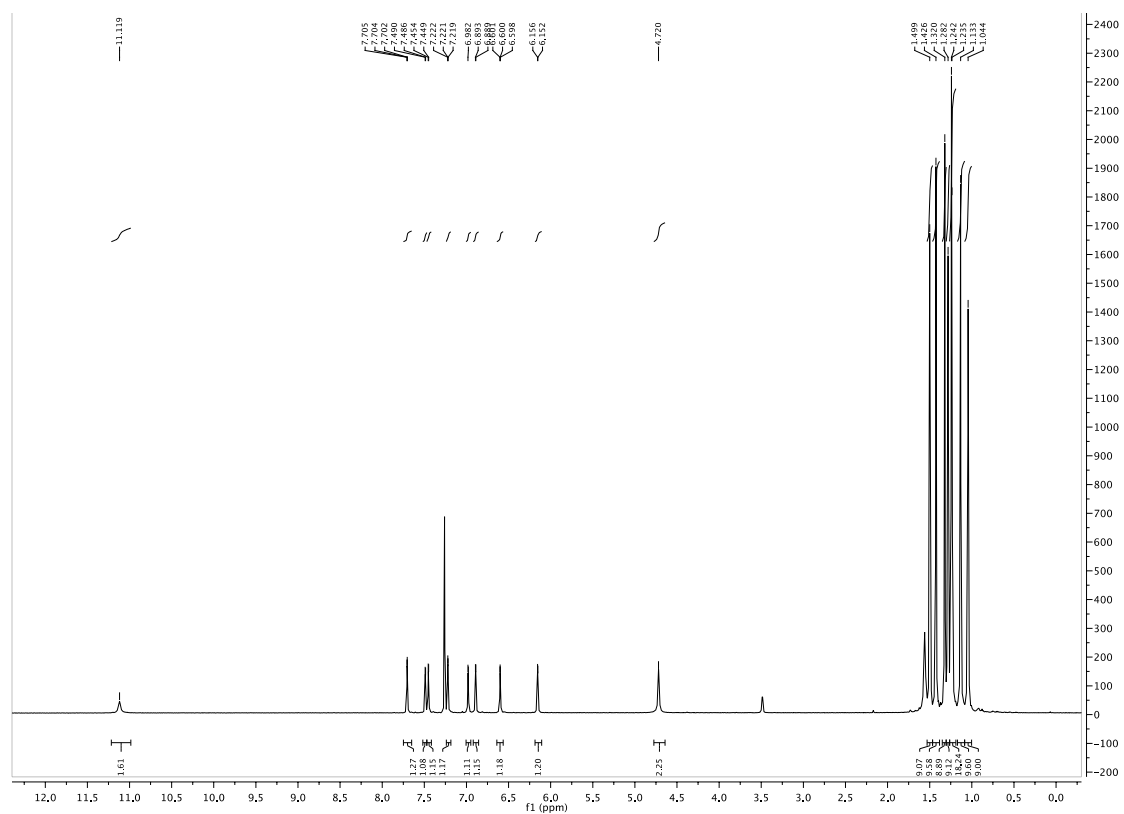


Fig. S1 ^1H NMR spectrum of $4^+ \cdot \text{SbF}_6^-$

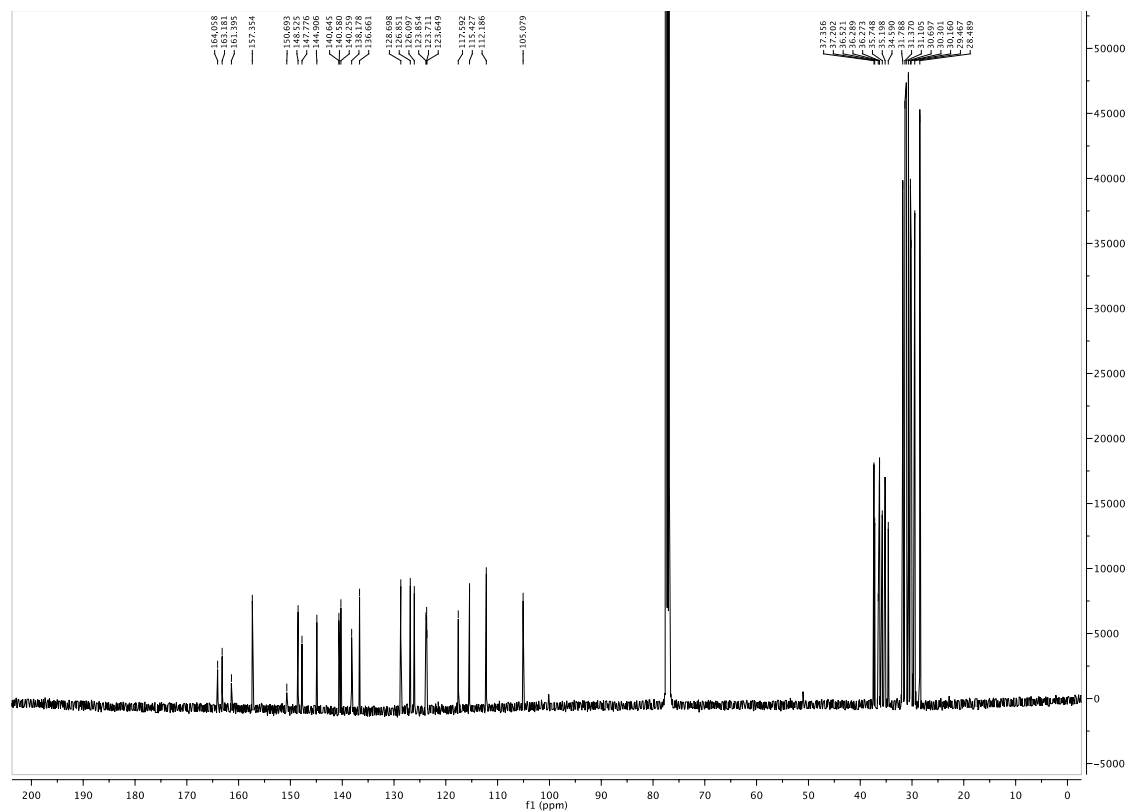


Fig. S2 ^{13}C NMR spectrum of $4^+ \cdot \text{SbF}_6^-$

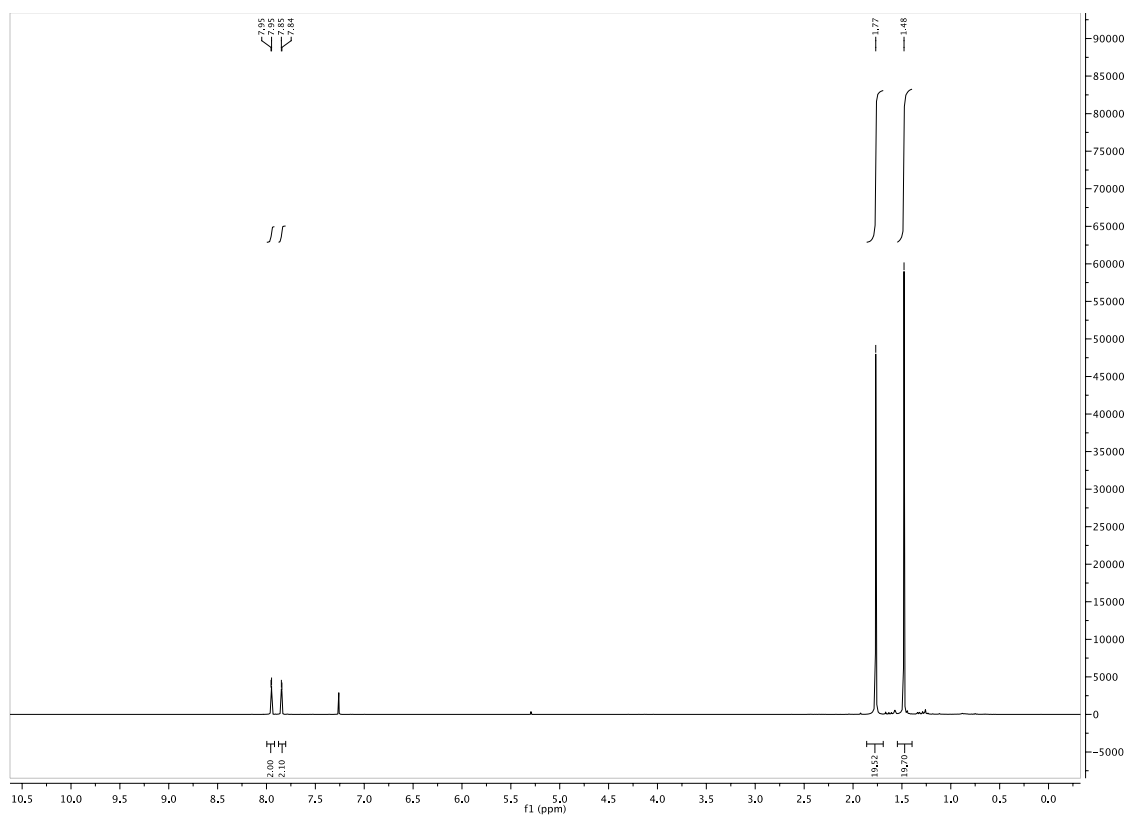


Fig. S3 ^1H NMR spectrum of **6**

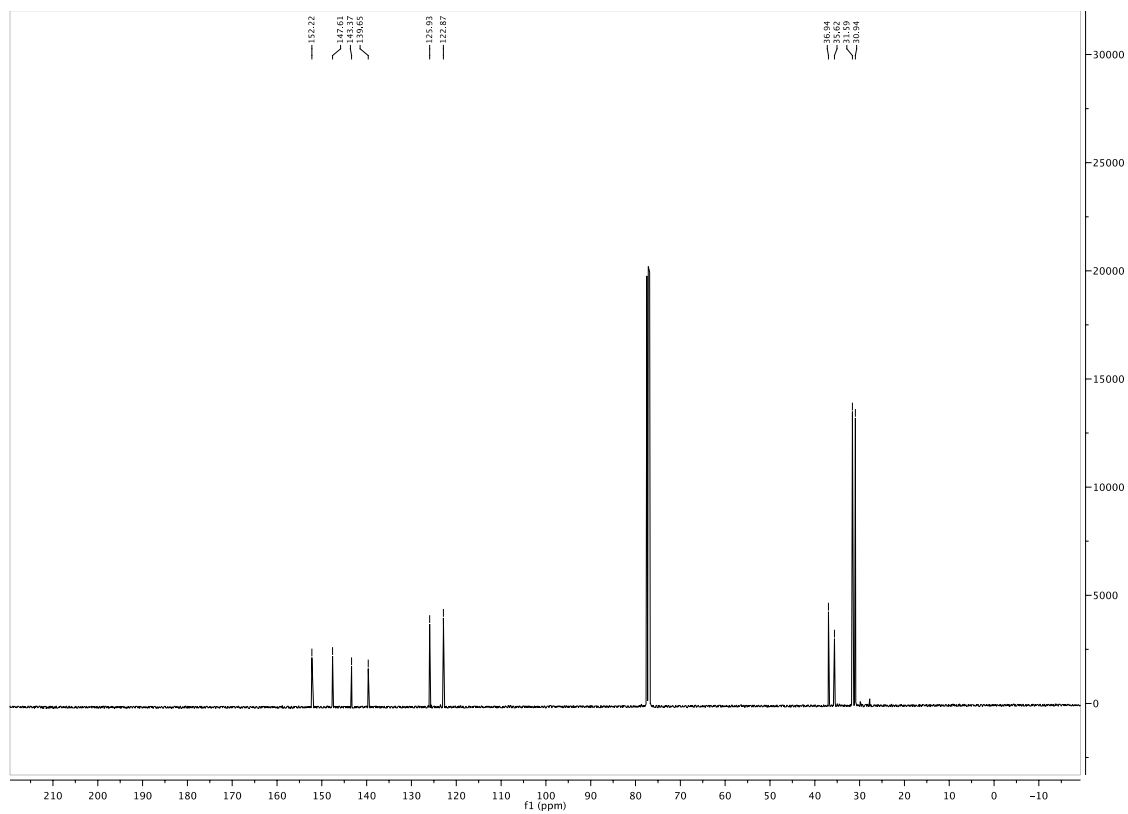


Fig. S4 ^{13}C NMR spectrum of **6**

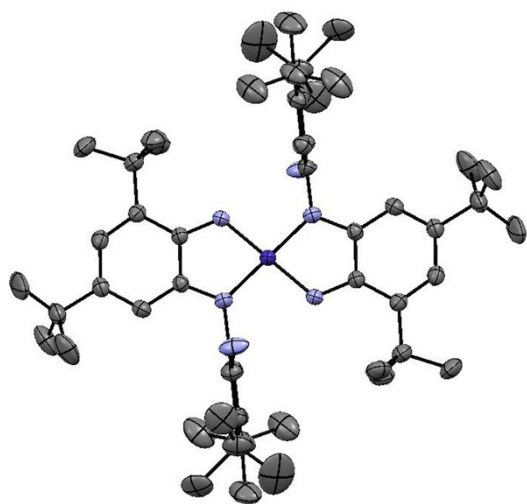


Fig. S5 ORTEP plot of **2** shown with 30% thermal ellipsoids

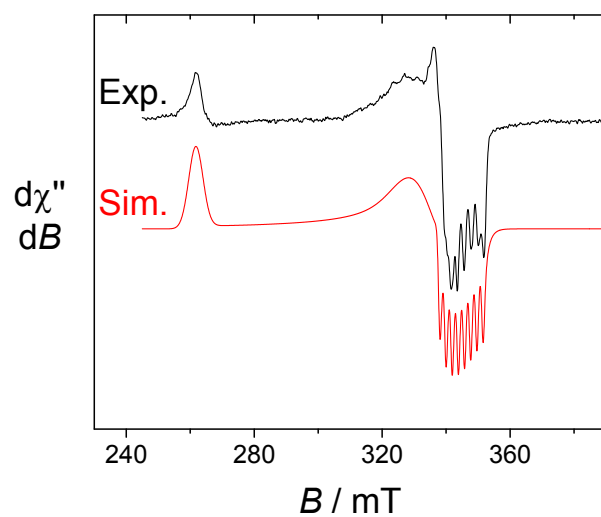


Fig. S6 X-Band EPR spectrum of a 0.5 mM toluene solution of **2**. Microwave Freq. 9.63 GHz, power 5 mW; Mod. Amp. 0.4 mT, Freq. 100 KHz; $T = 18$ K. The red line represents a simulation by using the following spin Hamiltonian parameters: ($S = \frac{1}{2}$), $g_1 = 2.628$, $g_2 = 2.050$, $g_3 = 1.997$, $A_3 = 56$ MHz.

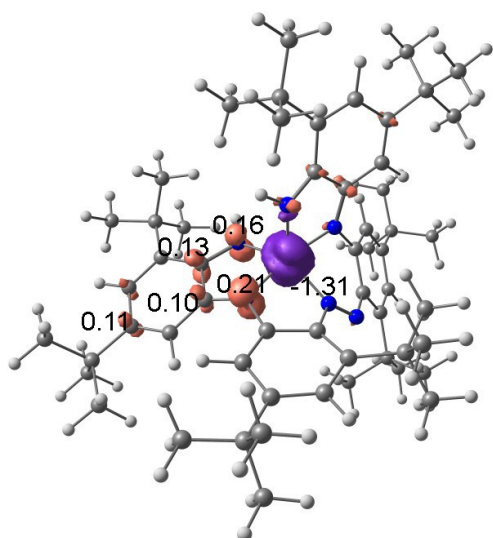


Fig. S7 Spin density plot for the broken symmetry singlet 3^+ (B3LYP/6-31g*)

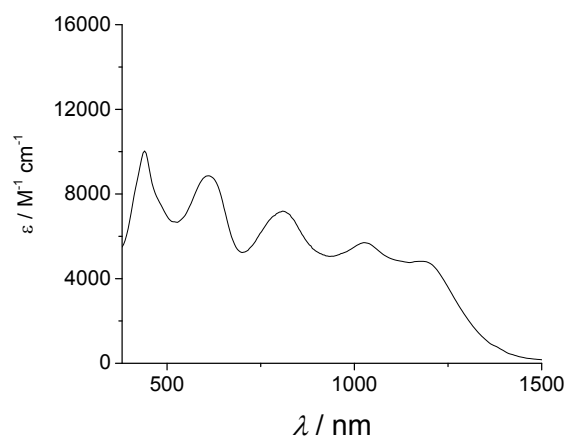


Fig. S8 UV-Vis-NIR spectrum of **2** in CH_2Cl_2 ; $T = 298 \text{ K}$.

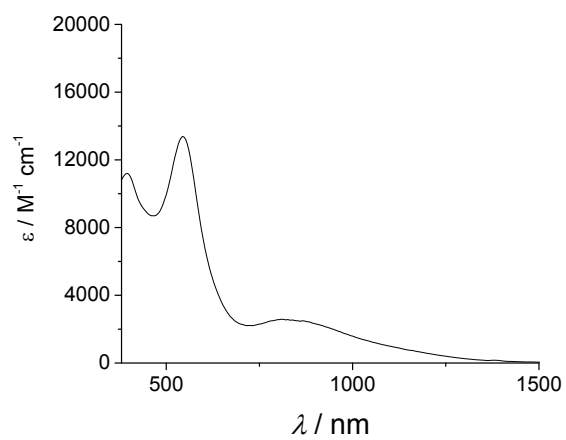


Fig. S9 UV-Vis-NIR spectrum of 3^+ in CH_2Cl_2 ; $T = 298 \text{ K}$.

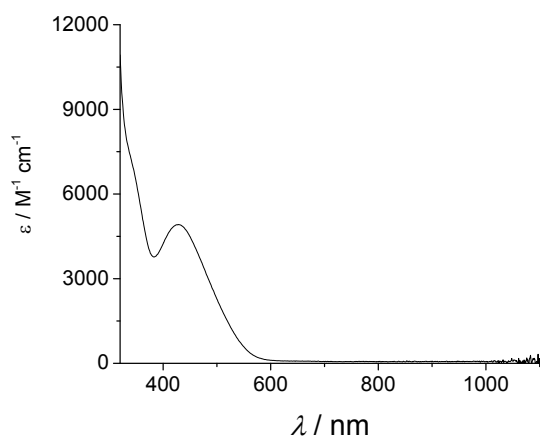


Fig. S10 UV-Vis-NIR spectrum of 4^+ in CH_2Cl_2 ; $T = 298 \text{ K}$.

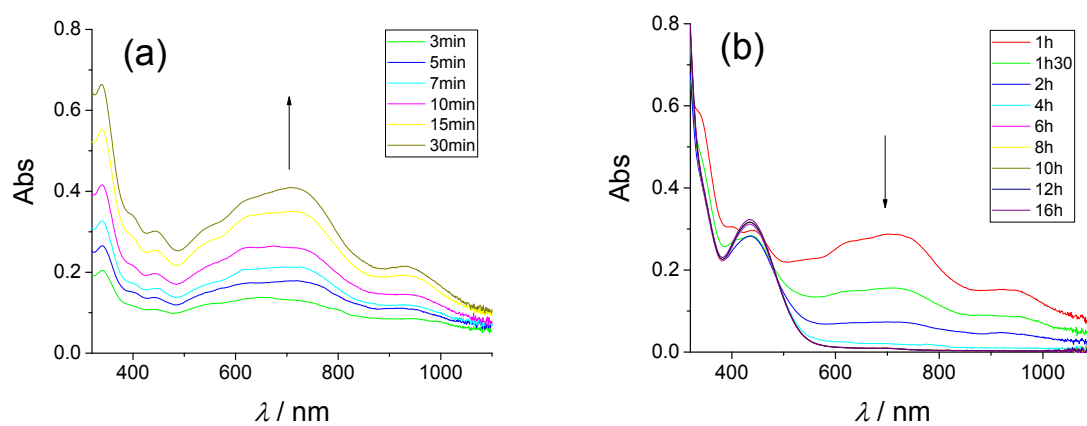


Fig. S11 Evolution of the UV-Vis spectrum of 1 (conversion of 1 to 4^+) in CH_2Cl_2 . (a) Slow solubilisation of the crystalline material; (b) conversion to 4^+ . $c = 0.5 \text{ mM}$; $l = 1.00 \text{ mm}$; $T = 298 \text{ K}$.

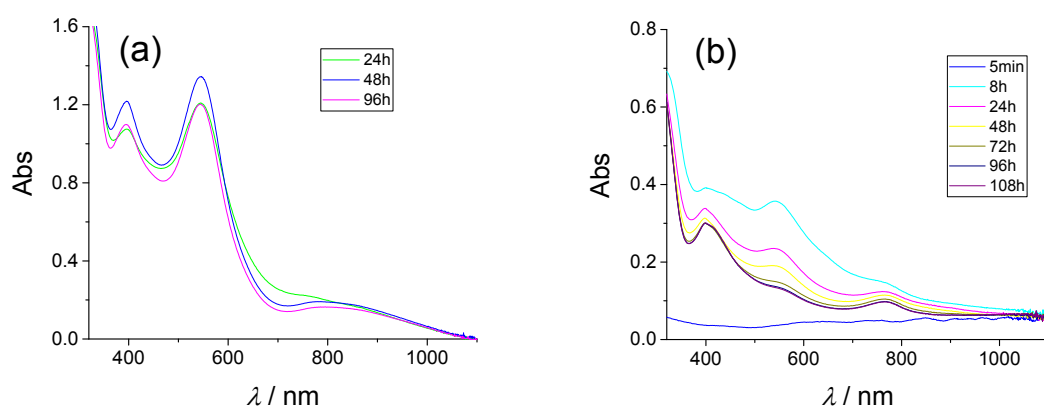


Fig. S12 Evolution of the UV-Vis spectrum of 2 in (a) CH_2Cl_2 and (b) CH_3CN . The deviation from the baseline and the lower intensity in the top spectra of (b) is explained by the presence of a microprecipitate inside the cell; It must be emphasized that complex 2 is poorly soluble in CH_3CN , explaining the featureless spectrum after 5 minutes. $c = 0.5 \text{ mM}$; $l = 1.00 \text{ mm}$; $T = 298 \text{ K}$.

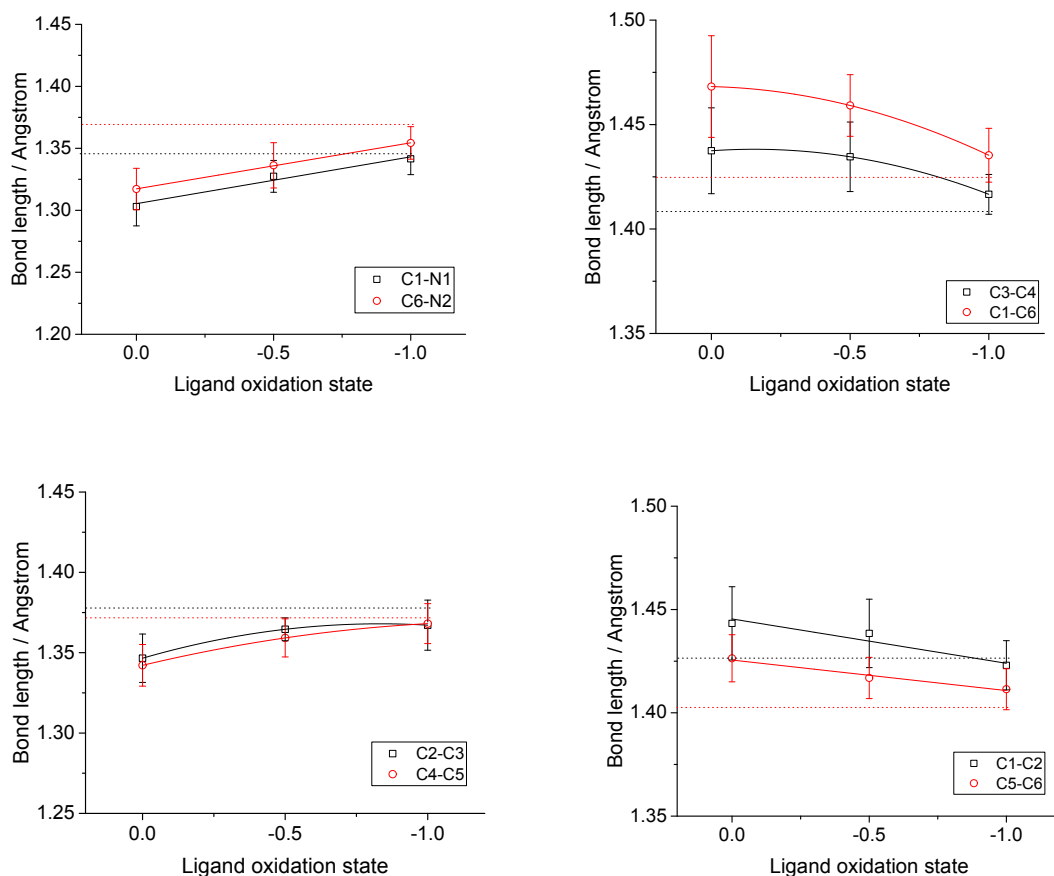
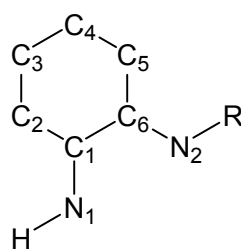


Fig. S13 Empirical “metric oxidation state” (MOS) for the o-phenylene diamine ligand in the oxidation states of -1 (iminosemiquinone), -0.5 (mixed valent iminosemiquinone-diiminoquinone) and 0 (diiminoquinone), based on the article of S. N. Brown (*Inorg. Chem.* 2012, **51**, 1251). 36 entries were used for the oxidation state of -1; 14 entries for -0.5; 24 entries for 0. References: *Dalton Trans.* **2009**, 7778; *Angew. Chem. Int. Ed.* **2003**, 42, 563; *Inorg. Chem.* **2005**, 44, 7087; *Inorg. Chim. Acta*, **1985**, 101, L31; *J. Coord. Chem.* **2003**, 56, 1049; *Inorg. Chem.* **2004**, 43, 6445; *Eur. J. Inorg. Chem.* 2007, 314; *J. Am. Chem. Soc.* **2003**, 125, 9116; *Chem. Commun.* **2014**, 50, 1918; *Inorg. Chem.* **2016**, 55, 649; *Eur. J. Inorg. Chem.* **2018**, 1752; *Inorg. Chem.* **1998**, 37, 35; *J. Am. Chem. Soc.* **1973**, 95, 3869; *J. Chem. Soc. Dalton Trans.* **2001**, 336; *Inorg. Chem.* **2017**, 56, 4966; *Inorg. Chim. Acta* **2003**, 350, 557. The data reported for the pincer ligands coordinated in tridentate fashion are omitted due to delocalization, but those of the same ligand coordinated in a bidentate fashion are included. The numbering is indicated above. The dotted lines represent the experimental bond lengths in complex **2**.

3. Tables

Table S1 Selected bond distances in **3⁺**

	Exp ^[a]	Singlet ^[b]	Triplet ^[b]
Co-N1	1.843	1.827	1.924
Co-N2	1.848	1.884	1.904
Co-N9	1.869	1.863	1.876
Co-N3	1.873	1.881	1.892
Co-N5	1.883	1.845	1.951
C-N1	1.32	1.346	1.341
C--N2	1.326/1.405	1.353/1.403	1.353/1.387
C-N9	1.469	1.432	1.423
C--N3	1.384/1.326	1.389/1.352	1.324/1.390
C-N5	1.305	1.344	1.328

^[a] From the X-Ray crystal structure

^[b] B3LYP/6-31g* level of theory

Table S2 Energy of the different spin configurations of **3⁺** ^[a]

Spin state ^[a,b]	Electronic energy	Electronic energy + ZPE	Electronic + thermal free energy	<S ² >
Closed-shell singlet / Ha	-3894.399553	-3893.116607	-3893.218058	0
Triplet / Ha	-3894.397332	-3893.116001	-3893.218101	2.179
BS(1,1) / Ha	-3894.401511			1.1124
$\Delta E(\text{BS}(1,1)\text{-triplet}) / \text{kcal/mol}$	-2.6			
$\Delta E(\text{CSS-triplet}) / \text{kcal/mol}$		-0.4		

^[a] CSS: Closed-shell singlet; BS: Broken-symmetry.

^[b] B3LYP/6-31g* calculation in the gas phase.

4. Computational details

XYZ coordinates for **2** (quartet):

Co	-0.038087000	0.044242000	-0.140021000
N	0.568844000	1.796496000	-0.031994000
H	-0.010191000	2.599387000	0.176299000
N	1.774652000	-0.322235000	-0.533941000
C	2.335519000	-1.583342000	-0.898052000
C	2.575158000	0.790994000	-0.592567000
C	1.877362000	2.020596000	-0.283817000
C	3.442162000	-3.992405000	-1.618623000
H	3.884468000	-4.940058000	-1.898151000
C	4.652060000	2.008686000	-0.895547000
C	2.593898000	3.261734000	-0.288593000
C	2.467362000	-1.917500000	-2.241525000
H	2.133636000	-1.185738000	-2.972012000
C	2.743223000	-2.482360000	0.130235000
C	3.946349000	0.810227000	-0.894609000
H	4.438462000	-0.127856000	-1.122630000
C	3.028382000	-3.137480000	-2.640713000
C	3.950824000	3.203777000	-0.592885000
H	4.508380000	4.127958000	-0.603597000
C	6.157959000	2.002121000	-1.222095000
C	3.322542000	-3.721885000	-0.241019000
C	1.287577000	4.610898000	1.430208000
H	0.544464000	3.826308000	1.591379000
H	0.798029000	5.572470000	1.626743000
H	2.073958000	4.473055000	2.181319000
C	1.901532000	4.608800000	0.006014000
C	0.818245000	4.892999000	-1.066879000
H	1.280867000	4.964312000	-2.058159000
H	0.324966000	5.850629000	-0.858004000
H	0.043781000	4.123544000	-1.125534000
C	3.848918000	-4.841990000	0.706569000
C	2.889036000	5.794945000	-0.041337000
H	3.688110000	5.695474000	0.701820000
H	2.348262000	6.722449000	0.178348000
H	3.348749000	5.909166000	-1.029197000
C	3.178969000	-3.469122000	-4.136614000
C	1.792868000	-3.425466000	-4.822357000
H	1.113822000	-4.162686000	-4.378598000
H	1.886106000	-3.649040000	-5.892592000
H	1.322950000	-2.440827000	-4.729037000
C	3.781768000	-4.866890000	-4.372388000
H	4.788467000	-4.955701000	-3.948042000
H	3.860901000	-5.058170000	-5.448603000
H	3.157356000	-5.657883000	-3.941007000
C	4.107753000	-2.425841000	-4.802718000
H	3.715540000	-1.408801000	-4.697170000
H	4.215295000	-2.633226000	-5.874885000
H	5.106402000	-2.447061000	-4.350825000
C	6.374014000	1.427818000	-2.643184000
H	7.443714000	1.400690000	-2.885829000
H	5.870633000	2.046378000	-3.395129000
H	5.983867000	0.408974000	-2.734739000
C	6.903956000	1.115439000	-0.195821000
H	6.539121000	0.083414000	-0.209036000
H	6.775662000	1.502979000	0.821513000
H	7.978112000	1.094073000	-0.418675000
C	6.786082000	3.408760000	-1.178241000
H	6.698704000	3.866408000	-0.186141000

H	6.327422000	4.084643000	-1.908912000
H	7.853699000	3.341625000	-1.416671000
N	2.477459000	-2.074237000	1.443610000
H	3.163427000	-2.322582000	2.138280000
H	2.233608000	-1.091397000	1.485089000
C	5.345325000	-5.106642000	0.401445000
H	5.730875000	-5.898560000	1.055815000
H	5.943520000	-4.204189000	0.573554000
H	5.512642000	-5.422089000	-0.632458000
C	3.757437000	-4.562403000	2.223090000
H	2.736120000	-4.353595000	2.551257000
H	4.415044000	-3.739706000	2.532758000
H	4.104921000	-5.450021000	2.764310000
C	3.038741000	-6.138570000	0.452670000
H	1.982101000	-5.990673000	0.701038000
H	3.423065000	-6.955416000	1.076534000
H	3.093585000	-6.463682000	-0.590542000
N	-0.659942000	-1.686520000	-0.365294000
H	-0.092123000	-2.468318000	-0.665446000
N	-1.834609000	0.387375000	0.350945000
C	-2.335573000	1.577294000	0.958432000
C	-2.641479000	-0.725208000	0.337496000
C	-1.967391000	-1.922421000	-0.112261000
C	-3.329617000	3.842211000	2.155932000
H	-3.727077000	4.733572000	2.623470000
C	-4.718323000	-1.954770000	0.592960000
C	-2.698019000	-3.149464000	-0.221875000
C	-2.430966000	1.651881000	2.344640000
H	-2.111131000	0.783065000	2.912693000
C	-2.724979000	2.671900000	0.133946000
C	-4.000289000	-0.767210000	0.688956000
H	-4.475432000	0.145469000	1.029664000
C	-2.931522000	2.791423000	2.983945000
C	-4.043032000	-3.114806000	0.136321000
H	-4.611755000	-4.029572000	0.063890000
C	-6.209764000	-1.973341000	0.980829000
C	-3.246048000	3.837892000	0.750002000
C	-1.470733000	-4.290300000	-2.135467000
H	-0.718338000	-3.502443000	-2.220594000
H	-1.006227000	-5.226727000	-2.468041000
H	-2.278625000	-4.046656000	-2.834979000
C	-2.035030000	-4.458302000	-0.700895000
C	-0.917336000	-4.885581000	0.284890000
H	-1.342841000	-5.080826000	1.275880000
H	-0.440275000	-5.808567000	-0.066883000
H	-0.133545000	-4.134388000	0.412089000
C	-3.746528000	5.136688000	0.048594000
C	-3.036516000	-5.631697000	-0.761952000
H	-3.859681000	-5.435455000	-1.458057000
H	-2.516723000	-6.530895000	-1.111543000
H	-3.463143000	-5.860521000	0.220816000
C	-3.025406000	2.839761000	4.519768000
C	-1.615657000	2.652096000	5.129304000
H	-0.939672000	3.451692000	4.805041000
H	-1.664740000	2.670570000	6.225340000
H	-1.169671000	1.697407000	4.831438000
C	-3.595614000	4.175488000	5.033799000
H	-4.612692000	4.353641000	4.665849000
H	-3.639006000	4.160829000	6.128861000
H	-2.971250000	5.027125000	4.739828000
C	-3.948369000	1.701676000	5.017260000
H	-3.575388000	0.716378000	4.718613000
H	-4.018593000	1.713777000	6.112270000

H	-4.960481000	1.813275000	4.611032000
C	-6.357964000	-1.561715000	2.465776000
H	-7.415645000	-1.555640000	2.757962000
H	-5.828811000	-2.264100000	3.120052000
H	-5.952598000	-0.562195000	2.653137000
C	-6.987423000	-0.970214000	0.095123000
H	-6.605428000	0.049696000	0.205317000
H	-6.912221000	-1.243095000	-0.963881000
H	-8.049762000	-0.961168000	0.369531000
C	-6.856140000	-3.361083000	0.805711000
H	-6.814830000	-3.703647000	-0.234578000
H	-6.375682000	-4.118609000	1.435260000
H	-7.912016000	-3.313698000	1.095320000
N	-2.493734000	2.513387000	-1.240687000
H	-3.175996000	2.921699000	-1.859566000
H	-2.304271000	1.544059000	-1.471620000
C	-5.228657000	5.383665000	0.429982000
H	-5.596903000	6.297048000	-0.053794000
H	-5.859371000	4.549153000	0.101822000
H	-5.369387000	5.501238000	1.508406000
C	-3.685556000	5.153947000	-1.494702000
H	-2.677430000	4.976857000	-1.877757000
H	-4.378659000	4.430933000	-1.944161000
H	-4.004350000	6.141419000	-1.847647000
C	-2.889108000	6.333550000	0.533023000
H	-1.840416000	6.200304000	0.245319000
H	-3.249409000	7.266368000	0.081209000
H	-2.923275000	6.456036000	1.619517000

XYZ coordinates for **2** (doublet):

Co	0.000001000	0.000003000	-0.000088000
N	0.422784000	1.771243000	-0.033472000
H	1.368192000	2.133233000	-0.022618000
N	-1.752216000	0.622163000	-0.032165000
C	-2.955675000	-0.152014000	0.016388000
C	-1.868995000	1.996013000	-0.048739000
C	-0.600107000	2.668160000	-0.048709000
C	-5.295584000	-1.579966000	0.152938000
H	-6.220155000	-2.140617000	0.202431000
C	-3.036063000	4.118560000	-0.091027000
C	-0.551148000	4.095180000	-0.061575000
C	-3.531330000	-0.429645000	1.250870000
H	-3.026636000	-0.045286000	2.132441000
C	-3.541246000	-0.614573000	-1.196525000
C	-3.066671000	2.728400000	-0.070745000
H	-4.006799000	2.188738000	-0.066195000
C	-4.726162000	-1.152492000	1.353382000
C	-1.774997000	4.762495000	-0.084795000
H	-1.763451000	5.841903000	-0.095303000
C	-4.360519000	4.907766000	-0.113297000
C	-4.751872000	-1.350416000	-1.125908000
C	1.636229000	4.533902000	-1.284431000
H	1.890398000	3.474192000	-1.366828000
H	2.578064000	5.095819000	-1.258864000
H	1.100854000	4.813097000	-2.199195000
C	0.781390000	4.873951000	-0.036458000
C	1.559461000	4.556927000	1.266628000
H	0.979060000	4.874193000	2.140508000
H	2.511730000	5.101576000	1.277132000
H	1.782409000	3.494753000	1.395837000
C	-5.559233000	-1.957683000	-2.312756000

C	0.564367000	6.401932000	-0.058981000
H	0.042448000	6.729987000	-0.964794000
H	1.537847000	6.904721000	-0.039076000
H	-0.003238000	6.749492000	0.811174000
C	-5.353340000	-1.420345000	2.733700000
C	-4.349455000	-2.193246000	3.621397000
H	-4.098911000	-3.162939000	3.175927000
H	-4.776706000	-2.375543000	4.615466000
H	-3.415420000	-1.638090000	3.757746000
C	-6.647167000	-2.251170000	2.641561000
H	-7.420758000	-1.739903000	2.057144000
H	-7.050810000	-2.417918000	3.646798000
H	-6.469510000	-3.233792000	2.189445000
C	-5.695561000	-0.071689000	3.411498000
H	-4.806211000	0.554183000	3.539358000
H	-6.132459000	-0.238990000	4.404060000
H	-6.418829000	0.494178000	2.812823000
C	-5.188743000	4.559911000	1.146983000
H	-6.142096000	5.103257000	1.141052000
H	-4.646241000	4.835060000	2.058747000
H	-5.413451000	3.489904000	1.203246000
C	-5.169049000	4.522409000	-1.375462000
H	-5.396773000	3.451751000	-1.400074000
H	-4.611242000	4.767273000	-2.286813000
H	-6.120759000	5.067810000	-1.402298000
C	-4.145630000	6.433399000	-0.134600000
H	-3.589458000	6.756440000	-1.022037000
H	-3.606734000	6.782928000	0.753337000
H	-5.116790000	6.941145000	-0.151314000
N	-2.825458000	-0.357163000	-2.373629000
H	-3.373836000	-0.124510000	-3.186435000
H	-2.076348000	0.308223000	-2.222477000
C	-6.999859000	-1.386190000	-2.298782000
H	-7.582811000	-1.809819000	-3.126145000
H	-6.987181000	-0.296411000	-2.417416000
H	-7.533063000	-1.611876000	-1.370685000
C	-5.003262000	-1.698771000	-3.730486000
H	-3.978116000	-2.056899000	-3.852185000
H	-5.052267000	-0.637504000	-4.007259000
H	-5.630273000	-2.231247000	-4.454850000
C	-5.617578000	-3.497022000	-2.140627000
H	-4.611882000	-3.930022000	-2.179706000
H	-6.213086000	-3.947290000	-2.944763000
H	-6.069534000	-3.789686000	-1.188231000
N	-0.422787000	-1.771236000	0.033315000
H	-1.368195000	-2.133227000	0.022478000
N	1.752215000	-0.622159000	0.032031000
C	2.955679000	0.152014000	-0.016478000
C	1.868990000	-1.996007000	0.048676000
C	0.600103000	-2.668154000	0.048636000
C	5.295599000	1.579954000	-0.152942000
H	6.220163000	2.140619000	-0.202401000
C	3.036057000	-4.118554000	0.091077000
C	0.551147000	-4.095176000	0.061587000
C	3.531398000	0.429610000	-1.250938000
H	3.026756000	0.045214000	-2.132521000
C	3.541189000	0.614596000	1.196454000
C	3.066664000	-2.728396000	0.070729000
H	4.006794000	-2.188736000	0.066181000
C	4.726243000	1.152444000	-1.353406000
C	1.774993000	-4.762491000	0.084860000
H	1.763443000	-5.841898000	0.095427000
C	4.360513000	-4.907758000	0.113429000

C	4.751825000	1.350426000	1.125881000
C	-1.636213000	-4.533931000	1.284489000
H	-1.890405000	-3.474231000	1.366921000
H	-2.578033000	-5.095875000	1.258935000
H	-1.100808000	-4.813133000	2.199232000
C	-0.781388000	-4.873953000	0.036494000
C	-1.559469000	-4.556937000	-1.266588000
H	-0.979065000	-4.874207000	-2.140466000
H	-2.511731000	-5.101597000	-1.277089000
H	-1.782417000	-3.494764000	-1.395809000
C	5.559094000	1.957768000	2.312752000
C	-0.564339000	-6.401929000	0.059015000
H	-0.042321000	-6.729959000	0.964782000
H	-1.537807000	-6.904743000	0.039209000
H	0.003188000	-6.749493000	-0.811189000
C	5.353507000	1.420238000	-2.733698000
C	4.349692000	2.193149000	-3.621466000
H	4.099168000	3.162865000	-3.176037000
H	4.776993000	2.375398000	-4.615523000
H	3.415642000	1.638023000	-3.757833000
C	6.647358000	2.251017000	-2.641513000
H	7.420895000	1.739741000	-2.057030000
H	7.051068000	2.417710000	-3.646733000
H	6.469714000	3.233663000	-2.189447000
C	5.695715000	0.071555000	-3.411448000
H	4.806350000	-0.554285000	-3.539348000
H	6.132677000	0.238821000	-4.403986000
H	6.418926000	-0.494328000	-2.812719000
C	5.188767000	-4.560005000	-1.146860000
H	6.142119000	-5.103353000	-1.140859000
H	4.646288000	-4.835233000	-2.058614000
H	5.413479000	-3.490005000	-1.203209000
C	5.169016000	-4.522299000	1.375583000
H	5.396741000	-3.451640000	1.400106000
H	4.611185000	-4.767084000	2.286939000
H	6.120724000	-5.067702000	1.402489000
C	4.145624000	-6.433389000	0.134845000
H	3.589443000	-6.756364000	1.022299000
H	3.606736000	-6.782983000	-0.753073000
H	5.116783000	-6.941135000	0.151607000
N	2.825315000	0.357259000	2.373522000
H	3.373639000	0.124657000	3.186380000
H	2.076222000	-0.308143000	2.222363000
C	6.999711000	1.386247000	2.298965000
H	7.582588000	1.809923000	3.126357000
H	6.987002000	0.296476000	2.417674000
H	7.533015000	1.611857000	1.370908000
C	5.002996000	1.698967000	3.730450000
H	3.977849000	2.057135000	3.852033000
H	5.051947000	0.637715000	4.007294000
H	5.629958000	2.231474000	4.454833000
C	5.617478000	3.497092000	2.140511000
H	4.611784000	3.930112000	2.179455000
H	6.212914000	3.947416000	2.944670000
H	6.069532000	3.789668000	1.188134000

XYZ coordinates for **3⁺** (singlet):

C	-3.953421000	5.309863000	1.589111000
H	-3.396350000	5.500801000	2.511835000
H	-4.761156000	6.048010000	1.530752000
H	-3.276233000	5.481662000	0.744712000

C	4.683054000	-5.301108000	1.245956000
H	3.980683000	-5.690438000	1.990088000
H	5.605994000	-5.886817000	1.324234000
H	4.253548000	-5.476786000	0.253162000
C	4.689499000	2.026595000	-1.552554000
C	2.705857000	0.737925000	-1.055269000
C	4.113627000	0.889609000	-1.027014000
H	4.724506000	0.110865000	-0.597269000
C	-2.625709000	-2.451884000	-2.707847000
C	-1.886302000	-1.542302000	-1.865151000
C	-2.054686000	1.042835000	0.728073000
C	2.310955000	-1.282731000	0.323589000
C	-2.590517000	-0.655593000	-0.958418000
C	-6.217237000	-1.866022000	-1.418646000
C	1.871778000	1.827522000	-1.523410000
C	6.209666000	2.250991000	-1.567837000
C	-3.991075000	-0.783189000	-0.777961000
H	-4.483837000	-0.175179000	-0.032872000
C	1.381011000	-2.581820000	2.209931000
C	2.623940000	-3.239803000	2.224460000
H	2.752884000	-4.037683000	2.945243000
C	2.464701000	2.996949000	-2.124024000
C	-4.697871000	-1.678841000	-1.549101000
C	3.495527000	-2.014080000	0.358218000
H	4.236780000	-1.855329000	-0.411981000
C	-3.989906000	-2.471185000	-2.515736000
H	-4.582924000	-3.143568000	-3.120163000
C	3.841921000	3.038904000	-2.114749000
H	4.332277000	3.900167000	-2.546985000
C	-1.489059000	1.979731000	2.955547000
C	-0.993674000	3.314076000	5.087319000
H	-0.899038000	4.259830000	4.541969000
H	-0.319227000	3.364221000	5.948035000
H	-2.012653000	3.238533000	5.482426000
C	-1.937080000	-3.361941000	-3.747218000
C	-1.230434000	1.032487000	1.908502000
C	-1.020122000	-4.394094000	-3.039311000
H	-0.206126000	-3.942405000	-2.463175000
H	-0.562601000	-5.055932000	-3.783014000
H	-1.600636000	-5.014285000	-2.347750000
C	-1.158382000	-2.648798000	2.828766000
H	-1.298990000	-1.637225000	3.208469000
H	-1.881503000	-3.293336000	3.339702000
H	-1.408437000	-2.657715000	1.761202000
C	-6.520002000	-3.335012000	-1.032115000
H	-6.150457000	-4.044781000	-1.779196000
H	-7.602325000	-3.482398000	-0.944162000
H	-6.063560000	-3.590534000	-0.069293000
C	0.677147000	3.589020000	-3.829808000
H	1.258928000	3.142990000	-4.643817000
H	0.081434000	4.406274000	-4.251167000
H	-0.020642000	2.824813000	-3.473685000
C	1.618918000	4.138143000	-2.727845000
C	3.687891000	-2.983464000	1.348719000
C	0.259891000	-3.194706000	3.092364000
C	1.290765000	-1.506610000	1.299229000
C	-2.963284000	-4.171168000	-4.568239000
H	-3.546967000	-4.854072000	-3.941797000
H	-2.432693000	-4.780810000	-5.306814000
H	-3.655554000	-3.521186000	-5.114211000
C	-4.542731000	3.878410000	1.549043000
C	-2.558330000	2.850008000	2.775088000
H	-2.758745000	3.581630000	3.544317000

C	0.883268000	2.285438000	3.827658000
H	1.283620000	1.415880000	3.302403000
H	1.485369000	2.439627000	4.730310000
H	1.009937000	3.166611000	3.187473000
C	2.502259000	5.212162000	-3.397430000
H	3.162255000	5.711441000	-2.679962000
H	1.861027000	5.981883000	-3.839356000
H	3.115915000	4.792721000	-4.201761000
C	-0.603348000	2.096201000	4.221073000
C	-3.399246000	2.855493000	1.641870000
C	-3.128971000	1.940147000	0.631396000
H	-3.707332000	1.935248000	-0.283463000
C	-6.829570000	-0.950070000	-0.342555000
H	-6.413443000	-1.149729000	0.651422000
H	-7.909386000	-1.121971000	-0.286233000
H	-6.679376000	0.110756000	-0.575304000
C	4.988423000	-3.799407000	1.463707000
C	-5.359432000	3.728989000	0.251394000
H	-6.165990000	4.469170000	0.238920000
H	-5.823182000	2.738772000	0.170737000
H	-4.747839000	3.898677000	-0.642251000
C	-1.128450000	-2.511852000	-4.760957000
H	-1.788183000	-1.819219000	-5.294744000
H	-0.657212000	-3.166879000	-5.502062000
H	-0.334339000	-1.914788000	-4.302531000
C	-6.892800000	-1.538371000	-2.773266000
H	-6.701889000	-0.500372000	-3.068154000
H	-7.977156000	-1.673531000	-2.690858000
H	-6.540983000	-2.187988000	-3.581138000
C	-5.500680000	3.681849000	2.749743000
H	-4.993368000	3.818949000	3.709914000
H	-5.943067000	2.679362000	2.742784000
H	-6.315815000	4.412285000	2.698729000
C	0.609940000	-2.997136000	4.585687000
H	1.560127000	-3.475355000	4.845730000
H	-0.169489000	-3.440526000	5.216037000
H	0.689879000	-1.935899000	4.839575000
C	6.981340000	1.081131000	-0.929031000
H	6.707227000	0.936127000	0.122378000
H	8.055670000	1.289432000	-0.961476000
H	6.814341000	0.139689000	-1.465096000
C	0.181894000	-4.717653000	2.788572000
H	-0.065037000	-4.895409000	1.735711000
H	-0.606273000	-5.168805000	3.401050000
H	1.109380000	-5.250995000	3.010430000
C	6.544244000	3.539085000	-0.775164000
H	6.066072000	4.425739000	-1.203792000
H	7.626443000	3.711654000	-0.782861000
H	6.221783000	3.453930000	0.268607000
C	-0.766864000	0.837826000	5.106184000
H	-1.812743000	0.702464000	5.404872000
H	-0.169979000	0.948462000	6.019014000
H	-0.434701000	-0.062667000	4.590186000
C	6.041247000	-3.367706000	0.424946000
H	6.954051000	-3.956360000	0.562726000
H	6.313533000	-2.311230000	0.532513000
H	5.698631000	-3.535028000	-0.602772000
C	0.807572000	4.859256000	-1.618837000
H	0.085263000	4.215622000	-1.106507000
H	0.246225000	5.694228000	-2.053194000
H	1.478520000	5.265310000	-0.854126000
C	6.692360000	2.405700000	-3.031327000
H	6.473054000	1.505329000	-3.616075000

H	7.776102000	2.567129000	-3.051710000
H	6.223625000	3.257106000	-3.535173000
C	5.590692000	-3.595387000	2.875139000
H	4.908302000	-3.924397000	3.665655000
H	5.828877000	-2.540919000	3.054539000
H	6.515949000	-4.174065000	2.974794000
N	1.958538000	-0.301114000	-0.615525000
N	0.573928000	1.596928000	-1.251501000
N	-1.742690000	0.176771000	-0.312503000
N	-0.554406000	-1.407570000	-1.747539000
N	-0.243101000	0.079717000	2.126054000
N	0.250830000	-0.536442000	1.133957000
Co	0.089820000	-0.062636000	-0.660562000
H	0.009567000	-2.000809000	-2.346637000
H	-0.078415000	2.330702000	-1.506273000

XYZ coordinates for 3^+ (triplet):

C	-4.624738000	0.233766000	-5.227456000
H	-4.189810000	1.126750000	-5.687486000
H	-5.487783000	-0.063916000	-5.833571000
H	-3.880492000	-0.568847000	-5.279824000
C	5.048857000	3.250641000	3.945964000
H	4.330928000	4.040181000	4.190328000
H	6.018750000	3.545944000	4.362021000
H	4.727521000	2.334386000	4.453993000
C	4.750942000	-2.063851000	-1.500465000
C	2.749947000	-1.071433000	-0.561333000
C	4.135224000	-1.014544000	-0.851448000
H	4.695536000	-0.134169000	-0.577294000
C	-2.263665000	-2.302090000	2.904978000
C	-1.633160000	-1.487939000	1.879594000
C	-2.263575000	0.567449000	-1.114168000
C	2.352176000	1.030252000	0.712790000
C	-2.475933000	-0.755502000	0.930260000
C	-5.952390000	-1.230989000	2.522247000
C	1.940248000	-2.172242000	-1.080386000
C	6.246918000	-2.066143000	-1.849272000
C	-3.869980000	-0.622077000	1.171363000
H	-4.452330000	0.020807000	0.526548000
C	1.402089000	3.168659000	1.538265000
C	2.702374000	3.454994000	1.979364000
H	2.852617000	4.382612000	2.516978000
C	2.593672000	-3.308014000	-1.686814000
C	-4.452908000	-1.315624000	2.204523000
C	3.605950000	1.359175000	1.244618000
H	4.393306000	0.620991000	1.229948000
C	-3.625784000	-2.170159000	3.020565000
H	-4.128847000	-2.730306000	3.796711000
C	3.957999000	-3.202088000	-1.863270000
H	4.476803000	-4.025221000	-2.335367000
C	-2.004290000	2.531206000	-2.602886000
C	-1.840459000	4.296288000	-4.457207000
H	-1.761891000	3.540715000	-5.246994000
H	-1.264569000	5.169288000	-4.780311000
H	-2.886028000	4.613670000	-4.379529000
C	-1.451066000	-3.217919000	3.844379000
C	-1.553664000	1.767039000	-1.471325000
C	-0.544431000	-2.373536000	4.778902000
H	0.190089000	-1.759887000	4.248288000
H	0.009486000	-3.034829000	5.454455000
H	-1.149373000	-1.696251000	5.391335000

C	-1.162456000	3.595501000	1.838189000
H	-1.483391000	3.653447000	0.799038000
H	-1.846453000	4.215961000	2.426995000
H	-1.280881000	2.561097000	2.182379000
C	-6.138376000	-0.714119000	3.971084000
H	-5.672703000	-1.373287000	4.710784000
H	-7.206053000	-0.653718000	4.209787000
H	-5.707262000	0.285977000	4.091420000
C	1.028250000	-5.180451000	-0.971966000
H	1.717644000	-5.509131000	-0.186290000
H	0.469409000	-6.057644000	-1.316867000
H	0.310768000	-4.496560000	-0.508365000
C	1.813724000	-4.556201000	-2.154632000
C	3.810011000	2.600043000	1.845496000
C	0.276613000	4.108517000	2.054183000
C	1.270153000	1.973079000	0.792151000
C	-2.369481000	-4.057583000	4.757440000
H	-2.957297000	-3.434779000	5.440059000
H	-1.753807000	-4.720325000	5.373812000
H	-3.056271000	-4.686934000	4.180800000
C	-5.068679000	0.488231000	-3.765951000
C	-3.125662000	2.068564000	-3.280020000
H	-3.464112000	2.620703000	-4.144498000
C	0.233337000	3.506280000	-3.345710000
H	0.754128000	3.259098000	-2.418743000
H	0.715190000	4.391358000	-3.776344000
H	0.366507000	2.677576000	-4.051346000
C	2.756570000	-5.658966000	-2.681494000
H	3.310558000	-5.339507000	-3.570676000
H	2.162941000	-6.533832000	-2.966152000
H	3.475433000	-5.981492000	-1.920496000
C	-1.270024000	3.797810000	-3.110451000
C	-3.850036000	0.908526000	-2.928990000
C	-3.400968000	0.175593000	-1.839839000
H	-3.882497000	-0.750864000	-1.555502000
C	-6.697590000	-0.275070000	1.572554000
H	-6.309327000	0.747869000	1.633436000
H	-7.757276000	-0.240284000	1.845219000
H	-6.639595000	-0.606663000	0.529154000
C	5.173249000	3.026359000	2.419303000
C	-5.730606000	-0.796331000	-3.232737000
H	-6.596954000	-1.047241000	-3.853348000
H	-6.090208000	-0.675464000	-2.203908000
H	-5.048337000	-1.653668000	-3.262775000
C	-0.606956000	-4.225106000	3.020817000
H	-1.256626000	-4.863436000	2.411818000
H	-0.038659000	-4.873080000	3.697007000
H	0.110756000	-3.750872000	2.345152000
C	-6.587016000	-2.638001000	2.390748000
H	-6.477591000	-3.026284000	1.371927000
H	-7.657221000	-2.585312000	2.619798000
H	-6.139799000	-3.363438000	3.077983000
C	-6.121014000	1.623774000	-3.737336000
H	-5.729147000	2.560109000	-4.147183000
H	-6.462482000	1.821118000	-2.714906000
H	-6.993273000	1.339503000	-4.336724000
C	0.427210000	5.505221000	1.408670000
H	1.393881000	5.959097000	1.651049000
H	-0.357114000	6.176296000	1.777362000
H	0.346739000	5.453234000	0.319374000
C	6.950740000	-0.766972000	-1.414958000
H	6.522014000	0.114216000	-1.905973000
H	8.009298000	-0.813309000	-1.691075000

H	6.902226000	-0.618336000	-0.329898000
C	0.435006000	4.248941000	3.595341000
H	0.347264000	3.275451000	4.090891000
H	-0.357988000	4.897974000	3.982371000
H	1.388564000	4.692279000	3.892372000
C	6.416546000	-2.217051000	-3.381504000
H	5.983412000	-3.150162000	-3.756313000
H	7.481161000	-2.219940000	-3.641800000
H	5.939630000	-1.386587000	-3.913964000
C	-1.440683000	4.947595000	-2.090491000
H	-2.500317000	5.187792000	-1.945955000
H	-0.940007000	5.849975000	-2.460550000
H	-1.009407000	4.691529000	-1.123497000
C	6.266213000	1.967846000	2.178304000
H	7.218592000	2.327090000	2.581516000
H	6.416058000	1.769934000	1.110513000
H	6.038671000	1.019667000	2.679287000
C	0.859110000	-4.195445000	-3.323450000
H	0.110094000	-3.440844000	-3.065795000
H	0.322394000	-5.090854000	-3.657121000
H	1.427997000	-3.806336000	-4.174769000
C	6.939580000	-3.253279000	-1.135136000
H	6.841309000	-3.169881000	-0.046913000
H	8.007982000	-3.264866000	-1.379125000
H	6.522728000	-4.219487000	-1.437651000
C	5.617609000	4.343276000	1.737777000
H	4.903055000	5.155686000	1.905313000
H	5.727508000	4.210476000	0.655647000
H	6.584827000	4.665976000	2.139562000
N	2.002881000	-0.177955000	0.127998000
N	0.622282000	-1.951761000	-0.964275000
N	-1.771210000	-0.223625000	-0.082695000
N	-0.339666000	-1.246528000	1.700676000
N	-0.503180000	2.279749000	-0.721115000
N	0.160762000	1.499104000	0.037519000
Co	0.112442000	-0.375665000	0.014242000
H	0.289305000	-1.784957000	2.288067000
H	0.012750000	-2.698357000	-1.271947000

XYZ coordinates for 4⁺:

N	0.514123000	-0.042290000	-1.177503000
N	1.444071000	0.573563000	-0.348944000
N	-0.250975000	0.823531000	-1.778935000
N	1.109346000	-0.490571000	2.232138000
C	0.186163000	2.054190000	-1.429692000
N	-1.399761000	-0.652242000	0.578889000
C	-0.880602000	-1.715061000	-0.172622000
C	2.349065000	-0.593680000	1.637745000
C	0.165682000	-1.443044000	-1.094512000
C	-5.019768000	-0.707908000	0.062040000
C	-3.709147000	-1.030670000	-0.116151000
H	-3.407845000	-1.762546000	-0.853251000
C	0.736457000	-2.446094000	-1.894300000
C	2.542446000	-0.063457000	0.339751000
C	1.265500000	1.912229000	-0.520581000
C	-0.274793000	3.346640000	-1.835570000
C	-1.256649000	-3.039454000	0.046081000
H	-2.024676000	-3.234756000	0.786543000
C	4.936455000	-0.447092000	0.382215000
C	1.516778000	4.261603000	-0.339850000
C	0.421180000	4.392310000	-1.263817000

H	0.126031000	5.399451000	-1.525263000
C	-4.513777000	1.001105000	1.818835000
C	3.497266000	-1.136900000	2.294706000
C	-2.672604000	-0.389218000	0.654686000
C	1.951144000	3.001714000	0.035516000
H	2.768514000	2.840253000	0.724653000
C	-5.389352000	0.288437000	1.066361000
H	-6.448012000	0.467585000	1.191696000
C	3.413186000	-1.794144000	3.696938000
C	1.728783000	-2.277666000	-3.073117000
H	5.592982000	-1.440528000	2.147159000
C	3.072698000	-2.945491000	-2.694926000
H	2.951529000	-4.010160000	-2.471657000
H	3.520868000	-2.466327000	-1.818877000
H	3.778482000	-2.859541000	-3.528965000
C	0.320359000	-3.761340000	-1.603535000
H	0.772454000	-4.561360000	-2.172023000
C	-0.639742000	-4.091092000	-0.645193000
C	2.006478000	-0.822932000	-3.499908000
H	2.497917000	-0.237540000	-2.720356000
H	1.095192000	-0.303149000	-3.810061000
H	2.684237000	-0.837360000	-4.359890000
C	1.136402000	-2.984431000	-4.321800000
H	0.169633000	-2.549845000	-4.599029000
H	0.994541000	-4.058373000	-4.176731000
H	1.819244000	-2.857506000	-5.168971000
C	-1.439210000	3.525630000	-2.817373000
C	-6.149706000	-1.349400000	-0.750575000
C	4.785211000	-2.317985000	4.177830000
H	5.520000000	-1.513463000	4.287979000
H	5.198461000	-3.078480000	3.506335000
H	4.663204000	-2.782683000	5.161711000
C	-1.050177000	-5.543629000	-0.341853000
C	-3.065824000	0.733942000	1.611776000
C	2.950982000	-0.763774000	4.761663000
H	1.982674000	-0.304140000	4.550721000
H	3.680622000	0.049765000	4.839771000
H	2.883903000	-1.247758000	5.742648000
C	2.479460000	-3.034504000	3.664622000
H	2.880390000	-3.791852000	2.981955000
H	1.455388000	-2.826448000	3.340429000
H	2.418444000	-3.480002000	4.663606000
C	6.329236000	-0.292429000	-0.259639000
C	-1.740483000	5.013005000	-3.080046000
H	-0.886372000	5.533733000	-3.527467000
H	-2.030889000	5.542151000	-2.165330000
H	-2.575704000	5.092565000	-3.783096000
C	-4.979368000	2.055920000	2.838696000
C	2.172730000	5.542137000	0.199395000
C	-1.081991000	2.856403000	-4.168418000
H	-0.917963000	1.780690000	-4.059532000
H	-0.180282000	3.302348000	-4.603227000
H	-1.903600000	3.000552000	-4.878881000
C	1.107912000	6.388502000	0.940736000
H	0.685511000	5.837526000	1.788183000
H	0.282674000	6.687116000	0.286328000
H	1.568791000	7.303970000	1.327546000
C	-2.713837000	2.867218000	-2.232375000
H	-2.982211000	3.316365000	-1.269443000
H	-2.587724000	1.790774000	-2.088802000
H	-3.552772000	3.019475000	-2.920761000
C	-7.105434000	-2.095605000	0.215584000
H	-7.550137000	-1.430589000	0.962354000

H	-6.581112000	-2.897406000	0.747381000
H	-7.925568000	-2.546614000	-0.353960000
C	2.749399000	6.355479000	-0.986365000
H	1.976791000	6.651016000	-1.703219000
H	3.510379000	5.781883000	-1.527274000
H	3.219467000	7.271370000	-0.611764000
C	3.319008000	5.240263000	1.182739000
H	4.125154000	4.666569000	0.711312000
H	2.968485000	4.689432000	2.062902000
C	-5.630734000	-2.357637000	-1.791737000
H	-5.093736000	-3.191161000	-1.324842000
H	-4.965751000	-1.883917000	-2.522694000
H	-6.476332000	-2.781354000	-2.342917000
C	-2.563120000	-5.717278000	-0.617812000
H	-2.869292000	-6.745993000	-0.397136000
H	-2.799127000	-5.512991000	-1.668363000
H	-3.173504000	-5.051883000	0.002294000
C	-6.932072000	-0.240123000	-1.498459000
H	-6.281190000	0.295689000	-2.198291000
H	-7.373827000	0.493997000	-0.817506000
H	-7.749607000	-0.690114000	-2.072459000
H	7.302751000	-1.976938000	0.767014000
H	8.411060000	-0.765239000	0.118566000
C	-4.459128000	1.696950000	4.254361000
H	-3.369107000	1.698281000	4.294918000
H	-4.822800000	0.710451000	4.566296000
H	-4.832680000	2.432565000	4.975872000
C	-0.760577000	-5.847368000	1.148341000
H	-1.319355000	-5.185973000	1.818959000
H	0.305843000	-5.734112000	1.373969000
H	-1.048195000	-6.877992000	1.384106000
N	-2.175886000	1.429751000	2.220876000
H	-1.242179000	1.102476000	1.946661000
C	6.634711000	1.212867000	-0.451918000
H	6.628122000	1.741729000	0.507994000
H	5.903432000	1.697457000	-1.108980000
H	7.623769000	1.346424000	-0.905058000
C	-4.463683000	3.459629000	2.428812000
H	-4.832127000	3.734022000	1.432635000
H	-3.373778000	3.499805000	2.425565000
H	-4.837477000	4.205788000	3.139533000
C	6.359238000	-0.996651000	-1.635980000
H	6.158402000	-2.069046000	-1.534360000
H	7.345250000	-0.880361000	-2.100606000
H	5.619095000	-0.579041000	-2.327457000
C	-0.282523000	-6.565759000	-1.200884000
H	0.798849000	-6.515433000	-1.030260000
H	-0.471737000	-6.427657000	-2.271391000
H	-0.607612000	-7.578295000	-0.940528000
C	-6.518068000	2.131068000	2.915938000
H	-6.964940000	1.178881000	3.224747000
H	-6.968388000	2.434952000	1.963754000
H	-6.801258000	2.880604000	3.661737000
C	3.802125000	0.037744000	-0.260103000
H	3.873944000	0.520549000	-1.229055000
C	4.728433000	-1.040485000	1.639670000
H	3.752264000	6.181000000	1.536799000
C	7.443541000	-0.900948000	0.613097000
H	7.507580000	-0.417516000	1.594458000
H	0.939437000	-1.063925000	3.041435000
H	0.286726000	-0.394507000	1.641407000

XYZ coordinates for 5:

N	-0.276874000	1.040050000	-1.547811000
N	-1.730571000	-0.690843000	0.511097000
N	0.468825000	0.101324000	-1.005498000
C	0.311323000	2.209501000	-1.219910000
N	-1.998194000	0.844508000	2.018658000
N	1.505138000	0.603501000	-0.244514000
C	1.440756000	1.950570000	-0.403326000
N	-1.109405000	0.115709000	1.437566000
C	2.499707000	-0.168528000	0.417986000
C	-3.242902000	0.545356000	1.499926000
C	2.116732000	-1.094174000	1.403938000
H	1.069575000	-1.158893000	1.667886000
C	-1.428856000	-2.979336000	-0.180710000
H	-2.261139000	-3.218587000	0.468955000
C	0.287845000	-3.554516000	-1.735295000
H	0.796677000	-4.310075000	-2.320699000
C	-4.152220000	-0.970067000	-0.222902000
H	-3.981930000	-1.724427000	-0.979755000
C	-1.008135000	-1.654784000	-0.243857000
C	0.088623000	-1.281517000	-1.049121000
C	-0.063110000	3.550221000	-1.557728000
C	3.871726000	0.097838000	0.029346000
C	2.242570000	2.968981000	0.140757000
H	3.101590000	2.711023000	0.739526000
C	-4.525206000	1.072199000	1.805891000
C	-3.083351000	-0.449406000	0.520418000
C	-1.273244000	3.849208000	-2.452187000
C	-4.714399000	2.149710000	2.881887000
C	1.896691000	4.265580000	-0.172513000
C	4.428188000	-1.632211000	1.682545000
H	5.180854000	-2.221400000	2.196071000
C	0.733190000	-2.227368000	-1.871115000
C	0.753145000	4.517588000	-1.013439000
H	0.527683000	5.553949000	-1.230450000
C	-0.763745000	-3.966932000	-0.912558000
C	3.072666000	-1.852417000	2.054663000
C	-5.566804000	0.533637000	1.062487000
H	-6.569258000	0.895552000	1.252649000
C	-5.416473000	-0.467284000	0.055297000
C	-1.149232000	-5.455233000	-0.839012000
C	1.836275000	-1.972954000	-2.934701000
C	-6.671362000	-0.956232000	-0.692289000
C	4.858481000	-0.719674000	0.736434000
C	-1.079648000	3.170100000	-3.830422000
H	-0.175356000	3.541308000	-4.326257000
H	-1.936470000	3.391998000	-4.478045000
H	-0.998536000	2.084208000	-3.736030000
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H	-6.597324000	2.988645000	2.112603000
H	-6.271441000	3.329234000	3.815652000
H	-6.823509000	1.720277000	3.337359000
C	2.705196000	5.469389000	0.339791000
C	-2.559280000	3.302585000	-1.784282000
H	-2.511400000	2.220361000	-1.640178000
H	-3.428564000	3.524402000	-2.415365000
H	-2.722158000	3.770613000	-0.806671000
C	-6.342424000	-2.028879000	-1.748427000
H	-5.660910000	-1.648850000	-2.517981000
H	-7.263211000	-2.344952000	-2.251102000
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C	2.733753000	-2.869764000	3.156630000

C	-3.893981000	3.406555000	2.500437000
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H	-4.231525000	3.816797000	1.540969000
C	-2.329845000	-5.704226000	0.118767000
H	-2.096086000	-5.398241000	1.144703000
H	-2.564530000	-6.773926000	0.140654000
H	-3.235941000	-5.176203000	-0.200647000
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H	-1.632133000	5.900512000	-1.745759000
H	-2.328029000	5.525442000	-3.326216000
H	-0.589272000	5.807983000	-3.182521000
C	-7.669732000	-1.569272000	0.319009000
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H	-8.568707000	-1.919706000	-0.202240000
H	-7.985802000	-0.844126000	1.075734000
C	6.351352000	-0.517177000	0.413229000
C	3.134107000	-2.691182000	-2.490994000
H	3.499062000	-2.297666000	-1.538111000
H	3.915444000	-2.532494000	-3.242976000
H	2.989870000	-3.772176000	-2.382675000
C	-4.214848000	1.606220000	4.243513000
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H	-3.154687000	1.344032000	4.203359000
C	3.894593000	5.037078000	1.217680000
H	3.564507000	4.497324000	2.112316000
H	4.444445000	5.924086000	1.551325000
H	4.594198000	4.397397000	0.669141000
C	0.065679000	-6.269066000	-0.332639000
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H	-6.653708000	0.688844000	-2.141827000
C	6.752765000	0.947213000	0.718914000
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H	7.812166000	1.108750000	0.479670000
H	6.610255000	1.173343000	1.783266000
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H	7.170086000	-1.256203000	2.319656000
H	8.312146000	-1.251106000	0.970319000
H	7.063524000	-2.499825000	1.055233000
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H	-2.418070000	-5.398148000	-2.628650000
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C	1.787337000	6.386198000	1.183975000
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H	2.354072000	7.250910000	1.549306000
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C	2.172082000	-0.494528000	-3.226942000
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H	2.700664000	0.011893000	-2.416455000
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H	3.926508000	5.636341000	-1.472799000

H	3.836708000	7.127560000	-0.514490000
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H	7.662064000	-0.629023000	-1.333451000
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C	3.237268000	-4.274524000	2.745846000
H	2.753510000	-4.604321000	1.818585000
H	3.015052000	-5.011145000	3.529010000
H	4.319290000	-4.285915000	2.576999000
C	3.414726000	-2.457539000	4.484015000
H	4.503536000	-2.400153000	4.380529000
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C	1.217403000	-2.964597000	3.410542000
H	0.797902000	-2.005693000	3.734899000
H	1.016154000	-3.699678000	4.198923000
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XYZ coordinates for **6**:

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C	1.163209000	-0.281564000	0.024109000
C	2.359819000	1.913149000	-0.081876000
H	2.251599000	2.990188000	-0.127165000
C	-1.163210000	-0.281565000	-0.024104000
C	3.574852000	-0.151299000	0.019702000
H	4.544479000	-0.629468000	0.053018000
C	3.572677000	1.280722000	-0.080024000
C	2.455651000	-0.950378000	0.091487000
C	-2.600726000	-2.474165000	-0.293611000
C	-2.359821000	1.913148000	0.081878000
H	-2.251601000	2.990188000	0.127165000
C	-2.455651000	-0.950378000	-0.091484000
C	-5.688731000	1.558337000	1.413768000
H	-5.885300000	0.481102000	1.399388000
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H	-5.125836000	1.783993000	2.326552000
C	-3.572679000	1.280721000	0.080022000
C	1.915705000	-3.256825000	-0.850108000
H	0.846268000	-3.060586000	-0.882782000
H	2.067410000	-4.334032000	-0.707781000
H	2.348402000	-2.982725000	-1.819954000
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C	1.984968000	-2.857923000	1.661822000
H	2.540606000	-2.382295000	2.478936000
H	2.034394000	-3.944128000	1.808463000
H	0.942072000	-2.548100000	1.738164000
C	-3.574853000	-0.151300000	-0.019703000
H	-4.544480000	-0.629469000	-0.053020000
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C	-1.915709000	-3.256825000	0.850115000
H	-0.846272000	-3.060585000	0.882795000
H	-2.067413000	-4.334032000	0.707788000
H	-2.348411000	-2.982724000	1.819959000
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C	-4.724131000	3.550521000	0.247716000
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H	5.125822000	1.784005000	-2.326559000

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