Supporting Information for

Communication Title: Functional nanosized trigonal prismatic and antiprismatic Cu^{II} coordination cages based on tricarboxylate linkers

Authors: Anna Company, Nans Roques, Mireia Güell, Veronica Mugnaini, Laura Gómez, Angela Datcu, Inhar Imaz, Miquel Solà, Josep M. Luis, Jaume Veciana,* Xavi Ribas* and Miquel Costas*

Experimental Section

Materials and synthesis. Solvents were purchased from SDS as reagent grade and used without further purification. Unless noted otherwise, all reagents were purchased from commercial sources and used as received.

Instrumentation and Measurements. IR spectra were recorded on a Mattson Satellite FT-IR using a MKII Golden Gate Single Reflection ATR System. UV-vis spectroscopy was performed in a Cary 50 Scan (Varian) UV-vis spectrophotometer. Luminescence measurements were performed in a Fluorescence Spectrometer LS 45 from Perkin Elmer. Spectroscopy measurements were performed using ROMIL-SpS Surper Purity Solvents with far UV gradient quality. Elemental analyses were performed using a CHNS-O Elemental Analyser EA-1108 from Fisons. The ESI-MS experiments were performed on a Bruker Daltonics Esquire 3000 spectrometer.

Ligand and linkers synthesis. Reported synthesis were followed to prepare 3,6,9,16,19,22-hexamethyl-3,6,9,16,19,22-hexaazatricyclo[22.2.2.2^{11,14}]triaconta-1(26),11(12),13,24,27,29-hexaene (Me2p ligand),[1] BTB (1,3,5-Tris-(4-carboxyphenyl)benzene), αH-PTMTC (tricarboxilated polychlorotriphenylmethane) and PTMTC radical.[2]

Complex synthesis

Caution: Perchlorate salts are potentially explosive and should be handled with care!

{[Cu_2^{II}(Me2p)]$_3$[BTB]$_2$}(ClO_4)$_6$ (1**(ClO_4)$_6$)**

In a 10 mL flask, Me2p ligand (30 mg, 61 μmol) was dissolved in CH_3CN (3 mL) and a CH_3CN solution (2 mL) of $Cu(H_2O)_6(ClO_4)_2$ (45 mg, 120 μmol) was added dropwise under vigorous stirring. A violet precipitate was formed but this was solubilised by the addition of H_2O (0.5 mL) which generated a reddish-blue solution. The mixture was stirred for 30 min and then, a suspension of the trisodium salt of BTB (18 mg, 41 μmol) in CH_3CN (1 mL) was added dropwise to the stirred solution. The trisodium salt of BTB slowly got solubilised which produced a color change of the solution turning dark blue (the trisodium salt of BTB was previously obtained by reaction of BTB with 3 equivalents of NaOH in water and evaporation to dryness of the resulting solution). After stirring for 2 h the solution was filtered through Celite. Ether diffusion afforded blue needles. The solvent was decanted and the crystalline solids dried under vacuum. (61 mg, 18 μmol, 88 %). Elemental analysis calcd for $C_{144}H_{180}Cl_6Cu_6N_{18}O_{36}\cdot 20H_2O$: N, 6.82; C, 46.83; H, 6.00 %. Found: N, 6.95; C, 46.93; H, 6.13 %. FT-IR (ATR) ν, cm^{-1}: 1620, 1351 (COO), 1085, 623 (ClO_4). ESI-MS (m/z): 1566 {**1**(ClO_4)$_6$-2ClO_4}$^{2+}$, 1011 {**1**(ClO_4)$_6$-3ClO_4}$^{3+}$, 734 {**1**(ClO_4)$_6$-4ClO_4}$^{4+}$, 567 {**1**(ClO_4)$_6$-5ClO_4}$^{5+}$and 456 {**1**(ClO_4)$_6$-6ClO_4}$^{6+}$.

{[Cu_2^{II}(Me2p)]$_3$[BTB]$_2$}(CF_3SO_3)$_6$ (1**(CF_3SO_3)$_6$)**

1(CF_3SO_3)$_6$ was prepared by the same synthetic procedure as for **1**(ClO_4)$_6$ but using the appropriate amount of $Cu(CF_3SO_3)_2$ instead of $Cu(H_2O)_6(ClO_4)_2$ as the copper source. Elemental analysis calcd for $C_{150}H_{180}Cu_6F_{18}N_{18}O_{30}S_6\cdot 20H_2O$: N, 6.32; C, 45.14; H, 5.56; S, 4.82 %. Found: N, 6.73; C, 44.40; H, 5.70; S, 4.54 %. FT-IR (ATR) ν, cm^{-1}: 1612, 1349 (COO), 1249, 1162, 1028, 772, 636 (CF_3SO_3). ESI-MS (m/z): 1666 {**1**(CF_3SO_3)$_6$-2CF_3SO_3}$^{2+}$, 1061 {**1**(CF_3SO_3)$_6$-3CF_3SO_3}$^{3+}$, 759 {**1**(CF_3SO_3)$_6$-4CF_3SO_3}$^{4+}$, 577 {**1**(CF_3SO_3)$_6$-5CF_3SO_3}$^{5+}$and 456 {**1**(CF_3SO_3)$_6$-6 CF_3SO_3}$^{6+}$.

{[Cu_2^{II}(Me2p)]$_3$[αH-PTMTC]$_2$}(CF_3SO_3)$_6$ (2**(CF_3SO_3)$_6$)**

Me2p ligand (13 mg, 26 μmol) was dissolved in CH_3CN (3 mL) and a CH_3CN solution (2 mL) of $Cu(CF_3SO_3)_2$ (19 mg, 52 μmol) was added dropwise under vigorous stirring. The addition of H_2O (0.5 mL) afforded the formation of a violet solution. The mixture was stirred for 30 min and then Na_3(αH-PTMTC) (15 mg, 18 μmol) was directly added as a solid to the stirred solution. The trisodium salt got slowly solubilised and the solution turned dark blue. After stirring for 12 h the mixture was

filtered through Celite. Ether diffusion afforded blue powder corresponding to **2**$(CF_3SO_3)_6$ (34 mg, 8 μmol, 90 %). Elemental analysis calcd for $C_{140}H_{152}Cl_{24}Cu_6F_{18}N_{18}O_{30}S_6{\cdot}20H_2O$: N, 5.37; C, 35.83; H, 4.12; S, 4.10 %. Found: N, 5.53; C, 35.66; H, 3.73; S, 4.82 %. FT-IR (ATR) ν, cm^{-1}: 1649, 1326 (COO), 1250, 1158, 1028, 636 (CF_3SO_3). ESI-MS (m/z): 1296 $\{\mathbf{2}(CF_3SO_3)_6\text{-}3CF_3SO_3\}^{3+}$, 934 $\{\mathbf{2}(CF_3SO_3)_6\text{-}4CF_3SO_3\}^{4+}$ and 718 $\{\mathbf{2}(CF_3SO_3)_6\text{-}5CF_3SO_3\}^{5+}$.

$\{[Cu_2^{II}(Me2p)]_3[PTMTC]_2\}(ClO_4)_6$ ($\mathbf{3}(ClO_4)_6$)

Me2p ligand (43 mg, 87 μmol) was dissolved in CH_3CN (5 mL) and a CH_3CN solution (5 mL) of $Cu(H_2O)_6(ClO_4)_2$ (65 mg, 175 μmol) was added dropwise under vigorous stirring. The addition of H_2O (2 mL) caused the solubilisation of the precipitate formed. The mixture was stirred for 30 min and then Na_3PTMTC (50 mg, 58 μmol) was directly added as a solid to the stirred solution. Complete dissolution of the trisodium salt was achieved after the addition of 3 mL of water. After stirring for 3 h the red solution was filtered through Celite. Ether diffusion afforded red needles. Light was avoided due to decomposition of the Na_3PTMTC radical in solution. The solvent was decanted and the crystalline solid dried under vacuum (40 mg, 10 μmol, 35 %). FT-IR (ATR) ν, cm^{-1}: 1620, 1320 (COO), 1114 (ClO_4). ESI-MS (m/z): 1245 $\{\mathbf{3}(ClO_4)_6\text{-}3ClO_4\}^{3+}$, 909 $\{\mathbf{3}(ClO_4)_6\text{-}4ClO_4\}^{4+}$, 707 $\{\mathbf{3}(ClO_4)_6\text{-}5ClO_4\}^{5+}$and 573 $\{\mathbf{3}(ClO_4)_6\text{-}6ClO_4\}^{6+}$.

EPR experimental details

All the EPR measurements have been performed on a Bruker Elexsys E500 equipped with a Bruker double cavity (type ER 4105 or 9105, system ZI810). The temperature was controlled with an Oxford Instruments Temperature Controller (Model ITC4) equipped with a Continuous Flow Cryostat (ESR 9).

EPR sample preparation.

To record EPR spectra in the solid state, the powder crystalline compounds have been accurately smashed inside an agatha mortar.

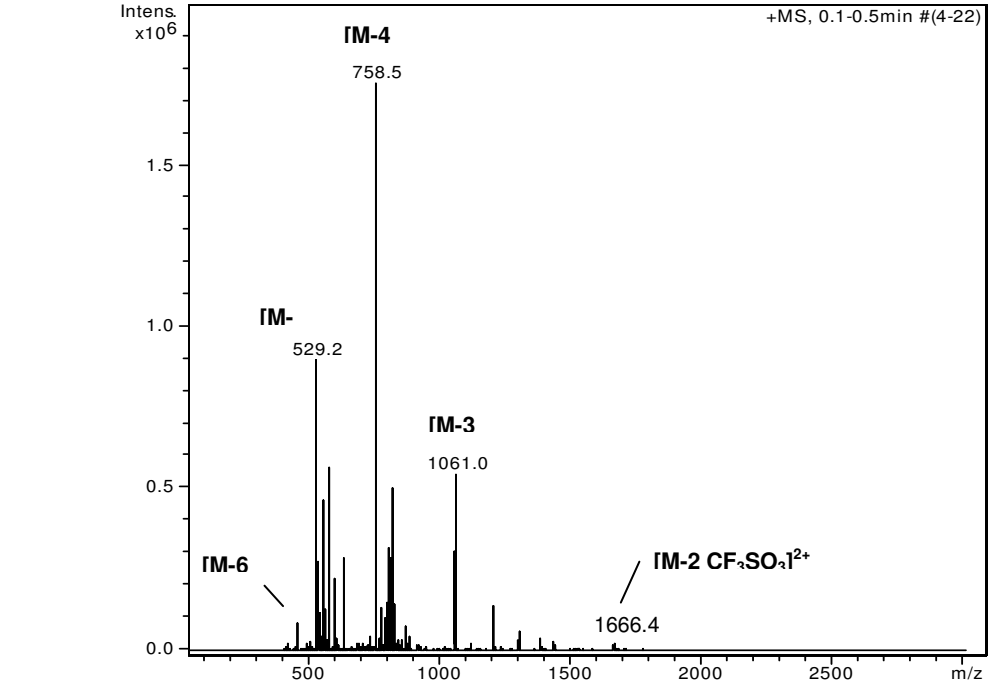
As solvents, pure or as mixtures, we have used butyronitrile, ACN: toluene 1:1, butryronitrile: toluene 1:1, toluene, acetone and CH_3CN. The compounds precipitated into the tube after a few minutes in all solvents except in pure CH_3CN. To record the spectra in CH_3CN solution, due to the high dielectric constant of this solvent, a capillary glass tube was filled with a few μl of the solution of compounds **1**-**3**, sealed at both end with a butane-oxygen flame and then inserted into the 5mm quartz EPR tube. A spectrum of the capillary inserted in the tube was recorded under the same experimental conditions to get rid of any spurious signals.

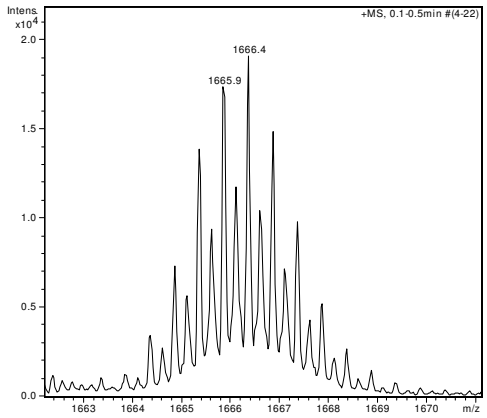
X-ray Diffraction Studies

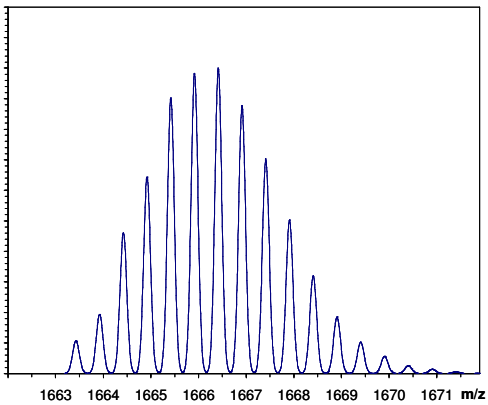
Crystal data for **1**$(ClO_4)_6$: $C_{144}H_{138}Cl_6Cu_6N_{18}O_{36}$, trigonal, *R*-3c, a = 45.210(2) Å, c = 15.024 (2) Å, V = 26594 (1) $Å^3$, Z = 6, D_c = 1.233 $g.cm^{-3}$, μ= 2.500 mm^{-1}, T = 150 K, crystal size = 0.3 × 0.2 × 0.2 mm^3, θ range = 4.03-28.54º, unique reflections = 2822, parameters = 226, GOF = 1.962, R1 [$I > 2\sigma(I)$] = 0.0965, wR2 [$I > 2\sigma(I)$] = 0.2405. Because the low diffraction intensity and the very low stability of crystals, the diffraction data collection has been performed with synchrotron radiation in BM16

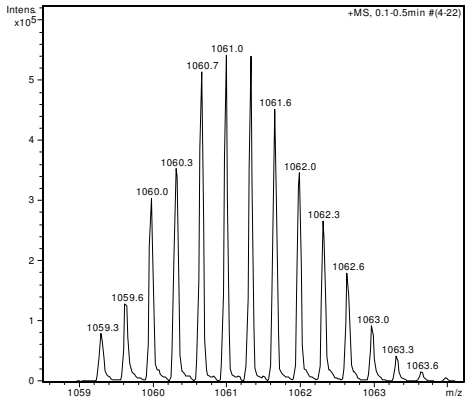
Spanish Beam-Line of the ESRF. However the solvent loos allowed us only to collect the data with a φ angle rotation before degradation of the crystal. The structure was solved from this data by direct methods (*SHELXS-97*)[3a] and refined using *SHELXL-97*.[3b] The high disorder observed on the external benzene rings of the BTB moieties obliged us to fix the atoms in two equivalent positions (0.5 site occupancy). These atoms have not been refined anisotropically. The second perchlorate shows also a high disorder. See CIF file for other details.

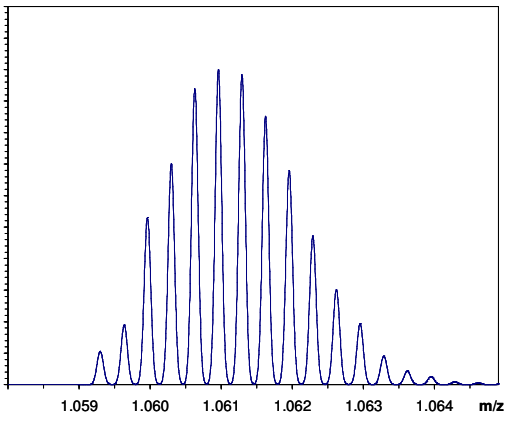
Figure S1. Experimental ESI-MS spectra for $\{[Cu_2^{II}(Me2p)]_3[BTB]_2\}(CF_3SO_3)_6$ (**1**$(CF_3SO_3)_6$).

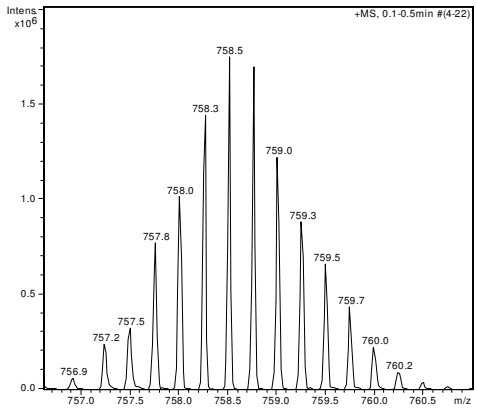








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758.3
759.0
758.0
759.3
757.8
759.5
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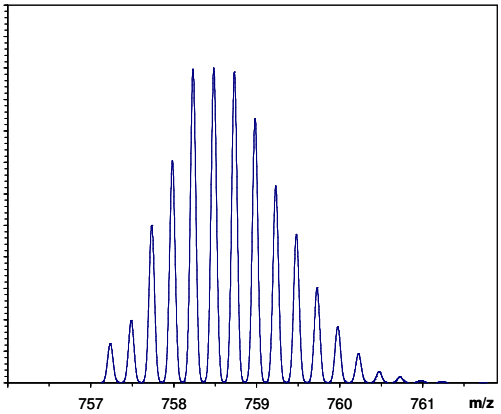
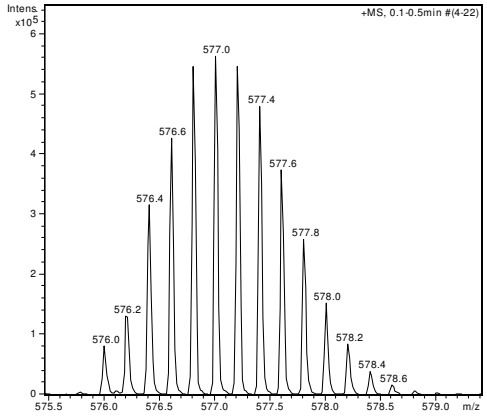
757.5
760.0
757.2
760.2
756.9
m/z


757
758
759
760
761
m/z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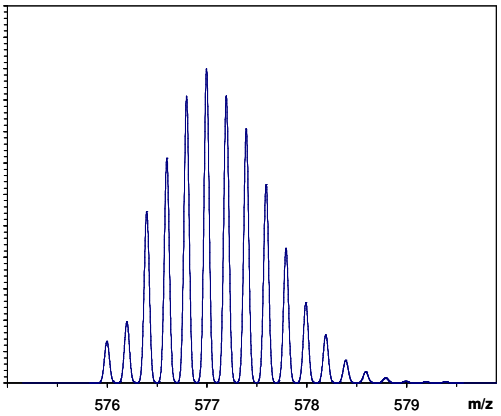
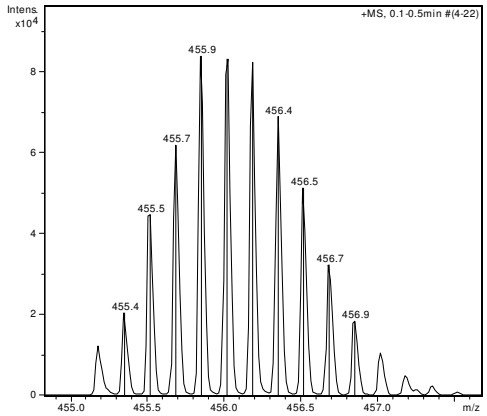
578.4
578.6
m/z


576
577
578
579
m/z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456.5
455.5
456.7
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456.9
m/z

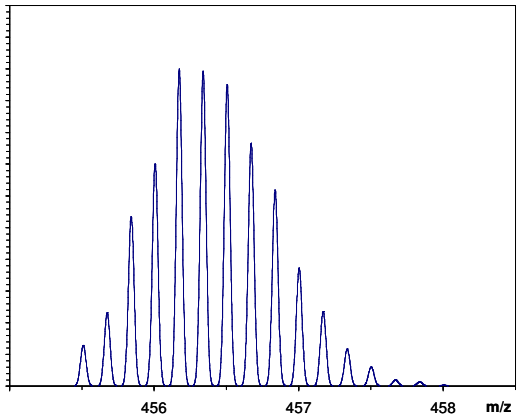

456
457
458
m/z

Figure S2. Experimental ESI-MS spectra for {[Cu_2^{II}(Me2p)]$_3$[αH-PTMTC]$_2$}(CF_3SO_3)$_6$ (**2**(CF_3SO_3)$_6$).

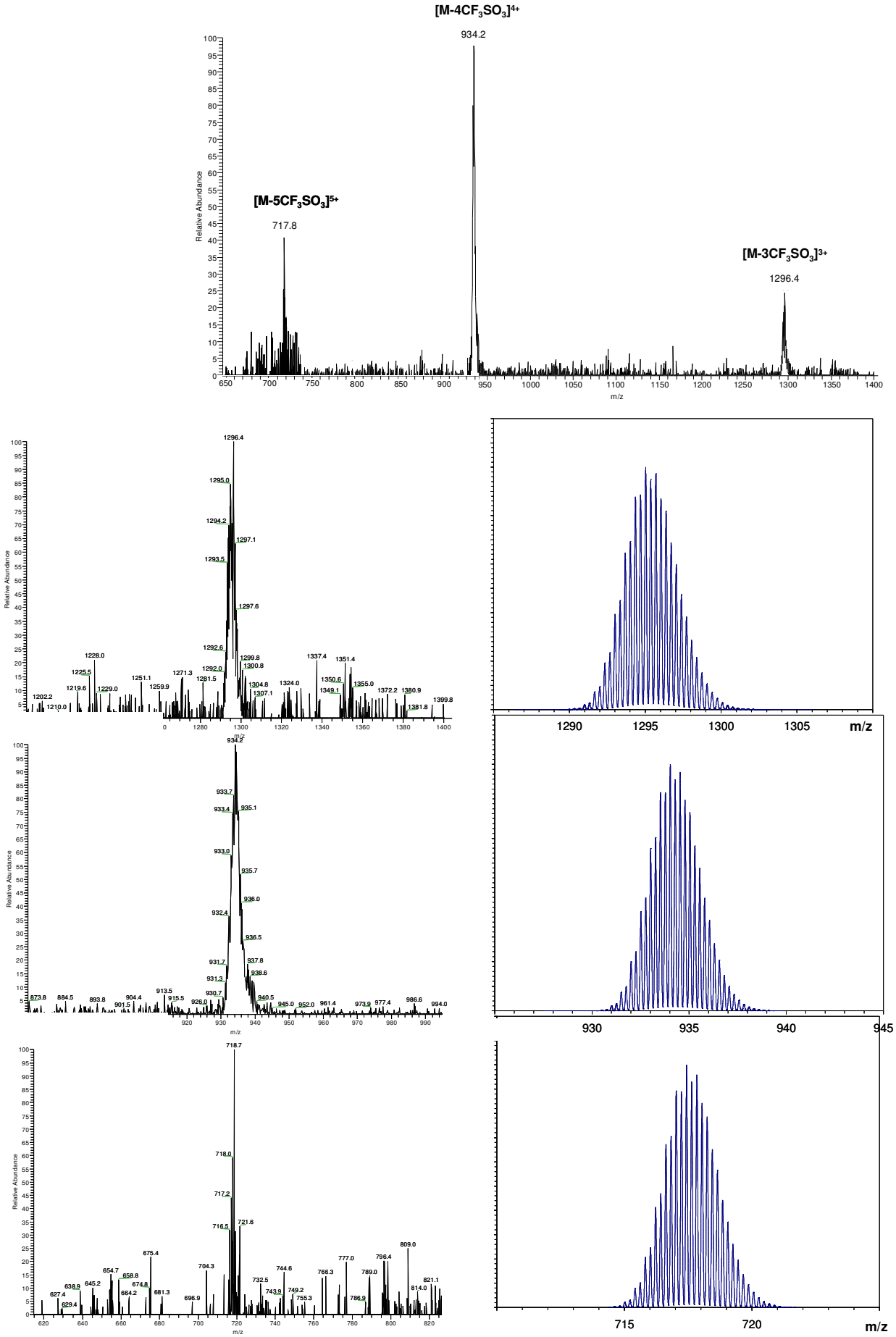
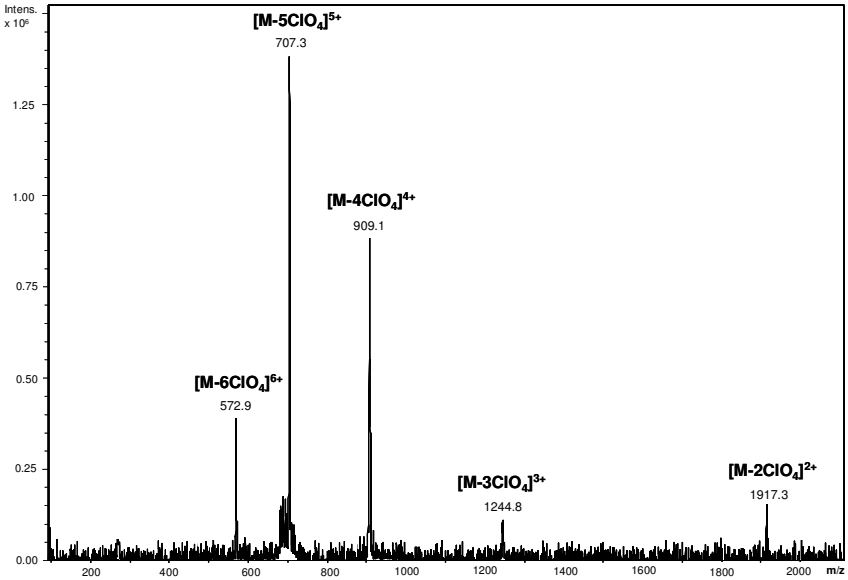
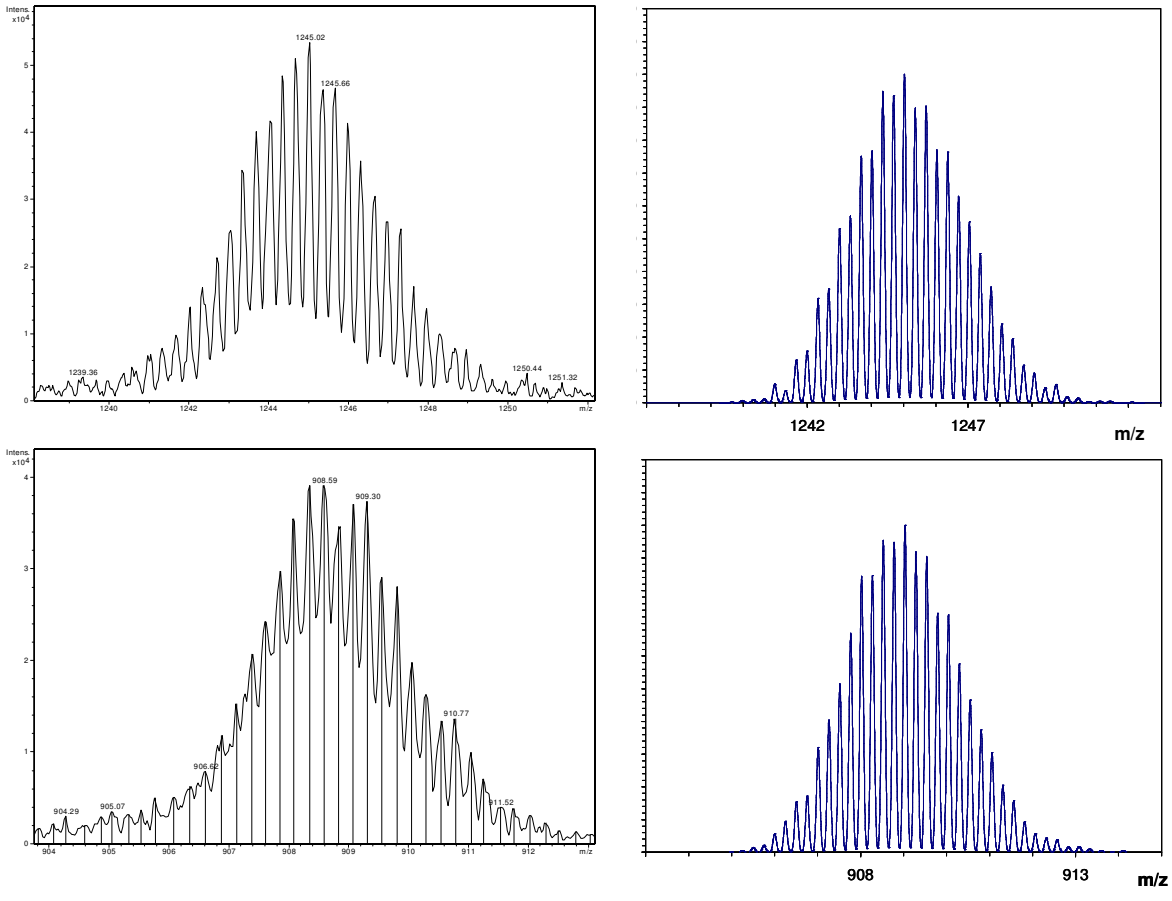
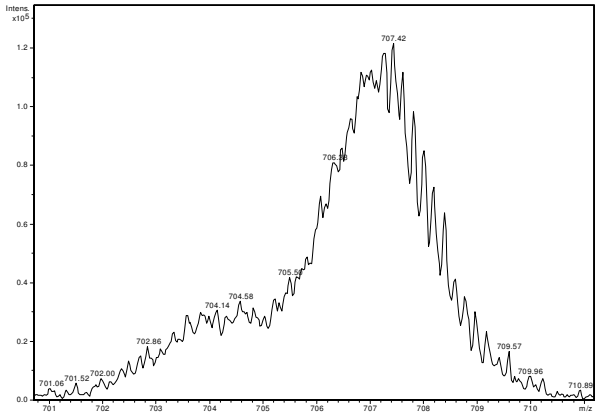


Figure S3. Experimental ESI-MS spectra for $\{[Cu_2^{II}(Me2p)]_3[PTMTC]_2\}(ClO_4)_6$ (**3**$(ClO_4)_6$)



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704.58
704.14
702.86
709.57
709.96
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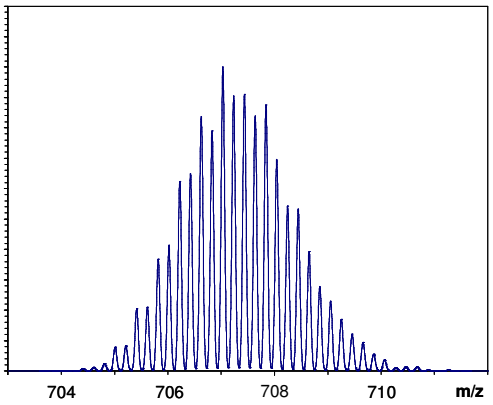
701.52
702.00
710.89
701
702
703
704
705
706
707
708
709
710
m/z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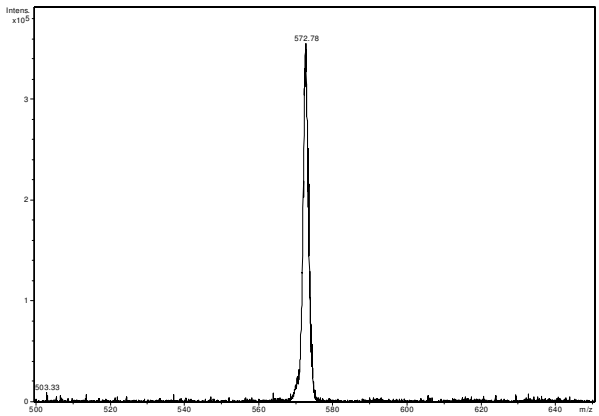
708
710
m/z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540
560
580
600
620
640
m/z

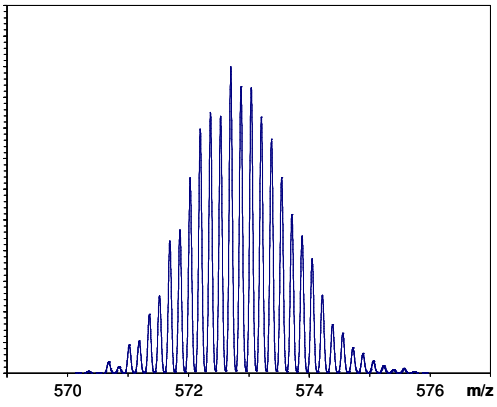

570
572
574
576
m/z

Figure S4. UV-Vis spectra for a) the BTB-based capsule **1**$(CF_3SO_3)_6$, b) the αH-PTMTC-based capsule **2**$(CF_3SO_3)_6$, and c) the radical PTMTC-based capsule **3**$(ClO_4)_6$ in acetonitrile. Otherwise indicated, [C = 10^{-4} M].

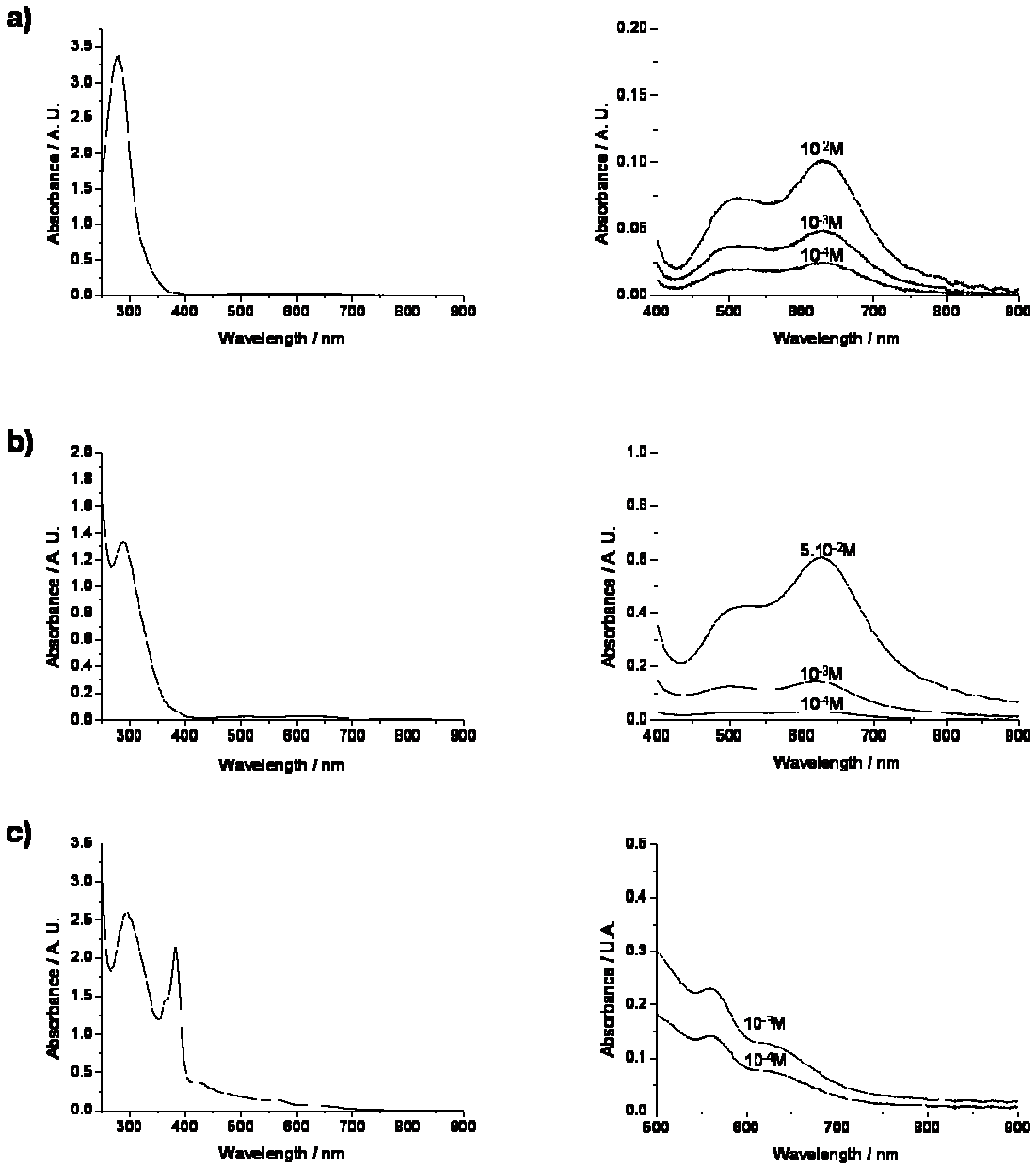
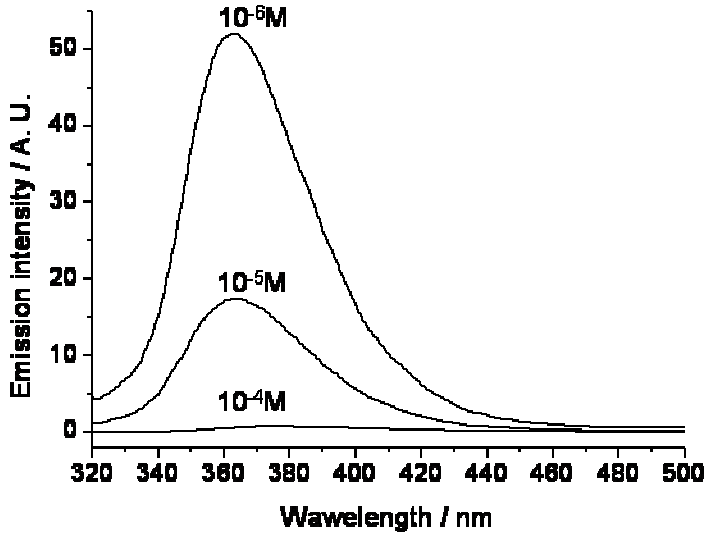
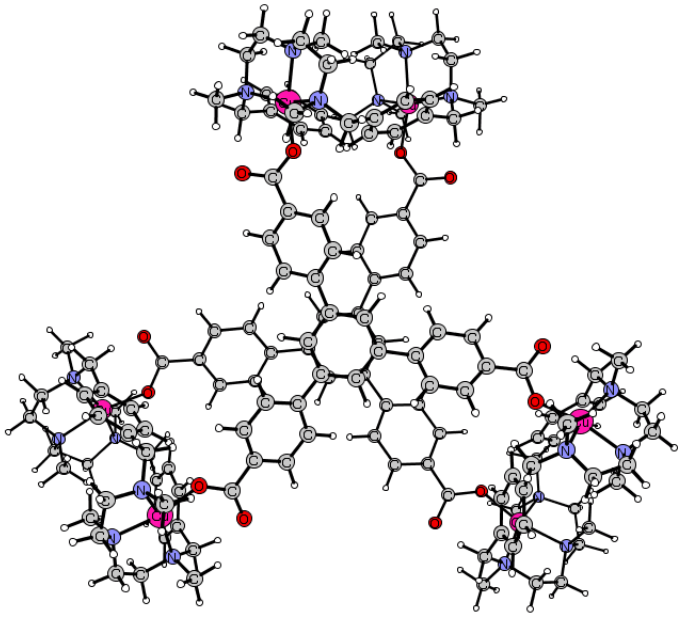


Figure S5. Emission spectra (excitation at 290 nm) of compound **1**$(ClO_4)_6$ (298 K) at different concentrations in CH_3CN.



Figures S6. DFT optimized structures for compound **1, 2a, 2b, 3a** and **3b** in a view along C3 axis.

1:



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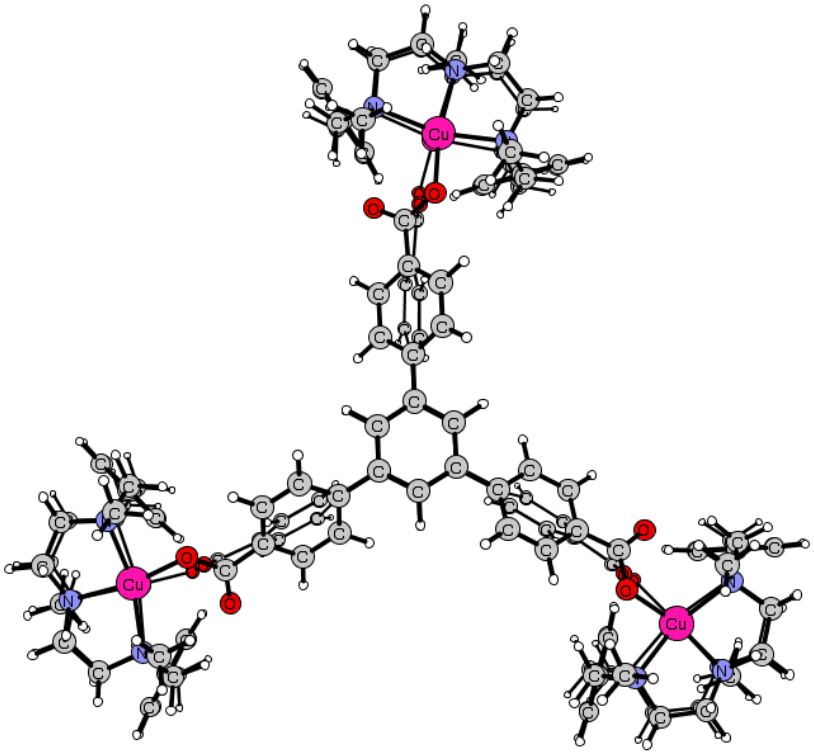

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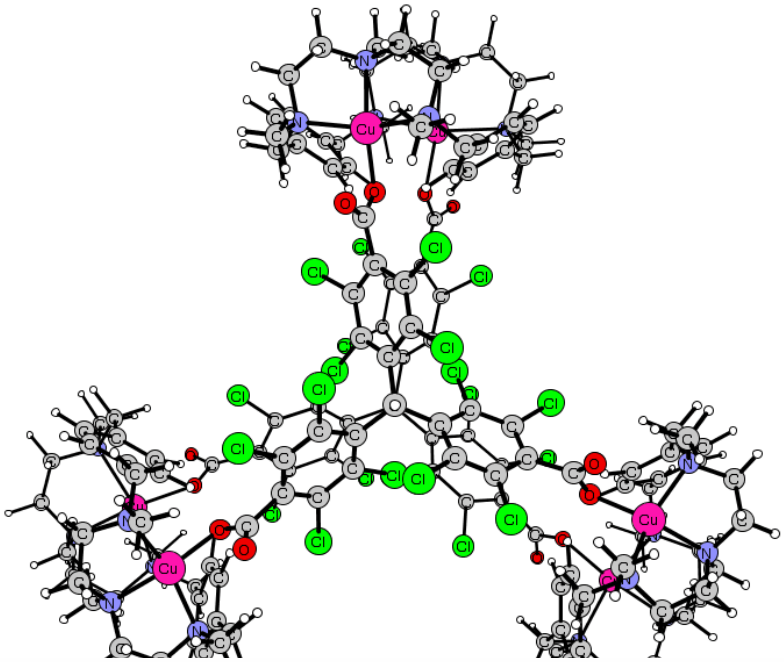
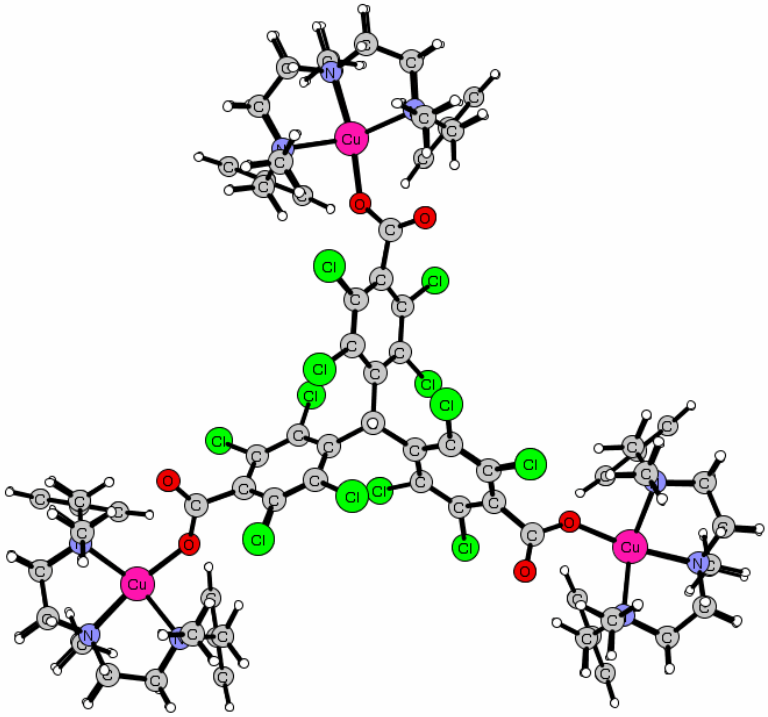
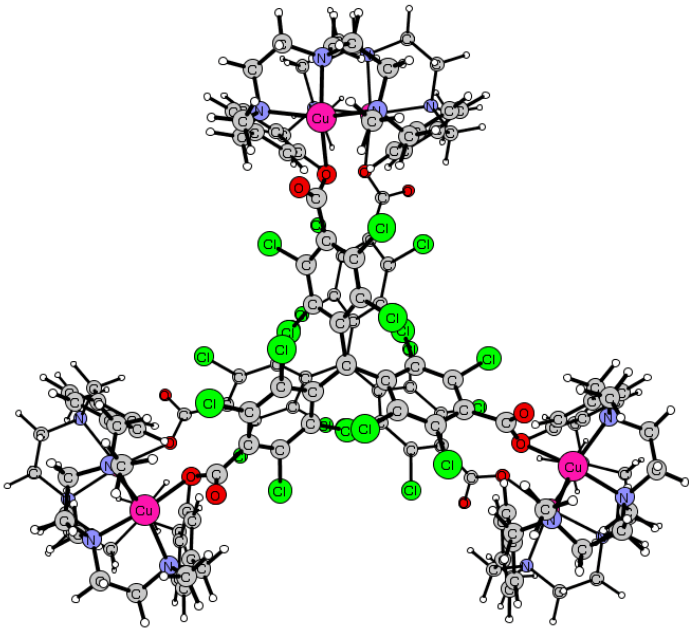


2b:



3a:



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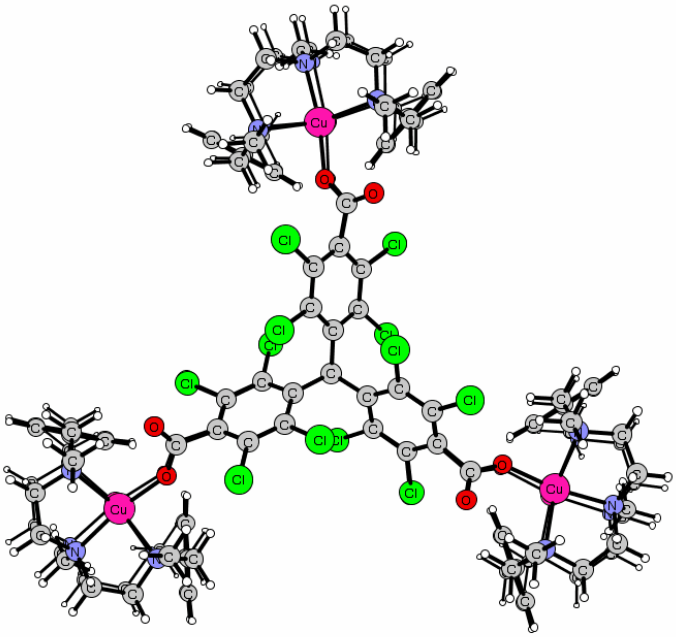
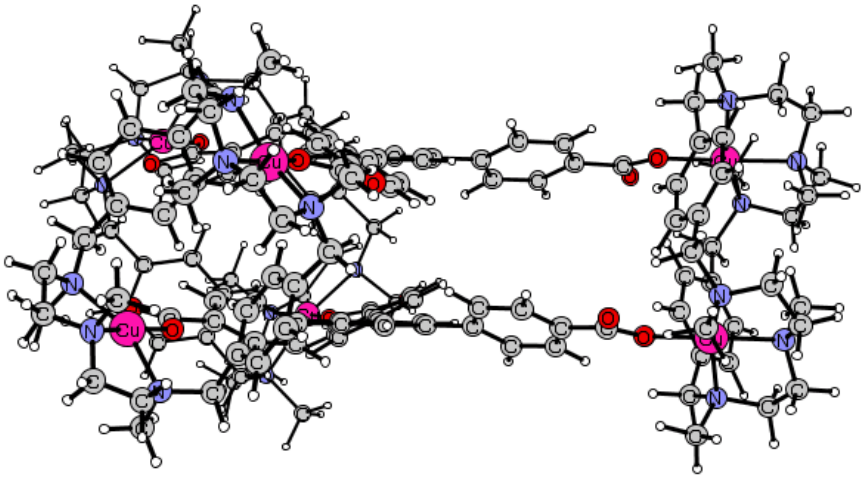


Figures S7. Lateral views of DFT optimized geometries for compounds **1, 2a, 2b, 3a** and **3b**.

1:



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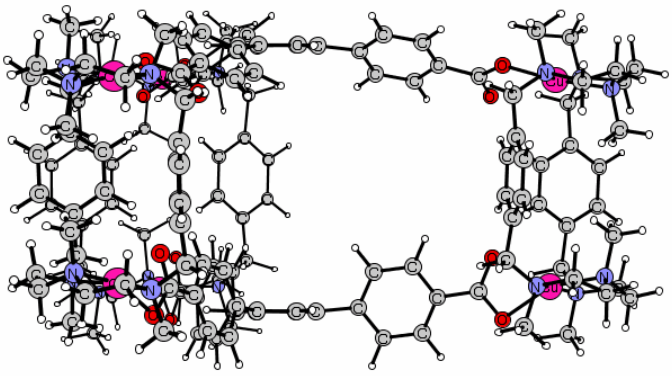

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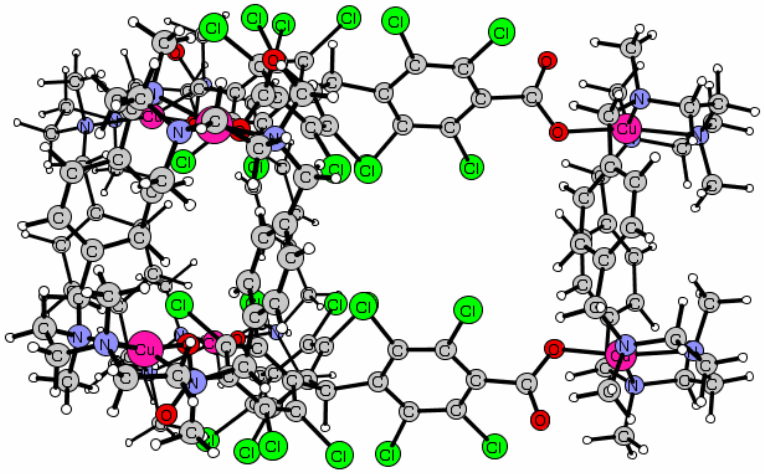
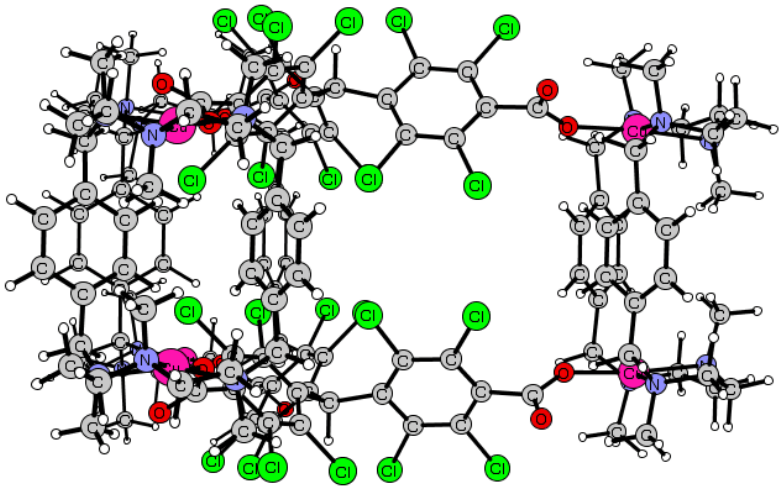


2b:



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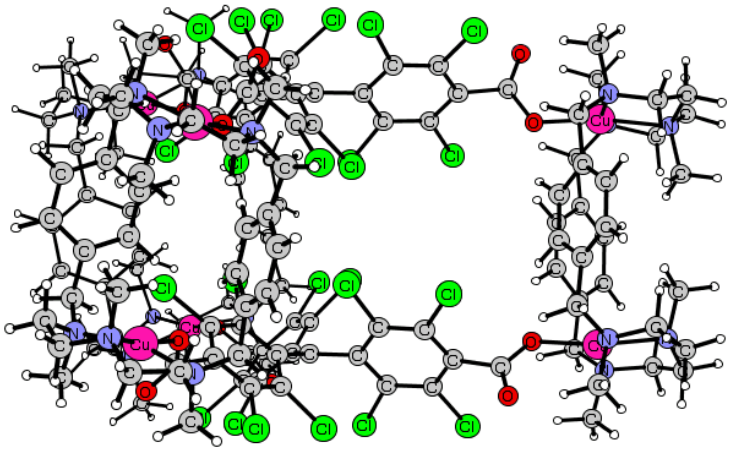


3b:

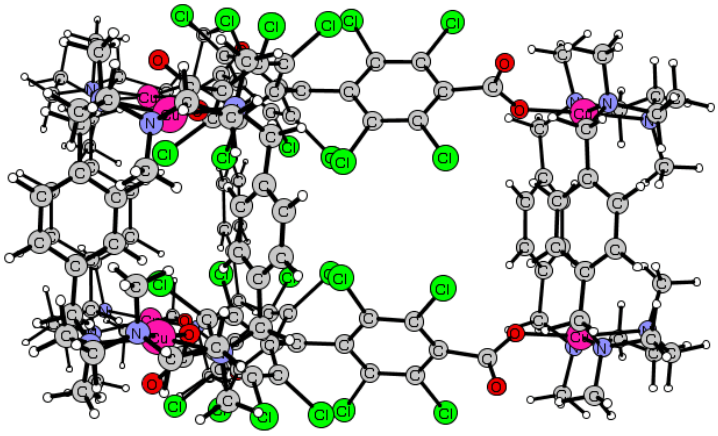


Figure S8. Experimental points and fitting of the Double Integral value (ESR intensity) *vs* T for compound **3** (θ=–0.66; *J*/*k*=-0.3K; r^2=0.85).

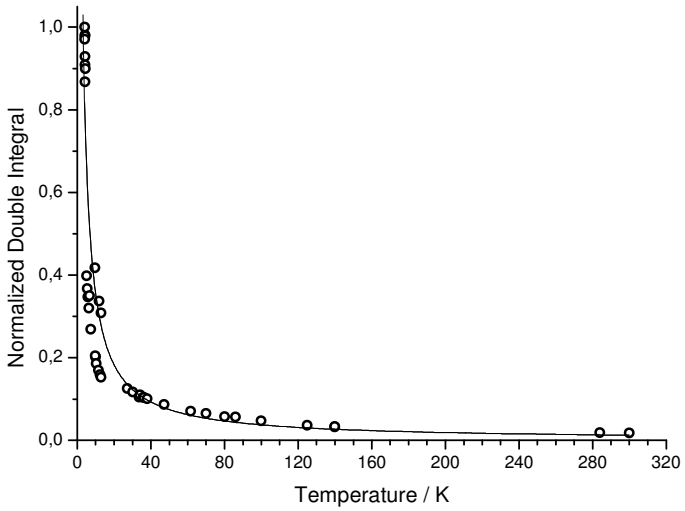


Figure S9. SQUID measurements of the Magnetic Susceptibility χ of compound **3** *vs* T (at 1 Tesla). The data have been fitted with a Curie Weiss equation (see Magnetic Measurements Section – *vide infra*-)

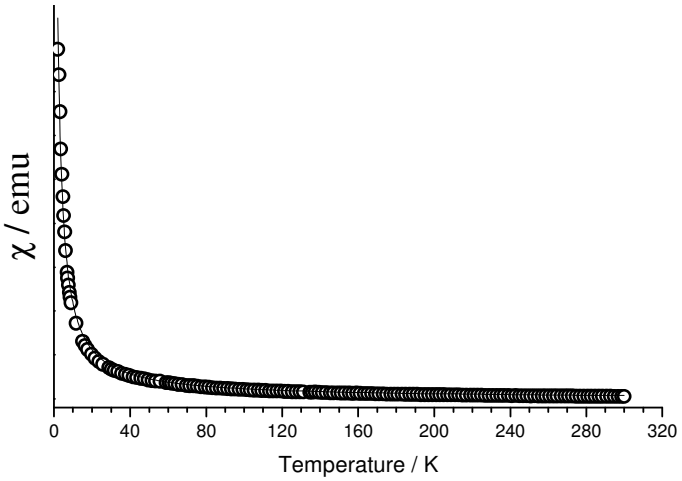


Table S1. EPR *g*-values and linewidth values of the investigated compounds.

Compound	Temperature / K	g_{iso}-value		ΔHpp / G	
		solid	ACN	solid	ACN
4	rt	[§]2.09(2)	[§]2.07(6)	19.8*	-
1	rt	2.08(3)	2.07(1)	91	-
2	rt	2.09(1)	2.07(1)	82.15	-
3	rt	2.07(4)	2.06(2)	77.2	-

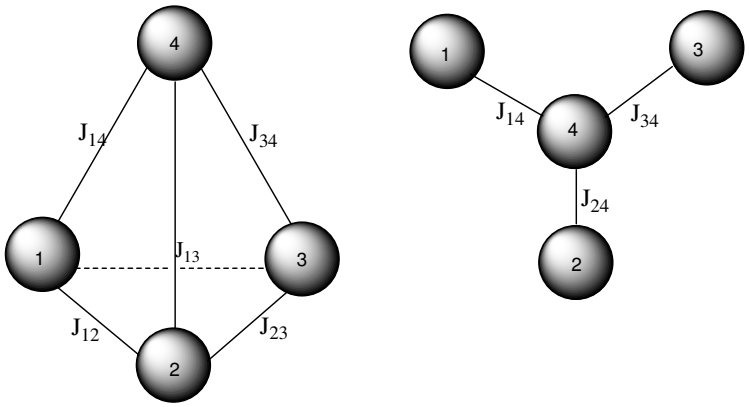
[*]**axial symmetry. The ΔHpp refers to the line in the perpendicular region.**

[§]$g_{iso} = (2g_{\perp}+g_{//})/3$

Magnetic measurements

The star-like 4 spin system (4●S=½) in Scheme S1b can be considered as a particular case of the pyramidal 4 spin system in Scheme S1a when $J_1 = J_{12}=J_{13}=J_{23} = 0$ and $J = J_{14}=J_{24}=J_{34} \neq 0$.

Scheme S1. a) On the left the 4 spin pyramidal system and b) on the right the star like 4 spin system



The general expression for the magnetization χ in a multispin system is

$$\chi = \frac{N\mu_B^2 g^2}{3kT} \frac{\sum_{S'} S'(S'+1)(2S'+1)\Omega(S') e^{\frac{[-W'(S')]}{kT}}}{\sum_{S'} (2S'+1)\Omega(S') e^{\frac{[-W'(S')]}{kT}}} \qquad \text{Eq.1}$$

where N, μ_B, g, k and T have the usual meaning, while the other parameters will be introduced.

S' is the quantum number describing the system and with values *n*S, *n*S-1 and *n*S-2, where *n* is the number of interacting spins. Let's assume, for the system under study, that $S'=S^* + S_4$ and $S^* = S_1 + S_2 + S_3$.

Ω(S') is the degeneracy of the quantum state S' and is defined as follows:

$$\Omega(S') = \omega(S') - \omega(S'+1) \qquad \text{Eq. 2}$$

where ω(S') is the coefficient of S' in the expansion $(x^S + x^{S-1} + \ldots + x^{-S+1} + x^{-S})^n$

W(S') is the energy of the quantum state with expression

$$W(S') = -J[S'(S'+1) - S^*(S^*+1) - S(S+1)] \qquad \text{Eq. 3}$$

By choosing as fundamental state S'=0, W'(S'_i) can be calculated using eq. 4

$$W'(S'_i) = W(S'_i) - W(S'_0) = W(S'_i) - {}^3/_2 J \qquad \text{Eq. 4}$$

In Table S2 are reported the values of all the parameters above defined and needed to solve Eq. 1.

Table S2. Values of the described parameters.

State i	S'	S*	Ω(S')	W'(S')
a	1	½	3	-2J
b	1	3/2	3	J
c	0	½	2	0
d	2	3/2	1	-3J

By substitution in equation 1, we find that the magnetization of the system is

$$\chi = \frac{N\mu_B^2 g^2}{3kT} \frac{18e^{\frac{-J}{kT}} + 18e^{\frac{-4J}{kT}} + 30}{9e^{\frac{-J}{kT}} + 9e^{\frac{-4J}{kT}} + 2e^{\frac{-3J}{kT}} + 5} \qquad \text{Eq. 5}$$

For T→ 0, $J/kT \to \infty$, $e^{-J/kT} \to 0$ and Eq. 5 becomes

$$\chi = \frac{N\mu_B^2 g^2}{3kT} \frac{30}{5} \qquad \text{Eq. 6}$$

By considering $2N\mu_B^2 g^2/k = C$, this is the expression of the Curie law.

When $kT >> J$, $J/kT << 1$, $e^{-J/kT} \approx 1 - J/kT \approx 1$, Eq. 5 becomes

$$\chi = \frac{22N\mu_B^2 g^2}{25k} \frac{1}{T - \frac{51J}{25k}} \qquad \text{Eq. 7}$$

By considering $22/25 N\mu_B^2 g^2/k = C$, the simplified expression corresponds to the Curie-Weiss equation. The condition $kT >> J$ is fulfilled in all the temperature range (4-300K) studied by EPR. Therefore the experimental data has been fitted with a Curie Weiss equation in the whole temperature range. From the fitting of the experimental points, we obtain the value of θ and hence, according to eq. 7, the value of J/k, as reported in the text.

Computational details

The geometry of the compounds was optimized at the B3LYP[4] level as implemented in the Gaussian 03 program.[5] The geometries were optimized using LANL2DZ[6] basis set with associated ECP for Cu and Cl, and 6-31G basis set[7] on the other atoms.

Since the macrocyclic dicopper complexes are symmetric, we have calculated conformers **2a** and **3a** in a *M*,*M* propeller helicities for the PTM moieties, which is thought to be equivalent as the P,P combination.

Table S3. Optimized xyz cartesian coordinates (Å) for structure **1a**.

Atom	X	Y	Z
Cu	-8.769334	-4.623348	-2.468532
Cu	-5.586192	-8.174619	2.467881
N	-7.248847	-9.426782	2.503863
N	-10.149763	-3.604231	-1.197745
N	-4.745503	-9.673834	1.198737
N	-10.212763	-6.126701	-2.487758
C	-11.508100	-5.520307	-2.021139
H	-11.945412	-4.977288	-2.862475
H	-12.219002	-6.306892	-1.735360
C	-6.808238	-10.787640	2.037479
H	-6.319365	-11.288000	2.876943
H	-7.677392	-11.397146	1.756268
C	-5.741901	-6.318972	-1.845257
H	-5.894088	-5.257235	-1.688284
C	-4.028105	-9.243327	-0.073927
H	-3.648334	-10.158136	-0.551037
H	-3.172630	-8.653624	0.262185
C	-9.619276	-2.937356	0.065565
H	-8.930522	-2.167133	-0.287261
H	-10.473285	-2.439401	0.546866
O	-4.308247	-6.703741	2.496062
C	-8.277822	-8.850238	1.575730
H	-7.884951	-8.836189	0.558596
H	-8.514132	-7.826687	1.867814
H	-9.191559	-9.458404	1.603607
C	-7.497188	-5.238958	3.090420
O	-7.152340	-3.537121	-2.493865
C	-4.851565	-8.456208	-1.073074
C	-9.764520	-7.215350	-1.557474
H	-9.705262	-6.825686	-0.540928
H	-8.776001	-7.571857	-1.847747
H	-10.477468	-8.049974	-1.585532
C	-8.930091	-3.843000	1.066283
O	-2.290155	-7.592561	1.894753
C	-10.300041	-6.624057	-3.904691
H	-10.887001	-7.551440	-3.950896
H	-10.834857	-5.868728	-4.487286
C	-6.082175	-6.875562	-3.093808
C	-5.855083	-10.633829	0.861800
H	-5.432947	-11.609783	0.585784
H	-6.374910	-10.244639	-0.016344
O	-7.804164	-1.422016	-1.928339

C	-10.687415	-2.515910	-2.102090
H	-9.872608	-1.825915	-2.321107
H	-11.506104	-1.984286	-1.600111
H	-11.072015	-2.949359	-3.028157
C	-11.235661	-4.587352	-0.850308
H	-12.152248	-4.048683	-0.573794
H	-10.909369	-5.147308	0.028583
C	-3.728474	-10.334023	2.103655
H	-4.199139	-10.646522	3.038778
H	-2.938359	-9.611160	2.306896
H	-3.310576	-11.221286	1.610720
N	-6.490476	-7.331655	4.224132
C	-7.747875	-9.450418	3.921994
H	-7.060183	-10.070485	4.504102
H	-8.738708	-9.922157	3.973208
C	-2.997451	-6.606512	2.224859
C	-6.903194	-2.244004	-2.235246
C	-9.538376	-4.160754	2.294725
H	-10.550591	-3.823828	2.498831
C	-1.350659	-0.153121	2.381420
H	-2.428944	-0.253002	2.378414
N	-8.046591	-5.630664	-4.220849
C	-5.218566	-9.020251	-2.308443
H	-4.987475	-10.060799	-2.516773
C	-8.283414	-4.595025	-5.290265
H	-7.726293	-3.693676	-5.034511
H	-9.347113	-4.354562	-5.356321
H	-7.950472	-4.970104	-6.266493
C	-6.897715	-4.944096	1.850498
H	-5.856132	-5.203104	1.699840
C	-5.488295	-7.684585	5.293630
H	-4.526816	-7.243487	5.031369
H	-5.379405	-8.769026	5.367302
H	-5.817902	-7.300966	6.267669
C	-0.296796	-1.353898	-2.375196
H	-0.514729	-2.414764	-2.373403
C	-5.138123	-7.096025	-0.853724
H	-4.828671	-6.629535	0.075096
C	-0.555627	-1.313358	2.382973
C	-8.898244	-6.847816	-4.457119
H	-8.417804	-7.695272	-3.965526
H	-8.946072	-7.077625	-5.530063
C	-1.362787	-0.436424	-2.372046
C	-1.183506	-2.666085	2.365245
C	-2.402810	-5.235812	2.294700
C	-7.602297	-4.259928	0.857083
H	-7.098966	-3.990713	-0.064600
C	-6.568745	-5.982701	-4.219701
H	-6.342862	-6.448386	-5.189794
H	-6.050575	-5.025030	-4.173558
C	-5.820873	-8.241288	-3.306064
H	-6.038263	-8.692234	-4.270252
C	-6.664848	-5.823121	4.216006
H	-7.097863	-5.538557	5.185897
H	-5.652998	-5.422649	4.165542
C	-5.471432	-1.818078	-2.294723

C	-8.832365	-4.844508	3.293691
H	-9.310356	-5.017840	4.253831
C	-2.776881	-0.908323	-2.353085
C	-7.800284	-8.030597	4.468666
H	-8.585554	-7.454927	3.976477
H	-8.030090	-8.045320	5.542386
C	-5.123695	-0.565388	-1.757226
H	-5.905225	0.047647	-1.323919
C	-3.055801	-4.146537	2.893858
H	-4.031867	-4.285495	3.340154
C	-1.126297	-5.029866	1.741392
H	-0.615397	-5.872493	1.290416
C	-2.451441	-2.890348	2.941466
H	-2.960624	-2.081865	3.453852
C	-4.459641	-2.605626	-2.867052
H	-4.706744	-3.568416	-3.295774
C	-3.800641	-0.128271	-1.772892
H	-3.556925	0.823728	-1.313969
C	-0.536845	-3.767380	1.763452
H	0.430575	-3.631301	1.292137
C	-3.140778	-2.152329	-2.909336
H	-2.392154	-2.760784	-3.404125
Cu	0.332750	9.910621	-2.485026
Cu	-4.281253	8.888025	2.500389
N	-4.562255	10.950265	2.546959
N	1.915011	10.612140	-1.229960
N	-6.015869	8.892609	1.248988
N	-0.259414	11.907394	-2.500100
C	0.912033	12.736527	-2.050563
H	1.590211	12.845703	-2.900339
H	0.582060	13.744063	-1.764505
C	-5.970159	11.231770	2.097886
H	-6.635349	11.042561	2.943951
H	-6.081369	12.289466	1.824451
C	-2.640664	8.076034	-1.845577
H	-1.648303	7.661904	-1.709679
C	-6.005865	8.058987	-0.027522
H	-6.993146	8.182333	-0.495328
H	-5.914727	7.023206	0.305082
C	2.243340	9.831546	0.036125
H	2.576659	8.850400	-0.307995
H	3.098278	10.335899	0.509060
O	-3.615712	7.058651	2.507775
C	-3.567712	11.572886	1.611305
H	-3.762838	11.235280	0.593055
H	-2.556033	11.272944	1.885314
H	-3.648614	12.667187	1.651981
C	-0.778154	9.125380	3.086950
O	0.466510	7.967468	-2.509519
C	-4.923040	8.386170	-1.036393
C	-1.412816	12.050064	-1.550812
H	-1.087840	11.801444	-0.540172
H	-2.215120	11.367622	-1.831966
H	-1.788202	13.081728	-1.568145
C	1.122793	9.684248	1.045328
O	-5.386630	5.739408	1.922521

C	-0.671898	12.231011	-3.909506
H	-1.192249	13.197934	-3.945508
H	0.239048	12.327297	-4.506933
C	-2.959414	8.684782	-3.075099
C	-6.313526	10.330853	0.920863
H	-7.373999	10.441023	0.656095
H	-5.727980	10.597972	0.038783
O	2.631919	7.471941	-1.969041
C	3.118749	10.540719	-2.144858
H	3.316158	9.491213	-2.362758
H	3.988690	10.993068	-1.651465
H	2.923857	11.086186	-3.071335
C	1.602751	12.043991	-0.885466
H	2.528499	12.574550	-0.624297
H	0.967126	12.042463	0.002560
C	-7.080925	8.325417	2.162110
H	-7.115709	8.888452	3.097822
H	-6.833537	7.283198	2.362856
H	-8.063324	8.393826	1.677329
N	-3.082129	9.259653	4.245951
C	-4.324694	11.389594	3.965509
H	-5.193949	11.085365	4.555394
H	-4.256024	12.484515	4.021933
C	-4.176318	5.869590	2.238410
C	1.465173	7.105102	-2.260627
C	1.175684	10.349016	2.284367
H	1.982612	11.046812	2.488368
C	0.621870	1.240615	2.383707
H	1.075242	2.224125	2.383164
N	-0.921301	9.780626	-4.224666
C	-5.234701	9.020697	-2.253006
H	-6.250683	9.354611	-2.442915
C	0.082292	9.478452	-5.308041
H	0.592265	8.546790	-5.062992
H	0.817305	10.283558	-5.378459
H	-0.420208	9.380253	-6.278895
C	-0.851302	8.485804	1.834205
H	-1.608153	7.725214	1.680400
C	-3.868930	8.548511	5.317255
H	-3.950325	7.495019	5.049479
H	-4.870311	8.977411	5.399369
H	-3.367634	8.645653	6.288784
C	-1.061303	0.937143	-2.374648
H	-1.871603	1.655698	-2.371371
C	-3.605918	7.927821	-0.846550
H	-3.352353	7.398125	0.064942
C	-0.780528	1.132471	2.379128
C	-1.564455	11.121289	-4.449443
H	-2.530911	11.119668	-3.942635
H	-1.756544	11.277162	-5.519515
C	0.266337	1.401441	-2.378354
C	-1.640161	2.350573	2.357792
C	-3.273453	4.679229	2.296067
C	0.083343	8.759437	0.833129
H	0.044059	8.206246	-0.098725
C	-1.957892	8.670854	-4.214203

H	-2.488889	8.711265	-5.176292
H	-1.382715	7.746063	-4.182963
C	-4.269412	9.164120	-3.259134
H	-4.559075	9.601472	-4.210532
C	-1.679711	8.678213	4.221604
H	-1.209784	8.915867	5.186790
H	-1.822357	7.599142	4.168826
C	1.119296	5.652038	-2.315424
C	0.242645	10.070916	3.292470
H	0.349859	10.554305	4.259532
C	0.563757	2.862522	-2.365505
C	-3.052684	10.742195	4.497642
H	-2.171519	11.150422	4.000102
H	-2.944783	10.944784	5.571495
C	2.035334	4.726770	-1.783575
H	2.960369	5.098644	-1.358792
C	-2.001283	4.709826	2.889430
H	-1.639250	5.626844	3.336313
C	-3.724870	3.468873	1.739800
H	-4.710944	3.441224	1.291249
C	-1.207183	3.563790	2.932875
H	-0.251883	3.606955	3.443743
C	-0.070808	5.167209	-2.880663
H	-0.783469	5.860764	-3.308252
C	1.754404	3.362115	-1.794751
H	2.461180	2.676946	-1.339246
C	-2.917858	2.333343	1.757538
H	-3.278447	1.426487	1.284744
C	-0.335752	3.797869	-2.919342
H	-1.239105	3.452328	-3.409118
Cu	8.376834	-5.248507	-2.483119
Cu	9.915164	-0.746275	2.459408
N	11.834873	-1.551430	2.473831
N	8.199223	-6.956517	-1.209296
N	10.776799	0.739309	1.184506
N	10.399026	-5.742243	-2.514998
C	10.534682	-7.164587	-2.044147
H	10.285759	-7.820059	-2.882298
H	11.574259	-7.376811	-1.761298
C	12.784135	-0.483955	2.002870
H	12.975271	0.188257	2.843012
H	13.746496	-0.926937	1.713806
C	8.340492	-1.791484	-1.852731
H	7.499052	-2.456150	-1.693823
C	10.028427	1.145482	-0.078157
H	10.620104	1.938112	-0.558342
H	9.091818	1.583809	0.272179
C	7.365663	-6.841610	0.061546
H	6.348804	-6.632693	-0.277142
H	7.371304	-7.833905	0.535005
O	7.999946	-0.395999	2.502335
C	11.843488	-2.726422	1.540705
H	11.627201	-2.388619	0.526803
H	11.076086	-3.442160	1.836409
H	12.827048	-3.214286	1.559724
C	8.338713	-3.873410	3.094045

O	6.629661	-4.387540	-2.494739
C	9.753263	0.042849	-1.079924
C	11.114724	-4.800412	-1.591374
H	10.754858	-4.945495	-0.572293
H	10.916909	-3.768349	-1.882433
H	12.195757	-4.990143	-1.625277
C	7.814067	-5.800061	1.066718
O	7.739147	1.799160	1.924896
C	10.864592	-5.571571	-3.934665
H	11.961072	-5.615783	-3.987038
H	10.474391	-6.413831	-4.512807
C	8.984938	-1.801052	-3.105314
C	12.161761	0.265277	0.834021
H	12.790825	1.121998	0.556163
H	12.080664	-0.377616	-0.045121
O	5.124324	-6.010033	-1.929823
C	7.528570	-7.970139	-2.111190
H	6.517468	-7.621257	-2.320774
H	7.492594	-8.946935	-1.611804
H	8.089401	-8.077917	-3.042618
C	9.597296	-7.398205	-0.869000
H	9.595257	-8.461258	-0.591990
H	9.920751	-6.833581	0.007994
C	10.843760	1.948770	2.091880
H	11.363909	1.698053	3.019531
H	9.823367	2.265029	2.307991
H	11.391725	2.758902	1.593746
N	9.661720	-1.958223	4.217717
C	12.121065	-1.977857	3.886697
H	12.317936	-1.075453	4.472540
H	13.027218	-2.597769	3.925122
C	7.249486	0.685442	2.241570
C	5.385141	-4.818970	-2.237416
C	8.383392	-6.180219	2.295830
H	8.580669	-7.229047	2.497725
C	0.843109	-1.164685	2.385789
H	1.467773	-2.049319	2.384441
N	8.875372	-4.116627	-4.240308
C	10.419372	0.011438	-2.318707
H	11.202935	0.733607	-2.528541
C	8.087361	-4.836351	-5.305101
H	7.029884	-4.797248	-5.044090
H	8.403501	-5.880042	-5.370870
H	8.244138	-4.363282	-6.283016
C	7.794874	-3.489052	1.852832
H	7.517824	-2.451739	1.704305
C	9.475405	-0.915098	5.289814
H	8.604830	-0.308498	5.040383
H	10.356518	-0.272400	5.349758
H	9.325429	-1.392733	6.266581
C	1.305329	0.453575	-2.379423
H	2.332464	0.797060	-2.379525
C	8.717691	-0.884369	-0.859555
H	8.163184	-0.852068	0.071608
C	1.450270	0.104367	2.385629
C	10.353312	-4.247195	-4.486850

H	10.851656	-3.406240	-4.001790
H	10.567649	-4.178472	-5.561705
C	1.044038	-0.928640	-2.376219
C	2.934685	0.243241	2.370256
C	5.767449	0.499504	2.308287
C	7.535975	-4.435747	0.858783
H	7.060138	-4.122960	-0.064019
C	8.445857	-2.660255	-4.232880
H	8.734734	-2.228091	-5.201829
H	7.357619	-2.685947	-4.183194
C	10.038724	-0.893749	-3.318601
H	10.531025	-0.850354	-4.286105
C	8.444139	-2.866085	4.223370
H	8.428129	-3.388029	5.191190
H	7.589475	-2.191076	4.188213
C	4.299394	-3.793232	-2.297391
C	8.638126	-5.232710	3.296645
H	9.021064	-5.567813	4.256541
C	2.160687	-1.917284	-2.359122
C	10.926882	-2.739702	4.443768
H	10.817941	-3.705748	3.948550
H	11.068151	-2.935381	5.515105
C	3.040598	-4.119535	-1.760750
H	2.902140	-5.101820	-1.324552
C	5.160051	-0.623889	2.893419
H	5.775150	-1.399040	3.331960
C	4.942812	1.500364	1.764452
H	5.409254	2.373698	1.323830
C	3.770690	-0.742248	2.936394
H	3.332402	-1.596525	3.439776
C	4.473188	-2.524301	-2.872677
H	5.429892	-2.256009	-3.302439
C	1.999592	-3.193287	-1.776803
H	1.054978	-3.459001	-1.314938
C	3.556339	1.366158	1.782565
H	2.949199	2.135524	1.318062
C	3.419487	-1.610870	-2.917366
H	3.571271	-0.659491	-3.414528

E = -8657.65517541 au

Table S4. Optimized xyz cartesian coordinates (Å) for structure **1b**.

Atom	X	Y	Z
Cu	-2.650419	9.545036	-3.573590
Cu	-2.540972	9.325604	3.732613
N	-3.538680	11.121847	3.387260
N	-0.828920	10.763221	-3.651232
N	-4.563317	8.490650	3.686600
N	-3.579241	11.382545	-3.286545
C	-2.699721	12.391146	-3.971581
H	-2.797864	12.235548	-5.049985

H	-3.042705	13.411900	-3.752591
C	-4.918153	10.937664	3.953301
H	-4.829731	10.924892	5.043441
H	-5.560176	11.788450	3.685421
C	-3.748169	7.621209	-0.926948
H	-2.827182	7.522171	-1.492814
C	-4.847847	7.327425	2.735256
H	-5.824585	6.916323	3.029954
H	-4.089723	6.575201	2.954489
C	0.385027	10.529855	-2.747127
H	0.760965	9.545277	-3.018144
H	1.127098	11.289460	-3.032621
C	-3.586502	11.435296	1.923089
H	-4.081913	10.624795	1.389130
H	-2.574724	11.524022	1.529338
H	-4.129751	12.375539	1.757341
C	0.197598	10.444407	1.603907
C	-4.874482	7.599612	1.238304
C	-3.685948	11.656733	-1.815065
H	-2.703638	11.582197	-1.348368
H	-4.339769	10.917105	-1.353039
H	-4.097303	12.661374	-1.649565
C	0.172394	10.574005	-1.243552
C	-4.942506	11.316979	-3.920657
H	-5.559661	12.161776	-3.586945
H	-4.810695	11.417391	-5.001160
C	-4.976329	7.708802	-1.606196
C	-5.513019	9.634749	3.439079
H	-6.475922	9.440561	3.930036
H	-5.702151	9.692824	2.367023
C	-0.388962	10.477177	-5.068363
H	-0.114039	9.426023	-5.145100
H	0.474291	11.101376	-5.331366
H	-1.200006	10.690575	-5.769002
C	-1.261112	12.203591	-3.519677
H	-0.594427	12.849155	-4.106669
H	-1.146650	12.488166	-2.472505
C	-4.746583	7.979886	5.096645
H	-4.595899	8.792528	5.809952
H	-4.008246	7.208523	5.304284
H	-5.760975	7.580743	5.223472
N	-0.826557	10.593252	3.993277
C	-2.755705	12.155930	4.148244
H	-2.931058	11.983449	5.213987
H	-3.118151	13.166013	3.911995
C	0.592335	11.675524	-0.471761
H	0.979431	12.565134	-0.961161
N	-4.672659	8.856861	-3.887135
C	-6.103451	7.713173	0.560112
H	-7.034182	7.706576	1.120668
C	-4.696220	8.534701	-5.358525
H	-3.917742	7.801190	-5.561770
H	-4.502189	9.435985	-5.944083
H	-5.679110	8.138368	-5.643873
C	-0.241133	9.355456	0.830559
H	-0.517439	8.433112	1.326608

C	-0.415292	10.371150	5.430276
H	-0.196589	9.316160	5.581543
H	-1.233145	10.652742	6.097019
H	0.462184	10.985427	5.666503
C	-3.695471	7.568758	0.468645
H	-2.746491	7.434828	0.969744
C	-5.606919	9.990923	-3.574138
H	-5.853495	9.941729	-2.512157
H	-6.545029	9.878772	-4.134110
C	-0.258236	9.419898	-0.563383
H	-0.506793	8.538677	-1.140913
C	-5.029735	7.599447	-3.116495
H	-6.037529	7.293047	-3.431847
H	-4.317438	6.846497	-3.459185
C	-6.153701	7.770054	-0.838839
H	-7.120164	7.810075	-1.333205
C	0.375547	10.279217	3.103148
H	1.200972	10.917989	3.449139
H	0.639444	9.244251	3.330095
C	0.607654	11.611704	0.929676
H	1.006100	12.453942	1.489095
C	-1.277788	12.021602	3.809788
H	-1.093946	12.307647	2.774421
H	-0.680006	12.688618	4.443937
Cu	9.597934	-2.411426	-3.596228
Cu	9.383078	-2.537977	3.705600
N	11.438691	-2.582296	3.353215
N	9.745803	-4.594912	-3.721543
N	9.687710	-0.377156	3.715283
N	11.656234	-2.529898	-3.317154
C	12.090855	-3.780490	-4.028635
H	12.004508	-3.594443	-5.103234
H	13.146882	-3.996863	-3.815013
C	11.981868	-1.310873	3.940896
H	11.936035	-1.402620	5.029824
H	13.038004	-1.180180	3.666179
C	8.493212	-0.550833	-0.887200
H	7.942998	-1.287447	-1.464058
C	8.818923	0.478072	2.791617
H	8.961350	1.521307	3.109023
H	7.788022	0.200622	3.013767
C	8.938023	-5.546132	-2.833859
H	7.896278	-5.376108	-3.100703
H	9.224496	-6.563452	-3.137942
C	11.727684	-2.673227	1.886591
H	11.289163	-1.818316	1.372336
H	11.279668	-3.577047	1.475515
H	12.813090	-2.690296	1.718439
C	8.960836	-5.422706	1.519120
C	9.056184	0.395728	1.290603
C	11.945603	-2.603681	-1.847060
H	11.392331	-3.428297	-1.397914
H	11.627114	-1.677941	-1.367773
H	13.021720	-2.748670	-1.682780
C	9.085210	-5.412170	-1.327964
C	12.277934	-1.302168	-3.925649

H	13.319050	-1.196011	-3.592593
H	12.295718	-1.440389	-5.009936
C	9.182300	0.478656	-1.553031
C	11.152822	-0.130157	3.457097
H	11.475934	0.790517	3.961190
H	11.287402	0.022507	2.385905
C	9.276852	-4.804689	-5.143004
H	8.229461	-4.515677	-5.216402
H	9.384857	-5.859211	-5.426668
H	9.868205	-4.197084	-5.832225
C	11.209866	-4.943363	-3.601526
H	11.434183	-5.829537	-4.209857
H	11.400827	-5.209753	-2.560888
C	9.355956	0.005803	5.139081
H	9.980674	-0.560559	5.832733
H	8.316127	-0.236159	5.347699
H	9.537412	1.077132	5.291781
N	9.608403	-4.662607	3.923376
C	11.933247	-3.796349	4.089194
H	11.874842	-3.580083	5.159867
H	12.987269	-3.991362	3.847426
C	9.818841	-6.349443	-0.574484
H	10.386830	-7.126165	-1.079309
N	10.010911	-0.311226	-3.858247
C	9.768519	1.412508	0.625976
H	10.234940	2.210177	1.197567
C	9.734044	-0.093541	-5.323059
H	8.707884	-0.395506	-5.525705
H	10.412604	-0.696712	-5.929891
H	9.879863	0.962858	-5.582869
C	8.247534	-4.474618	0.764237
H	7.590935	-3.780444	1.274496
C	9.211802	-4.934589	5.356508
H	8.191560	-4.593201	5.517901
H	9.869348	-4.383931	6.032721
H	9.299339	-6.006648	5.570980
C	8.429829	-0.593918	0.508500
H	7.843665	-1.356636	1.005048
C	11.461075	-0.073977	-3.546791
H	11.546311	0.137491	-2.479497
H	11.828865	0.808884	-4.086818
C	8.312868	-4.465014	-0.629481
H	7.682901	-3.790518	-1.195351
C	9.103308	0.608156	-3.060889
H	9.337770	1.640749	-3.357235
H	8.093481	0.372993	-3.402140
C	9.832551	1.452204	-0.772926
H	10.348026	2.276860	-1.256891
C	8.729048	-5.523581	3.016515
H	8.868369	-6.565322	3.340087
H	7.701417	-5.238095	3.250616
C	9.756583	-6.356538	0.827066
H	10.281021	-7.136794	1.372287
C	11.067690	-4.994431	3.728482
H	11.216487	-5.277070	2.686360
H	11.341205	-5.860331	4.344466

Cu	-6.892423	-7.012878	-3.636927
Cu	-6.909592	-6.896260	3.669992
N	-7.987104	-8.642238	3.297375
N	-8.847407	-6.027400	-3.742714
N	-5.199370	-8.246265	3.664854
N	-8.039595	-8.726219	-3.386483
C	-9.337883	-8.454389	-4.093977
H	-9.132857	-8.456984	-5.168593
H	-10.060638	-9.257495	-3.893484
C	-7.163211	-9.758474	3.875219
H	-7.221435	-9.683495	4.964896
H	-7.583148	-10.733346	3.590521
C	-4.754759	-7.058507	-0.924884
H	-5.113892	-6.202905	-1.488365
C	-4.026878	-7.913714	2.741379
H	-3.197894	-8.569369	3.045206
H	-3.745409	-6.887395	2.979007
C	-9.255725	-4.863525	-2.833797
H	-8.574222	-4.052799	-3.082274
H	-10.275431	-4.584212	-3.136149
C	-8.210566	-8.834404	1.828902
H	-7.251568	-8.876124	1.313165
H	-8.770672	-7.991726	1.425393
H	-8.767125	-9.765010	1.652958
C	-9.172721	-5.023851	1.517640
C	-4.222485	-8.052343	1.239179
C	-8.250714	-8.958243	-1.919320
H	-8.689431	-8.072874	-1.459159
H	-7.290950	-9.150329	-1.439798
H	-8.914456	-9.819797	-1.767904
C	-9.220235	-5.083735	-1.331314
C	-7.298481	-9.877095	-4.011235
H	-7.737983	-10.831979	-3.693098
H	-7.425621	-9.805466	-5.094549
C	-4.202192	-8.157687	-1.606677
C	-5.724368	-9.633751	3.394153
H	-5.093083	-10.380941	3.893085
H	-5.658075	-9.819111	2.321509
C	-8.784791	-5.490950	-5.154340
H	-8.002795	-4.735147	-5.209833
H	-9.746604	-5.042958	-5.433900
H	-8.558414	-6.296604	-5.857133
C	-9.892479	-7.112218	-3.644755
H	-10.767343	-6.844230	-4.251726
H	-10.223450	-7.160501	-2.606087
C	-4.696014	-8.167361	5.088023
H	-5.494875	-8.437757	5.781273
H	-4.389392	-7.147523	5.310060
H	-3.855487	-8.858826	5.228316
N	-8.852832	-6.017989	3.903361
C	-9.286606	-8.463434	4.032496
H	-9.073987	-8.538437	5.102901
H	-9.988651	-9.269197	3.777197
C	-10.402282	-5.251171	-0.583528
H	-11.359019	-5.334998	-1.091984
N	-5.290245	-8.432441	-3.919680

C	-3.695517	-9.166421	0.558092
H	-3.240802	-9.978559	1.118623
C	-4.958594	-8.283582	-5.381618
H	-4.697420	-7.243392	-5.569340
H	-5.821875	-8.552784	-5.993881
H	-4.121924	-8.941469	-5.649801
C	-7.992003	-4.878604	0.768094
H	-7.061553	-4.681428	1.286627
C	-8.890522	-5.564452	5.344814
H	-8.081378	-4.858924	5.520115
H	-8.747954	-6.421276	6.006477
H	-9.861119	-5.103124	5.564732
C	-4.766862	-7.004562	0.471539
H	-5.131880	-6.120651	0.977286
C	-5.825433	-9.805678	-3.629373
H	-5.686476	-10.003012	-2.565016
H	-5.253019	-10.563694	-4.180786
C	-8.013800	-4.911493	-0.626889
H	-7.110973	-4.700731	-1.186346
C	-4.041780	-8.128021	-3.112678
H	-3.268586	-8.847081	-3.418794
H	-3.733108	-7.131712	-3.435055
C	-3.687613	-9.219902	-0.841817
H	-3.231071	-10.072055	-1.337210
C	-9.141124	-4.804155	3.019993
H	-10.104512	-4.391180	3.352476
H	-8.364660	-4.077754	3.268317
C	-10.380312	-5.218389	0.818896
H	-11.320388	-5.281102	1.360435
C	-9.878085	-7.104469	3.687726
H	-10.191920	-7.076096	2.644546
H	-10.766435	-6.909315	4.301656
O	7.631260	-2.453867	4.872541
O	7.769294	-1.936696	-4.116201
O	7.289764	-2.320619	2.681645
O	6.718885	-3.621676	-3.031901
C	6.802966	-2.265740	3.878051
C	6.661418	-2.576278	-3.735933
C	0.207854	-1.446208	4.629218
H	0.375924	-2.517859	4.597530
C	1.115455	0.918242	-4.786196
H	1.960894	1.596407	-4.758621
C	1.308948	-0.571885	4.623769
C	1.349556	-0.468384	-4.779273
C	2.703219	-1.104468	4.474633
C	5.381460	-1.927442	4.102615
C	5.336276	-2.006003	-4.109245
C	2.733325	-0.994420	-4.610333
C	4.203067	-2.637540	-3.564876
H	4.349028	-3.508484	-2.938180
C	4.777369	-2.025681	5.368773
H	5.355319	-2.395724	6.207971
C	4.628325	-1.441384	3.018117
H	5.091348	-1.382194	2.040489
C	3.446125	-1.632309	5.547298
H	2.992024	-1.704440	6.529768

C	5.155072	-0.876845	-4.925341
H	6.015309	-0.393177	-5.373855
C	2.930595	-2.137368	-3.806133
H	2.077108	-2.615358	-3.338865
C	3.314841	-1.021832	3.207571
H	2.749369	-0.622548	2.372275
C	3.870266	-0.381411	-5.175565
H	3.749630	0.475983	-5.829407
O	-5.941563	-5.438963	4.871922
O	-5.565794	-5.674436	-4.148879
O	-5.667105	-5.200148	2.681710
O	-6.473746	-3.937200	-3.021634
C	-5.365745	-4.814063	3.879863
C	-5.549902	-4.403289	-3.743019
C	-1.313138	0.439855	4.632198
H	-2.325440	0.829809	4.603673
C	0.244181	-1.337479	-4.793783
H	0.409306	-2.408758	-4.770506
C	-1.106888	-0.951002	4.626453
C	-1.073948	-0.847389	-4.780964
C	-2.270662	-1.886492	4.477891
C	-4.348358	-3.765127	4.104064
C	-4.393309	-3.539206	-4.112873
C	-2.220208	-1.784604	-4.613485
C	-4.365322	-2.250604	-3.548619
H	-5.184833	-1.949776	-2.907991
C	-4.096813	-3.228887	5.379559
H	-4.690761	-3.560196	6.223740
C	-3.572224	-3.334842	3.012109
H	-3.778500	-3.738579	2.028190
C	-3.076424	-2.288264	5.559725
H	-2.885470	-1.886052	6.548833
C	-3.335124	-3.934981	-4.948210
H	-3.353839	-4.913999	-5.413224
C	-3.298799	-1.395515	-3.790550
H	-3.279976	-0.424410	-3.309032
C	-2.540077	-2.420292	3.201693
H	-1.929698	-2.111903	2.359473
C	-2.265435	-3.067318	-5.197301
H	-1.470755	-3.381895	-5.865654
O	-1.750356	7.757948	4.848409
O	-2.138550	7.733649	-4.115357
O	-1.661676	7.379666	2.661749
O	-0.167100	7.657261	-3.004816
C	-1.484183	6.938738	3.860266
C	-1.036309	7.091306	-3.723270
C	1.079743	0.813958	4.629243
H	1.923931	1.495290	4.599748
C	-1.273487	0.544591	-4.788497
H	-2.283462	0.937238	-4.762283
C	-0.227221	1.331059	4.628095
C	-0.189879	1.441354	-4.776235
C	-0.457558	2.806417	4.480793
C	-1.069853	5.538929	4.099263
C	-0.864636	5.659910	-4.098890
C	-0.430204	2.902317	-4.605988

C	0.247022	4.994888	-3.550233
H	0.924365	5.556559	-2.919052
C	-0.725865	5.059697	5.375665
H	-0.721091	5.741617	6.218477
C	-1.077076	4.648068	3.009905
H	-1.327280	5.024419	2.025528
C	-0.408937	3.708640	5.559777
H	-0.153292	3.347140	6.549980
C	-1.744598	4.939760	-4.924151
H	-2.590555	5.442938	-5.378406
C	0.455305	3.644636	-3.795684
H	1.295643	3.145458	-3.326693
C	-0.789982	3.300394	3.203429
H	-0.824319	2.614270	2.363812
C	-1.527228	3.580171	-5.176658
H	-2.203108	3.048405	-5.838049

E = -8657.62814552 au

Table S5. Optimized xyz cartesian coordinates (Å) for structure **2a**.

Atom	X	Y	Z
H	0.000000	0.000000	5.566007
C	0.000000	0.000000	4.469000
C	1.513927	-0.151761	4.187225
C	2.270033	0.559936	3.238826
C	2.249779	-1.006265	5.040560
C	3.667460	0.479765	3.205206
C	3.635507	-1.123637	4.962371
C	4.388254	-0.350194	4.067776
C	5.906487	-0.337204	4.151465
O	6.589197	-0.834095	3.131749
O	6.447063	0.122562	5.184952
Cl	1.461298	1.569475	1.981186
Cl	1.385911	-1.961717	6.306571
Cl	4.589464	1.514913	2.035968
Cl	4.487250	-2.295566	6.039027
C	-0.888392	-1.235219	4.187225
C	-0.650098	-2.245874	3.238826
C	-1.996340	-1.445233	5.040560
C	-1.418241	-3.415996	3.205206
C	-2.790851	-2.586623	4.962371
C	-2.497404	-3.625242	4.067776
C	-3.245271	-4.946566	4.151465
O	-4.016946	-5.289365	3.131749
O	-3.117389	-5.644602	5.184952
Cl	0.628557	-2.050259	1.981186
Cl	-2.391852	-0.219375	6.306571
Cl	-0.982778	-4.732049	2.035968
Cl	-4.231643	-2.738290	6.039027
C	-0.625535	1.386980	4.187225
C	-1.619935	1.685938	3.238826
C	-0.253438	2.451498	5.040560
C	-2.249219	2.936231	3.205206
C	-0.844656	3.710260	4.962371
C	-1.890850	3.975437	4.067776

C	-2.661216	5.283770	4.151465
O	-2.572251	6.123460	3.131749
O	-3.329674	5.522039	5.184952
Cl	-2.089854	0.480783	1.981186
Cl	1.005941	2.181092	6.306571
Cl	-3.606685	3.217136	2.035968
Cl	-0.255607	5.033855	6.039027
H	0.000000	0.000000	-5.566046
C	0.000000	0.000000	-4.468773
C	1.410079	-0.593338	-4.189315
C	2.460843	-0.185656	-5.042096
C	1.742113	-1.575604	-3.239014
C	3.738683	-0.733492	-4.963833
C	3.013080	-2.162049	-3.205314
C	4.038944	-1.768724	-4.067531
C	5.376137	-2.492699	-4.153198
O	5.639453	-3.147446	-5.186958
O	6.210855	-2.371375	-3.131553
Cl	2.147388	1.062224	-6.310775
Cl	0.553097	-2.082949	-1.982004
Cl	5.041851	-0.098374	-6.039116
Cl	3.339879	-3.506233	-2.033454
C	-1.218885	-0.924495	-4.189315
C	-1.391204	-2.038324	-5.042096
C	-2.235569	-0.720912	-3.239014
C	-2.504564	-2.871049	-4.963833
C	-3.378930	-1.528379	-3.205314
C	-3.551231	-2.613466	-4.067531
C	-4.846809	-3.409521	-4.153198
O	-5.545495	-3.310186	-5.186958
O	-5.159099	-4.193071	-3.131553
Cl	-0.153781	-2.390805	-6.310775
Cl	-2.080435	0.562478	-1.982004
Cl	-2.606120	-4.317183	-6.039116
Cl	-4.706426	-1.139304	-2.033454
C	-0.191193	1.517833	-4.189315
C	-1.069639	2.223980	-5.042096
C	0.493457	2.296516	-3.239014
C	-1.234119	3.604541	-4.963833
C	0.365849	3.690429	-3.205314
C	-0.487712	4.382190	-4.067531
C	-0.529328	5.902220	-4.153198
O	-0.093958	6.457632	-5.186958
O	-1.051757	6.564446	-3.131553
Cl	-1.993607	1.328581	-6.310775
Cl	1.527338	1.520470	-1.982004
Cl	-2.435731	4.415558	-6.039116
Cl	1.366547	4.645536	-2.033454
Cu	-3.397216	7.932620	3.274545
N	-1.660814	8.819617	4.175653
N	-5.486294	7.487593	2.956626
N	-4.036086	9.930105	3.101981
H	-2.393925	11.954427	-1.602315
H	-3.108300	10.326802	-1.455541
H	-1.420873	10.586638	-0.993330
C	1.515165	8.540701	-1.851372

C	0.910974	8.593766	-0.462284
H	-0.314763	6.845025	-0.758529
H	2.520037	8.987485	-1.837254
C	-0.437901	7.540877	1.278571
H	-1.086396	6.732136	1.598962
C	0.000000	7.602943	-0.048176
C	0.015306	8.473285	2.231808
C	0.902806	9.481165	1.811807
H	1.301279	10.189004	2.533373
C	1.348721	9.537687	0.485619
H	2.088830	10.283826	0.209949
C	-0.312079	8.297415	3.702139
H	0.455339	8.796594	4.310927
H	-0.299811	7.237404	3.960274
C	-1.809175	8.480680	5.640661
H	-1.010968	8.964103	6.217501
H	-2.771425	8.829772	6.017797
H	-1.760494	7.402996	5.778629
C	-1.763906	10.308032	3.975529
H	-1.156164	10.831458	4.724899
H	-1.346052	10.539733	2.994784
C	-3.217414	10.745298	4.064874
H	-3.317084	11.816254	3.844146
H	-3.617538	10.583528	5.068603
C	-3.837681	10.421178	1.697555
H	-4.224613	11.444616	1.603653
H	-2.775023	10.415697	1.453497
H	-4.356055	9.771556	0.992585
C	-5.497018	9.919247	3.466104
H	-5.568828	9.768120	4.546691
H	-5.957520	10.889826	3.238263
C	-6.191358	8.799375	2.709301
H	-6.178757	8.993114	1.636833
H	-7.241895	8.721593	3.016169
C	-5.969585	6.899815	4.266493
H	-7.045148	6.694712	4.201021
H	-5.420639	5.988811	4.489887
H	-5.795615	7.603895	5.081869
C	-5.792445	6.486884	1.854387
H	-6.882609	6.343894	1.839571
H	-5.338390	5.549003	2.175740
C	-5.305059	6.841034	0.463639
C	-4.012514	6.468065	0.049084
H	-3.349760	5.980022	0.756639
C	-3.606151	6.641025	-1.278507
H	-2.633006	6.285851	-1.600352
C	-4.479175	7.202373	-2.231388
C	-5.759826	7.604853	-1.810280
H	-6.467912	8.003073	-2.531775
C	-6.169368	7.421691	-0.483970
H	-7.188518	7.675277	-0.207818
C	-4.107554	7.223876	-3.701963
H	-5.023278	7.254696	-4.309585
H	-3.568439	6.312775	-3.961823
H	1.616702	7.502062	-2.171232
N	0.733341	9.233640	-2.959329

N	-1.775296	10.562294	-3.102363
C	1.455629	8.980620	-4.264996
C	0.651575	10.719381	-2.713842
H	0.944310	9.490673	-5.083560
H	2.481339	9.364928	-4.197313
H	1.461373	7.916975	-4.487888
N	-3.225867	8.371933	-4.173275
H	1.588644	11.201586	-3.021843
H	0.540447	10.881883	-1.641857
C	-0.525303	11.311308	-3.471481
C	-2.924076	8.160712	-5.640067
H	-0.636623	12.380876	-3.247543
H	-0.386366	11.215611	-4.551625
H	-3.858519	8.156574	-6.214891
H	-2.286077	8.960956	-6.017072
C	-3.913594	9.694500	-3.973306
H	-4.706698	9.826234	-4.721705
H	-4.391203	9.676372	-2.992045
C	-2.903933	10.828088	-4.064085
H	-3.376651	11.793303	-3.840787
H	-2.479250	10.901004	-5.068033
C	-2.199216	10.878039	-1.698222
H	-2.403331	7.216072	-5.777474
Cu	-1.283056	8.522780	-3.271666
Cu	-5.171242	-6.908385	3.274545
N	-6.807605	-5.848115	4.175653
N	-3.741299	-8.495066	2.956626
N	-6.581680	-8.460405	3.101981
H	-9.155875	-8.050413	-1.602315
H	-7.389123	-7.855267	-1.455541
H	-8.457861	-6.523831	-0.993330
C	-8.154047	-2.958179	-1.851372
C	-7.897906	-3.507956	-0.462284
H	-5.770584	-3.695105	-0.758529
H	-9.043409	-2.311327	-1.837254
C	-6.311641	-4.149672	1.278571
H	-5.287003	-4.306915	1.598962
C	-6.584342	-3.801472	-0.048176
C	-7.345733	-4.223387	2.231808
C	-8.662333	-3.958729	1.811807
H	-9.474576	-3.967561	2.533373
C	-8.934240	-3.600817	0.485619
H	-9.950470	-3.332933	0.209949
C	-7.029733	-4.418976	3.702139
H	-7.845743	-4.003961	4.310927
H	-6.117871	-3.878346	3.960274
C	-6.439897	-5.807132	5.640661
H	-7.257657	-5.357576	6.217501
H	-6.261095	-6.815011	6.017797
H	-5.530935	-5.226130	5.778629
C	-8.045065	-6.681604	3.975529
H	-8.802236	-6.416996	4.724899
H	-8.454650	-6.435582	2.994784
C	-7.696994	-8.159011	4.064874
H	-8.574634	-8.780806	3.844146
H	-7.356835	-8.424644	5.068603

C	-7.106164	-8.534118	1.697555
H	-7.799021	-9.380930	1.603653
H	-7.632746	-7.611089	1.453497
H	-6.284388	-8.658232	0.992585
C	-5.841811	-9.720181	3.466104
H	-5.675026	-9.706807	4.546691
H	-6.452106	-10.604276	3.238263
C	-4.524803	-9.761561	2.709301
H	-4.698887	-9.847518	1.636833
H	-3.932174	-10.632462	3.016169
C	-2.990622	-8.619720	4.266493
H	-2.275216	-9.448633	4.201021
H	-2.476143	-7.688816	4.489887
H	-3.687359	-8.821098	5.081869
C	-2.721584	-8.259847	1.854387
H	-2.052669	-9.132461	1.839571
H	-2.136383	-7.397682	2.175740
C	-3.271980	-8.014833	0.463639
C	-3.595251	-6.708972	0.049084
H	-3.503971	-5.890988	0.756639
C	-3.948221	-6.443531	-1.278507
H	-4.127204	-5.423175	-1.600352
C	-3.997850	-7.480266	-2.231388
C	-3.706083	-8.790582	-1.810280
H	-3.696908	-9.602913	-2.531775
C	-3.342689	-9.053675	-0.483970
H	-3.052726	-10.063077	-0.207818
C	-4.202283	-7.169184	-3.701963
H	-3.771112	-7.977634	-4.309585
H	-3.682803	-6.246746	-3.961823
H	-7.305327	-2.350926	-2.171232
N	-8.363238	-3.981728	-2.959329
N	-8.259567	-6.818599	-3.102363
C	-8.505260	-3.229699	-4.264996
C	-9.609044	-4.795410	-2.713842
H	-8.691319	-3.927540	-5.083560
H	-9.350934	-2.533562	-4.197313
H	-7.586988	-2.692902	-4.487888
N	-5.637373	-6.979649	-4.173275
H	-10.495180	-4.224987	-3.021843
H	-9.694211	-4.972901	-1.641857
C	-9.533228	-6.110580	-3.471481
C	-5.605346	-6.612680	-5.640067
H	-10.403842	-6.741769	-3.247543
H	-9.519821	-5.942408	-4.551625
H	-5.134541	-7.419862	-6.214891
H	-6.617377	-6.460279	-6.017072
C	-6.438886	-8.236522	-3.973306
H	-6.156419	-8.989237	-4.721705
H	-6.184383	-8.641080	-2.992045
C	-7.925433	-7.928924	-4.064085
H	-8.524974	-8.820917	-3.840787
H	-8.200922	-7.597596	-5.068033
C	-8.321050	-7.343596	-1.698222
H	-5.047636	-5.689382	-5.777474
Cu	-6.739416	-5.372549	-3.271666

Cu	8.568458	-1.024235	3.274545
N	8.468419	-2.971502	4.175653
N	9.227593	1.007474	2.956626
N	10.617766	-1.469699	3.101981
H	11.549800	-3.904014	-1.602315
H	10.497423	-2.471534	-1.455541
H	9.878734	-4.062807	-0.993330
C	6.638881	-5.582522	-1.851372
C	6.986932	-5.085809	-0.462284
H	6.085347	-3.149920	-0.758529
H	6.523372	-6.676159	-1.837254
C	6.749542	-3.391205	1.278571
H	6.373399	-2.425221	1.598962
C	6.584342	-3.801472	-0.048176
C	7.330427	-4.249898	2.231808
C	7.759527	-5.522436	1.811807
H	8.173297	-6.221443	2.533373
C	7.585519	-5.936870	0.485619
H	7.861639	-6.950893	0.209949
C	7.341812	-3.878439	3.702139
H	7.390404	-4.792632	4.310927
H	6.417681	-3.359058	3.960274
C	8.249072	-2.673548	5.640661
H	8.268625	-3.606527	6.217501
H	9.032520	-2.014762	6.017797
H	7.291429	-2.176865	5.778629
C	9.808971	-3.626429	3.975529
H	9.958400	-4.414462	4.724899
H	9.800702	-4.104151	2.994784
C	10.914408	-2.586287	4.064874
H	11.891718	-3.035447	3.844146
H	10.974373	-2.158884	5.068603
C	10.943845	-1.887060	1.697555
H	12.023634	-2.063685	1.603653
H	10.407770	-2.804608	1.453497
H	10.640443	-1.113323	0.992585
C	11.338829	-0.199066	3.466104
H	11.243855	-0.061314	4.546691
H	12.409625	-0.285549	3.238263
C	10.716161	0.962186	2.709301
H	10.877644	0.854403	1.636833
H	11.174069	1.910869	3.016169
C	8.960208	1.719905	4.266493
H	9.320364	2.753921	4.201021
H	7.896782	1.700005	4.489887
H	9.482974	1.217203	5.081869
C	8.514029	1.772963	1.854387
H	8.935277	2.788567	1.839571
H	7.474772	1.848679	2.175740
C	8.577039	1.173798	0.463639
C	7.607766	0.240907	0.049084
H	6.853731	-0.089034	0.756639
C	7.554372	-0.197495	-1.278507
H	6.760210	-0.862676	-1.600352
C	8.477025	0.277893	-2.231388
C	9.465908	1.185729	-1.810280

H	10.164821	1.599840	-2.531775
C	9.512057	1.631984	-0.483970
H	10.241244	2.387800	-0.207818
C	8.309838	-0.054692	-3.701963
H	8.794390	0.722939	-4.309585
H	7.251243	-0.066028	-3.961823
H	5.688625	-5.151136	-2.171232
N	7.629897	-5.251912	-2.959329
N	10.034863	-3.743696	-3.102363
C	7.049631	-5.750922	-4.264996
C	8.957468	-5.923971	-2.713842
H	7.747008	-5.563133	-5.083560
H	6.869596	-6.831366	-4.197313
H	6.125615	-5.224073	-4.487888
N	8.863240	-1.392283	-4.173275
H	8.906536	-6.976599	-3.021843
H	9.153764	-5.908983	-1.641857
C	10.058532	-5.200728	-3.471481
C	8.529422	-1.548032	-5.640067
H	11.040464	-5.639107	-3.247543
H	9.906187	-5.273203	-4.551625
H	8.993060	-0.736711	-6.214891
H	8.903454	-2.500677	-6.017072
C	10.352480	-1.457978	-3.973306
H	10.863117	-0.836997	-4.721705
H	10.575586	-1.035293	-2.992045
C	10.829366	-2.899165	-4.064085
H	11.901626	-2.972386	-3.840787
H	10.680172	-3.303409	-5.068033
C	10.520266	-3.534442	-1.698222
H	7.450967	-1.526690	-5.777474
Cu	8.022472	-3.150231	-3.271666

E = -8617.97241602 a.u.

Table S6. Optimized xyz cartesian coordinates (Å) for structure **2b**.

Atom	X	Y	Z
H	0.000000	0.000000	-5.579071
C	0.000000	0.000000	-4.483726
C	-1.173113	-0.972053	-4.203189
C	-2.161815	-0.824917	-3.214383
C	-1.342678	-2.047689	-5.101447
C	-3.269386	-1.671495	-3.165820
C	-2.452936	-2.888553	-5.043623
C	-3.451929	-2.711900	-4.082126
C	-4.769796	-3.482062	-4.142819
O	-4.836314	-4.639091	-3.493692
O	-5.690688	-2.963866	-4.802994
Cl	-2.018295	0.443384	-1.939707
Cl	-0.119676	-2.325742	-6.403903
Cl	-4.540968	-1.425286	-1.904231
Cl	-2.645798	-4.183497	-6.284448
C	1.428379	-0.529919	-4.203189
C	1.795306	-1.459728	-3.214383
C	2.444689	-0.138949	-5.101447

C	3.082250	-1.995624	-3.165820
C	3.728029	-0.680028	-5.043623
C	4.074539	-1.633508	-4.082126
C	5.400452	-2.389733	-4.142819
O	6.435728	-1.868826	-3.493692
O	5.412127	-3.446348	-4.802994
Cl	0.625166	-1.969587	-1.939707
Cl	2.073989	1.059229	-6.403903
Cl	3.504818	-3.219951	-1.904231
Cl	4.945914	-0.199580	-6.284448
C	-0.255266	1.501972	-4.203189
C	0.366509	2.284645	-3.214383
C	-1.102011	2.186638	-5.101447
C	0.187136	3.667119	-3.165820
C	-1.275092	3.568582	-5.043623
C	-0.622610	4.345408	-4.082126
C	-0.630657	5.871796	-4.142819
O	-1.599413	6.507916	-3.493692
O	0.278561	6.410213	-4.802994
Cl	1.393129	1.526203	-1.939707
Cl	-1.954314	1.266513	-6.403903
Cl	1.036150	4.645237	-1.904231
Cl	-2.300116	4.383077	-6.284448
H	0.000000	0.000000	5.603125
C	0.000000	0.000000	4.508358
C	-1.193234	-0.945395	4.224246
C	-2.165136	-0.788199	3.220192
C	-1.390118	-2.014004	5.124341
C	-3.270487	-1.635552	3.142935
C	-2.507091	-2.844827	5.048822
C	-3.477385	-2.673982	4.057686
C	-4.792018	-3.450785	4.076653
O	-4.796636	-4.661921	3.532131
O	-5.772270	-2.886324	4.602888
Cl	-1.999266	0.487578	1.955268
Cl	-0.192144	-2.301300	6.447895
Cl	-4.495256	-1.401079	1.835298
Cl	-2.747261	-4.114956	6.306368
C	1.415353	-0.560673	4.224246
C	1.765168	-1.480964	3.220192
C	2.439238	-0.196875	5.124341
C	3.051673	-2.014548	3.142935
C	3.717238	-0.748791	5.048822
C	4.054429	-1.674512	4.057686
C	5.384477	-2.424617	4.076653
O	6.435660	-1.823049	3.532131
O	5.385765	-3.555771	4.602888
Cl	0.577378	-1.975204	1.955268
Cl	2.089057	0.984248	6.447895
Cl	3.460998	-3.192467	1.835298
Cl	4.937287	-0.321720	6.306368
C	-0.222119	1.506068	4.224246
C	0.399968	2.269162	3.220192
C	-1.049120	2.210879	5.124341
C	0.218813	3.650101	3.142935
C	-1.210147	3.593618	5.048822

C	-0.577044	4.348494	4.057686
C	-0.592458	5.875402	4.076653
O	-1.639024	6.484969	3.532131
O	0.386505	6.442095	4.602888
Cl	1.421888	1.487626	1.955268
Cl	-1.896912	1.317052	6.447895
Cl	1.034258	4.593546	1.835298
Cl	-2.190026	4.436676	6.306368
Cu	-2.205696	8.394923	-3.461636
N	-4.201622	7.717608	-3.736045
N	-0.465270	9.578547	-3.733517
N	-3.157857	10.284202	-3.209426
H	-3.944890	11.514999	1.648052
H	-2.459917	10.600336	1.269801
H	-4.020030	9.767465	1.290351
C	-4.617070	6.434553	2.919946
C	-4.591500	6.600227	1.413139
H	-2.494731	6.145055	1.241024
H	-5.618476	6.115281	3.242546
C	-3.393217	6.397765	-0.704875
H	-2.483747	6.164581	-1.248587
C	-3.399538	6.386519	0.693834
C	-4.578136	6.623882	-1.430862
C	-5.768270	6.843479	-0.712524
H	-6.707359	6.968431	-1.244534
C	-5.774746	6.831095	0.687475
H	-6.719092	6.946075	1.212617
C	-4.591636	6.481823	-2.940378
H	-5.594589	6.182942	-3.277325
H	-3.881646	5.712398	-3.244057
C	-4.194647	7.354350	-5.199725
H	-5.194178	7.030075	-5.514700
H	-3.904051	8.215873	-5.805835
H	-3.483931	6.546442	-5.360441
C	-5.149816	8.859812	-3.490837
H	-6.078772	8.707029	-4.056007
H	-5.411362	8.862078	-2.431930
C	-4.495123	10.175228	-3.889750
H	-5.136186	11.026274	-3.622148
H	-4.329496	10.223197	-4.969221
C	-3.332212	10.599032	-1.754855
H	-3.820182	11.576953	-1.641119
H	-3.945485	9.833240	-1.279845
H	-2.361698	10.620753	-1.260339
C	-2.258492	11.293129	-3.868792
H	-2.381560	11.196042	-4.950416
H	-2.558619	12.314793	-3.597792
C	-0.821772	11.018240	-3.450806
H	-0.685925	11.202864	-2.384749
H	-0.134702	11.684697	-3.988473
C	-0.125146	9.430066	-5.202825
H	0.745410	10.052600	-5.441676
H	0.100704	8.384311	-5.408644
H	-0.965139	9.763974	-5.816681
C	0.748695	9.144956	-2.916860
H	1.588892	9.779680	-3.232648

H	0.965662	8.123904	-3.237233
C	0.596794	9.224040	-1.408953
C	0.000000	8.175666	-0.682738
H	-0.388496	7.313979	-1.215239
C	-0.013652	8.185501	0.717297
H	-0.412290	7.330461	1.252732
C	0.567580	9.243953	1.441223
C	1.149726	10.300195	0.714406
H	1.641919	11.112184	1.241913
C	1.165198	10.289539	-0.685277
H	1.670223	11.093272	-1.213866
C	0.698513	9.180856	2.951353
H	1.509319	9.848706	3.275329
H	0.944828	8.169762	3.281731
H	-3.897245	5.672497	3.219185
N	-4.253223	7.663937	3.737753
N	-3.244520	10.245208	3.220159
C	-4.252259	7.276962	5.195441
C	-5.217160	8.796232	3.504567
H	-3.990078	8.135719	5.818224
H	-5.247138	6.923617	5.493899
H	-3.523194	6.484133	5.349434
N	-0.541632	9.576689	3.747615
H	-6.140735	8.629438	4.074264
H	-5.485753	8.802325	2.447438
C	-4.575960	10.117029	3.907295
C	-0.226120	9.421992	5.221351
H	-5.228837	10.962293	3.648942
H	-4.403023	10.160182	4.985709
H	0.598497	10.091714	5.494431
H	-1.098363	9.688435	5.823245
C	-0.918922	11.009617	3.460253
H	-0.240173	11.687467	3.994393
H	-0.781768	11.188212	2.392804
C	-2.359386	11.271626	3.871637
H	-2.669376	12.286858	3.587400
H	-2.485189	11.186635	4.953947
C	-3.429376	10.551538	1.764493
H	0.060832	8.388228	5.410789
Cu	-2.261990	8.364807	3.469900
Cu	8.373065	-2.287273	-3.461636
N	8.784455	-0.220092	-3.736045
N	8.527900	-4.386338	-3.733517
N	10.485309	-2.407316	-3.209426
H	11.944726	-2.341125	1.648052
H	10.410118	-3.169817	1.269801
H	10.468888	-1.402285	1.290351
C	7.881021	0.781224	2.919946
C	8.011714	0.676242	1.413139
H	6.569139	-0.912027	1.241024
H	8.105227	1.808103	3.242546
C	7.237235	-0.260270	-0.704875
H	6.580557	-0.931303	-1.248587
C	7.230657	-0.249173	0.693834
C	8.025517	0.652841	-1.430862
C	8.810762	1.573729	-0.712524

H	9.388517	2.324528	-1.244534
C	8.803275	1.585529	0.687475
H	9.375024	2.345867	1.212617
C	7.909241	0.735562	-2.940378
H	8.151879	1.753585	-3.277325
H	6.887904	0.505405	-3.244057
C	8.466378	-0.044504	-5.199725
H	8.685312	0.983253	-5.514700
H	9.067180	-0.726929	-5.805835
H	7.411350	-0.256049	-5.360441
C	10.247731	0.029966	-3.490837
H	10.579895	0.910857	-4.056007
H	10.380466	0.255338	-2.431930
C	11.059567	-1.194723	-3.889750
H	12.117126	-1.065069	-3.622148
H	11.018296	-1.362145	-4.969221
C	10.845137	-2.413736	-1.754855
H	11.936026	-2.480102	-1.641119
H	10.488578	-1.499730	-1.279845
H	10.378691	-3.265086	-1.260339
C	10.909383	-3.690653	-3.868792
H	10.886837	-3.535529	-4.950416
H	11.944233	-3.941568	-3.597792
C	9.952962	-4.797445	-3.450806
H	10.044927	-5.007404	-2.384749
H	10.186595	-5.725693	-3.988473
C	8.229250	-4.606653	-5.202825
H	8.333102	-5.671844	-5.441676
H	7.210675	-4.279367	-5.408644
H	8.938419	-4.046152	-5.816681
C	7.545417	-5.220867	-2.916860
H	7.675006	-6.265861	-3.232648
H	6.552676	-4.898240	-3.237233
C	7.689856	-5.128858	-1.408953
C	7.080335	-4.087833	-0.682738
H	6.528340	-3.320542	-1.215239
C	7.095678	-4.080927	0.717297
H	6.554510	-3.308177	1.252732
C	7.721708	-5.113515	1.441223
C	8.345368	-6.145789	0.714406
H	8.802474	-6.978036	1.241913
C	8.328403	-6.153860	-0.685277
H	8.771944	-6.993091	-1.213866
C	7.601598	-5.195358	2.951353
H	7.774570	-6.231461	3.275329
H	6.602807	-4.903125	3.281731
H	6.861149	0.538865	3.219185
N	8.763776	-0.148569	3.737753
N	10.494870	-2.312767	3.220159
C	8.428163	0.044083	5.195441
C	10.226340	0.120077	3.504567
H	9.040778	-0.612351	5.818224
H	8.619597	1.082346	5.493899
H	7.377021	-0.190891	5.349434
N	8.564472	-4.319278	3.747615
H	10.543680	1.003313	4.074264

H	10.365913	0.349639	2.447438
C	11.049584	-1.095616	3.907295
C	8.272745	-4.515170	5.221351
H	12.108043	-0.952841	3.648942
H	11.000487	-1.266961	4.985709
H	8.440432	-5.564171	5.494431
H	8.939613	-3.893007	5.823245
C	9.994069	-4.708999	3.460253
H	10.241730	-5.635738	3.994393
H	10.080159	-4.917075	2.392804
C	10.941208	-3.592525	3.871637
H	11.975419	-3.831681	3.587400
H	10.930504	-3.441081	4.953947
C	10.852588	-2.305842	1.764493
H	7.234003	-4.246796	5.410789
Cu	8.375130	-2.223462	3.469900
Cu	-6.167369	-6.107650	-3.461636
N	-4.582833	-7.497515	-3.736045
N	-8.062630	-5.192209	-3.733517
N	-7.327452	-7.876886	-3.209426
H	-7.999837	-9.173874	1.648052
H	-7.950201	-7.430518	1.269801
H	-6.448858	-8.365180	1.290351
C	-3.263951	-7.215777	2.919946
C	-3.420214	-7.276469	1.413139
H	-4.074408	-5.233028	1.241024
H	-2.486750	-7.923383	3.242546
C	-3.844018	-6.137495	-0.704875
H	-4.096811	-5.233278	-1.248587
C	-3.831118	-6.137346	0.693834
C	-3.447382	-7.276722	-1.430862
C	-3.042491	-8.417208	-0.712524
H	-2.681158	-9.292959	-1.244534
C	-3.028529	-8.416624	0.687475
H	-2.655932	-9.291942	1.212617
C	-3.317605	-7.217385	-2.940378
H	-2.557290	-7.936527	-3.277325
H	-3.006259	-6.217803	-3.244057
C	-4.271730	-7.309846	-5.199725
H	-3.491134	-8.013328	-5.514700
H	-5.163129	-7.488944	-5.805835
H	-3.927420	-6.290393	-5.360441
C	-5.097914	-8.889778	-3.490837
H	-4.501122	-9.617886	-4.056007
H	-4.969104	-9.117417	-2.431930
C	-6.564444	-8.980505	-3.889750
H	-6.980940	-9.961205	-3.622148
H	-6.688800	-8.861052	-4.969221
C	-7.512925	-8.185296	-1.754855
H	-8.115844	-9.096851	-1.641119
H	-6.543093	-8.333510	-1.279845
H	-8.016992	-7.355667	-1.260339
C	-8.650891	-7.602477	-3.868792
H	-8.505276	-7.660512	-4.950416
H	-9.385614	-8.373225	-3.597792
C	-9.131190	-6.220796	-3.450806

H	-9.359002	-6.195460	-2.384749
H	-10.051893	-5.959004	-3.988473
C	-8.104104	-4.823413	-5.202825
H	-9.078512	-4.380756	-5.441676
H	-7.311378	-4.104944	-5.408644
H	-7.973280	-5.717822	-5.816681
C	-8.294112	-3.924089	-2.916860
H	-9.263898	-3.513819	-3.232648
H	-7.518338	-3.225664	-3.237233
C	-8.286650	-4.095181	-1.408953
C	-7.080335	-4.087833	-0.682738
H	-6.139843	-3.993437	-1.215239
C	-7.082026	-4.104574	0.717297
H	-6.142220	-4.022284	1.252732
C	-8.289288	-4.130438	1.441223
C	-9.495093	-4.154406	0.714406
H	-10.444393	-4.134148	1.241913
C	-9.493601	-4.135679	-0.685277
H	-10.442167	-4.100181	-1.213866
C	-8.300111	-3.985498	2.951353
H	-9.283889	-3.617244	3.275329
H	-7.547635	-3.266636	3.281731
H	-2.963904	-6.211362	3.219185
N	-4.510553	-7.515368	3.737753
N	-7.250350	-7.932441	3.220159
C	-4.175904	-7.321045	5.195441
C	-5.009180	-8.916309	3.504567
H	-5.050700	-7.523368	5.818224
H	-3.372459	-8.005963	5.493899
H	-3.853827	-6.293242	5.349434
N	-8.022840	-5.257411	3.747615
H	-4.402946	-9.632752	4.074264
H	-4.880160	-9.151964	2.447438
C	-6.473624	-9.021412	3.907295
C	-8.046625	-4.906822	5.221351
H	-6.879206	-10.009453	3.648942
H	-6.597464	-8.893221	4.985709
H	-9.038929	-4.527543	5.494431
H	-7.841249	-5.795428	5.823245
C	-9.075147	-6.300618	3.460253
H	-10.001557	-6.051729	3.994393
H	-9.298392	-6.271137	2.392804
C	-8.581822	-7.679102	3.871637
H	-9.306043	-8.455176	3.587400
H	-8.445315	-7.745554	4.953947
C	-7.423212	-8.245696	1.764493
H	-7.294834	-4.141432	5.410789
Cu	-6.113140	-6.141344	3.469900

E = -8617.97426327 a.u.

Table S7. Optimized xyz cartesian coordinates (Å) for structure **3a**.

Atom	X	Y	Z
C	0.000000	0.000000	-3.851895
C	-1.473692	0.181676	-3.859274

C	-2.125616	1.076497	-2.975500
C	-2.319197	-0.514476	-4.760020
C	-3.501479	1.283603	-3.016655
C	-3.698197	-0.313230	-4.772984
C	-4.323427	0.602149	-3.918923
C	-5.792520	0.971734	-4.086268
O	-6.668779	0.320568	-3.331039
O	-6.075208	1.854192	-4.919200
Cl	-1.178621	1.925859	-1.696968
Cl	-1.610947	-1.606307	-6.002628
Cl	-4.274363	2.467805	-1.884670
Cl	-4.722214	-1.211948	-5.960633
C	0.579510	-1.367092	-3.859274
C	0.130535	-2.379086	-2.975500
C	1.605148	-1.751245	-4.760020
C	0.639107	-3.674171	-3.016655
C	2.120363	-3.046117	-4.772984
C	1.640237	-4.045272	-3.918923
C	2.054713	-5.502337	-4.086268
O	3.056769	-5.935616	-3.331039
O	1.431827	-6.188380	-4.919200
Cl	-1.078532	-1.983645	-1.696968
Cl	2.196576	-0.591967	-6.002628
Cl	0.000000	-4.935609	-1.884670
Cl	3.410685	-3.483583	-5.960633
C	0.894182	1.185416	-3.859274
C	1.995082	1.302589	-2.975500
C	0.714049	2.265722	-4.760020
C	2.862372	2.390568	-3.016655
C	1.577833	3.359347	-4.772984
C	2.683190	3.443123	-3.918923
C	3.737807	4.530602	-4.086268
O	3.612009	5.615048	-3.331039
O	4.643381	4.334188	-4.919200
Cl	2.257153	0.057786	-1.696968
Cl	-0.585629	2.198275	-6.002628
Cl	4.274363	2.467805	-1.884670
Cl	1.311529	4.695531	-5.960633
C	0.000000	0.000000	3.967499
C	-1.451051	-0.294683	3.971338
C	-2.353814	0.357641	4.850037
C	-2.027872	-1.252849	3.102886
C	-3.717447	0.073619	4.842410
C	-3.385555	-1.561821	3.140141
C	-4.266942	-0.909813	4.007999
C	-5.722327	-1.328328	4.153028
O	-6.071084	-1.937002	5.186965
O	-6.549204	-1.000902	3.168550
Cl	-1.737692	1.506713	6.090095
Cl	-1.011828	-2.052657	1.844495
Cl	-4.815993	0.981719	5.951301
Cl	-4.035847	-2.856663	2.055013
C	0.980728	-1.109306	3.971338
C	0.867181	-2.217283	4.850037
C	2.098935	-1.129764	3.102886
C	1.794968	-3.256212	4.842410

C	3.045354	-2.151066	3.140141
C	2.921392	-3.240373	4.007999
C	4.011529	-4.291517	4.153028
O	4.713035	-4.289212	5.186965
O	4.141409	-5.171327	3.168550
Cl	-0.436006	-2.258242	6.090095
Cl	2.283567	0.150060	1.844495
Cl	1.557803	-4.661632	5.951301
Cl	4.491866	-2.066815	2.055013
C	0.470323	1.403988	3.971338
C	1.486633	1.859642	4.850037
C	-0.071063	2.382613	3.102886
C	1.922479	3.182594	4.842410
C	0.340200	3.712887	3.140141
C	1.345550	4.150186	4.007999
C	1.710798	5.619844	4.153028
O	1.358049	6.226214	5.186965
O	2.407796	6.172228	3.168550
Cl	2.173698	0.751529	6.090095
Cl	-1.271739	1.902598	1.844495
Cl	3.258191	3.679913	5.951301
Cl	-0.456019	4.923478	2.055013
Cu	4.687201	7.285568	-3.386233
N	3.055375	8.365646	-4.213926
N	6.688415	6.600171	-3.128804
N	5.535659	9.180140	-3.163340
H	5.134238	10.959501	1.609111
H	5.294009	9.183870	1.487435
H	3.773983	9.959311	1.024623
C	0.368099	8.663815	2.031252
C	0.854838	8.584606	0.596038
H	1.767572	6.646202	0.834486
H	-0.519337	9.310716	2.081619
C	1.851033	7.291226	-1.220115
H	2.317644	6.377524	-1.572195
C	1.540930	7.444258	0.135504
C	1.489593	8.274723	-2.161475
C	0.818339	9.422699	-1.699089
H	0.483047	10.177327	-2.405336
C	0.505870	9.574669	-0.342188
H	-0.064545	10.443940	-0.026456
C	1.683961	8.025203	-3.646056
H	0.944913	8.602908	-4.219415
H	1.530749	6.968666	-3.866271
C	3.096385	7.943116	-5.662557
H	2.292899	8.436270	-6.223885
H	4.052506	8.222114	-6.110473
H	2.971773	6.864384	-5.730033
C	3.346729	9.838661	-4.097780
H	2.842197	10.387897	-4.903625
H	2.931057	10.192680	-3.153449
C	4.849512	10.081022	-4.153884
H	5.083000	11.133422	-3.943220
H	5.249656	9.850052	-5.144734
C	5.292852	9.637888	-1.756159
H	5.724870	10.636681	-1.607150

H	4.221847	9.672025	-1.555401
H	5.750225	8.936287	-1.058419
C	7.008646	9.042752	-3.438063
H	7.142261	8.979623	-4.520820
H	7.548340	9.934450	-3.092057
C	7.529782	7.791446	-2.746198
H	7.493649	7.902737	-1.661723
H	8.577006	7.611974	-3.022863
C	7.115943	6.101695	-4.494573
H	8.160691	5.768891	-4.453445
H	6.463530	5.284695	-4.799745
H	7.037872	6.907739	-5.227776
C	6.864434	5.461332	-2.131677
H	7.915926	5.145483	-2.187189
H	6.253531	4.639049	-2.508529
C	6.505068	5.771104	-0.690479
C	5.174232	5.668549	-0.242867
H	4.397129	5.403678	-0.951209
C	4.858057	5.813037	1.112553
H	3.839989	5.661040	1.454589
C	5.861448	6.073269	2.065548
C	7.190198	6.193882	1.616874
H	7.992938	6.351190	2.332066
C	7.506541	6.043622	0.260819
H	8.547768	6.088622	-0.046324
C	5.536655	6.066911	3.548173
H	6.440106	5.819095	4.123304
H	4.786644	5.304427	3.759297
H	0.076698	7.671492	2.378746
N	1.358346	9.184809	3.064283
N	4.109883	9.854293	3.128049
C	0.677325	9.160901	4.416756
C	1.787415	10.595494	2.745760
H	1.340297	9.577748	5.177266
H	-0.237316	9.765686	4.378386
H	0.446472	8.135468	4.697544
N	4.979624	7.360048	4.127693
H	1.005317	11.302309	3.052651
H	1.897513	10.681789	1.663956
C	3.096167	10.917776	3.453505
C	4.647547	7.131272	5.584453
H	3.467800	11.907447	3.155422
H	2.964005	10.931550	4.538696
H	5.542222	6.793925	6.122860
H	4.296551	8.058980	6.040240
C	5.970855	8.488409	4.004764
H	6.735258	8.405194	4.788801
H	6.478264	8.390239	3.043616
C	5.252336	9.827863	4.106929
H	5.945246	10.657704	3.912160
H	4.837090	9.977860	5.107090
C	4.610786	10.000475	1.722201
H	3.863664	6.383440	5.677090
Cu	3.128587	8.023656	3.299006
Cu	3.965886	-7.702019	-3.386233
N	5.717175	-6.828856	-4.213926

N	2.371709	-9.092423	-3.128804
N	5.182405	-9.384091	-3.163340
H	6.924087	-9.926131	1.609111
H	5.306461	-9.176681	1.487435
H	6.738025	-8.248020	1.024623
C	7.319034	-4.650691	2.031252
C	7.007068	-5.032614	0.596038
H	4.871994	-4.853863	0.834486
H	8.322985	-4.205599	2.081619
C	5.388871	-5.248654	-1.220115
H	4.364275	-5.195901	-1.572195
C	5.676451	-5.056613	0.135504
C	6.421324	-5.427387	-2.161475
C	7.751127	-5.420052	-1.699089
H	8.572300	-5.506994	-2.405336
C	8.038971	-5.225431	-0.342188
H	9.076990	-5.166072	-0.026456
C	6.108049	-5.470954	-3.646056
H	6.977880	-5.119773	-4.219415
H	5.269668	-4.810000	-3.866271
C	5.330748	-6.653106	-5.662557
H	6.159575	-6.203844	-6.223885
H	5.094307	-7.620630	-6.110473
H	4.458844	-6.005823	-5.730033
C	6.847166	-7.817683	-4.097780
H	7.575084	-7.655363	-4.903625
H	7.361591	-7.634709	-3.153449
C	6.305665	-9.240312	-4.153884
H	7.100326	-9.968718	-3.943220
H	5.905567	-9.471361	-5.144734
C	5.700230	-9.402688	-1.756159
H	6.349201	-10.276223	-1.607150
H	6.265296	-8.492239	-1.555401
H	4.863939	-9.447984	-1.058419
C	4.326930	-10.591041	-3.438063
H	4.205451	-10.675191	-4.520820
H	4.829316	-11.504280	-3.092057
C	2.982699	-10.416705	-2.746198
H	3.097146	-10.441059	-1.661723
H	2.303659	-11.233892	-3.022863
C	1.726252	-9.213435	-4.494573
H	0.915661	-9.951812	-4.453445
H	1.344916	-8.239929	-4.799745
H	2.463342	-9.548845	-5.227776
C	1.297435	-8.675440	-2.131677
H	0.498156	-9.428134	-2.187189
H	0.890769	-7.735241	-2.508529
C	1.745388	-8.519106	-0.690479
C	2.321991	-7.315291	-0.242867
H	2.481158	-6.509864	-0.951209
C	2.605209	-7.113719	1.112553
H	2.982610	-6.156048	1.454589
C	2.328882	-8.112797	2.065548
C	1.768961	-9.323835	1.616874
H	1.503823	-10.097682	2.332066
C	1.480660	-9.522667	0.260819

H	0.999018	-10.446895	-0.046324
C	2.485771	-7.828339	3.548173
H	1.819431	-8.486843	4.123304
H	2.200446	-6.797569	3.759297
H	6.605358	-3.902168	2.378746
N	7.275105	-5.768767	3.064283
N	6.479127	-8.486409	3.128049
C	7.594910	-5.167031	4.416756
C	8.282259	-6.845694	2.745760
H	7.624424	-5.949605	5.177266
H	8.575990	-4.677321	4.378386
H	6.822285	-4.454390	4.697544
N	3.884176	-7.992505	4.127693
H	9.285428	-6.521785	3.052651
H	8.301945	-6.984189	1.663956
C	7.906988	-8.140247	3.453505
C	3.852089	-7.590530	5.584453
H	8.578252	-8.956926	3.155422
H	7.984998	-8.032679	4.538696
H	3.112600	-8.196668	6.122860
H	4.831006	-7.750412	6.040240
C	4.365750	-9.415117	4.004764
H	3.911483	-10.035501	4.788801
H	4.027028	-9.805461	3.043616
C	5.885011	-9.462588	4.106929
H	6.257219	-10.477586	3.912160
H	6.222535	-9.177973	5.107090
C	6.355272	-8.993296	1.722201
H	3.596390	-6.537751	5.677090
Cu	5.384397	-6.721264	3.299006
Cu	-8.653088	0.416451	-3.386233
N	-8.772550	-1.536791	-4.213926
N	-9.060124	2.492251	-3.128804
N	-10.718064	0.203951	-3.163340
H	-12.058325	-1.033370	1.609111
H	-10.600470	-0.007189	1.487435
H	-10.512008	-1.711290	1.024623
C	-7.687134	-4.013124	2.031252
C	-7.861906	-3.551992	0.596038
H	-6.639566	-1.792339	0.834486
H	-7.803648	-5.105117	2.081619
C	-7.239903	-2.042572	-1.220115
H	-6.681920	-1.181623	-1.572195
C	-7.217381	-2.387644	0.135504
C	-7.910917	-2.847336	-2.161475
C	-8.569467	-4.002647	-1.699089
H	-9.055347	-4.670333	-2.405336
C	-8.544842	-4.349238	-0.342188
H	-9.012444	-5.277867	-0.026456
C	-7.792010	-2.554249	-3.646056
H	-7.922794	-3.483135	-4.219415
H	-6.800416	-2.158666	-3.866271
C	-8.427133	-1.290010	-5.662557
H	-8.452474	-2.232426	-6.223885
H	-9.146812	-0.601484	-6.110473
H	-7.430617	-0.858561	-5.730033

C	-10.193895	-2.020978	-4.097780
H	-10.417281	-2.732533	-4.903625
H	-10.292648	-2.557970	-3.153449
C	-11.155178	-0.840710	-4.153884
H	-12.183326	-1.164704	-3.943220
H	-11.155223	-0.378691	-5.144734
C	-10.993082	-0.235200	-1.756159
H	-12.074071	-0.360458	-1.607150
H	-10.487142	-1.179786	-1.555401
H	-10.614164	0.511697	-1.058419
C	-11.335576	1.548289	-3.438063
H	-11.347712	1.695568	-4.520820
H	-12.377656	1.569829	-3.092057
C	-10.512481	2.625260	-2.746198
H	-10.590795	2.538322	-1.661723
H	-10.880666	3.621919	-3.022863
C	-8.842195	3.111740	-4.494573
H	-9.076352	4.182921	-4.453445
H	-7.808445	2.955233	-4.799745
H	-9.501214	2.641106	-5.227776
C	-8.161869	3.214109	-2.131677
H	-8.414082	4.282652	-2.187189
H	-7.144300	3.096192	-2.508529
C	-8.250456	2.748002	-0.690479
C	-7.496224	1.646742	-0.242867
H	-6.878287	1.106186	-0.951209
C	-7.463266	1.300682	1.112553
H	-6.822599	0.495008	1.454589
C	-8.190329	2.039528	2.065548
C	-8.959158	3.129953	1.616874
H	-9.496761	3.746492	2.332066
C	-8.987201	3.479044	0.260819
H	-9.546786	4.358273	-0.046324
C	-8.022426	1.761428	3.548173
H	-8.259537	2.667748	4.123304
H	-6.987090	1.493142	3.759297
H	-6.682056	-3.769324	2.378746
N	-8.633451	-3.416043	3.064283
N	-10.589009	-1.367884	3.128049
C	-8.272236	-3.993869	4.416756
C	-10.069674	-3.749800	2.745760
H	-8.964722	-3.628143	5.177266
H	-8.338674	-5.088364	4.378386
H	-7.268758	-3.681077	4.697544
N	-8.863800	0.632457	4.127693
H	-10.290745	-4.780524	3.052651
H	-10.199457	-3.697601	1.663956
C	-11.003155	-2.777529	3.453505
C	-8.499637	0.459258	5.584453
H	-12.046051	-2.950521	3.155422
H	-10.949003	-2.898872	4.538696
H	-8.654823	1.402743	6.122860
H	-9.127556	-0.308568	6.040240
C	-10.336606	0.926708	4.004764
H	-10.646741	1.630307	4.788801
H	-10.505292	1.415222	3.043616

C	-11.137347	-0.365275	4.106929
H	-12.202465	-0.180118	3.912160
H	-11.059625	-0.799887	5.107090
C	-10.966059	-1.007179	1.722201
H	-7.460053	0.154311	5.677090
Cu	-8.512984	-1.302392	3.299006

E = -8616.72101189 a.u.

Table S8. Optimized xyz cartesian coordinates (Å) for structure **3b**.

Atom	X	Y	Z
C	0.000000	0.000000	-3.802465
C	-1.480732	0.005281	-3.818413
C	-2.241546	0.850539	-2.973165
C	-2.231167	-0.810466	-4.702095
C	-3.630113	0.905875	-3.041543
C	-3.622994	-0.761880	-4.737520
C	-4.360266	0.111574	-3.929254
C	-5.860586	0.322223	-4.128853
O	-6.672776	-0.421913	-3.388711
O	-6.221968	1.169030	-4.966627
Cl	-1.415455	1.863532	-1.729445
Cl	-1.399074	-1.863121	-5.904134
Cl	-4.548711	2.042954	-1.975685
Cl	-4.511155	-1.810132	-5.909721
C	0.735792	-1.284992	-3.818413
C	0.384184	-2.366505	-2.973165
C	1.817468	-1.527015	-4.702095
C	1.030546	-3.596708	-3.041543
C	2.471305	-2.756665	-4.737520
C	2.083507	-3.831888	-3.929254
C	2.651240	-5.236527	-4.128853
O	3.701775	-5.567837	-3.388711
O	2.098575	-5.972898	-4.966627
Cl	-0.906139	-2.157586	-1.729445
Cl	2.313047	-0.280073	-5.904134
Cl	0.505105	-4.960776	-1.975685
Cl	3.823198	-3.001709	-5.909721
C	0.744940	1.279710	-3.818413
C	1.857361	1.515966	-2.973165
C	0.413700	2.337481	-4.702095
C	2.599568	2.690833	-3.041543
C	1.151690	3.518545	-4.737520
C	2.276759	3.720314	-3.929254
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