European Journal of Inorganic Chemistry

Supporting Information

Theoretical Investigation of Hydrogen-Bond-Assisted Tetradentate N4 Copper(I) Chloride and *trans*-1,2-Peroxodicopper Complexes

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Table S1. The matched DFT optimized structures with reported X-ray crystal structures. All non-hydrogen atoms are used to calculate the RMSD (in Å), X-ray crystal structures are presented in green.

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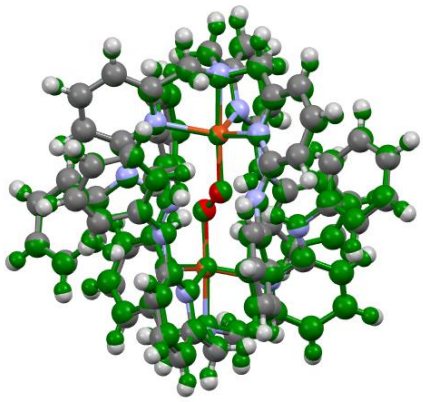
<td> 
9 [Cu₂-O₂]²⁺
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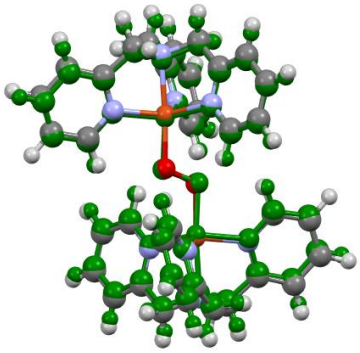
<td> 
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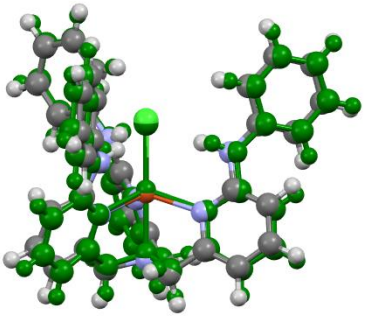
<td> 
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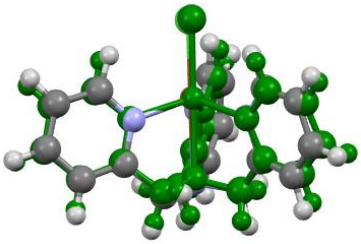
<td> 
1 [Cu^I-Cl]
RMSD = 0.2232
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Table S2. The calculated $\rho_{(BCP)}$ and CVB index of [Cu^{I}-Cl].

Parameter	**1**	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**
ρ(BCP)	0.0108	0.0397	0.0313	0.0320	0.0354	0.0313	0.0320	0.0329	0.0324
CVB	0.0478	-0.1135	-0.0542	-0.0642	-0.0821	-0.0544	-0.0573	-0.0628	-0.0602

Table S3. The calculated cone angles of [Cu^{I}]$^{+}$ and [Cu^{I}-Cl].

Cone Angle	**1**	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**
[Cu^{I}]$^{+}$	113.4	79.9	80.6	80.4	73.6	75.3	80.5	77.2	73.7
[Cu^{I}-Cl]	121.7	90.2	93.3	78.2	93.6	92.9	93.0	94.1	94.6

Table S4. The Cu-N and Cu-Cl bond distances of [Cu^{I}-Cl].

Bond	1	2	3	4	5	6	7	8	9
Cu-N	2.539	2.337	2.368	2.263	2.318	2.373	2.360	2.333	2.340
Cu-Cl	2.351	2.540	2.564	3.344	2.456	2.586	2.536	2.572	2.569

Table S5. The calculated APT, Mulliken and NBO charges charge of Cu atom in $[Cu^{I}]^{+}$.

[Cu^{I}-Cl]	1	2	3	4	5	6	7	8	9
APT	0.108	0.240	0.182	0.198	0.204	0.206	0.151	0.200	0.190
Mulliken	0.200	0.057	0.094	0.073	0.092	0.123	0.094	0.071	0.057
NBO	0.610	0.382	0.461	0.448	0.482	0.494	0.471	0.475	0.467

Table S6. The calculated APT, Mulliken and NBO charges charge of Cu atom in [Cu^{I}-Cl].

[Cu^{I}-Cl]	1	2	3	4	5	6	7	8	9
APT	0.095	0.351	0.371	0.286	0.393	0.382	0.321	0.387	0.384
Mulliken	0.241	0.257	0.337	0.231	0.309	0.332	0.331	0.334	0.331
NBO	0.516	0.498	0.543	0.582	0.522	0.543	0.548	0.547	0.545

ΔG^{1}_{RXN} = APT(–6.4198) + $\rho_{(BCP)}$(1506.5257) – 30.1145 **Eq. 1 (APT Charges)**

R^2 = 0.8611

ΔG^{1}_{RXN} = Mulliken(4.9284) + $\rho_{(BCP)}$(1531.7493) – 34.7802 **Eq. 1a (Mulliken Charges)**

R^2 = 0.8599

ΔG^{1}_{RXN} = NBO(11.7331) + $\rho_{(BCP)}$(1578.4976) – 41.1714 **Eq. 1b (NBO Charges)**

R^2 = 0.8596

ΔG^{2}_{RXN} = APT(–158.5495) + Vol(0.7968) + 1.9582 **Eq. 3**

R^2 = 0.7051

ΔG^{2}_{RXN} = Mulliken(132.9707) + Vol(0.1404) - 23.9108 **Eq. 3a (Mulliken Charges)**

R^2 = 0.3897

ΔG^{2}_{RXN} =NBO(115.9047) + Vol(1.3678) - 96.6186 **Eq. 3b (NBO Charges)**

R^2 = 0.5859

Scheme S1. The two-parameter fitting of the Gibbs reaction energies.
In Eq. 1, 1a and 1b, APT is APT charge of Cu atom in the [Cu^{I}-Cl], and $\rho_{(BCP)}$ is the electron densities of hydrogen bond critical points. In Eq. 3, 3a and 3b, APT is APT charge of Cu atom in the $[Cu^{I}]^{+}$, and Vol is the percentages of free volume (%V_{Free}) of $[Cu^{I}]^{+}$.

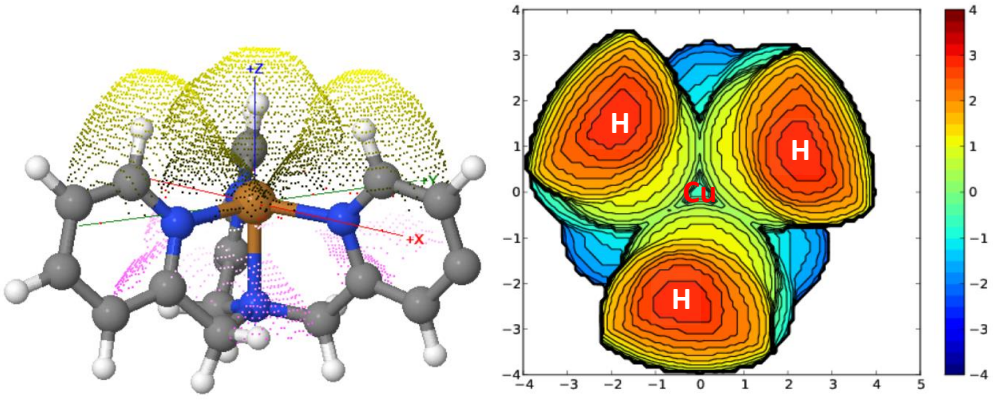
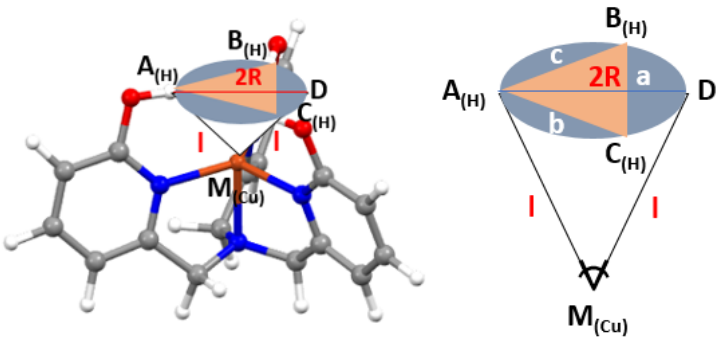


Figure S1. The representations of 3D and 2D steric maps.
Details on the calculation of percentage buried volume (%V_{Bur}) and the generation of steric map via SambVca (version 2.1): (1) Cu atom was coordinated to the center of the sphere, (2) H/H/H atoms were defined as the positive z axis, (3) N/N/N atoms of the coordinated pyridyl unit were defined as xz-plane, (4) Atomic Bondi radii were scaled by 1.17, (5) Sphere radius was set to 4.0 Å, (6) Mesh spacing for numerical integration was set to 0.10, (7) H atoms were included in the calculations, (8) Cl atom was removed in the calculation of Cu^1-Cl species.



(1) For an equilateral triangle (a = b = c), the radius of the circumcircle (R):

Radius $= \frac{\sqrt{3}\,a}{3} \approx 0.577a$

(2) The cosine of cone angle: $\cos(AMD) = \frac{l^2+l^2-(2R)^2}{2\times l\times l}$

(3) The cone angle = arccos(AMD)

Figure S2. The representation of calculation of cone angle.

Table S7. The calculated $\%V_{Free}$ and $\%V_{Buried}$ of $[Cu^{I}]^{+}$.
The calculated excluding hydrogen atoms are presented in parentheses.

Parameter	1	2	3	4	5	6	7	8	9
$\%V_{Free}$	35.0 (35.5)	27.3 (28.6)	26.0 (27.5)	25.8 (27.3)	24.1 (25.6)	26.0 (27.5)	26.1 (27.6)	21.1 (22.6)	21.6 (23.0)
$\%V_{Buried}$	65.0 (64.5)	72.7 (71.4)	74.0 (72.5)	74.2 (72.7)	75.9 (74.4)	74.0 (72.5)	73.9 (72.4)	78.9 (77.4)	78.4 (77.0)

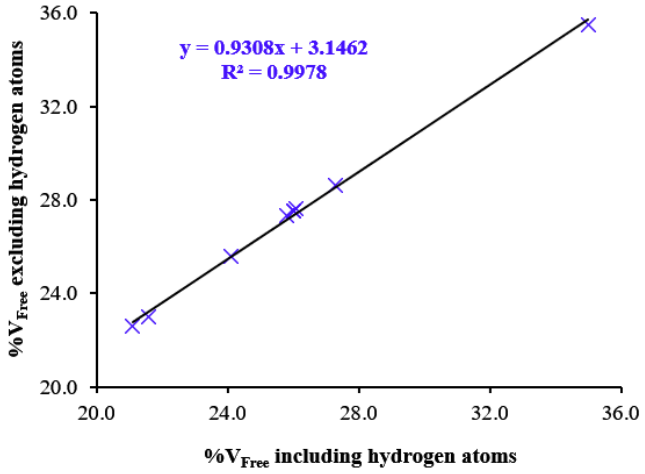


Figure S3. The linear relationship between the calculated $\%V_{Free}$ with and without hydrogen atoms.

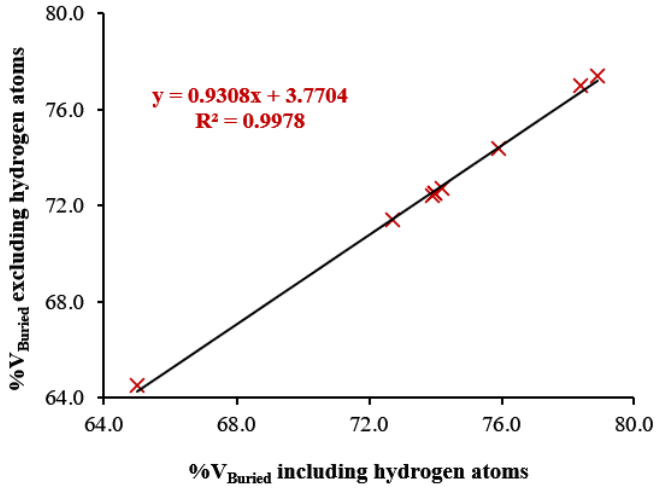
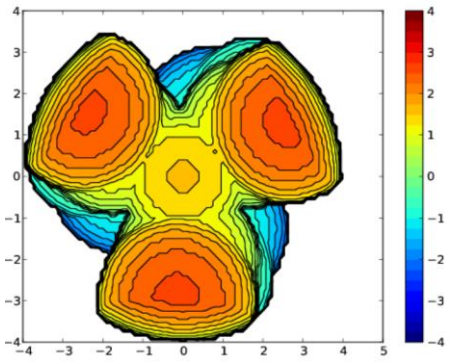
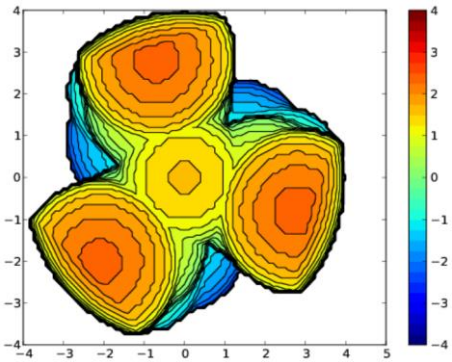
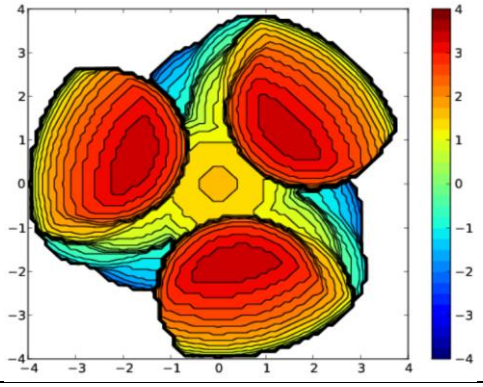
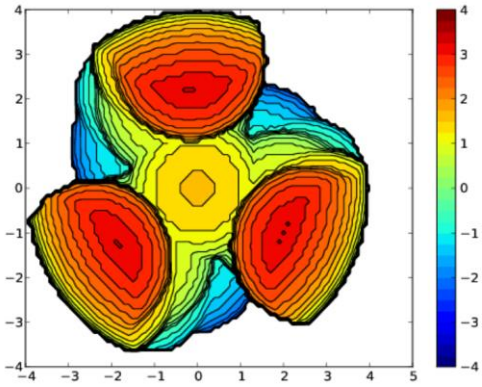
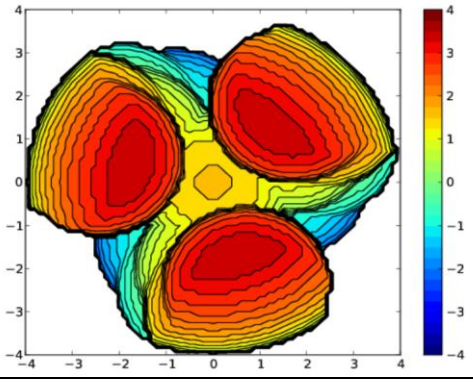
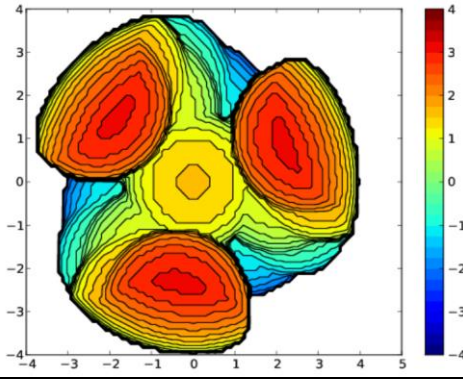
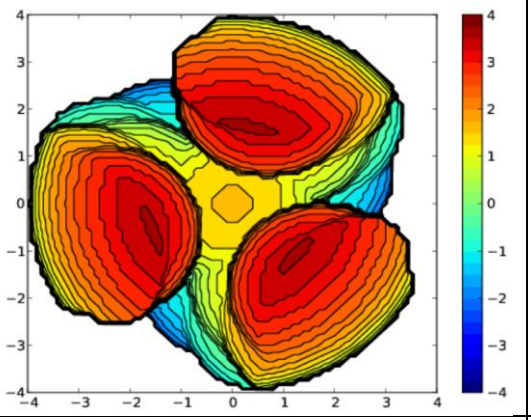


Figure S4. The linear relationship between the calculated $\%V_{Buried}$ with and without hydrogen atoms.

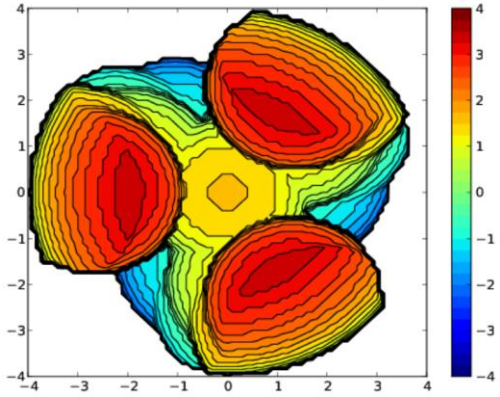
Table S8. The steric map of optimized $[Cu^{I}]^{+}$ and $[Cu^{I}$-Cl] without hydrogen atoms. Hydrogen atoms are excluded in the calculation of percentage buried volume ($\%V_{Bur}$), and X/X/X atoms (X= C or O or N, from the X-H···Cl hydrogen bond) were defined as the positive z axis.

1 $[Cu^{I}]^{+}$ **%V Free = 35.5** **%V Buried = 64.5** 	**1 $[Cu^{I}$-Cl]** **%V Free = 38.1** **%V Buried = 61.9** 
2 $[Cu^{I}]^{+}$ **%V Free = 28.6** **%V Buried = 71.4** 	**2 $[Cu^{I}$-Cl]** **%V Free = 32.4** **%V Buried = 67.6** 
3 $[Cu^{I}]^{+}$ **%V Free = 27.5** **%V Buried = 72.5** 	**3 $[Cu^{I}$-Cl]** **%V Free = 32.4** **%V Buried = 67.6** 

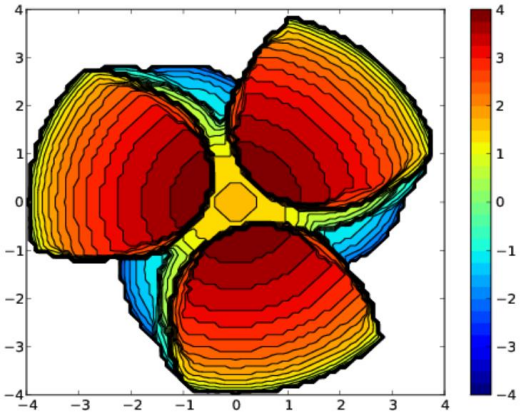
4 [Cu^{I}]$^{+}$
%V Free = 27.3
%V Buried = 72.7



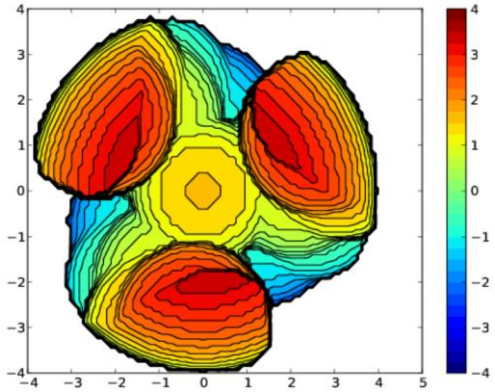
4 [Cu^{I}-Cl]
%V Free = 29.7
%V Buried = 70.3



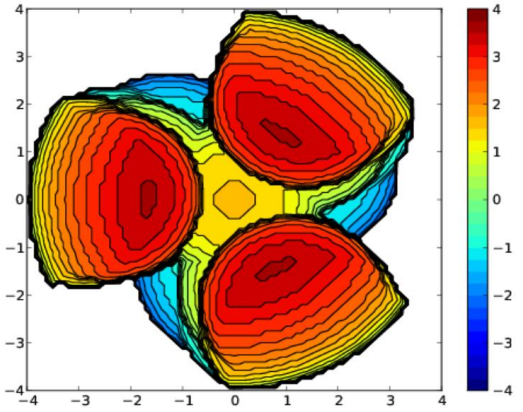
5 [Cu^{I}]$^{+}$
%V Free = 25.6
%V Buried = 74.4



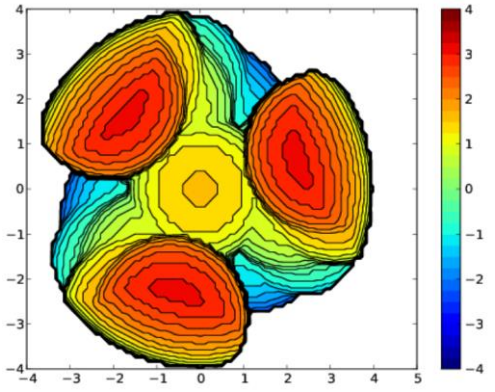
5 [Cu^{I}-Cl]
%V Free = 32.1
%V Buried = 67.9



6 [Cu^{I}]$^{+}$
%V Free = 27.5
%V Buried = 72.5



6 [Cu^{I}-Cl]
%V Free = 32.4
%V Buried = 67.6



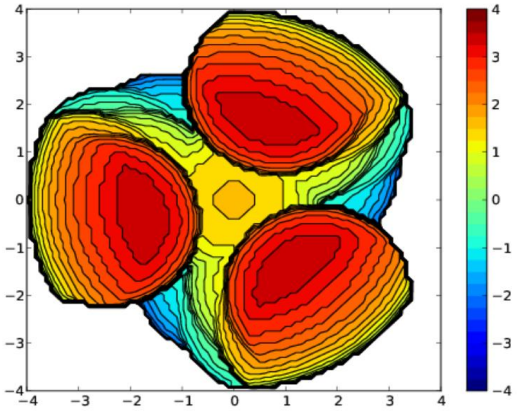
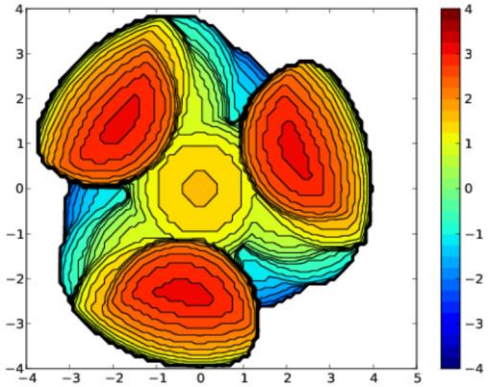
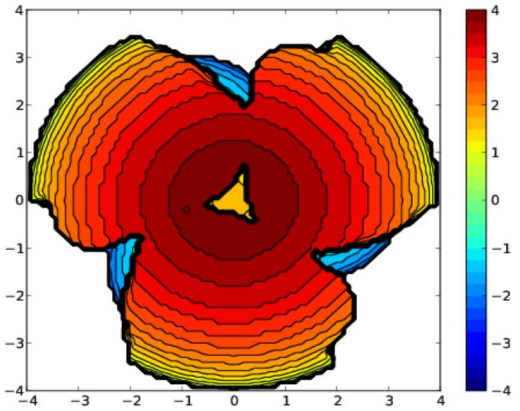
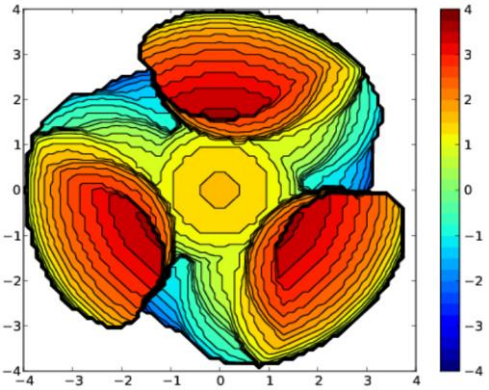
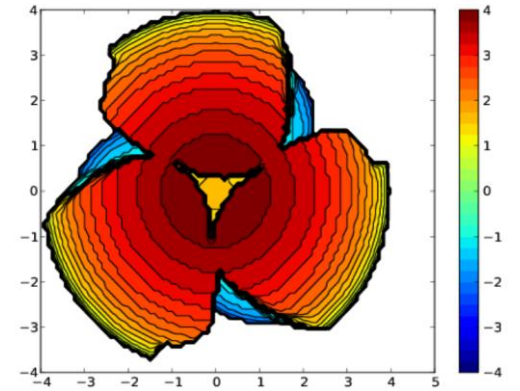
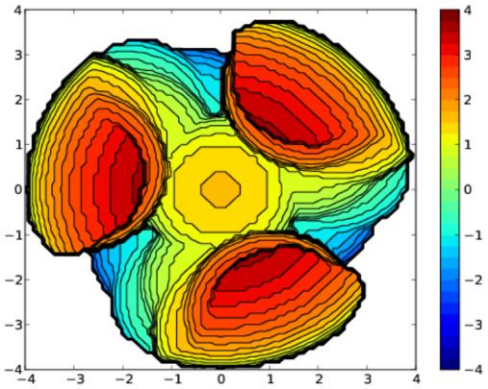
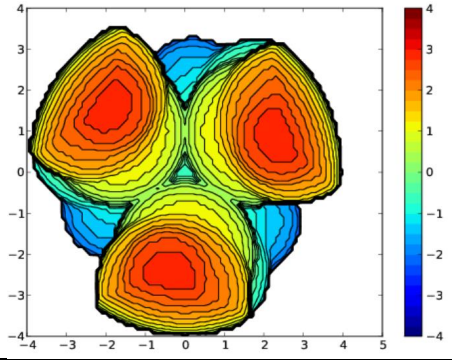
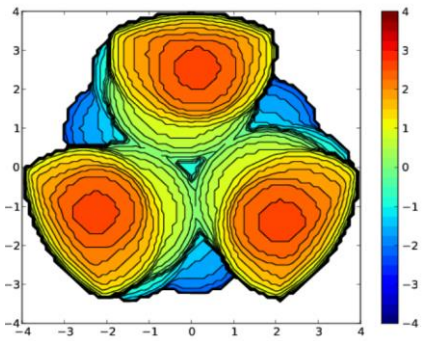
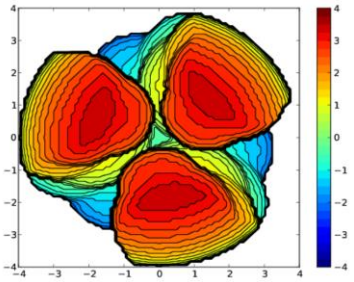
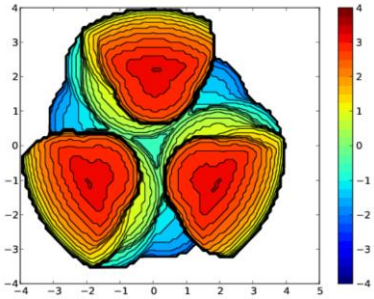
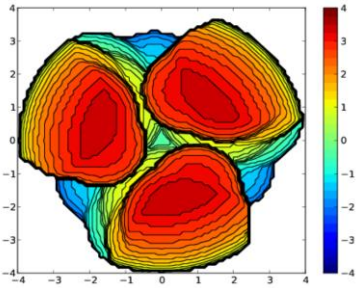
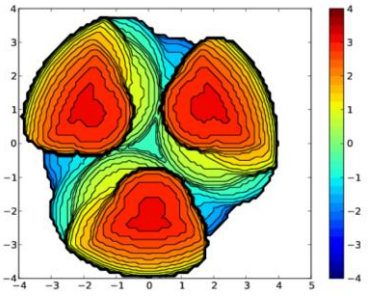
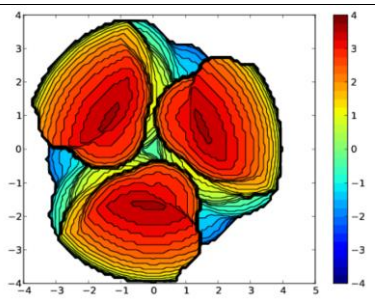
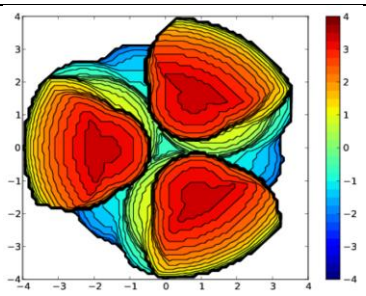
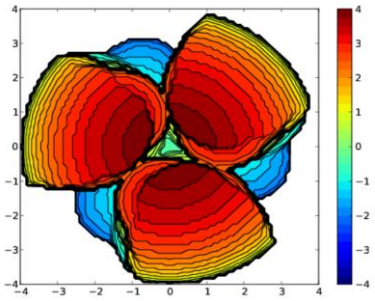
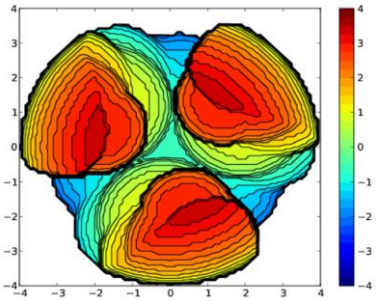
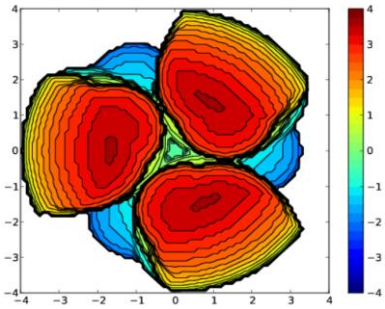
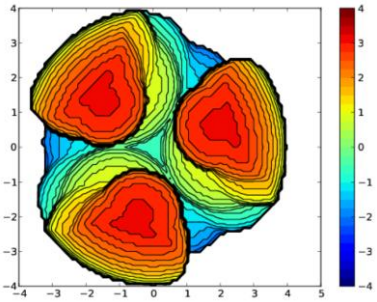
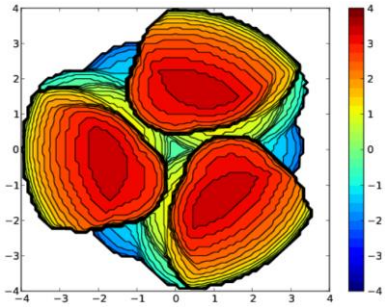
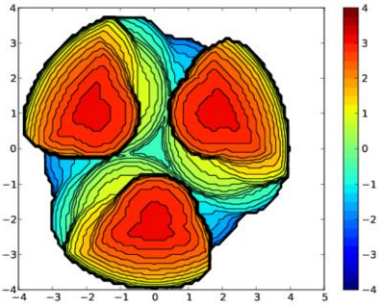
7 [Cu^{I}]$^{+}$ **%V Free = 27.6** **%V Buried = 72.4** 	**7 [Cu^{I}-Cl]** **%V Free = 32.4** **%V Buried = 67.6** 
8 [Cu^{I}]$^{+}$ **%V Free = 22.6** **%V Buried = 77.4** 	**8 [Cu^{I}-Cl]** **%V Free = 31.3** **%V Buried = 68.7** 
9 [Cu^{I}]$^{+}$ **%V Free = 23.0** **%V Buried = 77.0** 	**9 [Cu^{I}-Cl]** **%V Free = 31.5** **%V Buried = 68.5** 

Table S9. The steric map of optimized $[Cu^{I}]^{+}$ and $[Cu^{I}$-Cl] with hydrogen atoms.

1 $[Cu^{I}]^{+}$ **%V Free = 35.0** **%V Buried = 65.0** 	**1 $[Cu^{I}$-Cl]** **%V Free = 38.0** **%V Buried = 62.0** 
2 $[Cu^{I}]^{+}$ **%V Free = 27.3** **%V Buried = 72.7** 	**2 $[Cu^{I}$-Cl]** **%V Free = 31.6** **%V Buried = 68.4** 
3 $[Cu^{I}]^{+}$ **%V Free = 26.0** **%V Buried = 74.0** 	**3 $[Cu^{I}$-Cl]** **%V Free = 31.8** **%V Buried = 68.2** 
4 $[Cu^{I}]^{+}$ **%V Free = 25.8** **%V Buried = 74.2**	**4 $[Cu^{I}$-Cl]** **%V Free = 28.5** **%V Buried = 71.5**

	
5 [Cu^{I}]$^{+}$ **%V Free = 24.1** **%V Buried = 75.9** 	**5 [Cu^{I}-Cl]** **%V Free = 31.7** **%V Buried = 68.3** 
6 [Cu^{I}]$^{+}$ **%V Free = 26.0** **%V Buried = 74.0** 	**6 [Cu^{I}-Cl]** **%V Free = 31.7** **%V Buried = 68.3** 
7 [Cu^{I}]$^{+}$ **%V Free = 26.1** **%V Buried = 73.9** 	**7 [Cu^{I}-Cl]** **%V Free = 31.9** **%V Buried = 68.1** 
8 [Cu^{I}]$^{+}$ **%V Free = 21.1**	**8 [Cu^{I}-Cl]** **%V Free = 30.7**

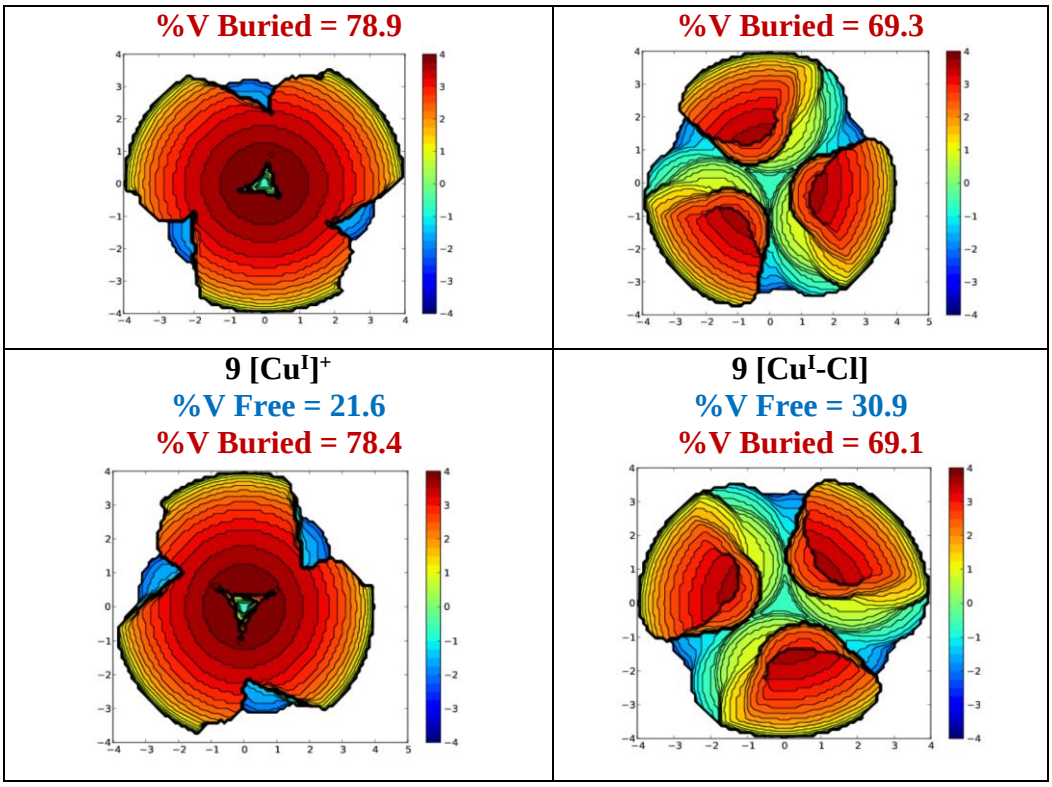
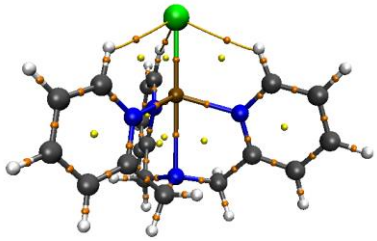
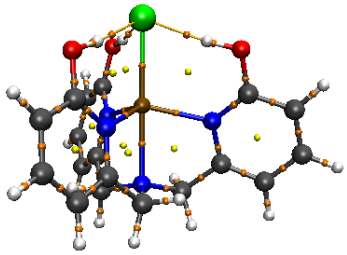
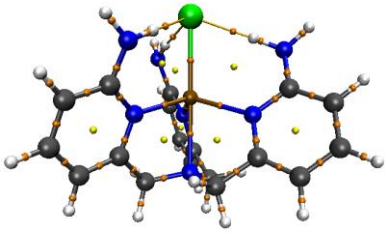
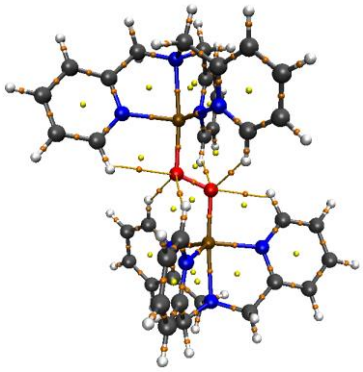
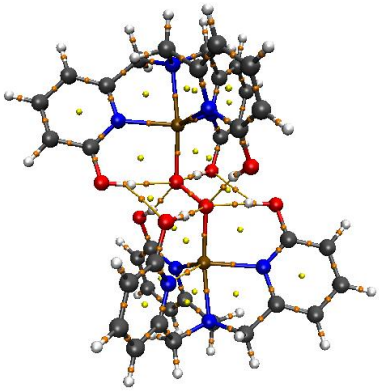
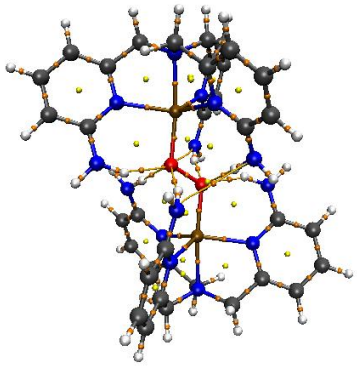
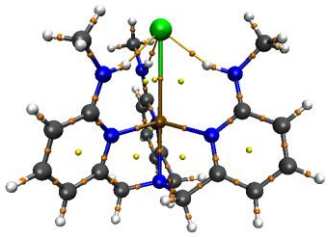
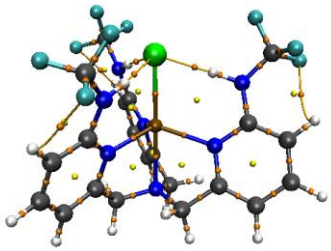
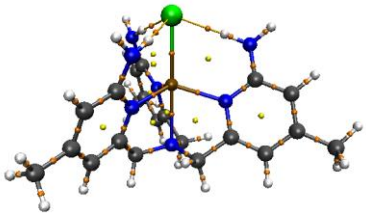
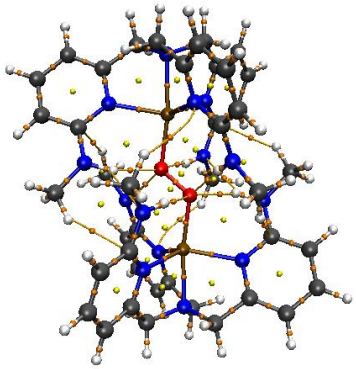
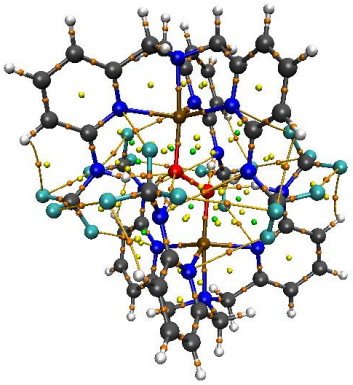
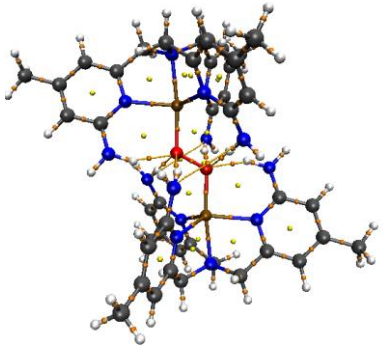
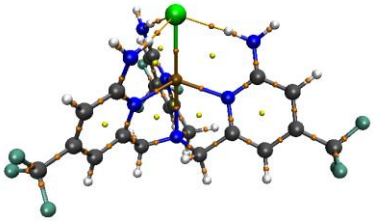
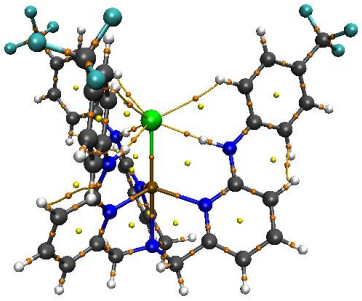
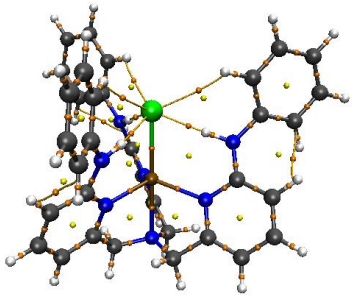


Table S10. The AIM (Atoms-In-Molecules) analysis of the optimized structures.
The orange balls represent the BCP (bond critical point), the yellow balls represent ring critical point (RCP), and the bond paths fo hydrogen bonds are shown in orange.

1 [Cu^{I}-Cl]	2 [Cu^{I}-Cl]	3 [Cu^{I}-Cl]
		

1 [Cu_2-O_2]$^{2+}$	**2 [Cu_2-O_2]$^{2+}$**	**3 [Cu_2-O_2]$^{2+}$**
		
4 [Cu^I-Cl]	**5 [Cu^I-Cl]**	**6 [Cu^I-Cl]**
		
4 [Cu_2-O_2]$^{2+}$	**5 [Cu_2-O_2]$^{2+}$**	**6 [Cu_2-O_2]$^{2+}$**
		
7 [Cu^I-Cl]	**8 [Cu^I-Cl]**	**9 [Cu^I-Cl]**
		
7 [Cu_2-O_2]$^{2+}$	**8 [Cu_2-O_2]$^{2+}$**	**9 [Cu_2-O_2]$^{2+}$**

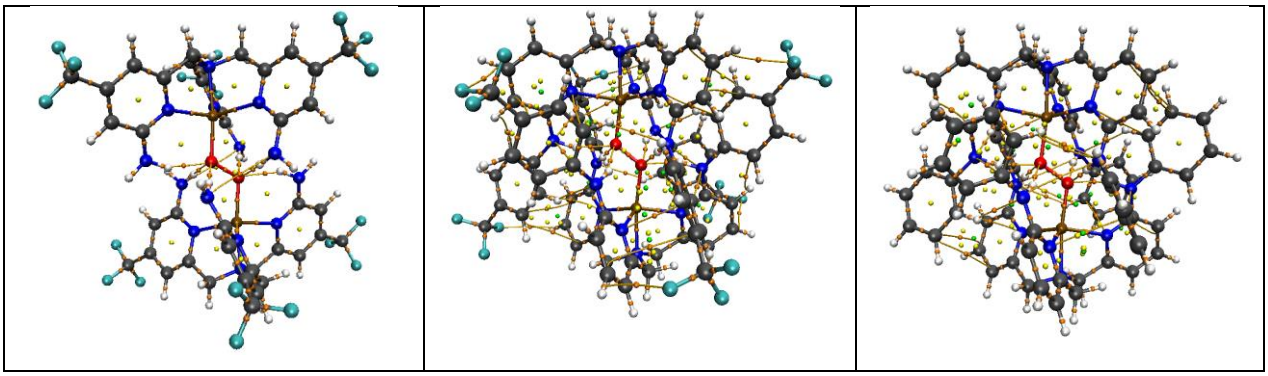
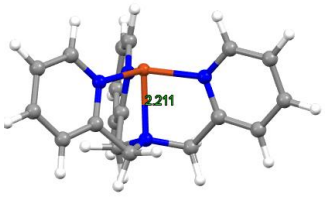
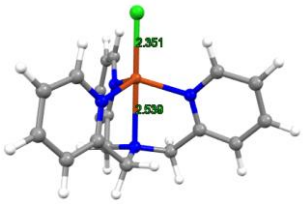
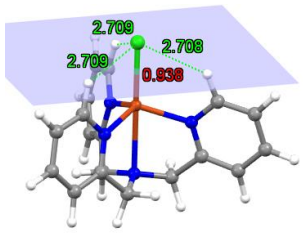
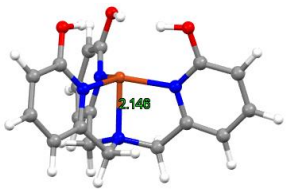
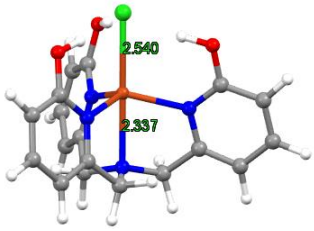
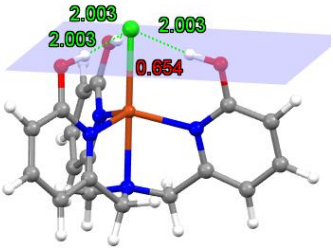
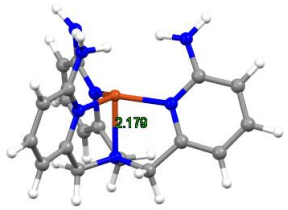
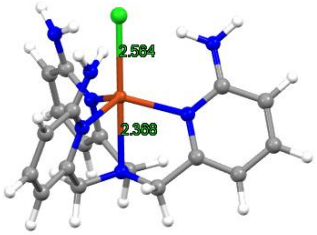
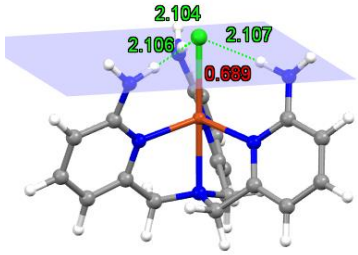
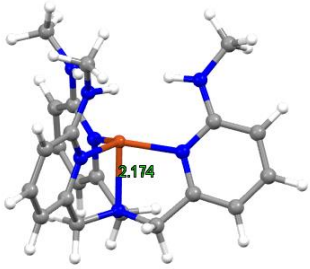
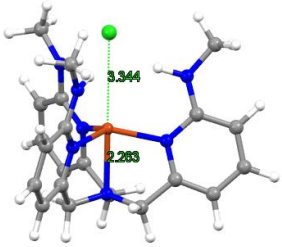
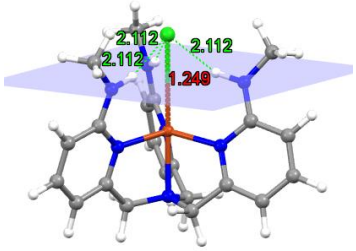
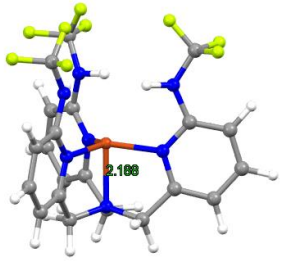
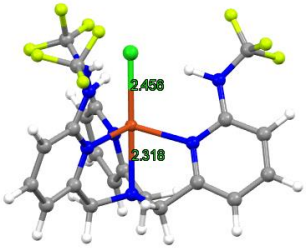
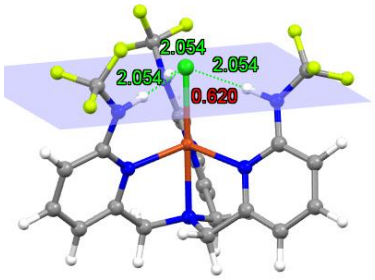
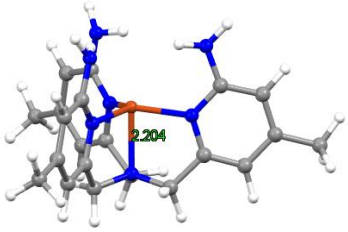
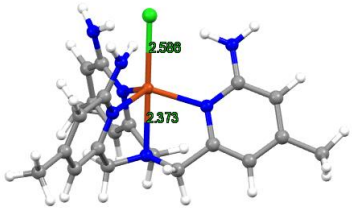
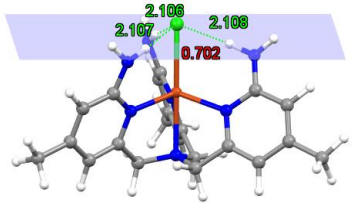
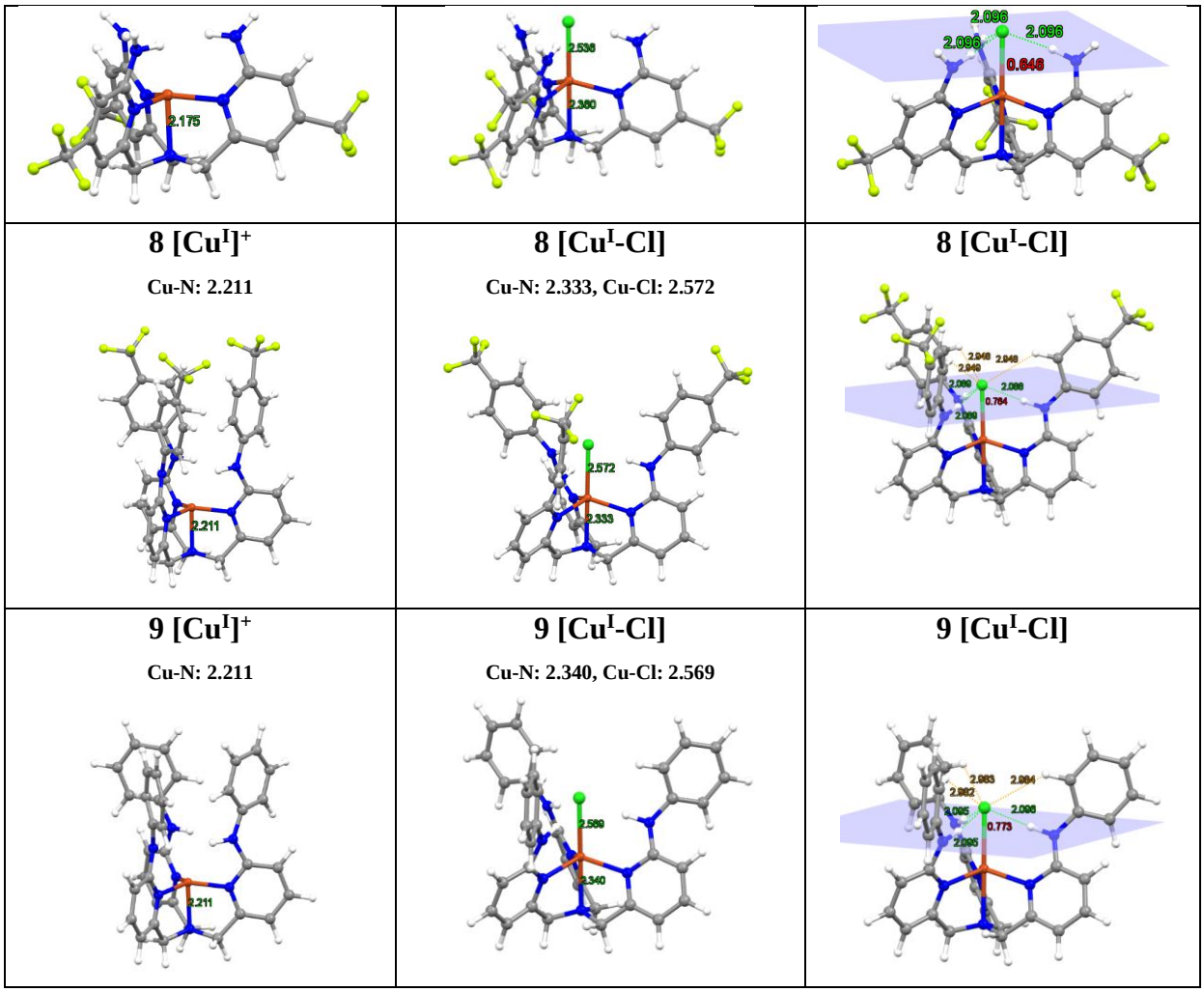


Table S11. Selected geometric parameters for the optimized structures.
"1 **[Cu^{I}]$^{+}$** "represents the Cu^{1+} of complex 1, and "1 **[Cu^{I}-Cl]**" represents the Cu^{1}-Cl of complex 1. The bond distances in green are given in Å, the Cl off plane (Cl-HHH) in red are given in Å, and the plane of HHH are shown in blue violet. Color codes for 3D structures: brown, Cu; blue N; gray, C; white, H; red, O; green, Cl; lime, F.

1 [Cu^{I}]$^{+}$ **Cu-N: 2.211** 	**1 [Cu^{I}-Cl]** **Cu-N: 2.539, Cu-Cl: 2.351** 	**1 [Cu^{I}-Cl]** 
2 [Cu^{I}]$^{+}$ **Cu-N: 2.146** 	**2 [Cu^{I}-Cl]** **Cu-N: 2.337, Cu-Cl: 2.540** 	**2 [Cu^{I}-Cl]** 
3 [Cu^{I}]$^{+}$ **Cu-N: 2.179**	**3 [Cu^{I}-Cl]** **Cu-N: 2.368, Cu-Cl: 2.564**	**3 [Cu^{I}-Cl]**

		
4 [Cu^{I}]$^{+}$ **Cu-N: 2.174** 	**4 [Cu^{I}-Cl]** **Cu-N: 2.263, Cu-Cl: 3.344** 	**4 [Cu^{I}-Cl]** 
5 [Cu^{I}]$^{+}$ **Cu-N: 2.188** 	**5 [Cu^{I}-Cl]** **Cu-N: 2.318, Cu-Cl: 2.456** 	**5 [Cu^{I}-Cl]** 
6 [Cu^{I}]$^{+}$ **Cu-N: 2.204** 	**6 [Cu^{I}-Cl]** **Cu-N: 2.373, Cu-Cl: 2.586** 	**6 [Cu^{I}-Cl]** 
7 [Cu^{I}]$^{+}$ **Cu-N: 2.175**	**7 [Cu^{I}-Cl]** **Cu-N: 2.360, Cu-Cl: 2.536**	**7 [Cu^{I}-Cl]**



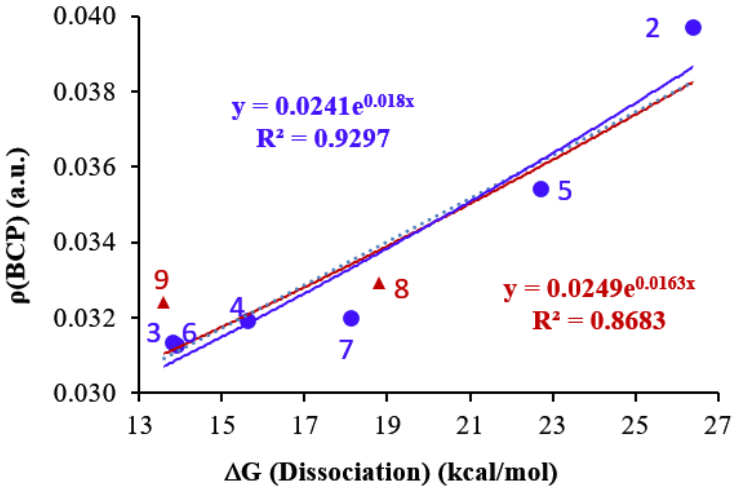


Figure S5. The curve fitting between $\rho_{(BCP)}$ and Gibbs energy of Cl^- dissociation of Cu^I(L)-Cl. Values from complex **1** are excluded due to its non-hydrogen bond.

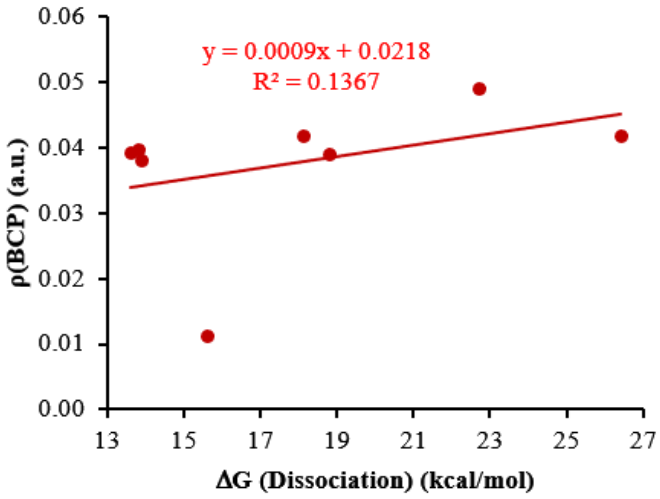


Figure S6. The fitting between electron density of Cu-Cl bond critical points $\rho_{(BCP)}$ and ΔG^{1}_{RXN} of [Cu^{I}-Cl].
Values from complex **1** are excluded due to its non-hydrogen bond.

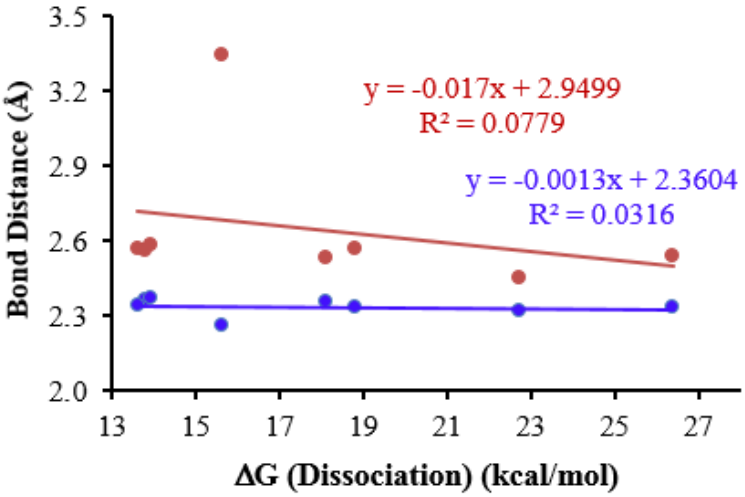


Figure S7. The fitting between bond distances and ΔG^{1}_{RXN} of [Cu^{I}-Cl].
The blue line and blue equation represent the Cu-N bond distances, and the red line and red equation represent the Cu-Cl bond distances. Values from complex 1 are excluded due to its non-hydrogen bond.

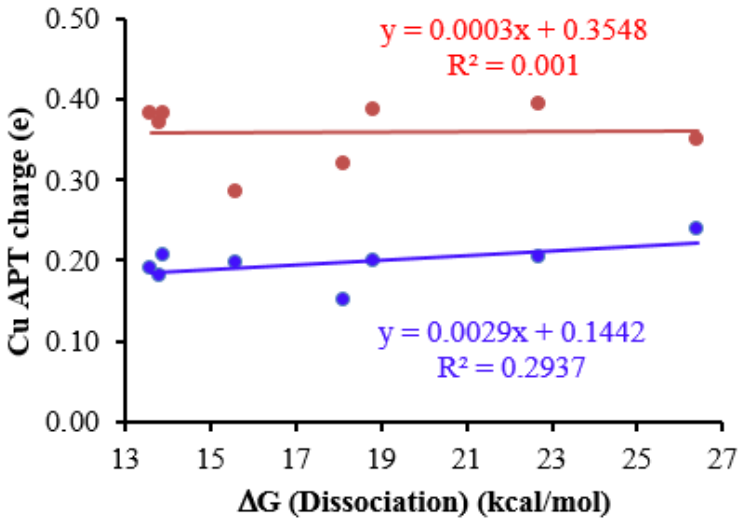


Figure S8. The fitting between APT charge of Cu atoms and ΔG^{1}_{RXN} of [Cu^{I}-Cl].
The blue line and blue equation represent the APT charge of Cu atom in Cu1+, and the red line and red equation represent the APT charge of Cu atom in Cu1-Cl. Values from complex 1 are excluded due to its non-hydrogen bond.

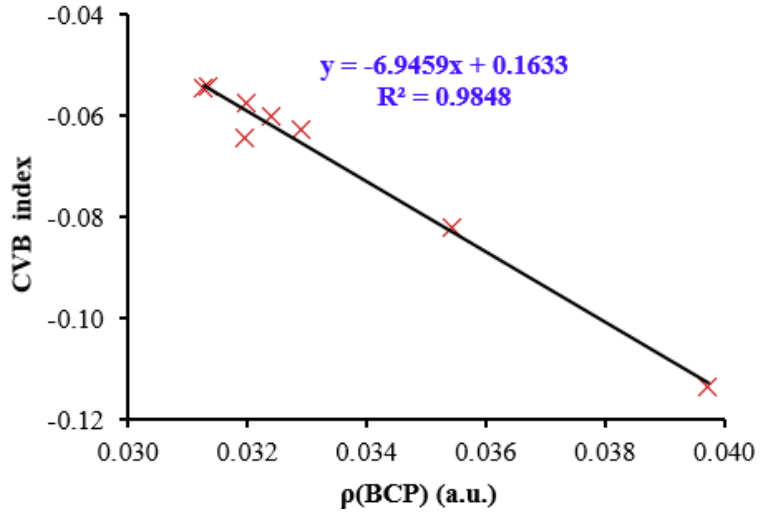


Figure S9. The linear relationship between ρ(BCP) and CVB index of [Cu^{I}-Cl].
Values from complex **1** are excluded due to its non-hydrogen bond.

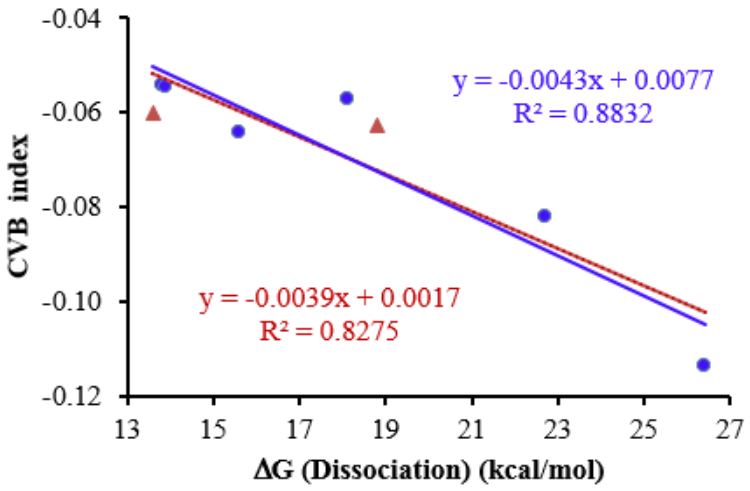


Figure S10. The linear relationship between CVB index and ΔG^{1}_{RXN} of [Cu^{I}-Cl].
The blue line and blue equation represent the values from structures 2 to 7, and the red line and red equation represent the values from structures 2 to 9. The two red triangles represent the values from structures 8 and 9. Values from complex 1 are excluded due to its non-hydrogen bond.

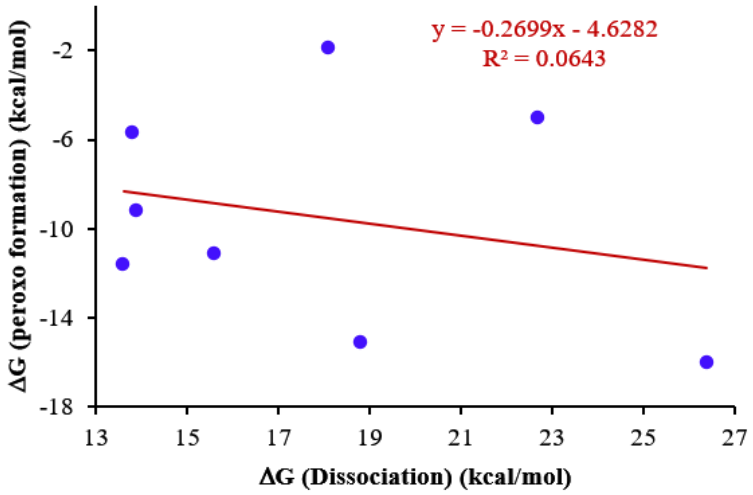


Figure S11. The fitting between ΔG^{1}_{RXN} of [Cu^{I}-Cl] and ΔG^{2}_{RXN} of $[Cu^{I}]^{+}$.
Values from complex 1 are excluded due to its non-hydrogen bond.

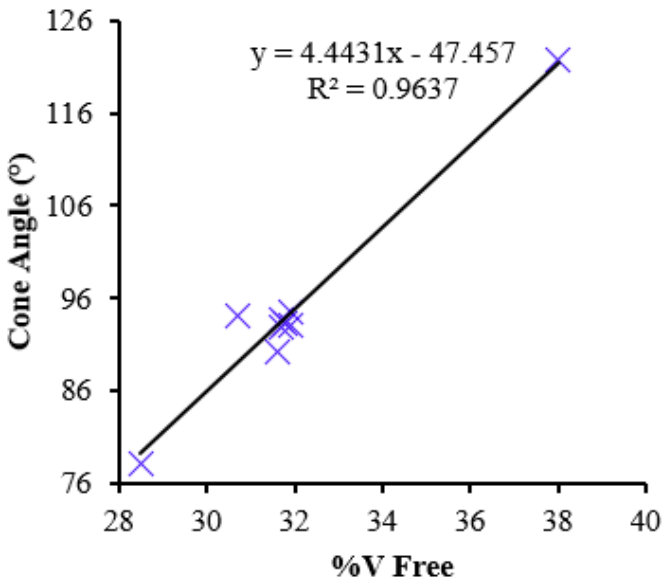


Figure S12. The linear relationship between calculated cone angles and percentages of free volume of [Cu^{I}-Cl].

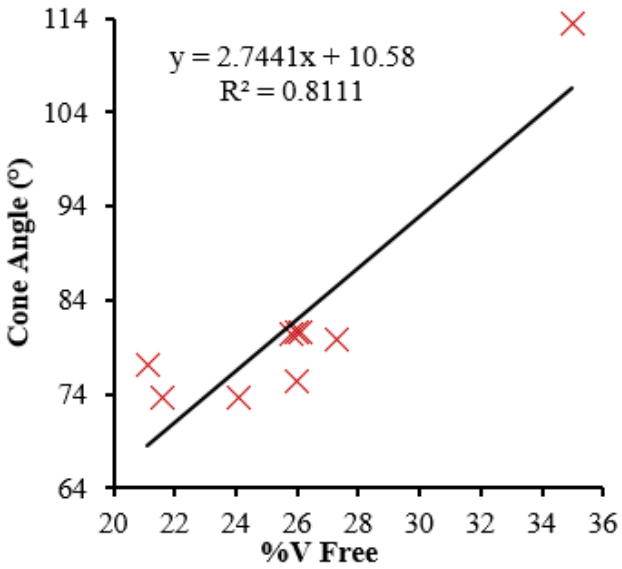


Figure S13. The linear relationship between calculated cone angles and percentages of free volume of $[Cu^{I}]^{+}$**.**

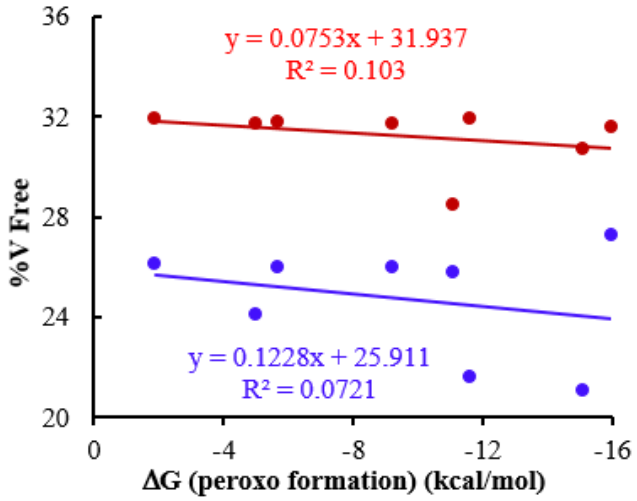


Figure S14. The fitting between percentages of free volume and ΔG^2_{RXN} of $[Cu^I]^+$.
The blue line and blue equation represent the values from **$[Cu^I]^+$**, and the red line and red equation represent the values from **$[Cu^I\text{-}Cl]$**. Values from complex 1 are excluded due to its non-hydrogen bond.

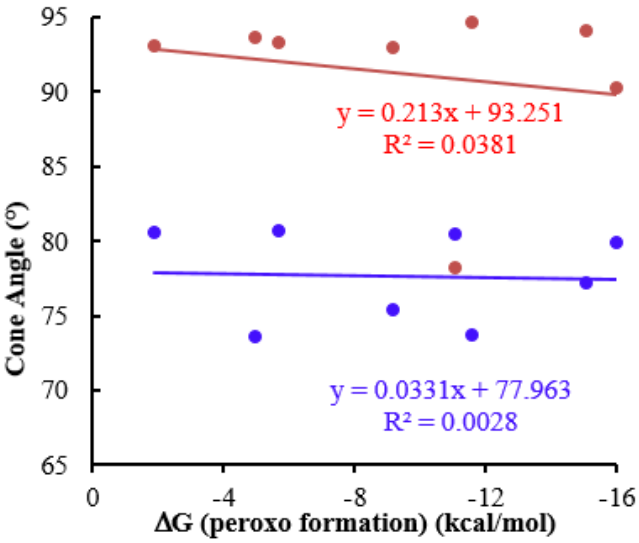


Figure S15. The fitting between calculated cone angles and ΔG^2_{RXN} of $[Cu^I]^+$.
The blue line and blue equation represent the values from **$[Cu^I]^+$**, and the red line and red equation represent the values from **$[Cu^I\text{-}Cl]$**. Values from complex 1 are excluded due to its non-hydrogen bond.

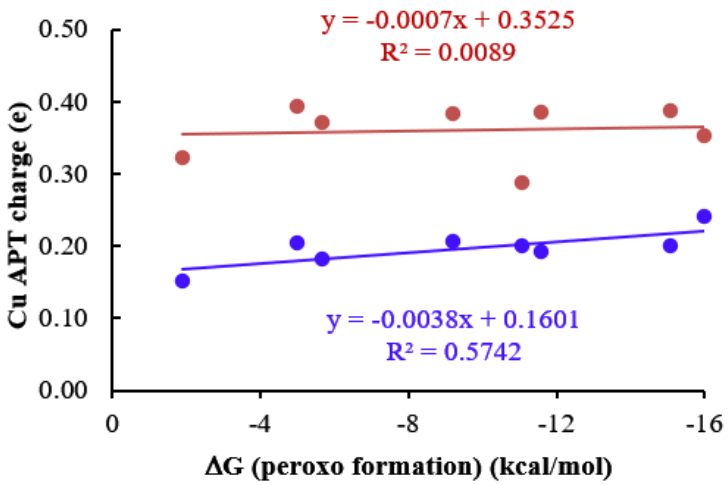


Figure S16. The fitting between APT charge of Cu atoms and ΔG^2_{RXN} of $[Cu^I]^+$.
The blue line and blue equation represent the APT charge of Cu atom in **$[Cu^I]^+$**, and the red line and red equation represent the APT charge of Cu atom in **$[Cu^I$-Cl$]$**. Values from complex 1 are excluded due to its non-hydrogen bond.

Scheme S2. The Cu-O and O-O bond distances of *trans*-1,2-peroxodicopper complex $[Cu_2$-$O_2]^{2+}$.
Bond distances are given in Å.

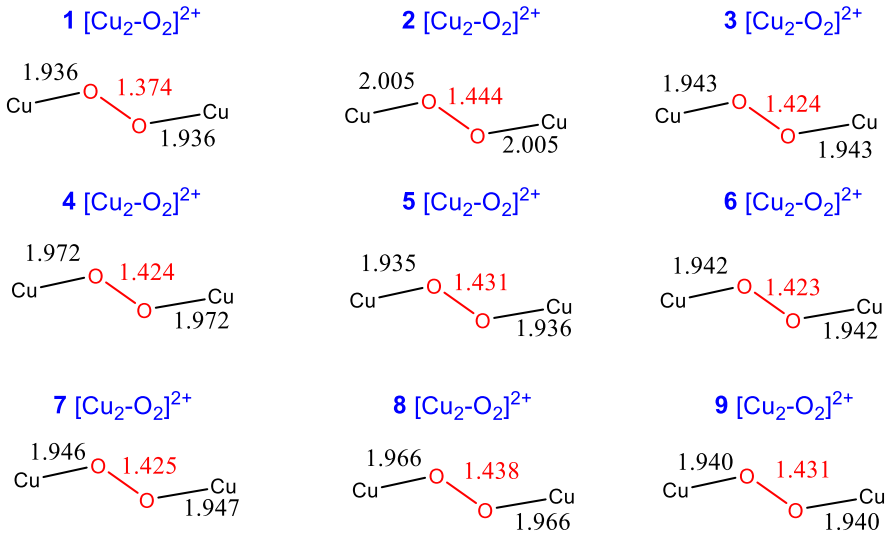


Table S12. DFT computed energies for species in **Scheme 2** at 1 atm and 298.15 K. Energies are given in Hartrees.

Species	**E** (PBEPBE-D3BJ/ Def-TZVP)	**G** (PBEPBE-D3BJ/ Def-TZVP)	**E_{soln}** (SMD-PBEPBE-D3BJ/ Def2-TZVP)
Cl^-	-460.077762	-460.092785	-460.178244
O_2	-150.241832	-150.258322	-150.249365
1 $[Cu^I]^+$	-2555.122324	-2554.847904	-2555.240171
1 $[Cu^I$-Cl]	-3015.364938	-3015.096082	-3015.447324
1 $[Cu_2$-$O_2]^{2+}$	-5260.488522	-5259.915746	-5260.772904
2 $[Cu^I]^+$	-2780.706961	-2780.423914	-2780.849165
2 $[Cu^I$-Cl]	-3240.992628	-3240.713233	-3241.080783
2 $[Cu_2$-$O_2]^{2+}$	-5711.693247	-5711.094795	-5712.011856
3 $[Cu^I]^+$	-2721.128990	-2720.809713	-2721.265696
3 $[Cu^I$-Cl]	-3181.384542	-3181.070034	-3181.476181
3 $[Cu_2$-$O_2]^{2+}$	-5592.509064	-5591.839965	-5592.827065
4 $[Cu^I]^+$	-2838.922217	-2838.527807	-2839.060677
4 $[Cu^I$-Cl]	-3299.179531	-3298.788430	-3299.275529
4 $[Cu_2$-$O_2]^{2+}$	-5828.110728	-5827.288852	-5828.427513
5 $[Cu^I]^+$	-3731.710965	-3731.398508	-3731.894927
5 $[Cu^I$-Cl]	-4191.991719	-4191.683444	-4192.120210
5 $[Cu_2$-$O_2]^{2+}$	-7613.690970	-7613.023900	-7614.093310
6 $[Cu^I]^+$	-2838.965403	-2838.575677	-2839.104014
6 $[Cu^I$-Cl]	-3299.217793	-3298.832016	-3299.315456
6 $[Cu_2$-$O_2]^{2+}$	-5828.192570	-5827.379935	-5828.511151
7 $[Cu^I]^+$	-3731.730371	-3731.420542	-3731.919689
7 $[Cu^I$-Cl]	-4192.006813	-4191.701836	-4192.136870
7 $[Cu_2$-$O_2]^{2+}$	-7613.699075	-7613.048838	-7614.128887
8 $[Cu^I]^+$	-4424.256168	-4423.728443	-4424.480983
8 $[Cu^I$-Cl]	-4884.523332	-4884.003259	-4884.696523
8 $[Cu_2$-$O_2]^{2+}$	-8998.802738	-8997.706269	-8999.280711
9 $[Cu^I]^+$	-3413.639420	-3413.108077	-3413.815621
9 $[Cu^I$-Cl]	-3873.893641	-3873.365952	-3874.026898
9 $[Cu_2$-$O_2]^{2+}$	-6977.571835	-6976.464361	-6977.947440

Table S13. Cartesian coordinates and absolute energies of the species in **Scheme 2**. Energies are given in Hartrees.

```
1
Cl-anion
el energy= -460.077761898
Cl    0.000000  0.000000  0.000000

2
O2
el energy= -150.241832165
O     0.000000  0.000000  0.611232
O     0.000000  0.000000 -0.611232

41
1 Cu1
el energy= -2555.12232423
```

```
Cu    0.000955 -0.000602 -0.809389
N    -1.332815 -1.476201 -0.577145
N     0.001547 -0.000482  1.401274
N    -0.612900  1.891567 -0.577748
N     1.946391 -0.414910 -0.577718
C    -2.530831 -3.479080 -1.175966
H    -2.833630 -4.174362 -1.958869
C    -1.711063 -1.655015  0.716777
C     0.155062  1.420872  1.709257
H     1.230748  1.654160  1.637419
H    -0.157598  1.676031  2.739674
C    -1.305577 -0.578347  1.711039
H    -2.045408  0.236896  1.642800
H    -1.367908 -0.978739  2.740805
C     1.155883 -0.843636  1.709759
H     0.820207 -1.892006  1.639557
H     1.533694 -0.699015  2.739802
C    -0.577894  2.308807  0.716105
C     2.290885 -0.654146  0.715828
C    -1.742057 -2.377622 -1.495959
H    -1.416786 -2.196935 -2.521300
C    -2.908073 -3.671003  0.153138
H    -3.516349 -4.528635  0.442972
C     3.622511 -0.780512  1.107815
H     3.860457 -0.959292  2.157749
C     2.931420 -0.315775 -1.496521
H     2.611977 -0.123772 -2.521637
C    -1.192453  2.695026 -1.495764
H    -1.199141  2.322934 -2.521082
C    -2.487459 -2.744134  1.109025
H    -2.760188 -2.861020  2.159218
C    -1.754864  3.927367 -1.175025
H    -2.208478  4.535920 -1.957289
C    -1.135495  3.524315  1.109070
H    -1.099582  3.819146  2.159181
C     4.279919 -0.446360 -1.176779
H     5.033255 -0.358633 -1.959614
C     4.635248 -0.678449  0.151957
H     5.682298 -0.775222  0.441533
C    -1.731581  4.350273  0.153968
H    -2.172324  5.304713  0.444357

42
1 Cu1-Cl
el energy= -3015.36493829
Cu   -0.000041 -0.000582  0.771609
N    -0.288449  1.953018  0.238660
N     0.000041 -0.000998 -1.767384
N    -1.548430 -1.226557  0.238903
N     1.836330 -0.727536  0.238092
C    -0.057702  4.269656  0.837406
H     0.104532  5.011272  1.620593
C    -0.468927  2.315191 -1.051875
C    -0.651529 -1.266925 -2.035053
H     0.111135 -2.055724 -1.919392
H    -1.041169 -1.352501 -3.072428
C    -0.770689  1.195973 -2.035367
H    -1.835026  0.929534 -1.919534
H    -0.650043  1.576072 -3.072779
C     1.421789  0.067676 -2.036385
H     1.723349  1.122853 -1.922773
H     1.689848 -0.228653 -3.073482
C    -1.771885 -1.564329 -1.051559
C     2.240788 -0.751922 -1.052219
C    -0.092972  2.915612  1.163751
H     0.033818  2.540205  2.185184
C    -0.224197  4.647596 -0.496966
H    -0.189897  5.698398 -0.789805
C     3.380874 -1.449277 -1.453335
H     3.666602 -1.457678 -2.507670
C     2.572506 -1.377356  1.163539
H     2.183147 -1.300195  2.184720
C    -2.480542 -1.536771  1.163839
H    -2.218964 -1.238757  2.185163
C    -0.433188  3.650969 -1.453526
H    -0.568218  3.902321 -2.508001
C    -3.671398 -2.182212  0.837512
H    -4.395306 -2.411174  1.620599
C    -2.947096 -2.200312 -1.453170
H    -3.097249 -2.443347 -2.507551
C     3.728558 -2.083437  0.837753
H     4.289848 -2.594236  1.621165
C     4.139930 -2.127527 -0.496406
H     5.033711 -2.681410 -0.788802
C    -3.915291 -2.516141 -0.496692
H    -4.842843 -3.011131 -0.789527
Cl    0.000781 -0.000778  3.123075

84
1 Cu2O2
el energy= -5260.48852236
Cu   -2.291059  0.039315 -0.015572
O    -0.421502  0.534060 -0.097010
N    -4.425835 -0.338597  0.010580
N    -2.449511 -0.983323  1.787808
N    -2.947689  1.954979 -0.154659
N    -2.422829 -1.251953 -1.634840
C    -1.443524 -1.571768  2.459952
C    -1.661391 -2.315073  3.618675
C    -2.968815 -2.464591  4.085124
C    -4.013927 -1.864946  3.378613
C    -3.717984 -1.123670  2.234967
C    -4.778866 -0.389626  1.441908
C    -2.198898  3.051207  0.066142
C    -2.744164  4.332625  0.065331
C    -4.114929  4.478976 -0.157279
C    -4.891551  3.340124 -0.381663
C    -4.274889  2.089638 -0.382376
C    -5.018107  0.810309 -0.698809
C    -1.460648 -1.451360 -2.554041
C    -1.680527 -2.201449 -3.707361
C    -2.946938 -2.750306 -3.919736
C    -3.943635 -2.547552 -2.962812
C    -3.643524 -1.799955 -1.823881
```

```
C    -4.628632 -1.621928 -0.687051
H    -0.450527 -1.429175  2.021496
H    -0.820804 -2.774933  4.138576
H    -3.175848 -3.047743  4.983556
H    -5.048008 -1.971649  3.710172
H    -4.829669  0.650605  1.803690
H    -5.773835 -0.840143  1.607281
H    -1.137856  2.863012  0.246641
H    -4.576201  5.467464 -0.152955
H    -5.965531  3.419737 -0.556744
H    -4.919613  0.612403 -1.779035
H    -6.096588  0.918645 -0.485791
H    -0.495203 -0.996116 -2.323959
H    -0.876025 -2.343148 -4.429173
H    -3.157779 -3.330438 -4.819200
H    -4.942112 -2.967012 -3.096243
H    -4.449062 -2.424993  0.046282
H    -5.667467 -1.737636 -1.043362
O     0.421394 -0.533644  0.096246
Cu    2.291122 -0.039239  0.015449
N     4.425896  0.338489 -0.010322
N     2.449902  0.983275 -1.787992
N     2.947501 -1.954936  0.154808
N     2.422577  1.252206  1.634511
C     4.779162  0.389397 -1.441597
C     5.017947 -0.810414  0.699239
C     4.628668  1.621849  0.687273
C     1.444096  1.571697 -2.460390
C     3.718474  1.123442 -2.234916
C     2.198665 -3.051139 -0.065975
C     4.274640 -2.089701  0.382843
C     1.460199  1.451762  2.553461
C     3.643313  1.800061  1.823863
H     4.829975 -0.650863 -1.803297
H     5.774185  0.839846 -1.606836
H     4.919353 -0.612409  1.779439
H     6.096446 -0.918892  0.486372
H     4.449394  2.424890 -0.046156
H     5.667431  1.737451  1.043830
C     1.662242  2.314824 -3.619186
H     0.451000  1.429286 -2.022093
C     4.014700  1.864533 -3.378607
C     2.743797 -4.332613 -0.064810
H     1.137684 -2.862898 -0.246781
C     4.891175 -3.340249  0.382493
C     1.679884  2.201841  3.706838
H     0.494744  0.996650  2.323164
C     3.943228  2.547604  2.962862
C     2.969765  2.464163 -4.085403
H     0.821793  2.774681 -4.139309
H     5.048851  1.971111 -3.709989
C     4.114495 -4.479070  0.158144
H     5.965110 -3.419935  0.557819
C     2.946311  2.750509  3.919542
H     0.875200  2.343660  4.428424
H     4.941730  2.966921  3.096561
H     3.177025  3.047172 -4.983876
H     4.575673 -5.467603  0.154103
H     3.157028  3.330609  4.819054
H    -2.105668  5.197272  0.246240
H     2.105248 -5.197221 -0.245721

44
2 Cu1
el energy= -2780.70696089
Cu   -0.000390 -0.000157  0.477719
N    -1.944602 -0.441806  0.240547
N     0.589747  1.904258  0.240426
O    -2.573736  0.005112  2.412670
O     1.290677  2.226625  2.412695
O     1.283665 -2.230605  2.412755
N     1.354899 -1.462614  0.240473
N    -0.000455 -0.000249 -1.667956
C     0.489859  2.340433 -1.048186
C     2.624939 -3.415611  0.855373
H     2.921457 -4.108557  1.641155
C     1.751189 -2.360961  1.158326
C     1.647789  3.979899  0.854781
H     2.100259  4.582961  1.640358
C    -4.271014 -0.563557  0.855573
H    -5.019309 -0.472998  1.641327
C     1.782306 -1.594474 -1.048164
C    -1.112103 -0.900391 -2.011637
H    -0.729455 -1.931349 -1.927926
H    -1.460620 -0.769125 -3.052081
C    -2.920641 -0.334931  1.158409
C     1.170414  2.696290  1.158059
C    -2.272667 -0.746407 -1.047933
C    -4.597760 -0.875575 -0.454741
H    -5.639319 -1.047110 -0.729262
C     2.625469 -2.627435 -1.428088
H     2.944683 -2.718573 -2.466218
C     1.334745 -0.512852 -2.012053
H     2.035984  0.334279 -1.929125
H     1.394828 -0.880684 -3.052387
C    -3.588932 -0.959791 -1.427671
H    -3.827593 -1.191167 -2.465656
C     1.540991  4.418536 -0.455678
H     1.913266  5.406220 -0.730517
C    -0.224201  1.412461 -2.011696
H    -1.308386  1.596378 -1.927781
H     0.063501  1.648436 -3.052251
C     0.963444  3.586829 -1.428331
H     0.882393  3.908916 -2.466412
C     3.057976 -3.542690 -0.455133
H     3.727611 -4.358648 -0.729793
H    -1.604540  0.184210  2.401795
H     0.643238 -1.481404  2.401866
H     0.960531  1.297945  2.402386

45
2 Cu1-Cl
el energy= -3240.99262817
Cu   -0.000094 -0.000393  0.488829
```

```
Cl    0.000015 -0.000516  3.029039
N     1.880789 -0.848602  0.030331
N    -1.675349 -1.204425  0.030087
O     2.309854 -1.711621  2.146517
O    -2.637395 -1.145130  2.146266
O     0.325521  2.855934  2.147108
N    -0.205647  2.052863  0.030456
N     0.000213  0.000061 -1.848404
C    -1.796719 -1.565353 -1.275790
C     0.107069  4.422992  0.418847
H     0.337146  5.204345  1.142147
C     0.071179  3.082903  0.861320
C    -3.884501 -2.118472  0.417808
H    -4.676476 -2.309718  1.140867
C     3.777501 -2.303881  0.418599
H     4.339113 -2.893963  1.141791
C    -0.457191  2.338768 -1.275392
C     1.413445  0.120710 -2.162558
H     1.699794  1.169303 -1.974056
H     1.644782 -0.092206 -3.227124
C     2.634307 -1.603668  0.860996
C    -2.706206 -1.479330  0.860562
C     2.254485 -0.772917 -1.275366
C     4.135943 -2.221542 -0.914172
H     5.010868 -2.759428 -1.283220
C    -0.428720  3.629865 -1.784676
H    -0.622607  3.799623 -2.844333
C    -0.810808  1.163704 -2.162634
H    -1.862172  0.887615 -1.974151
H    -0.741916  1.470426 -3.227209
C     3.358857 -1.442348 -1.784622
H     3.603030 -1.358807 -2.844187
C    -3.992496 -2.469465 -0.915102
H    -4.896006 -2.957617 -1.284410
C    -0.602018 -1.284092 -2.162782
H     0.162667 -2.056604 -1.974121
H    -0.901841 -1.377842 -3.227427
C    -2.928943 -2.186261 -1.785358
H    -2.978719 -2.439121 -2.845009
C    -0.142388  4.692321 -0.914110
H    -0.113271  5.718943 -1.283182
H     1.511927 -1.139112  2.374457
H     0.228025  1.878715  2.375081
H    -1.742515 -0.740743  2.374530

90
2 Cu2O2
el energy= -5711.69324718
Cu    2.438891 -0.045422  0.104869
O     0.481705 -0.392695  0.367886
N     4.512161  0.108759  0.093867
N     2.916867 -2.036461  0.429605
N     2.767576  0.747112 -1.905449
N     2.665205  1.447453  1.549986
H     0.683890 -2.020415 -0.230020
H     0.442528  1.263360 -1.567934
H     0.529941  0.588815  1.754915
C     4.953699 -0.904817  1.077381
H     6.044031 -1.065000  1.018614
H     4.728307 -0.507475  2.080359
C     4.203309 -2.191317  0.855932
C     4.765110 -3.437299  1.071180
H     5.801191 -3.524894  1.397267
C     3.972855 -4.576856  0.849649
H     4.386743 -5.572309  1.015575
C     2.668093 -4.432621  0.415228
H     2.016563 -5.284619  0.226009
C     2.164412 -3.135195  0.203068
C     4.918211 -0.208956 -1.290737
H     4.778059 -1.291662 -1.435049
H     5.988239  0.011496 -1.447247
C     4.068475  0.556331 -2.271806
C     4.592359  1.024740 -3.465032
H     5.642189  0.858970 -3.706379
C     3.746033  1.719536 -4.343493
H     4.125744  2.094402 -5.294762
C     2.429466  1.935746 -3.984510
H     1.731619  2.480290 -4.619049
C     1.975692  1.444770 -2.745062
C     4.843771  1.494401  0.491869
H     4.710049  2.129717 -0.397904
H     5.900608  1.573898  0.798819
C     3.922136  1.970719  1.583986
C     4.304862  2.910720  2.525974
H     5.322409  3.300940  2.533049
C     3.353395  3.345489  3.463607
H     3.623802  4.091560  4.211983
C     2.075129  2.816224  3.443155
H     1.308106  3.109997  4.158281
C     1.766315  1.843552  2.475457
O    -0.481699  0.392742 -0.367893
Cu   -2.438894  0.045450 -0.104913
N    -4.512160 -0.108762 -0.093866
N    -2.916892  2.036490 -0.429530
N    -2.767542 -0.747159  1.905420
N    -2.665194 -1.447418 -1.550024
H    -0.683912  2.020462  0.230082
H    -0.442485 -1.263360  1.567896
H    -0.529925 -0.588780 -1.754959
C    -4.953711  0.904844 -1.077343
H    -6.044046  1.065010 -1.018573
H    -4.728310  0.507546 -2.080337
C    -4.203342  2.191346 -0.855842
C    -4.765167  3.437326 -1.071028
H    -5.801252  3.524916 -1.397104
C    -3.972931  4.576889 -0.849453
H    -4.386842  5.572342 -1.015325
C    -2.668166  4.432657 -0.415048
H    -2.016651  5.284659 -0.225795
C    -2.164453  3.135231 -0.202951
C    -4.918198  0.208903  1.290749
H    -4.778058  1.291607  1.435096
H    -5.988222 -0.011567  1.447263
C    -4.068444 -0.556415  2.271781
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C    -4.592324 -1.024882  3.464988
H    -5.642157 -0.859136  3.706341
C    -3.745993 -1.719708  4.343418
H    -4.125699 -2.094617  5.294672
C    -2.429421 -1.935887  3.984428
H    -1.731571 -2.480453  4.618942
C    -1.975652 -1.444845  2.745006
C    -4.843762 -1.494394 -0.491905
H    -4.710045 -2.129731  0.397854
H    -5.900597 -1.573886 -0.798864
C    -3.922124 -1.970688 -1.584030
C    -4.304851 -2.910677 -2.526029
H    -5.322398 -3.300898 -2.533108
C    -3.353387 -3.345433 -3.463669
H    -3.623794 -4.091496 -4.212053
C    -2.075122 -2.816167 -3.443213
H    -1.308101 -3.109930 -4.158345
C    -1.766306 -1.843505 -2.475505
O     0.708547  1.711132 -2.412184
O    -0.551214 -1.291583 -2.468989
O    -0.915076  2.992046  0.237157
O     0.915037 -2.991998 -0.237058
O    -0.708499 -1.711176  2.412118
O     0.551225  1.291624  2.468937

47
3 Cu1
el energy= -2721.12899013
Cu   -0.000303 -0.000151  0.460044
N    -0.000057 -0.000095 -1.719316
N    -1.973046 -0.208323  0.220736
N    -2.366172 -0.803761  2.423172
H    -1.368362 -1.014315  2.467205
C    -1.339921  0.501387 -2.035598
H    -1.653700  0.269113 -3.070765
H    -1.299276  1.600633 -1.954238
C    -2.389608 -0.000355 -1.056555
C    -3.713505 -0.174331 -1.434773
H    -4.014397 -0.013131 -2.469834
C    -4.646041 -0.553283 -0.457249
H    -5.695471 -0.688304 -0.722651
C    -4.229791 -0.770651  0.845994
H    -4.933439 -1.080542  1.619271
C    -2.863931 -0.610966  1.156731
N     0.805962  1.812641  0.220556
N     0.487030  2.450760  2.423069
H    -0.194311  1.692000  2.467274
C     1.104196  0.909503 -2.035650
H     1.059949  1.297399 -3.070814
H     2.035826  0.324670 -1.954274
C     1.194499  2.069411 -1.056650
C     1.705922  3.302889 -1.434806
H     1.996159  3.482823 -2.469821
C     1.843940  4.299973 -0.457283
H     2.251923  5.276253 -0.722609
C     1.447411  4.048196  0.845901
H     1.530990  4.812447  1.619237
C     0.902615  2.785522  1.156542
N     1.167085 -1.604200  0.220580
N     1.879359 -1.646777  2.423069
H     1.562417 -0.677507  2.467321
C     0.235691 -1.411149 -2.035695
H     0.593945 -1.566659 -3.070807
H    -0.736591 -1.925614 -1.954607
C     1.195096 -2.069190 -1.056601
C     2.007777 -3.128705 -1.434743
H     2.018507 -3.470095 -2.469736
C     2.802439 -3.746550 -0.457227
H     3.444052 -4.587926 -0.722540
C     2.782735 -3.277141  0.845921
H     3.402974 -3.731477  1.619222
C     1.961481 -2.174114  1.156573
H     2.615233 -1.887819  3.079934
H     0.328112  3.208616  3.079949
H    -2.942926 -1.320570  3.079946

48
3 Cu1-Cl
el energy= -3181.38454178
Cu   -0.000351 -0.000359  0.541457
Cl   -0.000861  0.001797  3.105771
N     0.000006 -0.000773 -1.826114
N     1.289103 -1.623251  0.001629
N     2.426645 -1.663383  2.029471
H     1.693205 -1.045341  2.417127
C     0.110808 -1.413106 -2.128000
H     0.336079 -1.616343 -3.197097
H    -0.869163 -1.871335 -1.913785
C     1.155169 -2.089937 -1.263414
C     1.903319 -3.144139 -1.775639
H     1.761872 -3.461097 -2.809361
C     2.833714 -3.772642 -0.935662
H     3.428678 -4.613421 -1.297406
C     2.998051 -3.309264  0.355556
H     3.726987 -3.761104  1.030615
C     2.224323 -2.207421  0.802716
N    -2.050681 -0.304678  0.000769
N    -2.655927 -1.266347  2.029756
H    -1.753519 -0.941363  2.417568
C    -1.278366  0.609028 -2.129102
H    -1.566378  0.514696 -3.198284
H    -1.185682  1.686979 -1.915586
C    -2.387136  0.043675 -1.264702
C    -3.673966 -0.077004 -1.777432
H    -3.877039  0.203188 -2.811501
C    -4.684190 -0.567104 -0.937497
H    -5.709634 -0.661988 -1.299721
C    -4.365925 -0.939555  0.354395
H    -5.122258 -1.343720  1.029550
C    -3.025005 -0.820445  0.802184
N     0.761416  1.927528  0.000122
N     0.228838  2.933005  2.027935
H     0.059923  1.988783  2.415504
C     1.167364  0.801211 -2.129468
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H     1.229486  1.097723 -3.198693
H     2.054608  0.181933 -1.916220
C     1.232043  2.044263 -1.265146
C     1.771509  3.218876 -1.777745
H     2.116319  3.254469 -2.811614
C     1.852117  4.338808 -0.937803
H     2.283464  5.274042 -1.299787
C     1.369329  4.249905  0.353717
H     1.397300  5.107096  1.028744
C     0.800963  3.029479  0.801054
H     0.426082  3.667082  2.697891
H    -3.390639 -1.462324  2.699382
H     2.964595 -2.200576  2.699270

96
3 Cu2O2
el energy= -5592.50906415
Cu    2.361142 -0.009811 -0.012045
O     0.485761 -0.492461 -0.168061
N     4.414041  0.296745  0.037744
N     3.045794 -2.020233 -0.221239
N     2.622957  1.381487 -1.668704
N     2.562592  1.017986  1.908859
N     1.180742 -2.978802 -1.254309
H     0.654604 -2.129016 -1.049931
N     0.525805  2.411569 -1.720600
H     0.150290  1.727204 -1.052527
N     0.520060  0.445523  2.883352
H     0.105729  0.333885  1.951947
C     4.968202 -0.881748  0.727713
H     6.066538 -0.927558  0.622649
H     4.744424 -0.767221  1.800656
C     4.332171 -2.144184  0.210206
C     5.025550 -3.342492  0.197041
H     6.060440 -3.383082  0.535437
C     4.362729 -4.490296 -0.266251
H     4.871468 -5.455166 -0.276094
C     3.064962 -4.386005 -0.722258
H     2.530175 -5.255746 -1.106158
C     2.422005 -3.123373 -0.717615
C     4.816420  0.383977 -1.380038
H     4.734748 -0.627958 -1.806910
H     5.869379  0.701832 -1.476872
C     3.905909  1.330578 -2.120853
C     4.368752  2.083727 -3.186475
H     5.409986  2.016541 -3.500457
C     3.461010  2.933871 -3.840302
H     3.782546  3.530340 -4.695236
C     2.163951  3.025271 -3.380111
H     1.446525  3.700360 -3.848797
C     1.763595  2.254459 -2.258184
C     4.645015  1.547955  0.783468
H     4.358300  2.381878  0.124454
H     5.713286  1.670961  1.032634
C     3.799203  1.573942  2.029633
C     4.269458  2.143278  3.201732
H     5.275594  2.558964  3.247853
C     3.420856  2.158195  4.320581
H     3.754513  2.599246  5.260889
C     2.159639  1.607955  4.220663
H     1.477335  1.604235  5.071871
C     1.744218  1.032181  2.993578
O    -0.485799  0.492453  0.168425
Cu   -2.361170  0.009871  0.012059
N    -4.414061 -0.296710 -0.037839
N    -3.045846  2.020279  0.221316
N    -2.623062 -1.381587  1.668704
N    -2.562382 -1.017998 -1.908782
N    -1.180821  2.978840  1.254463
H    -0.654657  2.129086  1.050015
N    -0.525907 -2.411645  1.720702
H    -0.150334 -1.727216  1.052726
N    -0.519663 -0.445695 -2.882990
H    -0.105404 -0.334277 -1.951525
C    -4.968221  0.881819 -0.727748
H    -6.066558  0.927612 -0.622690
H    -4.744437  0.767352 -1.800696
C    -4.332205  2.144239 -0.210176
C    -5.025581  3.342551 -0.197018
H    -6.060459  3.383148 -0.535453
C    -4.362774  4.490346  0.266311
H    -4.871507  5.455219  0.276143
C    -3.065020  4.386046  0.722359
H    -2.530239  5.255782  1.106277
C    -2.422071  3.123414  0.717726
C    -4.816513 -0.384063  1.379920
H    -4.734872  0.627832  1.806892
H    -5.869479 -0.701927  1.476657
C    -3.906064 -1.330740  2.120721
C    -4.369016 -2.084028  3.186195
H    -5.410287 -2.016896  3.500067
C    -3.461340 -2.934257  3.840010
H    -3.782967 -3.530841  4.694829
C    -2.164233 -3.025594  3.379945
H    -1.446851 -3.700738  3.848620
C    -1.763757 -2.254631  2.258162
C    -4.644974 -1.547872 -0.783661
H    -4.358318 -2.381832 -0.124669
H    -5.713224 -1.670860 -1.032926
C    -3.799047 -1.573793 -2.029749
C    -4.269248 -2.142940 -3.201963
H    -5.275424 -2.558512 -3.248233
C    -3.420538 -2.157814 -4.320728
H    -3.754151 -2.598713 -5.261124
C    -2.159265 -1.607733 -4.220617
H    -1.476875 -1.603995 -5.071755
C    -1.743895 -1.032170 -2.993417
H     0.138728 -0.601830 -3.638394
H    -0.138275  0.601640  3.638808
H     0.162719 -2.908374  2.274496
H     0.642921 -3.816113 -1.446241
H    -0.162886  2.908178 -2.274425
H    -0.642999  3.816160  1.446354
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56
4 Cu1
el energy= -2838.92221721
Cu   -0.000382 -0.000401  0.088954
N    -0.000555 -0.003006 -2.085065
N     1.277862 -1.519700 -0.153625
N     2.019191 -1.472548  2.031534
H     1.545824 -0.566602  2.034112
C     0.326503 -1.396034 -2.402527
H     0.689915 -1.527286 -3.439122
H    -0.608966 -1.973786 -2.316326
C     1.332937 -1.984210 -1.426468
C     2.219518 -2.983390 -1.809135
H     2.247661 -3.326368 -2.843176
C     3.065479 -3.532812 -0.835871
H     3.767482 -4.323989 -1.103300
C     3.026147 -3.060165  0.467183
H     3.692945 -3.462429  1.227882
C     2.122656 -2.022771  0.784190
N    -1.955206 -0.347369 -0.154601
N    -2.287862 -1.005276  2.032472
H    -1.266598 -1.047586  2.036939
C    -1.370178  0.409843 -2.404414
H    -1.664796  0.159129 -3.440849
H    -1.402600  1.509010 -2.320028
C    -2.383711 -0.165736 -1.428256
C    -3.691989 -0.434664 -1.811559
H    -4.002098 -0.290025 -2.846247
C    -4.591797 -0.890185 -0.838074
H    -5.627692 -1.103242 -1.106054
C    -4.164269 -1.088911  0.465999
H    -4.846829 -1.463078  1.227056
C    -2.814469 -0.824252  0.783775
N     0.676642  1.865542 -0.156939
N     0.269489  2.487578  2.028098
H    -0.279341  1.625293  2.033159
C     1.042057  0.976255 -2.405078
H     0.972942  1.355093 -3.442163
H     2.010129  0.454903 -2.319274
C     1.049598  2.143381 -1.430781
C     1.471495  3.410022 -1.816083
H     1.752814  3.604191 -2.850892
C     1.526407  4.418800 -0.844450
H     1.860527  5.421797 -1.113984
C     1.138977  4.150497  0.459686
H     1.155633  4.930166  1.219221
C     0.692130  2.850089  0.779399
C     0.032455  3.448441  3.092658
H     0.968097  3.952390  3.375812
H    -0.712263  4.214722  2.816060
H    -0.333948  2.909147  3.973590
C    -2.999416 -1.689204  3.099546
H    -3.904431 -1.131737  3.381948
H    -3.288996 -2.718586  2.826058
H    -2.348334 -1.733223  3.980056
C     2.970305 -1.743629  3.096715
H     2.940368 -2.805163  3.382722
H     4.005866 -1.481176  2.819166
H     2.685826 -1.154667  3.976104

57
4 Cu1-Cl
el energy= -3299.17953109
Cu   -0.000028  0.000183 -0.015574
Cl    0.000559 -0.001832  3.327971
N    -0.000653  0.001420 -2.278112
N     1.625571  1.212599 -0.362998
N     1.758233  2.049829  1.791375
H     1.110770  1.290650  2.080026
C     1.407520  0.209031 -2.577398
H     1.591983  0.496695 -3.633014
H     1.917615 -0.754912 -2.411257
C     2.027296  1.242855 -1.656192
C     2.977057  2.136031 -2.140376
H     3.247770  2.125162 -3.196244
C     3.561644  3.038344 -1.239514
H     4.313074  3.752302 -1.582415
C     3.178144  3.024668  0.088335
H     3.615782  3.717294  0.805493
C     2.189270  2.097213  0.517997
N     0.236710 -2.013719 -0.364225
N     0.897292 -2.548589  1.789165
H     0.563696 -1.608511  2.078724
C    -0.525367 -1.321728 -2.577330
H    -0.370169 -1.624661 -3.633377
H    -1.614932 -1.281565 -2.409258
C     0.061326 -2.375882 -1.657572
C     0.360356 -3.644395 -2.143019
H     0.214922 -3.872620 -3.198962
C     0.850718 -4.602273 -1.243282
H     1.093737 -5.609564 -1.587190
C     1.031379 -4.264240  0.084701
H     1.413397 -4.989896  0.801000
C     0.722139 -2.944636  0.515634
N    -1.863038  0.801897 -0.362557
N    -2.654779  0.494939  1.791058
H    -1.673589  0.313673  2.079547
C    -0.884479  1.117410 -2.576330
H    -1.225471  1.134564 -3.632039
H    -0.304747  2.040918 -2.408843
C    -2.089936  1.136087 -1.655427
C    -3.338293  1.512356 -2.139464
H    -3.464053  1.753394 -3.195087
C    -4.412189  1.566283 -1.238756
H    -5.406177  1.860367 -1.581498
C    -4.208791  1.239429  0.088736
H    -5.027595  1.271152  0.805751
C    -2.911186  0.846337  0.518169
C    -3.625699  0.539122  2.859224
H    -4.045849  1.550548  3.003485
H    -4.460332 -0.162127  2.687770
H    -3.106711  0.245867  3.779710
C     1.344672 -3.412672  2.856290
H     0.679116 -4.282660  2.999390
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H     2.369437 -3.784295  2.684500
H     1.338860 -2.817716  3.777503
C     2.283157  2.867679  2.859616
H     3.369242  2.725400  3.002792
H     2.093336  3.941290  2.689098
H     1.770419  2.564365  3.780347

114
4 Cu2O2
el energy= -5828.11072841
Cu   -2.413206  0.028417  0.068845
O    -0.496312  0.480349  0.172742
N    -4.495060 -0.155497  0.094860
N    -2.986543  2.077804  0.051428
N    -2.797308 -1.146917 -1.772034
N    -2.672212 -1.188425  1.807914
N    -1.061562  2.988797 -0.880279
H    -0.692920  2.031564 -0.820300
N    -0.753931 -2.224239 -2.035239
H    -0.416295 -1.650225 -1.255983
N    -0.581271 -0.830866  2.738786
H    -0.441870 -0.213610  1.931741
C    -4.958192  0.971001  0.923793
H    -6.052488  1.100296  0.848664
H    -4.726537  0.723463  1.972328
C    -4.245550  2.239624  0.533217
C    -4.853985  3.477699  0.673131
H    -5.876516  3.551154  1.041908
C    -4.117697  4.619278  0.322447
H    -4.555543  5.612082  0.436143
C    -2.837469  4.483643 -0.178963
H    -2.254732  5.358091 -0.462442
C    -2.284881  3.185995 -0.337891
C    -4.914690 -0.051655 -1.314082
H    -4.763774  0.993067 -1.627444
H    -5.988537 -0.282189 -1.429011
C    -4.083220 -0.972311 -2.171183
C    -4.631029 -1.587890 -3.287145
H    -5.675035 -1.422990 -3.551739
C    -3.806506 -2.427745 -4.050091
H    -4.196382 -2.920227 -4.942147
C    -2.500295 -2.645028 -3.656327
H    -1.851334 -3.308501 -4.224857
C    -2.011718 -2.005676 -2.487224
C    -4.803679 -1.467535  0.691878
H    -4.616306 -2.232019 -0.077988
H    -5.868343 -1.536967  0.975541
C    -3.914060 -1.729492  1.879108
C    -4.346710 -2.502849  2.946387
H    -5.360020 -2.902749  2.963253
C    -3.446984 -2.743623  3.995536
H    -3.750130 -3.348861  4.851191
C    -2.177390 -2.198771  3.952149
H    -1.472977 -2.359424  4.766231
C    -1.804112 -1.400354  2.840184
O     0.496392 -0.480190 -0.172823
Cu    2.413286 -0.028407 -0.068875
N     4.495083  0.155307 -0.094920
N     2.986385 -2.077824 -0.051465
N     2.797437  1.146809  1.771977
N     2.672296  1.188454 -1.807941
N     1.061400 -2.988539  0.880468
H     0.692885 -2.031261  0.820577
N     0.754116  2.224219  2.035089
H     0.416442  1.650195  1.255860
N     0.581267  0.831173 -2.738641
H     0.441737  0.214131 -1.931463
C     4.958098 -0.971219 -0.923899
H     6.052388 -1.100587 -0.848860
H     4.726360 -0.723634 -1.972403
C     4.245382 -2.239773 -0.533257
C     4.853691 -3.477910 -0.673124
H     5.876216 -3.551486 -1.041890
C     4.117250 -4.619405 -0.322464
H     4.554959 -5.612263 -0.436214
C     2.837042 -4.483630  0.178950
H     2.254178 -5.358027  0.462320
C     2.284633 -3.185909  0.337968
C     4.914753  0.051427  1.314014
H     4.763882 -0.993308  1.627341
H     5.988589  0.282012  1.428918
C     4.083305  0.972060  2.171183
C     4.631086  1.587512  3.287228
H     5.675049  1.422483  3.551917
C     3.806593  2.427431  4.050133
H     4.196455  2.919828  4.942241
C     2.500434  2.644890  3.656277
H     1.851536  3.308481  4.224741
C     2.011864  2.005604  2.487139
C     4.803796  1.467349 -0.691952
H     4.616373  2.231827  0.077902
H     5.868484  1.536734 -0.975523
C     3.914240  1.729310 -1.879215
C     4.346958  2.502512 -2.946574
H     5.360324  2.902268 -2.963517
C     3.447196  2.743399 -3.995677
H     3.750397  3.348541 -4.851379
C     2.177497  2.198802 -3.952170
H     1.473033  2.359550 -4.766193
C     1.804172  1.400479 -2.840158
C     0.458796 -0.963104  3.739473
H     1.364603 -0.479872  3.359626
H     0.183355 -0.487010  4.695278
H     0.697836 -2.021111  3.930990
C    -0.151366  4.064982 -1.221748
H     0.767361  3.622580 -1.621639
H    -0.576915  4.722235 -1.995651
H     0.115448  4.681380 -0.346361
C    -0.237537  2.996429  2.759867
H     0.055450  4.054384  2.847746
H    -1.179411  2.951142  2.202075
H    -0.417929  2.598850  3.773021
C     0.151176 -4.064603  1.222234
H     0.577172 -4.722243  1.995554
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H    -0.767104 -3.622113  1.623051
H    -0.116500 -4.680585  0.346816
C     0.237833 -2.996056 -2.760288
H     1.179636 -2.951033 -2.202361
H    -0.055107 -4.053973 -2.848704
H     0.418319 -2.597971 -3.773230
C    -0.459121  0.964007 -3.738915
H    -0.184264  0.487900 -4.694882
H    -1.364992  0.481118 -3.358777
H    -0.697761  2.022142 -3.930218

56
5 Cu1
el energy= -3731.71096506
Cu   -0.864351 -0.001079 -0.001109
N    -3.052742 -0.006184 -0.004966
N    -1.062007 -0.943792 -1.747723
N     1.197456 -0.908823 -2.140487
H     1.267035 -1.107456 -1.138978
C    -3.379578 -1.051932 -0.984285
H    -4.394207 -0.938128 -1.407108
H    -3.362957 -2.015039 -0.447434
C    -2.357214 -1.137320 -2.106053
C    -2.708674 -1.455039 -3.411666
H    -3.756208 -1.589970 -3.681239
C    -1.692105 -1.598445 -4.364444
H    -1.938734 -1.845958 -5.397614
C    -0.361556 -1.440184 -3.995937
H     0.439134 -1.569243 -4.721241
C    -0.083041 -1.113802 -2.660741
N    -1.068066 -1.043824  1.686822
N     1.191179 -1.398583  1.862057
H     1.261020 -0.431779  1.533834
C    -3.385559 -0.332222  1.388771
H    -4.399856 -0.757387  1.496660
H    -3.373683  0.614146  1.954739
C    -2.364416 -1.259301  2.028088
C    -2.718344 -2.231834  2.954399
H    -3.766683 -2.399409  3.201601
C    -1.703230 -2.983906  3.559111
H    -1.951811 -3.755369  4.288892
C    -0.371692 -2.741992  3.243356
H     0.427831 -3.304585  3.720931
C    -0.090633 -1.748332  2.294445
N    -1.071488  1.981389  0.055902
N     1.186297  2.315148  0.284070
H     1.260544  1.547413 -0.388502
C    -3.385923  1.363230 -0.421120
H    -4.402129  1.667700 -0.111549
H    -3.369040  1.379993 -1.523621
C    -2.368655  2.382308  0.066324
C    -2.726539  3.670267  0.443407
H    -3.775515  3.966171  0.460495
C    -1.714546  4.572067  0.796076
H    -1.966259  5.589474  1.097826
C    -0.382074  4.180161  0.749908
H     0.415115  4.876752  1.001057
C    -0.096931  2.861900  0.365593
C     2.384980  3.059069  0.437285
C     2.391980 -1.897721  2.430133
C     2.399846 -1.147298 -2.855483
F     2.467314  3.598225  1.674864
F     2.512549  4.084997 -0.449890
F     3.421992  2.216325  0.248108
F     2.486764 -0.345347 -3.941019
F     2.530632 -2.428601 -3.299366
F     3.432632 -0.888649 -2.026132
F     3.426517 -1.308310  1.794731
F     2.518248 -1.641129  3.762068
F     2.480198 -3.238779  2.278935

57
5 Cu1-Cl
el energy= -4191.99171850
Cu    0.000754 -0.001032  0.450215
Cl    0.002395 -0.001599 -2.005615
N     0.002168 -0.005231  2.768540
N    -1.330209 -1.642773  0.986471
N    -2.409936 -1.687853 -1.054574
H    -1.647439 -1.057232 -1.386619
C    -0.126376 -1.413946  3.098334
H    -0.342002 -1.589950  4.172999
H     0.843121 -1.892264  2.881265
C    -1.192581 -2.084457  2.258636
C    -1.964992 -3.108453  2.796141
H    -1.823244 -3.410821  3.834279
C    -2.917188 -3.724321  1.978290
H    -3.534260 -4.539210  2.360104
C    -3.082216 -3.287138  0.674239
H    -3.823840 -3.744318  0.023260
C    -2.276899 -2.226388  0.208855
N     2.088910 -0.333111  0.988541
N     2.671443 -1.240186 -1.053869
H     1.742171 -0.899322 -1.384860
C     1.285472  0.586743  3.103344
H     1.544592  0.480837  4.177610
H     1.214184  1.667064  2.894223
C     2.401387  0.006089  2.261147
C     3.675642 -0.144526  2.797607
H     3.865645  0.128407  3.836203
C     4.687681 -0.653461  1.978161
H     5.702949 -0.774924  2.359064
C     4.392838 -1.014442  0.673656
H     5.161496 -1.422512  0.021409
C     3.070203 -0.854586  0.209584
N    -0.756807  1.968025  0.990414
N    -0.263828  2.928257 -1.051450
H    -0.095072  1.953548 -1.384396
C    -1.152592  0.809583  3.103595
H    -1.191940  1.084850  4.178318
H    -2.052396  0.208441  2.891918
C    -1.205733  2.067944  2.263642
C    -1.709516  3.246982  2.802310
H    -2.039937  3.274078  3.841229
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C    -1.773298  4.379308  1.984643
H    -2.173468  5.319520  2.367354
C    -1.314874  4.305431  0.679537
H    -1.345165  5.176044  0.028463
C    -0.794792  3.079814  0.213036
C    -0.252536  3.918626 -2.038148
C     3.523289 -1.739747 -2.043550
C    -3.273445 -2.170325 -2.042602
F     0.442212  5.036481 -1.652719
F    -1.502669  4.374304 -2.386557
F     0.325910  3.430084 -3.151328
F    -4.589150 -2.125082 -1.658314
F    -3.045559 -3.480921 -2.392193
F    -3.136941 -1.424195 -3.154854
F     2.809386 -1.997531 -3.155451
F     4.538465 -0.880022 -2.392930
F     4.149788 -2.898385 -1.661639

114
5 Cu2O2
el energy= -7613.69096969
Cu    2.295077 -0.516000 -0.067162
O     0.592171  0.402397 -0.013156
N     4.188537 -1.305990 -0.125937
N     3.444516  1.325275 -0.123772
N     2.309893 -1.813003  1.815984
N     2.111802 -1.836697 -1.885049
N     1.793226  2.845425  0.472052
H     1.141538  2.074450  0.295968
N     0.040584 -2.016323  2.299859
H    -0.140328 -1.344148  1.539406
N     0.041431 -1.190192 -2.730316
H    -0.199615 -0.928544 -1.763803
C     5.004051 -0.353903 -0.906028
H     6.077547 -0.595438 -0.821812
H     4.719902 -0.465646 -1.965207
C     4.732142  1.055827 -0.468010
C     5.731113  2.016744 -0.479057
H     6.750768  1.744744 -0.750434
C     5.393841  3.330874 -0.136407
H     6.152996  4.113838 -0.128505
C     4.084429  3.635772  0.188631
H     3.799250  4.652340  0.450840
C     3.120684  2.608530  0.177340
C     4.639267 -1.404296  1.277478
H     4.784674 -0.378428  1.652108
H     5.610857 -1.924026  1.339721
C     3.603496 -2.104004  2.112028
C     3.981592 -2.949600  3.144235
H     5.035850 -3.150654  3.333109
C     2.977371 -3.532953  3.924086
H     3.230748 -4.214068  4.737297
C     1.652685 -3.244922  3.651324
H     0.856882 -3.698492  4.237878
C     1.347716 -2.362735  2.593786
C     4.114232 -2.627887 -0.781769
H     3.655206 -3.328096 -0.066921
H     5.124246 -3.002752 -1.019083
C     3.263558 -2.546983 -2.016511
C     3.630256 -3.199229 -3.183816
H     4.568647 -3.750856 -3.234597
C     2.772107 -3.116930 -4.286028
H     3.034434 -3.593503 -5.231275
C     1.577331 -2.430620 -4.166934
H     0.892816 -2.365266 -5.009505
C     1.257594 -1.824032 -2.934656
O    -0.591799 -0.401666  0.013894
Cu   -2.294807  0.516300  0.067558
N    -4.188297  1.306077  0.124693
N    -3.443957 -1.325098  0.125090
N    -2.309003  1.812163 -1.816980
N    -2.112817  1.837804  1.884411
N    -1.792392 -2.845577 -0.468992
H    -1.140569 -2.074664 -0.293256
N    -0.039539  2.016563 -2.299969
H     0.141495  1.345171 -1.538853
N    -0.043633  1.190113  2.731547
H     0.198222  0.928833  1.765115
C    -5.003938  0.354576  0.905428
H    -6.077434  0.595901  0.820624
H    -4.720162  0.467348  1.964600
C    -4.731713 -1.055504  0.468745
C    -5.730604 -2.016493  0.480221
H    -6.750376 -1.744375  0.751036
C    -5.393098 -3.330869  0.138727
H    -6.152169 -4.113918  0.131271
C    -4.083566 -3.635926 -0.185646
H    -3.798217 -4.652717 -0.446801
C    -3.119926 -2.608574 -0.174965
C    -4.638554  1.402998 -1.278940
H    -4.783810  0.376761 -1.652630
H    -5.610172  1.922579 -1.342003
C    -3.602646  2.102016 -2.113948
C    -3.980803  2.946017 -3.147452
H    -5.035103  3.146195 -3.337025
C    -2.976616  3.528921 -3.927659
H    -3.230048  4.208757 -4.741920
C    -1.651874  3.242131 -3.653870
H    -0.856104  3.695473 -4.240639
C    -1.346805  2.361567 -2.595007
C    -4.114370  2.628606  0.779274
H    -3.655104  3.328182  0.063961
H    -5.124515  3.003639  1.015792
C    -3.264245  2.548885  2.014470
C    -3.631097  3.202718  3.180835
H    -4.569250  3.754847  3.230581
C    -2.773422  3.121357  4.283478
H    -3.035813  3.599377  5.227976
C    -1.579023  2.434122  4.165794
H    -0.894906  2.369520  5.008741
C    -1.259204  1.825652  2.934488
C    -1.076793 -1.392324 -3.573999
C     1.193196  4.123353  0.540455
C     1.031702  2.185798 -3.203225
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C    -1.192566 -4.123442 -0.539681
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F    -1.658988 -4.859675 -1.573816
F     0.142478 -3.937729 -0.709273
F    -1.368164 -4.869789  0.582789
F    -1.381928 -3.486586  3.370770
F    -0.779142 -1.691583  4.443874
F    -2.109326 -1.525096  2.706524
F     2.111003  1.526805 -2.704951
F     1.382031  3.486630 -3.372417
F     0.781495  1.689478 -4.443177
F    -0.927363 -0.801980 -4.784733
F    -2.165886 -0.849970 -2.973144
F    -1.351480 -2.703289 -3.812038
F     2.162848  0.846445  2.976944
F     0.922470  0.803692  4.787428
F     1.351088  2.702623  3.812096
F     1.369065  4.867888 -0.583220
F     1.659106  4.861359  1.573498
F    -0.141905  3.937729  0.709870

56
6 Cu1
el energy= -2838.96540333
Cu   -0.000104 -0.000048  0.547128
N     0.000067 -0.000414 -1.656982
N     0.868737 -1.789807  0.321838
N     1.316763 -2.064309  2.575818
H     0.405099 -1.631164  2.726010
C     0.156204 -1.421389 -1.982728
H     0.535537 -1.586771 -3.008447
H    -0.848150 -1.874417 -1.933579
C     1.037360 -2.146467 -0.980071
C     1.908995 -3.151877 -1.361832
H     2.025661 -3.397912 -2.418529
C     2.638243 -3.855267 -0.378325
C     2.432639 -3.509312  0.952464
H     2.961928 -4.036015  1.748614
C     1.534703 -2.474026  1.276417
N    -1.984546  0.142914  0.321290
N    -2.446778 -0.106335  2.575323
H    -1.616196  0.467265  2.725185
C    -1.308516  0.574839 -1.983206
H    -1.641132  0.328774 -3.008952
H    -1.198549  1.671137 -1.934338
C    -2.377333  0.174626 -0.980725
C    -3.683753 -0.077730 -1.362751
H    -3.954873 -0.056229 -2.419534
C    -4.657768 -0.357244 -0.379385
C    -4.255725 -0.351463  0.951538
H    -4.976728 -0.546212  1.747557
C    -2.910322 -0.091089  1.275756
N     1.115049  1.647313  0.321727
N     1.127746  2.174014  2.575456
H     1.208311  1.168029  2.726426
C     1.152749  0.845091 -1.982677
H     1.106524  1.256148 -3.008464
H     2.047118  0.201623 -1.933385
C     1.340259  1.970952 -0.980265
C     1.775975  3.228092 -1.362526
H     1.931264  3.451469 -2.419286
C     2.020416  4.211796 -0.379479
C     1.822590  3.861606  0.951392
H     2.013723  4.583802  1.747212
C     1.374457  2.566658  1.275896
H     1.544219  2.740590  3.308927
H    -3.145661 -0.028017  3.308724
H     1.598689 -2.708248  3.309502
C     2.486924  5.584008 -0.769766
H     1.748383  6.075188 -1.421524
H     2.648781  6.223465  0.106910
H     3.429071  5.530115 -1.335904
C     3.594351 -4.944706 -0.768097
H     4.391094 -4.549289 -1.416452
H     4.064483 -5.406599  0.109001
H     3.078339 -5.732339 -1.337650
C    -6.079202 -0.640686 -0.769421
H    -6.713896 -0.819353  0.107449
H    -6.504034  0.201115 -1.336825
H    -6.134722 -1.526840 -1.419912

57
6 Cu1-Cl
el energy= -3299.21779346
Cu   -0.001811 -0.000588  0.688252
Cl   -0.001641  0.001262  3.273968
N     0.000102 -0.000975 -1.684860
N     0.983707  1.817554  0.152313
N     0.587716  2.881257  2.180331
H     0.309973  1.963671  2.569962
C     1.253607  0.660701 -1.982446
H     1.355020  0.948915 -3.051078
H     2.061257 -0.058249 -1.765356
C     1.458557  1.886867 -1.115501
C     2.121111  2.993279 -1.628148
H     2.459200  2.988251 -2.666341
C     2.345999  4.111035 -0.799951
C     1.855196  4.055915  0.494010
H     1.982750  4.903192  1.171967
C     1.155959  2.908623  0.947708
N     1.082149 -1.760965  0.153719
N     2.197486 -1.950383  2.184163
H     1.539711 -1.252925  2.573925
C    -0.053399 -1.417432 -1.981863
H     0.145487 -1.649789 -3.050399
H    -1.079846 -1.757356 -1.764443
C     0.906547 -2.206998 -1.114331
C     1.535864 -3.332791 -1.626564
H     1.363631 -3.623421 -2.664845
C     2.392496 -4.084736 -0.797852
C     2.587992 -3.632152  0.496434
H     3.258499 -4.165084  1.174796
C     1.940669 -2.454781  0.950195
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N    -2.067331 -0.054699  0.153263
N    -2.791575 -0.923797  2.183336
H    -1.858341 -0.704512  2.573213
C    -1.199514  0.753661 -1.982731
H    -1.499651  0.697613 -3.051419
H    -0.980532  1.812490 -1.765160
C    -2.364124  0.318140 -1.115894
C    -3.653133  0.335488 -1.629753
H    -3.817218  0.627618 -2.668929
C    -4.733871 -0.027970 -0.801537
C    -4.441440 -0.421027  0.493894
H    -5.239149 -0.733258  1.172081
C    -3.098622 -0.449949  0.948867
H    -3.547786 -1.026203  2.849759
H     2.663879 -2.553779  2.851159
H     0.876779  3.586838  2.847474
C    -6.146034  0.008607 -1.316163
H    -6.247663 -0.595379 -2.230851
H    -6.857371 -0.372843 -0.571602
H    -6.441575  1.037401 -1.575054
C     3.087789  5.314087 -1.312605
H     2.620960  5.703216 -2.230434
H     3.110055  6.121916 -0.569106
H     4.127612  5.054042 -1.565474
C     3.066947 -5.326845 -1.310435
H     3.754769 -5.749462 -0.566026
H     2.323819 -6.098512 -1.565566
H     3.638794 -5.115057 -2.226897

114
6 Cu2O2
el energy= -5828.19257047
Cu    2.358215 -0.053673 -0.001733
O     0.496296  0.394755  0.322413
N     4.405137 -0.382542 -0.166683
N     3.095155  1.740803  0.870606
N     2.577380 -1.928808  1.080650
N     2.530988 -0.377492 -2.150392
N     1.258113  2.352515  2.178621
H     0.704827  1.647591  1.690792
N     0.457547 -2.867509  0.799554
H     0.102078 -1.984676  0.412312
N     0.508748  0.539922 -2.867217
H     0.092070  0.332072 -1.952892
C     4.991507  0.945659 -0.417157
H     6.090896  0.924749 -0.313712
H     4.762796  1.209972 -1.462219
C     4.389120  1.969942  0.507873
C     5.116170  3.064839  0.932289
H     6.155858  3.180726  0.623143
C     4.502502  4.024329  1.768856
C     3.192264  3.789445  2.151542
H     2.676572  4.487882  2.813469
C     2.508697  2.629117  1.716750
C     4.800014 -0.958661  1.133472
H     4.743872 -0.150153  1.879154
H     5.843705 -1.318749  1.109999
C     3.860264 -2.075975  1.512754
C     4.298768 -3.159104  2.249525
H     5.344396 -3.227526  2.552996
C     3.378695 -4.173991  2.599974
C     2.080135 -4.045283  2.136691
H     1.339297 -4.818258  2.351005
C     1.700094 -2.930572  1.348448
C     4.599467 -1.310255 -1.295984
H     4.285694 -2.309361 -0.956553
H     5.663985 -1.372124 -1.581937
C     3.753681 -0.886004 -2.468494
C     4.209279 -1.030163 -3.765282
H     5.208005 -1.427526 -3.951616
C     3.372982 -0.651581 -4.839826
C     2.124178 -0.142616 -4.524027
H     1.437476  0.164639 -5.315417
C     1.719679 -0.005716 -3.173824
O    -0.496300 -0.394760 -0.322379
Cu   -2.358210  0.053692  0.001783
N    -4.405143  0.382523  0.166728
N    -3.095145 -1.740757 -0.870638
N    -2.577383  1.928811 -1.080633
N    -2.531003  0.377481  2.150429
N    -1.258111 -2.352350 -2.178711
H    -0.704837 -1.647429 -1.690866
N    -0.457547  2.867530 -0.799574
H    -0.102068  1.984697 -0.412341
N    -0.508747 -0.539905  2.867223
H    -0.092077 -0.332013  1.952902
C    -4.991493 -0.945692  0.417170
H    -6.090882 -0.924796  0.313727
H    -4.762775 -1.210030  1.462224
C    -4.389097 -1.969937 -0.507896
C    -5.116129 -3.064834 -0.932346
H    -6.155810 -3.180758 -0.623192
C    -4.502451 -4.024272 -1.768964
C    -3.192225 -3.789340 -2.151665
H    -2.676530 -4.487735 -2.813635
C    -2.508678 -2.629015 -1.716832
C    -4.800029  0.958661 -1.133414
H    -4.743905  0.150160 -1.879105
H    -5.843717  1.318756 -1.109922
C    -3.860277  2.075972 -1.512711
C    -4.298790  3.159088 -2.249496
H    -5.344424  3.227507 -2.552949
C    -3.378723  4.173964 -2.599985
C    -2.080153  4.045264 -2.136725
H    -1.339320  4.818236 -2.351067
C    -1.700101  2.930568 -1.348470
C    -4.599507  1.310205  1.296051
H    -4.285781  2.309335  0.956649
H    -5.664029  1.372015  1.582005
C    -3.753704  0.885961  2.468551
C    -4.209298  1.030088  3.765342
H    -5.208031  1.427429  3.951689
C    -3.372991  0.651491  4.839876
C    -2.124185  0.142548  4.524059
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H    -1.437475 -0.164723  5.315437
C    -1.719685  0.005692  3.173849
H     0.151555 -0.654014  3.628463
H    -0.151550  0.654005 -3.628464
H     0.246108  3.496685 -1.169224
H     0.744524  3.097965  2.634340
H    -0.246106 -3.496702  1.169139
H    -0.744515 -3.097749 -2.634504
C    -5.257040 -5.235979 -2.227102
H    -5.590955 -5.834269 -1.365856
H    -6.161592 -4.942939 -2.781309
H    -4.647646 -5.875976 -2.876693
C    -3.813240  5.348540 -3.424913
H    -2.993314  6.058397 -3.589161
H    -4.185651  5.017311 -4.406216
H    -4.640432  5.883605 -2.934473
C    -3.834107  0.798950  6.259051
H    -4.082037  1.847950  6.480946
H    -4.748861  0.212066  6.432649
H    -3.071378  0.465714  6.973419
C     3.834099 -0.799082 -6.258996
H     4.748857 -0.212208 -6.432611
H     4.082022 -1.848090 -6.480862
H     3.071372 -0.465861 -6.973375
C     5.257112  5.236037  2.226954
H     6.161644  4.942999  2.781195
H     5.591062  5.834278  1.365687
H     4.647720  5.876081  2.876500
C     3.813198 -5.348583  3.424885
H     4.185598 -5.017374  4.406199
H     2.993268 -6.058441  3.589110
H     4.640395 -5.883641  2.934447

56
7 Cu1
el energy= -3731.73037078
Cu   -0.001664 -0.000189  0.771160
N    -0.000974 -0.000496 -1.403695
N    -1.983519 -0.090041  0.534321
N    -2.425991 -0.672826  2.731248
H    -1.441655 -0.932561  2.792978
C    -1.307730  0.581236 -1.724701
H    -1.634279  0.364115 -2.758478
H    -1.202848  1.676413 -1.647639
C    -2.385069  0.146998 -0.743872
C    -3.713615  0.059721 -1.125755
H    -4.008195  0.241930 -2.158961
C    -4.668313 -0.260582 -0.145695
C    -4.274196 -0.509197  1.156640
H    -5.003112 -0.774468  1.921742
C    -2.899470 -0.438952  1.467384
N     0.912219  1.761317  0.534443
N     0.629220  2.435982  2.731480
H    -0.087771  1.713340  2.793694
C     1.156719  0.839807 -1.723913
H     1.133527  1.230414 -2.758007
H     2.052287  0.200977 -1.644978
C     1.318950  1.990239 -0.743551
C     1.908512  3.184019 -1.125350
H     2.214134  3.347757 -2.158436
C     2.108407  4.171035 -0.145345
C     1.695424  3.954363  1.156839
H     1.830104  4.718359  1.921842
C     1.068406  2.728905  1.467558
N     1.068058 -1.671660  0.534900
N     1.793394 -1.763645  2.732160
H     1.524346 -0.781907  2.794865
C     0.148537 -1.423241 -1.723873
H     0.498884 -1.598179 -2.757856
H    -0.852250 -1.880004 -1.645397
C     1.064137 -2.138064 -0.743261
C     1.805382 -3.244002 -1.125226
H     1.795527 -3.590003 -2.158506
C     2.561170 -3.909591 -0.145249
C     2.578474 -3.444205  1.157152
H     3.173454 -3.941964  1.922202
C     1.828621 -2.289845  1.468037
H     2.497732 -2.067882  3.397079
H     0.541375  3.198223  3.396346
H    -3.041971 -1.130496  3.395999
C     3.363106 -5.132484 -0.547682
C    -6.128404 -0.342260 -0.548165
C     2.769078  5.475724 -0.547620
F     4.248347 -4.821789 -1.530385
F     2.545124 -6.104052 -1.028528
F     4.059413 -5.651130  0.490358
F     2.056746  6.090284 -1.527831
F     2.874880  6.336398  0.491332
F     4.017698  5.250323 -1.031757
F    -6.557293  0.849725 -1.037455
F    -6.927087 -0.676587  0.491884
F    -6.304122 -1.270590 -1.524534

57
7 Cu1-Cl
el energy= -4192.00681281
Cu   -0.001834 -0.000900  1.033968
Cl   -0.003325 -0.002886  3.570097
N    -0.001109 -0.001400 -1.326018
N     0.596061  1.985808  0.498468
N     0.009036  2.942347  2.535043
H    -0.094431  1.989230  2.924595
C     1.088175  0.903038 -1.637351
H     1.116592  1.203587 -2.705574
H     2.030192  0.368991 -1.428970
C     1.043498  2.144975 -0.770943
C     1.465827  3.360654 -1.290475
H     1.797652  3.434172 -2.325774
C     1.445288  4.483286 -0.446744
C     0.987081  4.356934  0.848959
H     0.944799  5.217118  1.516624
C     0.543116  3.086006  1.300848
N     1.422165 -1.511397  0.498894
N     2.544093 -1.480608  2.535405
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H     1.769367 -0.916095  2.925367
C     0.237808 -1.397175 -1.636428
H     0.482623 -1.572929 -2.704805
H    -0.695199 -1.946109 -1.426257
C     1.336991 -1.977901 -0.770777
C     2.180462 -2.949448 -1.291099
H     2.078407 -3.273543 -2.326430
C     3.163877 -3.491869 -0.447690
C     3.282763 -3.032579  0.848299
H     4.049209 -3.425590  1.515812
C     2.402302 -2.014423  1.300894
N    -2.021544 -0.479304  0.496670
N    -2.556707 -1.468374  2.531880
H    -1.679825 -1.081328  2.921933
C    -1.328930  0.489454 -1.638193
H    -1.602662  0.363689 -2.706615
H    -1.337721  1.572303 -1.429880
C    -2.382636 -0.170361 -0.772569
C    -3.646581 -0.411544 -1.292633
H    -3.875935 -0.159793 -2.327710
C    -4.609102 -0.990363 -0.449353
C    -4.270950 -1.325290  0.846121
H    -4.995277 -1.791706  1.513420
C    -2.948140 -1.075761  1.298270
H    -3.268040 -1.759227  3.191869
H     3.152419 -1.950414  3.195237
H     0.112829  3.703604  3.195246
C    -5.998288 -1.237410 -0.983054
C     1.926126  5.810170 -0.979524
C     4.077454 -4.566430 -0.982845
F    -5.968896 -2.016165 -2.102814
F    -6.610164 -0.069849 -1.333823
F    -6.803400 -1.858160 -0.082038
F     4.748377 -4.140457 -2.091823
F     5.008628 -4.962252 -0.076436
F     3.375820 -5.676399 -1.351789
F     3.246937  5.760322 -1.316814
F     1.778340  6.819832 -0.082789
F     1.247016  6.168231 -2.107174

114
7 Cu2O2
el energy= -7613.69907510
Cu    2.350878  0.212430  0.150381
O     0.532439 -0.134790 -0.451183
N     4.356839  0.550685  0.563446
N     3.246346 -0.799210 -1.502209
N     2.404721  2.391031  0.225166
N     2.488888 -0.638891  2.162986
N     1.465978 -0.777418 -3.016437
H     0.852614 -0.445624 -2.272697
N     0.200852  2.878431  0.831080
H    -0.081176  1.899037  0.700702
N     0.539944 -1.923018  2.199871
H     0.115406 -1.310622  1.495518
C     5.062799 -0.660117  0.104559
H     6.154985 -0.501766  0.079752
H     4.862749 -1.456525  0.839466
C     4.555564 -1.083276 -1.247534
C     5.382934 -1.728862 -2.146657
H     6.428713 -1.917656 -1.906061
C     4.835979 -2.127634 -3.379233
C     3.520862 -1.840201 -3.670181
H     3.084806 -2.125110 -4.627794
C     2.736465 -1.144160 -2.715240
C     4.707396  1.756259 -0.214929
H     4.728131  1.469097 -1.277969
H     5.714460  2.122736  0.049147
C     3.674914  2.832247  0.006514
C     4.024920  4.169111 -0.018125
H     5.057428  4.475514 -0.183056
C     3.006198  5.118757  0.182853
C     1.719091  4.701061  0.438584
H     0.924949  5.423792  0.626791
C     1.438025  3.309720  0.484989
C     4.473595  0.751149  2.020740
H     4.079640  1.753006  2.250955
H     5.528788  0.726256  2.342369
C     3.665876 -0.288112  2.752283
C     4.111595 -0.821521  3.947708
H     5.069503 -0.521175  4.371264
C     3.296144 -1.769412  4.591524
C     2.096375 -2.137981  4.023891
H     1.451393 -2.871407  4.508184
C     1.705625 -1.552863  2.791660
O    -0.532994  0.123762  0.458612
Cu   -2.350642 -0.217444 -0.148314
N    -4.356247 -0.547757 -0.569315
N    -3.248514  0.794892  1.502037
N    -2.411704 -2.394761 -0.223254
N    -2.479628  0.638834 -2.161055
N    -1.474111  0.762251  3.022899
H    -0.859500  0.428746  2.280981
N    -0.205795 -2.889390 -0.815731
H     0.078183 -1.910277 -0.687996
N    -0.528054  1.919310 -2.189341
H    -0.106337  1.303050 -1.486523
C    -5.059395  0.665207 -0.111669
H    -6.152253  0.510956 -0.091134
H    -4.853570  1.461715 -0.844853
C    -4.555571  1.084693  1.242868
C    -5.383568  1.732348  2.139930
H    -6.427671  1.925849  1.895820
C    -4.839498  2.126863  3.375165
C    -3.526752  1.833239  3.670709
H    -3.093192  2.114589  4.630504
C    -2.741778  1.135339  2.717608
C    -4.714457 -1.752875  0.206251
H    -4.739619 -1.466634  1.269440
H    -5.721345 -2.115914 -0.063175
C    -3.684303 -2.832000 -0.010642
C    -4.038484 -4.167773  0.012919
H    -5.072723 -4.470929  0.172920
C    -3.021647 -5.120629 -0.182266
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C    -1.731902 -4.707020 -0.431221
H    -0.938950 -5.432275 -0.614672
C    -1.446340 -3.316560 -0.476920
C    -4.468223 -0.746350 -2.027233
H    -4.075626 -1.748845 -2.257045
H    -5.522209 -0.718783 -2.352590
C    -3.655706  0.292090 -2.754553
C    -4.096774  0.828995 -3.950136
H    -5.054156  0.531747 -4.377049
C    -3.277373  1.776465 -4.589560
C    -2.078553  2.141254 -4.017539
H    -1.430581  2.874388 -4.498271
C    -1.692667  1.552645 -2.785416
H     0.112931  2.496449 -2.722570
H    -0.097976 -2.501531  2.735244
H     0.539740 -3.575275 -0.848083
H     1.033424 -1.156675 -3.850649
H    -0.546612  3.562119  0.866365
H    -1.042873  1.138052  3.859356
C    -5.720785  2.872987  4.363873
C    -3.374876 -6.597110 -0.117992
C    -3.735145  2.375675 -5.908797
C     3.759288 -2.365116  5.910485
C     5.716853 -2.871197 -4.370223
C     3.354396  6.596359  0.116938
F    -3.855997  1.404978 -6.848242
F    -2.866871  3.302756 -6.371348
F    -4.946714  2.965889 -5.763706
F    -5.079056  3.117162  5.527736
F    -6.836356  2.154283  4.636997
F    -6.109556  4.061184  3.838288
F    -3.796858 -6.922879  1.129626
F    -4.378223 -6.882759 -0.982885
F    -2.318414 -7.383883 -0.422314
F     6.114848 -4.055874 -3.843653
F     5.071125 -3.121798 -5.530507
F     6.827033 -2.146794 -4.650273
F     3.765950  6.924164 -1.133667
F     2.297819  7.379677  0.429645
F     4.363333  6.884632  0.974383
F     2.893400 -3.291686  6.378516
F     4.970696 -2.954875  5.762173
F     3.883051 -1.392125  6.847140

86
8 Cu1
el energy= -4424.25616774
Cu   -2.946426  0.000608  0.000233
N    -5.157604 -0.001446 -0.001312
N    -3.128353 -1.231447 -1.525546
N    -0.859941 -1.444506 -1.704236
H    -0.920195 -1.463429 -0.683821
C    -5.482207 -1.127761 -0.894404
H    -6.460879 -1.001182 -1.390987
H    -5.561084 -2.028866 -0.264162
C    -4.405375 -1.407280 -1.937672
C    -4.688268 -1.872081 -3.216606
H    -5.720289 -1.988342 -3.547768
C    -3.615689 -2.193161 -4.063982
H    -3.810074 -2.569500 -5.069309
C    -2.303840 -2.063217 -3.623000
H    -1.463401 -2.358175 -4.249367
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C     0.422679 -1.265397 -2.242656
C     0.639589 -0.653612 -3.487991
H    -0.202524 -0.346464 -4.108563
C     1.941665 -0.391384 -3.912530
H     2.108262  0.094020 -4.874359
C     3.032076 -0.731692 -3.106132
C     2.817216 -1.352965 -1.868777
H     3.662482 -1.636478 -1.239881
C     1.523560 -1.628249 -1.444966
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H    -6.463537 -0.704893  1.557151
H    -5.563334  0.784302  1.885420
C    -4.408977 -0.976458  2.185054
C    -4.693623 -1.852605  3.225784
H    -5.726097 -2.081244  3.490316
C    -3.622234 -2.426953  3.928471
H    -3.817997 -3.110154  4.756126
C    -2.309776 -2.110183  3.597536
H    -1.470331 -2.505924  4.167081
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C     0.636598 -2.697057  2.312369
H    -0.205192 -3.388399  2.357337
C     1.938802 -3.195390  2.296637
H     2.105668 -4.271028  2.357305
C     3.029045 -2.326628  2.187508
C     2.813726 -0.944533  2.106828
H     3.658823 -0.258002  2.037228
C     1.519907 -0.440277  2.134018
H     1.354741  0.637531  2.074372
N    -3.131672  1.937127 -0.304654
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H    -0.922809  1.326888 -0.924985
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H    -6.463648  1.699719 -0.171553
H    -5.564410  1.238895 -1.625651
C    -4.409448  2.379820 -0.251962
C    -4.694698  3.719693 -0.017036
H    -5.727337  4.062916  0.047095
C    -3.623738  4.616137  0.127618
H    -3.819992  5.674871  0.302734
C    -2.311061  4.171361  0.020649
H    -1.471875  4.862888  0.077460
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H    -0.208881  3.741626  1.750266
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C     2.813034  2.296044 -0.231158
H     3.659039  1.890482 -0.788116
C     1.520099  2.066289 -0.683046
H     1.356479  1.472938 -1.585083
C     4.433035 -2.861586  2.067427
C     4.430634  3.226886  1.445686
C     4.436471 -0.362515 -3.510127
F     5.324532 -2.112734  2.763016
F     4.536408 -4.142367  2.500675
F     4.845426 -2.848911  0.756863
F     5.318116  3.472674  0.449639
F     4.852090  2.080822  2.074839
F     4.529830  4.232611  2.349760
F     4.855530  0.758125 -2.835045
F     5.324602 -1.345973 -3.220655
F     4.537285 -0.086204 -4.833857

87
8 Cu1-Cl
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C    -0.010022 -1.423053  4.563256
H    -0.224348 -1.633859  5.632159
H     1.002520 -1.807763  4.357228
C    -0.997771 -2.182108  3.700846
C    -1.638787 -3.308727  4.207045
H    -1.455596 -3.624205  5.234642
C    -2.498705 -4.021226  3.363286
H    -2.978697 -4.939481  3.706152
C    -2.736300 -3.553268  2.082408
H    -3.379944 -4.098379  1.395031
C    -2.102708 -2.363455  1.657567
C    -3.326572 -2.057363 -0.496940
C    -4.628043 -2.444645 -0.123130
H    -4.885234 -2.558420  0.929243
C    -5.608823 -2.635860 -1.091343
H    -6.615738 -2.925607 -0.788704
C    -5.322291 -2.426152 -2.444878
C    -4.036720 -2.014474 -2.820444
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C     5.092938 -3.534505 -1.080318
H     5.846461 -4.262072 -0.776430
C     4.773563 -3.387904 -2.434947
C     3.775340 -2.480168 -2.812282
H     3.510804 -2.369058 -3.864358
C     3.118166 -1.720371 -1.852967
H     2.335206 -1.017500 -2.142558
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C    -1.395694  1.940498  3.704105
C    -2.053702  3.056675  4.211668
H    -2.420197  3.052865  5.238662
C    -2.241382  4.159148  3.370049
H    -2.798873  5.032144  3.713882
C    -1.715047  4.134746  2.090003
H    -1.865626  4.965997  1.404239
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H     0.221995  5.504326  0.945287
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H     0.770028  7.192266 -0.766765
C     0.560870  5.826772 -2.427441
C     0.277572  4.508367 -2.807244
H     0.320494  4.224287 -3.859203
C    -0.056823  3.558442 -1.850480
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C     5.533792 -4.156018 -3.476919
C     0.851023  6.870784 -3.466431
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F    -0.287993  7.506780 -3.888447
F    -7.631569 -2.487102 -3.020818
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174
8 Cu2O2
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N	-0.787252	-2.759464	-0.827552
H	-0.473444	-1.865540	-0.445270
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H	3.650234	2.338087	-5.528640
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H	5.581964	2.720348	-3.954463
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C	1.231397	-1.193564	-4.816182
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H	1.203295	-1.378716	-5.904181
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C	0.666205	-3.640611	-4.595181
H	1.046586	-3.817128	-5.601020
C	0.179812	-4.691700	-3.803863
H	0.203799	-5.716867	-4.174281
C	-0.310279	-4.424071	-2.540329
H	-0.668578	-5.222895	-1.893739
C	-0.310003	-3.092229	-2.068108
C	-0.888501	0.025599	-4.970829
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H	-0.916310	0.230265	-6.055281
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H	-2.950071	1.531643	-5.924512
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H	-4.436715	3.040320	-4.556298
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H	-3.965283	3.307451	-2.122686
C	-2.238508	2.001100	-2.170210
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C	6.258162	-0.131316	1.314194
H	7.235130	-0.584996	1.142497
C	5.875405	0.233093	2.610693
C	4.618688	0.804564	2.829715
H	4.325974	1.098017	3.837951
C	3.753483	1.016219	1.761178
H	2.773436	1.467291	1.922672
C	-1.495586	-3.610609	0.051030
C	-2.638376	-4.306386	-0.377292
H	-2.969900	-4.226532	-1.413205
C	-3.370654	-5.065283	0.529368
H	-4.266687	-5.591749	0.197111
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C	-2.486857	3.077404	0.044153
C	-2.990955	2.665142	1.285191
H	-3.032809	1.600604	1.515328
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H	-3.827501	3.285705	3.175334
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C	-3.597448	-2.025114	4.486196
H	-3.650545	-2.337604	5.528731
C	-4.675130	-2.222272	3.610089
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C    -4.617098 -0.805293 -2.830604
H    -4.323294 -1.097683 -3.838851
C    -3.751985 -1.015833 -1.761839
H    -2.770987 -1.464891 -1.923193
C     1.495832  3.611050 -0.051493
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H     2.969914  4.227795  1.412580
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H     4.266262  5.593045 -0.198180
C     2.977827  5.129858 -1.874364
C     1.836244  4.448736 -2.299134
H     1.524516  4.513995 -3.341481
C     1.095309  3.694857 -1.390848
H     0.204864  3.156173 -1.713173
C     2.486164 -3.076606 -0.043403
C     2.989823 -2.664966 -1.284852
H     3.030798 -1.600582 -1.515871
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77
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C     3.278056  2.413601 -2.834711
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H     0.059110  3.009148 -3.829612
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C    -2.048241  1.272376 -3.454863
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C    -4.450536  1.411564 -3.125266
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78
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156
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