

# **Density Functional Theory Study of the Reaction of N<sub>2</sub>O and CO with Small Copper Clusters**

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Supporting Information

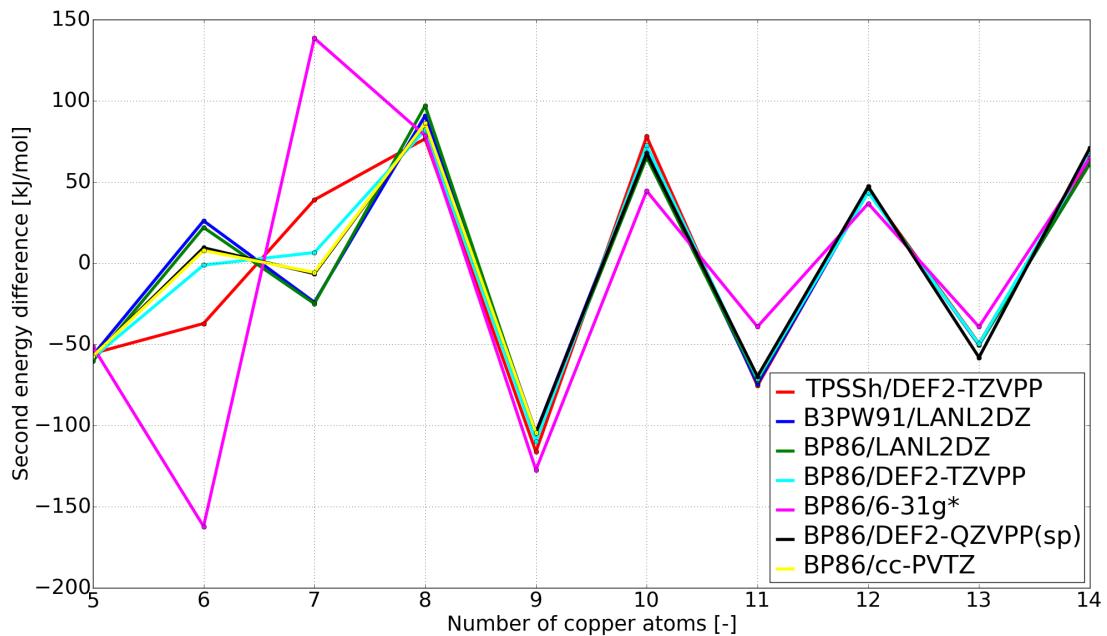


Figure S1: Second energy difference as function of size of copper clusters

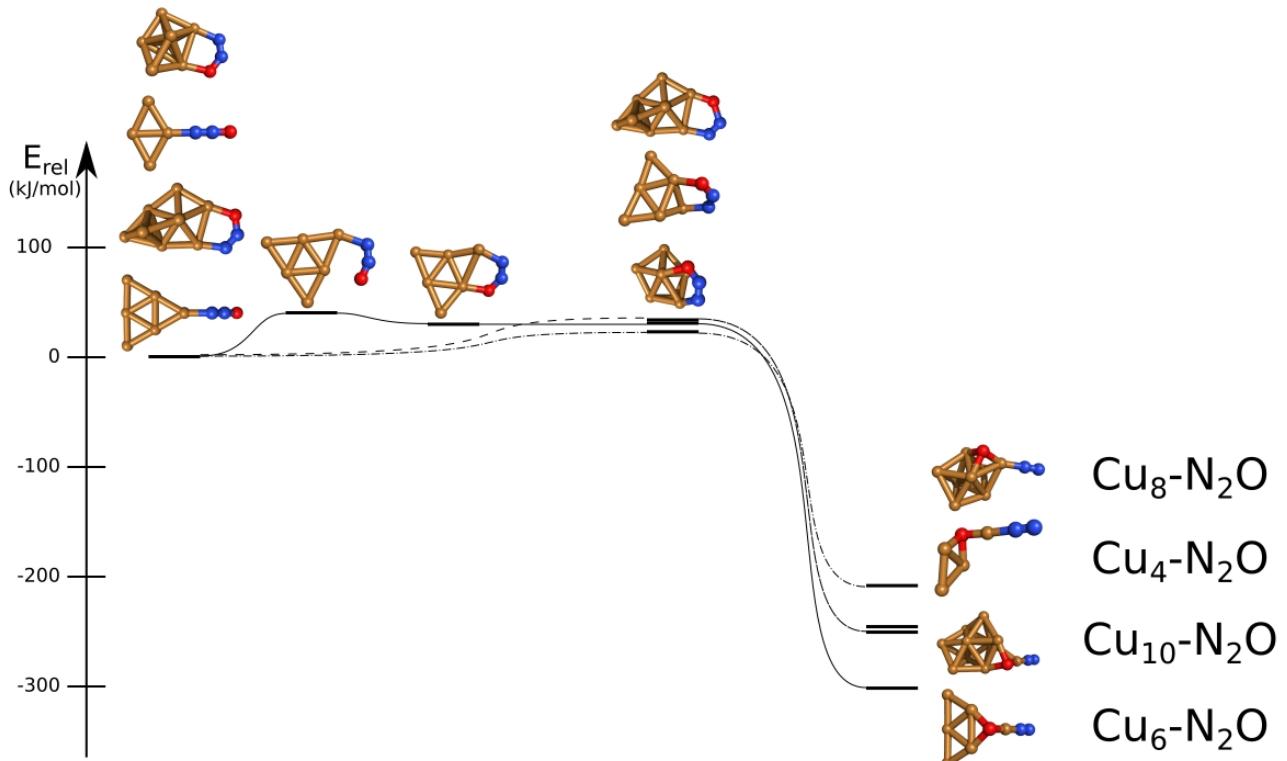


Figure S2: Isomerization of the ring isomers of  $Cu_x-N_2O$  ( $x=6, 8$  or  $10$ ) clusters to the more stable structure, where the oxygen-nitrogen bond is broken. Cu, yellow brown ; O, red; N, blue. (Method: TPSSh/DEF2-TZVPP)

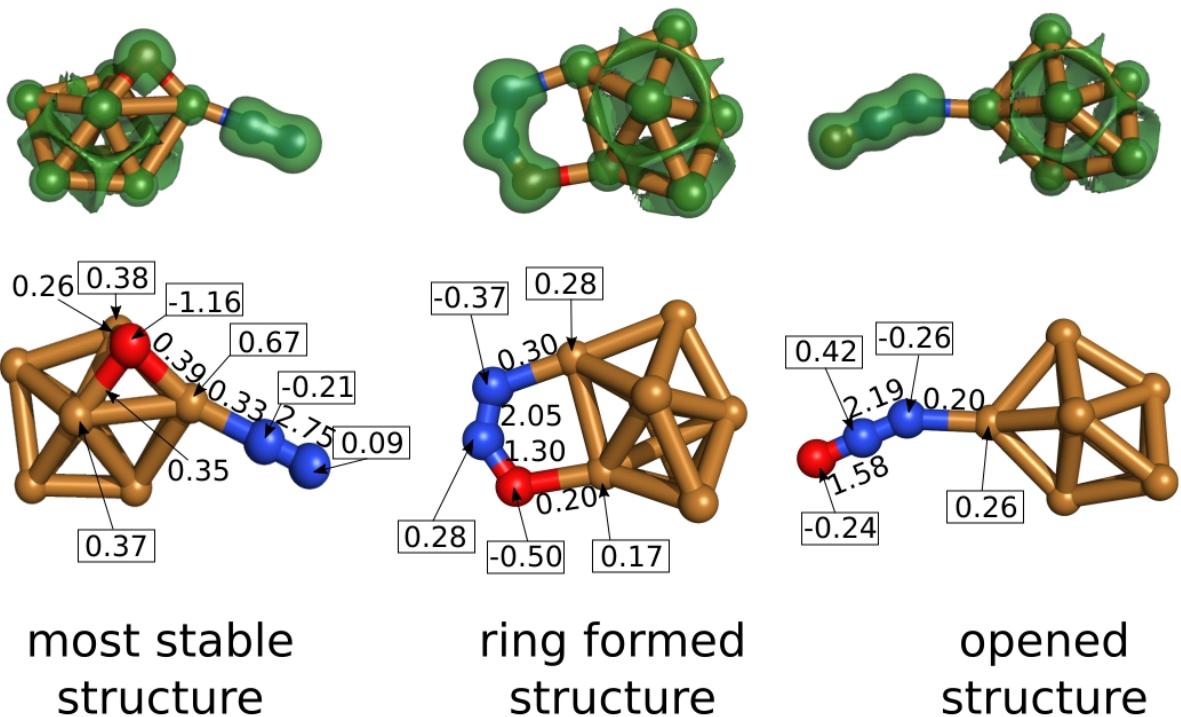


Figure S3: Localized-orbital locator profiles, natural charges and bond indices of the different structures of  $\text{Cu}_8$  clusters. Cu, yellow brown; O, red; N, blue. Method: BP86/LANL2DZ.

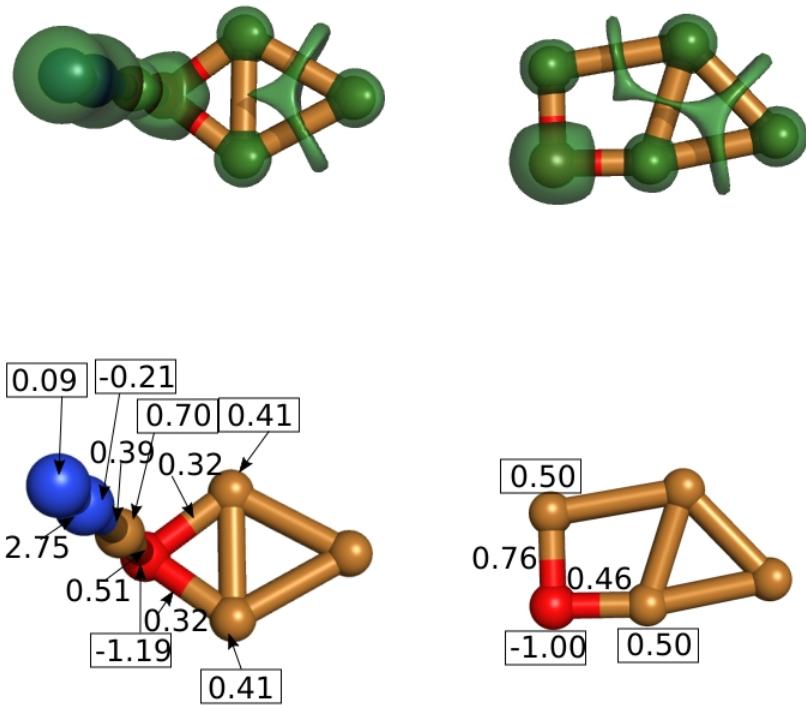


Figure S4: Localized-orbital locator profiles, natural charges and bond indices of  $\text{Cu}_4\text{-N}_2\text{O}$  and  $\text{Cu}_4\text{O}$  clusters. Cu, yellow brown; O, red; N, blue. Method: BP86/LANL2DZ.

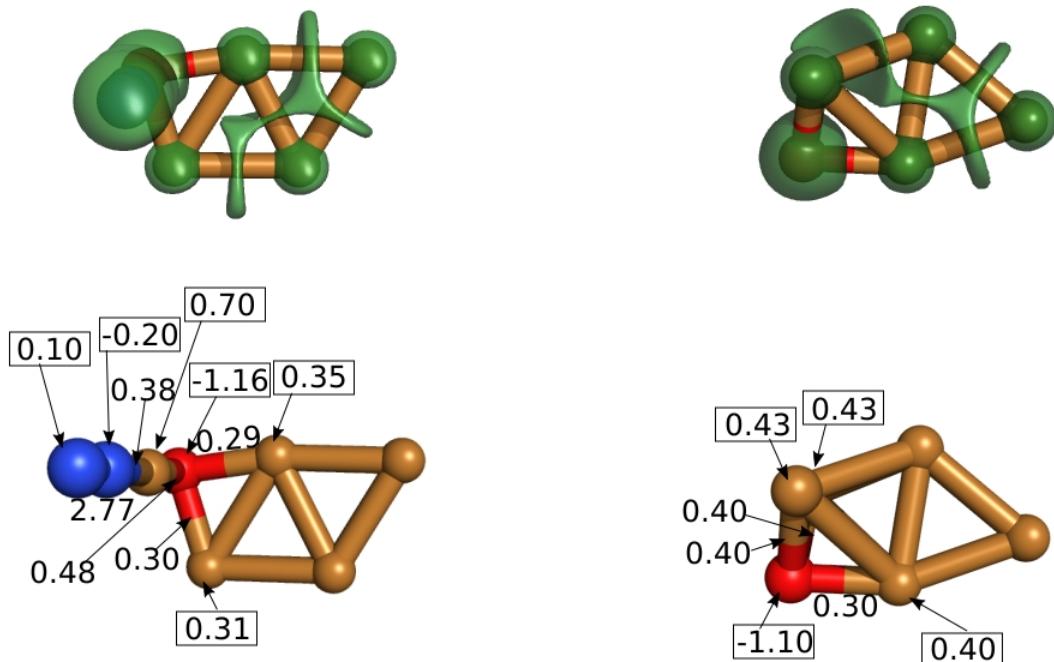


Figure S5: Localized-orbital locator profiles, natural charges and bond indices of  $\text{Cu}_5\text{-N}_2\text{O}$  and  $\text{Cu}_5\text{O}$  clusters. Cu, yellow brown; O, red; N, blue. Method: BP86/LANL2DZ.

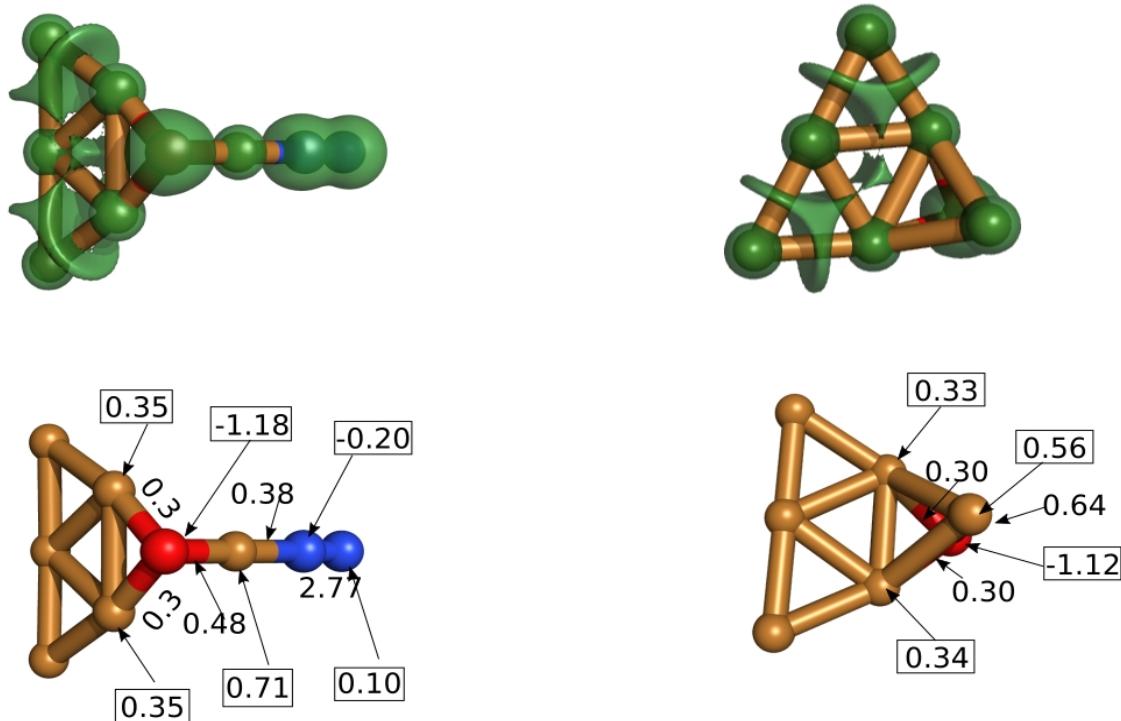


Figure S6: Localized-orbital locator profiles, natural charges and bond indices of  $\text{Cu}_6\text{-N}_2\text{O}$  and  $\text{Cu}_6\text{O}$  clusters. Cu, yellow brown; O, red; N, blue. Method: BP86/LANL2DZ.

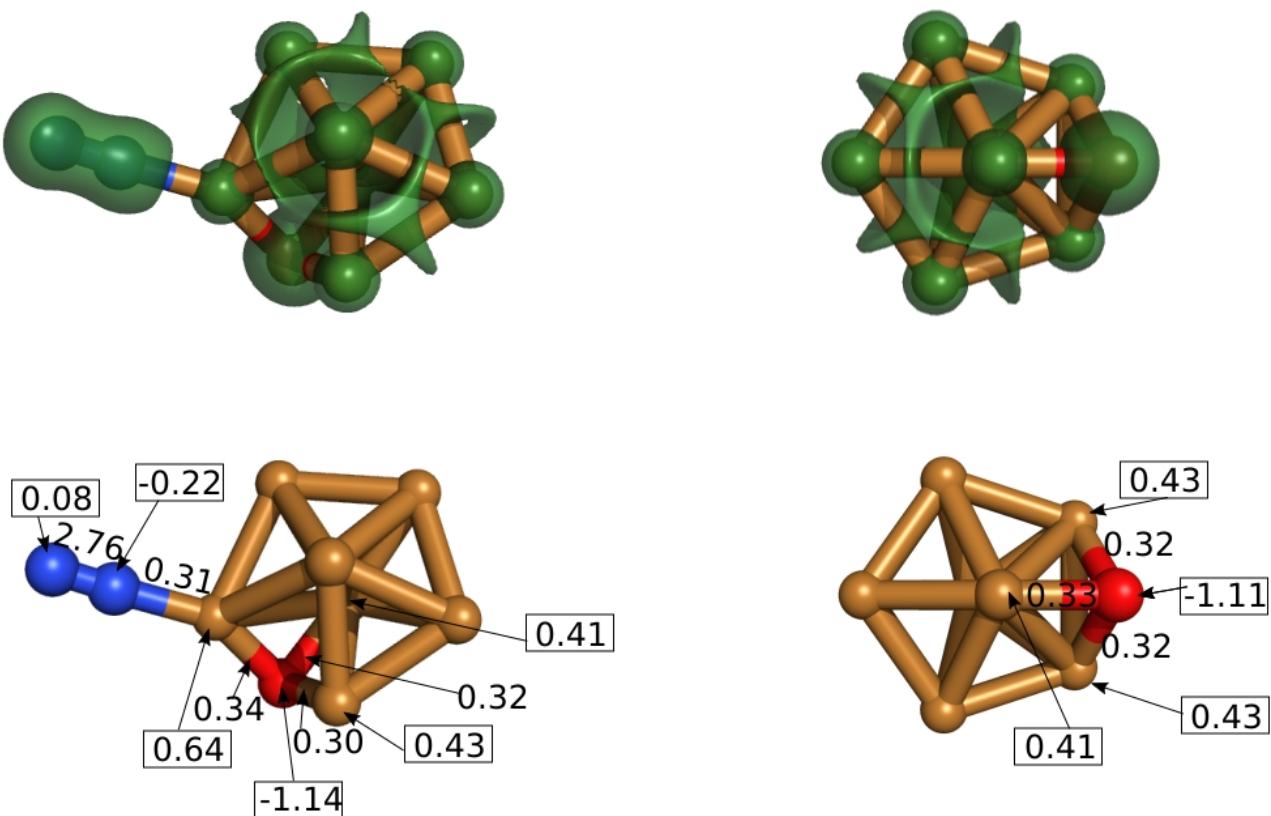


Figure S7: Localized-orbital locator profiles, natural charges and bond indices of  $\text{Cu}_7\text{-N}_2\text{O}$  and  $\text{Cu}_7\text{O}$  clusters. Cu, yellow brown; O, red; N, blue. Method: BP86/LANL2DZ.

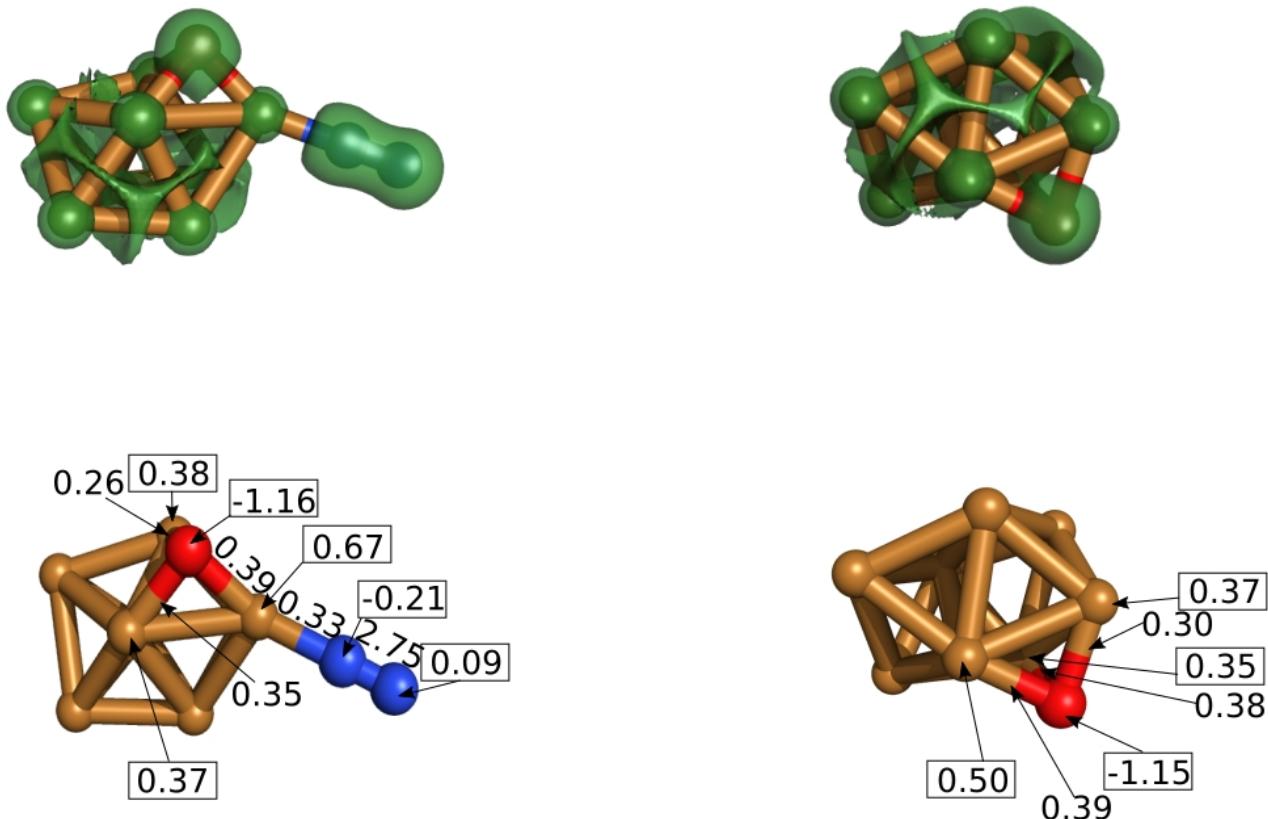


Figure S8: Localized-orbital locator profiles, natural charges and bond indices of  $\text{Cu}_8\text{-N}_2\text{O}$  and  $\text{Cu}_8\text{O}$  clusters. Cu, yellow brown; O, red; N, blue. Method: BP86/LANL2DZ.

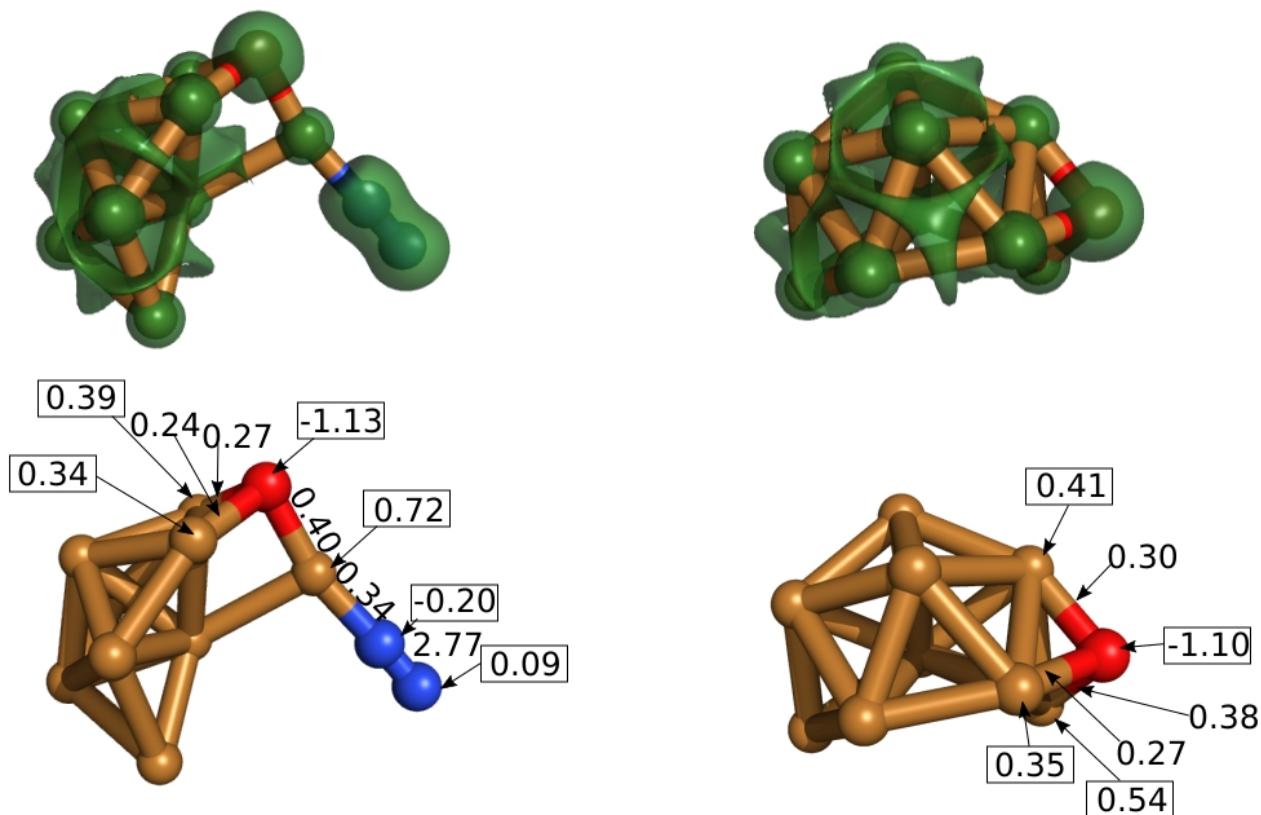


Figure S9: Localized-orbital locator profiles, natural charges and bond indices of  $\text{Cu}_9\text{-N}_2\text{O}$  and  $\text{Cu}_9\text{O}$  clusters. Cu, yellow brown; O, red; N, blue. Method: BP86/LANL2DZ.

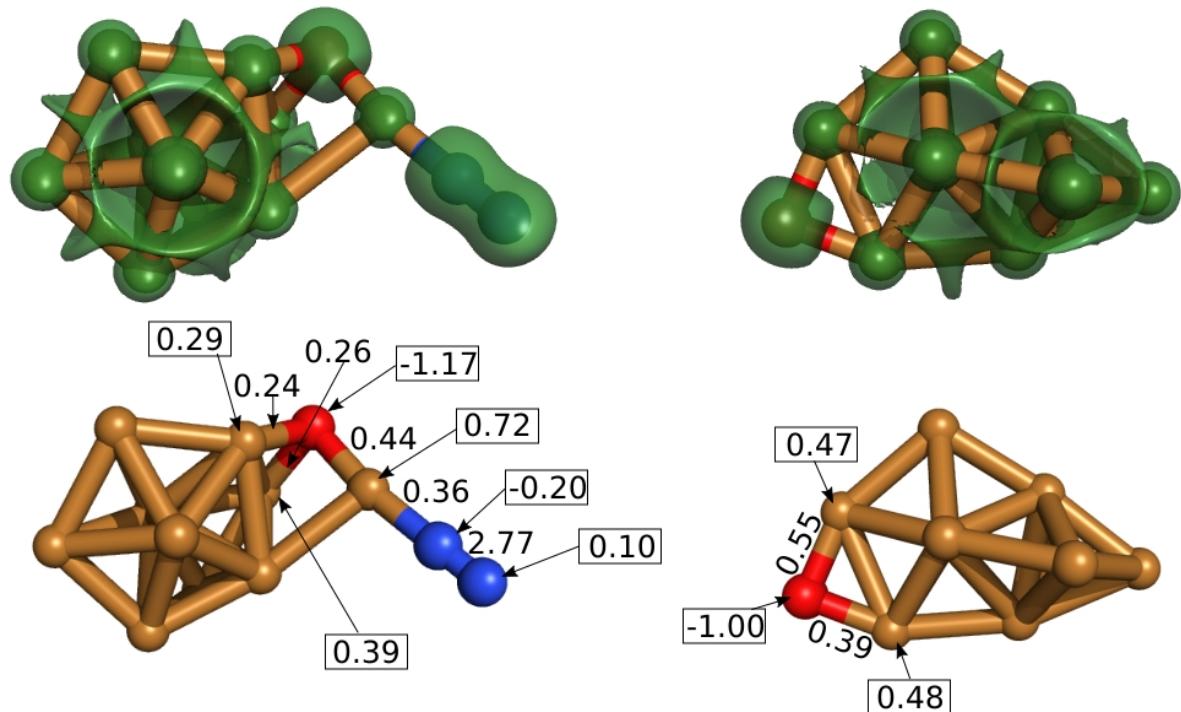


Figure S10: Localized-orbital locator profiles, natural charges and bond indices of  $\text{Cu}_{10}\text{-N}_2\text{O}$  and  $\text{Cu}_{10}\text{O}$  clusters. Cu, yellow brown; O, red; N, blue. Method: BP86/LANL2DZ.

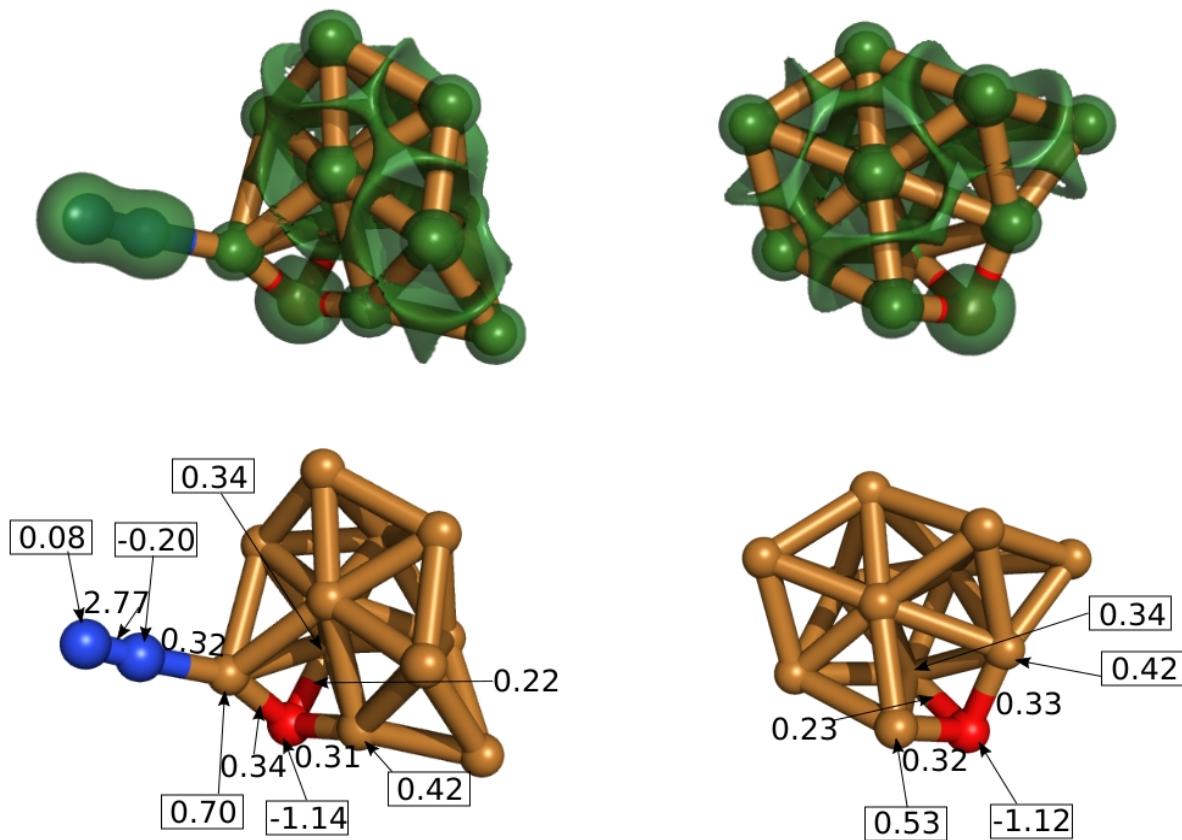


Figure S11: Localized-orbital locator profiles, natural charges and bond indices of  $\text{Cu}_{11}\text{-N}_2\text{O}$  and  $\text{Cu}_{11}\text{O}$  clusters. Cu, yellow brown; O, red; N, blue. Method: BP86/LANL2DZ.

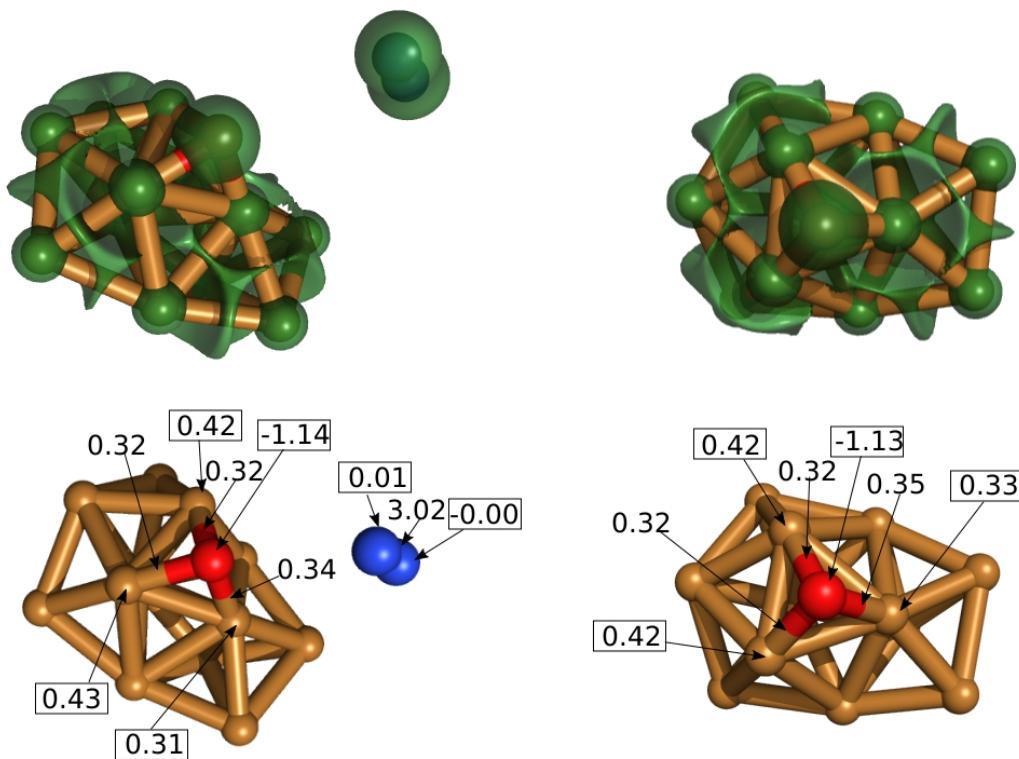


Figure S12: Localized-orbital locator profiles, natural charges and bond indices of  $\text{Cu}_{12}\text{-N}_2\text{O}$  and  $\text{Cu}_{12}\text{O}$  clusters. Cu, yellow brown; O, red; N, blue. Method: BP86/LANL2DZ.

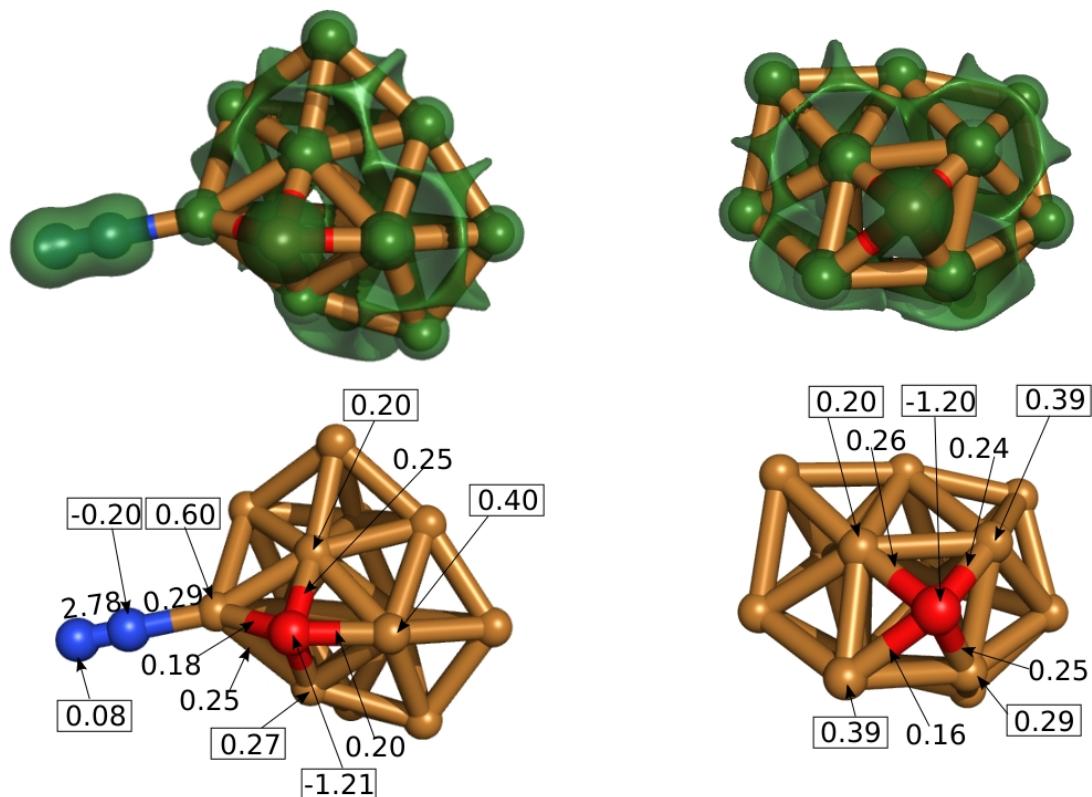


Figure S13: Localized-orbital locator profiles, natural charges and bond indices of  $\text{Cu}_{13}\text{-N}_2\text{O}$  and  $\text{Cu}_{13}\text{O}$  clusters. Cu, yellow brown; O, red; N, blue. Method: BP86/LANL2DZ.

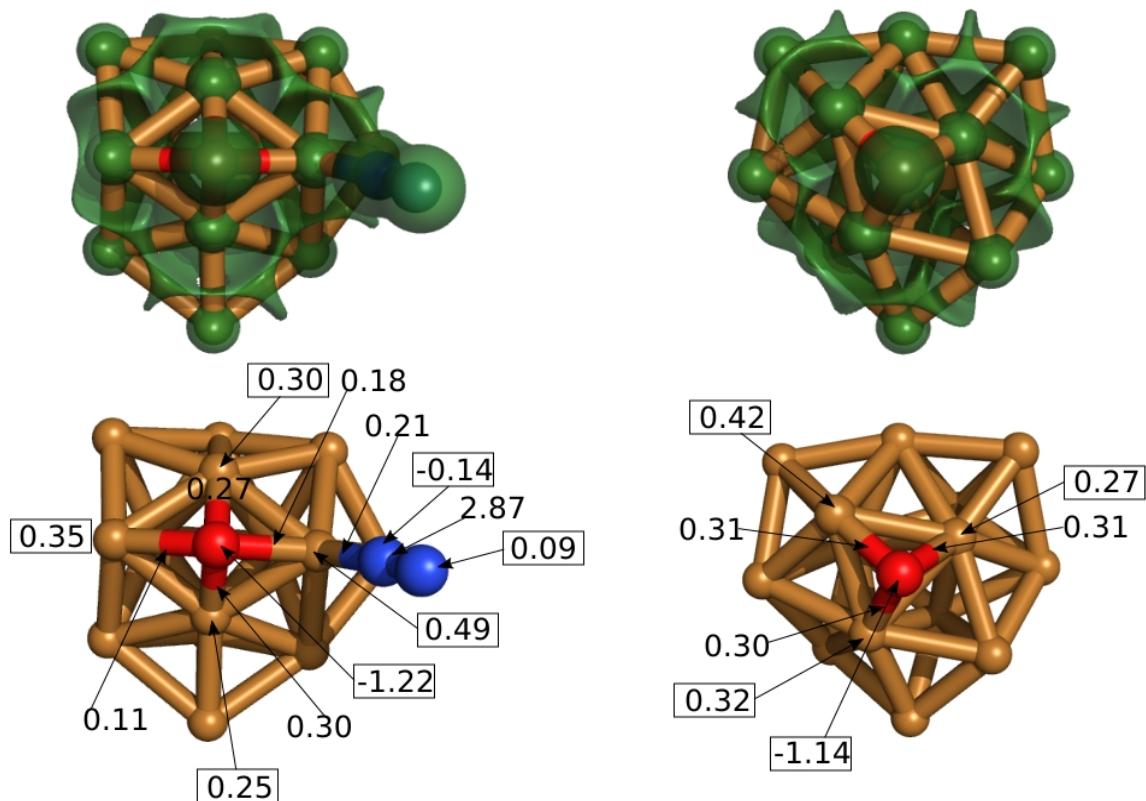


Figure S14: Localized-orbital locator profiles, natural charges and bond indices of  $\text{Cu}_{14}\text{-N}_2\text{O}$  and  $\text{Cu}_{14}\text{O}$  clusters. Cu, yellow brown; O, red; N, blue. Method: BP86/LANL2DZ.

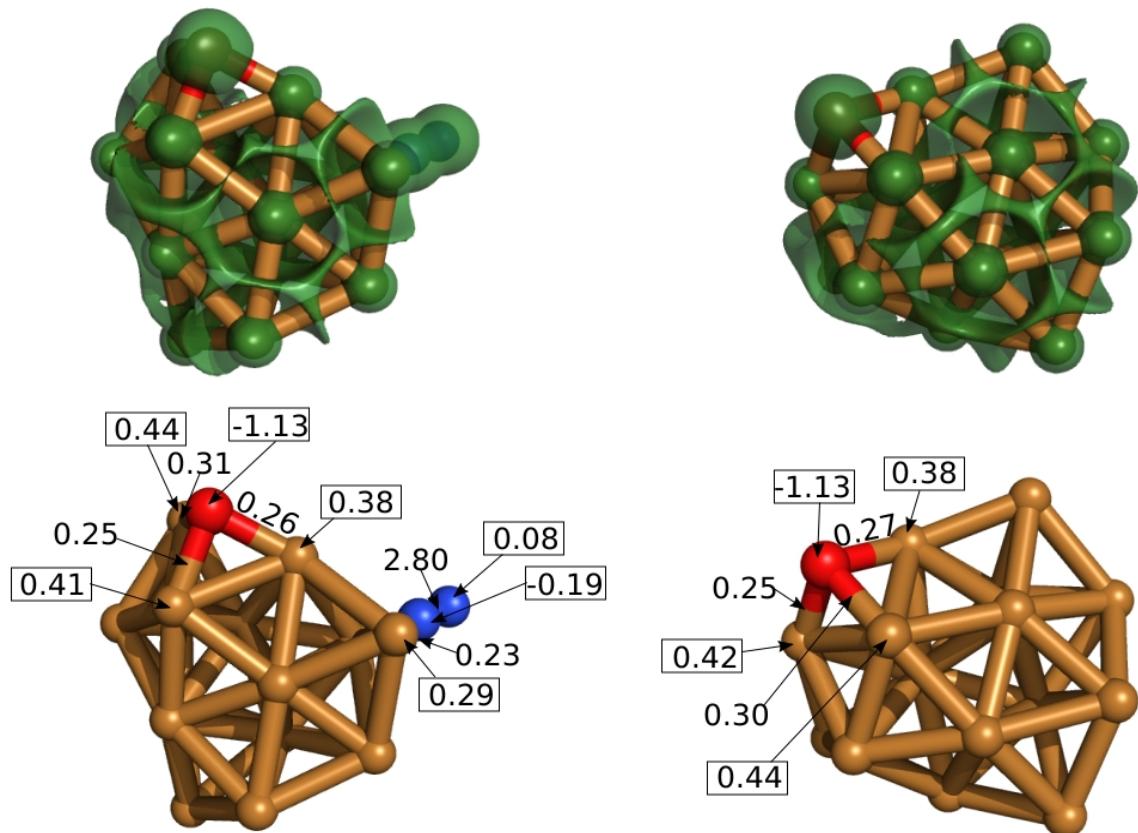
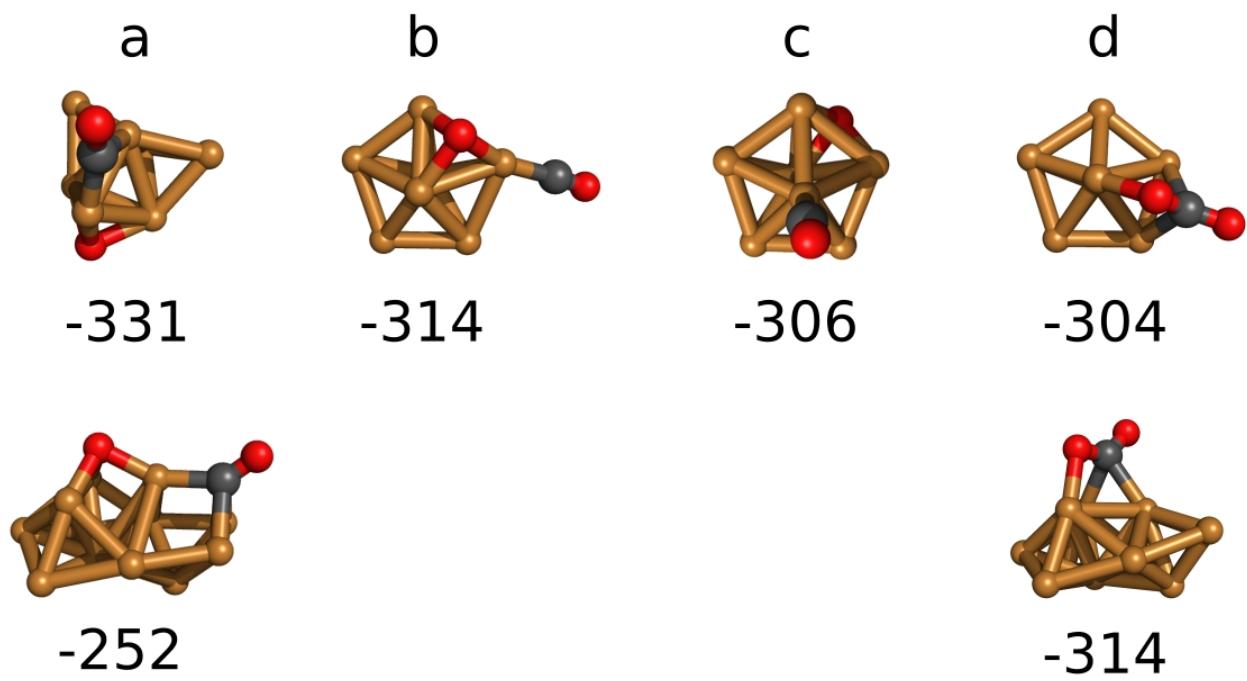


Figure S15: Localized-orbital locator profiles, natural charges and bond indices of  $\text{Cu}_{15}\text{-N}_2\text{O}$  and  $\text{Cu}_{15}\text{O}$  clusters. Cu, yellow brown; O, red; N, blue. Method: BP86/LANL2DZ.



*Figure S16: The lowest energy Cu<sub>7</sub>O-CO and Cu<sub>12</sub>O-CO systems, calculated with TPSSh functional and DEF2-TZVPP basis set. Cu, yellow brown; O, red; C, grey.*

It is well visible that carbon-monoxide attaches with the carbon site to the copper cluster. However, in contrary to the pure clusters, carbon-monoxide tends to form chemical bonds to more than one copper atoms, clearly shown by the relative energies of the different isomers. Addition of carbon monoxide results in the change of the cluster geometry of the lowest energy structure (cluster **a**), while there is no geometry change in the case of larger energy clusters. This step is again a barrierless process, nevertheless subsequent reaction steps are necessary for the further stabilization and for the formation of carbon-dioxide (structure **d**).

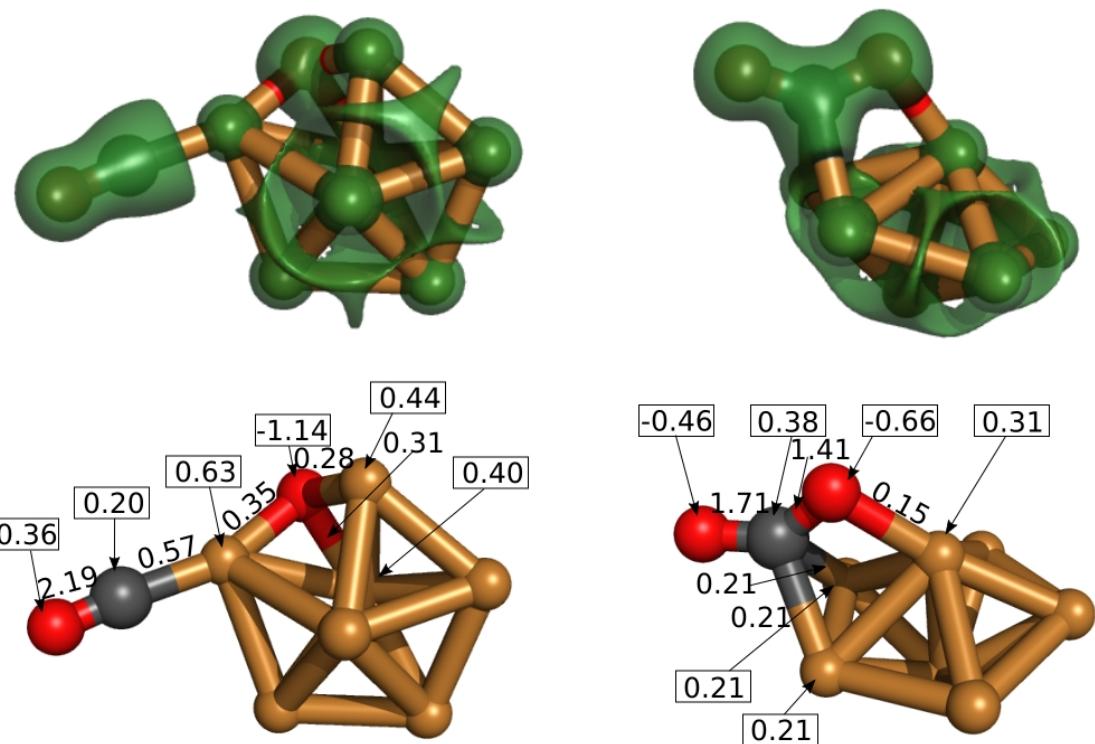


Figure S17: Localized orbital locators, Wiberg bond indices and natural charges of Cu<sub>12</sub>O-CO and Cu<sub>12</sub>-CO<sub>2</sub> clusters. Cu, yellow brown; O, red; C, grey. Method: BP86/LANL2DZ.

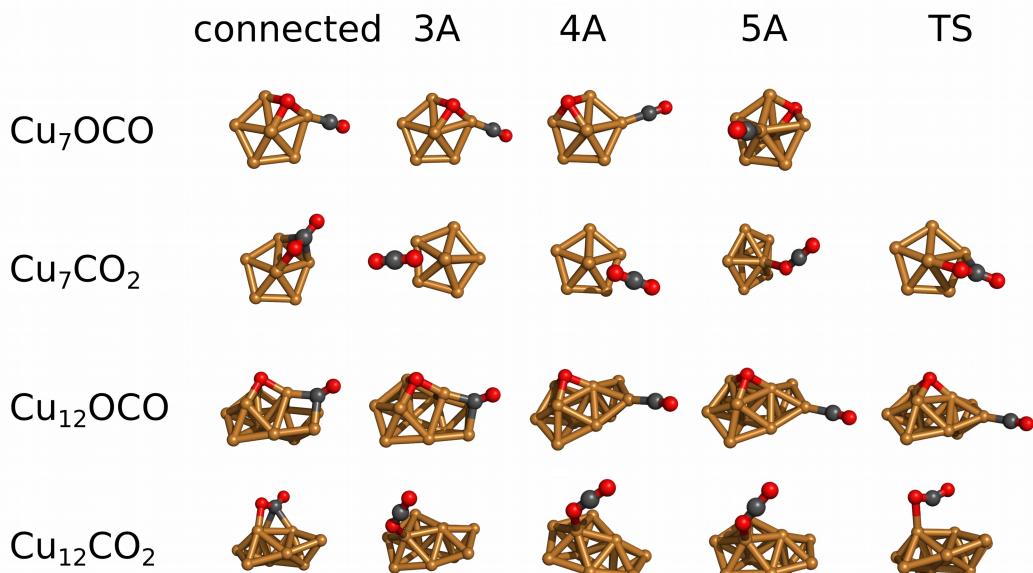
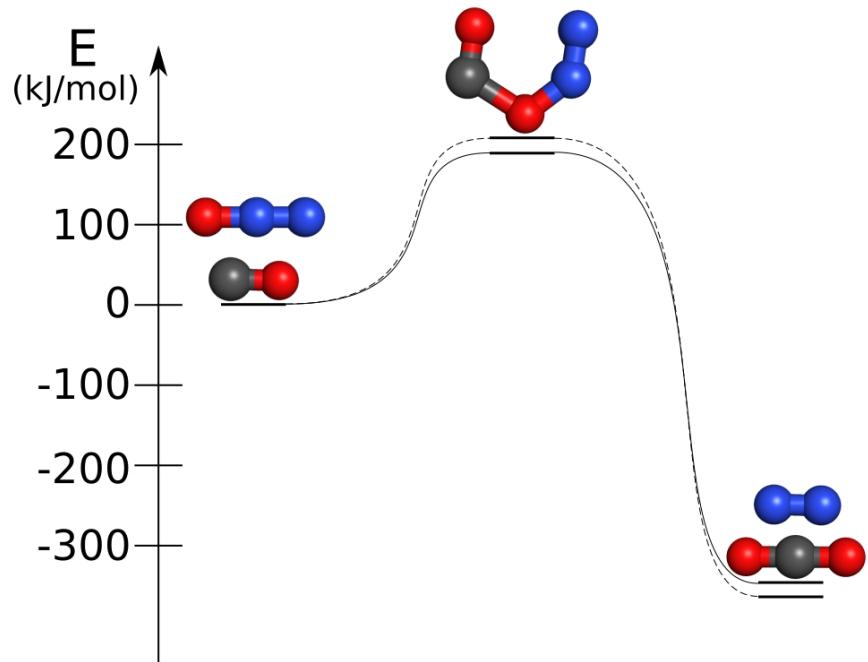


Figure S18: Optimized structures of Cu<sub>x</sub>-CO<sub>2</sub> and Cu<sub>x</sub>-OCO systems. Cu, yellow brown; O, red; C, grey. Method: BP86/LANL2DZ.

In the case of the Cu<sub>x</sub>O + CO → Cu<sub>x</sub>OCO reaction and Cu<sub>x</sub>CO<sub>2</sub> → Cu<sub>x</sub> + CO<sub>2</sub> desorption geometry optimization was performed from 3 Å, 4 Å and 5 Å distance of CO and CO<sub>2</sub> from the copper cluster to investigate whether the reactions have energy barriers on the potential energy surface.



*Figure S19: Activation and reaction energy of the  $\text{CO} + \text{N}_2\text{O} \rightarrow \text{CO}_2 + \text{N}_2$  reaction without catalyst. Calculated with TPSSh/DEF2-TZVPP and CCSD(T)/aug-cc-pVTZ (dashed line) methods.*

## 1. XYZ coordinates and total energies of CO, CO<sub>2</sub>, N<sub>2</sub>O and N<sub>2</sub> on BP86/LANL2DZ level

CO

E = -113.262248397942

O	0.0000000000	0.0000000000	0.4668910586
C	0.0000000000	0.0000000000	-0.7029732683

CO<sub>2</sub>

E = -188.518034825369

C	0.0000000000	0.0000000000	0.0000000000
O	0.0000000000	0.0000000000	1.2008282653
O	0.0000000000	0.0000000000	-1.2008282653

N<sub>2</sub>O

E = -184.606378972790

N	1.2544312195	-0.0001302420	0.0000000000
N	0.0862644639	0.0007498095	0.0000000000
O	-1.1464444908	-0.0004503540	0.0000000000

N<sub>2</sub>

E = -109.478583197086

N	0.0000000000	0.0000000000	-0.5656494464
N	0.0000000000	0.0000000000	0.5656494464

## 2. XYZ coordinates and total energies of CO, CO<sub>2</sub>, N<sub>2</sub>O and N<sub>2</sub> on TPSSh/DEF2-TZVPP level

CO

E = -113.359536065441  
 O 0.0000000000 0.0000000000 0.4466064731  
 C 0.0000000000 0.0000000000 -0.6826886828

CO<sub>2</sub>  
 E = -188.668329181925  
 C -0.0000008790 0.0000000000 0.0000021668  
 O -0.0000022600 0.0000000000 1.1632535348  
 O -0.0000022600 0.0000000000 -1.1632548357

N<sub>2</sub>O  
 E = -184.750013496356  
 N 0.0000001270 0.0000000000 -1.2008114242  
 N -0.0000002475 0.0000000000 -0.0741787479  
 O 0.0000001036 0.0000000000 1.1098350824

N<sub>2</sub>  
 E = -109.573207014820  
 N 0.0000000000 0.0000000000 -0.5474398249  
 N 0.0000000000 0.0000000000 0.5474398249

### 3. XYZ coordinates and total energies of copper clusters on BP86/DEF2-TZVPP level

Cu<sub>4</sub>  
 E = -6563.21346951231  
 Cu 0.0000000000 -1.1444602352 0.0001484234  
 Cu -2.1194292667 0.0000000000 -0.0001484234  
 Cu 0.0000000000 1.1444602352 0.0001484234  
 Cu 2.1194292667 0.0000000000 -0.0001484234

Cu<sub>5</sub>  
 E = -8204.04040514956  
 Cu 0.0122497205 -0.8363974786 0.0000000000  
 Cu -0.0061833951 -0.8350329820 -2.3629185727  
 Cu 0.0000585349 1.2532317213 -1.2082854981  
 Cu 0.0000585349 1.2532317213 1.2082854981  
 Cu -0.0061833951 -0.8350329820 2.3629185727

Cu<sub>6</sub>  
 E = -9844.88951901839  
 Cu 1.1943594042 0.7433020662 0.0026127962  
 Cu -0.0883815240 2.7341385075 -0.0003433232  
 Cu -1.2403974846 0.6634699498 -0.0035066743  
 Cu 0.0456972870 -1.4055265362 0.0035431685  
 Cu 2.4115448814 -1.2898067804 -0.0027716988  
 Cu -2.3228225640 -1.4455772068 0.0004657317

Cu<sub>7</sub>

E = -11485.7390509326

Cu	2.0632029960	-0.3059009880	0.0000000000
Cu	0.9274164973	1.8686015405	0.0000000000
Cu	-1.4909274638	1.4596637853	0.0000000000
Cu	-1.8489002748	-0.9652829842	0.0000000000
Cu	0.3469699804	-2.0567147974	0.0000000000
Cu	0.0011191324	-0.0001832782	-1.2783506415
Cu	0.0011191324	-0.0001832782	1.2783506415

Cu<sub>8</sub>

E = -13126.5860693714

Cu	0.1840916216	-1.5711625267	0.5151394484
Cu	0.1459091434	-1.2593894292	-1.8735289096
Cu	-0.1459091434	1.2593894292	-1.8735289096
Cu	-0.1840916216	1.5711625267	0.5151394484
Cu	-1.2593894186	-0.1459092330	1.8735288781
Cu	-1.5711624102	-0.1840915567	-0.5151394169
Cu	1.5711624102	0.1840915567	-0.5151394169
Cu	1.2593894186	0.1459092330	1.8735288781

Cu<sub>9</sub>

E = -14767.4018085174

Cu	-0.7040900133	-1.2452652327	-1.2103040884
Cu	-2.1892957021	0.6373354289	-0.9920840693
Cu	-1.0251604797	1.8153318984	0.9277694714
Cu	0.7727435755	0.1975421669	1.2622500546
Cu	0.2504140412	-2.1726817408	0.8493504256
Cu	-1.5631766269	-0.5721998552	1.0108083835
Cu	0.2398165451	1.0399365513	-0.9999551511
Cu	1.6667508094	-0.9236134061	-0.7621983789
Cu	2.5519978509	1.2236141893	-0.0856366474

Cu<sub>10</sub>

E = -16408.2593487501

Cu	0.0000000000	1.2743583566	-0.8615072613
Cu	0.0000000000	1.9559558405	1.5162340371
Cu	0.0000000000	0.0000000000	3.0338003702
Cu	0.0000000000	-1.9559558405	1.5162340371
Cu	0.0000000000	-1.2743583566	-0.8615072613
Cu	1.2743893391	0.0000000000	0.8615410334
Cu	-1.2743893391	0.0000000000	0.8615410334
Cu	1.9560669402	0.0000000000	-1.5162615936
Cu	0.0000000000	0.0000000000	-3.0338128013
Cu	-1.9560669402	0.0000000000	-1.5162615936

Cu<sub>11</sub>

E = -18049.0892567622

Cu	-0.6227086335	-2.3673021187	0.9481475914
Cu	-2.4981305490	-1.0044480904	-0.0754867625
Cu	-2.5417639595	1.3576706273	0.6203560673

Cu	-0.1932346721	2.2854740290	0.2428486776
Cu	1.8006729441	1.1060186006	1.0996905057
Cu	1.5715814438	-1.3428353734	0.4004361267
Cu	-0.4734278739	0.0183744930	0.8767485150
Cu	-0.3013062093	-1.4154990190	-1.2618452148
Cu	-1.3184192583	0.7776590150	-1.3897513445
Cu	1.1446097731	0.5855062085	-1.1516440048
Cu	3.4321269945	-0.0006183718	-0.3095001572

### Cu<sub>12</sub>

$$E = -19689.9462193662$$

Cu	-1.9787255231	0.7307503444	2.0808627296
Cu	-2.9708516440	-0.1802339690	0.0000000000
Cu	-1.9787255231	0.7307503444	-2.0808627296
Cu	0.6165850764	0.3370260580	-2.0000645613
Cu	1.6415978655	1.3485599938	0.0000000000
Cu	0.6165850764	0.3370260580	2.0000645613
Cu	-0.7693298396	0.8770036866	0.0000000000
Cu	-1.0783703580	-1.3334221539	1.2144484588
Cu	-1.0783703580	-1.3334221539	-1.2144484588
Cu	1.0661792422	-1.0998324786	0.0000000000
Cu	2.9567129926	-0.2071028648	1.2802751291
Cu	2.9567129926	-0.2071028648	-1.2802751291

### Cu<sub>13</sub>

$$E = -21330.7865810838$$

Cu	-0.9883748923	-0.9263635604	0.2104513602
Cu	1.3283456234	-1.4968565678	0.8105668493
Cu	-2.9902128089	0.2496537436	-0.4909068660
Cu	-1.7135946296	-1.1157002950	-2.1304218427
Cu	0.7562142769	-1.0067680059	-1.5279758093
Cu	2.9902128089	-0.2496537436	-0.4909068660
Cu	2.5188543419	0.2570740076	1.9722557485
Cu	0.0000000000	0.0000000000	2.3120611198
Cu	-2.5188543419	-0.2570740076	1.9722557485
Cu	-1.3283456234	1.4968565678	0.8105668493
Cu	-0.7562142769	1.0067680059	-1.5279758093
Cu	0.9883748923	0.9263635604	0.2104513602
Cu	1.7135946296	1.1157002950	-2.1304218427

### Cu<sub>14</sub>

$$E = -22971.6458666407$$

Cu	-0.9930182550	0.4754619216	0.9315176381
Cu	1.3086504783	1.0711408501	1.4662852974
Cu	-3.0028100452	-0.2044329177	-0.2186655645
Cu	-1.7165808574	-1.9340419830	1.0243887750
Cu	0.7402644835	-1.2726012625	1.0532783018
Cu	3.0028107448	-0.2044246520	0.2186652852
Cu	2.5118942668	2.2615827038	-0.2590415111
Cu	-0.0000035965	2.5945985633	-0.0000000754
Cu	-2.5119005907	2.2615758320	0.2590415059

Cu	-1.3086531884	1.0711373567	-1.4662851558
Cu	-0.7402608568	-1.2726034258	-1.0532784158
Cu	0.9930169701	0.4754644797	-0.9315174663
Cu	1.7165859570	-1.9340374325	-1.0243889411
Cu	0.0000044896	-3.3888200338	0.0000003224

### Cu<sub>15</sub>

E = -24612.4798136604

Cu	-0.8515418860	-0.4524549445	-0.6933051283
Cu	1.3332238917	-1.1227506817	-1.5467065580
Cu	-2.6281088343	0.3789457788	0.9141394902
Cu	-1.5961546218	1.8872641280	-0.8041141096
Cu	0.8941442375	1.2474782737	-1.0723199999
Cu	3.1495748471	0.1335174089	-0.5204485516
Cu	2.6634773640	-2.3405272286	0.0700550967
Cu	0.1386228219	-2.5880834889	0.1096492474
Cu	-2.4222854699	-2.0621321428	0.1130882490
Cu	-0.9008703056	-1.0559987066	1.7839647242
Cu	-0.3205744064	1.3101157131	1.2187414674
Cu	1.3171341066	-0.4962201850	0.8986533420
Cu	2.0999959798	1.9057427962	0.9034668366
Cu	0.2600842049	3.3618826547	0.0050328163
Cu	-3.1367219293	-0.1067793754	-1.3798969224

#### 4. XYZ coordinates and total energies of copper clusters on BP86/6-31g\* level

Cu<sub>4</sub>

E = -6561.90380126036

Cu	0.0000000000	-1.0730983794	0.0000004585
Cu	-1.8723158242	0.0000000000	-0.0000004585
Cu	0.0000000000	1.0730983794	0.0000004585
Cu	1.8723158242	0.0000000000	-0.0000004585

Cu<sub>5</sub>

E = -8202.43414301123

Cu	0.4127064140	-0.7364781526	0.0000000000
Cu	-0.2130231610	-0.7697562384	-2.0523165855
Cu	0.0066699540	1.1379953147	-1.0891278065
Cu	0.0066699540	1.1379953147	1.0891278065
Cu	-0.2130231610	-0.7697562384	2.0523165855

Cu<sub>6</sub>

E = -9842.98399944124

Cu	1.0903288126	0.6778636432	0.3058291820
Cu	-0.0777307018	2.3802106118	-0.3049015364
Cu	-1.1322337078	0.6052760411	0.3065528554
Cu	0.0416860358	-1.2825382348	0.3055368573
Cu	2.1000556325	-1.1231645584	-0.3063263118
Cu	-2.0221060714	-1.2576475029	-0.3066910464

Cu<sub>7</sub>

E = -11483.5955858380

Cu	1.8901213793	-0.2796917197	0.0000000000
Cu	0.8498900378	1.7112440065	0.0000000000
Cu	-1.3648982560	1.3371898424	0.0000000000
Cu	-1.6935338290	-0.8846256355	0.0000000000
Cu	0.3180676853	-1.8840614580	0.0000000000
Cu	0.0001764913	-0.0000275179	-1.1943698345
Cu	0.0001764913	-0.0000275179	1.1943698345

Cu<sub>8</sub>

E = -13124.1543676367

Cu	0.1679049382	-1.4382779045	0.4800273953
Cu	0.1330655083	-1.1420887221	-1.7433971702
Cu	-0.1330655083	1.1420887221	-1.7433971702
Cu	-0.1679049382	1.4382779045	0.4800273953
Cu	-1.1420886853	-0.1330655358	1.7433971543
Cu	-1.4382777592	-0.1679049014	-0.4800273794
Cu	1.4382777592	0.1679049014	-0.4800273794
Cu	1.1420886853	0.1330655358	1.7433971543

Cu<sub>9</sub>

E = -14764.6831973765

Cu	-0.6671987038	-1.1882461307	-1.1656926873
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Cu	-2.0371444718	0.6185533393	-0.9142256980
Cu	-0.9412119177	1.7014511200	0.8529388618
Cu	0.7556494366	0.1833505455	1.2226570509
Cu	0.2427174566	-2.0012822994	0.7672642521
Cu	-1.3756613755	-0.4874812516	0.8778051084
Cu	0.1870384269	0.9062146557	-0.8808444387
Cu	1.5426846492	-0.8687856967	-0.6802614286
Cu	2.2931264994	1.1362257178	-0.0796410207

### Cu<sub>10</sub>

E = -16405.2604937033

Cu	0.0000000000	1.1880347445	-0.7921031124
Cu	0.0000000000	1.8010964594	1.4164131157
Cu	0.0000000000	0.0000000000	2.7697032004
Cu	0.0000000000	-1.8010964594	1.4164131157
Cu	0.0000000000	-1.1880347445	-0.7921031124
Cu	1.1880780821	0.0000000000	0.7921236927
Cu	-1.1880780821	0.0000000000	0.7921236927
Cu	1.8010973814	0.0000000000	-1.4164245577
Cu	0.0000000000	0.0000000000	-2.7697214772
Cu	-1.8010973814	0.0000000000	-1.4164245577

### Cu<sub>11</sub>

E = -18045.8208234023

Cu	-0.6150094111	-2.2019562378	0.8829129062
Cu	-2.2914608289	-0.9251153093	-0.0763940643
Cu	-2.2779698472	1.2512060565	0.6194453138
Cu	-0.1632759324	2.1315613089	0.1687121923
Cu	1.6339791438	0.9999847257	1.0537335972
Cu	1.4543452565	-1.2485942244	0.3592108976
Cu	-0.4127337345	0.0069382809	0.7844794820
Cu	-0.2796237023	-1.3319992883	-1.1607774671
Cu	-1.2417552002	0.7220855441	-1.3013051742
Cu	1.0511060252	0.5411951955	-1.0606619143
Cu	3.1423982312	0.0546939481	-0.2693557692

### Cu<sub>12</sub>

E = -19686.3960402464

Cu	-1.8033663566	0.7008855359	1.9186835635
Cu	-2.7195753641	-0.1866584950	0.0000000000
Cu	-1.8033663566	0.7008855359	-1.9186835635
Cu	0.5597799016	0.2927729901	-1.8693204922
Cu	1.5089209948	1.2828224458	0.0000000000
Cu	0.5597799016	0.2927729901	1.8693204922
Cu	-0.6876147519	0.7814931924	0.0000000000
Cu	-1.0116336733	-1.2456961064	1.1441970719
Cu	-1.0116336733	-1.2456961064	-1.1441970719
Cu	0.9696183920	-1.0040445033	0.0000000000
Cu	2.7195454928	-0.1847687396	1.1629137419
Cu	2.7195454928	-0.1847687396	-1.1629137419

**Cu<sub>13</sub>**

E = -21326.9572377315

Cu	-0.8940721719	-0.8374078970	0.1893548004
Cu	1.2275152910	-1.4128710359	0.7726183189
Cu	-2.7520556150	0.2470209657	-0.4522625851
Cu	-1.5863661208	-1.0629269496	-1.9448471065
Cu	0.7113077554	-0.9245819797	-1.4345245194
Cu	2.7520556150	-0.2470209657	-0.4522625851
Cu	2.3275639665	0.2465533198	1.7950656715
Cu	0.0000000000	0.0000000000	2.1491908404
Cu	-2.3275639665	-0.2465533198	1.7950656715
Cu	-1.2275152910	1.4128710359	0.7726183189
Cu	-0.7113077554	0.9245819797	-1.4345245194
Cu	0.8940721719	0.8374078970	0.1893548004
Cu	1.5863661208	1.0629269496	-1.9448471065

**Cu<sub>14</sub>**

E = -22967.5333368396

Cu	-0.8989321101	0.4305235558	0.8493081301
Cu	1.2245476137	1.0369801634	1.3952277475
Cu	-2.7518152459	-0.2029253795	-0.2405214933
Cu	-1.5809689618	-1.7764392807	0.9765525201
Cu	0.7045705675	-1.1798185655	0.9776238034
Cu	2.7518158269	-0.2029178550	0.2405214704
Cu	2.3274177949	2.0467464475	-0.2675737827
Cu	-0.0000032257	2.3967128331	0.0000001563
Cu	-2.3274234548	2.0467401359	0.2675734072
Cu	-1.2245503435	1.0369768628	-1.3952277625
Cu	-0.7045674556	-1.1798204220	-0.9776236843
Cu	0.8989309120	0.4305259385	-0.8493081120
Cu	1.5809738131	-1.7764350350	-0.9765523735
Cu	0.0000042695	-3.1068493994	-0.0000000269

**Cu<sub>15</sub>**

E = -24608.0846626130

Cu	-0.7739064685	-0.4148692846	-0.6361542252
Cu	1.2476882396	-1.0803535031	-1.4581341461
Cu	-2.4357702953	0.3442982671	0.8526240674
Cu	-1.4815817255	1.7472423665	-0.7405638076
Cu	0.8239894812	1.1537186520	-1.0009782952
Cu	2.9024783133	0.1303270532	-0.5008808628
Cu	2.4771702616	-2.1197697458	0.0976992956
Cu	0.1258559612	-2.3909787385	0.0873186578
Cu	-2.2600047856	-1.8790630680	0.1065241062
Cu	-0.8331939392	-1.0176033299	1.6730735649
Cu	-0.3068649070	1.2226556433	1.1373859307
Cu	1.1923012891	-0.4480093229	0.8138261489
Cu	1.9452276611	1.7517533402	0.8393560654
Cu	0.2604270191	3.0975038937	0.0080279956
Cu	-2.8838161050	-0.0968522232	-1.2791244956

## 5. XYZ coordinates and total energies of copper clusters on BP86/cc-PVTZ level

Cu<sub>4</sub>

E = -6563.38905808121

Cu	0.0000000000	-1.1418640655	0.0001486587
Cu	-2.1139892700	0.0000000000	-0.0001486587
Cu	0.0000000000	1.1418640655	0.0001486587
Cu	2.1139892700	0.0000000000	-0.0001486587

Cu<sub>5</sub>

E = -8204.25942239222

Cu	0.0133840700	-0.8402830698	0.0000000000
Cu	-0.0066997485	-0.8303475564	-2.3590377344
Cu	0.0000077135	1.2504890913	-1.2068526541
Cu	0.0000077135	1.2504890913	1.2068526541
Cu	-0.0066997485	-0.8303475564	2.3590377344

Cu<sub>6</sub>

E = -9845.15160813977

Cu	1.1957787440	0.7440649746	0.0047802600
Cu	-0.0890783395	2.7299618249	-0.0005855387
Cu	-1.2412558043	0.6639235871	-0.0050108982
Cu	0.0459195367	-1.4060195454	0.0027689243
Cu	2.4074753061	-1.2887319818	-0.0035270828
Cu	-2.3188394430	-1.4431988593	0.0015743355

Cu<sub>7</sub>

E = -11486.0407974776

Cu	2.0609210394	-0.3058711221	0.0000000000
Cu	0.9267699269	1.8661659037	0.0000000000
Cu	-1.4897753011	1.4585284646	0.0000000000
Cu	-1.8464405963	-0.9645792133	0.0000000000
Cu	0.3468866296	-2.0544859663	0.0000000000
Cu	0.0008191507	0.0001209667	-1.2900812342
Cu	0.0008191507	0.0001209667	1.2900812342

Cu<sub>8</sub>

E = -13126.9321413876

Cu	0.1849879288	-1.5782153069	0.5157659799
Cu	0.1458956927	-1.2599932278	-1.8699842761
Cu	-0.1458956927	1.2599932278	-1.8699842761
Cu	-0.1849879288	1.5782153069	0.5157659799
Cu	-1.2599931809	-0.1458957775	1.8699842915
Cu	-1.5782151371	-0.1849878636	-0.5157659953
Cu	1.5782151371	0.1849878636	-0.5157659953
Cu	1.2599931809	0.1458957775	1.8699842915

Cu<sub>9</sub>

E = -14767.7906322808

Cu	-0.7067166295	-1.2494584596	-1.2177714705
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Cu	-2.1919334399	0.6308272438	-0.9914802520
Cu	-1.0213707855	1.8147696661	0.9261324536
Cu	0.7758870874	0.2023500120	1.2719025315
Cu	0.2506609998	-2.1678748750	0.8477549387
Cu	-1.5672800280	-0.5735176908	1.0151117014
Cu	0.2400710716	1.0455208205	-1.0047825374
Cu	1.6649467435	-0.9213443958	-0.7655359117
Cu	2.5557349807	1.2187276788	-0.0813314535

### Cu<sub>10</sub>

E = -16408.6888822847

Cu	0.0000000000	1.2819013171	-0.8632375526
Cu	0.0000000000	1.9521693291	1.5158884411
Cu	0.0000000000	0.0000000000	3.0403925788
Cu	0.0000000000	-1.9521693291	1.5158884411
Cu	0.0000000000	-1.2819013171	-0.8632375526
Cu	1.2819351560	0.0000000000	0.8632565203
Cu	-1.2819351560	0.0000000000	0.8632565203
Cu	1.9522848230	0.0000000000	-1.5159168121
Cu	0.0000000000	0.0000000000	-3.0403737721
Cu	-1.9522848230	0.0000000000	-1.5159168121

## 6. XYZ coordinates and total energies of copper clusters on B3PW91/LANL2DZ level

### Cu<sub>4</sub>

E = -784.809405395921

Cu	0.0000000000	-1.1497140594	-0.0006912781
Cu	-2.1628167420	0.0000000000	0.0006912781
Cu	0.0000000000	1.1497140594	-0.0006912781
Cu	2.1628167420	0.0000000000	0.0006912781

### Cu<sub>5</sub>

E = -981.033668986766

Cu	0.0040986792	-0.8464643167	0.0000000000
Cu	-0.0019885273	-0.8475481652	-2.3973135807
Cu	-0.0000608123	1.2707803236	-1.2370752003
Cu	-0.0000608123	1.2707803236	1.2370752003
Cu	-0.0019885273	-0.8475481652	2.3973135807

### Cu<sub>6</sub>

E = -1177.27954315420

Cu	1.1910914766	-0.8018337742	0.0035538166
Cu	2.4917584725	1.2193479131	-0.0008581074
Cu	0.0996102498	1.4324436070	-0.0018584752
Cu	-1.2888422058	-0.6306210978	0.0014328563
Cu	-0.1929529278	-2.7677209343	-0.0024890038
Cu	-2.3006650653	1.5483842862	0.0002189135

### Cu<sub>7</sub>

E = -1373.51545156190

Cu	1.8150374045	1.1099865964	0.0000000000
Cu	-0.4920686427	2.0701265232	0.0000000000
Cu	-2.1206891284	0.1726546527	0.0000000000
Cu	-0.8191413920	-1.9650080764	0.0000000000
Cu	1.6176788282	-1.3836207764	0.0000000000
Cu	-0.0004085348	-0.0020694598	-1.3144895048
Cu	-0.0004085348	-0.0020694598	1.3144895048

### Cu<sub>8</sub>

E = -1569.76049627045

Cu	0.5906376380	-1.5049288511	0.5234831703
Cu	0.4867150449	-1.2223159259	-1.8927870474
Cu	-0.4867150449	1.2223159259	-1.8927870474
Cu	-0.5906376380	1.5049288511	0.5234831703
Cu	-1.2223159680	-0.4867151290	1.8927870249
Cu	-1.5049288068	-0.5906375827	-0.5234831479
Cu	1.5049288068	0.5906375827	-0.5234831479
Cu	1.2223159680	0.4867151290	1.8927870249

### Cu<sub>9</sub>

E = -1765.97092063351

Cu	-0.7094767616	-1.2732332789	-1.2727767295
Cu	-2.2765723641	0.5937685721	-1.0213033151
Cu	-1.0318684285	1.8416692615	0.9884162767
Cu	0.8014444017	0.2033711651	1.3054611104
Cu	0.2730008595	-2.2123675466	0.8542059074
Cu	-1.5649707185	-0.5893741215	1.0096273391
Cu	0.2006072901	1.0550265891	-1.0027981089
Cu	1.7009941073	-0.8910049715	-0.8019167574
Cu	2.6068416141	1.2721443308	-0.0589157227

### Cu<sub>10</sub>

E = -1962.22102152540

Cu	0.0000000000	1.2924823760	-0.8775531043
Cu	0.0000000000	1.9954582055	1.5484557826
Cu	0.0000000000	0.0000000000	3.1226996225
Cu	0.0000000000	-1.9954582055	1.5484557826
Cu	0.0000000000	-1.2924823760	-0.8775531043
Cu	1.2924813526	0.0000000000	0.8775554135
Cu	-1.2924813526	0.0000000000	0.8775554135
Cu	1.9954580762	0.0000000000	-1.5484563411
Cu	0.0000000000	0.0000000000	-3.1227031238
Cu	-1.9954580762	0.0000000000	-1.5484563411

### Cu<sub>11</sub>

E = -2158.44465553783

Cu	-0.6259549532	-2.3775935476	0.9906547746
Cu	-2.5820823343	-1.0194694340	-0.0988610145
Cu	-2.6256760726	1.3684277109	0.6520823290
Cu	-0.1754856489	2.3299953819	0.2929096414

Cu	1.8610327601	1.1092086868	1.1201691699
Cu	1.6109817526	-1.3761521058	0.3931729374
Cu	-0.5008464753	0.0280645063	0.8700788304
Cu	-0.3209104699	-1.4302417640	-1.3123016253
Cu	-1.3433303498	0.8135566595	-1.4192185379
Cu	1.1782407216	0.5878454556	-1.1769313509
Cu	3.5240310698	-0.0336415495	-0.3117551540

$\text{Cu}_{12}$

E = -2354.69660657323

Cu	-2.0589975379	0.7657468586	2.0958243826
Cu	-3.0644719699	-0.1718212233	0.0000000000
Cu	-2.0589975379	0.7657468586	-2.0958243826
Cu	0.6513771628	0.3621106150	-2.0270044257
Cu	1.6891865224	1.3623504005	0.0000000000
Cu	0.6513771628	0.3621106150	2.0270044257
Cu	-0.7848721845	0.8645143089	0.0000000000
Cu	-1.0948843485	-1.3637535000	1.2377107207
Cu	-1.0948843485	-1.3637535000	-1.2377107207
Cu	1.0997979463	-1.1231591534	0.0000000000
Cu	3.0326845664	-0.2300461399	1.3191425392
Cu	3.0326845664	-0.2300461399	-1.3191425392

$\text{Cu}_{13}$

E = -2550.93156867191

Cu	-1.0122701174	-0.9211879354	0.2076833298
Cu	1.3561375298	-1.5286912202	0.8213784112
Cu	-3.0756528798	0.2525536796	-0.4927049807
Cu	-1.7762965744	-1.1432846120	-2.1663025397
Cu	0.7748174217	-1.0219271602	-1.5566479757
Cu	3.0756528798	-0.2525536796	-0.4927049807
Cu	2.5769361768	0.3008747269	2.0115705333
Cu	0.0000000000	0.0000000000	2.3500464435
Cu	-2.5769361768	-0.3008747269	2.0115705333
Cu	-1.3561375298	1.5286912202	0.8213784112
Cu	-0.7748174217	1.0219271602	-1.5566479757
Cu	1.0122701174	0.9211879354	0.2076833298
Cu	1.7762965744	1.1432846120	-2.1663025397

$\text{Cu}_{14}$

E = -2747.18570700653

Cu	-1.0141136706	0.9267838877	-0.4856639448
Cu	1.3272946371	1.4888438524	-1.0857251256
Cu	-3.0826961928	-0.2116288605	0.2052022491
Cu	-1.7562709495	1.0541982781	1.9767999609
Cu	0.7558396674	1.0596614365	1.2984886872
Cu	3.0826961928	0.2116288605	0.2052022491
Cu	2.5689701336	-0.2897675483	-2.3175226021
Cu	0.0000000000	0.0000000000	-2.6592176279
Cu	-2.5689701336	0.2897675483	-2.3175226021
Cu	-1.3272946371	-1.4888438524	-1.0857251256

Cu	-0.7558396674	-1.0596614365	1.2984886872
Cu	1.0141136706	-0.9267838877	-0.4856639448
Cu	1.7562709495	-1.0541982781	1.9767999609
Cu	0.0000000000	0.0000000000	3.4760591939

Cu<sub>15</sub>

E = -2943.41642468972

Cu	-0.8723370986	-0.4546690801	-0.6446041313
Cu	1.3105039851	-1.1307427238	-1.5915956154
Cu	-2.6927753844	0.4040296947	0.9264616849
Cu	-1.6098457510	1.9314164218	-0.8255972790
Cu	0.9155923798	1.2768741447	-1.0731954655
Cu	3.2076490452	0.1186309212	-0.5691700127
Cu	2.6971097483	-2.4156302332	0.0566231264
Cu	0.1266899278	-2.6457078755	0.1145598678
Cu	-2.4763568562	-2.1147144965	0.1328129974
Cu	-0.9218410923	-1.0399980661	1.8481251260
Cu	-0.3189690298	1.3535288812	1.2370615090
Cu	1.3370991179	-0.5112336031	0.8692267512
Cu	2.1673118548	1.9200250460	0.9427584830
Cu	0.2903262665	3.4534300857	0.0092405366
Cu	-3.1601571132	-0.1452391171	-1.4327075784

## 7. XYZ coordinates and total energies of copper clusters on TPSSh/DEF2-TZVPP level

Cu<sub>4</sub>

E = -6562.16783496893

Cu	0.0000000000	-1.1370550939	0.0001462496
Cu	-2.1212572184	0.0000000000	-0.0001462496
Cu	0.0000000000	1.1370550939	0.0001462496
Cu	2.1212572184	0.0000000000	-0.0001462496

Cu<sub>5</sub>

E = -8202.73340395565

Cu	0.0077020012	-0.8176023460	0.0000000000
Cu	-0.0040502896	-0.8385422590	-2.3613348799
Cu	0.0001992890	1.2473434319	-1.2111017122
Cu	0.0001992890	1.2473434319	1.2111017122
Cu	-0.0040502896	-0.8385422590	2.3613348799

Cu<sub>6</sub>

E = -9843.32012733808

Cu	1.1862729729	0.7380062561	0.0037710783
Cu	-0.0884308066	2.7335662569	-0.0009185486
Cu	-1.2321590376	0.6590306474	-0.0039441161
Cu	0.0454365465	-1.3960608151	0.0036135251
Cu	2.4111789632	-1.2894489574	-0.0032892632
Cu	-2.3222986384	-1.4450933878	0.0007673245

Cu<sub>7</sub>

E = -11483.9209814540

Cu	2.0622387850	-0.3056204147	0.0000000000
Cu	0.9269144763	1.8675910070	0.0000000000
Cu	-1.4899775660	1.4589222660	0.0000000000
Cu	-1.8480059037	-0.9647474614	0.0000000000
Cu	0.3468564595	-2.0556858776	0.0000000000
Cu	0.0009868745	-0.0002297597	-1.2493072628
Cu	0.0009868745	-0.0002297597	1.2493072628

Cu<sub>8</sub>

E = -13124.5069459596

Cu	0.1811672970	-1.5496006125	0.5115479995
Cu	0.1462186328	-1.2579066401	-1.8735952033
Cu	-0.1462186328	1.2579066401	-1.8735952033
Cu	-0.1811672970	1.5496006125	0.5115479995
Cu	-1.2579065575	-0.1462187696	1.8735952209
Cu	-1.5496005805	-0.1811672590	-0.5115480172
Cu	1.5496005805	0.1811672590	-0.5115480172
Cu	1.2579065575	0.1462187696	1.8735952209

Cu<sub>9</sub>

E = -14765.0636938934

Cu	-0.6993317323	-1.2385677354	-1.1968381992
Cu	-2.1914967065	0.6383238985	-0.9916277453
Cu	-1.0013527746	1.8164278862	0.9272072497
Cu	0.7667573064	0.1783959068	1.2419564361
Cu	0.2448326839	-2.1766591626	0.8516154061
Cu	-1.5448778896	-0.5547023517	0.9922937087
Cu	0.2276909636	1.0142140333	-0.9902779423
Cu	1.6693427135	-0.9149576513	-0.7573564485
Cu	2.5284354356	1.2375251761	-0.0769724654

Cu<sub>10</sub>

E = -16405.6646660546

Cu	0.0000000000	1.2501164000	-0.8652013907
Cu	0.0000000000	1.9587669725	1.5014544975
Cu	0.0000000000	0.0000000000	3.0226832529
Cu	0.0000000000	-1.9587669725	1.5014544975
Cu	0.0000000000	-1.2501164000	-0.8652013907
Cu	1.2501353459	0.0000000000	0.8652252911
Cu	-1.2501353459	0.0000000000	0.8652252911
Cu	1.9588184666	0.0000000000	-1.5014622738
Cu	0.0000000000	0.0000000000	-3.0227155011
Cu	-1.9588184666	0.0000000000	-1.5014622738

Cu<sub>11</sub>

E = -18046.2359168784

Cu	-0.6234417799	-2.3448927504	0.9634019191
Cu	-2.4931518138	-1.0031025516	-0.0869825735
Cu	-2.5277710751	1.3457297767	0.6347632812

Cu	-0.1869814207	2.2781064205	0.2375185747
Cu	1.7913417296	1.0802727034	1.1069435889
Cu	1.5671521383	-1.3255131092	0.4002670202
Cu	-0.4736993772	0.0181063144	0.8236823759
Cu	-0.2991484516	-1.4122004222	-1.2498874587
Cu	-1.3202639331	0.7744620806	-1.3815922755
Cu	1.1386639006	0.5834502862	-1.1310252788
Cu	3.4273000829	0.0055812518	-0.3170891736

### Cu<sub>12</sub>

E = -19686.8358909331

Cu	-1.9705979528	0.7464659705	2.0640385025
Cu	-2.9605735159	-0.1940092931	0.0000000000
Cu	-1.9705979528	0.7464659705	-2.0640385025
Cu	0.6133135436	0.3396397424	-1.9920647381
Cu	1.6335585291	1.3341099439	0.0000000000
Cu	0.6133135436	0.3396397424	1.9920647381
Cu	-0.7636143877	0.8231629141	0.0000000000
Cu	-1.0761148468	-1.3249477727	1.2124511392
Cu	-1.0761148468	-1.3249477727	-1.2124511392
Cu	1.0589632338	-1.0687568572	0.0000000000
Cu	2.9492323263	-0.2084112941	1.2764276034
Cu	2.9492323263	-0.2084112941	-1.2764276034

### Cu<sub>13</sub>

E = -21327.4186417582

Cu	-0.9812950006	-0.8835229332	0.2018280570
Cu	1.3192143245	-1.4893834109	0.8132195431
Cu	-2.9794200008	0.2599231384	-0.4927428271
Cu	-1.7032982356	-1.1303698917	-2.1137890459
Cu	0.7605682875	-0.9889168353	-1.5186390545
Cu	2.9794200008	-0.2599231384	-0.4927428271
Cu	2.5106013999	0.2636124606	1.9609632172
Cu	0.0000000000	0.0000000000	2.2983202204
Cu	-2.5106013999	-0.2636124606	1.9609632172
Cu	-1.3192143245	1.4893834109	0.8132195431
Cu	-0.7605682875	0.9889168353	-1.5186390545
Cu	0.9812950006	0.8835229332	0.2018280570
Cu	1.7032982356	1.1303698917	-2.1137890459

### Cu<sub>14</sub>

E = -22968.0202145201

Cu	-0.9853888769	0.4742055128	0.8921404839
Cu	1.2991349762	1.0722801222	1.4611039432
Cu	-2.9837534150	-0.2155245739	-0.2360541163
Cu	-1.6924390799	-1.9160280652	1.0522563301
Cu	0.7440799280	-1.2651756748	1.0212962494
Cu	2.9837540321	-0.2155165854	0.2360539922
Cu	2.5102837854	2.2468789086	-0.2573176585
Cu	-0.0000034371	2.5857751063	0.0000000625

Cu	-2.5102900532	2.2468720414	0.2573174282
Cu	-1.2991376162	1.0722766106	-1.4611039733
Cu	-0.7440766925	-1.2651778668	-1.0212962271
Cu	0.9853874961	0.4742081385	-0.8921402855
Cu	1.6924441997	-1.9160233376	-1.0522564432
Cu	0.0000047532	-3.3790503365	0.0000002143

**Cu<sub>15</sub>**

E = -24608.5969961572

Cu	-0.8469888085	-0.4455586351	-0.6342150400
Cu	1.3041654683	-1.1179079531	-1.5414312251
Cu	-2.6205845962	0.3766263209	0.8918685387
Cu	-1.5778127672	1.8738544682	-0.8138453142
Cu	0.8874944388	1.2446302063	-1.0365719807
Cu	3.1272011553	0.1359924491	-0.5407788817
Cu	2.6557106374	-2.3274873746	0.0558863295
Cu	0.1347142361	-2.5756197037	0.1132600676
Cu	-2.4166352279	-2.0525532391	0.1292407246
Cu	-0.8931385856	-1.0415893544	1.7869482359
Cu	-0.3205133499	1.3087277268	1.1981272560
Cu	1.3009862851	-0.4930005921	0.8535808510
Cu	2.0914597869	1.8862485175	0.9239847353
Cu	0.2661981123	3.3587219608	0.0158928423
Cu	-3.0922567851	-0.1310847975	-1.4019471392

## **8. XYZ coordinates and total energies of copper clusters on BP86/LANL2DZ level**

Cu<sub>4</sub>

E = -785.050980641802

Cu	0.0000000000	-1.1475175059	-0.0000199990
Cu	-2.1301174175	0.0000000000	0.0000198267
Cu	0.0000000000	1.1475175059	-0.0000199990
Cu	2.1301174175	0.0000000000	0.0000198267

Cu<sub>5</sub>

E = -981.337163080531

Cu	-0.0875293524	-0.8423980387	0.0000000000
Cu	-0.0505795193	-0.8376176874	2.3695166603
Cu	0.0943442326	1.2588163164	1.2187183207
Cu	0.0943442326	1.2588163164	-1.2187183207
Cu	-0.0505795193	-0.8376176874	-2.3695166603

Cu<sub>6</sub>

E = -1177.64626824945

Cu	1.3846935721	-0.3570698149	0.0623734782
Cu	1.9167682951	1.9560527775	-0.0637016275
Cu	-0.3850341464	1.3772076478	0.0616381902
Cu	-0.9882262035	-1.0086396083	0.0092802977
Cu	0.7308335661	-2.6448931002	-0.0346342012
Cu	-2.6590350833	0.6773420981	-0.0349561374

Cu<sub>7</sub>

E = -1373.94697585624

Cu	1.3517771343	-1.6078474090	0.0000000000
Cu	-1.1095500527	-1.7814197465	0.0000000000
Cu	-2.0389440473	0.5015268050	0.0000000000
Cu	-0.1543211833	2.0944107981	0.0000000000
Cu	1.9450237317	0.7922485383	0.0000000000
Cu	0.0030068653	0.0005407022	1.3391936970
Cu	0.0030068653	0.0005407022	-1.3391936970

Cu<sub>8</sub>

E = -1570.25714779841

Cu	0.0976780350	-1.6046847983	0.5170340243
Cu	0.0753859633	-1.2872025553	-1.8873209310
Cu	-0.0753859633	1.2872025553	-1.8873209310
Cu	-0.0976780350	1.6046847983	0.5170340243
Cu	-1.2872023545	-0.0753861022	1.8873201054
Cu	-1.6046847307	-0.0976779632	-0.5170349594
Cu	1.6046847307	0.0976779632	-0.5170349594
Cu	1.2872023545	0.0753861022	1.8873201054

Cu<sub>9</sub>

E = -1766.53034599445

Cu	-0.6911257142	-1.2018628177	-1.3047274383
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Cu	-2.1909752332	0.6857666554	-1.0384541080
Cu	-1.0378511316	1.8081562001	0.9935549490
Cu	0.7480052517	0.1501752392	1.3181401844
Cu	0.2192440839	-2.2225816324	0.7798394938
Cu	-1.6160113295	-0.6108204437	0.9603160237
Cu	0.2695276035	1.0992157268	-0.9680625582
Cu	1.6930427623	-0.9072876501	-0.7804716530
Cu	2.6061437072	1.1992387226	0.0398651066

$\text{Cu}_{10}$

E = -1962.84379365458

Cu	0.0000000000	1.3105124873	-0.8624121000
Cu	0.0000000000	1.9644169457	1.5413581791
Cu	0.0000000000	0.0000000000	3.0863178781
Cu	0.0000000000	-1.9644169457	1.5413581791
Cu	0.0000000000	-1.3105124873	-0.8624121000
Cu	1.3105972035	0.0000000000	0.8633399621
Cu	-1.3105972035	0.0000000000	0.8633399621
Cu	1.9646651969	0.0000000000	-1.5412570969
Cu	0.0000000000	0.0000000000	-3.0883748777
Cu	-1.9646651969	0.0000000000	-1.5412570969

$\text{Cu}_{11}$

E = -2159.13238927043

Cu	-0.6708861905	-2.3788486471	0.9279281640
Cu	-2.5624403194	-0.9540470939	-0.0877582764
Cu	-2.5537019994	1.4078197547	0.6663841218
Cu	-0.1333060457	2.3066804474	0.2933451609
Cu	1.8633508365	1.0675048091	1.1149278763
Cu	1.5604449935	-1.4131053177	0.3599245348
Cu	-0.4798758529	0.0244548939	0.9379820073
Cu	-0.3492945795	-1.3972587382	-1.3218040770
Cu	-1.3184926350	0.8476566461	-1.3940567233
Cu	1.1722575914	0.5834548208	-1.1790613390
Cu	3.4719442010	-0.0943115751	-0.3178114493

$\text{Cu}_{12}$

E = -2355.44841977539

Cu	-2.0129223185	0.7596857470	2.0944776697
Cu	-3.0234370672	-0.1372482463	0.0000000000
Cu	-2.0129223185	0.7596857470	-2.0944776697
Cu	0.6393537114	0.3383432588	-2.0121051860
Cu	1.6838885167	1.3568570738	0.0000000000
Cu	0.6393537114	0.3383432588	2.0121051860
Cu	-0.7680266910	0.9287487717	0.0000000000
Cu	-1.1003869300	-1.3469406013	1.2270016745
Cu	-1.1003869300	-1.3469406013	-1.2270016745
Cu	1.0744658070	-1.1531272423	0.0000000000
Cu	2.9905095733	-0.2487036176	1.2995113887
Cu	2.9905095733	-0.2487036176	-1.2995113887

**Cu<sub>13</sub>**

E = -2551.74741676093

Cu	-0.9878446964	-0.9604987564	0.2133979074
Cu	1.3614631789	-1.5159078703	0.8158722882
Cu	-3.0372147584	0.2218995049	-0.4882343431
Cu	-1.7370237546	-1.1402896198	-2.1533541244
Cu	0.7772837990	-1.0204502515	-1.5483845273
Cu	3.0372147584	-0.2218995049	-0.4882343431
Cu	2.5434467937	0.3071140982	1.9934913178
Cu	0.0000000000	0.0000000000	2.3344249658
Cu	-2.5434467937	-0.3071140982	1.9934913178
Cu	-1.3614631789	1.5159078703	0.8158722882
Cu	-0.7772837990	1.0204502515	-1.5483845273
Cu	0.9878446964	0.9604987564	0.2133979074
Cu	1.7370237546	1.1402896198	-2.1533541244

**Cu<sub>14</sub>**

E = -2748.06550255686

Cu	-0.9859378126	0.4783638136	0.9642091475
Cu	1.3467716789	1.0799348305	1.4682589768
Cu	-3.0538438068	-0.2009509491	-0.1614496799
Cu	-1.7299711756	-1.9620107934	1.0550030786
Cu	0.7691123542	-1.2885210414	1.0672505808
Cu	3.0538450380	-0.2009340115	0.1614493222
Cu	2.5323333416	2.2925652011	-0.3203640074
Cu	-0.0000073943	2.6337137774	0.0000001976
Cu	-2.5323461794	2.2925511676	0.3203638297
Cu	-1.3467774228	1.0799275461	-1.4682588220
Cu	-0.7691052492	-1.2885254326	-1.0672509944
Cu	0.9859350712	0.4783691613	-0.9642090811
Cu	1.7299820180	-1.9620017568	-1.0550030747
Cu	0.0000095388	-3.4324815130	0.0000005200

**Cu<sub>15</sub>**

E = -2944.36022182628

Cu	-0.8530359011	-0.4373004319	-0.6751617298
Cu	1.3075675154	-1.1551867989	-1.5795683678
Cu	-2.6697418745	0.4390241474	0.9288667519
Cu	-1.5779478869	1.9349080695	-0.8258664462
Cu	0.9367323047	1.2463263616	-1.1029812122
Cu	3.1806717643	0.0742040211	-0.5415222338
Cu	2.6373247548	-2.4230200946	0.0756120926
Cu	0.0914753325	-2.6237723552	0.1261330961
Cu	-2.4754624563	-2.0538975750	0.1234117593
Cu	-0.9386716469	-1.0281127506	1.8320040465
Cu	-0.3084887431	1.3419070838	1.2348682707
Cu	1.3215336187	-0.5206121574	0.9131177667
Cu	2.1622749672	1.8875268382	0.9156399699
Cu	0.3232513340	3.4018040850	-0.0094086390
Cu	-3.1374830829	-0.0837984428	-1.4151451250

## 9. XYZ coordinates and total energies of Cu<sub>x</sub>-N<sub>2</sub>O clusters on BP86/LANL2DZ level

Cu<sub>4</sub>-N<sub>2</sub>O.1

E = -969.688198078324

Cu	0.5064584556	0.0069252290	-0.0101948290
Cu	-0.7440847056	2.1177868183	0.0009688890
Cu	-1.8088050323	-0.0087611532	0.0068304611
Cu	-0.7200671491	-2.1221439892	0.0008145272
N	2.4003483993	0.0101436571	-0.0186739036
N	3.5716037064	0.0129193345	0.0011479805
O	4.8067706082	0.0062693762	0.0226208215

Cu<sub>4</sub>-N<sub>2</sub>O.2

E = -969.674538648581

Cu	-0.0603412079	-0.7658726867	-0.8300687049
Cu	-1.7072645982	1.0549915066	0.8560996881
Cu	0.6583097376	0.9231392074	0.6747314678
Cu	2.2559622936	-0.3929181795	-0.5218988637
N	-3.9932348207	-0.0651003537	-0.1594182990
N	-2.8020218973	-0.1840114444	-0.2784712156
O	-2.0029911945	-1.0118041242	-1.0431632589

Cu<sub>4</sub>-N<sub>2</sub>O.3

E = -969.672475152246

Cu	0.4995607363	0.2582009882	0.1314444807
Cu	-1.1274939412	2.0808887701	0.2893265732
Cu	-1.7520470973	-0.1976658761	-0.0688564661
Cu	-0.2333477306	-2.0441019565	-0.2646300224
N	4.3936858372	-0.5499414102	-0.5957367086
N	3.4995855184	0.0424154243	-0.1388672328
O	2.5287212099	0.6631237728	0.3387590549

Cu<sub>4</sub>-N<sub>2</sub>O.4

E = -969.673651738882

Cu	0.7760449036	-1.1390538829	-0.0007491539
Cu	-1.2714080178	-0.0000951122	0.7031579661
Cu	0.7756402027	1.1390200292	-0.0005609264
Cu	2.8296727188	0.0004599798	-0.6208108244
N	-3.2349981582	-0.0010631248	1.0667326270
N	-4.1985139409	-0.0004647192	0.3667312817
O	-4.9304551998	0.0013492588	-0.6403883810

Cu<sub>4</sub>-N<sub>2</sub>O.5

E = -969.788635147579

Cu	1.0954286903	-1.1702084994	-0.1770145373
Cu	-2.2259574452	-0.0479211512	-0.1327677544
Cu	1.0755303723	1.1963550443	-0.1648816862
Cu	3.1725999660	0.0314305597	-0.1624709329
N	-5.1806286002	-0.1322535969	-0.0662457180
N	-4.0338352213	-0.0996759539	-0.0900750538

O -0.4600885283 -0.0002047664 -0.1786102925

Cu<sub>5</sub>-N<sub>2</sub>O.1

E = -1165.97778823279

Cu	-0.6497351296	-0.1770145656	0.3272895253
Cu	-2.6013747410	1.2608582476	0.1115721090
Cu	-0.4751331550	2.1343395570	-0.3242084173
Cu	1.5833765872	0.8584329091	0.0356806015
Cu	1.6026136338	-1.4877534052	0.3136525856
N	0.5579493295	-3.0987966034	0.7526238409
N	-0.6423076715	-3.0030334426	0.9223276150
O	-1.4842546949	-1.9401897469	0.8510513744

Cu<sub>5</sub>-N<sub>2</sub>O.2

E = -1165.96497355250

Cu	-0.4218767052	0.2700907798	0.2081498861
Cu	1.7740136499	-0.4778430292	-0.3576000439
Cu	-0.1475190769	-1.6426099842	-1.2423833437
Cu	-2.3903096150	-0.8350946446	-0.6566011743
Cu	-2.6074586171	1.0573203386	0.7666231309
N	3.6183240213	0.0214175405	0.0377851339
N	4.2677594436	0.7845059810	0.6710019178
O	4.6419925183	1.6944998991	1.4275007875

Cu<sub>5</sub>-N<sub>2</sub>O.3

E = -1165.98087241608

Cu	0.6219131772	-1.0416021823	0.2524384605
Cu	-0.7663971420	-2.8361877849	0.9822249635
Cu	-1.8176653207	-0.8514438069	0.2692117101
Cu	-0.1342956794	1.1736536679	-0.5053971081
Cu	2.1492637605	0.6745582254	-0.3908602820
N	-2.7121009323	0.7518518135	-0.2833613689
N	-2.0263863388	1.7587590886	-0.6576738497
O	-2.3522191325	2.9376705766	-1.0689122342

Cu<sub>5</sub>-N<sub>2</sub>O.4

E = -1166.04270091846

Cu	0.4480843447	-0.4635967517	0.3716089637
Cu	-1.4473555459	-1.8473598594	0.3169332627
Cu	-1.9963906019	0.4622489803	-0.4141676479
Cu	0.8290728520	1.5165369982	-0.9083014007
Cu	2.6478444302	0.5367592464	0.2086904128
N	-4.7669787264	0.2482735521	0.8367991055
N	-3.7347741857	0.3229390352	0.3495399343
O	-0.9177517528	1.4818487073	-1.4694791216

Cu<sub>6</sub>-N<sub>2</sub>O.1

E = -1362.26340445270

Cu	0.2082846852	-1.3776191945	0.0989132657
Cu	-2.0551578703	-0.6436575617	-0.1431246436

Cu	-0.3097098697	0.9895681646	-0.1850673999
Cu	2.0387133131	0.2856055374	0.0813050067
Cu	2.4901717165	-2.0267178725	0.3613651379
Cu	1.4704413072	2.5727825475	-0.2114441831
N	-5.7181020839	1.0007459809	-0.3964995142
N	-5.0320607831	0.0570092609	-0.3315822324
O	-4.1573695737	-0.8383917209	-0.2595542957

#### Cu<sub>6</sub>-N<sub>2</sub>O.2

E = -1362.27643103152

Cu	0.6660630625	-1.0091499862	-0.1400460543
Cu	-1.0142320105	-2.6629272159	0.2934524253
Cu	-1.7357227005	-0.4406950536	0.0600709350
Cu	-0.0954318318	1.3607527842	-0.2116416628
Cu	2.1411247771	1.4028605711	0.5286000774
Cu	-2.4052429871	1.8487782341	-0.1632087923
N	3.7077924610	0.3947673468	-0.0844372462
N	3.5531506066	-0.7297925871	-0.5165134523
O	2.5161545477	-1.5258796116	-0.7298204811

#### Cu<sub>6</sub>-N<sub>2</sub>O.3

E = -1362.26424232742

Cu	1.0157574230	-0.0127117211	-0.2208821906
Cu	0.8837570766	2.3478508574	0.3168715136
Cu	-1.1595686332	1.2291351141	0.0038664300
Cu	-1.2040380867	-1.1952051843	-0.0363027438
Cu	0.8021801169	-2.3741895506	0.2824977892
Cu	-3.2096006254	0.0577943056	-0.2967756476
N	2.8349265553	-0.0266239570	-1.1636968128
N	3.9785990024	-0.0299786911	-0.8738943433
O	5.1138864380	-0.0293744595	-0.3797248261

#### Cu<sub>6</sub>-N<sub>2</sub>O.4

E = -1362.27135692455

Cu	-0.0747805315	-1.2131501176	0.1918161522
Cu	-2.1106255721	-0.0262832503	0.6765985039
Cu	-0.0951724661	1.2016460281	0.2025025633
Cu	2.0156401006	0.0163668874	-0.3007486416
Cu	1.9672815146	-2.3580518155	-0.2835957154
Cu	1.9269933225	2.3880837730	-0.2461026502
N	-4.0895204849	-0.0289082609	0.6854617497
N	-5.0064381911	-0.0131212956	-0.0560662379
O	-5.8436381202	0.0107625917	-0.9627126200

#### Cu<sub>6</sub>-N<sub>2</sub>O.5

E = -1362.38648055723

Cu	-0.0741371173	-1.2914148514	0.5225772545
Cu	-1.9365258118	-2.4112112955	-0.3780712200
Cu	-1.9418155861	-0.0081427207	-0.3990377642
Cu	-0.0906526736	1.3057251664	0.5140964264

Cu	2.8622430803	0.0116344634	0.6046244412
Cu	-1.9649004590	2.3966522277	-0.3901438170
N	4.5973157700	-0.0021579161	0.0817573270
N	5.6887307709	-0.0184507191	-0.2668996768
O	1.1722535954	0.0163324325	1.1659734734

#### Cu<sub>7</sub>-N<sub>2</sub>O.1

E = -1558.57262398116

Cu	1.5370887464	-0.0519200543	0.4205856868
Cu	0.0956558750	2.0094382427	0.3186978529
Cu	-2.2701797827	1.3386436617	-0.0670579276
Cu	-2.3655514786	-1.1023357746	-0.1454303948
Cu	-0.0599969441	-1.9790515157	0.1851276558
Cu	-0.7748840768	0.0075835150	1.4455643579
Cu	-0.4102801469	0.0774200858	-1.1413199026
N	3.5048727917	-0.1249489448	0.3006652568
N	4.4499839013	-0.1276790300	-0.4029655948
O	5.3160387070	-0.1170450542	-1.2843606082

#### Cu<sub>7</sub>-N<sub>2</sub>O.2

E = -1558.56396937794

Cu	1.5980541412	0.2941942601	-0.3858713985
Cu	-0.1341214712	2.0733131034	-0.1427928535
Cu	-2.3237808256	0.9955008081	0.2770709303
Cu	-2.0005666415	-1.4380729304	0.2413449770
Cu	0.4030538058	-1.8801573919	-0.1706089231
Cu	-0.7041814165	-0.0074079220	-1.3412195005
Cu	-0.2575473682	0.0270583788	1.2678441369
N	5.3723492178	-0.5980279737	0.7388894652
N	4.6342150616	-0.0000193701	0.0594171785
O	3.7143291354	0.5599248238	-0.5806996228

#### Cu<sub>7</sub>-N<sub>2</sub>O.3

E = -1558.65878491304

Cu	1.8816098191	1.4044708108	0.2557260213
Cu	1.7688931372	-0.9124028974	1.1563850261
Cu	-0.4522086156	-1.8754991101	0.6188248695
Cu	-2.2617549098	0.0160764393	0.0650659245
Cu	-0.4166155154	2.1673879883	-0.2907235234
Cu	-0.1505525800	0.4701114298	1.6002393514
Cu	0.3043443342	-0.1265526236	-0.8671872530
N	-4.3745872032	-1.6819450936	-1.2680919973
N	-3.6109511044	-1.0233451568	-0.7253115105
O	-1.7181446799	1.5617056307	1.0248876893

#### Cu<sub>7</sub>-N<sub>2</sub>O.4

E = -1558.57254762467

Cu	1.6317141914	0.4067027007	0.3149374798
Cu	-0.2113117399	2.1115139341	0.1261142419
Cu	-2.3767233340	0.9345582852	-0.2065342107

Cu	-1.9610503992	-1.4749781627	-0.1872864801
Cu	0.4765985734	-1.8221508011	0.1597310224
Cu	-0.6420705703	0.0175449508	1.3436303897
Cu	-0.2941030789	0.0551272360	-1.2500939156
N	3.6061289551	0.4828767733	0.3720166948
N	4.6082250817	-0.0201158493	0.0087576934
O	5.5510971154	-0.6592604213	-0.4704668807

### Cu<sub>7</sub>-N<sub>2</sub>O.5

E = -1558.59050231932

Cu	-0.1435572757	1.9967861488	-0.0953315049
Cu	-1.3657634080	0.4433091520	1.4770121204
Cu	-0.5108680869	-1.8691087452	0.8964600009
Cu	1.0538267150	-1.7154860393	-1.0412037114
Cu	1.2852427863	0.6714939991	-1.6534308650
Cu	-0.9368604566	-0.2469334888	-1.0566475933
Cu	0.9673768620	0.0308851042	0.7537106833
N	-2.8889543657	-0.0844202096	-1.1387863800
N	-3.6107282387	0.2305719617	-0.2089517370
O	-3.3599300482	0.5429282764	1.0782542361

### Cu<sub>8</sub>-N<sub>2</sub>O.1

E = -1754.89993868963

Cu	1.4113477230	-0.9584320736	-0.0241898863
Cu	1.2894276477	1.7548929176	0.0019351545
Cu	-1.2192341743	1.9225565705	0.1201537885
Cu	-1.7131011534	-0.4635802989	0.1327842484
Cu	-0.4429287172	-2.0026339380	-1.2767129738
Cu	-0.1232532215	0.4001662143	-1.5290228864
Cu	0.0313694208	0.3773484388	1.6391172447
Cu	-0.3107125300	-2.0236349170	1.3831763160
N	3.2480810009	1.6834611491	-0.1071716569
N	3.8204416855	0.6071525182	-0.1456547695
O	3.3994677315	-0.6646200717	-0.1307020219

### Cu<sub>8</sub>-N<sub>2</sub>O.2

E = -1754.89469766866

Cu	0.7849628045	-1.3328357046	-0.6076742366
Cu	-1.5287271537	-1.8797656632	0.0917184000
Cu	-2.4372835197	0.4531688231	0.7136499585
Cu	-0.4961500302	1.8853324779	0.1698108298
Cu	0.9877452486	1.0027215237	-1.6059827220
Cu	-1.1639423112	0.0082691242	-1.3976734047
Cu	-0.2426860989	-0.2428628908	1.4161807108
Cu	1.7433648159	0.9904014724	0.8483414378
N	3.3685800503	-0.1030643933	1.0302266838
N	3.4346042878	-1.2204080518	0.5539241377
O	2.5780384353	-2.0507800137	-0.0436387279

**Cu<sub>8</sub>-N<sub>2</sub>O.3**

E = -1754.87794554125

Cu	1.2933463729	0.7025996349	-0.3959368213
Cu	-0.6468009633	2.2584986252	-0.1817017656
Cu	-2.5775814282	0.4971855842	0.3523461826
Cu	-1.2304088619	-1.5223342614	0.2739669602
Cu	1.0939085193	-1.3313560453	1.1303357595
Cu	-0.3978733239	0.5005835661	1.4801290181
Cu	-0.9466533335	0.2331849623	-1.4849320222
Cu	0.6472848333	-1.5451136131	-1.3652266043
N	3.2649614098	1.1927169603	-0.5348931131
N	4.2641745431	0.8336632095	-0.0176713257
O	5.1471068639	0.3141001266	0.6781425953

**Cu<sub>8</sub>-N<sub>2</sub>O.4**

E = -1754.88215522045

Cu	0.5531947446	-1.6680898435	0.0000265251
Cu	-1.7568170705	-0.7972859303	-0.0009238302
Cu	-1.0287265958	1.7768217353	-0.0005939020
Cu	1.3886963177	1.5053908486	0.0002953153
Cu	2.2931431789	-0.4056498777	1.2765544892
Cu	-0.0462882317	0.1487320102	1.5486029046
Cu	-0.0450998897	0.1487776081	-1.5490778789
Cu	2.2940385975	-0.4057968037	-1.2752477026
N	-3.7240284035	-1.0084777752	-0.0012873251
N	-4.7692683923	-0.4699747035	0.0002675936
O	-5.8073766136	0.1956343355	0.0022120530

**Cu<sub>8</sub>-N<sub>2</sub>O.5**

E = -1754.96710606240

Cu	-0.5390448558	0.2077526856	1.5608872023
Cu	2.0674534778	0.4291312956	0.9262105131
Cu	1.3303482442	-0.0154486622	-1.6528432677
Cu	-1.0337074345	-0.2232894991	-1.4353528585
Cu	-1.9625690986	-1.4675382318	0.5858243311
Cu	0.4496855920	-1.5579544052	0.0727703659
Cu	0.0147408150	1.7316614798	-0.3572694547
Cu	-2.4056339517	1.0421864367	0.0349347120
N	3.7676499845	-0.3357810863	0.9470761279
N	4.8073995673	-0.8139114627	0.9706453943
O	0.7754316277	1.6733538964	1.4831543168

**Cu<sub>9</sub>-N<sub>2</sub>O.1**

E = -1951.26935287917

Cu	-0.4548957679	-1.2976277066	0.5182504539
Cu	-2.6800003163	-0.0315694835	-0.1592763675
Cu	-0.8798482768	1.9051183810	-1.0669765710
Cu	1.3412357220	0.7961150422	-1.2513841827
Cu	1.4828448477	-1.5897972480	-0.9781660669
Cu	-0.6145769256	-0.5989531444	-1.9107923029

Cu	-0.7007428825	0.9527236392	1.2684800747
Cu	1.5730478429	0.0075587095	1.0798289818
Cu	1.0400648056	2.4793481136	0.4426398218
N	-4.8127519998	-0.9557664079	1.7844297209
N	-4.0592459691	-0.5996807305	1.0000921353
O	-2.1298930904	0.6313731230	-1.8523090822

### Cu<sub>9</sub>-N<sub>2</sub>O.2

E = -1951.26378531910

Cu	-0.7567905385	2.0731522921	0.0798263880
Cu	-2.6693332535	0.0440854932	-0.0160381069
Cu	-0.5334297164	-1.5021260817	0.4224671583
Cu	1.4208762616	-0.4645252585	1.4391937452
Cu	1.1275030253	1.9326697703	1.7797463853
Cu	-0.8574275817	0.3787286561	2.0222453303
Cu	-0.4370222068	0.1189210055	-1.4249685137
Cu	1.5305301721	1.2237403368	-0.5206481989
Cu	1.5890604207	-1.2255412977	-0.9031228188
N	-4.5277725156	-1.7342468478	-1.6171890903
N	-3.8901818213	-1.0273062202	-0.9818656651
O	-2.2740003680	1.4599763285	1.1744472144

### Cu<sub>9</sub>-N<sub>2</sub>O.3

E = -1951.26429480655

Cu	-0.9642039121	-1.5193062380	-1.5787995228
Cu	-2.4566075930	-0.3554390741	0.0439174087
Cu	-1.2771317000	1.7601885056	0.8187676007
Cu	2.6141340786	-0.2161379680	0.2826002002
Cu	1.0834221289	-2.2414752326	-0.3078127275
Cu	-0.0502609368	-0.3295011141	0.5405514257
Cu	-1.0997383191	0.9275683258	-1.5877871463
Cu	1.1230109927	-0.2085343453	-1.9279558397
Cu	0.8786663731	1.9006546204	-0.3613882624
N	4.3914359696	-1.2418698095	2.5119546455
N	3.7653028467	-0.8353684694	1.6442758046
O	2.4236848934	1.0563813894	-1.1480494260

### Cu<sub>9</sub>-N<sub>2</sub>O.4

E = -1951.26784818654

Cu	1.1805699992	-1.1978603919	0.9546417491
Cu	-1.1969584880	-0.8990175773	1.6272293226
Cu	-2.8320920888	-0.1483346310	-0.5423177044
Cu	-0.3007689323	0.5595281365	-0.3918022304
Cu	1.4201597899	-0.8633860334	-1.5256960575
Cu	-0.6948534563	-1.8611739399	-0.7483927121
Cu	0.4321304060	0.9006194453	1.9979942719
Cu	2.1475724799	0.9108359750	0.0744562801
Cu	0.5276055197	2.7243136979	0.2268778303
N	-4.1835510395	2.1675557373	-1.8865359862
N	-3.7217060792	1.2562627028	-1.3706785815

O -2.3682402776 -1.7462871256 0.2840713344

Cu<sub>9</sub>-N<sub>2</sub>O.5

E = -1951.26363053773

Cu	0.0798759950	-1.2012881631	0.6972118856
Cu	-2.0027143956	-0.1323209264	1.4334970859
Cu	-1.3113673656	1.4455050798	-0.4110554037
Cu	0.4507152312	0.0902121277	-1.4504493127
Cu	0.1082051886	-2.3321578900	-1.4325762942
Cu	-1.8180814264	-0.8761151180	-0.9749975595
Cu	0.1615183181	0.9895071985	1.7505367826
Cu	2.4150935712	0.0532738627	0.6296126722
Cu	1.0358998307	2.2059722219	-0.4355615536
N	4.4368154164	-2.1495890773	0.1370429342
N	3.7227596257	-1.2802730839	0.3445073250
O	1.8886072857	1.7792570232	1.2515380058

Cu<sub>9</sub>-N<sub>2</sub>O.6

E = -1951.26945590631

Cu	1.2188720072	-0.9919851325	1.3979056431
Cu	1.7270934580	1.4738715019	0.7768288053
Cu	-0.0879725101	1.6214383781	-0.9332767306
Cu	-0.6651771620	-0.8008307607	-1.8417291169
Cu	0.7765491294	-2.4818977294	-0.6770909980
Cu	1.5843605236	-0.2270676510	-0.9296542399
Cu	-0.5456639586	0.7404371820	1.3940216463
Cu	-1.0692805220	-1.4387328259	0.5767973787
Cu	-2.5614887645	0.5451778416	-0.3131362373
N	-5.1079600418	0.5809698183	1.3279003132
N	-4.1844142763	0.5925770146	0.6523838781
O	-1.6113245544	0.9042845706	-1.9200305979

Cu<sub>9</sub>-N<sub>2</sub>O.7

E = -1951.26946297353

Cu	1.0799370723	0.4674154721	-2.0237932903
Cu	-0.1188344729	2.5407485106	-1.2857025412
Cu	-1.1759357158	1.4443199255	0.8274696450
Cu	0.1431619802	-0.6036409164	1.2424917222
Cu	2.3805214642	-1.0355838119	-0.0820787461
Cu	1.2493440204	1.3117521291	0.3539098681
Cu	-1.3411700113	0.4757288691	-1.4446433566
Cu	-0.1498506826	-1.6722240598	-1.0344615433
Cu	-2.1194821774	-0.9385404286	0.3387935187
N	4.5755015113	-1.3934874031	1.9755845056
N	3.7862545213	-1.2964645736	1.1525533132
O	1.6272715188	-1.3911326392	-1.7904967121

Cu<sub>10</sub>-N<sub>2</sub>O.1

E = -2147.49142555797

Cu	-0.7583537899	-0.4411442748	1.2049854946
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Cu	1.5047115526	0.2888774460	1.9763051322
Cu	3.0208169494	0.7465026529	0.0302913338
Cu	1.5623807843	0.4606273269	-1.9879922985
Cu	-0.7206237960	-0.3302337122	-1.3469510838
Cu	0.4751725363	1.3927678000	0.0224248596
Cu	1.3400705285	-1.0704372415	-0.0707729604
Cu	-2.0140020246	1.3507123342	-0.0134567264
Cu	-2.7647898536	-1.2932416502	-0.1404427777
Cu	-0.6402350615	-2.5351189368	-0.1655913754
N	-3.9546769647	1.5951322340	-0.0221877359
N	-4.7837214958	0.7035137854	-0.0696829037
O	-4.6449908579	-0.6546137438	-0.1296192956

#### Cu<sub>10</sub>-N<sub>2</sub>O.2

E = -2147.49152880349

Cu	-1.3132156394	0.0063044826	-1.0239024863
Cu	0.6354020808	0.0661877463	-2.5176456581
Cu	2.7836055771	0.0491249631	-1.3053369874
Cu	2.0276487541	0.0146492775	1.3903293339
Cu	-0.4450269619	-0.0288057326	1.4274874805
Cu	0.7887098771	-1.2542843905	-0.3797214089
Cu	0.7587962950	1.2963474833	-0.3368441155
Cu	-1.4776215713	-2.0088530784	0.3728609210
Cu	-2.9902373427	-0.0470960939	0.7975431733
Cu	-1.5243332404	1.9633641680	0.4463830860
N	4.6323922955	0.0343323101	-0.6085728668
N	4.8258276369	0.0356891239	0.5991641722
O	3.9981415051	0.0409770317	1.6657162581

#### Cu<sub>10</sub>-N<sub>2</sub>O.3

E = -2147.47108620125

Cu	-0.4800479606	-0.4331360079	1.2906087343
Cu	1.5058922449	0.8839528173	1.9924706162
Cu	2.9782744632	1.4775044139	0.0590768139
Cu	1.8059011927	0.4785467207	-1.9068681736
Cu	-0.2811047601	-0.7090083353	-1.2521751859
Cu	0.3970270239	1.4271856119	-0.1336424444
Cu	1.8080414875	-0.7819378467	0.2088298247
Cu	-2.0413589274	0.7423079821	-0.2489203453
Cu	-2.2217787925	-1.7670211941	0.0149631844
Cu	0.1487225272	-2.5967387606	0.2810319779
N	-3.7444106453	1.7013949045	-0.3365228034
N	-4.8443888119	1.9112262285	0.0263396076
O	-5.9994782121	1.9370874837	0.4667836030

#### Cu<sub>10</sub>-N<sub>2</sub>O.4

E = -2147.46679884542

Cu	-0.6471033946	0.1692653076	1.1019125905
Cu	1.6380503535	-0.1618314947	2.0373152867
Cu	3.4066338609	-0.3195396321	0.2529152396

Cu	2.1025117275	-0.1637800798	-1.8740900635
Cu	-0.3411001476	0.1554460526	-1.4785511108
Cu	1.3961853817	1.2231921640	0.0250377398
Cu	1.0344121361	-1.3701994300	-0.0139431645
Cu	-0.8659276108	2.2143994550	-0.2426143993
Cu	-2.7000648266	0.4780640526	-0.4335647772
Cu	-1.4256300952	-1.6897806579	-0.2812997330
N	-4.7065000167	0.5587925775	-0.5607573041
N	-5.5424368775	-0.1496845831	-0.0816154980
O	-6.0047413988	-1.1095474987	0.5741705037

### Cu<sub>10</sub>-N<sub>2</sub>O.5

E = -2147.46132169530

Cu	1.0212525355	-1.0856528811	-0.0017635096
Cu	-1.8044049036	-1.8413175231	-0.0006927265
Cu	-3.0696853588	0.1954081561	0.0036106774
Cu	-1.5111492567	2.2466591692	0.0037338186
Cu	0.8085061134	1.5904274037	0.0008713537
Cu	-0.8807723532	0.1724578280	-1.2537669929
Cu	-0.8786358237	0.1708293200	1.2561275667
Cu	1.4776426228	0.3466798242	-2.0006689970
Cu	3.0174240147	0.4353496349	-0.0016024169
Cu	1.4810805654	0.3423495194	1.9994786364
N	1.6918472567	-3.6048914418	0.0019421951
N	0.6181530543	-3.0437133977	0.0022903391
O	-0.6853667625	-3.5079055539	0.0045620694

### Cu<sub>10</sub>-N<sub>2</sub>O.6

E = -2147.46607500242

Cu	-0.9343669018	-0.3436996254	1.2688783909
Cu	1.3121788269	0.4663379521	1.9503668971
Cu	2.5795111065	1.4979782981	0.0632534335
Cu	1.0329749624	1.2324362474	-1.8789359818
Cu	-1.1204773027	0.1713500090	-1.2480543233
Cu	1.1187664465	-0.6687004364	-0.2634800843
Cu	0.0554557497	1.7501204429	0.2995481156
Cu	-0.9780884231	-2.1256642168	-0.4126457887
Cu	-3.0911351372	-0.9110406760	-0.0035296848
Cu	-2.4096077715	1.4560613543	0.4324936877
N	2.5115035058	-2.1046693278	-0.4811182395
N	2.9700524325	-3.1397148907	-0.1652168921
O	3.2985011927	-4.2633252989	0.2345419926

### Cu<sub>10</sub>-N<sub>2</sub>O.7

E = -2147.49196046045

Cu	-0.5516981212	-0.2142110792	1.2754687102
Cu	1.8009307899	0.2121261284	1.9912965705
Cu	3.3321691193	0.3916140352	0.0078900017
Cu	1.8081101099	0.2290608720	-1.9802524416
Cu	-0.5477975709	-0.2028744183	-1.2786456957

Cu	0.9018990535	1.3793015648	0.0088390388
Cu	1.4161635043	-1.1842962618	-0.0011627662
Cu	-1.5680858483	1.6894397566	0.0029547905
Cu	-2.6808368387	-0.8241360410	-0.0055860423
Cu	-0.7532725582	-2.3545895582	-0.0108801557
N	-3.4568002885	2.1997256526	0.0137850307
N	-4.4021454889	1.4315420956	0.0141306402
O	-4.4570447437	0.0671796949	0.0072673282

### Cu<sub>10</sub>-N<sub>2</sub>O.8

E = -2147.49155482665

Cu	0.8305124142	-1.5140970576	-0.0829882848
Cu	-1.6142400146	-1.8761443984	-0.1087168759
Cu	-2.7972487253	0.6497764618	0.0473194101
Cu	-0.8762820884	2.1964409902	0.1521348191
Cu	1.2963459895	1.0426535490	0.0868424026
Cu	-0.6576316790	0.1296439174	-1.2551328566
Cu	-0.6603749629	-0.0319455402	1.2895651047
Cu	1.7075240875	-0.2149139232	-1.9884942570
Cu	3.2367443903	-0.5007708028	-0.0150597724
Cu	1.7028854665	-0.4721810601	1.9792416557
N	-4.5095955618	-0.3313931593	-0.0533899687
N	-4.5036997353	-1.5520435902	-0.1316896163
O	-3.5134700594	-2.4685384357	-0.1691352122

### Cu<sub>10</sub>-N<sub>2</sub>O.9

E = -2147.49189857313

Cu	-0.5078014221	-0.0141270043	1.4152939580
Cu	1.9788553336	-0.0183658576	1.4207424996
Cu	2.7775416973	0.0364491536	-1.2104508227
Cu	0.6734188837	0.0640954368	-2.4936438974
Cu	-1.3270092878	0.0342964571	-1.0596534286
Cu	0.7374193419	-1.2593338302	-0.3654100149
Cu	0.7398934455	1.2981692520	-0.3116561997
Cu	-1.5498736694	-1.9771649874	0.3447588921
Cu	-3.0471723365	0.0016546724	0.7229680846
Cu	-1.5480313080	1.9898118862	0.4224036283
N	3.9145882634	-0.0418771813	1.6988282353
N	4.7591473786	-0.0314440515	0.8209457512
O	4.6464876523	0.0003167248	-0.5395184626

### Cu<sub>10</sub>-N<sub>2</sub>O.10

E = -2147.45888481505

Cu	-1.1219930586	-0.1416723862	1.2872629988
Cu	1.0700356677	0.7929336550	1.9806350231
Cu	2.5636170342	1.3385608778	0.0518522268
Cu	1.2225917297	0.5926105003	-1.9196473991
Cu	-1.0189839515	-0.2766737264	-1.3054815746
Cu	1.0390029646	-0.8137097310	0.1046443448
Cu	0.0249113840	1.6461158991	-0.0610523827

Cu	-1.0121489390	-2.2825569901	0.1042836063
Cu	-3.1494035066	-1.0120582258	-0.0458618146
Cu	-2.4472885080	1.3730566406	-0.1497881321
N	4.9754502354	-1.6482434196	-0.3388910648
N	3.9132039362	-2.0399307891	-0.0601229783
O	2.7279268733	-2.3135182040	0.2132883000

### Cu<sub>10</sub>-N<sub>2</sub>O.11

E = -2147.57782762511

Cu	-0.5218591989	0.4035380485	1.7173742458
Cu	1.8675569492	-0.0357279564	2.1302072084
Cu	3.1626915649	-0.4064351369	-0.0433159214
Cu	1.5614926528	0.0820381375	-1.8468885650
Cu	-0.6818529490	0.5823069316	-0.9401066544
Cu	1.2737764758	1.4083526363	0.2332588462
Cu	0.8953794051	-1.2202449861	0.2315806170
Cu	-2.9264690822	1.1576757668	0.5159235369
Cu	-1.6213576056	-1.4645135781	0.2281972271
Cu	-0.2644854292	-1.8125267151	-1.7797267576
N	-3.6974402331	2.5680901352	-0.3836392442
N	-4.1606395558	3.4386053011	-0.9630113967
O	-2.3901085375	-0.2532896040	1.5515761018

### Cu<sub>11</sub>-N<sub>2</sub>O.1

E = -2343.86829050796

Cu	2.5085275810	-1.4062240756	-0.0942516945
Cu	2.2665632211	1.3296827832	0.5807589057
Cu	0.8334207957	2.6121758621	-0.9545027735
Cu	-1.4543212074	1.5819669593	-0.8538143146
Cu	-1.5594595038	-0.9119860963	-1.3590168074
Cu	-0.2450139542	-2.2239049612	0.3555113604
Cu	0.5288142922	0.1660268230	-0.6973877170
Cu	0.9016852038	-0.3874755926	1.8667719180
Cu	-0.1025464472	1.7937856757	1.2788305515
Cu	-1.5543943452	-0.1543016879	1.0272690929
Cu	-2.6359999241	-2.3716515074	0.3009642808
N	4.6772352552	-1.1699384107	-2.1774631988
N	3.8943967063	-1.3132868104	-1.3548598135
O	1.4525786135	-2.1912666564	1.2532674186

### Cu<sub>11</sub>-N<sub>2</sub>O.2

E = -2343.86436860247

Cu	-2.7227646628	-1.0611600060	-0.1722562018
Cu	-2.2893190184	1.4439203172	-1.4236905182
Cu	-1.1873110095	3.1395004294	-0.1155466758
Cu	1.2254136987	2.0187406654	0.6461428439
Cu	1.1481157939	-0.1631472092	1.7738913177
Cu	-0.2394654901	-1.6651743998	0.3377285506
Cu	-0.8410206887	0.7385651289	0.5261354293
Cu	-0.6602124276	-0.6075389583	-1.9269407138

Cu	0.2339985878	1.7369852407	-1.6189504596
Cu	1.4893479151	-0.1557013182	-0.7265404583
Cu	2.0992273088	-2.1778603240	0.6556450549
N	-3.5930227344	-1.8866329726	1.2846414365
N	-4.0043586420	-2.3601871239	2.2419642205
O	-2.6177749444	-0.4021408706	-1.9377268967

### Cu<sub>11</sub>-N<sub>2</sub>O.3

E = -2343.86218485971

Cu	-0.0955365343	-2.3348696457	1.1398442616
Cu	-1.9564260523	-1.5219806153	-0.3953873126
Cu	-3.1560358853	0.8889580571	-0.1426804954
Cu	-0.6252197879	2.2470017400	-0.1788129801
Cu	1.3888517015	1.6625071076	1.1311196347
Cu	1.8824177819	-0.9445744295	0.7058456999
Cu	-0.4399249834	0.0308182473	0.7804923193
Cu	0.3800865582	-1.5547966507	-1.2723017880
Cu	-1.1071358826	0.3207261914	-1.8888341698
Cu	1.2950820395	0.7034323394	-1.1391225752
Cu	3.4831668750	0.7206067827	0.0513042599
N	-5.2072385702	-0.0729530870	1.8333496159
N	-4.4392046869	0.2949164421	1.0681103595
O	-2.1706526302	1.8939364276	-1.3426819191

### Cu<sub>11</sub>-N<sub>2</sub>O.4

E = -2343.86650759454

Cu	0.9309106525	1.5277240572	-0.3633426748
Cu	-0.4147055732	3.3489962718	0.7515781858
Cu	-1.5381322802	1.9520488896	-0.7911817657
Cu	-2.6118427470	-0.5303793275	-0.1741575940
Cu	0.5958074567	-2.6267258578	-1.3208878615
Cu	1.9111142253	-0.5981832492	-0.8891024907
Cu	-0.3778035712	-0.2985757912	-1.7907229294
Cu	1.6034428605	-0.0226127397	1.5223813401
Cu	-0.7639523789	0.9351031167	1.3554786095
Cu	-0.2603942111	-1.2809603908	0.5461191506
Cu	1.8400226673	-2.4688524969	0.8342802568
N	-4.3250394239	-2.0960480263	1.7617586099
N	-3.7511876250	-1.4935957556	0.9758637466
O	-2.1937533807	0.4281340929	-1.7526833278

### Cu<sub>12</sub>-N<sub>2</sub>O.1

E = -2540.09482806119

Cu	2.8807194154	-1.0707813034	0.7558703462
Cu	2.9910834245	1.2320076656	-0.1671036721
Cu	1.3123817905	2.7872353523	0.7637203997
Cu	-1.1509706173	1.7305246541	0.4002157718
Cu	-1.3531603549	-0.6059391492	1.3144717411
Cu	0.4846809978	-1.9898697337	0.3915972118
Cu	0.8982336106	0.3943896398	0.9281288615

Cu	1.7024044537	-0.6268930757	-1.3721408038
Cu	0.7202265998	1.6139396664	-1.3382562400
Cu	-0.7873146240	-0.3557767284	-1.1141902674
Cu	-1.9241883095	-2.4374840782	-0.2701295992
Cu	-3.1808625094	-0.2967113931	-0.3357514078
N	-4.3204826996	1.2839648002	-0.3700678098
N	-3.9495541121	2.4076036499	-0.0681680728
O	-2.7755440018	2.9013729534	0.3455333368

#### Cu<sub>12</sub>-N<sub>2</sub>O.2

E = -2540.09439148027

Cu	-1.3502080450	-2.4739564499	0.8337546812
Cu	-2.7398036134	-0.7621837099	-0.2840763472
Cu	-1.8998238479	1.8764679223	0.6742074260
Cu	0.5923082870	2.0388108821	0.2035433704
Cu	1.8558667184	0.3008881397	1.3925031651
Cu	1.2021445032	-1.9202864769	0.4780890070
Cu	-0.5484544701	-0.1575611806	0.8575096444
Cu	-0.5650228183	-1.5575478463	-1.3216223056
Cu	-1.0106463358	0.8668677963	-1.4240731146
Cu	1.3415735818	0.0575141200	-1.1527682313
Cu	3.3852427117	-0.8557597352	-0.1224703960
Cu	3.0357271051	1.6972797368	-0.2823160308
N	-3.8261909525	2.1853574622	0.6440009768
N	-4.6404440623	1.3768626203	0.2300072005
O	-4.5178796291	0.1266294797	-0.2603526218

#### Cu<sub>12</sub>-N<sub>2</sub>O.3

E = -2540.15322758673

Cu	-1.8144955873	-2.1389102588	1.0352268697
Cu	-3.1472201480	-0.1830068947	-0.0793231764
Cu	-2.2751086521	1.9984847846	0.6266335707
Cu	0.6270460220	2.0309258951	0.0149651086
Cu	1.9341240729	0.0496629473	0.9834580389
Cu	0.6220490556	-2.0237457569	0.2054272567
Cu	-0.7648988995	0.0178858684	0.9769720993
Cu	-1.2601725905	-1.3525622684	-1.2605492072
Cu	-1.4016387124	1.0276509422	-1.5130804888
Cu	0.8292143015	-0.0559905691	-1.3812109345
Cu	2.8434314987	-1.4098137943	-0.7230419328
Cu	2.7677666082	1.3566705525	-0.9544647517
N	2.3598738067	0.2164740066	2.8557906689
N	2.6040892377	0.3470531026	3.9616722820
O	-0.5678608356	1.9823617423	1.5243215373

#### Cu<sub>12</sub>-N<sub>2</sub>O.4

E = -2540.15550445354

Cu	-2.3250279516	-2.0295357001	0.6658155646
Cu	-3.1193487627	0.1505745628	-0.3833891658
Cu	-2.1974180531	2.2737780472	0.6742452360

Cu	0.4151177490	2.0517517860	0.7836221757
Cu	1.2301076911	0.0136746007	1.8631289354
Cu	0.2934503984	-1.9653138661	0.7747000220
Cu	-1.0995425365	0.0878561466	1.0631753817
Cu	-1.1867573140	-1.2006383010	-1.2919577073
Cu	-1.1080779458	1.3914572453	-1.2868127045
Cu	1.1552093570	0.0220313267	-0.7623735153
Cu	2.7248164623	-1.3588976942	0.4982274652
Cu	2.8034975796	1.3054680190	0.5020001147
N	3.0101939569	-1.0748761527	-3.5747526825
N	3.0170299603	-0.1829627177	-4.2697588986
O	-0.0661657333	0.0658719767	-2.2664342961

### Cu<sub>13</sub>-N<sub>2</sub>O.1

E = -2736.47750039960

Cu	-0.2196296714	0.4031924578	-1.3800179111
Cu	1.0844457044	-1.7546186911	-1.1199515317
Cu	-1.0082629625	2.5080101773	-0.4583066242
Cu	1.5678281863	2.0669904798	-0.9432851443
Cu	2.2859499058	-0.0647643892	0.3776530671
Cu	2.0120971578	-2.4308502147	1.2279639529
Cu	-0.0574666226	-3.4153268061	0.1795963985
Cu	-1.5319113246	-1.6045493942	-0.8312341979
Cu	-2.5589382126	0.5920535061	-1.7132524006
Cu	-1.8641718507	0.4337291523	0.6407954943
Cu	0.3600025150	1.3430302277	1.2752095890
Cu	-0.0911717053	-1.1529216788	1.2113444576
Cu	1.7332901090	-0.3441236445	2.6699676203
N	3.0191233251	4.7341248310	-1.0342268485
N	2.5186993110	3.7086233808	-1.1203792734
O	1.7688801040	0.1040176682	-1.5469888342

### Cu<sub>13</sub>-N<sub>2</sub>O.2

E = -2736.45985775577

Cu	0.0510894672	0.8060282743	1.1477060965
Cu	-0.6398615203	-1.4349194035	1.9477244820
Cu	0.7126724256	2.8358546189	-0.0567383794
Cu	-1.6898896434	2.1986553130	0.0233093115
Cu	-1.9679482271	-0.3145503721	0.1661209794
Cu	-1.5549198724	-2.8626591665	0.0231029096
Cu	0.7249334983	-3.3047244848	1.0932474072
Cu	1.8300880094	-1.0139774613	1.6048087039
Cu	2.2681116751	1.8828636584	1.6163593941
Cu	2.2450611384	0.4783671050	-0.5657099950
Cu	-0.2134742923	0.8081504516	-1.3943924154
Cu	0.4121207605	-1.3596752528	-0.3842309539
Cu	-1.3815816744	-1.4107032088	-1.9866790113
N	3.8340454068	0.5997750908	-3.2178571227
N	3.2705171587	0.6294103568	-2.2264745471
O	3.2193699263	0.2686774052	1.2498245529

Cu<sub>13</sub>-N<sub>2</sub>O.3

E = -2736.45481844944

Cu	-1.2320038002	-0.1081313336	-0.6987322741
Cu	1.1485958312	-0.7337381393	-1.7997196115
Cu	-2.6520017494	0.5467950359	1.1848072407
Cu	-1.7526643032	2.3346686548	-0.2709657950
Cu	0.7056454274	1.7421583322	-0.9494859487
Cu	3.0572952081	0.5559562966	-0.7443687066
Cu	2.6212481402	-1.9699930134	-0.3746386523
Cu	0.0796149274	-2.2113535043	-0.0188520577
Cu	-2.4318023688	-1.8999929871	0.4179735511
Cu	-0.7445223249	-0.8700775680	1.9025534153
Cu	-0.2755949047	1.5156079841	1.4603314126
Cu	1.3743962964	-0.2210418568	0.8490965454
Cu	2.1385284649	2.1490747276	0.9526739883
N	-3.3235726245	-0.6258593769	-3.2675679722
N	-2.8712128744	-0.7980398847	-4.2896995967
O	-0.2099558656	0.5596451453	-2.2410297326

Cu<sub>13</sub>-N<sub>2</sub>O.4

E = -2736.45648315709

Cu	0.6421113621	0.8149745224	-0.9433357872
Cu	-0.0621898943	-1.4226669640	-1.7260762528
Cu	1.0475080344	3.0024702730	0.2071822862
Cu	-0.9470823878	2.6499309016	-1.2081382783
Cu	-1.7867096845	0.2496045539	-1.0307407660
Cu	-2.2031445774	-2.1475172571	-0.1918181009
Cu	-0.0120666258	-3.2706094858	0.0617784995
Cu	2.0319466965	-1.1631649217	-0.0785928924
Cu	2.9284360298	1.4571914050	-0.3333721187
Cu	1.3677310769	0.7724933202	1.4632780931
Cu	-0.9657168667	1.5769583717	1.0218275131
Cu	-0.3871517484	-0.8773127855	0.8887158919
Cu	-2.7690416411	-0.1922916880	1.2094500626
N	4.7145767478	-2.2276094301	1.0998842862
N	3.7543027785	-1.7429379255	0.7222253394
O	1.3402378924	-2.7076329542	-1.1686163814

Cu<sub>13</sub>-N<sub>2</sub>O.5

E = -2736.46901100330

Cu	-1.6991359357	-0.3173199491	-0.4628254251
Cu	0.3297787634	-0.0106566460	-2.0106365166
Cu	-2.8730210529	0.1223735633	1.6946186332
Cu	-2.2473901597	2.0032770348	0.1683793889
Cu	0.2620363216	2.0764592954	-0.4127846782
Cu	2.4979689684	1.0527414908	-0.8717459135
Cu	2.1698907121	-1.4175978586	-1.1214801684
Cu	-0.1316189310	-2.1800562700	-0.3969044284
Cu	-2.5404500067	-2.3075400789	0.5043119915

Cu	-0.8139518985	-1.2426017021	1.8929973022
Cu	-0.6116792732	1.2264986147	1.9021607260
Cu	1.0261913248	-0.2038886743	0.6518207921
Cu	1.7824654536	2.0286728169	1.4128545169
N	0.1750127833	-0.6138236820	-5.0531915062
N	0.2728976286	-0.3914567906	-3.9400173811
O	-1.2021536631	1.3401487910	-1.5005901441

#### Cu<sub>14</sub>-N<sub>2</sub>O.1

E = -2932.71123411402

Cu	-0.9859483160	-0.1865395402	0.9029961815
Cu	1.2654150756	-1.0500229860	1.4827756145
Cu	-2.8910787563	0.9181062882	-0.2982139374
Cu	-1.3404875594	2.3416822352	1.0668626742
Cu	1.0028346429	1.3726969020	1.0380150917
Cu	3.1046787539	0.0493046660	0.1993316829
Cu	2.4069617067	-2.3737510537	-0.2836210230
Cu	-0.1278699666	-2.4635412754	-0.0311001919
Cu	-2.5549667301	-2.0547272799	0.3317286174
Cu	-1.3772657519	-0.7597423893	-1.4596972595
Cu	-0.5228530748	1.5532320803	-1.0847116911
Cu	1.0228970373	-0.4238838172	-0.9822944164
Cu	2.0264101550	1.9326669290	-1.0974863023
Cu	0.5138667081	3.6043347694	-0.0402457269
N	-4.5089500267	-1.9065446301	0.3721082564
N	-5.1383815139	-0.8846599743	0.1642459475
O	-4.7977326721	0.3869375831	-0.1241850026

#### Cu<sub>14</sub>-N<sub>2</sub>O.2

E = -2932.78654288820

Cu	0.4272331750	-1.1973484112	-0.9818149119
Cu	-1.9209373398	-0.0781702492	-1.1759594883
Cu	2.7827942184	-1.3130286514	-0.2530611873
Cu	1.9647783287	0.6805700368	-1.5927248836
Cu	-0.1480475755	1.8219344188	-0.8220689741
Cu	-2.2215574854	1.9140104621	0.5488993033
Cu	-3.0220769742	-0.4726357057	0.9913354404
Cu	-1.2593998792	-2.1719423224	0.5197966945
Cu	0.9128264771	-3.3647861334	-0.1653076852
Cu	1.0088565474	-1.5689015805	1.5191976528
Cu	1.7739807882	0.6677455376	0.8992733106
Cu	-0.6783281776	0.1800903025	1.2895486711
Cu	0.1352171899	2.5470442354	1.4281732148
Cu	2.0829490215	2.7960232106	-0.2716568642
N	-3.2895348890	-0.4608158116	-2.5674372640
N	-3.9747249436	-0.7440176824	-3.4312712909
O	-0.1048319852	0.3143206858	-2.1103166230

#### Cu<sub>14</sub>-N<sub>2</sub>O.3

E = -2932.70869589336

Cu	0.7341922601	0.6636826707	-0.8824039187
Cu	0.1489687958	-1.6722765330	-1.4557179721
Cu	0.8758347454	2.8615342037	0.3361633375
Cu	-1.1154287632	2.4335685496	-1.1060611674
Cu	-1.6787257889	-0.0578680060	-1.1120407347
Cu	-1.8829069357	-2.5509335864	-0.2754651185
Cu	0.4570605861	-3.3822915649	0.3141323130
Cu	2.0779287309	-1.3823510707	0.1330391289
Cu	2.9537007615	1.6026259007	-0.1679291845
Cu	1.3469549385	0.6582691470	1.4987775005
Cu	-1.0261308466	1.2627612360	1.0570468653
Cu	-0.2890538582	-1.1203139347	0.9588138067
Cu	-2.8047730460	-0.6035654734	0.9772747807
Cu	-3.2162274360	1.6607578853	-0.0495131605
N	4.6805952581	0.7118691699	-0.3989989833
N	4.8445941855	-0.4937645437	-0.3573526092
O	4.0437063115	-1.5527345691	-0.1640321842

#### Cu<sub>14</sub>-N<sub>2</sub>O<sub>4</sub>

E = -2932.77667184890

Cu	-1.1813780290	0.2828529431	-0.7525983893
Cu	1.1122638508	1.1297524444	-1.7221503653
Cu	-2.6167997119	-0.6805201667	0.9634136762
Cu	-1.3912028021	-2.2652313838	-0.5188005774
Cu	1.0021110532	-1.4336058115	-1.1080503992
Cu	3.1488757772	0.0765018827	-0.6572916018
Cu	2.3596104503	2.5405692171	-0.2541567506
Cu	-0.1630130190	2.5034402451	0.0499144809
Cu	-2.6173746126	1.8773088952	0.3474890069
Cu	-0.8945026702	0.9141299245	1.8192176988
Cu	-0.1498925152	-1.3730778361	1.3731033863
Cu	1.3268929653	0.5963038787	0.8776222945
Cu	2.3418476170	-1.6939451213	0.9024279926
Cu	0.6624327262	-3.4605906495	0.2280847760
N	-3.8733820691	0.3793067433	-3.2356976532
N	-3.5124182053	1.2183630718	-3.9022826626
O	-0.0920427925	-0.2933397318	-2.2701616841

#### Cu<sub>14</sub>-N<sub>2</sub>O<sub>5</sub>

E = -2932.71135049068

Cu	-0.9340678516	-0.3271463292	0.7555292679
Cu	1.2986329747	-1.2518137072	1.2945077297
Cu	-2.8041935042	0.9350992936	-0.3479016858
Cu	-1.3409836400	2.1468507022	1.2893479193
Cu	1.0176624483	1.2115127705	1.2269629721
Cu	3.1743121096	0.0492374712	0.2850909963
Cu	2.5397573845	-2.2708876345	-0.6039104214
Cu	-0.0030546536	-2.4303398733	-0.4804766222
Cu	-2.4489879115	-2.1013018941	-0.1554762094
Cu	-1.2212712195	-0.5422716695	-1.6804622698

Cu	-0.4146225300	1.6923111921	-0.9159431898
Cu	1.1538412320	-0.2560619128	-1.0507668303
Cu	2.1240443972	2.0980950632	-0.7528854105
Cu	0.5389863756	3.5735918894	0.4639419750
N	-4.4046160226	-1.9736689559	-0.1970742963
N	-5.0398632785	-0.9378365205	-0.2812573968
O	-4.7075859504	0.3657536779	-0.3559537087

### Cu<sub>14</sub>-N<sub>2</sub>O.6

E = -2932.71055168618

Cu	1.1205665365	-0.1213378221	-0.8345811843
Cu	-0.6209109697	-1.7483626576	-1.4969816714
Cu	2.4443582411	1.5981129669	0.4185995374
Cu	0.5612883021	2.3579745934	-1.0858476832
Cu	-1.2789541630	0.6134167596	-1.1435799626
Cu	-2.8123943907	-1.3608733671	-0.3639834333
Cu	-1.3257906169	-3.3642419494	0.2524107981
Cu	1.0906274752	-2.5444979915	0.1395548326
Cu	3.2058163752	-1.2955249031	-0.1209497834
Cu	1.5445914598	-0.4776968947	1.5691010273
Cu	-0.0592401825	1.3612753559	1.0465002625
Cu	-0.7781042579	-1.0403143154	0.9494533913
Cu	-2.5712241958	0.8040653375	0.9123704486
Cu	-1.6891507835	2.8866116617	-0.1281206772
N	4.4048119640	1.7467597603	0.3744135155
N	5.1728265013	0.8256710568	0.1633250842
O	5.0211890042	-0.4852877436	-0.0941625490

### Cu<sub>15</sub>-N<sub>2</sub>O.1

E = -3129.08414040237

Cu	-0.9280447039	-0.2036775964	0.7312718177
Cu	1.1044265134	-1.5791815790	1.0082580104
Cu	-2.6252864856	1.5283722326	-0.2303684665
Cu	-0.9364603297	2.1038939538	1.6440401015
Cu	1.2444224417	0.9030248723	1.1800755800
Cu	3.0614736165	-0.4547246534	-0.0833654953
Cu	1.8838688299	-2.4723077535	-1.2067515384
Cu	-0.5926142034	-2.1447275820	-0.7923768664
Cu	-2.9531995981	-1.1798780073	-0.1150636238
Cu	-1.4076753551	-0.0634238370	-1.8901290895
Cu	-0.1185106287	2.1367726193	-0.7965845957
Cu	0.9536744777	-0.1866214643	-1.1861977797
Cu	2.4113706328	1.8972848647	-0.7331752523
Cu	1.1377409943	3.3641783610	0.9200553596
Cu	-2.9526008838	0.5046332069	1.9067923341
N	-5.3130545105	-3.1091708405	-0.5150614937
N	-4.5390693836	-2.2688053391	-0.4986486375
O	-1.6955816870	1.8556074498	-1.9194041528

### Cu<sub>15</sub>-N<sub>2</sub>O.2

E = -3129.08396709965

Cu	-0.8007918554	-0.5126362429	0.4596857795
Cu	1.2877822461	-1.7827037056	0.7230318693
Cu	-2.4869434023	1.2618975809	-0.2893337852
Cu	-1.4496084191	1.2000215223	2.1078335190
Cu	0.9833167142	0.3862085126	1.8986123200
Cu	3.2215981102	-0.2339594052	0.7383443956
Cu	2.6571838753	-1.6238032672	-1.3834036172
Cu	0.1350455734	-1.6663628002	-1.5381752581
Cu	-2.3618855626	-1.1771307451	-1.2183891687
Cu	-0.7179639395	0.6856988034	-2.2353167902
Cu	-0.0800333126	2.2420069774	0.2023413135
Cu	1.3678466000	0.3640853604	-0.7170225753
Cu	2.3494961221	2.1267372948	0.8529306948
Cu	0.5075632276	2.7361011046	2.5383049061
Cu	-3.1610847413	-0.4833364269	1.1800913002
N	-0.5120711629	0.3858683419	-4.1424565847
N	-0.2906145505	0.2655775866	-5.2561947938
O	-1.2544116351	2.3343171020	-1.3298137971

Cu<sub>15</sub>-N<sub>2</sub>O.3

E = -3129.08409941860

Cu	-1.0562660080	-0.4920394368	-0.8069986410
Cu	1.0229436478	-0.9172320364	-1.9730706319
Cu	-2.8363878424	-0.0481008159	0.9965077293
Cu	-1.7557783096	1.8305722624	-0.3778480351
Cu	0.7835254918	1.2177128243	-0.7415306059
Cu	2.9869316619	0.0778021702	-0.7430816293
Cu	2.4317727918	-2.6755948207	-0.9967951979
Cu	-0.1291992595	-2.8025024043	-0.6711075891
Cu	-2.6044210380	-2.2699195055	-0.1860622830
Cu	-0.9460955182	-1.6284558420	1.5515382644
Cu	-0.6117570669	0.9174506405	1.5741149772
Cu	1.3387156947	-1.1689664514	0.5115197730
Cu	1.9338245212	1.0663587721	1.5458868814
Cu	0.2281837713	3.0497248205	0.7450028466
Cu	-3.3249860279	0.0297331697	-1.4023300485
N	4.1849723671	2.3553173350	3.1801862297
N	3.3259997464	1.8336346339	2.6368761237
O	0.6255110593	-0.5086598224	2.2388928258

Cu<sub>15</sub>-N<sub>2</sub>O.4

E = -3129.08796241582

Cu	1.2610119140	-0.4071069135	0.2600514342
Cu	0.6876872526	1.6909039919	1.4481805907
Cu	1.2592784889	-2.3360576808	-1.3846976385
Cu	0.1056177674	-2.5527234915	0.8222585366
Cu	-0.9304259528	-0.3114174371	1.4201442059
Cu	-1.8417482046	2.0937710287	1.1405305293
Cu	0.0171818212	3.4844261301	-0.0988261677

Cu	1.7780819686	1.9224860274	-0.9383668674
Cu	3.1985722800	-0.6061187938	-1.2934431281
Cu	0.8244294460	-0.0787326963	-2.3743594726
Cu	-0.9806741102	-1.2927567684	-1.0850334033
Cu	-0.5870686951	1.1329502172	-0.6768754455
Cu	-2.8591104933	0.0920329555	-0.0666539314
Cu	-2.3787571302	-2.2447671942	0.7447789590
Cu	2.8432931776	-2.2807707048	0.4886688520
N	1.6568813582	2.2228099243	3.0349240276
N	2.3263454467	2.5009213429	3.9182749626
O	2.5704776453	0.8659976667	-2.3681690201

## 10. XYZ coordinates and total energies of Cu<sub>x</sub>-N<sub>2</sub>O clusters on TPSSh/DEF2-TZVPP level

### Cu<sub>4</sub>-N<sub>2</sub>O.1

E = -6746.94293314854

Cu	0.5248002369	0.0048097357	-0.0085505556
Cu	-0.7075026813	2.1095500673	-0.0007012898
Cu	-1.7718199162	-0.0086027018	0.0076574937
Cu	-0.6848858628	-2.1146057491	-0.0008312819
N	2.4019466624	0.0095812030	-0.0163913635
N	3.5323629593	0.0115388441	0.0017148470
O	4.7158220267	0.0130222812	0.0192898126

### Cu<sub>4</sub>-N<sub>2</sub>O.2

E = -6746.91017326097

Cu	0.1840565660	-0.8831827665	-0.0038381608
Cu	-1.6144147646	0.9243435987	-0.0031681954
Cu	0.7823517017	1.3471695959	0.0010439382
Cu	2.4824557441	-0.3311372190	0.0020563277
N	-3.5972049268	-0.7987492124	-0.0052387160
N	-2.4409631860	-0.9268249095	-0.0045330156
O	-1.5594214183	-1.8697172883	-0.0048187471

### Cu<sub>4</sub>-N<sub>2</sub>O.3

E = -6746.92679040510

Cu	0.4069760551	0.4317070094	-0.0423431791
Cu	-1.6849349074	1.6473097410	0.1753667819
Cu	-1.5530153755	-0.7272857068	0.0676108101
Cu	0.4625148477	-1.9944231765	-0.1534826809
N	4.3233236509	0.4015548428	0.0332849200
N	3.3221160945	0.9015345115	-0.0489358477
O	2.2628090779	1.4503276488	-0.1381190575

### Cu<sub>4</sub>-N<sub>2</sub>O.4

E = -6746.92437166677

Cu	0.8204284575	-1.1251204725	0.0789548217
Cu	-1.3049004991	-0.0004040333	0.4684459717
Cu	0.8201066883	1.1249707092	0.0801041596
Cu	2.9298532557	0.0003370194	-0.2978331685

N	-3.3395689061	-0.0011680912	0.4912361858
N	-4.1551662845	0.0000354770	-0.3023681353
O	-4.9495740780	0.0014685729	-1.1783964711

#### Cu<sub>4</sub>-N<sub>2</sub>O.5

E = -6747.03664440640

Cu	0.5039591110	-1.1526549254	-0.2804879715
Cu	-2.0003984508	0.0130402101	-0.5341645387
Cu	0.4920961652	1.1621357139	-0.2163698719
Cu	1.9224896664	-0.0316095917	1.2982452455
N	-4.5374005664	-0.0217513524	0.8716591971
N	-3.5711034299	-0.0074080687	0.3354373286
O	-0.4962204583	0.0324227235	-1.4590605992

#### Cu<sub>5</sub>-N<sub>2</sub>O.1

E = -8387.49878272790

Cu	-0.0204735762	-0.5307437186	0.0582384869
Cu	-2.3354382734	-1.2404265062	-0.0085330662
Cu	-1.7940643988	1.0242912586	-0.1216510470
Cu	0.4823962150	1.8481169908	0.1484444209
Cu	2.3148522725	0.3868063297	-0.0853529885
N	2.9287700866	-1.4485381137	-0.1110565828
N	2.1430242696	-2.3236359888	0.0205242902
O	0.8471330955	-2.3026624550	0.1516137950

#### Cu<sub>5</sub>-N<sub>2</sub>O.2

E = -8387.49629814652

Cu	0.4424983335	-0.6189344873	-0.0880095738
Cu	-1.7659312151	0.2677549915	-0.1368207346
Cu	0.1451129390	1.7206951594	0.0735494575
Cu	2.3843964510	0.7692767145	0.1335323116
Cu	2.6070371599	-1.5858974244	-0.0346189966
N	-3.6844829498	-0.0810891900	-0.1455728476
N	-4.5383014666	-0.8101910408	0.0176228373
O	-5.4096661026	-1.5864812497	0.1932309305

#### Cu<sub>5</sub>-N<sub>2</sub>O.3

E = -8387.50650216854

Cu	-0.6331531123	-1.0938763617	-0.0002587248
Cu	-2.7833516395	-0.0795585322	-0.0024708323
Cu	-0.8821751219	1.2988635014	0.0000635521
Cu	1.4288406040	0.1868687660	0.0004398809
Cu	1.4921549657	-2.1527157334	0.0009285655
N	0.5759715456	2.4844883716	0.0017621153
N	1.7634482178	2.1269226111	0.0023380191
O	2.8284461639	2.7497775051	0.0035033608

#### Cu<sub>5</sub>-N<sub>2</sub>O.4

E = -8387.60236722384

Cu	-1.5134642444	-0.6853187918	-1.2093089553
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Cu	0.5858264019	-1.6371744281	-0.5115483448
Cu	1.9310730440	0.4750270856	0.4217884990
Cu	-0.6552870435	-0.0302281784	0.9090182148
Cu	-2.7213318229	0.8353904853	0.2113533926
N	3.4885768886	2.6592977709	-0.6928636442
N	2.9037303621	1.8279048775	-0.2623171075
O	1.0295645643	-0.8663191551	1.1796243695

#### Cu<sub>6</sub>-N<sub>2</sub>O.1

E = -10028.0736824891

Cu	0.2106471048	-1.3144373540	-0.0297193642
Cu	-2.0451612207	-0.5945873247	-0.2107642944
Cu	-0.3056035262	1.0245513863	-0.1069280587
Cu	2.0029598586	0.3129929634	0.0684841886
Cu	2.4779290723	-2.0043120122	0.1342663959
Cu	1.4547143123	2.6148050007	-0.0020183394
N	-5.7394962453	0.7292879859	0.7297897665
N	-5.0521241372	-0.0027293845	0.2258006054
O	-4.3108601222	-0.7736665443	-0.3063283311

#### Cu<sub>6</sub>-N<sub>2</sub>O.2

E = -10028.0706653480

Cu	0.7253885819	-1.0270793703	-0.1246244458
Cu	-0.9419202730	-2.6218880434	0.4937179017
Cu	-1.6024360376	-0.4040082190	0.1631925865
Cu	-0.0316495156	1.3203790639	-0.3783362650
Cu	1.9669992936	1.0598079551	0.8571369920
Cu	-2.3322046482	1.8119810308	-0.3477981013
N	3.5775674692	0.4624549510	-0.0286896661
N	3.4724590320	-0.5301544751	-0.6653319241
O	2.5156241623	-1.2987695067	-0.9789892520

#### Cu<sub>6</sub>-N<sub>2</sub>O.3

E = -10028.0738294025

Cu	0.9834290397	-0.0023958305	0.0983989271
Cu	0.7555099644	2.2843272153	0.8352687735
Cu	-1.1551108517	1.2011959117	0.0128063360
Cu	-1.1665646239	-1.1866856941	0.0121972753
Cu	0.7352115183	-2.2879313080	0.8313184465
Cu	-3.0149752584	0.0165850091	-0.8660638571
N	2.7606402824	-0.0102124771	-0.8465214329
N	3.8909915562	-0.0152991549	-0.7700622036
O	5.0699699654	-0.0207716986	-0.6650538465

#### Cu<sub>6</sub>-N<sub>2</sub>O.4

E = -10028.0819228060

Cu	-0.0286917509	-1.1839984357	0.1135980784
Cu	-2.1048773649	-0.0031381958	0.3482321529
Cu	-0.0329286606	1.1876494520	0.1223338382
Cu	2.0749299961	0.0059701919	-0.0972394137

Cu	2.0293037109	-2.3607087414	-0.0993849063
Cu	2.0216273545	2.3723464009	-0.0791169092
N	-4.0672013188	-0.0054276428	0.2545120917
N	-4.9885716133	-0.0071152172	-0.4065279748
O	-5.9388649277	-0.0087924834	-1.1051046820

### Cu<sub>6</sub>-N<sub>2</sub>O.5

E = -10028.1969753263

Cu	0.1968983220	-1.2461302256	0.7331279208
Cu	-1.3521033446	-2.4008943645	-0.5965186476
Cu	-1.3365155041	-0.0112533696	-0.6537706198
Cu	0.1885998438	1.2516795064	0.7165149930
Cu	2.5459234482	0.0102966439	0.4124181487
Cu	-1.3666414062	2.3788547617	-0.6295504592
N	3.8935253200	0.0092393432	-0.7794495040
N	4.7086740121	0.0087087046	-1.5241949608
O	1.2731722442	0.0124669305	1.6601881176

### Cu<sub>7</sub>-N<sub>2</sub>O.1

E = -11668.6826117372

Cu	1.6149307005	-0.0004215096	0.3383817550
Cu	0.1158424403	1.9821023333	0.1266577766
Cu	-2.2052282489	1.2117970603	-0.2277582188
Cu	-2.2054768173	-1.2090284131	-0.2328031674
Cu	0.1154134871	-1.9812469158	0.1186789462
Cu	-0.6742963066	-0.0016617648	1.2411924526
Cu	-0.3137894092	0.0030757094	-1.1845990175
N	3.5732729899	-0.0016031998	0.2941008330
N	4.5699061802	-0.0019063887	-0.2449704093
O	5.6007084136	-0.0022396144	-0.8218120693

### Cu<sub>7</sub>-N<sub>2</sub>O.2

E = -11668.6739300392

Cu	1.5534144589	0.4485244395	-0.0741997937
Cu	-0.2900454054	2.0859937139	-0.0944175101
Cu	-2.4211074266	0.8623982344	0.0165111645
Cu	-1.9223777471	-1.5227415298	0.1103717252
Cu	0.5204415289	-1.7890644826	0.0572459855
Cu	-0.5357664595	-0.0358577162	-1.2344658888
Cu	-0.4703999668	0.0747250668	1.2416248411
N	5.3669333929	-0.8686123033	0.3935322598
N	4.6286152346	-0.0479348186	0.1823246012
O	3.8331715090	0.8134680289	-0.0400578051

### Cu<sub>7</sub>-N<sub>2</sub>O.3

E = -11668.7627191536

Cu	2.2500185513	-0.7504095196	0.3463373926
Cu	1.7056074443	1.6012080986	-0.0849122127
Cu	-0.7294644601	1.8930087360	-0.1007662252
Cu	-1.9260438385	-0.4298474816	-0.2732886005

Cu	0.1676931436	-2.0468413827	0.1669075735
Cu	0.3913861040	-0.0313877706	-1.2019044308
Cu	0.1731118824	0.1306850372	1.2363926809
N	-4.5820637843	0.3146836546	0.7881967570
N	-3.6084995822	0.0242641647	0.3520665363
O	-0.8502433535	-1.5123199054	-1.3401520208

### Cu<sub>7</sub>-N<sub>2</sub>O.4

E = -11668.6825707301

Cu	1.5970739921	0.2631389285	0.1257173280
Cu	-0.1720970295	2.0188978963	-0.0404076012
Cu	-2.3907869362	0.9296356539	-0.1354430609
Cu	-2.0637348238	-1.4668157288	-0.0312714637
Cu	0.3630140413	-1.9042768828	0.1359887414
Cu	-0.5870645421	0.0175118824	1.2347064978
Cu	-0.4408374343	-0.0721849596	-1.2095352716
N	3.5457691969	0.3868402851	0.1164496725
N	4.6194396104	0.1292648378	-0.1344560470
O	5.7363624142	-0.1476308908	-0.4015632304

### Cu<sub>7</sub>-N<sub>2</sub>O.5

E = -11668.6889574312

Cu	-0.3132010654	-1.9951888361	-0.4051725640
Cu	-1.7532649550	0.0033398307	-0.8454805838
Cu	-0.3111057733	1.9974706351	-0.3918147896
Cu	1.8871126997	1.2221972933	0.4477319924
Cu	1.8857584296	-1.2278353042	0.4395394315
Cu	-0.1072746904	-0.0038456419	1.0801021633
Cu	0.6347299073	0.0035182678	-1.2655591920
N	-1.7448697644	-0.0067263541	2.0877528449
N	-2.8452329884	-0.0050054182	1.6455556604
O	-3.2915911716	-0.0008500999	0.4310357944

### Cu<sub>8</sub>-N<sub>2</sub>O.1

E = -13309.2703932342

Cu	-0.3129680362	-1.4267901907	-0.0027875587
Cu	-2.0345302080	0.5275819585	-0.0036952792
Cu	-0.3745950837	2.3741819725	0.0008426872
Cu	1.5969506480	0.9899018958	0.0032810717
Cu	1.7023006827	-1.0372922909	1.2883752319
Cu	-0.1607662483	0.4870511515	1.5502388119
Cu	-0.1554462169	0.4897634105	-1.5508585362
Cu	1.7066632673	-1.0348755041	-1.2856688277
N	-3.3686305697	-0.8619071890	0.0015084959
N	-3.0402435635	-2.0015936142	0.0030173526
O	-1.9173057088	-2.6068247197	0.0024471343

### Cu<sub>8</sub>-N<sub>2</sub>O.2

E = -13309.2652949169

Cu	0.8301104932	-1.2921410291	-0.6120500312
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Cu	-1.4903791466	-1.8921205036	0.0850429506
Cu	-2.4326891436	0.4384221017	0.7310656761
Cu	-0.4923607764	1.8981362824	0.1797623310
Cu	0.9694368154	1.0258910259	-1.6054894624
Cu	-1.1136962656	0.0178431168	-1.2616808777
Cu	-0.2484074346	-0.2297828399	1.2948614721
Cu	1.7305356514	0.9393696383	0.7671213712
N	3.3150313641	-0.1383734309	1.0255988893
N	3.3775319354	-1.2256777930	0.5675363791
O	2.5827357905	-2.0327681225	-0.0069415237

### Cu<sub>8</sub>-N<sub>2</sub>O.3

E = -13309.2635298171

Cu	1.3926636008	0.1178720646	-0.0871956361
Cu	-0.1409239081	2.0867193026	0.1899929615
Cu	-2.5195382416	0.7983421046	0.2508324148
Cu	-1.6797159009	-1.4759041334	-0.0019845790
Cu	0.5142376411	-1.9529166512	1.0457585792
Cu	-0.5417847215	0.1086648810	1.4292591320
Cu	-0.7362663024	0.3398044696	-1.2942351905
Cu	0.3383587699	-1.7446838030	-1.4136449415
N	3.3658366362	0.4884717872	-0.1388047957
N	4.1984005958	1.2472061372	-0.0149000682
O	5.0454036020	2.0610228686	0.1212042609

### Cu<sub>8</sub>-N<sub>2</sub>O.4

E = -13309.2695506153

Cu	0.0583448925	-1.4977501590	0.0046128610
Cu	-1.8750907069	0.0317934847	0.0084167252
Cu	-0.4301050647	2.2372274403	0.0002671359
Cu	1.7875448877	1.2429544433	-0.0049653314
Cu	2.0850453927	-0.8250367146	1.2419321433
Cu	0.0412483558	0.3992171320	1.4687519868
Cu	0.0319631045	0.3945124802	-1.4650604261
Cu	2.0776018225	-0.8283581792	-1.2479606495
N	-3.8221378873	-0.1228559957	0.0099174495
N	-4.7974783430	-0.6988562746	-0.0014877870
O	-5.8054688123	-1.3127660536	-0.0135958656

### Cu<sub>8</sub>-N<sub>2</sub>O.5

E = -13309.3498605390

Cu	-0.4046407462	-0.0666139191	1.4316290582
Cu	2.0319663033	0.3027788716	0.7065387589
Cu	1.1827175536	0.2758212818	-1.7677226419
Cu	-1.0974230877	-0.0658950281	-1.3199416679
Cu	-1.8732842753	-1.6119628201	0.4145462117
Cu	0.4951348862	-1.5708051214	-0.2854683388
Cu	-0.0160149870	1.7256970108	-0.1313201387
Cu	-2.3951489574	0.9263360504	0.3520597754
N	3.7125798752	-0.4059558779	0.4800433407

N 4.7195244733 -0.8419919682 0.3471680230

O 0.8308179847 1.3895826717 1.5760704363

Cu<sub>9</sub>-N<sub>2</sub>O.1

E = -14949.9328286696

Cu -0.5216082312 -1.2092811323 1.0876363639

Cu -2.3338692503 0.0209261582 -0.2750509667

Cu -0.2775328476 1.2923281971 -1.2999355287

Cu 1.7746406343 0.0128447982 -0.9190686088

Cu 1.4751571069 -2.1387274794 0.0672724276

Cu -0.2930145514 -1.2198200767 -1.3655101016

Cu -0.5079897053 1.1563394578 1.1488118037

Cu 1.5714458494 -0.0483938203 1.4800706712

Cu 1.5009479382 2.1137009882 0.1797456638

N -4.7933128669 -0.0084058553 1.3802475738

N -3.9007888897 0.0042142585 0.7293085818

O -1.5595995624 0.0602384907 -1.9642632860

Cu<sub>9</sub>-N<sub>2</sub>O.2

E = -14949.9263836678

Cu -0.1024682238 -1.3849625069 1.2104430616

Cu -2.3037812026 -0.5938846379 0.0032443942

Cu -0.7080886664 1.0807558893 -1.1970600749

Cu 1.5968092538 0.4319182676 -1.2376616974

Cu 2.0346817072 -1.6200189399 -0.0622735355

Cu -0.1346021481 -1.2968313139 -1.2462637036

Cu -0.6726594342 0.9890411257 1.2156748473

Cu 1.6333930802 0.3604034863 1.2489357263

Cu 0.9632366938 2.3895788654 0.0605455623

N -4.8704792772 0.8911559850 0.0504642752

N -3.9434621609 0.2904022439 0.0311298403

O -1.3348398633 -2.1694055940 -0.0290462750

Cu<sub>9</sub>-N<sub>2</sub>O.3

E = -14949.9333407949

Cu -1.0447729640 -1.9370705483 -0.3722450967

Cu -2.3949798148 -0.5421709143 1.1583418164

Cu -1.5498011880 1.8323616652 0.9591740026

Cu 2.3525470760 0.4239020406 -0.0202139134

Cu 1.3125298072 -1.9021973024 0.4282000992

Cu -0.0529461761 -0.0368436804 0.8851020330

Cu -1.7084019097 0.3046201908 -0.9939420634

Cu 0.5797976424 -0.5279058739 -1.5320108452

Cu 0.2062010531 1.8302920811 -0.7352091653

N 4.6376922504 0.5189972581 1.8638454992

N 3.8138728263 0.4998364799 1.1273244662

O 1.6491596083 1.0647526006 -1.6518255838

Cu<sub>9</sub>-N<sub>2</sub>O.4

E = -14949.9359069770

Cu -1.2131931200 -1.4018582210 -0.6001192337

Cu	0.8461914238	-0.6269104179	-1.6714436686
Cu	2.6612933886	0.2334619768	0.0450839679
Cu	0.0910891745	0.4875932007	0.4699516712
Cu	-0.9867239539	-1.2243242942	1.8335083811
Cu	1.0243966321	-1.7414386639	0.5479373189
Cu	-1.1280939371	0.7916538957	-1.6208301922
Cu	-2.3375134463	0.4186008178	0.5558572950
Cu	-1.1557452040	2.4912417323	0.2118195372
N	3.7596318568	2.6759621691	1.2361362555
N	3.3704517206	1.7504964206	0.7764890004
O	2.3797563683	-1.3668048021	-0.7616700194

### Cu<sub>9</sub>-N<sub>2</sub>O.5

E = -14949.9358907366

Cu	-0.1493298654	0.5860606005	0.2668514947
Cu	1.5844490166	-0.2910123141	1.7413724921
Cu	1.5092517364	-1.1441590981	-0.5544513845
Cu	0.6103973245	0.5335205127	-2.0513965078
Cu	0.3717305282	2.6618229934	-0.7584627872
Cu	2.1681489868	1.1663305457	-0.1770420672
Cu	-0.3293317290	-1.6731427462	1.1124285212
Cu	-2.5487251603	-0.4313572505	0.5078440546
Cu	-0.8192652118	-1.2837296073	-1.2963348928
N	-4.1697269136	1.8943782438	1.2506628617
N	-3.5817428869	1.0027706792	0.9694445959
O	-1.9046149612	-2.0750411471	0.0909153593

### Cu<sub>9</sub>-N<sub>2</sub>O.6

E = -14949.9328213224

Cu	1.5622553209	0.0327980201	1.4866989170
Cu	1.4812876312	2.1331013936	0.0872882835
Cu	-0.2836369975	1.2307605023	-1.3597390122
Cu	-0.2786921577	-1.2818206482	-1.3121594372
Cu	1.4893115012	-2.1204649581	0.1706698155
Cu	1.7766478400	-0.0132539029	-0.9117713473
Cu	-0.5243024199	1.2050273144	1.0919131343
Cu	-0.5201134896	-1.1609309415	1.1360631704
Cu	-2.3350950831	-0.0089281356	-0.2885301760
N	-4.8001102721	0.0119179381	1.3585029914
N	-3.9057882176	0.0052226058	0.7099574154
O	-1.5525581337	-0.0398428996	-1.9739212846

### Cu<sub>9</sub>-N<sub>2</sub>O.7

E = -14949.9328284248

Cu	-0.2850603788	1.2576609023	1.3304939874
Cu	1.4930288103	2.1200983935	-0.1247305015
Cu	1.5716129732	-0.0097421086	-1.4766593385
Cu	-0.5187695696	-1.1860616194	-1.1162185549
Cu	-2.3364951149	0.0054969853	0.2740438176
Cu	-0.5116583030	1.1806763078	-1.1210622381

Cu	1.7724645855	-0.0055304473	0.9235510209
Cu	-0.2925112725	-1.2549725130	1.3356971178
Cu	1.4802026559	-2.1335809438	-0.1163229854
N	-4.7917440076	0.0178691331	-1.3873472055
N	-3.9008561543	0.0109822714	-0.7340738669
O	-1.5638341525	0.0063258807	1.9641537247

### Cu<sub>10</sub>-N<sub>2</sub>O.1

E = -16590.4341684288

Cu	-0.5571561737	-0.2128790169	1.2301770293
Cu	1.7557062922	0.2343051272	1.9740511326
Cu	3.2502905107	0.4324457998	0.0012737284
Cu	1.7610052020	0.2160719110	-1.9731361663
Cu	-0.5543619965	-0.2234212741	-1.2311365621
Cu	0.8948485756	1.3325688025	-0.0058192149
Cu	1.3868184609	-1.1198157902	0.0060854621
Cu	-1.5650756677	1.6303681478	-0.0100095499
Cu	-2.6424096046	-0.7666498144	-0.0000013996
Cu	-0.7435444794	-2.3204496050	0.0081861664
N	-3.4197207509	2.1035406886	-0.0050092955
N	-4.3504043844	1.3677658091	0.0004098919
O	-4.4271661691	0.0731467055	0.0037832436

### Cu<sub>10</sub>-N<sub>2</sub>O.2

E = -16590.4331832162

Cu	1.3908113302	1.1102556585	-0.0018889701
Cu	-0.7086311013	2.3621796750	-0.0027223045
Cu	-2.6419496968	0.8404654219	0.0005285703
Cu	-1.5692125014	-1.6155810874	0.0028412008
Cu	0.8680583138	-1.3239575913	0.0023500729
Cu	-0.5685208216	0.2478542348	1.2289974755
Cu	-0.5694213142	0.2443598484	-1.2284436087
Cu	1.7430673903	-0.2287802456	1.9753871019
Cu	3.2325581164	-0.4726306815	-0.0001278257
Cu	1.7414976219	-0.2352150132	-1.9750461791
N	-4.3517791306	-0.0809083782	0.0055698288
N	-4.3705606231	-1.2699163860	0.0084504273
O	-3.4555452595	-2.1732941711	0.0087576937

### Cu<sub>10</sub>-N<sub>2</sub>O.3

E = -16590.4278666213

Cu	-0.5017750062	-0.5826207024	1.2029342726
Cu	1.3560371044	0.8494554900	1.9583724662
Cu	2.7542127594	1.5619683434	0.0409008329
Cu	1.6991286422	0.4689301848	-1.9182817836
Cu	-0.2826458010	-0.8294139849	-1.2311740718
Cu	0.2877996941	1.3014459165	-0.1539660038
Cu	1.7698020898	-0.7164513976	0.1770140827
Cu	-2.0933496805	0.5192178944	-0.2889569877
Cu	-2.1065930585	-1.9838088856	-0.0379946795

Cu	0.2923625685	-2.6535581153	0.2481281521
N	-3.6954713861	1.6096227286	-0.3686931388
N	-4.5923322161	2.2131449302	-0.0318772975
O	-5.5286783136	2.8409781761	0.3221402790

#### Cu<sub>10</sub>-N<sub>2</sub>O.4

E = -16590.4192828131

Cu	-0.5519426157	-0.7131546216	0.8361057457
Cu	1.7272858966	-1.2935414664	1.6023146242
Cu	3.4736874272	-0.1749949149	0.2110722022
Cu	2.1502931073	1.1275182747	-1.4378779834
Cu	-0.2811722341	0.8256659969	-1.0874945356
Cu	1.3102307937	0.9329120617	0.8062977023
Cu	1.3307756271	-1.0242587204	-0.7507185812
Cu	-1.0611175276	1.6174368798	1.0416914480
Cu	-2.5990675281	0.1779675788	-0.3140951018
Cu	-1.0237600543	-1.4384986471	-1.3980194129
N	-4.6824286127	0.2138077871	-0.4389447374
N	-5.4967821981	-0.3264702411	0.1443396495
O	-6.2801393592	-0.9278535278	0.7956865490

#### Cu<sub>10</sub>-N<sub>2</sub>O.5

E = -16590.4051184727

Cu	0.9458325976	-1.1206278479	-0.0002656714
Cu	-1.6212065979	-1.7500223743	-0.0006654194
Cu	-2.9911525354	0.2541290991	0.0006616446
Cu	-1.4603401916	2.2729101633	0.0018228509
Cu	0.8421825024	1.4720609507	0.0012157294
Cu	-0.8717692750	0.2339331653	-1.2126238253
Cu	-0.8716424171	0.2324461374	1.2137050674
Cu	1.4545977632	0.2582146637	-1.9828392053
Cu	2.9585148093	0.2117029287	0.0003812605
Cu	1.4547978019	0.2559790393	1.9838277492
N	1.5553521661	-3.2114226961	-0.0010993776
N	0.3877714872	-3.0503082118	-0.0010280327
O	-0.7184510787	-3.6713495114	-0.0012018461

#### Cu<sub>10</sub>-N<sub>2</sub>O.6

E = -16590.4217427303

Cu	-1.0081061575	-0.3121009864	1.2204551547
Cu	1.1914187887	0.5141201977	1.9672649160
Cu	2.4942396519	1.4231515762	0.0654672057
Cu	1.0238081802	1.0562355108	-1.8969075348
Cu	-1.1165523013	0.0354968428	-1.2188919628
Cu	1.0786839930	-0.6694869744	-0.1677859395
Cu	0.0398019221	1.6490186645	0.2032360317
Cu	-0.9691961472	-2.1753180405	-0.2960131685
Cu	-3.0657379670	-0.9289941762	-0.0211490973
Cu	-2.4166190370	1.4344683027	0.2887521251
N	2.5413953220	-2.0245678822	-0.3116496434

N 3.2512546238 -2.8777232163 -0.0971143219  
O 3.9889263413 -3.7740762677 0.1347621534

#### Cu<sub>10</sub>-N<sub>2</sub>O.7

E = -16590.4341686588

Cu	-0.5565449229	-0.2172018299	1.2304889654
Cu	1.7568555928	0.2295263551	1.9741391347
Cu	3.2499747566	0.4355299080	0.0010335728
Cu	1.7593274724	0.2234604988	-1.9729276962
Cu	-0.5550837612	-0.2210524205	-1.2307846466
Cu	0.8933121327	1.3329218449	-0.0016747706
Cu	1.3877381368	-1.1186636872	0.0024864266
Cu	-1.5666696867	1.6286134096	-0.0039306897
Cu	-2.6419484103	-0.7694052804	-0.0004555094
Cu	-0.7415764021	-2.3216053313	0.0029472637
N	-3.4216361214	2.1006342231	0.0007409755
N	-4.3516125537	1.3639563561	0.0042108114
O	-4.4273277875	0.0693185469	0.0049422806

#### Cu<sub>10</sub>-N<sub>2</sub>O.8

E = -16590.4331825094

Cu	0.8691021220	-1.3238320490	0.0049479882
Cu	-1.5678938628	-1.6170612338	0.0114616411
Cu	-2.6423741217	0.8380394393	0.0000560171
Cu	-0.7101975850	2.3612415129	-0.0122737262
Cu	1.3901010581	1.1106949456	-0.0072745034
Cu	-0.5710756946	0.2387275663	-1.2294294160
Cu	-0.5669644752	0.2519677089	1.2281453010
Cu	1.7395684717	-0.2405524824	-1.9766580850
Cu	3.2330851971	-0.4707682878	-0.0025190749
Cu	1.7454607186	-0.2222078794	1.9736606223
N	-4.3514545023	-0.0846829703	-0.0094757490
N	-4.3693867659	-1.2737037659	-0.0051510702
O	-3.4537581721	-2.1763860672	0.0051635047

#### Cu<sub>10</sub>-N<sub>2</sub>O.9

E = -16590.4341681730

Cu	0.8941932533	-1.3326613151	-0.0075942676
Cu	-1.5655976909	-1.6288234869	-0.0127162814
Cu	-2.6421987340	0.7684586452	0.0015350243
Cu	-0.7420263643	2.3211896074	0.0136162253
Cu	1.3877633298	1.1192251837	0.0087098906
Cu	-0.5568792721	0.2112839263	1.2311322418
Cu	-0.5541039087	0.2268236801	-1.2299557050
Cu	1.7560188859	-0.2386477554	1.9738866504
Cu	3.2500552844	-0.4346021009	0.0002040051
Cu	1.7603913019	-0.2133742267	-1.9731152991
N	-3.4202607276	-2.1025298200	-0.0086314538
N	-4.3505628521	-1.3663205841	0.0006002479
O	-4.4268140738	-0.0716542616	0.0079624253

Cu<sub>10</sub>-N<sub>2</sub>O.10

E = -16590.4157894922

Cu	-1.2527764787	0.0347168511	1.2112465776
Cu	0.8430390971	1.0237123601	2.0652890584
Cu	2.4618687709	1.4102307506	0.2281679443
Cu	1.2947658194	0.5927076224	-1.7956672518
Cu	-0.9623389331	-0.2430913282	-1.2507483876
Cu	0.9607874176	-0.5975434355	0.2797989354
Cu	0.0125245927	1.7030645324	-0.0889791999
Cu	-0.9809949574	-2.1441345616	0.2267326134
Cu	-3.0967629118	-0.9215481393	-0.1603706196
Cu	-2.4266981578	1.4536986117	-0.3531705859
N	4.7679973117	-2.3229676085	-0.8583622098
N	3.8942723982	-2.3779818980	-0.1513076421
O	2.9691830502	-2.4299234684	0.5910152261

Cu<sub>10</sub>-N<sub>2</sub>O.11

E = -16590.5297829965

Cu	-0.8653277452	0.9863796035	1.3347487733
Cu	3.0703870925	0.4951687080	0.0175925971
Cu	1.2445093419	-0.6870175060	-1.5935110244
Cu	-0.1507022163	-2.4363034842	-0.6461920969
Cu	-1.0657252371	-0.2712217278	-0.8145153884
Cu	0.8068793350	-0.6591448641	0.8344705025
Cu	0.6984346626	1.5169069754	-0.5234479161
Cu	-1.4637580237	-1.3912673022	1.3299501414
Cu	-3.0707063235	0.1938852094	0.3930520741
Cu	-1.7097234942	2.0262145593	-0.6657876723
N	4.1189960511	0.1653665676	1.4613424532
N	4.7485284077	-0.0394555623	2.3448244569
O	2.2600593883	0.9321675560	-1.5244734165

Cu<sub>11</sub>-N<sub>2</sub>O.1

E = -18231.1020436979

Cu	-1.4811990410	-2.1375320140	0.1682217386
Cu	-2.4635363019	0.2913057246	-0.6499199579
Cu	-1.8262126161	2.1617846167	0.7878607046
Cu	0.6494706542	2.2613197299	0.8103881249
Cu	1.7767565994	0.1183555711	1.5383311259
Cu	1.2024157251	-1.6955647424	-0.0470276777
Cu	-0.4729417478	0.1560831475	0.6804671908
Cu	-0.4314982558	-0.7053871302	-1.6936261899
Cu	-0.5426844771	1.6901826467	-1.2873769010
Cu	1.5759052496	0.6119370025	-0.8369176307
Cu	3.4249162893	-0.8486593766	0.0613388500
N	-3.5823795212	-2.7842273841	2.1415158468
N	-2.8052959586	-2.5825703654	1.3828472751
O	-0.1529237536	-2.5057141301	-1.0586757880

Cu<sub>11</sub>-N<sub>2</sub>O.2

E = -18231.0977637624

Cu	-1.0141641648	-2.3997498710	0.1002097187
Cu	-2.5272956115	-0.2312542099	-0.4082555980
Cu	-2.2542374216	1.6282517228	1.0776616266
Cu	0.3323462632	2.3063129829	0.9244615734
Cu	1.9586452158	0.5286795346	1.3433256634
Cu	1.3680040757	-1.3632360878	-0.1145471794
Cu	-0.3975582161	0.0475599755	0.7907379754
Cu	-0.4016823359	-0.6726928864	-1.7111405969
Cu	-1.0032689778	1.6394273450	-1.0200466081
Cu	1.3063190044	0.9415443393	-0.9719272487
Cu	3.4360989613	-0.2194835456	-0.4600970565
N	-0.6393986971	-3.6436791720	1.4285046588
N	-0.3583508455	-4.3269341689	2.2497328313
O	-1.9389982395	-1.7604525477	-1.3616980741

### Cu<sub>11</sub>-N<sub>2</sub>O.3

E = -18231.0958646939

Cu	-0.0228956378	-2.5276795752	0.8405553938
Cu	-1.8640778385	-1.5185867670	-0.5398278943
Cu	-2.8261303175	0.8789815422	0.1561274957
Cu	-0.4621598840	2.1379292724	0.1617222529
Cu	1.5170928805	1.3259990913	1.3604090057
Cu	1.9453684731	-1.0996456952	0.6067431140
Cu	-0.3102041051	-0.1667566454	0.7255129779
Cu	0.4319116192	-1.4307210700	-1.3583181388
Cu	-1.0209752898	0.5140690421	-1.6634433668
Cu	1.3781123221	0.7389707716	-0.9623180313
Cu	3.5632598878	0.5758687462	0.1280288769
N	-4.7415553434	-0.2529473551	2.0789593754
N	-4.0232177544	0.1681206699	1.3533712993
O	-1.9997445989	2.0329389085	-0.9841268650

### Cu<sub>11</sub>-N<sub>2</sub>O.4

E = -18231.0971650284

Cu	-0.7234785015	-1.6095956763	0.5467781804
Cu	-3.0257781017	-1.6200935232	-0.3901455462
Cu	-2.3128308898	0.2299479388	0.8722654015
Cu	-0.9226255218	2.2605614992	-0.0013075433
Cu	2.5632123129	0.9436249059	1.0259026078
Cu	1.5959852945	-1.2535520732	0.8880870957
Cu	0.1279348597	0.5460090084	1.6845903240
Cu	0.8011093899	-1.6488733858	-1.4114572009
Cu	-1.2746199833	-0.1607304824	-1.3047226217
Cu	0.8756873419	0.6084273663	-0.6436161944
Cu	2.9841135738	-0.4436863988	-0.9847000239
N	-0.6529771635	4.2549899429	-2.1707297720
N	-0.7796425911	3.5514713634	-1.3286144389
O	-1.4229454959	1.6580688186	1.6778171817

Cu<sub>12</sub>-N<sub>2</sub>O.1

E = -19871.6030165434

Cu	2.6763533808	-1.5255998746	0.7626048604
Cu	3.0285812199	0.7010827994	-0.2404230559
Cu	1.5337371978	2.4154053169	0.6878950174
Cu	-0.9556080606	1.6564258566	0.3419956059
Cu	-1.3700930911	-0.5878240865	1.3307054077
Cu	0.2354269733	-2.1834333010	0.4103222917
Cu	0.9136582552	0.1169996708	0.8044199265
Cu	1.5728515873	-1.0102538331	-1.3311645751
Cu	0.8545869794	1.2980830596	-1.3591713698
Cu	-0.8316383088	-0.4652769698	-1.0352113286
Cu	-2.2182294438	-2.3028342486	-0.1610951650
Cu	-3.1140683776	-0.0031075171	-0.2405614440
N	-4.0441753321	1.6640682355	-0.2687171476
N	-3.5422930534	2.7148306887	-0.0299003450
O	-2.3523367153	3.0585274291	0.2898602890

Cu<sub>12</sub>-N<sub>2</sub>O.2

E = -19871.6025237589

Cu	-1.3401044033	-2.4156117239	0.8405448795
Cu	-2.6845252741	-0.6750433839	-0.2640252512
Cu	-1.9029484652	1.8118984867	0.6730465057
Cu	0.5683415943	2.0165475013	0.2087387481
Cu	1.8321901884	0.2926438412	1.3411534135
Cu	1.1617047729	-1.9038753394	0.4684401432
Cu	-0.5277772655	-0.1517450781	0.7942027780
Cu	-0.5792171520	-1.5208084296	-1.2718576061
Cu	-0.9998834043	0.8750269606	-1.3877811465
Cu	1.3028643784	0.0597521583	-1.0756938271
Cu	3.3297864668	-0.8526706595	-0.1363768034
Cu	2.9936320668	1.6611416455	-0.2890918213
N	-3.7913959920	2.1177570226	0.6304905263
N	-4.5806013822	1.3356154083	0.2136727277
O	-4.4755486613	0.1505693220	-0.2635404566

Cu<sub>12</sub>-N<sub>2</sub>O.3

E = -19871.6682943483

Cu	-1.7997584535	-2.1000224708	1.0441856147
Cu	-3.0745129505	-0.1564525745	-0.0521323101
Cu	-2.1375720922	1.9791970305	0.6515307830
Cu	0.5709541453	1.9783513285	0.0030099649
Cu	1.8721604426	0.0577217008	0.9508446156
Cu	0.6340535388	-1.9989836230	0.2138255438
Cu	-0.7389924734	0.0179288466	0.8720329891
Cu	-1.2461676304	-1.3382858821	-1.1826982045
Cu	-1.3632758642	1.0197281769	-1.4623285955
Cu	0.8278327551	-0.0680092020	-1.3224253226
Cu	2.8311467813	-1.3300213341	-0.7350368776
Cu	2.7294571869	1.3280695349	-0.9391555242

N	2.2609040246	0.2349759302	2.8107760145
N	2.4792713569	0.3585860928	3.8831090838
O	-0.4948821297	1.8799617760	1.5426764285

### Cu<sub>12</sub>-N<sub>2</sub>O.4

E = -19871.6783112425

Cu	-2.0225157514	-2.1135842890	0.8057120559
Cu	-2.9081056392	-0.2770950508	-0.6608777836
Cu	-2.3663169964	2.0548732176	0.0909104720
Cu	0.1758639946	2.1961854740	0.4751818165
Cu	1.0864556450	0.4929165587	1.9203470929
Cu	0.5012746821	-1.7127714804	1.1407581515
Cu	-1.0965700130	0.1367733505	0.8905439351
Cu	-0.7542677724	-1.4394918458	-1.0797309791
Cu	-0.9533061677	1.0057795966	-1.4982549509
Cu	1.2289288842	0.0856244366	-0.5390511370
Cu	2.8450319629	-0.8375413118	0.9882740849
Cu	2.6323193591	1.7076626056	0.5559318815
N	3.4160580300	-1.8514282961	-3.6109925501
N	2.9682563739	-1.4488429727	-4.5251389749
O	0.2928222577	-0.2695581804	-2.1379671872

### Cu<sub>13</sub>-N<sub>2</sub>O.1

E = -21512.2743962598

Cu	-0.9014609328	0.6667118897	0.7537947989
Cu	1.2982348864	0.1134413663	1.6729418625
Cu	-2.7646890698	0.6035468685	-0.7158933154
Cu	-2.0918636639	-1.4099435320	0.8433679286
Cu	0.3759242800	-1.8622806185	0.5016575256
Cu	2.7879672951	-1.3491280702	0.2069189822
Cu	3.0606605668	1.1156618918	0.4710750106
Cu	0.8400791412	2.2843850734	0.3341598981
Cu	-1.6461368080	2.8310354987	0.2042703897
Cu	-0.6300765997	1.5180423327	-1.5391701686
Cu	-0.9314676786	-0.9168728866	-1.3838560858
Cu	1.2623874251	0.1527247171	-0.8791830129
Cu	1.2754060582	-2.1599551006	-1.6337136317
N	-4.3388316978	-3.3343559951	1.1977852525
N	-3.5018678603	-2.6162716950	1.1407814815
O	-0.4315776254	-0.8306926010	1.9214575088

### Cu<sub>13</sub>-N<sub>2</sub>O.2

E = -21512.2598057694

Cu	-0.7129417576	-0.2217831917	1.1213851708
Cu	1.5485852006	0.5770797093	1.5962390284
Cu	-2.7845770522	-1.0237348055	0.2314661953
Cu	-1.0815539045	-2.6215775334	1.0212174727
Cu	1.2096802864	-1.6686594683	0.6632623882
Cu	3.1650143186	-0.2530091017	-0.1153843306
Cu	2.4087239420	2.1513427250	-0.0130725951

Cu	-0.0811443843	2.1508330950	0.5722582313
Cu	-2.6445767283	1.2876102716	1.0762051213
Cu	-1.5513576418	0.9461880883	-1.1161236923
Cu	-0.6362791259	-1.4328235989	-1.0432443307
Cu	0.9261237859	0.4081637389	-0.7800927801
Cu	1.8190528000	-1.5882571192	-1.6865399270
N	-2.5249684975	1.2098578352	-3.9911672670
N	-2.2242265418	1.1138572062	-2.9358339111
O	-1.8249614063	2.5992604180	0.0657016755

### Cu<sub>13</sub>-N<sub>2</sub>O.3

E = -21512.2577993513

Cu	1.2209801889	0.2227298679	-0.3022089636
Cu	-0.8832834569	1.3693906831	-1.2102252967
Cu	2.5857321065	-1.1261007987	1.1305235891
Cu	1.6747756577	-2.1306482692	-0.9156670311
Cu	-0.6636829401	-1.1461817014	-1.3373313489
Cu	-2.9145165406	-0.0058132545	-0.8453204491
Cu	-2.3845607773	2.1374124072	0.4328666555
Cu	0.0978622175	2.0715195930	0.9792409863
Cu	2.5424415403	1.4193417373	1.2988130731
Cu	0.7611986287	0.0734732361	2.2096809417
Cu	0.1861505634	-1.9160251660	0.9293927489
Cu	-1.2964160283	0.0166443294	0.9143036485
Cu	-2.1919989809	-2.1414320377	0.1797353112
N	3.0309777052	1.4404344376	-4.1197292439
N	2.3643557843	2.2873774612	-4.3115398998
O	0.4028425386	0.2880840515	-2.0346927325

### Cu<sub>13</sub>-N<sub>2</sub>O.4

E = -21512.2560978928

Cu	-0.9637557889	-0.0415608552	-0.8833161683
Cu	1.2765659008	0.6064769456	-1.5815588346
Cu	-3.0008866009	-0.8105052288	0.1866813795
Cu	-1.6106290119	-2.3295202316	-1.1438164727
Cu	0.8196555442	-1.7105128603	-0.8882223420
Cu	2.9743639059	-0.7060189317	-0.0918345477
Cu	2.6372740109	1.7216829272	0.1235709594
Cu	-0.0901801841	2.1938770552	-0.1110208467
Cu	-2.6959530046	1.5665331343	-0.4173850766
Cu	-1.3887625372	0.6684904732	1.4085755575
Cu	-0.7744364152	-1.6947880000	1.0413017611
Cu	0.9314671321	0.0704348273	0.9093309571
Cu	1.6702476434	-2.2137250646	1.3305589425
N	-0.6322763128	4.9785673025	1.0691972247
N	-0.5017848707	3.9510871905	0.6953073029
O	1.5455782791	2.4700604352	-1.1733474379

### Cu<sub>13</sub>-N<sub>2</sub>O.5

E = -21512.2648415721

Cu	0.9601885601	-0.6641672339	0.7717817258
Cu	-1.4842446252	-1.0249854261	0.9742469242
Cu	3.0423897237	0.4761378959	0.2604024541
Cu	1.4308066795	1.3571290143	1.9521947770
Cu	-0.9233913674	1.4330931905	1.0723686600
Cu	-2.8781106814	0.7586006726	-0.2698448173
Cu	-2.3596182031	-1.4709208369	-1.2366868227
Cu	0.0545396817	-2.0931402840	-0.9275569261
Cu	2.5174680768	-2.0617420188	-0.2907657146
Cu	1.6347443621	-0.2493982409	-1.6037053253
Cu	1.0741395732	1.8217259003	-0.4368968941
Cu	-0.6980230938	0.2583635648	-1.1513618177
Cu	-1.2756018595	2.6132562191	-0.9180377451
N	-2.7086782415	-3.0342737113	2.9231579683
N	-2.2848562220	-2.3079875553	2.2136255410
O	-0.1512595481	0.1006105063	2.1803321147

### Cu<sub>14</sub>-N<sub>2</sub>O.1

E = -23152.7862541958

Cu	-0.8648281511	0.1734164734	-0.8613705930
Cu	1.1354747268	1.4370515791	-1.4522778550
Cu	-2.5170629609	-1.2184756573	0.2764879719
Cu	-0.7700994218	-2.3179600315	-1.1147264622
Cu	1.3247904057	-0.9741856423	-1.0318917605
Cu	3.1187111847	0.6694745796	-0.2460333869
Cu	2.0135532281	2.8857003110	0.2859851694
Cu	-0.4736513362	2.5028365803	0.0515183238
Cu	-2.7671244989	1.5961561050	-0.2773717087
Cu	-1.3449597710	0.6293388350	1.4473280855
Cu	-0.1021461653	-1.4446874131	0.9903892989
Cu	1.0287235544	0.7418467089	0.9068189115
Cu	2.4104797826	-1.3463799343	1.0523056936
Cu	1.2555844466	-3.2292187353	-0.0321153781
N	-4.6284024081	1.1046554088	-0.2698579570
N	-5.0282789962	0.0058037620	-0.0793738332
O	-4.4799975968	-1.1268942584	0.1623878468

### Cu<sub>14</sub>-N<sub>2</sub>O.2

E = -23152.8663260585

Cu	0.1701491872	-1.1954664267	-0.8327840093
Cu	-1.8926358525	0.2062760389	-1.0446262906
Cu	2.4114279734	-1.8486446884	-0.2221064073
Cu	1.9976128750	0.1929798019	-1.6406865358
Cu	0.1746609904	1.6428324112	-0.8681367619
Cu	-1.7951204601	2.2778622041	0.4756344831
Cu	-3.0295012331	0.1575210358	1.0784771792
Cu	-1.6416598812	-1.8551051079	0.6275927610
Cu	0.2527554586	-3.4132489640	-0.0710536722
Cu	0.6814859961	-1.6727020441	1.5391560217
Cu	1.8035175740	0.3289926224	0.7772551908

Cu	-0.6296582026	0.3354297039	1.2320085897
Cu	0.6214661175	2.4734294552	1.2675567825
Cu	2.5057251606	2.2880564757	-0.4347180202
N	-3.2767355535	0.0729810361	-2.4662811494
N	-4.0015711677	-0.0515956786	-3.2836844832
O	-0.1065168827	0.1994244137	-2.0891631625

#### Cu<sub>14</sub>-N<sub>2</sub>O.3

E = -23152.7828102939

Cu	0.7116233136	0.6607894797	-0.8314044876
Cu	0.1589815900	-1.6437975644	-1.4296259413
Cu	0.8631408218	2.8070654677	0.3351933523
Cu	-1.0902723773	2.3746943296	-1.1152292030
Cu	-1.6556492027	-0.0610189500	-1.0557791105
Cu	-1.8313498682	-2.5040519967	-0.2750988345
Cu	0.4908866359	-3.3036201364	0.2992897327
Cu	2.0643799187	-1.2965437525	0.1132044837
Cu	2.9111354781	1.5045163638	-0.1416031424
Cu	1.3185611582	0.6634667081	1.4905025466
Cu	-1.0116403637	1.2509887327	1.0012365941
Cu	-0.2753086369	-1.0848885214	0.8922079621
Cu	-2.7343811821	-0.5843543635	0.9971033744
Cu	-3.1696994075	1.6309250829	-0.0563554930
N	4.6269066824	0.6610872142	-0.3635833178
N	4.7692850194	-0.5134273455	-0.3506990956
O	4.0077171756	-1.5259178392	-0.2011852348

#### Cu<sub>14</sub>-N<sub>2</sub>O.4

E = -23152.8640666340

Cu	1.3788706971	0.0834431708	0.1673909281
Cu	-0.2060466101	1.6736230482	1.3194538754
Cu	2.1787254786	-1.4966212029	-1.4349528200
Cu	1.0081024144	-2.3751877735	0.5577011711
Cu	-0.8356926223	-0.7750383453	1.2692942523
Cu	-2.5888543063	1.1329615065	0.9745162110
Cu	-1.3921420204	3.1209791138	-0.1077378852
Cu	0.8839609266	2.3285340163	-0.8492960855
Cu	2.9547160640	0.9624960070	-1.3878308616
Cu	0.7989256719	0.3407199032	-2.2653102162
Cu	-0.3591821214	-1.4926763529	-1.1800060516
Cu	-1.1152048071	0.8315947922	-0.8858269506
Cu	-2.6396986677	-1.0050046316	-0.2642964825
Cu	-1.3714262436	-3.0004030354	0.4968719286
N	3.3987700885	-0.6992187300	4.0002402122
N	3.4577961173	0.3473681653	4.3150699536
O	0.6926266528	0.1427613289	1.9426457317

#### Cu<sub>14</sub>-N<sub>2</sub>O.5

E = -23152.7862547027

Cu	-0.8638073521	0.1729658170	-0.8620958550
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Cu	1.1380744933	1.4335065332	-1.4538462058
Cu	-2.5182897747	-1.2156343737	0.2765467508
Cu	-0.7718370908	-2.3190340825	-1.1118694938
Cu	1.3245029914	-0.9774946604	-1.0299115474
Cu	3.1199507975	0.6649601370	-0.2458449785
Cu	2.0173698089	2.8831066435	0.2831256545
Cu	-0.4702058649	2.5030888877	0.0479894694
Cu	-2.7647118375	1.5985543977	-0.2805675162
Cu	-1.3443998560	0.6323330153	1.4458280273
Cu	-0.1041135844	-1.4438039543	0.9923983020
Cu	1.0295988248	0.7413595112	0.9063423176
Cu	2.4086989995	-1.3480778659	1.0551943820
Cu	1.2522288586	-3.2312496377	-0.0272235169
N	-4.6268089738	1.1106849250	-0.2662927290
N	-5.0282512512	0.0129827949	-0.0723292933
O	-4.4813793382	-1.1202994116	0.1696900508

#### Cu<sub>14</sub>-N<sub>2</sub>O.6

E = -23152.7858649961

Cu	-0.8690903077	0.1303387057	-0.8526657963
Cu	1.0831333287	1.4542817255	-1.4530997480
Cu	-2.4905248591	-1.2797872434	0.2909973303
Cu	-0.7031145988	-2.3552933700	-1.1001093142
Cu	1.3533386503	-0.9500691607	-1.0326192709
Cu	3.0961759890	0.7530345957	-0.2571152145
Cu	1.9176148382	2.9351188623	0.2785576462
Cu	-0.5585086349	2.4706211551	0.0529500646
Cu	-2.8041970784	1.5006851190	-0.2597838332
Cu	-1.3495348628	0.5738101572	1.4639735376
Cu	-0.0439610200	-1.4617824473	0.9988332787
Cu	1.0108170893	0.7598324140	0.9039678498
Cu	2.4663074529	-1.2864006870	1.0424988127
Cu	1.3609626511	-3.2038693184	-0.0308393515
N	-4.4116039710	-1.1774690698	0.1687208225
N	-5.0249702292	-0.1918986101	-0.0661347805
O	-4.7163808332	1.0278173128	-0.3072537712

#### Cu<sub>15</sub>-N<sub>2</sub>O.1

E = -24793.4511847653

Cu	-0.7821117515	0.0028827613	-0.7697203959
Cu	0.8427627929	1.6211107413	-1.5933396322
Cu	-1.9648193613	-1.6095875081	0.7626794391
Cu	-0.2750156435	-2.3721764235	-0.9536335569
Cu	1.5420062122	-0.6737165775	-1.0297340514
Cu	3.0045548760	1.3375880098	-0.4658001840
Cu	1.4355066447	3.2807136892	0.0997285010
Cu	-0.8784082016	2.3125710712	0.0568675214
Cu	-2.9381468674	0.6966489678	-0.0810814979
Cu	-1.1477718681	0.5316100034	1.7053718921
Cu	0.5228809994	-1.4382262850	1.2291275293

Cu	1.0662619007	1.0028750694	0.8207630773
Cu	2.9043174663	-0.7279552552	0.9340622773
Cu	2.0096817954	-2.8448945906	-0.0542124398
Cu	-2.5748874599	-1.4310460734	-1.5082442312
N	-5.7177528774	1.8742754021	0.2125758094
N	-4.7243077392	1.3986217547	0.1870422937
O	-1.0015909657	-1.2311522873	2.3508687787

### Cu<sub>15</sub>-N<sub>2</sub>O.2

E = -24793.4485399849

Cu	-0.7599093150	0.0334627984	0.9110836561
Cu	1.2516503593	-0.9554752630	1.8643500189
Cu	-2.4473898822	0.8729246929	-0.6982717369
Cu	-0.8886433347	2.4268454642	0.5820782326
Cu	1.3299391306	1.2550558630	0.8002881145
Cu	3.1760633336	-0.4728934265	0.4577117140
Cu	2.0693372571	-2.7904054982	0.4747854466
Cu	-0.3952617135	-2.3756243906	0.6519474154
Cu	-2.7050576727	-1.2565193050	0.6998450259
Cu	-1.2796976407	-1.2639223935	-1.4362883040
Cu	-0.0407313801	1.2059754113	-1.4325209559
Cu	1.0906711205	-0.8676685537	-0.6111332901
Cu	2.4365567377	1.1235435661	-1.3092930322
Cu	1.1345457867	3.1830386010	-0.6665280241
Cu	-2.8152044816	1.1379693715	1.6062018836
N	-1.5596862532	-2.9143111633	-2.4145647923
N	-1.6686545107	-3.8365072178	-3.0080678377
O	-1.5364551864	0.4453270512	-2.2806866123

### Cu<sub>15</sub>-N<sub>2</sub>O.3

E = -24793.4489463318

Cu	1.1969683855	0.2773704994	-0.5723524359
Cu	-0.4380414167	1.7128454377	-1.5680891841
Cu	2.3399927586	-1.2789834722	0.9800190213
Cu	1.1973672405	-2.0837305285	-1.0602564567
Cu	-0.8933982083	-0.6838520204	-1.4416266902
Cu	-2.7349154216	0.9908767590	-1.1370022019
Cu	-1.6529404207	3.1081113554	-0.0417026090
Cu	0.7710515181	2.4629025886	0.4426298072
Cu	2.9594273473	1.1335556791	0.7723104700
Cu	0.9409915947	0.4722541958	1.9674798212
Cu	-0.1851113081	-1.5376484780	0.8729879743
Cu	-1.1732029051	0.8666479606	0.6577057904
Cu	-2.6173609626	-1.1933631208	0.1500374603
Cu	-1.1210529752	-3.0083637422	-0.7900082709
Cu	3.3250584873	-0.6428690215	-1.1156161351
N	-4.8254835427	-1.8464503314	2.1142685324
N	-4.0148681317	-1.6091500767	1.4080426847
O	-0.8057378444	-0.2649418711	2.1464025151

**Cu<sub>15</sub>-N<sub>2</sub>O<sub>4</sub>**

E = -24793.4550595352

Cu	-0.7839979548	-0.4877619860	0.5879729672
Cu	1.4720737887	-1.2154728705	1.2151527262
Cu	-2.7131372455	0.4721153377	-0.6122114937
Cu	-1.5760207580	1.7389319928	1.1683808262
Cu	0.8708370374	1.2469936272	1.0411141632
Cu	3.1146310324	0.3915141730	0.1844665992
Cu	2.7252923529	-2.0216442562	-0.6726409311
Cu	0.2782391233	-2.4466080934	-0.7045433298
Cu	-2.4306122504	-2.0290413516	-0.2934898977
Cu	-1.0513214478	-0.7229928903	-1.9610546937
Cu	-0.5560084977	1.5511659833	-1.0715384359
Cu	1.1646629229	-0.1749217900	-1.0119554080
Cu	1.8287555121	2.2606427802	-0.9074377116
Cu	0.0246716233	3.4449982532	0.3469572834
Cu	-3.0023848252	-0.5184462137	1.5580517460
N	1.8645030939	-1.9539953933	2.9383911444
N	2.0290152245	-2.3727429033	3.9455867713
O	-1.3255678296	-2.6109089127	-1.6926797318

**11. XYZ coordinates and total energies of Cu<sub>7</sub>-OCO clusters on BP86/LANL2DZ level**

**Cu<sub>7</sub>-OCO.1**

E = -1562.46517191245

Cu	1.9493441602	-0.0000010368	0.9977009143
Cu	0.6428354260	2.0381800587	0.3092309457
Cu	-1.6471499882	1.3763972331	-0.4105258898
Cu	-1.6471524236	-1.3763951448	-0.4105241149
Cu	0.6428316139	-2.0381810121	0.3092337946
Cu	-0.4794785758	0.0000012172	1.3838041700
Cu	0.4613862514	-0.0000008263	-1.0588849364
O	-2.4036821403	0.0000028439	0.7323148345
C	1.2763814166	-0.0000029401	-2.7185293402
O	1.7235323178	-0.0000042885	-3.8098300450

**Cu<sub>7</sub>-OCO.2**

E = -1562.47704908513

Cu	1.0905736078	0.0000034788	0.5195124524
Cu	0.8212433259	2.1349628008	-0.8049930227
Cu	-1.3193125439	1.2867096386	-0.0482302068
Cu	-1.3193153878	-1.2867060529	-0.0482348654
Cu	0.8212445200	-2.1349575145	-0.8049902585
Cu	-0.7091770435	-0.0000042506	2.2067324967
Cu	0.0674972145	0.0000025836	-1.6996416112
O	-2.2546295274	0.0000006990	1.1014378453
C	1.1621752693	-0.0000087291	2.5936136218
O	2.0961023196	-0.0000153380	3.3558063334

**Cu<sub>7</sub>-OCO.3**

E = -1562.45087507975

Cu	0.4258318715	-2.0137818235	0.2957718948
Cu	-2.0843703208	-1.5407555419	-0.4689969555
Cu	-2.1972964538	0.8601437657	-0.0794635325
Cu	0.3207871964	2.0204153885	-0.2883719225
Cu	1.9419376776	-0.0106300179	-0.0398695238
Cu	-0.1984044883	0.0744080424	1.3007017185
Cu	-0.2552917115	-0.1908880112	-1.2566774723
O	-1.0214952975	1.8888729687	1.1024362662
C	3.8037319012	0.2037438713	-0.2161547778
O	4.9474074827	0.3153107299	-0.4734385174

Cu<sub>7</sub>-OCO.4

E = -1562.45160748641

Cu	1.9454536295	0.0000019419	0.0383367589
Cu	0.4683765008	2.0198395904	-0.1681207486
Cu	-1.9627364665	1.3428699478	-0.1670828066
Cu	-1.9627338915	-1.3428739444	-0.1670820580
Cu	0.4683800231	-2.0198391153	-0.1681204946
Cu	-0.2544272429	-0.0000002593	1.1906064292
Cu	-0.2261237427	-0.0000002180	-1.3923961414
O	-2.3313464118	-0.0000018119	1.1762367678
C	3.8151454218	0.0000020519	-0.2020860646
O	4.9884203325	0.0000018354	-0.0888553789

Cu<sub>7</sub>-OCO.5

E = -1562.46797503664

Cu	1.7931054250	1.3795626337	-0.0753910316
Cu	-0.6343215776	1.7994042460	-0.2910985804
Cu	-2.1189196052	-0.2931432036	0.3643895916
Cu	0.0162701086	-2.2485359372	0.0878355147
Cu	2.1918990254	-1.0858882918	-0.1992280670
Cu	0.3514550937	-0.0080101825	1.2578420546
Cu	0.1692481037	-0.2296398765	-1.3255704581
O	-1.0688421383	-1.3982243907	1.4630837783
C	-3.5967146355	0.5136683151	-0.3497729558
O	-4.4878413571	1.0778067082	-0.8803844266

Cu<sub>7</sub>-OCO.6

E = -1562.46895355316

Cu	2.2339791877	-0.5942608650	0.0000000000
Cu	0.8377771681	0.0630204527	-2.0009844501
Cu	-1.4465928577	0.7366195126	-1.2229337733
Cu	-1.4465928577	0.7366195126	1.2229337733
Cu	0.8377771681	0.0630204527	2.0009844501
Cu	-0.0436207835	-1.2468620866	0.0000000000
Cu	0.5831029955	1.4091934892	0.0000000000
O	-2.0118109541	-1.7269077027	0.0000000000
C	-2.6806580847	-0.5895710042	0.0000000000
O	-3.9021803468	-0.3219818305	0.0000000000

### Cu<sub>7</sub>-OCO.7

E = -1562.42409690939

Cu	1.8361967465	0.1662203343	-1.3308381184
Cu	0.5333780833	2.0812169431	-0.3702578231
Cu	-1.6470040840	1.2528009606	0.5095860542
Cu	-1.5058278099	-1.4904614762	0.3325616234
Cu	0.7480216698	-1.9776924798	-0.6103983801
Cu	-0.5940676434	0.0469544521	-1.4782942224
Cu	0.5127786198	-0.0363388092	0.8800789809
O	-2.4412813091	-0.0955606436	-0.6471716228
O	1.6215848544	-0.0860659462	2.6920953166
C	1.9342472627	-0.1322206472	3.8278917074

### Cu<sub>7</sub>-OCO.8

E = -1562.42249174299

Cu	1.9548359849	0.7082104594	-0.8311437719
Cu	0.0756858348	2.2384834330	-0.2370519638
Cu	-1.9475594906	0.8718793676	0.3350314913
Cu	-1.2623772059	-1.7191519822	-0.2751469789
Cu	1.0735931548	-1.6032127060	-1.1632555413
Cu	0.3947148078	-0.1034552445	0.8981393071
Cu	-0.4419707573	0.2574513988	-1.5534746979
O	-1.5341046973	-0.7156196505	1.3551799310
O	1.3060339067	-0.4668828523	2.9060314139
C	1.1409731390	-0.9067675783	3.9837472265

### Cu<sub>7</sub>-OCO.9

E = -1562.42091834577

Cu	0.5970453402	-2.0089726969	0.3340271804
Cu	-1.8869308542	-1.7392374225	-0.0323917617
Cu	-2.3953700344	0.6835754926	-0.1196464901
Cu	0.0189354997	1.9690038960	-0.3139629282
Cu	1.7757191413	0.1562584450	-0.1840910630
Cu	-0.3767169616	-0.0006919172	1.2861978162
Cu	-0.3682361636	-0.2849665933	-1.2745168991
O	-1.3181548185	1.7817955240	1.0826965954
O	3.9664168461	0.4884209954	-0.1399420514
C	5.0049660132	0.4829461398	-0.6981234788

### Cu<sub>7</sub>-OCO.10

E = -1562.42071598747

Cu	1.8016997679	0.0272461209	-0.3072649985
Cu	0.3228598623	1.9923677923	0.1916042239
Cu	-2.0784487355	1.2562668508	0.2533872741
Cu	-2.0066184966	-1.4480593989	0.1090232730
Cu	0.4276996244	-2.0492064304	-0.0235427459
Cu	-0.4305870141	0.0259260462	-1.2870905061
Cu	-0.2529591933	-0.1088978747	1.2952203269
O	-2.4628462628	-0.0357941031	-1.1505937430

O	3.9815367392	0.0407908780	0.2376503669
C	4.8040715119	0.0154422651	1.0791493784

### Cu<sub>7</sub>-OCO.11

E = -1562.42473391185

Cu	2.0904942541	1.3158806266	-0.2439381792
Cu	-0.2889730537	2.0076499638	0.0282831017
Cu	-1.8392764056	-0.0346265793	-0.0777726209
Cu	-0.0083941096	-2.1447503533	0.1279989779
Cu	2.2703006412	-1.1255602615	0.1799382950
Cu	0.4343714390	-0.0746117447	-1.3294613570
Cu	0.3795839882	0.0310345925	1.2535854412
O	-1.0931685827	-1.3687780076	-1.2834705315
O	-3.7647387600	0.4451866836	0.5223709025
C	-4.7843582147	0.5245633284	1.1142317240

### Cu<sub>7</sub>O-OC\_O

E = -1562.45495650622

Cu	1.3937261997	-0.0000888515	-1.7016496502
Cu	0.4929669005	2.0486151998	-0.4794043923
Cu	-0.9771254555	1.3665746564	1.4380497682
Cu	-0.9771256549	-1.3666701514	1.4374615405
Cu	0.4929829129	-2.0477758082	-0.4792692824
Cu	-0.9342498253	-0.0000931062	-0.8015378041
Cu	1.0060440762	-0.0006568547	0.7667111841
O	-1.8311417568	-0.0000175036	2.3599687133
O	-3.3947988574	0.0000676891	-2.5580985145
C	-2.4241469342	0.0000456410	-1.8941332893

## 12. XYZ coordinates and total energies of the four most stable Cu<sub>7</sub>OCO clusters on TPSSh/DEF2-TZVPP level

### Cu<sub>7</sub>-OCO.1

E = -11672.5729718386

Cu	2.3076228139	-0.5033579465	0.0000000000
Cu	0.9076539754	0.0386444715	-1.9970983646
Cu	-1.3776508525	0.6119883812	-1.2002809951
Cu	-1.3776508525	0.6119883812	1.2002809951
Cu	0.9076539754	0.0386444715	1.9970983646
Cu	0.0338051090	-1.1237627975	0.0000000000
Cu	0.6044658154	1.3157567754	0.0000000000
O	-1.8033649591	-1.9215558615	0.0000000000
C	-2.5402253090	-0.8868786630	0.0000000000
O	-3.7326167594	-0.6892369009	0.0000000000

### Cu<sub>7</sub>-OCO.2

E = -11672.5767707816

Cu	1.5184320937	-1.7435857951	-0.1553468285
Cu	-0.9283185358	-1.7670179464	-0.1345104262
Cu	-1.8960574176	0.6418987319	-0.3001588688

Cu	0.3759375058	2.0330167316	0.2387770153
Cu	2.3207165724	0.5303950442	0.3421916794
Cu	0.3939809732	0.0617222805	-1.2002969958
Cu	0.1802882483	-0.1628279933	1.2443217416
O	-0.7079915434	1.6571009387	-1.2750595515
C	-3.4880639431	0.0682738655	0.3404610485
O	-4.4415163139	-0.3609621608	0.7973665286

### Cu<sub>7</sub>-OCO.3

E = -11672.5737943486

Cu	1.7553439892	1.2601868030	0.0000000000
Cu	0.5646184672	0.4235733615	-2.0123715155
Cu	-1.5504583578	-0.6138231810	-1.3022569428
Cu	-1.5504583578	-0.6138231810	1.3022569428
Cu	0.5646184672	0.4235733615	2.0123715155
Cu	-0.6532181282	1.2453647012	0.0000000000
Cu	0.5915222696	-0.9116117716	0.0000000000
O	-2.4487437555	0.4130000579	0.0000000000
C	1.6429691893	-2.4166033645	0.0000000000
O	2.2478967334	-3.3822635501	0.0000000000

### Cu<sub>7</sub>-OCO.4

E = -11672.5833486080

Cu	-0.2760890020	-0.0000053321	-1.0735164319
Cu	1.0212475318	-2.0954347833	-0.7977063816
Cu	0.0351030521	-1.2334497123	1.1983636436
Cu	0.0350533339	1.2334442129	1.1983711748
Cu	1.0211560846	2.0954790980	-0.7976981642
Cu	-2.0798662539	-0.0000423030	0.4963336315
Cu	1.8350938997	0.0000381650	0.0789505922
O	-1.1341617303	-0.0000290096	2.0783582342
C	-2.3628169260	-0.0000398783	-1.3518210649
O	-2.9747636903	-0.0000453776	-2.3407919118

## 13. XYZ coordinates and total energies of Cu<sub>12</sub>O-CO and Cu<sub>12</sub>-CO<sub>2</sub> clusters on BP86/LANL2DZ level

### Cu<sub>12</sub>O-CO

E = -2543.96247793505

Cu	-2.0360589905	-2.1539227241	0.8684404690
Cu	-3.1928624990	-0.0029237377	0.1618092797
Cu	-2.0439414077	2.1542473748	0.8602950419
Cu	0.5252229400	1.9141211368	0.2251157509
Cu	1.5180618566	0.0080892960	1.5555666555
Cu	0.5339469327	-1.9079904541	0.2331466867
Cu	-0.8664250029	0.0009590459	0.8658431977
Cu	-1.4401556603	-1.3131488834	-1.3075200587
Cu	-1.4469053483	1.3062805330	-1.3117155907
Cu	0.9717826642	-0.0023397160	-1.8173384603
Cu	2.9005419316	-1.2721757238	0.0438106402

Cu	2.8899598110	1.2783353009	0.0246240516
O	-0.7837619603	-0.0031424213	-2.5773968372
C	2.8893662021	-0.0090318151	-1.6255477499
O	3.8488286685	-0.0162431624	-2.3925233841

### Cu<sub>12</sub>-CO<sub>2</sub>

E = -2543.97468255647

Cu	-1.9265453694	-2.0591117689	1.0972821270
Cu	-3.0017551501	-0.1026667311	0.0031711006
Cu	-2.0643824187	2.1569845360	0.6999568407
Cu	0.5786627414	2.0655792414	0.2904697593
Cu	1.6411542032	0.2524898077	1.6071982304
Cu	0.7176788847	-1.9130446768	0.8955993769
Cu	-0.7681882287	0.1109087625	1.0652843987
Cu	-0.9435280508	-1.4188099593	-1.0290173892
Cu	-1.2820214122	1.2089736898	-1.3390369192
Cu	1.1621718121	-0.1648710023	-0.9201419816
Cu	3.0712344401	-1.2175852465	0.2958640102
Cu	2.9477852270	1.3437705477	-0.1635811907
O	-0.7001752398	0.3482487788	-3.0476723842
C	0.1404070431	-0.6397762815	-2.7516762966
O	0.8071387749	-1.3915895972	-3.4900150268

## 14. XYZ coordinates and total energies of Cu<sub>12</sub>O-CO and Cu<sub>12</sub>-CO<sub>2</sub> clusters on TPSSh/DEF2-TZVPP level

### Cu<sub>12</sub>O-CO

E = -19875.4683783124

Cu	-2.0162724224	-2.1227592065	0.8322149287
Cu	-3.1319685362	-0.0004655726	0.0802491555
Cu	-2.0164781412	2.1252718898	0.8212103369
Cu	0.5048558917	1.9092308038	0.2548010241
Cu	1.4710046373	0.0033886113	1.5065385001
Cu	0.5047870989	-1.9093481182	0.2645446118
Cu	-0.8707193309	0.0015174331	0.8218267877
Cu	-1.3625843310	-1.2544486671	-1.2706354112
Cu	-1.3629471991	1.2464967585	-1.2768452980
Cu	0.9529916444	-0.0042708590	-1.6854349572
Cu	2.8352697747	-1.2361637841	0.0168640723
Cu	2.8360685592	1.2362408558	0.0126238367
O	-0.7244226873	-0.0070792670	-2.5308306942
C	2.8543213202	-0.0025055480	-1.6652688638
O	3.7936938594	-0.0039912805	-2.3752483371

### Cu<sub>12</sub>-CO<sub>2</sub>

E = -19875.4918752996

Cu	-1.8825195396	-2.0234878457	1.1310252590
Cu	-2.9395081595	-0.1136340805	-0.0256546196

Cu	-2.0238758116	2.1137158078	0.6542497658
Cu	0.5625123224	2.0427860488	0.2968163380
Cu	1.6201010142	0.2333100627	1.5502780612
Cu	0.6823485718	-1.8943873737	0.8704644625
Cu	-0.7593067128	0.1031327272	1.0004856765
Cu	-0.9528812185	-1.3941321015	-0.9870652055
Cu	-1.1702625376	1.1168107967	-1.3038558773
Cu	1.1044902932	-0.1359146317	-0.8609308027
Cu	3.0063972267	-1.2064575796	0.2432539220
Cu	2.9086395950	1.3161367677	-0.1616609689
O	-0.7238655249	0.3216667796	-3.0715025432
C	0.1197990301	-0.5790373470	-2.7429399126
O	0.8275687078	-1.3210079309	-3.3792788996

**15. XYZ coordinates and total energies of Cu<sub>7</sub>O-CO, Cu<sub>7</sub>-CO<sub>2</sub>, Cu<sub>12</sub>O-CO and Cu<sub>12</sub>-CO<sub>2</sub> clusters on BP86/LANL2DZ level**

**Cu<sub>7</sub>O-CO-3A**

E = -1562.46792408739

Cu	1.1047236039	-2.1556426569	-0.6128323354
Cu	-1.2855072303	-1.6002887959	-0.3288895128
Cu	-1.7131333990	1.0061381108	-0.0130277753
Cu	1.0189590224	1.6709041017	0.6873806851
Cu	2.4804459396	-0.3042329574	0.3488974129
Cu	0.4565654784	0.0785467878	-1.2167088116
Cu	0.2088744743	-0.5888230883	1.2772214498
O	-0.2443927708	1.8975281115	-0.7789149076
C	-3.4244957875	0.6906676051	0.5506303968
O	-4.4921647723	0.3999226306	0.9621766979

**Cu<sub>7</sub>O-CO-4A**

E = -1562.45080031091

Cu	-0.2705167731	-2.0528363506	-0.1382423558
Cu	-1.8886690944	-0.1365818940	0.2068207906
Cu	-0.4120098568	1.9884725872	0.4004586447
Cu	2.1878447045	1.0290790696	0.1634695112
Cu	2.2243769824	-1.3841526194	0.4989844875
Cu	0.2500651539	0.0548993096	-1.1645606254
Cu	0.3359522511	-0.1694547812	1.3770041268
O	0.9113417869	1.9469519686	-1.0112843803
C	-3.7604697306	0.0006019682	0.3763175718
O	-4.9007663533	0.0708967204	0.6623866278

**Cu<sub>7</sub>O-CO-5A**

E = -1562.46516887602

Cu	1.1977978838	-1.3494313700	1.5693669485
Cu	1.2439081819	1.1616078115	1.6958735113
Cu	-0.3908367320	2.1275879832	0.0871572656
Cu	-1.3441761068	-0.0113643244	-1.3548402871
Cu	-0.1726470664	-2.0067906420	-0.4398026188

Cu	-0.8993255846	-0.1336809133	1.1472988415
Cu	1.1125141526	0.0931149138	-0.5169617019
O	-2.0534172016	1.1253581840	0.0519188437
C	2.6227053510	0.1244264687	-1.5824714423
O	3.5495015903	0.1890882139	-2.3086579522

### Cu<sub>7</sub>-CO<sub>2</sub>-3A

E = -1562.46977589703

Cu	2.2837776374	-0.8410579272	0.0000000000
Cu	1.0319611094	-0.1005900052	-1.9952863919
Cu	-1.0052615483	1.0585982160	-1.2325427545
Cu	-1.0052615483	1.0585982160	1.2325427545
Cu	1.0319611094	-0.1005900052	1.9952863919
Cu	-0.1916957694	-0.9494312517	0.0000000000
Cu	1.1384548108	1.3830957878	0.0000000000
O	-2.8464660529	-2.4786830223	0.0000000000
C	-3.5219305355	-1.4837623145	0.0000000000
O	-4.2050611797	-0.4965888825	0.0000000000

### Cu<sub>7</sub>-CO<sub>2</sub>-4A

E = -1562.46983048554

Cu	1.9636061737	-1.3462249730	0.0000000000
Cu	0.8705514802	-0.3940124468	-1.9930461014
Cu	-0.9064383575	1.1374740171	-1.2327200168
Cu	-0.9064383575	1.1374740171	1.2327200168
Cu	0.8705514802	-0.3940124468	1.9930461014
Cu	-0.5004148040	-0.9934771307	0.0000000000
Cu	1.2565291401	1.0470086361	0.0000000000
O	-3.1911703705	-2.0032482491	0.0000000000
C	-3.8074442455	-0.9693538102	0.0000000000
O	-4.4190593098	0.0625743779	0.0000000000

### Cu<sub>7</sub>-CO<sub>2</sub>-5A

E = -1562.47139398074

Cu	-0.8722867509	-2.0219639359	0.0000000000
Cu	-0.5117769935	-0.6284552504	1.9905823498
Cu	0.1083357216	1.6209988947	1.2273144317
Cu	0.1083357216	1.6209988947	-1.2273144317
Cu	-0.5117769935	-0.6284552504	-1.9905823498
Cu	0.9998286613	-0.3689505408	0.0000000000
Cu	-1.6443955871	0.3466067539	0.0000000000
O	3.1861202437	-1.0502859749	0.0000000000
C	4.2820496772	-0.5429223352	0.0000000000
O	5.3400692207	0.0182233267	0.0000000000

### Cu<sub>7</sub>-CO<sub>2</sub>\_TS

E = -1562.46842098354

Cu	2.3239152463	-0.2493770946	-0.5597031070
Cu	1.0088071107	1.8743024981	-0.2362437777
Cu	-1.3641220697	1.2629743894	0.3810677983

Cu	-1.4136065323	-1.1564518590	0.8115231064
Cu	0.8196751859	-2.0983847446	0.2577771174
Cu	0.0628596711	-0.2797288730	-1.2940935875
Cu	0.6066129585	0.0944255669	1.3408631650
O	-1.8457437667	-0.1605643356	-1.9631607709
C	-2.5907449570	0.2134696681	-0.9497416470
O	-3.8190668671	0.2963578834	-0.7590596797

### Cu<sub>7</sub>O-CO\_TS

E = -1562.44344538429

Cu	2.2093148712	0.6744993323	0.6360072816
Cu	0.3960549292	2.1628425634	-0.2466890396
Cu	-1.6458027080	0.8717532257	-0.6642009342
Cu	-0.8285174499	-1.8490308505	-0.3953036924
Cu	1.6193219309	-1.6830769221	0.1979283868
Cu	-0.0412238375	0.0004925039	1.2058841221
Cu	0.6014810979	-0.0106618106	-1.3027067316
O	-1.7649839623	-0.9220167719	1.0032054599
C	-3.1672586730	0.3354012906	0.3754534046
O	-4.1777711999	0.1533751994	0.9750074046

### Cu<sub>12</sub>O-CO-3A

E = -2543.96250347562

Cu	-2.0291396250	-2.1548905627	0.6184986613
Cu	-3.0808526710	0.0009051095	-0.2246170058
Cu	-2.0276650412	2.1560574068	0.6180090233
Cu	0.5967985217	1.9256630681	0.3476500841
Cu	1.3929717947	-0.0005380098	1.7821569920
Cu	0.5956006497	-1.9261532387	0.3476758235
Cu	-0.8616638844	0.0001772962	0.7641365104
Cu	-1.1380060070	-1.3100121908	-1.4510808181
Cu	-1.1369398336	1.3100626394	-1.4513057917
Cu	1.3286683962	-0.0002491757	-1.6440284846
Cu	2.9628746801	-1.2742613645	0.4619653124
Cu	2.9637971309	1.2731850373	0.4631612674
O	-0.3157593424	-0.0004915672	-2.6207849638
C	3.1992362347	0.0001767340	-1.1865627539
O	4.2605787903	0.0005660073	-1.8040006262

### Cu<sub>12</sub>O-CO-4A

E = -2543.97173322325

Cu	-2.4697825360	-1.5264874439	1.4216289608
Cu	-3.1041568625	0.2921209558	-0.2183759233
Cu	-1.6328959433	2.4004534982	-0.1491842217
Cu	0.8797185523	1.5998540349	-0.4136714800
Cu	1.5512333025	-0.0771022723	1.2183474892
Cu	0.0620797143	-1.9965271151	1.1762474221
Cu	-0.8574253211	0.2873306477	0.8497822877
Cu	-1.6467936018	-1.6720858692	-0.8366497846
Cu	-1.1805363444	0.6898637792	-1.8014417001

Cu	0.9399334653	-0.8268754250	-1.1782236394
Cu	2.4275435623	-2.1370450033	0.2435422215
Cu	3.0804052335	0.2665752801	-0.7134340371
O	-0.5780598380	-1.0899179568	-2.3497856921
C	4.7481083280	1.0397760940	-1.1622638973
O	5.5951470933	1.7250716869	-1.6123514297

### Cu<sub>12</sub>O-CO-5A

E = -2543.97175759391

Cu	-2.4469877788	-1.4942436387	1.3638774224
Cu	-3.0311071130	0.2114668177	-0.4131789691
Cu	-1.5988680189	2.3478429722	-0.3995708901
Cu	0.9303986245	1.5849291698	-0.5107622146
Cu	1.5552156570	0.0355610720	1.2571174481
Cu	0.1034772758	-1.9125978964	1.2794215458
Cu	-0.8435897899	0.3195665768	0.7624877703
Cu	-1.5139940703	-1.7558984094	-0.8377380606
Cu	-1.0459660276	0.5496622799	-1.9281277983
Cu	1.0646936208	-0.8863542899	-1.1012727667
Cu	2.5134010199	-2.0702512958	0.4682897774
Cu	3.1643956597	0.2767292484	-0.6286391565
O	-0.3827278854	-1.2505005230	-2.3318985159
C	4.8419299278	1.0097909804	-1.1026039884
O	5.7080702879	1.6286200459	-1.6093432894

### Cu<sub>12</sub>O-CO\_TS

E = -2543.94912773789

Cu	2.3916998847	-1.9321671632	-0.3055705278
Cu	3.0056284671	0.3653642939	0.5547079168
Cu	1.8437893053	2.3257707591	-0.6875485154
Cu	-0.6611138208	1.8173783642	-1.0536860675
Cu	-1.2657256039	-0.3905811656	-1.8884370476
Cu	-0.1841745216	-2.1708972574	-0.4222449328
Cu	0.9928532727	-0.0155274582	-0.8500998300
Cu	1.1291312125	-1.0275858888	1.5553935871
Cu	0.6727045636	1.4899276631	1.2182452268
Cu	-1.4554902269	-0.2915011697	0.9424382991
Cu	-2.6840960525	-1.8378349287	-0.5565966932
Cu	-2.9568074431	0.7702434735	-0.6991526988
O	-0.1967004903	0.1709662477	2.3554102607
C	-3.2146406524	0.9465798805	1.2644511951
O	-3.7735715007	1.2115209441	2.2805669071

### Cu<sub>12</sub>O-CO\_TS

E = -2543.94585571415

Cu	-2.1115235353	-2.1379249083	0.8077509012
Cu	-3.1344015073	-0.0014351254	-0.0991228322
Cu	-2.1100470943	2.1545966268	0.7591782115
Cu	0.5456993278	2.0224044114	0.5337725790
Cu	1.4444607559	0.0158672894	1.6278782975

Cu	0.5438697887	-2.0132032749	0.5778075071
Cu	-0.9146240243	0.0094696814	0.9428256677
Cu	-1.1707753123	-1.3175916738	-1.2566918036
Cu	-1.1691391062	1.2871274051	-1.2858753771
Cu	1.2824051164	-0.0116608047	-0.9634192078
Cu	2.9922763021	-1.3163011673	0.3745023791
Cu	2.9936184163	1.3193122390	0.3461074643
O	-0.4547791946	-0.0295126052	-2.4800360695
C	1.8448490063	-0.0323993397	-2.8093826820
O	2.0245910362	-0.0445051976	-3.9734919713

### Cu<sub>12</sub>-CO<sub>2</sub>-3A

E = -2543.97577173636

Cu	-1.9381842257	-2.2645474966	1.3157460339
Cu	-2.9419863545	-0.3787744075	0.0140581123
Cu	-2.0490111773	1.8658836779	0.6265680700
Cu	0.6181107124	1.8183726293	0.3870989149
Cu	1.6380427109	0.0355595077	1.7966058925
Cu	0.7180404785	-2.1556878045	1.0561239965
Cu	-0.7640275448	-0.1267185768	1.1730428042
Cu	-0.9160788564	-1.7054102650	-0.8536403372
Cu	-0.9900802367	0.7296928402	-1.2905340801
Cu	1.1989062982	-0.3959033976	-0.7142696504
Cu	3.0851033821	-1.4546224466	0.5071359468
Cu	3.0139559227	1.1050130370	0.0759340182
O	-1.0259460243	1.7000753916	-3.3279886721
C	-0.2852573943	1.5505891097	-4.2694654279
O	0.4663187032	1.3726271947	-5.1822040018

### Cu<sub>12</sub>-CO<sub>2</sub>-4A

E = -2543.97574364110

Cu	-1.7106392465	-2.4796058437	-0.9956431990
Cu	-2.9452595544	-0.4568490283	-0.2012265689
Cu	-2.0929327342	0.4877288476	1.9407263441
Cu	0.5421780844	0.9619100178	1.6773992173
Cu	1.7945585943	-1.0891334326	1.0155366265
Cu	0.8806438971	-1.8862357775	-1.1542498810
Cu	-0.6587793434	-0.9671270694	0.6148437000
Cu	-0.9824921207	-0.2867412753	-1.8483188541
Cu	-1.2070235841	1.4805776299	-0.1291241973
Cu	1.0764110296	0.6244983264	-0.7807146929
Cu	3.1313108936	-0.7481034798	-1.0059285871
Cu	2.9146299943	1.0793655320	0.8282820810
O	-1.5158358492	3.6727350696	-0.5963947054
C	-0.8902621905	4.3783221085	-1.3504327107
O	-0.2498734866	5.0451734197	-2.1086185238

### Cu<sub>12</sub>-CO<sub>2</sub>-5A

E = -2543.97578359242

Cu	-0.8323249379	-2.8110230383	-1.0201652642
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Cu	-2.6694682757	-1.3906484640	-0.1011438870
Cu	-2.1066104918	-0.2507464596	2.0422406927
Cu	0.1636824730	1.1544223447	1.6933027266
Cu	2.0312870626	-0.3007804641	0.9163382165
Cu	1.3646994724	-1.3278302158	-1.2508545619
Cu	-0.3171858538	-1.0550709904	0.6030831440
Cu	-0.9781521465	-0.4867479411	-1.8179074635
Cu	-1.7412647360	1.0412989528	-0.0226721206
Cu	0.6656367260	1.0782578994	-0.7916089127
Cu	3.0660125308	0.5365446298	-1.1322605683
Cu	2.2946581452	2.1318033467	0.7598623560
O	-2.8795348783	2.9678989829	-0.3635643671
C	-2.6356723785	3.8571132387	-1.1430963929
O	-2.3653003941	4.7159090754	-1.9297734915

### Cu<sub>12</sub>-CO<sub>2</sub>\_TS

E = -2543.97041542181

Cu	-1.8020812434	-2.5241059747	0.8281708575
Cu	-3.0324731914	-0.4108554574	0.2204719428
Cu	-2.0913617791	1.6411818923	1.2992620159
Cu	0.5184708878	1.7933927367	0.7527285549
Cu	1.7609916120	-0.2639028265	1.3592931652
Cu	0.7612459566	-2.1927478909	0.1704772311
Cu	-0.7090778270	-0.3602143213	1.0951690623
Cu	-1.1667713872	-1.3368120236	-1.2351744261
Cu	-1.3103917822	1.1211904012	-0.9719702886
Cu	0.9402969810	0.0532796783	-1.0720561800
Cu	2.9833499437	-1.2198962402	-0.5419123730
Cu	2.8566704145	1.3420537590	-0.1115357584
O	-1.1778307655	2.4954249164	-2.8028740188
C	-0.2297631420	1.7026934112	-2.9623449902
O	0.7109337608	1.2702223711	-3.6127665212

## 16. XYZ coordinates and total energies of the transition states of Cu<sub>7</sub>O-CO and Cu<sub>12</sub>O-CO clusters on TPSSh/DEF2-TZVPP level

### Cu<sub>7</sub>O-CO\_TS

E = -11672.5421402919

Cu	2.1861825573	0.6345502193	0.5874945971
Cu	0.3415661339	2.1520003987	-0.0553737348
Cu	-1.6486885016	0.8711958064	-0.6255384218
Cu	-0.8368163066	-1.7403188252	-0.5002720130
Cu	1.5917871730	-1.6704749951	0.0612768240
Cu	-0.0333220236	-0.0704436852	1.1017554419
Cu	0.5983514424	0.1014915759	-1.2615927119
O	-1.7084078804	-1.0090034576	0.9988259873
C	-3.0155765421	0.1300122076	0.5191022616
O	-3.9913709085	-0.0709782458	1.1116862597

**Cu<sub>12</sub>O-CO\_TS1**

E = -19875.4646346678

Cu	2.3155180440	-1.9522356537	-0.4033356654
Cu	2.9790457460	0.3006110582	0.4797340698
Cu	1.8598606733	2.2615203579	-0.6593222471
Cu	-0.6509974659	1.8092723902	-0.8809916225
Cu	-1.2414392694	-0.3554730477	-1.8068428519
Cu	-0.2442639179	-2.1084663772	-0.3944341900
Cu	0.9706955535	-0.0075959156	-0.8084659539
Cu	1.1154737327	-1.0664616841	1.4475269381
Cu	0.7591832943	1.3794036580	1.2285202969
Cu	-1.3557713080	-0.1116394916	0.9094810475
Cu	-2.6887835432	-1.7276082503	-0.5106314881
Cu	-2.9464366496	0.7831462596	-0.6731980848
O	-0.0711305901	0.0950725593	2.3367257654
C	-3.0660064879	0.8147787498	1.3529316554
O	-3.7781478778	1.1218503091	2.2019973295

**Cu<sub>12</sub>O-CO\_TS2**

E = -19875.4617262982

Cu	-2.0577982713	-2.1155189235	0.7777762087
Cu	-3.0597073609	0.0004435775	-0.1177577647
Cu	-2.0572851238	2.1154199702	0.7795176744
Cu	0.5251666702	1.9950137544	0.5247232883
Cu	1.4403978032	-0.0007785952	1.5576201368
Cu	0.5246838452	-1.9955035126	0.5230840959
Cu	-0.8909107287	-0.0002341722	0.8932120361
Cu	-1.1388053960	-1.2449951329	-1.2364770275
Cu	-1.1384652835	1.2463347499	-1.2354330686
Cu	1.1812026527	0.0002778261	-0.9142105911
Cu	2.9490719229	-1.2865925989	0.2822723332
Cu	2.9493721250	1.2857409098	0.2833412111
O	-0.5922455204	0.0011092592	-2.4877832012
C	1.8496046740	0.0008608549	-2.7140736442
O	2.1113201193	0.0012021962	-3.8193573240

**17. XYZ coordinates and total energies of Cu<sub>x</sub>O clusters on BP86/LANL2DZ level****Cu<sub>4</sub>O**

E = -860.257196245862

Cu	0.2144932501	-1.1870171943	-0.2701540177
Cu	-2.3189613378	-0.0041221661	0.4784476616
Cu	0.2115186139	1.1843744172	-0.2868127662
Cu	2.2187627368	0.0055245142	0.3444824883
O	-1.2239207758	-0.0078423127	-0.9759068537

**Cu<sub>5</sub>O**

E = -1056.54804029516

Cu	0.2901454853	-0.8431331878	0.9102067922
Cu	-1.6992277946	-0.4090534207	-0.9312380333
Cu	-1.2398283086	1.4097117133	0.6333821995
Cu	0.6113247018	0.6539378818	-0.9305319863
Cu	2.4738880687	-0.6159220500	0.0033481285
O	-1.6130396036	-0.4714484158	1.0232267213

### Cu<sub>6</sub>O

E = -1252.85656606940

Cu	0.5886286908	-1.3118720629	-0.4833846094
Cu	-1.4182482302	-2.3973107788	0.1033602434
Cu	-1.3836619293	-0.0000048770	0.1552731035
Cu	0.5886196338	1.3118764261	-0.4833843805
Cu	2.5859286348	0.0000089425	0.8046061049
Cu	-1.4182651894	2.3973007959	0.1033603410
O	1.9647093762	0.0000069164	-0.9370465141

### Cu<sub>7</sub>O

E = -1449.15148823935

Cu	-1.4557661477	-1.6259814201	-0.1183197502
Cu	-2.0437657449	0.7714410436	0.2590995075
Cu	-0.0214197306	2.1791900148	-0.1339596794
Cu	2.0067157996	0.7059836044	-0.1761472066
Cu	1.0341301202	-1.8620662633	-0.1486558886
Cu	0.0226248063	0.0017638882	1.2949625773
Cu	-0.1220238585	0.0382961639	-1.3074000449
O	1.9131491194	-0.7115142325	1.1529005162

### Cu<sub>8</sub>O

E = -1645.45435610224

Cu	-0.5321545487	0.3020118387	1.5139997404
Cu	1.9826385996	0.0697709379	1.0536944061
Cu	1.8236286663	-0.4160856039	-1.3828096081
Cu	-0.5556667439	-0.2793361084	-1.5149468204
Cu	-1.9889185957	-1.2565883036	0.3631810431
Cu	0.4307170018	-1.7266356136	0.2732100631
Cu	0.5175207642	1.6517398625	-0.3725788113
Cu	-1.9754724217	1.2350228151	-0.3923964268
O	0.9538527018	1.6125770549	1.5858915674

### Cu<sub>9</sub>O

E = -1841.75533474374

Cu	-0.2805259130	1.0907538181	1.4050993383
Cu	1.3459182517	-0.7663567217	1.4425078688
Cu	2.1615916342	-1.2229363840	-1.0925648826
Cu	-0.0741403405	-0.2891648165	-0.9024019770
Cu	-0.4051374965	2.1964646928	-0.8464052068
Cu	1.7824762365	1.2363362009	-0.1816125220
Cu	-1.0630280566	-1.2311572437	1.2313514189
Cu	-2.2160611875	0.6407398906	-0.0841927026

Cu	-2.0867969487	-1.5748131186	-1.0854512828
O	2.9332350337	-0.2709930856	0.3761755711

### $\text{Cu}_{10}\text{O}$

E = -2038.06792950671

Cu	-0.4139746479	0.7817187550	1.2581491706
Cu	2.1206852422	0.7883739113	1.1762252123
Cu	1.8244182212	-0.6538960315	-1.0971585905
Cu	0.1543443842	-2.4583736244	-0.9524242197
Cu	-0.6767009754	-0.1776824466	-1.0572190028
Cu	0.9183827563	-1.3077375745	1.1839451988
Cu	0.9290908690	1.8021497146	-0.8500698023
Cu	-1.4583344493	-1.5668839002	0.9111165619
Cu	-2.7520244467	0.3087881877	0.2110726488
Cu	-1.4063631108	2.2145817091	-0.6771628752
O	2.7054997544	1.0320235626	-0.6736524397

### $\text{Cu}_{11}\text{O}$

E = -2234.36130704136

Cu	-0.7358961111	-2.3905367251	0.9463951256
Cu	-2.5170177642	-0.9115964942	-0.0739767781
Cu	-2.5849095799	1.4303886753	0.6947241006
Cu	-0.2648071757	2.3573742936	0.3303875883
Cu	1.7008171183	1.0272635015	1.2628594746
Cu	1.7759131824	-1.3038987155	0.2080022252
Cu	-0.5304095592	0.0537171262	0.9751904687
Cu	-0.2962861155	-1.3803612359	-1.4172689055
Cu	-1.3355095737	0.8646926094	-1.4375427862
Cu	1.0920704511	0.7388120682	-1.1233710331
Cu	3.4882561891	0.3066870933	-0.2540852537
O	0.6536723194	-2.7693260351	-0.3219625913

### $\text{Cu}_{12}\text{O}$

E = -2430.67176840577

Cu	-1.9528426852	-2.1557072313	0.8075934941
Cu	-2.9800738031	-0.0007246085	-0.0813794498
Cu	-1.9554298163	2.1531562984	0.8130134611
Cu	0.6418220333	2.0093512449	0.4799234215
Cu	1.6901729006	-0.0016903896	1.3977687293
Cu	0.6424229406	-2.0107518868	0.4749890886
Cu	-0.7445752395	-0.0007571145	1.0038496928
Cu	-1.1880094939	-1.2951182631	-1.3127898349
Cu	-1.1887071782	1.2999101282	-1.3100521672
Cu	1.1698451027	0.0002791630	-1.1786583637
Cu	2.9717310905	-1.3324304708	-0.2091126938
Cu	2.9700177447	1.3347911400	-0.2065140894
O	-0.2842705302	0.0033012250	-2.4562846194

### $\text{Cu}_{13}\text{O}$

E = -2626.97326499380

Cu	-1.3007752557	-0.3380303676	-1.0813470818
Cu	1.1322968705	-0.8260890910	-1.5849306656
Cu	-2.8511237613	0.9810751478	0.3337253568
Cu	-1.2673186185	2.1078407008	-1.2547264367
Cu	1.1913130788	1.6141107332	-0.8213921214
Cu	3.0828497553	0.0885013886	-0.1276687437
Cu	2.1951623431	-2.2697125885	0.0205780586
Cu	-0.3476615584	-2.3065093041	0.0367554271
Cu	-2.8823682735	-1.7449469850	-0.0193906652
Cu	-1.4134660286	-0.6092896374	1.5809002117
Cu	-0.5404604469	1.6539366540	1.1025981577
Cu	0.9588980998	-0.3728897905	1.0345702843
Cu	2.0227598644	1.8237297644	1.4063785359
O	0.0192196922	0.7397523059	-2.1962201681

### Cu<sub>14</sub>O

E = -2823.29387075291

Cu	1.3826286575	-0.2685420659	1.0675408663
Cu	-0.2539309225	1.6402464546	1.4578102424
Cu	1.8954245777	-2.3203267075	-0.1659586194
Cu	-0.1750442674	-2.1958651891	1.3170286010
Cu	-1.7928363737	-0.3221802644	0.9850708534
Cu	-2.3553406610	1.9211630789	-0.0064404414
Cu	-0.2048459197	3.3288765287	-0.2279739151
Cu	1.8366426667	1.8630301587	-0.1315967995
Cu	3.5325013413	-0.0658074902	0.0957921349
Cu	1.6970920573	-0.2261497242	-1.5256031080
Cu	-0.3152336829	-1.5346528191	-1.0799324769
Cu	-0.3740640868	1.0000861072	-1.1178465406
Cu	-2.5288479321	-0.2762068292	-1.2878404654
Cu	-2.2917377061	-2.5194711725	-0.0134512404
O	-0.2182522984	-0.2017114073	2.2330717168

### Cu<sub>15</sub>O

E = -3019.58540647643

Cu	-0.8718581569	0.2795709772	-0.7583920372
Cu	1.1835808351	1.2515207352	-1.5989825448
Cu	-2.5280835257	-0.8059574092	0.8014045738
Cu	-1.2624352702	-2.1930136737	-0.8354074902
Cu	1.0929653282	-1.2081964176	-1.0766836234
Cu	3.2200168561	0.1871958870	-0.4995630955
Cu	2.4458752391	2.6459337655	-0.0413749137
Cu	-0.0468696215	2.6820912970	0.1454148130
Cu	-2.7818263374	1.6755473296	0.0109768863
Cu	-1.0159404825	0.9054439478	1.8506611423
Cu	-0.1521139488	-1.4047736987	1.2839403784
Cu	1.2469929637	0.5990245987	0.8286520346
Cu	2.3693507582	-1.7019077345	0.9592866376
Cu	0.7144930065	-3.4108487352	0.0936584490
Cu	-3.1636627443	-0.2359260370	-1.4985068418

O -1.6637850325 2.6664065255 1.2318137008

## 18. XYZ coordinates and total energies of Cu<sub>x</sub>O clusters on TPSSh/DEF2-TZVPP level

Cu<sub>4</sub>O

E = -6637.41995439710

Cu	0.1503277171	-1.1610838057	-0.3510748410
Cu	-2.0027798865	-0.0001940750	0.5440742175
Cu	0.1526523652	1.1630338698	-0.3468384687
Cu	2.0679195232	-0.0025246550	0.5132272477
O	-1.2428893107	0.0037737364	-1.0772952173

Cu<sub>5</sub>O

E = -8277.99395117338

Cu	0.4352004639	-1.1248684409	-0.0113043542
Cu	-1.4776395737	0.1386772833	-1.1869599543
Cu	-1.4747621912	0.1150378143	1.1925115489
Cu	0.4168704749	1.2352505146	0.0102822547
Cu	2.5064797142	0.0097280217	-0.0022546491
O	-1.4395233537	-1.3597573430	-0.0120329677

Cu<sub>6</sub>O

E = -9918.58047261319

Cu	-0.5380189772	-0.5647804221	1.2562803976
Cu	0.1832627918	1.3578364899	2.3908205147
Cu	0.2596967738	1.3270431189	0.0000000000
Cu	-0.5380189772	-0.5647804221	-1.2562803976
Cu	0.7362166187	-2.3888413669	0.0000000000
Cu	0.1832627918	1.3578364899	-2.3908205147
O	-1.0116227893	-1.9105539133	0.0000000000

Cu<sub>7</sub>O

E = -11559.1691344737

Cu	-0.7413258964	-2.0168456719	-0.0966155781
Cu	-2.1452727406	-0.0096250209	0.2165162781
Cu	-0.7599166085	2.0097101016	-0.0988497381
Cu	1.6109115959	1.3084640529	-0.1496196081
Cu	1.6218642830	-1.2932661720	-0.1460012431
Cu	0.0340328593	0.0021252621	1.2099339045
Cu	-0.1428212136	-0.0014753129	-1.2559814408
O	2.0006444947	0.0111227459	1.1658581591

Cu<sub>8</sub>O

E = -13199.7506017709

Cu	-0.5079654246	0.5379183992	1.2977000969
Cu	1.9139577937	0.2680757060	0.9629084070
Cu	1.8272703178	-0.6455214911	-1.2731164046
Cu	-0.5120045805	-0.5103547181	-1.2574017485
Cu	-1.9719403680	-1.1827190504	0.5754202093
Cu	0.4634151389	-1.6728601296	0.6109695173

Cu	0.5342073786	1.5732719482	-0.6468000267
Cu	-1.9778814222	1.1624956069	-0.5969139439
O	0.9187594471	1.8288569582	1.2451062826

### Cu<sub>9</sub>O

E = -14840.3356336694

Cu	-0.1509011515	1.0921183206	1.3515451328
Cu	1.3684891518	-0.8004824685	1.2737225436
Cu	2.0104283593	-1.2552379662	-1.1577217172
Cu	-0.1330777403	-0.2504134783	-0.7920062643
Cu	-0.3492197058	2.1703385117	-0.8366658616
Cu	1.8076803646	1.1212241983	-0.2557077784
Cu	-1.0428360734	-1.1577444437	1.2874631903
Cu	-2.1711391377	0.7003971361	0.0290648439
Cu	-2.1279271411	-1.5094689499	-0.9452425670
O	2.9178254588	-0.3837697097	0.2042632808

### Cu<sub>10</sub>O

E = -16480.9312510324

Cu	-0.5695444830	0.5874163541	1.2787057736
Cu	1.9079254736	0.9312786075	1.2803939357
Cu	1.9106506859	-0.2481767900	-1.0047827593
Cu	0.5452355031	-2.2749431744	-1.1443754376
Cu	-0.5788685315	-0.1700610757	-1.0095219994
Cu	1.0101851792	-1.2484694023	1.0535126674
Cu	0.7078089309	1.9193295650	-0.6116851869
Cu	-1.2424723012	-1.8302853417	0.6651985995
Cu	-2.7315426878	-0.0735424013	0.1475866872
Cu	-1.6443493835	2.0076086333	-0.5321994458
O	2.5348610385	1.4524745114	-0.4413519506

### Cu<sub>11</sub>O

E = -18121.5085346936

Cu	-0.6359582886	-2.3007214665	1.0267650940
Cu	-2.4628372202	-0.9696703850	-0.0556039118
Cu	-2.5636613456	1.3851025406	0.6031604879
Cu	-0.3036458246	2.3490822024	0.1830120543
Cu	1.6489229313	1.1019987851	1.1983355666
Cu	1.7045627421	-1.2299088654	0.3110840476
Cu	-0.5189431160	0.0950456805	0.8391345404
Cu	-0.2490621991	-1.4363561621	-1.2654129773
Cu	-1.3266170983	0.7437349700	-1.4369771490
Cu	1.0783777468	0.6844420750	-1.1123330178
Cu	3.4254901419	0.3142256794	-0.2376769690
O	0.7175881723	-2.7446543873	-0.1737430358

### Cu<sub>12</sub>O

E = -19762.1041282390

Cu	-1.9262264551	-2.1222220098	0.7949762363
Cu	-2.9372203681	-0.0013545953	-0.0956775888

Cu	-1.9282229709	2.1200520027	0.7958393735
Cu	0.6210854456	1.9894230573	0.4580138031
Cu	1.6607583164	0.0005345828	1.3390363764
Cu	0.6230116789	-1.9889830736	0.4572002664
Cu	-0.7436926448	-0.0005630600	0.9264691235
Cu	-1.1323350304	-1.2453848012	-1.2602803417
Cu	-1.1334562361	1.2447888322	-1.2597484569
Cu	1.0955697615	0.0007569473	-1.0937842235
Cu	2.9325070503	-1.2929970273	-0.2234487649
Cu	2.9311980112	1.2960204242	-0.2229469692
O	-0.2686898589	0.0003478670	-2.3944022196

### Cu<sub>13</sub>O

E = -21402.6833490291

Cu	-1.1611094455	-0.2366762636	-0.8866492515
Cu	1.1052212924	-0.9051509648	-1.5163641094
Cu	-2.8121110098	1.0450150639	0.2960955195
Cu	-1.2030070402	2.0889860759	-1.3208288644
Cu	1.1649334321	1.4780845560	-0.8625299065
Cu	3.0313697287	0.0103090859	-0.1466519040
Cu	2.1177454103	-2.3014657579	0.1031110480
Cu	-0.3964833056	-2.2864078794	0.1133207315
Cu	-2.8643030818	-1.6079250513	-0.0257209207
Cu	-1.4211579481	-0.5316318400	1.5645701872
Cu	-0.5089994288	1.6639990580	0.9997645565
Cu	0.9222831534	-0.3514526768	0.9545327405
Cu	2.0120308348	1.7959404573	1.3018031632
O	0.0431843175	0.6179609808	-2.1834049722

### Cu<sub>14</sub>O

E = -23043.2897793730

Cu	1.1202193018	-0.3525448195	0.9474423529
Cu	-0.2383297672	1.7152601228	1.4227765628
Cu	1.9918261752	-2.2216164329	-0.2557532083
Cu	-0.0926615431	-2.5548547969	1.0320248845
Cu	-1.4985415047	-0.4349225829	0.9954375956
Cu	-2.3212598378	1.8658173841	0.1014086133
Cu	-0.2563957439	3.3254829928	-0.2930519603
Cu	1.7754009277	1.8480733789	-0.0780079034
Cu	3.3764753743	-0.0985649528	0.2148842607
Cu	1.6805571983	-0.1383659143	-1.4971531859
Cu	-0.3075856277	-1.4584557353	-1.0694908260
Cu	-0.3838130899	1.0016945358	-1.0014705223
Cu	-2.5017989132	-0.2559065777	-1.1534286615
Cu	-2.3084277341	-2.4659263018	-0.0324290529
O	-0.1773482522	0.0439454413	2.2825589437

### Cu<sub>15</sub>O

E = -24683.8663197588

Cu	-0.8589984989	0.2731936101	-0.7126405827
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Cu	1.1737116441	1.2107185646	-1.5776525974
Cu	-2.4935351262	-0.7485194565	0.8131734818
Cu	-1.2800031890	-2.1258862145	-0.8186385503
Cu	1.0542033221	-1.2126563958	-1.0251600043
Cu	3.1611925192	0.1519937454	-0.5332874683
Cu	2.4194796396	2.5770701789	-0.0641053868
Cu	-0.0612202701	2.5994456233	0.1216607878
Cu	-2.6761908230	1.6736865656	0.0606338440
Cu	-0.9741828995	0.9295884494	1.7711480798
Cu	-0.1475511946	-1.3601837444	1.2283812649
Cu	1.2463745083	0.5837348121	0.7845107887
Cu	2.3193144669	-1.6888529609	0.9466025687
Cu	0.6565753014	-3.3627659929	0.1085191846
Cu	-3.1195117189	-0.2143868571	-1.4426844001
O	-1.5949096106	2.6622435698	1.2318486081

**19. XYZ coordinates and total energies of transition states by the Cu<sub>4</sub>-N<sub>2</sub>O, Cu<sub>6</sub>-N<sub>2</sub>O, Cu<sub>8</sub>-N<sub>2</sub>O and Cu<sub>10</sub>-N<sub>2</sub>O clusters on TPSSh/DEF2-TZVPP level**

Cu<sub>6</sub>\_TS1

E = -10028.0666399466

Cu	0.9082556867	-0.5996321996	-0.0775229159
Cu	1.7934150105	1.7592513182	-0.1594115543
Cu	-0.5326789418	1.3498589613	0.0265660715
Cu	-1.5037141228	-0.8568468399	-0.0136852549
Cu	-0.1163946469	-2.7534260203	-0.1189074767
Cu	-2.8773505643	1.0778689500	0.1281765363
N	3.7225753715	1.1487647549	-0.0437091204
N	3.8348059595	0.0026689546	0.0325708142
O	3.3722008730	-1.1126727744	0.0920474221

Cu<sub>6</sub>\_TS2

E = -10028.0703003734

Cu	1.0750460928	0.7826176320	0.2271872340
Cu	-0.0802272898	2.7396787376	-0.4972208239
Cu	-1.2936769470	0.7579601947	-0.2236893343
Cu	-0.3536669504	-1.2771469709	0.5805466123
Cu	1.2176770258	-1.3258155463	-1.1807576723
Cu	-2.6959894081	-1.0465470175	0.4794267320
N	3.0145410612	-1.5818111810	-0.5295056743
N	3.3811245261	-0.8283766306	0.3157134656
O	2.7976968340	0.1181169163	0.9482378778

Cu<sub>8</sub>\_TS

E = -13309.2617545962

Cu	0.1090037234	-1.0724912421	0.8473904965
Cu	-2.0133244727	0.2847456952	0.5647328305
Cu	-0.9734885806	1.8926498024	-0.9463776127
Cu	1.1827685334	0.9471000339	-0.8327689912
Cu	2.1599354823	0.0608151721	1.1877115026

Cu	0.0630404694	1.3525212521	1.2618972317
Cu	-0.6240668421	-0.5440978547	-1.3916946443
Cu	1.7233975734	-1.3365547477	-0.9735926070
N	-3.0277088843	-1.3643533490	0.6393248126
N	-2.4312894616	-2.3635283458	0.3980428291
O	-1.1241011569	-2.4815772790	0.1071285065

### Cu<sub>10</sub>\_TS

E = -16590.4214097409

Cu	-0.5647473572	-0.2519281863	1.2419794279
Cu	1.7351421628	0.2518648894	1.9870599115
Cu	3.1854693911	0.4815909133	-0.0008429306
Cu	1.7342076426	0.2574309553	-1.9888138489
Cu	-0.5652568683	-0.2486633999	-1.2441280586
Cu	0.8345746626	1.3329497667	0.0008296059
Cu	1.3728701728	-1.1022317273	-0.0026839691
Cu	-1.5961509851	1.6139232118	0.0016667157
Cu	-2.5670929662	-0.8770486835	-0.0017780439
Cu	-0.6943916057	-2.3952551667	-0.0036699925
N	-3.4232359248	2.2904586280	0.0033113857
N	-4.3452742617	1.6021253280	0.0020362820
O	-4.1298373219	-0.0339066828	-0.0013334190