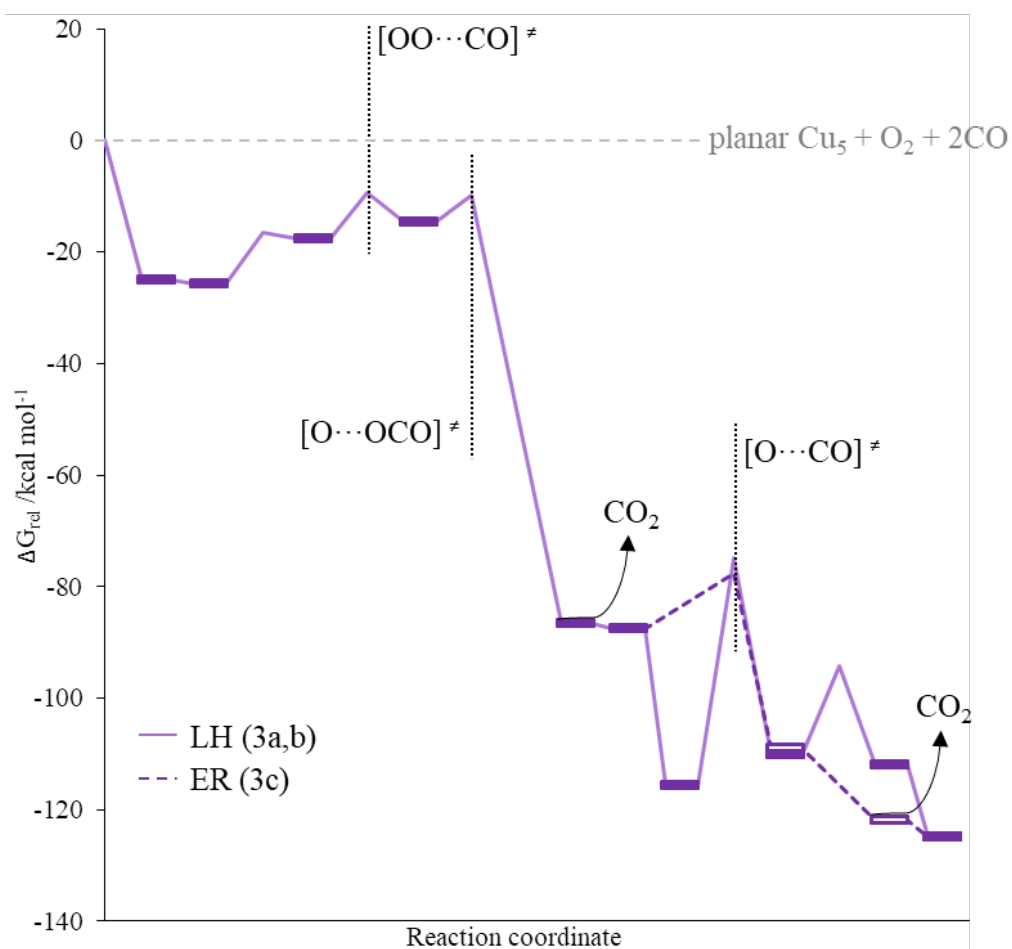


## Electronic Supplementary Information

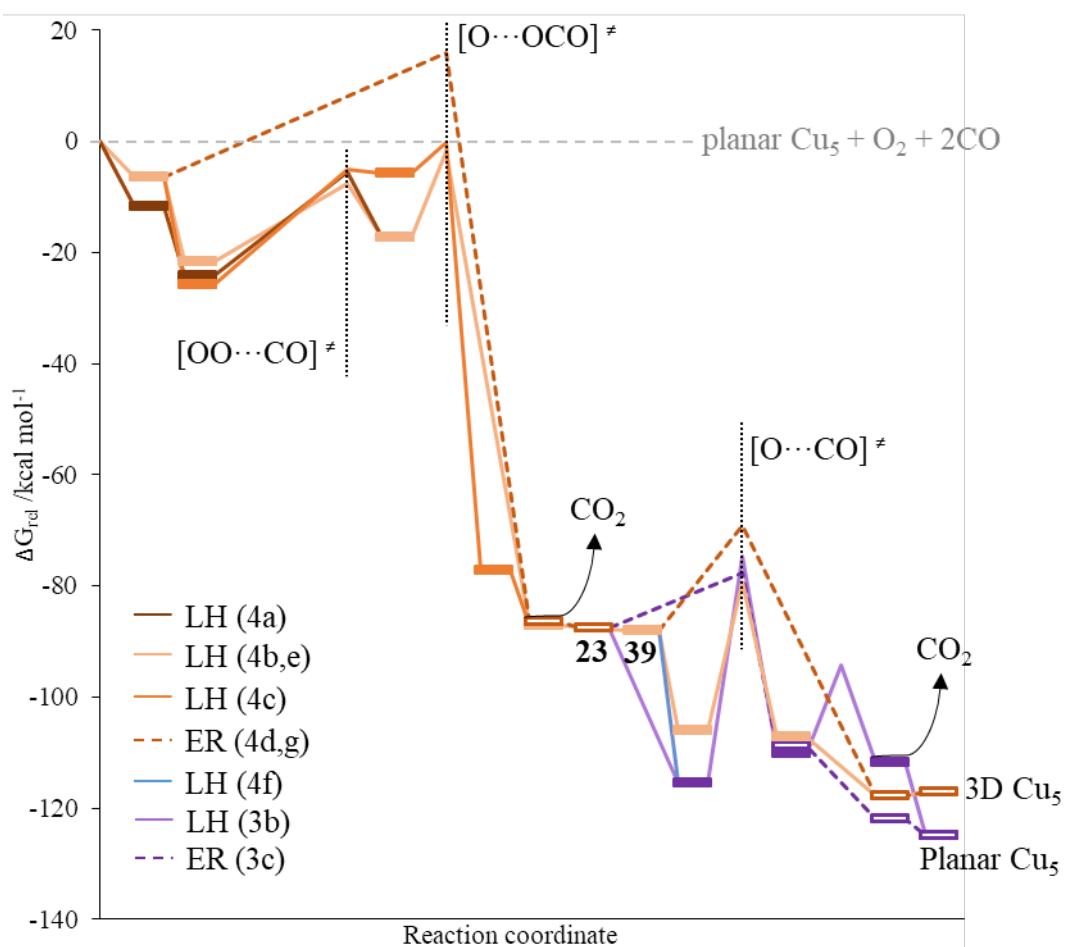
### **2D or 3D morphology of sub-nanometer Cu<sub>5</sub> and Cu<sub>8</sub> clusters changes the mechanism of CO oxidation**

Estefanía Fernández,<sup>[a]</sup> Mercedes Boronat,<sup>\*[a]</sup> and Avelino Corma<sup>[a]</sup>

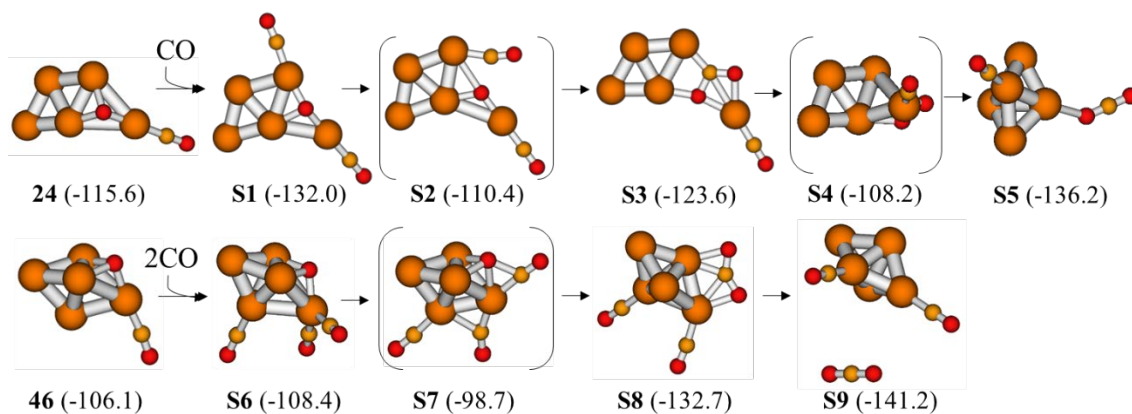
<sup>[a]</sup> Instituto de Tecnología Química, Universitat Politècnica de València–Consejo Superior de Investigaciones Científicas (UPV-CSIC), Av. de los Naranjos s/n, 46022 Valencia, Spain.



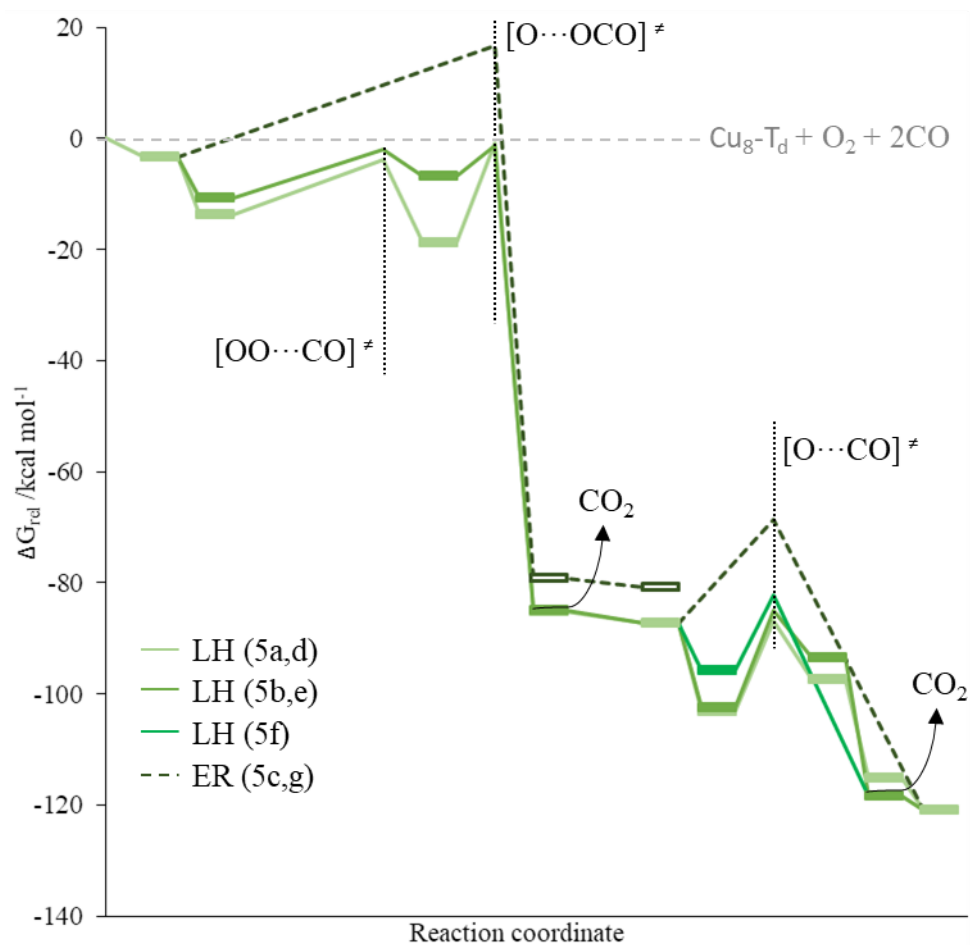
**Figure S1.** Energy profile for the CO oxidation by molecular O<sub>2</sub> in planar Cu<sub>5</sub>. a) and b,c) correspond to the first and second part of the catalytic cycle, respectively (Figure 3). Dashed lines correspond to ER paths. Key transition states of the reaction indicated by vertical dotted lines.



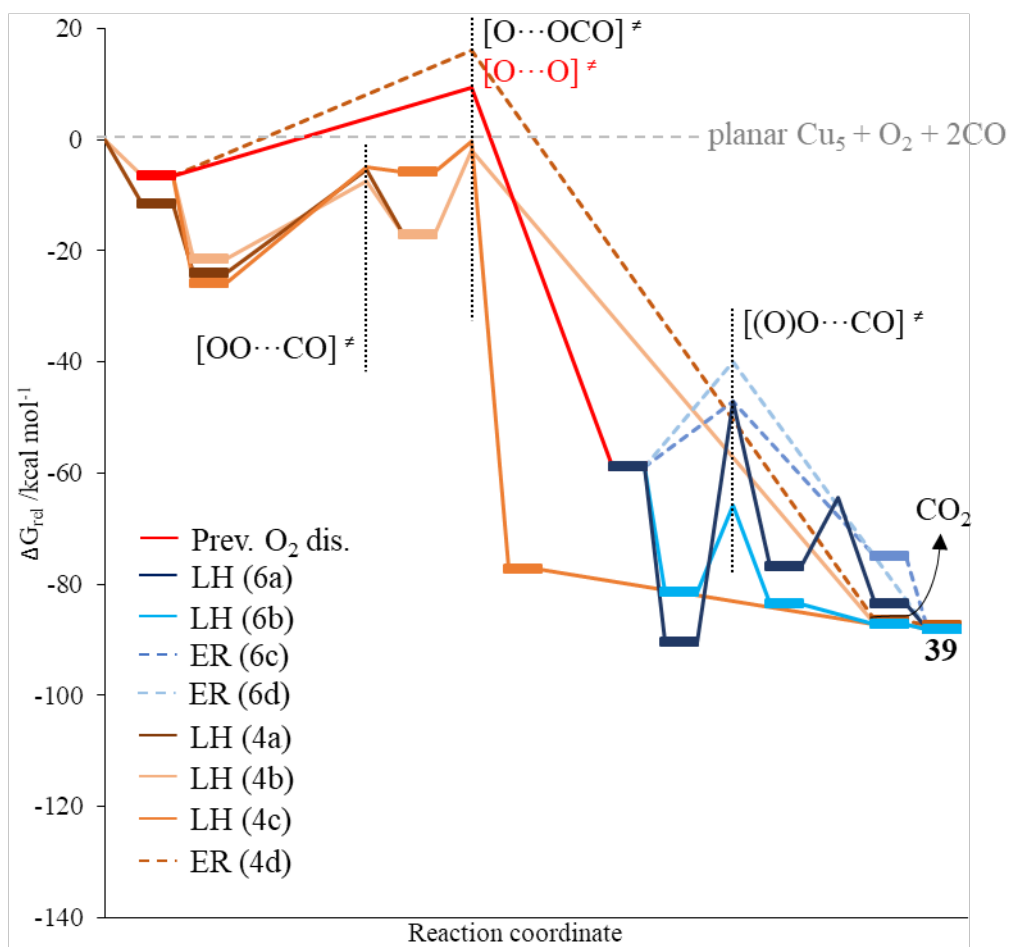
**Figure S2.** Energy profile for the CO oxidation by molecular O<sub>2</sub> in 3D Cu<sub>5</sub>. a-d) and e-f) correspond to the first and second part of the catalytic cycle, respectively (Figure 4). Dashed lines correspond to ER paths. Key transition states of the reaction indicated by vertical dotted lines. The paths from Figure 3b,c (S1) are also shown.



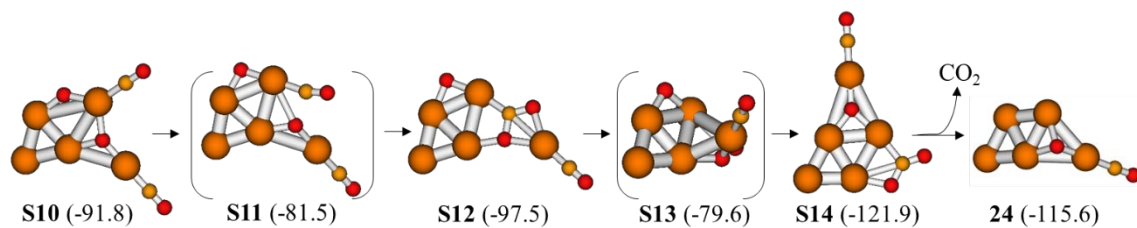
**Figure S3.** Mechanism for the second part of the  $2\text{CO} + \text{O}_2$  catalytic cycle (CO oxidation by atomic O), from structures **24** and **46** when more CO molecules are adsorbed. Relative Gibbs free energies with respect to separate planar  $\text{Cu}_5 + \text{O}_2 + 3/4\text{CO}$  in  $\text{kcal mol}^{-1}$  are given in parenthesis. Cu in orange, C in amber, O in red.



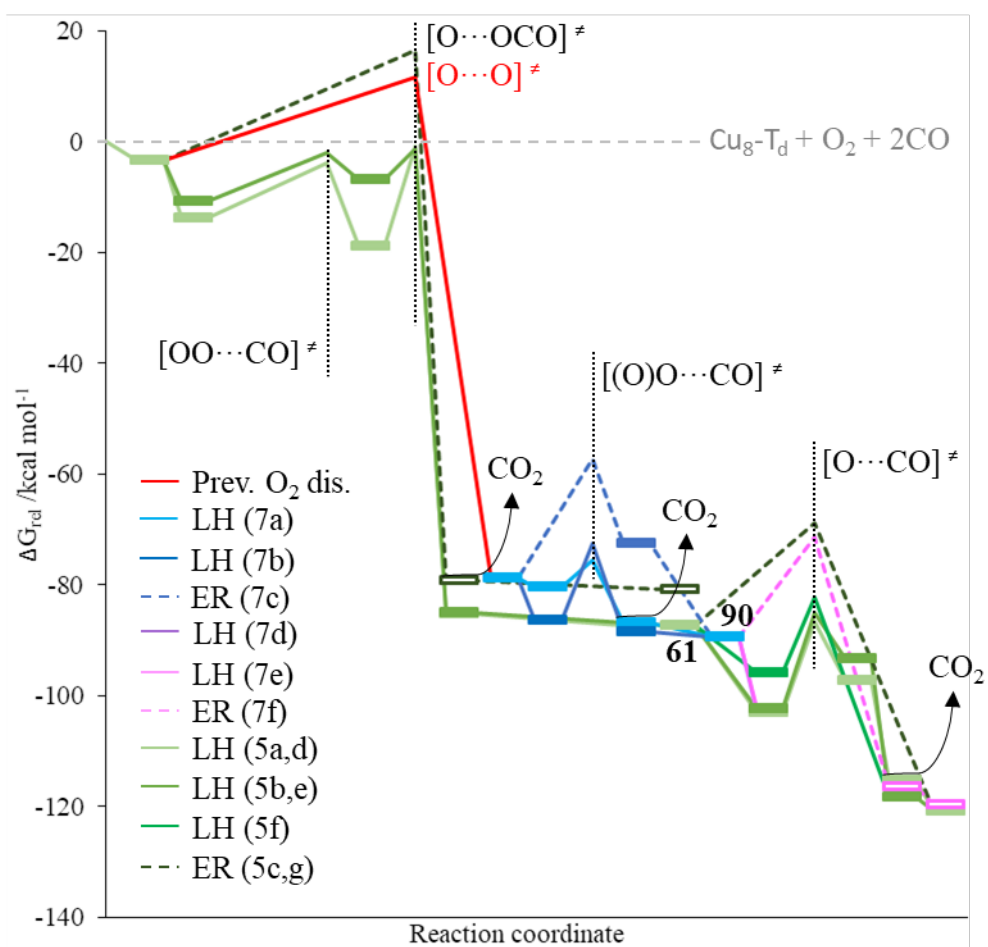
**Figure S4.** Energy profile for the CO oxidation by molecular O<sub>2</sub> in Cu<sub>8</sub>-T<sub>d</sub>. a-c) and d-g) correspond to the first and second part of the catalytic cycle, respectively (Figure 5). Dashed lines correspond to ER paths. Key transition states of the reaction indicated by vertical dotted lines.



**Figure S5.** Energy profile of the first part of the catalytic cycle for CO oxidation by previously dissociated O<sub>2</sub> on Cu<sub>5</sub> (Figure 6). The second part of the cycle follows the paths shown for structure **39** (Figures 4, S2). The energy profile for the reaction with molecular O<sub>2</sub> up to structure **39** is kept for comparison (Figures 4, S2). Dashed lines correspond to ER paths. Key transition states indicated by vertical dotted lines.



**Figure S6.** Mechanism for CO oxidation from structure **85** when another CO is adsorbed. Relative Gibbs free energies with respect to separate planar  $\text{Cu}_5 + \text{O}_2 + 3\text{CO}$  in  $\text{kcal mol}^{-1}$  are given in parenthesis. Cu in orange, C in amber, O in red.



**Figure S7.** Energy profile of the catalytic cycle for CO oxidation by previously dissociated O<sub>2</sub> on Cu<sub>8</sub> (Figure 7). The energy profile for the reaction with molecular O<sub>2</sub> is kept for comparison (Figures 5, S4). Dashed lines correspond to ER paths. Key transition states indicated by vertical dotted lines.



**Table S1.** Cartesian coordinates of all structures presented, optimized at the B3PW91/Def2TZVP level. Charge and multiplicity are also indicated, along with the number of the first figure the structure is shown in.

Figure	#Structure	Charge Multiplicity Coordinates
1	#1	0 2 Cu -2.148782 -0.069273 -0.000209 Cu 0.199133 -0.669338 -0.000029 Cu -0.387932 1.651398 0.000733 Cu 2.006057 0.952404 -0.001119 Cu 2.507291 -1.391348 0.000348 C -3.953919 -0.644819 0.000240 O -4.921720 -1.234064 0.000823
1	#2	0 2 Cu -1.432704 2.071715 0.002112 Cu 0.654202 0.913780 -0.007964 Cu -1.407074 -0.361104 -0.000436 Cu 0.850853 -1.479477 -0.011510 Cu 2.852081 -0.091878 0.012584 C -2.753807 -1.661094 0.009232 O -3.435068 -2.571435 0.011979
1	#3	0 2 Cu 2.413671 -1.144943 -0.002124 Cu -0.000120 -1.164092 0.003550 Cu 1.274664 0.965184 0.000768 Cu -1.274342 0.965187 -0.005297 Cu -2.413879 -1.144642 0.001078 C -0.000068 2.484678 0.000413 O 0.000074 3.658473 0.007029
1	#4	0 2 Cu -0.415879 -2.024329 -0.000829 Cu 1.040365 -0.020292 -0.000850 Cu -0.988244 0.016425 1.254799 Cu -0.346076 2.035159 -0.000868 Cu -0.990655 0.016417 -1.252056 C 2.872785 -0.041654 -0.000666 O 4.009682 -0.053512 -0.000211
1	#5	0 2 Cu -2.054178 -0.339977 -0.000048 Cu 0.000549 0.493603 1.184483 Cu 0.000578 0.493360 -1.184149 Cu 2.053002 -0.345949 -0.000031 Cu -0.002440 -1.649930 -0.000033 C 0.003811 2.133905 -0.000815 O 0.006166 3.289304 -0.000192
1	#6	0 1 Cu 1.619812 0.373920 -0.000461

		Cu	-0.572891	0.494392	1.258090
		Cu	0.710090	-1.559648	1.307334
		Cu	0.708657	-1.559479	-1.307764
		Cu	-0.573559	0.495269	-1.258761
		Cu	0.227090	2.413758	0.000365
		Cu	-1.394792	-1.455447	0.000188
		Cu	-2.726055	0.541419	0.000892
		C	3.499520	0.481560	-0.000085
		O	4.631337	0.566158	0.000488
<b>1</b>	<b>#7</b>	O 1			
		Cu	-0.205121	0.224312	-1.521974
		Cu	0.133550	-1.638389	-0.002385
		Cu	-2.057684	-0.463425	-0.002564
		Cu	-0.981670	1.971264	0.001475
		Cu	1.396100	1.371020	0.002650
		Cu	2.062128	-0.627978	-1.259665
		Cu	-0.207366	0.220471	1.521381
		Cu	2.060038	-0.631585	1.260495
		C	-3.927425	-0.731932	-0.000158
		O	-5.029338	-0.994173	0.002248
<b>1</b>	<b>#8</b>	O 1			
		Cu	0.215150	-1.403766	0.159746
		Cu	0.237004	0.560599	-1.287774
		Cu	2.298698	-0.017237	0.015669
		Cu	-1.171504	-0.934143	2.137509
		Cu	-1.867443	0.013370	-0.010859
		Cu	-1.146961	-1.382826	-1.889843
		Cu	0.223701	0.830579	1.139507
		Cu	-1.126443	2.334387	-0.264064
		C	4.196371	-0.009556	0.008019
		O	5.327247	0.003673	-0.005620
<b>1</b>	<b>#9</b>	O 1			
		Cu	-0.755263	1.411170	-0.049961
		Cu	-0.756650	-0.660997	1.245326
		Cu	0.587528	1.248100	1.995978
		Cu	0.591498	1.106100	-2.076947
		Cu	-0.755550	-0.746020	-1.197973
		Cu	-2.796538	0.001844	-0.000638
		Cu	1.400283	-0.004065	0.000748
		Cu	0.581899	-2.354973	0.082342
		C	3.292707	-0.003371	0.002123
		O	4.428094	-0.001672	0.002485
<b>1</b>	<b>#10</b>	O 2			
		Cu	2.463773	-0.928936	-0.000032
		Cu	-0.000015	-0.811873	0.000010
		Cu	1.279251	1.221370	0.000046
		Cu	-1.279225	1.221398	-0.000010
		Cu	-2.463805	-0.928880	0.000024
		C	4.229147	-1.622807	-0.000134
		O	5.361010	-1.711240	-0.000177
		C	1.982404	2.951996	0.000132

		O	2.357872	4.029513	0.000198
		C	-0.000037	-2.666145	0.000083
		O	-0.000053	-3.808369	0.000136
		C	-1.982305	2.952053	-0.000125
		O	-2.357725	4.029587	-0.000209
		C	-4.229183	-1.622738	-0.000013
		O	-5.361047	-1.711173	-0.000044
<b>1</b>	<b>#11</b>	O 2			
		Cu	2.418971	-0.862810	0.153734
		Cu	0.000009	-0.853748	0.000037
		Cu	1.190772	1.257954	-0.140956
		Cu	-1.190733	1.258018	0.140934
		Cu	-2.418950	-0.862717	-0.153751
		C	4.058983	-1.773203	0.360134
		O	4.985015	-2.409817	0.495231
		C	2.865045	1.948823	-0.563812
		O	3.945987	2.240024	-0.783978
		C	-0.000093	-2.697922	0.000054
		O	-0.000143	-3.842773	0.000042
		C	-2.865077	1.948648	0.563869
		O	-3.946044	2.239747	0.784060
		C	-4.058963	-1.773089	-0.360201
		O	-4.985003	-2.409670	-0.495401
		C	-0.000050	2.866984	0.000007
		O	0.000055	4.021783	0.000016
<b>1</b>	<b>#12</b>	O 2			
		Cu	2.153036	0.123782	-0.000406
		Cu	0.000272	-0.641980	1.211646
		Cu	-0.000017	-0.642574	-1.211407
		Cu	-2.153049	0.123180	0.000097
		Cu	-0.000221	1.368834	-0.000422
		C	0.000276	-2.015945	2.456969
		O	0.000250	-2.757208	3.320998
		C	4.058595	0.167914	-0.000394
		O	5.191715	0.175292	0.000056
		C	-0.000097	-2.017530	-2.455606
		O	-0.000163	-2.759565	-3.318976
		C	-4.058595	0.167471	0.000002
		O	-5.191707	0.175807	-0.000291
		C	-0.000194	3.197652	-0.000407
		O	-0.000161	4.340247	-0.000427
<b>1</b>	<b>#13</b>	O 2			
		Cu	2.295273	-0.000087	0.074308
		Cu	-0.000060	1.196617	-0.794786
		Cu	0.000000	0.000507	1.437515
		Cu	-2.295223	0.000130	0.074276
		Cu	-0.000133	-1.197254	-0.793868
		C	0.000176	3.051026	-0.994530
		O	0.000278	4.147034	-1.310440
		C	2.906363	0.000985	1.868547
		O	3.260451	0.001575	2.949137
		C	0.000183	1.652825	2.373766

		O	0.000325	2.701638	2.813232
		C	-2.906367	0.001200	1.868479
		O	-3.260600	0.001834	2.949023
		C	-0.000367	-3.051690	-0.993122
		O	-0.000609	-4.147779	-1.308748
		C	-2.846960	1.559247	-0.876368
		O	-3.247446	2.473003	-1.420377
		C	0.000067	-0.000765	-2.458124
		O	0.000246	-0.001371	-3.624914
		C	-2.847326	-1.559895	-0.874621
		O	-3.247969	-2.474166	-1.417645
		C	2.847210	1.558854	-0.876567
		O	3.247709	2.472455	-1.420814
		C	2.847347	-1.560189	-0.874536
		O	3.247839	-2.474503	-1.417586
		C	0.000005	-1.651185	2.374893
		O	0.000041	-2.699716	2.815033
<b>1</b>	<b>#14</b>	O 1			
		Cu	0.670787	1.213778	-0.249591
		Cu	0.669309	-1.214749	-0.248768
		Cu	2.763281	-0.001822	-0.590244
		Cu	-1.460552	2.324673	0.095857
		Cu	-1.119992	0.001054	0.839106
		Cu	1.273851	-0.000089	1.842190
		Cu	-1.189535	0.000204	-1.579593
		Cu	-1.462834	-2.323158	0.099176
		C	1.501908	2.784879	-0.722645
		O	2.000114	3.765218	-1.044033
		C	4.554356	-0.003223	-1.181702
		O	5.545417	-0.004131	-1.731784
		C	-2.719129	0.002246	1.740812
		O	-3.693731	0.002969	2.342392
		C	-2.499370	3.892855	0.184734
		O	-3.081705	4.859212	0.287152
		C	1.987529	0.000117	3.597414
		O	2.157952	0.000641	4.719206
		C	1.498777	-2.787035	-0.720675
		O	1.995892	-3.768140	-1.041422
		C	-1.928812	-0.000782	-3.317104
		O	-2.273782	-0.001755	-4.397710
		C	-2.505149	-3.889030	0.186676
		O	-3.090885	-4.853640	0.286082
<b>1</b>	<b>#15</b>	O 1			
		Cu	0.513189	1.298199	0.000281
		Cu	0.866682	-1.092989	-0.002573
		Cu	2.796387	0.414719	-0.003472
		Cu	-1.755558	2.216726	0.005307
		Cu	-1.380153	-0.202891	0.003636
		Cu	0.005855	-0.002404	2.294671
		Cu	-0.005107	0.001209	-2.293578
		Cu	-1.040725	-2.628096	-0.000661
		C	1.187228	3.002079	0.000742

		O	1.609328	4.068074	0.001115
		C	4.658200	0.689043	-0.007607
		O	5.778570	0.853034	-0.012007
		C	-3.193002	-0.470448	0.007370
		O	-4.327220	-0.637833	0.009743
		C	-2.927438	3.689033	0.002101
		O	-3.634197	4.573680	-0.003681
		C	2.005808	-2.528377	-0.005782
		O	2.717893	-3.426935	-0.007696
		C	-1.733695	-4.377681	-0.002133
		O	-2.150610	-5.430453	-0.002993
		C	-1.794192	-0.274000	2.908611
		C	-1.807788	-0.266908	-2.900846
		C	0.674062	1.691566	2.906417
		C	0.663638	1.695201	-2.904821
		C	1.141224	-1.428529	2.900807
		C	1.126272	-1.425258	-2.906615
		O	-2.836103	-0.432153	3.336373
		O	1.798862	-2.254451	3.323818
		O	1.061053	2.672376	3.332797
		O	1.780960	-2.251462	-3.333648
		O	-2.851727	-0.422819	-3.324446
		O	1.050882	2.675941	-3.331152
<b>2, 3</b>	<b>Cu<sub>5</sub> planar</b>	O 2			
		Cu	2.400123	-0.848182	-0.003618
		Cu	0.000064	-0.831915	-0.002211
		Cu	1.230425	1.264249	0.009205
		Cu	-1.230628	1.264166	-0.009188
		Cu	-2.399984	-0.848318	0.005812
<b>2, 4</b>	<b>Cu<sub>5</sub>-3D</b>	O 2			
		Cu	2.036971	0.001381	-0.040587
		Cu	0.002371	1.301657	-0.621365
		Cu	-0.001238	-0.008061	1.335126
		Cu	-2.037194	0.003482	-0.041835
		Cu	-0.000911	-1.298459	-0.631339
<b>2, 5</b>	<b>Cu<sub>8</sub>-D<sub>2d</sub></b>	O 1			
		Cu	-0.520515	1.596124	-0.015788
		Cu	0.519500	-0.015855	-1.588585
		Cu	-1.887079	-0.012439	-1.291447
		Cu	-1.888416	0.012149	1.291147
		Cu	0.518573	0.015604	1.589082
		Cu	1.888501	1.294323	-0.012338
		Cu	-0.520051	-1.596376	0.014655
		Cu	1.889487	-1.293529	0.013274
<b>2</b>	<b>Cu<sub>8</sub>-T<sub>d</sub></b>	O 1			
		Cu	-0.700365	-1.185445	0.658534
		Cu	0.952636	-0.509425	-1.077663
		Cu	1.709445	-1.504427	1.037665
		Cu	-1.567917	0.831874	1.762973
		Cu	-1.038116	0.920519	-0.634446
		Cu	-1.295023	-1.267195	-1.724137

		Cu 0.786301 0.773870 1.054672
		Cu 1.153039 1.940229 -1.077600
<b>3</b>	<b>Cu<sub>5</sub>-O<sub>2</sub></b>	Cu -2.412242 -1.166601 -0.001093
		Cu -0.000490 -1.088334 0.009931
		Cu -1.357724 0.947458 -0.006313
		Cu 1.359117 0.946972 0.006167
		Cu 2.410723 -1.168504 -0.008569
		O -0.663724 2.771551 -0.003146
		O 0.665958 2.771105 0.002704
<b>3</b>	<b>#16</b>	O 2
		Cu -1.872325 -1.451819 -0.884953
		Cu -1.288015 0.689446 0.167038
		Cu 0.358615 -1.177246 -0.126438
		Cu 1.381356 1.015350 -0.418180
		Cu 2.603782 -0.695764 0.648794
		O -0.935842 2.260252 -1.021780
		O 0.361029 2.471221 -1.199232
		C -1.898896 0.734145 1.938045
		O -2.290889 0.590538 2.992283
<b>3</b>	<b>#17</b>	O 2
		Cu -1.018111 2.477857 0.321905
		Cu -1.330682 0.187240 -0.311232
		Cu 0.911294 1.099154 -0.014158
		Cu 0.701423 -1.303049 0.410031
		Cu 2.727960 -0.406586 -0.454503
		O -1.916661 -2.084599 1.181432
		O -0.645722 -2.345668 1.306094
		C -2.317275 -1.263932 -1.024461
		O -2.920240 -2.069764 -1.545340
<b>3</b>	<b>#18</b>	O 2
		Cu 0.525748 2.699502 -0.243282
		Cu 1.309985 0.458363 0.122646
		Cu -1.083740 0.953195 0.001323
		Cu -0.475872 -1.409028 -0.238816
		Cu -2.695243 -0.785506 0.339078
		O 2.157456 -2.558991 -0.467467
		O 0.911129 -2.654121 -0.781278
		C 2.680451 -0.867916 0.469326
		O 3.690395 -1.083356 0.965814
<b>3</b>	<b>#19</b>	O 2
		Cu -0.779732 2.637684 -0.188888
		Cu -1.361812 0.309447 0.015725
		Cu 0.999530 1.041229 0.060593
		Cu 0.552939 -1.337836 -0.287199
		Cu 2.734947 -0.595775 0.318387
		O -1.926691 -2.567965 -0.157758
		O -0.788430 -2.507235 -0.928600
		C -2.354255 -1.346174 0.371475
		O -3.297970 -1.363634 1.102761
<b>3</b>	<b>#20</b>	O 2
		Cu -1.348246 2.271098 -0.003694

		Cu -1.344745 -0.053615 -0.489416
		Cu 0.773406 1.101959 0.096571
		Cu 1.001244 -1.312740 -0.220739
		Cu 2.910785 -0.031610 0.306217
		O -1.583473 -2.522522 0.189756
		O -0.704692 -2.003787 -0.878144
		C -2.318699 -1.481470 0.577943
		O -3.195419 -1.522295 1.382526
<b>3</b>	<b>#21</b>	O 2
		Cu -1.268096 2.299116 -0.009982
		Cu -1.310657 -0.030444 -0.488904
		Cu 0.815305 1.083298 0.120137
		Cu 0.975312 -1.353071 -0.153158
		Cu 2.934760 -0.101910 0.259971
		O -1.796301 -2.538740 0.248159
		O -0.704876 -1.930626 -0.863959
		C -2.472192 -1.507269 0.525577
		O -3.426193 -1.276769 1.207384
<b>3</b>	<b>#22</b>	O 2
		Cu 1.610756 2.432770 0.150155
		Cu -0.439968 1.302894 -0.258918
		Cu 1.617652 -0.000153 0.079420
		Cu -0.440291 -1.302676 -0.258769
		Cu 1.610142 -2.433099 0.150171
		O -4.589757 -1.159006 0.279681
		O -1.750164 0.000285 -0.266323
		C -4.558597 0.000245 0.274665
		O -4.589933 1.159491 0.280683
<b>3</b>	<b>#23</b>	O 2
		Cu 2.434776 -0.966092 0.000503
		Cu -0.000184 -0.976925 -0.000579
		Cu 1.288530 1.115399 -0.000525
		Cu -1.288381 1.115660 -0.000426
		Cu -2.434819 -0.965992 0.000451
		O 0.000285 2.457570 0.002088
<b>3</b>	<b>#24</b>	O 2
		Cu 0.168097 1.729334 0.146827
		Cu -0.555343 -0.656969 0.539082
		Cu 2.569193 -0.233724 0.176486
		Cu -2.709077 -1.392135 -0.145911
		Cu -2.021805 0.915512 -0.567283
		O 1.065173 0.250453 0.972808
		C 4.113829 -0.718397 -0.586186
		O 5.089342 -1.023970 -1.074022
<b>3</b>	<b>#25</b>	O 2
		Cu 0.306927 1.683422 -0.056658
		Cu -0.386563 -0.712908 0.047883
		Cu 3.145132 -0.587187 -0.756758
		Cu -2.686846 -1.311808 0.004062
		Cu -2.046466 1.043928 -0.089462
		O 1.377250 0.064003 0.004007

		C 2.774036 -0.353270 1.115327 O 2.588056 -0.217543 2.244126
<b>3</b>	<b>#26</b>	O 2 Cu 0.093264 1.687067 -0.000447 Cu -0.531722 -0.753066 0.000613 Cu 4.100661 -0.592293 -0.000030 Cu -2.852193 -1.349685 -0.000710 Cu -2.217272 0.985796 0.000612 O 2.003857 1.154562 -0.000642 C 2.252122 -0.078223 -0.000092 O 1.408382 -1.015489 0.000574
<b>3</b>	<b>#27</b>	O 2 Cu -0.798796 1.213278 0.474271 Cu 0.681592 -0.984529 0.122922 Cu -3.133550 -0.207976 -0.776684 Cu 3.014881 -0.600313 -0.149260 Cu 1.476096 1.262482 -0.328360 O -1.135079 -1.737860 0.268755 C -1.918946 -0.803661 0.602949 O -1.921517 -0.135062 1.661060
<b>3</b>	<b>#28</b>	O 2 Cu 0.284527 -1.956657 -0.000194 Cu -0.054600 0.514937 -0.000102 Cu 2.243644 -0.505720 0.000313 Cu -2.347111 1.437827 0.000115 Cu -1.950739 -0.899063 0.000028 O 1.261206 2.048264 -0.000332 C 2.403696 1.545907 -0.000131 O 3.549033 1.898752 -0.000151
<b>3</b>	<b>#29</b>	O 2 Cu -1.321488 2.432765 0.128238 Cu 0.715445 1.283197 -0.271492 Cu 0.714531 -1.283709 -0.271444 Cu -1.323208 -2.431854 0.128224 Cu -1.335586 0.000464 0.143754 O 2.049890 -0.000741 -0.653654 C 3.487027 -0.001171 0.842503 O 4.579698 -0.001506 0.539136
<b>3</b>	<b>#30</b>	O 2 Cu 0.887504 2.594052 0.000082 Cu 1.468027 0.305691 -0.000278 Cu -0.547263 -1.476087 -0.000230 Cu -2.743423 -0.632665 0.000149 Cu -0.894579 0.947631 0.000138 O 1.416055 -1.700136 -0.000550 C 2.301578 -2.638509 0.000233 O 3.490543 -2.623486 0.000878
<b>3</b>	<b>#31</b>	O 2 Cu -2.827296 -1.114088 -0.004527 Cu -1.253199 0.697539 -0.002164 Cu 1.138607 0.317244 0.005133



		Cu 0.243694 2.566897 -0.000151 Cu -0.450010 -1.586874 0.006195 O 3.568377 -0.156051 -0.006190 C 4.152108 -1.163354 -0.005924 O 4.729779 -2.164036 -0.005632
4	3D-Cu <sub>5</sub> -O <sub>2</sub>	O 2 Cu -2.086217 -0.392718 -0.004224 Cu -0.005425 0.508761 1.197430 Cu 0.006123 0.509013 -1.196657 Cu 2.087713 -0.388278 0.002663 Cu 0.000892 -1.597537 0.000638 O -0.007106 2.466197 0.657040 O -0.004082 2.466555 -0.656499
4	#32	O 2 Cu -0.201462 -2.075714 -0.407636 Cu 0.845523 0.001949 0.769038 Cu -1.547297 -0.003325 0.165817 Cu -0.210016 2.074914 -0.408054 Cu 0.043035 0.000055 -1.602928 O -0.319307 0.000064 2.433558 O -1.613582 -0.002643 2.168804 C 2.681133 0.004918 0.547213 O 3.801574 0.006575 0.365871
4	#33	O 2 Cu 0.042412 -2.055929 -0.056253 Cu 0.455060 0.221407 -1.064272 Cu -0.035746 0.079169 1.226481 Cu -1.262262 1.810021 -0.040396 Cu -1.834189 -0.533648 -0.278270 O 2.748916 0.468678 0.807617 O 1.764182 0.280643 1.737236 C 2.351299 0.462397 -0.593962 O 3.274303 0.640181 -1.328308
4	3D-Cu <sub>5</sub> -O <sub>2</sub> -h	O 2 Cu 1.918322 0.672634 -0.062891 Cu -0.023961 -0.440069 1.252132 Cu -0.193553 -0.808838 -1.150695 Cu -2.184897 -0.113623 0.144151 Cu -0.342916 1.516128 -0.237550 O 1.748703 -1.115069 0.674169 O 1.249192 -1.880023 -0.475324
4	#34	O 2 Cu 1.721188 -0.945611 -0.699236 Cu 0.846405 1.099024 0.681874 Cu -0.641126 -0.881308 0.575338 Cu -1.436262 1.609597 0.166581 Cu -0.011219 0.514106 -1.524558 O 2.052135 -0.497961 1.162556 O 0.790130 -0.664622 1.890862 C -2.101773 -1.884287 0.107642 O -3.002260 -2.484007 -0.234144

4	#35	O 2 Cu 1.148391 1.532889 -0.238374 Cu -0.171466 -0.153066 1.306329 Cu 0.156776 -0.625323 -1.066662 Cu -2.036999 -1.072485 0.092319 Cu -1.267957 1.253073 -0.416973 O 1.791669 0.504751 1.315210 O 1.803767 -0.913198 1.157039 C 1.907356 -1.341427 -0.609821 O 2.844849 -1.975175 -0.842701
4	#36	O 2 Cu 1.061847 1.530609 -0.277286 Cu -0.222970 -0.073544 1.330449 Cu 0.225963 -0.742883 -0.941961 Cu -2.080279 -1.076948 0.145806 Cu -1.354882 1.149567 -0.541427 O 1.683733 0.500370 1.333176 O 2.528289 -0.558027 0.829174 C 2.084242 -1.133779 -0.365060 O 2.817214 -1.944163 -0.857534
4	#37	O 2 Cu 1.221813 1.317468 -0.470776 Cu -0.372979 0.287364 1.325685 Cu 0.242783 -0.965596 -0.734397 Cu -2.138857 -0.992577 0.201502 Cu -1.250429 1.037615 -0.794278 O 1.406391 0.908404 1.399927 O 2.441085 -0.579962 1.036938 C 2.140613 -1.137849 -0.128076 O 2.876113 -1.955549 -0.628852
4	#38	O 2 Cu 0.555482 -2.070817 -0.267132 Cu 1.216585 0.007728 1.252682 Cu -0.850337 0.119340 0.055489 Cu 0.864941 2.079608 0.001051 Cu 1.321865 0.014653 -1.248244 O -0.203301 -1.307284 1.265340 O -5.088424 -0.055467 0.122035 C -4.026269 0.272735 -0.184516 O -2.957021 0.612594 -0.501683
4	#39	O 2 Cu -2.029685 0.330659 0.000712 Cu 0.077347 -0.739640 1.190191 Cu 0.111188 1.480469 0.001881 Cu 2.130268 0.051052 -0.000714 Cu 0.074903 -0.735974 -1.192078 O -1.319580 -1.401299 0.000026
4	#40	O 2 Cu -1.813366 0.432385 0.000273 Cu 0.733965 0.606717 1.215927 Cu 0.736669 0.609446 -1.214844

		Cu 2.424348 -0.660443 -0.000246 Cu 0.024130 -1.441282 -0.000354 O -0.654759 1.890962 0.754764 O -0.654832 1.890685 -0.753887 C -3.166002 -0.749006 -0.001301 O -3.949240 -1.577126 -0.002643
4	#41	O 2 Cu -1.683037 -1.117866 0.028417 Cu 0.470040 -0.441384 1.275590 Cu 0.312213 1.402539 -0.325048 Cu 2.415766 0.275955 -0.147651 Cu 0.565488 -1.128021 -1.018919 O -1.206794 0.460230 1.671962 O -1.449073 1.416931 0.614519 C -2.458989 0.599533 -0.522544 O -3.041597 1.330002 -1.214481
4	#42	O 2 Cu -1.757079 -1.136953 0.076207 Cu 0.349887 -0.298117 1.301805 Cu 0.428086 1.388452 -0.474554 Cu 2.412878 0.128348 -0.111345 Cu 0.514060 -1.238069 -0.882824 O -1.132999 0.907355 1.660131 O -1.439418 1.552018 0.396279 C -2.253494 0.675530 -0.473186 O -2.798354 1.225711 -1.372695
4	#43	O 2 Cu -1.939457 -0.988955 -0.288069 Cu 0.394068 -1.221620 0.735728 Cu 0.934664 1.243894 0.775582 Cu 2.276171 -0.295631 -0.525726 Cu -0.064616 0.244855 -1.241194 O -1.249648 -0.471950 1.533285 O -1.080344 1.139404 1.148066 C -1.520656 1.250860 -0.259270 O -2.332519 2.082681 -0.516062
4	#44	O 2 Cu -2.049558 -0.650272 0.034237 Cu 0.507881 -1.348421 0.477784 Cu 0.850772 1.136134 0.901716 Cu 2.389636 -0.136557 -0.418629 Cu -0.094615 0.303137 -1.176676 O -1.132818 -2.116168 0.465131 O -0.839359 2.284556 0.538259 C -1.498119 1.481714 -0.156577 O -2.719155 1.243253 -0.227770
4	#45	O 2 Cu -1.343319 1.329824 -0.200600 Cu 0.001553 -0.661264 -1.077304 Cu 0.169128 -0.268431 1.312276 Cu 2.198844 -0.787083 0.068531

		Cu 1.097309 1.389282 -0.296207 O -2.357404 -0.217559 0.486957 O -1.659392 -0.590639 1.718235 C -2.608063 -1.547726 -0.393760 O -1.724898 -1.664444 -1.209143
4	#46	O 2 Cu 1.773186 -0.554787 -0.000072 Cu -0.690980 -0.726949 1.183821 Cu -0.691027 -0.727239 -1.183657 Cu -2.350187 0.674970 -0.000082 Cu 0.031314 1.384260 -0.000064 O 0.440777 -1.794590 0.000232 C 3.248933 0.495229 -0.000048 O 4.110413 1.240993 -0.000001
4	#47	O 2 Cu -1.546064 1.067124 -0.000006 Cu 0.147861 -0.653548 -1.184308 Cu 0.147858 -0.653530 1.184314 Cu 2.347576 -0.507347 0.000002 Cu 0.882990 1.456734 -0.000005 O -1.260494 -1.243796 0.000005 C -2.866263 -0.348143 0.000000 O -3.768108 -1.066793 0.000004
4	#48	O 2 Cu -1.671746 1.127588 0.102595 Cu -0.172669 -0.219854 -1.177267 Cu 0.507923 -0.994663 1.022710 Cu 2.244741 -0.327679 -0.485171 Cu 0.720875 1.414314 0.471637 O -1.396910 -1.621954 0.907685 C -1.980604 -1.049344 -0.052595 O -3.023211 -1.214971 -0.630819
4	#49	O 2 Cu 1.300195 1.402783 0.000003 Cu -0.051115 -0.546369 1.184311 Cu -0.051120 -0.546346 -1.184323 Cu -2.200141 -0.905348 -0.000002 Cu -1.121664 1.366082 0.000011 O 1.601549 -0.544821 -0.000005 C 2.887268 -1.578360 -0.000001 O 3.931939 -1.065567 0.000003
4	#50	O 2 Cu -0.026431 2.029302 -0.001300 Cu 1.083623 0.266676 1.330085 Cu 1.265673 0.314489 -1.227183 Cu 1.304735 -1.813787 0.020955 Cu -0.699574 -0.354867 -0.100738 O -2.764758 -0.949824 -0.145510 C -3.862496 -0.576334 -0.027448 O -4.952465 -0.219501 0.087002
5	Cu <sub>8</sub> -O <sub>2</sub>	O 1

		Cu -1.306410 -1.679114 -0.106332
		Cu 1.235577 0.506450 1.109948
		Cu -1.235569 0.506466 1.109947
		Cu -2.447017 0.207331 -1.046127
		Cu 0.000001 0.288310 -1.031324
		Cu 1.306391 -1.679123 -0.106337
		Cu 0.000014 2.444156 0.188405
		Cu 2.447018 0.207312 -1.046127
		O -0.000005 -0.794851 2.061168
		O -0.000010 -2.111627 1.302636
<b>5</b>	<b>#51</b>	0 1
		Cu -1.972220 -1.291699 0.205991
		Cu 1.559470 -0.161710 0.858240
		Cu -0.830750 0.677894 1.291124
		Cu -2.843726 0.917423 -0.144380
		Cu -0.649417 0.391360 -1.105330
		Cu 0.461308 -1.811443 -0.756158
		Cu 0.757018 2.081724 -0.013681
		Cu 1.664424 0.082378 -1.654215
		O 0.072512 -1.030660 1.829075
		O -0.410431 -2.190642 0.983732
		C 3.389356 -0.059433 1.074621
		O 4.516261 0.054394 1.160460
<b>5</b>	<b>#52</b>	0 1
		Cu 1.326130 1.456550 -0.949089
		Cu -1.429214 -0.382959 0.881247
		Cu 1.013289 0.258388 1.240196
		Cu 2.671556 -0.456319 -0.482321
		Cu 0.291227 -0.852187 -0.864355
		Cu -1.297667 1.124158 -1.028328
		Cu 0.302278 -2.101846 1.247838
		Cu -2.031112 -1.141023 -1.456852
		O -0.043049 2.132102 1.273845
		O -0.157175 2.510123 -0.149970
		C -1.363628 1.411217 1.733088
		O -1.845576 1.894597 2.693591
<b>5</b>	<b>#53</b>	0 1
		Cu 0.254405 1.771273 -0.051972
		Cu -0.908338 -0.397661 0.905203
		Cu 1.497966 0.039346 1.353393
		Cu 2.531685 1.250449 -0.577416
		Cu 0.824287 -0.478618 -0.944337
		Cu -1.493694 0.400709 -1.411493
		Cu 0.690891 -2.233245 0.846803
		Cu -1.022061 -1.976846 -1.117788
		O -2.447407 2.101121 0.653513
		O -1.607988 2.208642 -0.511902
		C -2.214045 0.982226 1.426321
		O -2.893954 0.842717 2.404971
<b>5</b>	<b>#54</b>	0 1
		Cu -0.663785 -1.714773 -0.365986

		Cu 1.109679 0.070724 0.804181
		Cu -1.252846 -0.065695 1.497014
		Cu -2.811033 -0.611987 -0.387762
		Cu -0.800464 0.695365 -0.812695
		Cu 1.273812 -0.446689 -1.656934
		Cu -0.155382 2.122647 1.106147
		Cu 1.198420 1.957026 -1.062304
		O 2.135803 -2.545016 0.592054
		O 1.090434 -2.172844 -0.862262
		C 2.163204 -1.568877 1.381607
		O 2.769656 -1.379473 2.417980
<b>5</b>	<b>#55</b>	O 1
		Cu -0.189481 -1.758878 -0.414978
		Cu 1.016730 0.218279 0.670361
		Cu -1.244409 -0.498996 1.541733
		Cu -2.582799 -1.505663 -0.333980
		Cu -1.176815 0.507469 -0.680427
		Cu 1.017545 0.107473 -1.813598
		Cu -0.584922 1.858211 1.414373
		Cu 0.351135 2.313595 -0.979460
		O 4.406108 -2.064771 0.431394
		O 1.606616 -1.223453 -0.560582
		C 3.862705 -1.197429 0.967248
		O 3.389931 -0.314105 1.564165
<b>5</b>	<b>#56</b>	O 1
		Cu -0.168180 -2.034710 0.120362
		Cu 0.212878 1.279092 1.099018
		Cu -1.739928 -0.241342 0.945861
		Cu -2.071759 -1.465847 -1.207283
		Cu -0.293763 0.196892 -1.024397
		Cu 2.010027 -0.478286 0.294183
		Cu -1.847415 1.943680 -0.158303
		Cu 1.593300 1.708005 -0.851234
		O -0.112142 -0.376202 2.177253
		O 0.882143 -1.363779 1.637693
		C 3.741270 -0.841010 -0.300265
		O 4.779096 -0.918889 -0.755754
<b>5</b>	<b>#57</b>	O 1
		Cu 0.576232 -1.882654 -0.454566
		Cu 0.439463 1.061425 1.141341
		Cu -1.067345 -0.877399 1.214324
		Cu -1.803658 -1.918418 -0.916720
		Cu -0.649372 0.184423 -1.009539
		Cu 1.821875 0.566273 -0.845467
		Cu -1.948615 1.422083 0.718718
		Cu 0.130501 2.409870 -0.879632
		O 0.890172 -0.723863 1.892067
		O 1.800353 -1.537953 1.082483
		C 3.034450 -0.492806 0.290697
		O 4.099470 -0.868890 0.546767
<b>5</b>	<b>#58</b>	O 1

		Cu -1.435461 1.193604 -0.594022
		Cu 0.419816 -1.261836 1.101658
		Cu 0.418058 1.262340 1.101628
		Cu 0.579933 2.424896 -1.113779
		Cu 0.774321 0.000779 -0.976561
		Cu -1.433177 -1.195495 -0.594551
		Cu 2.523238 0.001585 0.780118
		Cu 0.583897 -2.423667 -1.114197
		O -0.769728 -0.000738 2.149844
		O -2.214060 -0.002191 1.969361
		C -2.644478 -0.002221 0.671184
		O -3.843870 -0.003400 0.487588
<b>5</b>	<b>#59</b>	0 1
		Cu -1.448686 1.204735 -0.545046
		Cu 0.440311 -1.275976 1.105581
		Cu 0.440541 1.275905 1.105579
		Cu 0.621972 2.422996 -1.085740
		Cu 0.714138 -0.000075 -0.994450
		Cu -1.448933 -1.204478 -0.544972
		Cu 2.509134 -0.000217 0.716432
		Cu 0.621477 -2.423129 -1.085745
		O -0.601497 0.000059 2.093567
		O -2.356241 0.000258 1.916792
		C -2.718455 0.000243 0.685622
		O -3.884503 0.000364 0.290734
<b>5</b>	<b>#60</b>	0 1
		Cu 0.045375 -1.959546 -0.994615
		Cu 0.155453 1.608732 0.943659
		Cu -0.183109 -0.897902 1.148685
		Cu -2.479995 -1.266649 -0.569641
		Cu -0.833248 0.406249 -0.985620
		Cu 1.521909 -0.035738 -0.493172
		Cu -2.229350 0.497628 1.097291
		Cu 0.797528 2.239884 -1.295135
		O -0.712134 0.598464 2.278803
		O 3.900280 -0.267104 -0.001231
		C 4.485162 -1.000980 0.688359
		O 5.067693 -1.729006 1.369642
<b>5</b>	<b>#61</b>	0 1
		Cu 1.005122 2.067020 0.237400
		Cu -1.317177 -1.258234 0.556425
		Cu 0.756628 -0.040741 1.377482
		Cu 2.298246 0.137971 -0.950210
		Cu -0.082245 0.151858 -1.077600
		Cu -1.271318 1.294133 0.729317
		Cu 1.113885 -1.884902 -0.236915
		Cu -2.560181 0.060463 -1.037176
		O 0.206770 -1.912431 1.454633
<b>5</b>	<b>#62</b>	0 1
		6 0 3.912856 -0.002187 0.263602
		O 4.708733 -0.001572 1.097322

		O 2.276570 -0.001883 0.562011
		O 1.045664 -0.000883 1.778858
		Cu -0.369916 -1.234181 1.172943
		Cu -2.513855 0.001862 0.849228
		Cu -0.829755 0.000559 -0.936074
		Cu -0.791508 2.425740 -0.952775
		Cu 1.322758 1.294117 -0.678428
		Cu -0.367975 1.234730 1.172843
		Cu 1.320714 -1.296517 -0.678202
		Cu -0.795459 -2.424660 -0.952541
<b>5</b>	<b>#63</b>	0 1
		6 0 3.954854 -1.156151 0.720065
		O 4.322475 -1.300428 1.804134
		O 3.684644 -1.044127 -0.411647
		O 1.484823 -0.278321 1.314472
		Cu -0.250692 -1.015483 1.018495
		Cu -1.964952 0.879560 1.368755
		Cu -0.957043 0.595123 -0.822192
		Cu 0.732867 2.168568 -1.346030
		Cu 1.421652 -0.187979 -0.690438
		Cu 0.525777 1.376965 1.038221
		Cu -0.488169 -1.697481 -1.459625
		Cu -2.456151 -1.156516 -0.002912
<b>5</b>	<b>#64</b>	0 1
		8 0 -0.920508 0.004928 2.144485
		Cu 0.818302 -0.002753 1.336738
		Cu 0.966803 -2.050867 -0.227322
		Cu 0.004101 0.001606 -1.083676
		Cu -2.359090 0.001602 -1.236185
		Cu -1.268336 1.246832 0.686845
		Cu -1.276230 -1.237960 0.690291
		Cu 0.981090 2.047335 -0.228267
		Cu 2.387295 -0.007154 -0.530006
<b>5</b>	<b>#65</b>	0 1
		Cu -0.432081 1.204361 -1.202320
		Cu 0.194406 -1.285038 1.275700
		Cu -2.050809 0.008995 0.555846
		Cu 1.630764 2.423363 -0.287443
		Cu 1.553438 -0.006872 -0.336127
		Cu -0.443054 -1.199150 -1.202209
		Cu 0.206647 1.283993 1.275500
		Cu 1.607578 -2.437937 -0.286976
		O -0.955397 0.005126 2.063734
		C -3.627229 0.013171 -0.361734
		O -4.541658 0.015024 -1.038330
<b>5</b>	<b>#66</b>	0 1
		Cu 0.270740 -1.224527 1.427127
		Cu -0.490350 1.274219 -1.021763
		Cu -1.793141 0.000040 0.982517
		Cu 1.550359 -2.431483 -0.389207



		Cu 1.509951 -0.000066 -0.367555 Cu 0.270782 1.224527 1.427100 Cu -0.490493 -1.274175 -1.021778 Cu 1.550590 2.431352 -0.389193 O -1.804453 0.000101 -1.456914 C -3.331394 0.000143 -0.176902 O -4.318837 0.000208 -0.756679
5	#67	O 1 Cu 1.212154 0.395032 1.441182 Cu -1.289540 -0.584805 -0.952253 Cu 0.000160 -1.742529 1.145430 Cu 2.446504 1.457422 -0.508111 Cu -0.000135 1.475822 -0.412712 Cu -1.212226 0.394811 1.441180 Cu 1.289643 -0.584576 -0.952251 Cu -2.446771 1.456982 -0.508106 O 0.000179 -1.996022 -1.527441 C 0.000266 -2.880632 -0.476900 O 0.000383 -4.065581 -0.631933
5	#68	O 1 Cu 0.327388 -1.215714 1.370477 Cu -0.226348 1.211813 -1.171212 Cu -1.637983 -0.013686 0.458227 Cu 1.776012 -2.386603 -0.268694 Cu 1.727017 0.009919 -0.253485 Cu 0.311085 1.212140 1.373849 Cu -0.210333 -1.214206 -1.175755 Cu 1.745347 2.406794 -0.260981 O -5.886793 0.016290 -0.869517 C -5.027223 -0.013759 -0.097304 O -4.161960 -0.043877 0.679951
5	#69	O 1 Cu -0.850137 2.311726 -0.134806 Cu -0.580293 -1.632982 0.739720 Cu 0.134400 0.715537 1.337964 Cu 1.528055 1.526694 -0.708404 Cu -0.246970 0.001075 -1.075068 Cu -2.181075 0.337041 0.450778 Cu 2.043285 -0.794902 0.446113 Cu -2.063833 -1.647686 -1.150243 O 0.832564 -1.014900 1.839001 C 3.587371 -1.053776 -0.482260 O 4.511964 -1.154596 -1.136755
5	#70	O 1 Cu -1.105181 2.157077 0.568856 Cu -0.045624 -1.758856 0.388079 Cu 0.559482 0.540909 1.213021 Cu 1.010130 2.022443 -0.908369 Cu -0.537912 0.222839 -1.056049 Cu -1.894234 -0.129305 0.954477 Cu 1.909768 -0.256878 -0.849406

		Cu -2.016420 -1.734274 -1.000696 O 1.443801 -1.149753 1.347846 C 3.102534 -1.236581 0.315758 O 3.914267 -1.779644 0.916900
5	#71	O 1 Cu -0.939432 2.177892 0.645654 Cu -0.098472 -1.766807 0.301167 Cu 0.605148 0.468701 1.251190 Cu 1.077454 2.003940 -0.930417 Cu -0.534740 0.294400 -1.057269 Cu -1.856249 -0.066542 1.001979 Cu 1.904720 -0.348530 -0.951872 Cu -2.074636 -1.580155 -1.045959 O 1.465467 -1.342630 1.475842 C 2.544305 -1.383231 0.607891 O 3.572551 -1.907952 0.915775
5	#72	O 1 Cu -1.862503 -1.632231 0.588624 Cu 1.709842 0.831567 0.493727 Cu -0.742427 0.333331 1.339961 Cu -2.586869 0.556509 -0.607983 Cu -0.432780 -0.306618 -1.133253 Cu 0.596458 -1.654955 0.612876 Cu -0.642167 2.047805 -0.457643 Cu 1.850242 -0.934316 -1.401980 O 0.344920 1.913427 1.174552 C 3.532158 0.578346 0.509863 O 4.655449 0.403853 0.493608
5	#73	O 1 Cu -1.991217 -1.039254 1.037075 Cu 1.784118 0.159908 -0.079655 Cu -0.452674 0.780301 1.190041 Cu -2.347272 0.803644 -0.755728 Cu -0.441461 -0.602611 -0.997734 Cu 0.392986 -1.609498 1.074921 Cu -0.148107 1.865279 -1.020259 Cu 1.551435 -1.975372 -1.145218 O 0.806897 2.114593 0.614576 C 2.618067 1.668934 0.792136 O 3.218747 2.497514 1.316337
5	#74	O 1 Cu 2.231334 0.500613 1.183554 Cu -1.488260 0.080770 -0.296603 Cu 0.232926 -0.943266 1.147226 Cu 2.298394 -1.391177 -0.428974 Cu 0.893123 0.463322 -0.906460 Cu -0.045583 1.485494 1.149890 Cu -0.078694 -1.794870 -1.128565 Cu -0.610327 2.283980 -1.181834 O -3.953436 -0.179456 -0.096674 C -4.525868 -0.904850 0.611136

		O	-5.096473	-1.624547	1.312225
5	#75	O 1			
		Cu	1.924131	1.250740	0.934849
		Cu	-1.715647	-0.342927	-0.008727
		Cu	0.539983	-0.678419	1.230684
		Cu	2.374353	-0.676844	-0.740064
		Cu	0.372617	0.576382	-1.039136
		Cu	-0.496237	1.623467	1.001753
		Cu	0.274112	-1.912347	-0.949647
		Cu	-1.749863	1.767859	-1.173207
		O	-0.742422	-2.051856	0.692696
		C	-2.284933	-2.647266	1.275965
		O	-3.066380	-1.791375	1.045493
6	$\text{Cu}_5(\text{O})_2$	O 2			
		Cu	2.070914	-0.025849	-0.064927
		Cu	-0.244897	-0.873890	-1.135759
		Cu	-0.141256	1.417225	-0.058905
		Cu	-2.214261	0.194204	-0.027985
		Cu	-0.236129	-0.745025	1.233146
		O	1.115216	-1.586184	0.087483
		O	1.660190	1.707025	0.109820
6	#76	O 2			
		Cu	-0.109720	1.519196	0.000588
		Cu	0.488355	-0.925172	0.003482
		Cu	2.287918	0.784896	-0.002237
		Cu	2.788779	-1.554905	-0.001660
		Cu	-2.937241	-0.228183	0.000557
		O	-1.191409	0.025579	0.003864
		O	1.419288	2.464106	0.000604
		C	-4.706118	-0.493376	-0.002806
		O	-5.826370	-0.654541	-0.005009
6	#77	O 2			
		Cu	0.488123	1.377652	0.115148
		Cu	-0.434549	-0.955999	-0.064076
		Cu	3.337690	-0.246971	-0.750800
		Cu	-2.800619	-1.286862	-0.152914
		Cu	-1.999166	0.960734	-0.011602
		O	1.391417	-0.254689	-0.007286
		C	2.800307	-0.748501	1.016310
		O	2.545399	-1.110330	2.080430
		O	-0.931154	2.475387	0.297509
6	#78	O 2			
		Cu	0.329851	1.790882	-0.000146
		Cu	-0.468440	-0.803106	0.000074
		Cu	4.166907	-0.684624	0.000030
		Cu	-2.728373	-1.607270	-0.000140
		Cu	-2.372080	0.732547	0.000130
		O	2.081201	1.068890	-0.000188
		C	2.322126	-0.171169	0.000010
		O	1.459591	-1.088574	0.000164
		O	-1.395898	2.220006	0.000205

6	#79	O 2 Cu -1.117941 1.252655 0.500422 Cu 0.838648 -1.214405 0.245065 Cu -2.999614 -0.503748 -0.859730 Cu 3.062704 -0.545707 -0.225737 Cu 1.374585 1.128305 -0.267714 O -1.010779 -1.906506 0.395531 C -1.815159 -0.962872 0.594548 O -1.868458 -0.208327 1.608692 O 0.041475 2.412498 -0.247241
6	#80	O 2 Cu 1.617893 0.630672 -1.003066 Cu -0.628182 -1.201440 0.196948 Cu 1.000003 0.463350 1.369668 Cu -2.806791 -0.380740 -0.298293 Cu -0.979551 1.159361 -0.158958 O 1.320458 -1.592808 0.681408 C 2.036110 -1.237728 -0.344857 O 2.924210 -1.806221 -0.919535 O 0.741022 1.894215 0.111434
6	#81	O 2 Cu -1.678646 -0.365002 0.000272 Cu 0.839673 0.002585 -1.200202 Cu 0.841007 0.003923 1.200820 Cu 2.690326 -0.944070 -0.000475 Cu -0.676131 1.966448 -0.000522 O -0.855946 0.815755 -1.438710 O -0.855506 0.815949 1.437861 C -2.805527 -1.792563 0.000531 O -3.493231 -2.693861 0.000835
6	#82	O 2 Cu -1.568958 -0.483446 -1.103639 Cu 0.603330 1.125093 0.405539 Cu 1.025260 -1.145798 -0.248758 Cu 2.805781 0.453641 -0.252646 Cu -1.157241 -0.665514 1.301098 O -1.258687 1.173704 0.868602 O -0.704894 -1.873303 -0.077302 C -2.105983 1.297251 -0.600431 O -2.649055 2.322248 -0.709258
6	#83	O 2 Cu -1.618530 -0.630088 -1.002842 Cu 0.627794 1.201202 0.197211 Cu 0.979372 -1.159251 -0.160189 Cu 2.806601 0.380981 -0.298063 Cu -0.999053 -0.464378 1.369971 O -1.319969 1.592344 0.682034 O -0.741105 -1.894324 0.110671 C -2.035767 1.238155 -0.344400 O -2.923266 1.807677 -0.918975
6	#84	O 2

		Cu 1.120384 -1.471871 -0.044365 Cu -1.129174 -0.590893 -1.145857 Cu 0.519807 1.023956 -0.042000 Cu -1.833059 1.536791 -0.031944 Cu -1.065910 -0.514511 1.221524 O -0.621517 -2.036368 0.077813 O 2.119574 0.048311 0.107725 C 3.958417 0.545271 -0.152375 O 4.189457 1.639015 0.083318
6	#85	O 2 Cu 1.344187 1.049658 0.095988 Cu -0.852646 0.638448 -1.258789 Cu -1.071708 0.785163 1.099961 Cu -2.125592 -1.183720 -0.062747 Cu 0.250438 -1.213563 0.152967 O 2.200315 -0.712391 0.314474 O -0.196613 2.050882 -0.090007 C 3.353073 -1.208844 -0.001819 O 4.382034 -0.707305 -0.322353
6	#86	O 2 Cu 1.433578 1.230784 -0.000003 Cu -0.080810 -0.661004 -1.187605 Cu -1.187535 1.222460 -0.000078 Cu -2.262039 -0.942127 0.000147 Cu -0.080801 -0.660885 1.187704 O 1.581453 -0.679619 0.000049 O 0.134332 2.467202 -0.000506 C 2.940467 -1.710021 0.000204 O 3.972692 -1.191022 -0.000294
7	$\text{Cu}_8(\text{O})_2$	O 1 Cu 1.328177 -0.318493 1.279914 Cu -1.328273 -0.319057 -1.279940 Cu -0.000157 -2.031849 0.000244 Cu 2.477920 1.413016 -0.000311 Cu -0.000020 1.344844 -0.000309 Cu -1.328306 -0.318413 1.280116 Cu 1.328453 -0.319306 -1.279479 Cu -2.477810 1.413002 -0.000334 O 0.000036 -1.565843 -1.843562 O 0.000027 -1.565231 1.843925
7	#87	O 1 Cu 0.002516 1.321968 -1.232995 Cu -0.003760 -1.321121 -1.232993 Cu -2.218693 0.004173 0.000333 Cu 1.739831 2.503272 0.000148 Cu 0.002191 1.321862 1.232753 Cu 1.694151 -0.003608 0.000057 Cu -0.004087 -1.321054 1.232762 Cu 1.727913 -2.510664 0.000116 O -1.203429 0.003251 -1.752477 O -1.203706 0.003219 1.752711

		C	-4.065791	0.006316	-0.000324
		O	-5.201246	0.007537	-0.000645
<b>7</b>	<b>#88</b>	O 1			
		Cu	0.376936	-1.296071	-1.121771
		Cu	0.405689	1.286949	-1.121977
		Cu	2.022103	-0.022860	0.930695
		Cu	-1.615193	-2.482908	-0.342820
		Cu	-0.279901	-1.318361	1.300257
		Cu	-1.568096	0.017688	-0.341925
		Cu	-0.248516	1.324141	1.300642
		Cu	-1.558257	2.518527	-0.342309
		O	1.588591	-0.017826	-1.711242
		O	0.699682	-0.008971	2.244110
		C	3.279250	-0.035627	-0.450832
		O	4.188770	-0.044735	-1.140114
<b>7</b>	<b>#89</b>	O 1			
		Cu	1.297240	0.618583	-0.935208
		Cu	-1.298223	0.616693	-0.935390
		Cu	-0.001273	1.759154	1.016622
		Cu	2.475721	-1.476796	-0.551017
		Cu	1.325282	-0.434906	1.318604
		Cu	0.001109	-1.484955	-0.507415
		Cu	-1.324503	-0.436642	1.318652
		Cu	-2.473537	-1.480395	-0.550739
		O	-0.001633	1.935196	-1.734987
		O	-0.000173	0.420280	2.357619
		C	-0.002126	2.774737	-0.646279
		O	-0.003182	3.970802	-0.769074
<b>7</b>	<b>#90</b>	O 1			
		Cu	-1.224507	0.231759	1.416164
		Cu	1.296358	0.509562	-1.176981
		Cu	0.000001	2.069223	0.369482
		Cu	-2.429130	-1.376962	-0.145625
		Cu	-0.000295	-1.309206	-0.127092
		Cu	1.226125	0.231190	1.415490
		Cu	-1.297321	0.508933	-1.178429
		Cu	2.428884	-1.377174	-0.147572
		O	-0.000413	1.858451	-1.542207
<b>7</b>	<b>#91</b>	O 1			
		Cu	1.117664	0.876568	-1.323729
		Cu	-0.544771	-0.441485	1.749746
		Cu	0.180736	1.784628	0.833892
		Cu	2.619063	-1.018121	-1.164155
		Cu	0.251549	-1.225414	-0.420406
		Cu	-1.697242	0.756053	-0.712160
		Cu	1.931306	0.010417	0.948048
		Cu	-2.003781	-1.687576	0.289843
		O	0.810051	0.779352	2.298492
		O	-0.338486	2.032358	-0.957556
		C	-3.482758	0.461061	-1.062052
		O	-4.582148	0.267866	-1.273304

7	#92	O 1 Cu 0.946020 1.364345 -0.744288 Cu -0.758342 -1.218085 1.284497 Cu -0.244097 1.290660 1.459934 Cu 2.718159 -0.250858 -1.141469 Cu 0.399187 -1.063848 -0.877896 Cu -1.684030 0.322567 -0.493932 Cu 1.688377 -0.257745 1.086089 Cu -1.828336 -2.093914 -0.723001 O 0.339335 -0.205613 2.449225 O -0.517049 2.353831 -0.071829 C -2.203940 2.143124 -0.872895 O -2.653236 3.156872 -1.178732
7	#93	O 1 Cu 1.198734 0.752489 -0.880108 Cu -1.308106 -0.610652 1.274721 Cu -0.004078 1.639477 1.412791 Cu 2.480703 -1.370352 -0.689502 Cu 0.003776 -1.401708 -0.686711 Cu -1.202245 0.746121 -0.879324 Cu 1.311726 -0.603518 1.274119 Cu -2.473142 -1.383204 -0.689112 O 0.000062 0.104359 2.448232 O -0.009194 3.004096 0.077763 C -0.008478 2.509031 -1.124231 O -0.011217 3.098408 -2.178993
7	#94	O 1 Cu 1.014403 1.258401 -0.846502 Cu -0.832074 -1.063976 1.351110 Cu -0.231040 1.414050 1.390736 Cu 2.723022 -0.455852 -1.071653 Cu 0.360946 -1.144252 -0.798569 Cu -1.606191 0.398076 -0.582048 Cu 1.655690 -0.233016 1.119969 Cu -1.928877 -2.018107 -0.604935 O 0.315224 -0.034137 2.465370 O -0.519455 2.266383 -0.291032 C -1.838808 3.038684 -0.981094 O -2.606717 2.175695 -1.286651
7	#95	O 1 Cu 0.353389 1.243378 -1.077321 Cu -0.421749 -1.011020 1.450758 Cu -1.127863 1.455582 0.966592 Cu 2.794513 0.620227 -0.859262 Cu 1.069070 -1.061600 -0.500103 Cu -1.358124 -0.547007 -0.870319 Cu 1.428738 0.768474 1.141224 Cu -0.569305 -2.824171 -0.150639 O -0.070102 0.657976 2.300350 O -2.562979 2.315579 -0.166128 C -3.085358 1.682319 -1.057348 O -2.914328 0.680706 -1.707085

7	#96	O 1 Cu -1.590371 -0.127050 1.256858 Cu 1.560378 0.294930 -0.544027 Cu 0.300179 1.381802 1.511489 Cu -2.708639 -0.319264 -1.023203 Cu -0.445731 -1.142041 -0.729415 Cu 0.680596 -1.031836 1.484577 Cu -0.918018 1.286663 -0.777798 Cu 1.764248 -2.112396 -0.531339 O 0.680939 2.186857 -0.216065 C 2.008594 2.921706 -1.045887 O 2.733031 2.035187 -1.345414
7	#97	O 1 Cu -1.412795 1.220102 1.051166 Cu 0.891932 -1.219379 -0.229604 Cu 0.562474 -0.000244 1.891327 Cu -1.101741 2.398342 -1.105820 Cu -1.078966 0.000248 -1.066437 Cu -1.413526 -1.219378 1.051203 Cu 0.892697 1.218671 -0.229614 Cu -1.103246 -2.397811 -1.105795 O 4.962298 1.158635 -0.337620 C 4.955621 -0.000725 -0.337737 O 4.962483 -1.160086 -0.338621
7	$\text{Cu}_8\text{-C}_1(97)$	O 1 Cu -1.218975 0.432323 1.321794 Cu 1.219010 0.432322 -1.321605 Cu -0.000322 2.124830 -0.000169 Cu -2.397225 -1.300609 0.000111 Cu 0.000105 -1.253265 0.000114 Cu 1.218987 0.432696 1.321576 Cu -1.219056 0.432120 -1.321874 Cu 2.397477 -1.300417 0.000053
8	#98	O 2 Cu 1.912525 -0.440882 -0.046350 Cu -0.740598 -0.537029 1.284475 Cu -0.730889 -0.743390 -1.146833 Cu -2.460273 0.605383 -0.167150 Cu -0.156602 1.427377 0.068367 O 0.779885 -1.601872 1.072984 O 0.774528 -1.798855 -0.788201 C 3.173686 0.825208 -0.122070 O 3.952730 1.652776 -0.166075
8	#99	O 2 Cu 1.661536 1.110663 0.529584 Cu 0.888972 -1.204636 -0.434577 Cu -0.632053 0.735856 -0.824127 Cu -1.420258 -1.641725 0.067429 Cu -0.102057 -0.183934 1.564732 O 2.146269 0.200973 -1.005546 O 0.483164 -0.114629 -2.047196



		C	-1.875063	1.978242	-0.325262
		O	-2.659147	2.721161	0.023164
<b>8</b>	<b>#100</b>	O 2			
		Cu	2.552058	1.465459	0.676355
		Cu	0.321901	0.548728	-0.618664
		Cu	-2.933873	0.116959	0.008741
		Cu	0.056791	-1.664660	0.444734
		Cu	2.308146	-0.959674	-0.279868
		O	2.129063	0.849574	-0.988272
		O	-1.232859	-0.319492	-0.067072
		C	-4.660883	0.554741	0.094635
		O	-5.756251	0.841669	0.145911
<b>8</b>	<b>#101</b>	O 1			
		Cu	-1.945672	1.337701	0.025810
		Cu	1.657921	0.367055	-1.012412
		Cu	-0.882514	-0.401107	-1.359609
		Cu	-2.878063	-0.914739	-0.003422
		Cu	-0.741119	-0.542081	1.115572
		Cu	0.540491	1.574267	0.927017
		Cu	0.700263	-1.956377	-0.270598
		Cu	1.651560	-0.490154	1.553242
		O	0.169971	1.069158	-1.842035
		O	-0.489510	2.441991	-0.364672
		C	3.471938	0.202834	-0.823308
		O	4.592688	0.053927	-0.712363
<b>8</b>	<b>#102</b>	O 1			
		Cu	-1.371974	-2.136099	-0.419692
		Cu	0.782522	0.880378	1.253310
		Cu	-1.468136	-0.165680	1.318257
		Cu	-2.614589	-0.000392	-0.803364
		Cu	-0.149225	-0.109408	-0.939539
		Cu	2.095949	-0.937550	-0.096291
		Cu	-1.104059	1.939791	0.070099
		Cu	1.438773	1.667823	-0.931474
		O	0.253316	-0.850873	1.941204
		O	0.411405	-1.747828	0.367373
		C	3.930799	-0.935192	-0.110711
		O	5.053608	-0.828286	-0.236534
<b>8</b>	<b>#103</b>	O 1			
		Cu	1.091224	2.179844	-0.284177
		Cu	-1.233194	-0.954644	0.757236
		Cu	0.995053	0.449448	1.493466
		Cu	2.654163	0.331785	-0.238031
		Cu	0.172664	0.048599	-1.077372
		Cu	-1.986944	1.351906	-0.335175
		Cu	1.018186	-1.778840	0.422989
		Cu	-0.633114	-2.213610	-1.362040
		O	0.132898	-1.109484	2.090084
		O	-0.538993	1.890554	-1.241381
		C	-3.524617	0.930196	0.500989
		O	-4.483333	0.643766	1.034306

<b>S3</b>	<b>#S1</b>	
<b>S3</b>	<b>#S2</b>	O 2 Cu 0.965857 1.948948 -0.000117 Cu 0.358554 -0.502204 0.000118 Cu -2.718720 -0.308182 0.000013 Cu 2.083528 -2.138252 0.000124 Cu 2.684539 0.214779 -0.000194 O -1.176147 0.574181 0.000217 C -4.291151 -1.172839 -0.000195 O -5.275485 -1.732082 -0.000322 C -0.891003 2.466539 0.000179 O -1.891624 3.032929 0.000322
<b>S3</b>	<b>#S3</b>	O 2 Cu 0.651333 1.916611 0.000000 Cu 0.744016 -0.700305 0.000228 Cu -3.236494 -0.093924 0.000089 Cu 2.849498 -1.790388 -0.000130 Cu 2.760151 0.646507 -0.000161 O -1.167106 -0.123178 0.000341 C -4.770760 -1.051225 -0.000196 O -5.736750 -1.640498 -0.000390 C -1.162709 1.208987 0.000206 O -2.306869 1.723289 -0.000052
<b>S3</b>	<b>#S4</b>	O 2 Cu -0.337356 -1.842655 0.835925 Cu 0.451343 -0.101345 -0.947047 Cu -1.767221 1.017538 -0.173588 Cu 2.480426 1.078334 -0.644725 Cu 1.687295 -0.452928 1.094550 O -1.510612 -0.478680 -1.248718 C -2.075146 2.503653 0.821970 O -2.247910 3.435343 1.435429 C -1.688272 -1.708349 -0.583657 O -2.533927 -2.461810 -0.963986
<b>S3</b>	<b>#S5</b>	O 2 Cu 0.089873 -1.853650 0.681069 Cu 0.971455 0.219755 -0.318252 Cu -1.333353 -0.270999 -0.566514 Cu -0.659810 2.055165 -0.108761 Cu -0.567338 0.323098 1.648646 O 3.234422 0.523784 -0.378979 C -2.921944 -0.743932 -1.349212 O -3.895346 -1.039129 -1.859376 C 4.192411 -0.046319 -0.717834 O 5.142574 -0.607931 -1.055047
<b>S3</b>	<b>#S6</b>	O 2 Cu -1.770985 -0.380673 -0.332075 Cu 1.133375 -0.453112 -1.468225 Cu 0.415807 -1.370090 0.641215 Cu 2.644690 -0.151187 0.422765 Cu 0.514725 1.026149 0.528440

		O -0.422650 -1.497333 -1.131813 C 0.126177 2.836001 0.691537 O -0.141695 3.917575 0.919539 C -2.438801 1.255752 -0.950640 O -2.834668 2.259903 -1.307559 C -2.843977 -1.340913 0.947810 O -3.382380 -1.925969 1.756868
<b>S3</b>	<b>#S7</b>	O 2 Cu 1.287694 1.088379 0.000014 Cu 0.406936 -1.041837 1.216319 Cu 0.406980 -1.041868 -1.216274 Cu -1.587800 -1.777906 -0.000005 Cu -1.129119 0.611402 -0.000025 O 1.994822 -0.833687 0.000047 C -2.874697 1.323615 -0.000078 O -3.963774 1.646407 -0.000110 C 0.086011 2.472496 -0.000044 O -0.301983 3.552693 -0.000074 C 3.126107 0.514041 0.000054 O 4.248360 0.238610 0.000080
<b>S3</b>	<b>#S8</b>	O 2 Cu 1.644655 0.465678 -0.039890 Cu 0.067901 -1.303032 0.608636 Cu -0.435721 -0.371792 -1.605287 Cu -2.262562 -1.160770 -0.075247 Cu -0.901609 0.845126 0.418207 O 1.688802 -2.715261 0.880947 C -1.564104 2.509068 0.849262 O -1.991463 3.516895 1.152584 C 2.005565 2.255799 -0.416317 O 2.091516 3.355757 -0.676652 C 2.095742 -1.595126 0.601155 O 3.149837 -1.007334 0.381775
<b>S3</b>	<b>#S9</b>	O 2 Cu 0.925671 1.294227 0.220274 Cu -0.430532 0.005962 -1.463758 Cu -1.600892 1.367182 0.195578 Cu -2.650898 -0.753396 -0.581527 Cu -0.568881 -0.667667 0.784794 O 3.387484 -2.903533 -1.382559 C -0.171038 -1.884849 2.084263 O 0.088654 -2.637547 2.898138 C 2.440335 2.411741 0.505367 O 3.329921 3.076144 0.727375 C 3.837281 -1.945529 -0.911102 O 4.294063 -0.988954 -0.440029
<b>S6</b>	<b>#S10</b>	O 2 Cu -0.513059 1.927057 0.000593 Cu 0.636120 -0.759488 -0.079069 Cu -2.410678 -1.093446 -0.011462 Cu 2.827877 -1.729409 -0.047717

		Cu 2.578833 0.636810 0.101773 O -1.052096 0.018655 -0.118031 C -3.800906 -2.207826 0.091538 O -4.679314 -2.920810 0.158615 C -1.844961 3.173675 -0.052975 O -2.675426 3.947224 -0.086251 O 1.334527 1.922520 0.146818
<b>S6</b>	<b>#S11</b>	O 2 Cu 0.758434 2.023627 0.176841 Cu 0.282508 -0.629203 -0.195545 Cu -2.833223 -0.330038 0.043165 Cu 2.024261 -2.273855 -0.159702 Cu 2.609250 0.009830 0.110948 O -1.250320 0.428576 -0.236630 C -4.446393 -1.064926 0.324925 O -5.458552 -1.539156 0.501140 C -0.985002 2.333150 -0.454987 O -1.951318 2.823745 -0.834322 O 2.434279 1.684357 0.755422
<b>S6</b>	<b>#S12</b>	O 2 Cu -0.578586 1.882117 -0.000046 Cu -0.596146 -0.858448 0.000015 Cu 3.338542 -0.059436 -0.000019 Cu -2.696427 -1.994065 0.000099 Cu -2.690452 0.380549 -0.000338 O 1.263924 -0.175854 0.000131 C 4.903468 -0.965720 0.000077 O 5.887815 -1.523447 0.000136 C 1.206706 1.156896 -0.000096 O 2.336135 1.706596 -0.000303 O -2.386881 2.202978 0.001099
<b>S6</b>	<b>#S13</b>	O 2 Cu -0.346993 -1.886881 0.604663 Cu 0.474583 0.182269 -1.021990 Cu -1.987121 0.919967 -0.174995 Cu 2.534607 1.316319 -0.606131 Cu 1.766271 -0.303080 0.964984 O -1.419980 -0.314479 -1.441777 C -2.579956 2.158558 1.016352 O -2.931412 2.925972 1.763223 C -1.483548 -1.639021 -0.936288 O -2.158138 -2.435439 -1.523797 O 0.707273 -1.394358 1.988630
<b>S6</b>	<b>#S14</b>	O 2 Cu 0.074288 1.389783 -0.000132 Cu -2.249193 0.193346 0.000111 Cu 3.044420 -0.203506 -0.000062 Cu -2.356173 -2.192911 0.000090 Cu -0.229330 -1.163124 -0.000164 O -2.570035 2.136791 0.000176 C 4.825542 -0.362077 0.000218

O	5.953119	-0.459687	0.000416
C	-1.426173	2.669148	0.000076
O	-0.999411	3.800957	0.000073
O	1.287254	-0.043870	-0.000316