

The geometries of the clusters with the adsorbates used for calculating the core electron binding energies are given on the following pages in .xyz file format. The file names given are not part of the files themselves; the first line denotes the number of atoms in the “molecule” (= cluster + adsorbate in this context), the second line is an arbitrary comment, and the following lines contain the element symbol followed by the x, y, and z coordinates in Angstroms.

## CO\_on\_Cu\_pos1.xyz

91

Atoms

Cu	-2.544967634	-4.420202696	-2.092520700
Cu	-3.818387734	-5.154734196	-0.033176709
Cu	-0.000042434	-4.419561296	-2.093244300
Cu	-1.272494134	-5.155437896	-0.036419736
Cu	-5.088939569	-0.011387077	-2.094876800
Cu	-5.088893369	-2.953558200	-0.035997863
Cu	-6.358789069	-0.748967430	-0.037288865
Cu	-5.088837069	1.455487500	-0.037299869
Cu	2.544801134	-4.420366896	-2.093164500
Cu	1.272420934	-5.155656296	-0.036564380
Cu	5.088659585	-4.419456296	-2.093393600
Cu	3.818167434	-5.154875196	-0.033608018
Cu	-0.000056198	-2.924066000	-6.186217600
Cu	-2.544251500	1.482645300	-6.186926300
Cu	-2.545184800	-1.456645300	-4.130715600
Cu	-1.272121600	-0.720978490	-6.185779300
Cu	-1.272432400	-3.659078100	-4.130829800
Cu	-3.815270500	0.746499940	-4.132001800
Cu	-3.815696000	-2.216670800	-2.090890700
Cu	2.544052000	1.482795300	-6.186295400
Cu	2.545048300	-1.456413400	-4.130225000
Cu	3.815922600	-0.720994140	-6.186433500
Cu	1.272052500	-0.720814190	-6.185350400
Cu	2.544259300	-2.924167700	-6.186847800
Cu	3.816307800	-3.660069500	-4.131191000
Cu	1.272270600	-3.659034300	-4.130555300
Cu	-0.000123835	2.950693500	-4.131303200
Cu	1.271641300	3.686905800	-6.186074300
Cu	-1.271813200	3.686710000	-6.186456100
Cu	-0.000005185	1.483522100	-6.186608300
Cu	0.000018490	-0.011637597	-2.089379200
Cu	1.271141900	0.746897940	-4.128909900
Cu	-1.271522900	0.746741140	-4.129273600
Cu	-0.000128405	-1.455984700	-4.129009300
Cu	0.000237678	-2.953147600	-0.035996314
Cu	1.272203600	-2.215956900	-2.091063400
Cu	-1.272382000	-2.216250900	-2.091161300
Cu	-2.543967600	4.393639100	-2.093164500
Cu	-2.544665700	2.950358000	-4.132583100
Cu	-2.543471400	1.458133800	-0.036558444
Cu	-1.272448100	2.192089100	-2.092975600
Cu	-3.816294900	2.191110700	-2.093538200
Cu	-2.545739500	-0.012827658	-2.090107000
Cu	-1.272924600	-0.748787210	-0.038399287
Cu	-3.819359100	-0.749144870	-0.038018136
Cu	-2.543892800	-2.954890300	-0.035544046
Cu	-3.816347800	3.658349700	-0.036564380

Cu	5.088666000	2.950065500	-4.131733900
Cu	3.816695700	3.686431900	-6.187846300
Cu	5.088639800	1.482938000	-6.187687900
Cu	5.088597900	-0.011387077	-2.094876800
Cu	3.815326000	0.746812640	-4.131865900
Cu	5.088706300	-1.457467500	-4.129957200
Cu	5.088644100	-2.953558200	-0.035997863
Cu	3.815551500	-2.216576400	-2.090505500
Cu	2.543801100	4.393803300	-2.092520700
Cu	2.544575000	2.950607600	-4.132159500
Cu	2.543089400	1.457860600	-0.035718549
Cu	3.816124000	2.191095000	-2.092995300
Cu	1.272314000	2.192301900	-2.092778600
Cu	2.545605200	-0.012556271	-2.089983400
Cu	3.818748400	-0.748967430	-0.037288865
Cu	1.273166100	-0.748680460	-0.036928042
Cu	2.543484900	-2.954147800	-0.034778924
Cu	-0.000109149	4.394549700	-2.093393600
Cu	1.270381000	3.659271800	-0.033176709
Cu	-1.270601300	3.659130800	-0.033608018
Cu	0.000181029	1.456430000	-0.037166062
Cu	5.088726300	4.394444700	-2.093244300
Cu	3.816274600	3.658568100	-0.036419736
Cu	5.088700400	1.455487500	-0.037299869
C	-0.003336171	-0.725139150	3.079423600
O	1.169404000	-0.721925790	3.091052200
O	-1.176464800	-0.728109490	3.076017100
Cu	-1.272460934	5.153936496	-4.131191000
Cu	-0.000124634	5.860447796	-0.035997863
Cu	-1.273217234	6.597429596	-2.090505500
Cu	-2.545283834	5.859858196	-0.034778924
Cu	6.362266969	0.746499940	-4.132001800
Cu	6.361841469	-2.216670800	-2.090890700
Cu	7.634066069	1.458133800	-0.036558444
Cu	6.361242569	2.191110700	-2.093538200
Cu	7.631797969	-0.012827658	-2.090107000
Cu	6.358178369	-0.749144870	-0.038018136
Cu	6.361189669	3.658349700	-0.036564380
Cu	3.816336334	5.154927896	-4.130829800
Cu	1.272292734	5.153773396	-4.131473600
Cu	1.273072734	6.597335196	-2.090890700
Cu	5.089006412	5.860858396	-0.035996314
Cu	3.816386734	6.597755096	-2.091161300
Cu	2.544875934	5.859115696	-0.035544046

## CO\_on\_Cu\_pos2.xyz

91

Atoms

Cu	1.274089266	-3.660440496	-4.131733900
Cu	0.002118966	-2.924074096	-6.187846300
Cu	-1.270775634	-2.216702696	-2.092520700
Cu	-1.270001734	-3.659898396	-4.132159500
Cu	-1.271487334	-5.152645396	-0.035718549
Cu	0.001547266	-4.419410996	-2.092995300
Cu	-2.542262734	-4.418204096	-2.092778600
Cu	-3.814685834	-2.215956296	-2.093393600
Cu	-2.544195734	-2.951234196	-0.033176709
Cu	-5.085178034	-2.951375196	-0.033608018
Cu	-3.814395734	-5.154075996	-0.037166062
Cu	1.274149566	-2.216061296	-2.093244300
Cu	0.001697866	-2.951937896	-0.036419736
Cu	1.274123666	-5.155018496	-0.037299869
Cu	-3.814747569	2.192112900	-2.094876800
Cu	-3.814639169	0.746032500	-4.129957200
Cu	-3.814701369	-0.750058200	-0.035997863
Cu	-5.087793969	-0.013076400	-2.090505500
Cu	-5.084597069	1.454532600	-0.037288865
Cu	-6.359860569	-0.750647800	-0.034778924
Cu	-3.814645069	3.658987500	-0.037299869
Cu	2.546098534	-2.924269296	-6.188094600
Cu	3.818993134	-2.216866896	-2.093164500
Cu	3.818295034	-3.660147996	-4.132583100
Cu	3.819489334	-5.152372196	-0.036558444
Cu	5.090512634	-4.418416896	-2.092975600
Cu	2.546665834	-4.419395296	-2.093538200
Cu	2.546612934	-2.952156296	-0.036564380
Cu	6.362851634	-2.215956296	-2.093393600
Cu	5.092359434	-2.951375196	-0.033608018
Cu	1.274135800	-0.720566000	-6.186217600
Cu	-1.270059500	3.686145300	-6.186926300
Cu	-1.270992800	0.746854700	-4.130715600
Cu	0.002070400	1.482521500	-6.185779300
Cu	-2.542013500	1.482366000	-6.186962700
Cu	-1.270240600	-0.721023700	-6.187424600
Cu	0.001759600	-1.455578100	-4.130829800
Cu	-2.542284000	-1.456732600	-4.131473600
Cu	-2.541078500	2.949999900	-4.132001800
Cu	-2.541504000	-0.013170800	-2.090890700
Cu	3.818244000	3.686295300	-6.186295400
Cu	3.819240300	0.747086600	-4.130225000
Cu	5.090114600	1.482505900	-6.186433500
Cu	2.546244500	1.482685800	-6.185350400
Cu	3.818451300	-0.720667700	-6.186847800
Cu	5.090499800	-1.456569500	-4.131191000
Cu	2.546462600	-1.455534300	-4.130555300

Cu	1.274068200	5.154193500	-4.131303200
Cu	1.274186800	3.687022100	-6.186608300
Cu	1.274210500	2.191862400	-2.089379200
Cu	2.545333900	2.950397900	-4.128909900
Cu	0.002669100	2.950241100	-4.129273600
Cu	1.274063600	0.747515300	-4.129009300
Cu	1.274429700	-0.749647600	-0.035996314
Cu	2.546395600	-0.012456900	-2.091063400
Cu	0.001810000	-0.012750900	-2.091161300
Cu	-1.269775600	6.597139100	-2.093164500
Cu	-1.270473700	5.153858000	-4.132583100
Cu	-1.269279400	3.661633800	-0.036558444
Cu	0.001743900	4.395589100	-2.092975600
Cu	-2.542102900	4.394610700	-2.093538200
Cu	-1.271547500	2.190672300	-2.090107000
Cu	0.001267400	1.454712800	-0.038399287
Cu	-2.545167100	1.454355100	-0.038018136
Cu	-1.269700800	-0.751390300	-0.035544046
Cu	-2.542155800	5.861849700	-0.036564380
Cu	6.362789900	2.192112900	-2.094876800
Cu	5.089518000	2.950312600	-4.131865900
Cu	6.362898300	0.746032500	-4.129957200
Cu	6.362836100	-0.750058200	-0.035997863
Cu	5.089743500	-0.013076400	-2.090505500
Cu	3.817993100	6.597303300	-2.092520700
Cu	3.818767000	5.154107600	-4.132159500
Cu	3.817281400	3.661360600	-0.035718549
Cu	5.090316000	4.394595000	-2.092995300
Cu	2.546506000	4.395801900	-2.092778600
Cu	3.819797200	2.190943700	-2.089983400
Cu	5.092940400	1.454532600	-0.037288865
Cu	2.547358100	1.454819500	-0.036928042
Cu	3.817676900	-0.750647800	-0.034778924
Cu	1.274082900	6.598049700	-2.093393600
Cu	2.544573000	5.862771800	-0.033176709
Cu	0.003590700	5.862630800	-0.033608018
Cu	1.274373000	3.659930000	-0.037166062
Cu	5.090466600	5.862068100	-0.036419736
Cu	6.362892400	3.658987500	-0.037299869
C	1.270855800	1.478360900	3.079423600
O	2.443596000	1.481574200	3.091052200
O	0.097727200	1.475390500	3.076017100
Cu	7.636033469	-0.013170800	-2.090890700
Cu	7.632370369	1.454355100	-0.038018136

## CO\_on\_Cu\_pos1.xyz

90

Atoms

Cu	-5.088768469	0.002217893	-2.069854068
Cu	-5.088768469	-2.932066787	0.003917049
Cu	-6.363951087	-0.731657725	0.026342104
Cu	-5.088768469	1.473581672	0.031416005
Cu	-2.541446745	-4.402000603	-2.084258761
Cu	-3.818760304	-5.134180428	0.028151722
Cu	2.541446745	-4.402000603	-2.084258761
Cu	0.000000000	-4.419335717	-2.088898946
Cu	1.284521937	-5.141387633	0.038112461
Cu	-1.284521937	-5.141387633	0.038112461
Cu	5.088769000	-4.400042926	-2.090528480
Cu	3.818760304	-5.134180428	0.028151722
Cu	0.000000000	-2.949130104	-6.268580725
Cu	-2.553811918	1.469005719	-6.272164391
Cu	-2.541238878	-1.474222398	-4.149060958
Cu	-1.273819498	-0.740698280	-6.274401378
Cu	-1.282964793	-3.671075865	-4.156269962
Cu	-3.815071059	0.726852564	-4.140865955
Cu	-3.815266442	-2.198802880	-2.080382089
Cu	2.553811918	1.469005719	-6.272164391
Cu	2.541238878	-1.474222398	-4.149060958
Cu	3.817366788	-0.741558694	-6.263756387
Cu	1.273819498	-0.740698280	-6.274401378
Cu	2.548683123	-2.944070523	-6.286853345
Cu	3.819783676	-3.678613726	-4.158888428
Cu	1.282964793	-3.671075865	-4.156269962
Cu	0.000000000	2.935438130	-4.162947836
Cu	1.274213729	3.669677473	-6.276427430
Cu	-1.274213729	3.669677473	-6.276427430
Cu	0.000000000	1.465022417	-6.275445200
Cu	0.000000000	0.001633676	-2.139374884
Cu	1.282921986	0.734647356	-4.177603567
Cu	-1.282921986	0.734647356	-4.177603567
Cu	0.000000000	-1.477596256	-4.176280077
Cu	0.000000000	-2.971702346	0.014630765
Cu	1.266117352	-2.190246319	-2.065777051
Cu	-1.266117352	-2.190246319	-2.065777051
Cu	-2.541446745	4.412005393	-2.084258761
Cu	-2.547476859	2.935796537	-4.151979425
Cu	-2.563291966	1.486948352	0.022195893
Cu	-1.266182032	2.191119497	-2.082641257
Cu	-3.818012513	2.209877998	-2.079741135
Cu	-2.529180515	0.003253259	-2.061557293
Cu	-1.275880936	-0.745672202	0.094974154
Cu	-3.813586382	-0.731657725	0.026342104
Cu	-2.542983066	-2.933269422	0.034875697
Cu	-3.818760304	3.679825568	0.028151722

Cu	5.088769000	2.934158222	-4.157197710
Cu	3.815354947	3.668367345	-6.284972070
Cu	5.088769000	1.467956862	-6.263081721
Cu	5.088769000	0.002217893	-2.069854068
Cu	3.815071059	0.726852564	-4.140865955
Cu	5.088769000	-1.477308784	-4.148144298
Cu	5.088769000	-2.932066787	0.003917049
Cu	3.815266442	-2.198802880	-2.080382089
Cu	2.541446745	4.412005393	-2.084258761
Cu	2.547476859	2.935796537	-4.151979425
Cu	2.563291966	1.486948352	0.022195893
Cu	3.818012513	2.209877998	-2.079741135
Cu	1.266182032	2.191119497	-2.082641257
Cu	2.529180515	0.003253259	-2.061557293
Cu	3.813586382	-0.731657725	0.026342104
Cu	1.275880936	-0.745672202	0.094974154
Cu	2.542983066	-2.933269422	0.034875697
Cu	0.000000000	4.394670279	-2.088898946
Cu	1.284521937	3.672618363	0.038112461
Cu	-1.284521937	3.672618363	0.038112461
Cu	0.000000000	1.488243806	0.077264072
Cu	5.088769000	4.413963070	-2.090528480
Cu	3.818760304	3.679825568	0.028151722
Cu	5.088769000	1.473581672	0.031416005
C	0.000000000	0.036994544	1.484629476
O	0.000000000	0.017824695	2.663295458
Cu	-1.282964793	5.142930131	-4.156269962
Cu	3.819783676	5.135392270	-4.158888428
Cu	1.282964793	5.142930131	-4.156269962
Cu	0.000000000	5.842303650	0.014630765
Cu	1.266117352	6.623759677	-2.065777051
Cu	-1.266117352	6.623759677	-2.065777051
Cu	-2.542983066	5.880736574	0.034875697
Cu	5.088769000	5.881939209	0.003917049
Cu	3.815266442	6.615203116	-2.080382089
Cu	2.542983066	5.880736574	0.034875697
Cu	6.362466410	0.726852564	-4.140865955
Cu	6.362271027	-2.198802880	-2.080382089
Cu	7.614245503	1.486948352	0.022195893
Cu	6.359524956	2.209877998	-2.079741135
Cu	7.648356954	0.003253259	-2.061557293
Cu	6.363951087	-0.731657725	0.026342104
Cu	6.358777165	3.679825568	0.028151722

## CO\_on\_Cu\_pos2.xyz

90

Atoms

Cu	-3.816576469	-2.196541926	-2.090528480
Cu	-5.086585165	-2.930679428	0.028151722
Cu	-3.816576469	-5.136923324	0.031416005
Cu	-3.816576469	2.205718893	-2.069854068
Cu	-3.816576469	0.726192216	-4.148144298
Cu	-3.816576469	-0.728565787	0.003917049
Cu	-5.090079027	0.004698120	-2.080382089
Cu	-5.091759087	1.471843275	0.026342104
Cu	-6.362362403	-0.729768422	0.034875697
Cu	-3.816576469	3.677082672	0.031416005
Cu	1.272192000	-3.675066866	-4.162947836
Cu	2.546405729	-2.940827523	-6.276427430
Cu	-0.002021729	-2.940827523	-6.276427430
Cu	-1.269254745	-2.198499603	-2.084258761
Cu	-1.275284859	-3.674708459	-4.151979425
Cu	-1.291099966	-5.123556644	0.022195893
Cu	0.006009968	-4.419385499	-2.082641257
Cu	-2.545820513	-4.400626998	-2.079741135
Cu	-2.546568304	-2.930679428	0.028151722
Cu	3.813638745	-2.198499603	-2.084258761
Cu	3.819668859	-3.674708459	-4.151979425
Cu	3.835483966	-5.123556644	0.022195893
Cu	5.090204513	-4.400626998	-2.079741135
Cu	2.538374032	-4.419385499	-2.082641257
Cu	1.272192000	-2.215834717	-2.088898946
Cu	2.556713937	-2.937886633	0.038112461
Cu	-0.012329937	-2.937886633	0.038112461
Cu	1.272192000	-5.122261190	0.077264072
Cu	6.360961000	-2.196541926	-2.090528480
Cu	5.090952304	-2.930679428	0.028151722
Cu	1.272192000	-0.745629104	-6.268580725
Cu	-1.281619918	3.672506719	-6.272164391
Cu	-1.269046878	0.729278602	-4.149060958
Cu	-0.001627498	1.462802720	-6.274401378
Cu	-2.545174788	1.461942306	-6.263756387
Cu	-1.276491123	-0.740569523	-6.286853345
Cu	-0.010772793	-1.467574865	-4.156269962
Cu	-2.547591676	-1.475112726	-4.158888428
Cu	-2.542879059	2.930353564	-4.140865955
Cu	-2.543074442	0.004698120	-2.080382089
Cu	3.826003918	3.672506719	-6.272164391
Cu	3.813430878	0.729278602	-4.149060958
Cu	5.089558788	1.461942306	-6.263756387
Cu	2.546011498	1.462802720	-6.274401378
Cu	3.820875123	-0.740569523	-6.286853345
Cu	5.091975676	-1.475112726	-4.158888428
Cu	2.555156793	-1.467574865	-4.156269962



Cu	1.272192000	5.138939130	-4.162947836
Cu	1.272192000	3.668523417	-6.275445200
Cu	1.272192000	2.205134676	-2.139374884
Cu	2.555113986	2.938148356	-4.177603567
Cu	-0.010729986	2.938148356	-4.177603567
Cu	1.272192000	0.725904744	-4.176280077
Cu	1.272192000	-0.768201346	0.014630765
Cu	2.538309352	0.013254681	-2.065777051
Cu	0.006074648	0.013254681	-2.065777051
Cu	-1.269254745	6.615506393	-2.084258761
Cu	-1.275284859	5.139297537	-4.151979425
Cu	-1.291099966	3.690449352	0.022195893
Cu	0.006009968	4.394620497	-2.082641257
Cu	-2.545820513	4.413378998	-2.079741135
Cu	-1.256988515	2.206754259	-2.061557293
Cu	-0.003688936	1.457828798	0.094974154
Cu	-2.541394382	1.471843275	0.026342104
Cu	-1.270791066	-0.729768422	0.034875697
Cu	-2.546568304	5.883326568	0.028151722
Cu	6.360961000	2.205718893	-2.069854068
Cu	5.087263059	2.930353564	-4.140865955
Cu	6.360961000	0.726192216	-4.148144298
Cu	6.360961000	-0.728565787	0.003917049
Cu	5.087458442	0.004698120	-2.080382089
Cu	3.813638745	6.615506393	-2.084258761
Cu	3.819668859	5.139297537	-4.151979425
Cu	3.835483966	3.690449352	0.022195893
Cu	5.090204513	4.413378998	-2.079741135
Cu	2.538374032	4.394620497	-2.082641257
Cu	3.801372515	2.206754259	-2.061557293
Cu	5.085778382	1.471843275	0.026342104
Cu	2.548072936	1.457828798	0.094974154
Cu	3.815175066	-0.729768422	0.034875697
Cu	1.272192000	6.598171279	-2.08898946
Cu	2.556713937	5.876119363	0.038112461
Cu	-0.012329937	5.876119363	0.038112461
Cu	1.272192000	3.691744806	0.077264072
Cu	5.090952304	5.883326568	0.028151722
Cu	6.360961000	3.677082672	0.031416005
C	1.272192000	2.240495544	1.484629476
O	1.272192000	2.221325695	2.663295458
Cu	7.634463027	0.004698120	-2.080382089
Cu	7.636143087	1.471843275	0.026342104

## CO\_on\_Cu\_top\_pos.xyz

90

Atoms

Cu	-5.084483159	-0.003536166	-2.103755725
Cu	-5.081224156	-2.943025226	-0.041360513
Cu	-6.331310791	-0.737847117	-0.051704229
Cu	-5.082300635	1.468921528	-0.040405588
Cu	-2.543867882	-4.412420577	-2.095385949
Cu	-3.816575879	-5.144660052	-0.043240001
Cu	2.544015698	-4.418866824	-2.102400810
Cu	0.000367056	-4.418868723	-2.102399110
Cu	1.272190354	-5.139855037	-0.044951761
Cu	-1.283023538	-5.144049508	-0.035709792
Cu	5.088251236	-4.412419935	-2.095385193
Cu	3.827405920	-5.144049491	-0.035710543
Cu	-0.000719597	-2.940336988	-6.197915002
Cu	-2.544640443	1.468246621	-6.191488710
Cu	-2.545254605	-1.460185026	-4.130196163
Cu	-1.277390060	-0.734146579	-6.195495860
Cu	-1.272189098	-3.662919210	-4.135331277
Cu	-3.816579737	0.748674192	-4.138958920
Cu	-3.816580068	-2.212284627	-2.092067316
Cu	2.545149151	1.474235467	-6.200493764
Cu	2.547358888	-1.460498019	-4.143768435
Cu	3.821773454	-0.734144280	-6.195497220
Cu	1.272188470	-0.733890811	-6.190091260
Cu	2.545101369	-2.940335734	-6.197916157
Cu	3.816571672	-3.662919142	-4.135333055
Cu	1.272190603	-3.655951223	-4.134871447
Cu	-0.000099747	2.943691813	-4.134841384
Cu	1.272192467	3.674079874	-6.191457308
Cu	-1.269806257	3.673362705	-6.187744129
Cu	-0.000767820	1.474235439	-6.200495248
Cu	0.006738176	-0.015559225	-2.079532636
Cu	1.272193963	0.743933182	-4.143074109
Cu	-1.262524489	0.739230832	-4.134979682
Cu	-0.002976666	-1.460496545	-4.143767210
Cu	-0.019721083	-2.966249985	-0.051584695
Cu	1.272193012	-2.200228316	-2.081376213
Cu	-1.266289198	-2.207269466	-2.095999255
Cu	-2.543867882	4.401585419	-2.095385949
Cu	-2.544735294	2.946130008	-4.135815520
Cu	-2.550850331	1.468921204	-0.040403011
Cu	-1.277625131	2.193901748	-2.101545105
Cu	-3.816575212	2.199102483	-2.095286265
Cu	-2.548668939	-0.003535881	-2.103757197
Cu	-1.301838441	-0.737846824	-0.051701969
Cu	-3.816567560	-0.735562798	-0.035174086
Cu	-2.551927403	-2.943024773	-0.041364601
Cu	-3.816575879	3.669345944	-0.043240001

Cu	5.089118422	2.946129847	-4.135817361
Cu	3.814189291	3.673362406	-6.187744895
Cu	5.089024368	1.468246860	-6.191489688
Cu	5.093054310	-0.003536166	-2.103755725
Cu	3.806906844	0.739230943	-4.134979397
Cu	5.089636910	-1.460183824	-4.130198752
Cu	5.096313313	-2.943025226	-0.041360513
Cu	3.810671210	-2.207268431	-2.096000559
Cu	2.544015698	4.395139172	-2.102400810
Cu	2.544482890	2.943692930	-4.134839724
Cu	2.561402914	1.495443514	-0.052506729
Cu	3.822007649	2.193902917	-2.101546773
Cu	1.272191099	2.183157975	-2.098206209
Cu	2.537643637	-0.015559919	-2.079535438
Cu	3.846226678	-0.737847117	-0.051704229
Cu	1.272192000	-0.734500000	0.011352187
Cu	2.564109579	-2.966249782	-0.051584641
Cu	0.000367056	4.395137273	-2.102399110
Cu	1.272190354	3.674150959	-0.044951761
Cu	-1.283023538	3.669956488	-0.035709792
Cu	-0.017012938	1.495444311	-0.052503112
Cu	5.088251236	4.401586061	-2.095385193
Cu	3.827405920	3.669956505	-0.035710543
Cu	5.095236834	1.468921528	-0.040405588
C	1.272192000	-0.734500000	1.846487463
O	1.272192000	-0.734500000	3.000741735
Cu	-1.272189098	5.151086786	-4.135331277
Cu	3.816571672	5.151086854	-4.135333055
Cu	1.272190603	5.158054773	-4.134871447
Cu	-0.019721083	5.847756011	-0.051584695
Cu	1.272193012	6.613777680	-2.081376213
Cu	-1.266289198	6.606736530	-2.095999255
Cu	-2.551927403	5.870981223	-0.041364601
Cu	5.096313313	5.870980770	-0.041360513
Cu	3.810671210	6.606737565	-2.096000559
Cu	2.564109579	5.847756214	-0.051584641
Cu	6.360957732	0.748674192	-4.138958920
Cu	6.360957401	-2.212284627	-2.092067316
Cu	7.626687138	1.468921204	-0.040403011
Cu	6.360962257	2.199102483	-2.095286265
Cu	7.628868530	-0.003535881	-2.103757197
Cu	6.360969909	-0.735562798	-0.035174086
Cu	6.360961590	3.669345944	-0.043240001

## Ethene\_on\_Cu.xyz

94

Atoms

H	0.932171426	2.718373826	2.368643939
H	-0.932171426	2.718373826	2.368643939
H	0.932273354	0.217323902	2.367179621
H	-0.932273354	0.217323902	2.367179621
C	0.000000000	2.157745046	2.239792571
C	0.000000000	0.778072516	2.238905720
Cu	0.000000000	1.465492234	0.139122933
Cu	-5.088768469	1.468497375	-0.032872568
Cu	5.088769000	1.468497375	-0.032872568
Cu	-2.549503221	-2.941531310	-0.039343737
Cu	2.549503221	-2.941531310	-0.039343737
Cu	-2.549503221	5.872474686	-0.039343737
Cu	2.549503221	5.872474686	-0.039343737
Cu	-6.356703573	-0.738804222	-0.039671597
Cu	-3.820833896	-0.738804222	-0.039671597
Cu	3.820833896	-0.738804222	-0.039671597
Cu	6.356703573	-0.738804222	-0.039671597
Cu	-5.088768469	-2.941784893	-0.039793734
Cu	5.088769000	-2.941784893	-0.039793734
Cu	5.088769000	5.872221103	-0.039793734
Cu	-3.818331118	-5.143871176	-0.040988095
Cu	3.818331118	-5.143871176	-0.040988095
Cu	-3.818331118	3.670134820	-0.040988095
Cu	3.818331118	3.670134820	-0.040988095
Cu	6.359206351	3.670134820	-0.040988095
Cu	0.000000000	-2.935674172	-0.056166809
Cu	0.000000000	5.878331824	-0.056166809
Cu	-2.578736575	1.461950616	-0.067283609
Cu	2.578736575	1.461950616	-0.067283609
Cu	7.598800894	1.461950616	-0.067283609
Cu	-1.292199668	-0.755358235	-0.071544186
Cu	1.292199668	-0.755358235	-0.071544186
Cu	1.282732200	-5.119915627	-0.073885327
Cu	-1.282732200	-5.119915627	-0.073885327
Cu	1.282732200	3.694090369	-0.073885327
Cu	-1.282732200	3.694090369	-0.073885327
Cu	0.000000000	0.012233935	-2.064651070
Cu	-1.255976980	2.181842376	-2.065144120
Cu	1.255976980	2.181842376	-2.065144120
Cu	-5.088768469	-0.006371146	-2.096981482
Cu	5.088769000	-0.006371146	-2.096981482
Cu	5.088769000	-4.408156449	-2.098586059
Cu	5.088769000	4.405849547	-2.098586059
Cu	-3.818375451	-2.209139523	-2.098916429
Cu	3.818375451	-2.209139523	-2.098916429
Cu	3.818375451	6.604866473	-2.098916429
Cu	6.359162018	-2.209139523	-2.098916429

Cu	-2.544977641	-0.007611137	-2.106466714
Cu	2.544977641	-0.007611137	-2.106466714
Cu	7.632559828	-0.007611137	-2.106466714
Cu	-3.820829502	2.201540936	-2.107299921
Cu	3.820829502	2.201540936	-2.107299921
Cu	6.356707967	2.201540936	-2.107299921
Cu	-2.549566829	-4.416897200	-2.107708286
Cu	2.549566829	-4.416897200	-2.107708286
Cu	-2.549566829	4.397108796	-2.107708286
Cu	2.549566829	4.397108796	-2.107708286
Cu	1.274227847	-2.216460422	-2.109323434
Cu	-1.274227847	-2.216460422	-2.109323434
Cu	1.274227847	6.597545574	-2.109323434
Cu	-1.274227847	6.597545574	-2.109323434
Cu	0.000000000	-4.421393683	-2.114878112
Cu	0.000000000	4.392612313	-2.114878112
Cu	0.000000000	-1.448548384	-4.127516692
Cu	-2.532763198	2.940085888	-4.129781879
Cu	2.532763198	2.940085888	-4.129781879
Cu	-3.816204053	0.743536084	-4.133466668
Cu	3.816204053	0.743536084	-4.133466668
Cu	6.361333416	0.743536084	-4.133466668
Cu	1.270600147	0.743529934	-4.133915502
Cu	-1.270600147	0.743529934	-4.133915502
Cu	5.088769000	-1.458959812	-4.136071392
Cu	0.000000000	2.941689171	-4.137125113
Cu	3.816373854	-3.663501926	-4.137319326
Cu	3.816373854	5.150504070	-4.137319326
Cu	5.088769000	2.953803212	-4.137646564
Cu	-2.544558651	-1.460528703	-4.138293806
Cu	2.544558651	-1.460528703	-4.138293806
Cu	-1.272891338	-3.665836466	-4.141727126
Cu	1.272891338	-3.665836466	-4.141727126
Cu	-1.272891338	5.148169530	-4.141727126
Cu	1.272891338	5.148169530	-4.141727126
Cu	5.088769000	1.471599267	-6.184029688
Cu	3.814970021	3.672577417	-6.189345307
Cu	0.000000000	1.469666765	-6.191736651
Cu	3.817197061	-0.731117496	-6.192689942
Cu	-2.545483757	1.469350362	-6.192911068
Cu	2.545483757	1.469350362	-6.192911068
Cu	0.000000000	-2.932552318	-6.193016291
Cu	2.541950166	-2.935753927	-6.193670438
Cu	-1.271182760	-0.734066038	-6.195810059
Cu	1.271182760	-0.734066038	-6.195810059
Cu	1.270609134	3.677052443	-6.198798358
Cu	-1.270609134	3.677052443	-6.198798358

# H2O\_layer\_on\_Cu.xyz

106

Atoms

O3	-0.21309684	-2.9080808	2.9582285
O3	1.3702311	3.7619994	2.9066158
H	0.77494179	4.5914178	2.9063808
O3	5.3932614	1.5389801	2.8704632
H	0.31324803	-2.0901607	2.7190321
H	4.5263366	0.17765818	2.5493874
H	0.57044062	2.5339815	2.5170967
H	4.8739872	2.3035264	2.5149796
H	-0.87276509	1.7514874	2.5108639
H	4.5205991	-1.4335534	2.4994446
H	2.2496744	-0.66149836	2.4231233
H	0.85437544	0.18706282	2.3933623
O3	3.9684818	-0.64339094	2.3029024
H	-0.91847428	-2.9514921	2.2642285
O	0.067247715	1.6563463	2.2387234
H	6.146552	1.500709	2.2190795
H	2.0544457	3.943784	2.2117518
O	1.2729137	-0.70967671	2.1935918
Cu	-0.008102171	1.4961207	0.024227366
Cu	-6.332219	-0.73650622	0.021716688
Cu	3.8453185	-0.73650622	0.021716688
Cu	1.2674004	-0.77013725	0.021340658
Cu	1.2732562	-5.1521207	-0.007057577
Cu	-3.8155125	3.6618853	-0.007057577
Cu	6.362025	3.6618853	-0.007057577
Cu	-2.5509841	-2.9466371	-0.012553735
Cu	2.5377846	5.8673689	-0.012553735
Cu	3.820988	3.670119	-0.015295562
Cu	-1.2677807	-5.143887	-0.015295562
Cu	-5.070914	-2.9636327	-0.033447027
Cu	0.017854766	5.8503733	-0.033447027
Cu	5.1066235	-2.9636327	-0.033447027
Cu	-2.5670745	1.4626615	-0.042834878
Cu	7.610463	1.4626615	-0.042834878
Cu	-3.8005442	-0.73955976	-0.042970929
Cu	6.3769933	-0.73955976	-0.042970929
Cu	-1.3083429	-0.75561156	-0.051373324
Cu	-1.3000673	3.6868603	-0.053558403
Cu	3.7887014	-5.1271457	-0.053558403
Cu	-2.5231197	5.8352368	-0.060821865
Cu	2.565649	-2.9787692	-0.060821865
Cu	2.5663357	1.5031683	-0.089355359
Cu	-0.019054143	-2.9643205	-0.092330587
Cu	5.0697146	5.8496855	-0.092330587
Cu	5.0941726	1.4893015	-0.10275543
Cu	-5.0833649	1.4893015	-0.10275543
Cu	1.2786505	3.6887886	-0.10995456

Cu	-3.8101182	-5.1252174	-0.10995456
Cu	0.006097735	-0.007367742	-2.0382649
Cu	2.5482564	-0.026550144	-2.046403
Cu	-1.2639554	6.6125595	-2.0745294
Cu	3.8248133	-2.2014465	-2.0745294
Cu	-1.2636089	2.1885005	-2.0762711
Cu	1.2785429	-2.2035972	-2.0794983
Cu	-5.0920913	-0.011106636	-2.0891758
Cu	5.0854462	-0.011106636	-2.0891758
Cu	-3.8173508	-2.2122449	-2.0916883
Cu	6.3601867	-2.2122449	-2.0916883
Cu	1.2714179	6.6017611	-2.0916883
Cu	5.0924068	4.396036	-2.0937158
Cu	0.003638066	-4.41797	-2.0937158
Cu	1.2577229	2.1800499	-2.0980626
Cu	-2.5527554	4.4041106	-2.1025998
Cu	2.5360133	-4.4098954	-2.1025998
Cu	3.8067129	6.6034891	-2.1061827
Cu	-1.2820558	-2.2105169	-2.1061827
Cu	-2.5482838	6.6741e-05	-2.1082381
Cu	7.6292537	6.6741e-05	-2.1082381
Cu	6.3695314	2.2095615	-2.1185378
Cu	-3.8080061	2.2095615	-2.1185378
Cu	3.8174631	2.2033879	-2.1251293
Cu	-2.5363142	-4.4166461	-2.1254417
Cu	2.5524545	4.3973599	-2.1254417
Cu	-0.008470832	4.3911785	-2.127307
Cu	5.0802979	-4.4228275	-2.127307
Cu	0.001199753	-1.4548397	-4.1221697
Cu	1.2789134	0.73023277	-4.1238624
Cu	-1.2591637	0.74073558	-4.1242744
Cu	2.5465502	-1.4624263	-4.1299266
Cu	3.8053318	0.73407563	-4.1311985
Cu	3.8186656	-3.6550199	-4.1312901
Cu	-1.2701031	5.1589861	-4.1312901
Cu	5.0883345	-1.4592031	-4.1336507
Cu	-2.5466409	-1.460365	-4.1337052
Cu	-2.5298387	2.9441776	-4.1361324
Cu	1.2701228	5.1520932	-4.137024
Cu	6.3531772	0.74530413	-4.1370902
Cu	-3.8243603	0.74530413	-4.1370902
Cu	1.2720984	-3.6542549	-4.1397182
Cu	5.0878871	2.9523062	-4.1443887
Cu	2.5323936	2.9392637	-4.1451563
Cu	3.8169303	5.1508531	-4.1478868
Cu	-1.2718384	-3.6631529	-4.1478868
Cu	0.00089724	2.9400295	-4.1486793
Cu	-1.2698003	-0.73066546	-6.1809111
Cu	-2.5395705	1.4693615	-6.181616
Cu	5.0834333	1.4728463	-6.1863838

Cu	3.8129855	3.678651	-6.1882022
Cu	1.271877	-0.73361753	-6.1902918
Cu	0.002254778	1.4704062	-6.1908016
Cu	3.8143664	-0.73183611	-6.1939976
Cu	0.001202717	-2.9289915	-6.197116
Cu	2.5418408	1.4724854	-6.197573
Cu	2.5416578	-2.9328591	-6.1983888
Cu	1.2711131	3.6823332	-6.2001023
Cu	-1.2683739	3.6775691	-6.2022893



## HCOO\_on\_Cu.xyz

92

Atoms

H	1.9337868	0.37836646	3.679952
C	1.9282263	0.37469549	2.5682538
O	1.3473925	-0.60822679	2.0194661
O	2.5026267	1.3542863	2.0061444
Cu	1.2523825	-0.76631669	0.025121599
Cu	2.5593332	1.4937753	0.012662949
Cu	6.3634708	-0.73867081	-0.039481306
Cu	-3.8140667	-0.73867081	-0.039481306
Cu	-2.5462876	1.4666405	-0.040479623
Cu	7.6312499	1.4666405	-0.040479623
Cu	-2.5488883	-2.9457916	-0.044386542
Cu	2.5398804	5.8682144	-0.044386542
Cu	1.275692	-5.144229	-0.044797914
Cu	6.3644608	3.669777	-0.044797914
Cu	-3.8130767	3.669777	-0.044797914
Cu	0.011010366	5.871421	-0.04486358
Cu	-5.0777584	-2.942585	-0.04486358
Cu	5.0997791	-2.942585	-0.04486358
Cu	-1.2822613	3.6654395	-0.045460367
Cu	3.8065074	-5.1485665	-0.045460367
Cu	5.1177066	1.4642956	-0.058811468
Cu	-5.0598309	1.4642956	-0.058811468
Cu	-1.3013834	-0.74575503	-0.061826563
Cu	-0.025251557	-2.9684036	-0.06364488
Cu	5.0635172	5.8456024	-0.06364488
Cu	-2.5269057	5.8526429	-0.068127812
Cu	2.561863	-2.9613631	-0.068127812
Cu	3.8372296	3.6933237	-0.068145599
Cu	-1.2515391	-5.1206823	-0.068145599
Cu	-3.8294857	-5.1241841	-0.074246607
Cu	1.259283	3.6898219	-0.074246607
Cu	-6.324216	-0.76105894	-0.078208043
Cu	3.8533215	-0.76105894	-0.078208043
Cu	-0.033899519	1.4822451	-0.080681359
Cu	2.5360411	-0.006805613	-2.0614337
Cu	1.2721113	-2.1938436	-2.0751238
Cu	3.8035105	2.1841026	-2.0769244
Cu	0.013271497	-0.018769667	-2.0803677
Cu	1.2841718	2.1814778	-2.0877332
Cu	-3.8142378	-2.2094509	-2.0980476
Cu	6.3632997	-2.2094509	-2.0980476
Cu	1.2745309	6.6045551	-2.0980476
Cu	2.5438803	-4.4099365	-2.0991451
Cu	-2.5448884	4.4040695	-2.0991451
Cu	6.3603244	2.2039962	-2.1014789
Cu	-3.8172131	2.2039962	-2.1014789
Cu	7.6325304	-0.002455374	-2.1019966

Cu	-2.5450071	-0.002455374	-2.1019966
Cu	-1.270561	-2.2094406	-2.1024076
Cu	3.8182077	6.6045654	-2.1024076
Cu	5.0868933	-0.001948857	-2.1038397
Cu	-5.0906442	-0.001948857	-2.1038397
Cu	-1.2727437	6.6024771	-2.1078168
Cu	3.816025	-2.2115289	-2.1078168
Cu	5.0922772	4.4011073	-2.1081439
Cu	0.003508466	-4.4128987	-2.1081439
Cu	-1.2720529	2.1966474	-2.1081783
Cu	-2.5435305	-4.4213058	-2.1134752
Cu	2.5452382	4.3927002	-2.1134752
Cu	-0.002691627	4.3952009	-2.1137121
Cu	5.0860771	-4.4188051	-2.1137121
Cu	5.074284	2.9384648	-4.1280764
Cu	-1.2626481	0.73537234	-4.1297254
Cu	6.357925	0.74560432	-4.1311302
Cu	-3.8196125	0.74560432	-4.1311302
Cu	-2.5435473	2.9472912	-4.1314223
Cu	1.2704826	-3.6537141	-4.1316197
Cu	-2.5425041	-1.4600037	-4.1322842
Cu	5.0867744	-1.4607347	-4.132344
Cu	3.8074625	0.73860044	-4.1328774
Cu	1.2728283	5.1495618	-4.1343866
Cu	2.5437756	-1.455624	-4.1352329
Cu	-1.2697987	-3.6646842	-4.1359321
Cu	3.81897	5.1493218	-4.1359321
Cu	0.010319913	2.9399644	-4.1367134
Cu	1.2728188	0.73863279	-4.1376493
Cu	0.000894593	-1.4636773	-4.1400033
Cu	-1.2742463	5.1490263	-4.1408209
Cu	3.8145224	-3.6649797	-4.1408209
Cu	2.543151	2.9434963	-4.1416055
Cu	-2.5414203	1.4696426	-6.1731964
Cu	-1.2710665	3.6749621	-6.1821492
Cu	5.0884259	1.4717207	-6.185422
Cu	-1.2722733	-0.73055525	-6.1902638
Cu	2.5437179	1.474192	-6.1908701
Cu	3.8180924	-0.7310716	-6.191467
Cu	1.2716836	-0.73359655	-6.1923167
Cu	-0.001363334	1.4730589	-6.1927503
Cu	1.272981	3.6804951	-6.1941262
Cu	0.00240214	-2.9341346	-6.1942418
Cu	3.8154557	3.6774971	-6.1947518
Cu	2.5436904	-2.9349165	-6.195325

## Methoxy\_on\_Cu.xyz

93

Atoms

H	0.38471084	0.22228902	3.087579
H	1.2844463	1.7810314	3.0833007
H	2.1844433	0.22181979	3.0751948
C	1.2819691	0.74222735	2.7090163
O	1.2735041	0.74245431	1.2745381
Cu	-0.094672184	1.5111831	0.00571133
Cu	2.6418691	1.5105105	0.003997042
Cu	1.2733572	-0.8419113	0.001429628
Cu	1.2725184	-5.1427744	-0.034323241
Cu	6.3612872	3.6712316	-0.034323241
Cu	-3.8162503	3.6712316	-0.034323241
Cu	0.005690466	5.8696167	-0.036878197
Cu	-5.0830783	-2.9443893	-0.036878197
Cu	5.0944592	-2.9443893	-0.036878197
Cu	5.1188086	1.4657042	-0.037968243
Cu	-5.0587289	1.4657042	-0.037968243
Cu	-2.549992	-2.9444651	-0.038700163
Cu	2.5387767	5.8695409	-0.038700163
Cu	6.3612118	-0.7369192	-0.039973081
Cu	-3.8163257	-0.7369192	-0.039973081
Cu	3.8394014	3.6883173	-0.040516641
Cu	-1.2493673	-5.1256887	-0.040516641
Cu	-1.2922889	3.6888078	-0.040603688
Cu	3.7964798	-5.1251982	-0.040603688
Cu	-2.5715966	1.4654159	-0.040999075
Cu	7.6059409	1.4654159	-0.040999075
Cu	-2.5211106	5.8457187	-0.045899106
Cu	2.5676581	-2.9682873	-0.045899106
Cu	-0.021282444	-2.9674448	-0.047791518
Cu	5.0674863	5.8465612	-0.047791518
Cu	-6.3226603	-0.76506291	-0.059020767
Cu	3.8548772	-0.76506291	-0.059020767
Cu	-1.3068434	-0.76397727	-0.061453636
Cu	1.274278	3.7048838	-0.07812484
Cu	-3.8144907	-5.1091222	-0.07812484
Cu	2.5361323	-0.006983571	-2.0694323
Cu	-1.2587491	2.1870422	-2.070132
Cu	0.008839396	-0.007174904	-2.0710709
Cu	1.2723531	-2.200807	-2.0714465
Cu	3.8060054	2.1876754	-2.0715609
Cu	1.2736641	2.1762968	-2.0741417
Cu	-3.8163463	-2.2090365	-2.0945161
Cu	1.2724224	6.6049695	-2.0945161
Cu	6.3611912	-2.2090365	-2.0945161
Cu	-5.0907356	-0.000999929	-2.0948923
Cu	5.0868019	-0.000999929	-2.0948923
Cu	7.6352494	-0.001564023	-2.0956185

Cu	-2.5422881	-0.001564023	-2.0956185
Cu	5.091656	4.4044743	-2.0981096
Cu	0.002887266	-4.4095317	-2.0981096
Cu	2.5427173	-4.4105671	-2.0984961
Cu	-2.5460514	4.4034389	-2.0984961
Cu	-3.816423	2.206966	-2.1009038
Cu	6.3611145	2.206966	-2.1009038
Cu	-1.2716877	6.6022096	-2.1025863
Cu	3.817081	-2.2117964	-2.1025863
Cu	3.8162991	6.6021684	-2.1035185
Cu	-1.2724696	-2.2118376	-2.1035185
Cu	-2.5391238	-4.4242263	-2.1117308
Cu	2.5496449	4.3897797	-2.1117308
Cu	-0.003748858	4.3895834	-2.1119997
Cu	5.0850199	-4.4244226	-2.1119997
Cu	-2.525819	2.9401463	-4.1173247
Cu	5.0708907	2.9408271	-4.1188788
Cu	-1.2668057	0.73945516	-4.1243777
Cu	3.8115624	0.73905539	-4.1245367
Cu	-3.8178407	0.74670983	-4.1261657
Cu	6.3596968	0.74670983	-4.1261657
Cu	1.2736359	-3.6534699	-4.1281144
Cu	1.2735959	0.73908184	-4.1281594
Cu	-2.5428619	-1.4600522	-4.130743
Cu	5.0862923	-1.4592716	-4.1308151
Cu	0.006136067	2.9415984	-4.131515
Cu	2.5466919	-1.4597183	-4.1315382
Cu	-0.000982286	-1.4606602	-4.1326164
Cu	2.5392537	2.9423026	-4.1326311
Cu	1.2717612	5.1496956	-4.1327753
Cu	-1.2699004	-3.6658874	-4.137061
Cu	3.8188683	5.1481186	-4.137061
Cu	-1.2745922	5.1492214	-4.1371287
Cu	3.8141765	-3.6647846	-4.1371287
Cu	-2.5389956	1.4750472	-6.1745095
Cu	5.0829598	1.4750476	-6.1755077
Cu	1.272769	-0.72935909	-6.1835982
Cu	0.002007465	1.4741776	-6.1837886
Cu	2.5431707	1.4736472	-6.1861247
Cu	-1.2741877	-0.72514966	-6.188037
Cu	1.2718479	3.6839421	-6.1883083
Cu	3.8158975	3.6763049	-6.1887245
Cu	-1.2713868	3.6767298	-6.1888619
Cu	3.8182702	-0.72514947	-6.1903481
Cu	0.002173078	-2.92886	-6.196003
Cu	2.5423459	-2.9286779	-6.1974053

## OH\_on\_Cu.xyz

90

Atoms

H	1.2838623	0.75018588	2.2485371
O	1.2763271	0.74585161	1.2682127
Cu	-0.10271879	1.5171486	0.012081334
Cu	1.2736849	-0.84787446	0.010844196
Cu	2.6523081	1.5200322	0.010373088
Cu	0.010548766	5.870527	-0.038002168
Cu	-5.07822	-2.943479	-0.038002168
Cu	5.0993175	-2.943479	-0.038002168
Cu	2.5344004	5.8686037	-0.038061463
Cu	-2.5543683	-2.9454023	-0.038061463
Cu	1.273883	-5.1397921	-0.038351665
Cu	6.3626518	3.6742139	-0.038351665
Cu	-3.8148857	3.6742139	-0.038351665
Cu	6.3610344	-0.73921572	-0.038837577
Cu	-3.8165031	-0.73921572	-0.038837577
Cu	-2.5731629	1.4693206	-0.043883536
Cu	7.6043746	1.4693206	-0.043883536
Cu	5.1200305	1.4703787	-0.044849099
Cu	-5.057507	1.4703787	-0.044849099
Cu	-1.2960168	3.6897678	-0.046345535
Cu	3.7927519	-5.1242382	-0.046345535
Cu	-0.024671077	-2.9667751	-0.046456672
Cu	5.0640977	5.8472309	-0.046456672
Cu	3.8413989	3.6923843	-0.04658767
Cu	-1.2473698	-5.1216217	-0.04658767
Cu	-2.5208205	5.849383	-0.047404966
Cu	2.5679482	-2.964623	-0.047404966
Cu	-6.3241508	-0.76247596	-0.066736252
Cu	3.8533867	-0.76247596	-0.066736252
Cu	-1.3122163	-0.76646948	-0.067103258
Cu	1.2713794	3.7056417	-0.086674796
Cu	-3.8173893	-5.1083643	-0.086674796
Cu	2.5341854	-0.002385281	-2.0698608
Cu	1.2723651	-2.1970838	-2.0702473
Cu	0.010970814	-0.00299906	-2.0716863
Cu	3.8041085	2.1885845	-2.0720309
Cu	-1.2585888	2.1872143	-2.072845
Cu	1.2718617	2.1790763	-2.0770067
Cu	-3.8167028	-2.2115289	-2.0932596
Cu	6.3608347	-2.2115289	-2.0932596
Cu	1.2720659	6.6024771	-2.0932596
Cu	-5.0900646	-0.001272708	-2.0975115
Cu	5.0874729	-0.001272708	-2.0975115
Cu	7.6346541	-0.002110107	-2.098356
Cu	-2.5428834	-0.002110107	-2.098356
Cu	0.004017666	-4.4106244	-2.1027405
Cu	5.0927864	4.4033816	-2.1027405

Cu	2.5407911	-4.4116265	-2.1039707
Cu	-2.5479776	4.4023795	-2.1039707
Cu	-1.273345	6.602829	-2.104433
Cu	3.8154237	-2.211177	-2.104433
Cu	-3.8154683	2.2069246	-2.1056191
Cu	6.3620692	2.2069246	-2.1056191
Cu	-1.2707627	-2.2128777	-2.1060569
Cu	3.818006	6.6011283	-2.1060569
Cu	-2.5387798	-4.4228153	-2.1160859
Cu	2.5499889	4.3911907	-2.1160859
Cu	-0.005565057	4.3910491	-2.1161162
Cu	5.0832037	-4.4229569	-2.1161162
Cu	5.0736322	2.9393416	-4.1228193
Cu	-2.5287309	2.9387913	-4.1249712
Cu	6.3619109	0.74428961	-4.1291847
Cu	-3.8156266	0.74428961	-4.1291847
Cu	3.811141	0.73834471	-4.1294525
Cu	-1.2665995	0.73733021	-4.1295679
Cu	5.087573	-1.4617623	-4.1297195
Cu	1.2713557	-3.6535015	-4.1306244
Cu	-2.5422582	-1.4621641	-4.1314434
Cu	1.2714999	0.73895105	-4.1357234
Cu	1.2728014	5.1481391	-4.1360993
Cu	-0.00198405	-1.4587358	-4.136296
Cu	2.5455124	-1.4588907	-4.1371986
Cu	-1.2740027	5.1486101	-4.1385443
Cu	3.814766	-3.6653959	-4.1385443
Cu	2.5395887	2.941259	-4.1387349
Cu	3.8187189	5.1479766	-4.1401938
Cu	-1.2700498	-3.6660294	-4.1401938
Cu	0.004481723	2.9413631	-4.1403342
Cu	5.0858529	1.4735592	-6.1792149
Cu	-2.5401267	1.4727295	-6.1792852
Cu	2.5440405	1.471173	-6.1919185
Cu	1.2714265	-0.73466091	-6.1921998
Cu	3.8185803	3.6757972	-6.192521
Cu	1.2722303	3.6803794	-6.192869
Cu	3.8196067	-0.7282982	-6.1937584
Cu	-1.2740218	3.675718	-6.1943707
Cu	-0.000792618	1.4707125	-6.1947788
Cu	-1.2743504	-0.72837303	-6.195601
Cu	2.5418838	-2.9346947	-6.1973732
Cu	0.002364551	-2.9338517	-6.1982995

# Oxide\_on\_Cu.xyz

103

Atoms

Cu	-5.090931734	-2.912665996	-0.010579000
Cu	-3.830532734	-5.117905996	0.022691000
Cu	-2.516032734	-2.904592996	0.064104000
Cu	-2.574180734	-4.362678996	-2.033358000
Cu	-1.281305734	-3.636114996	-4.035563000
Cu	-1.334487734	-5.112595996	-0.047264000
Cu	-0.007885734	-4.376468996	-2.023859000
Cu	-3.994388734	-1.056495996	2.336269000
Cu	-6.375607469	-0.677008000	0.067023000
Cu	-5.115734469	1.472192000	0.061024000
Cu	-5.102481469	0.030223000	-2.021791000
Cu	-3.820101469	-2.171563000	-2.023801000
Cu	-3.796267469	-0.655085000	-0.046194000
Cu	-3.823489469	0.768413000	-4.041797000
Cu	-3.828905469	2.226283000	-2.013725000
Cu	-2.544196469	-1.438006000	-4.035656000
Cu	-2.526359469	0.042715000	-2.033625000
Cu	-1.276979469	-2.174267000	-1.992536000
O	-3.170787469	0.370328000	3.046655000
Cu	-3.728050469	1.927089000	2.280080000
Cu	-0.007249266	-2.907613996	-6.094804000
Cu	-0.024780266	-2.885310996	0.068815000
Cu	1.262541734	-3.646699996	-4.050422000
Cu	1.268477734	-5.109520996	-0.010567000
Cu	2.536399734	-2.904240996	-6.095119000
Cu	2.544930734	-2.916661996	0.021593000
Cu	2.542786734	-4.387113996	-2.014328000
Cu	3.801797734	-3.647821996	-4.042300000
Cu	3.811606734	-5.113134996	0.049242000
Cu	5.086605734	-2.912665996	-0.010579000
Cu	5.073048734	-4.375796996	-2.013949000
O	1.915900734	-1.837049996	3.043189000
Cu	1.362734734	-3.394426996	2.273185000
Cu	3.542142734	-2.136683996	2.276711000
Cu	-3.820291000	3.704485000	-0.010567000
Cu	-2.544199000	1.504446000	0.022923000
Cu	-2.551936000	1.498646000	-6.095365000
Cu	-2.543838000	5.897344000	0.021593000
Cu	-2.540427000	2.965111000	-4.042648000
Cu	-2.545982000	4.426892000	-2.014328000
Cu	-1.289447000	-0.739491000	0.062109000
Cu	-1.286971000	5.166184000	-4.042300000
Cu	-1.272762000	0.765306000	-4.049566000
Cu	-1.277421000	-0.702611000	-6.094006000
Cu	-1.277162000	3.700871000	0.049242000
Cu	-1.271100000	2.241434000	-2.013159000
Cu	-1.278644000	3.704520000	-6.114894000

Cu	-0.009376000	-1.443770000	-4.036922000
Cu	-0.008812000	1.495645000	-0.008145000
Cu	-0.004351000	1.504303000	-6.083802000
Cu	-0.002163000	5.901340000	-0.010579000
Cu	-0.007957000	2.979804000	-4.042489000
Cu	-0.005356000	0.027259000	-2.025557000
Cu	-0.015720000	4.438209000	-2.013949000
Cu	1.264182000	-0.706285000	-6.078233000
Cu	1.298259000	-0.756154000	-0.053964000
Cu	1.263505000	5.178232000	-4.049135000
Cu	1.267736000	3.704656000	-6.095074000
Cu	1.271422000	0.769531000	-4.045372000
Cu	1.258236000	3.696100000	0.022691000
Cu	1.265534000	-2.202734000	-2.035365000
Cu	1.275800000	2.229977000	-2.014150000
Cu	2.541301000	1.506048000	-6.099090000
Cu	2.572736000	5.909413000	0.064104000
Cu	2.541165000	-1.438544000	-4.042489000
Cu	2.514588000	4.451327000	-2.033358000
Cu	2.535838000	2.967512000	-4.042266000
Cu	2.573190000	1.490122000	0.060294000
Cu	2.543851000	0.036829000	-2.023566000
Cu	3.807463000	5.177891000	-4.035563000
Cu	3.804064000	-0.701937000	-6.099152000
Cu	3.807541000	3.707436000	-6.077617000
Cu	3.754281000	3.701410000	-0.047264000
Cu	3.810603000	0.765983000	-4.046139000
Cu	3.801930000	-0.677008000	0.067023000
Cu	3.814872000	2.227935000	-2.023202000
Cu	3.808360000	-2.163677000	-2.013172000
Cu	5.084751000	1.495566000	-6.098965000
Cu	5.061803000	1.472192000	0.061024000
Cu	5.080883000	4.437537000	-2.023859000
Cu	5.083445000	2.962374000	-4.044779000
Cu	5.075056000	0.030223000	-2.021791000
Cu	5.076146000	-1.434555000	-4.043806000
Cu	6.357436000	-2.171563000	-2.023801000
Cu	6.381270000	-0.655085000	-0.046194000
Cu	6.354048000	0.768413000	-4.041797000
Cu	6.348632000	2.226283000	-2.013725000
Cu	7.651178000	0.042715000	-2.033625000
O	0.195339000	1.145040000	1.984120000
O	5.990127000	3.672657000	1.986157000
O	2.548821000	3.672945000	3.046346000
Cu	-1.547868000	0.672202000	2.272541000
Cu	1.092870000	-0.409336000	2.331869000
Cu	1.474969000	2.418702000	2.274608000
Cu	1.480372000	4.934491000	2.277606000
Cu	4.196187000	3.670423000	2.335556000
Cu	6.449487000	1.927089000	2.280080000



Cu	-1.280408734	6.650328996	-2.013172000
Cu	1.268667266	6.642442996	-2.023801000
Cu	3.811789266	6.639738996	-1.992536000
Cu	5.063988469	5.928695000	0.068815000
Cu	6.357246469	3.704485000	-0.010567000
Cu	7.633338469	1.504446000	0.022923000

## Oxide\_on\_Cu\_pos2.xyz

103

Atoms

Cu	-3.789731469	-0.720139000	0.055869000
Cu	-6.362582469	-0.728028000	-0.023513000
Cu	-5.101737469	-2.929898000	0.008647000
Cu	6.387806000	-0.720139000	0.055869000
Cu	5.084763000	-1.454298000	-4.063368000
Cu	3.812356000	-0.725169000	-6.096451000
Cu	3.814955000	-0.728028000	-0.023513000
Cu	1.271619000	-0.733137000	0.009977000
Cu	1.270465000	-0.723536000	-6.108311000
Cu	5.075800000	-2.929898000	0.008647000
Cu	2.534706000	-1.466736000	-4.055594000
Cu	3.803423000	-2.192816000	-2.027274000
Cu	-1.299063000	-0.697815000	0.049163000
Cu	3.814163000	-3.652797000	-4.055246000
Cu	-0.004214000	-1.464663000	-4.062512000
Cu	-1.273137000	-0.726670000	-6.106952000
Cu	2.540260000	-2.928635000	0.036296000
Cu	1.273320000	-2.204167000	-2.026105000
Cu	2.544161000	-2.929176000	-6.127840000
Cu	-2.549023000	-1.454250000	-4.049868000
Cu	-0.003696000	-2.924446000	-0.021091000
Cu	0.001571000	-2.932638000	-6.096748000
Cu	3.808423000	-5.133051000	-0.023525000
Cu	1.281195000	-3.667266000	-4.055435000
Cu	-1.277084000	-2.193246000	-2.038503000
Cu	2.548093000	-4.389745000	-2.026895000
Cu	-2.607347000	-2.930503000	-0.066910000
Cu	-1.272647000	-3.670104000	-4.058318000
Cu	1.268430000	-5.121969000	0.009745000
Cu	-3.843760000	-2.178872000	-2.048311000
Cu	-0.010052000	-4.404118000	-2.027096000
Cu	-1.299481000	-5.157763000	0.047348000
Cu	-2.543400000	-4.405709000	-2.036512000
Cu	-3.790640000	-5.138318000	0.054077000
O	-0.409405000	-2.925943000	1.971174000
Cu	5.253141000	-1.667204000	2.260239000
Cu	0.052709000	-1.179862000	2.259595000
Cu	-2.204299000	-2.926040000	2.318923000
Cu	0.053804000	-4.670966000	2.261662000
Cu	-0.012968734	5.884107996	0.008647000
Cu	-1.285345734	6.621189996	-2.027274000
Cu	-1.274605734	5.161208996	-4.055246000
Cu	-2.548508734	5.885370996	0.036296000
Cu	-1.269683734	3.684516996	-6.095108000
Cu	-1.280345734	3.680954996	-0.023525000
Cu	-2.540675734	4.424260996	-2.026895000
Cu	-2.539409734	2.946407996	-4.062081000

Cu	-3.820338734	3.692036996	0.009745000
Cu	-2.543428734	1.477844996	-6.106575000
Cu	-2.560803734	1.446989996	0.051158000
Cu	-3.794469734	2.226390996	-2.046304000
Cu	-3.811683734	0.743445996	-4.048509000
Cu	-5.063763734	1.527743996	-0.060210000
Cu	-5.089558734	0.010808996	-2.036805000
O	-1.116968734	3.357392996	1.974030000
Cu	0.163906266	4.630507996	2.263765000
Cu	-0.221126734	1.803234996	2.323323000
Cu	-2.858928734	2.880465996	2.264660000
Cu	6.333777469	-2.178872000	-2.048311000
Cu	5.096189469	-4.400552000	-2.026118000
Cu	5.085072734	5.889559996	-0.021091000
Cu	3.811684734	6.620759996	-2.038503000
Cu	2.481421734	5.883502996	-0.066910000
Cu	3.816121734	5.143901996	-4.058318000
Cu	6.357198734	3.692036996	0.009745000
Cu	1.245008734	6.635133996	-2.048311000
Cu	5.078716734	4.409887996	-2.027096000
Cu	3.819025734	3.675895996	-6.112036000
Cu	7.616733734	1.446989996	0.051158000
Cu	1.269001734	5.148309996	-4.055435000
Cu	6.383067734	2.226390996	-2.046304000
Cu	5.087421734	2.949894996	-4.055212000
Cu	3.789287734	3.656242996	0.047348000
Cu	2.545368734	4.408296996	-2.036512000
Cu	6.365853734	0.743445996	-4.048509000
Cu	1.275471734	3.686303996	-6.112098000
Cu	5.092363734	1.478605996	-6.090563000
Cu	5.113773734	1.527743996	-0.060210000
Cu	2.543458734	2.946680996	-4.059085000
Cu	1.298128734	3.675687996	0.054077000
Cu	3.807411734	2.212007996	-2.036148000
Cu	0.007420734	4.413453996	-2.026118000
Cu	2.538222734	1.478444996	-6.111911000
Cu	2.529453734	1.510005996	0.048078000
Cu	5.087978734	0.010808996	-2.036805000
Cu	3.809168734	0.746171996	-4.057725000
Cu	1.274045734	2.219511996	-2.034737000
Cu	0.004965734	2.950956996	-4.056752000
Cu	-1.273947266	2.209831996	-2.036747000
Cu	0.027444734	1.430951996	-0.059140000
Cu	1.273840734	0.742777996	-4.054743000
Cu	-0.001793266	1.474382996	-6.090144000
Cu	2.539101734	0.018532996	-2.026671000
Cu	-1.276620266	0.738087996	-4.048602000
Cu	-0.003197266	-0.017720004	-2.046571000
Cu	-2.547849266	0.008776996	-2.005482000
O	3.970950734	-0.394179004	1.973211000

O	5.691852734	2.585934996	3.033400000
O	0.602738734	0.376563996	3.033709000
Cu	5.142572734	4.143039996	2.261662000
Cu	4.865985734	1.160534996	2.322610000
Cu	2.229564734	0.080786996	2.267134000
Cu	7.629688203	0.008776996	-2.005482000

# Single\_H2O\_on\_Cu.xyz

91

Atoms

H	1.0610212	0.26642008	2.4407989
H	2.3083411	-0.66838736	2.4356672
O	1.3316533	-0.67120799	2.2936871
Cu	1.2662171	-0.74679151	0.021331955
Cu	6.3606638	-0.73574908	-0.031033666
Cu	-3.8168737	-0.73574908	-0.031033666
Cu	-2.5435087	1.4662557	-0.033873738
Cu	7.6340288	1.4662557	-0.033873738
Cu	5.0872939	1.4670606	-0.035135096
Cu	-5.0902436	1.4670606	-0.035135096
Cu	0.000739466	5.8758089	-0.035318046
Cu	-5.0880293	-2.9381971	-0.035318046
Cu	5.0895082	-2.9381971	-0.035318046
Cu	3.8194409	3.6685373	-0.035561171
Cu	-1.2693278	-5.1454687	-0.035561171
Cu	-1.2748576	3.6649537	-0.038817719
Cu	3.8139111	-5.1490523	-0.038817719
Cu	2.5415836	5.8726106	-0.039611675
Cu	-2.5471851	-2.9413954	-0.039611675
Cu	1.2720068	3.6650398	-0.042908977
Cu	-3.8167619	-5.1489662	-0.042908977
Cu	1.2716961	-5.1431907	-0.043182145
Cu	6.3604649	3.6708153	-0.043182145
Cu	-3.8170726	3.6708153	-0.043182145
Cu	2.549866	1.4787987	-0.048084402
Cu	-1.2914574	-0.73800014	-0.048716792
Cu	-0.011292211	-2.9603233	-0.051266754
Cu	5.0774765	5.8536827	-0.051266754
Cu	-6.3442645	-0.73788794	-0.05258344
Cu	3.833273	-0.73788794	-0.05258344
Cu	-2.5303703	5.8582719	-0.053777952
Cu	2.5583984	-2.9557341	-0.053777952
Cu	-0.007935079	1.4826629	-0.054905726
Cu	0.008117278	-0.01619761	-2.0761778
Cu	1.2719151	-2.2040382	-2.0790459
Cu	2.5370997	-0.013738838	-2.0796852
Cu	6.362042	2.1954748	-2.092505
Cu	-3.8154955	2.1954748	-2.092505
Cu	1.2718797	6.6020839	-2.0933773
Cu	-3.816889	-2.2119221	-2.0933773
Cu	6.3606485	-2.2119221	-2.0933773
Cu	-0.001012034	-4.4129931	-2.0969921
Cu	5.0877567	4.4010129	-2.0969921
Cu	-1.2706152	-2.2119626	-2.0972401
Cu	3.8181535	6.6020434	-2.0972401
Cu	2.54605	-4.4150189	-2.098331
Cu	-2.5427187	4.3989871	-2.098331

Cu	-2.5477792	-0.005826796	-2.0984259
Cu	7.6297583	-0.005826796	-2.0984259
Cu	3.8178192	2.1966463	-2.0999203
Cu	-1.2730478	6.6037924	-2.1004955
Cu	3.8157209	-2.2102136	-2.1004955
Cu	-5.0855806	-0.004199886	-2.1010946
Cu	5.0919569	-0.004199886	-2.1010946
Cu	-2.5457507	-4.4181318	-2.1031516
Cu	2.543018	4.3958742	-2.1031516
Cu	0.000595314	4.3951072	-2.1033294
Cu	5.089364	-4.4188988	-2.1033294
Cu	1.2724961	2.1906205	-2.1040655
Cu	-1.275339	2.1953617	-2.1060812
Cu	-1.263289	0.73680152	-4.1300487
Cu	3.80892	0.73975122	-4.1302321
Cu	5.0887557	-1.461599	-4.1314667
Cu	-2.5421777	-1.4614691	-4.132079
Cu	1.268564	0.73883416	-4.1346804
Cu	0.000404132	-1.4595884	-4.1347392
Cu	2.5418005	-1.4607013	-4.135251
Cu	1.2710836	-3.6574281	-4.1352837
Cu	5.0898918	2.9462013	-4.135391
Cu	6.3633607	0.74549796	-4.1354893
Cu	-3.8141768	0.74549796	-4.1354893
Cu	-1.273789	5.149557	-4.136231
Cu	3.8149797	-3.664449	-4.136231
Cu	1.2733238	5.1504262	-4.1367814
Cu	2.543349	2.9448417	-4.1378611
Cu	-1.2706047	-3.6636298	-4.1379907
Cu	3.818164	5.1503762	-4.1379907
Cu	-2.5450492	2.9459939	-4.1383116
Cu	0.000391429	2.9438276	-4.140034
Cu	5.0879241	1.4698343	-6.1860312
Cu	3.8170221	-0.732633	-6.1883548
Cu	3.8156713	3.6752656	-6.1902909
Cu	-2.543264	1.4704713	-6.1903604
Cu	-1.2714864	3.6742033	-6.1931713
Cu	1.2727796	3.6741691	-6.193414
Cu	2.5441651	1.4723176	-6.1942561
Cu	2.5451833	-2.9368089	-6.1952788
Cu	1.2721905	-0.73377216	-6.195442
Cu	-1.2727521	-0.73335636	-6.1956336
Cu	2.049e-06	1.4716956	-6.1993714
Cu	-0.000520232	-2.9380491	-6.1996097