SUPPORTING INFORMATION

for

$[Cu_2O]^{2+}$ Active Site Formation in Cu-ZSM-5: Geometric and Electronic Structure Requirements for N_2O Activation

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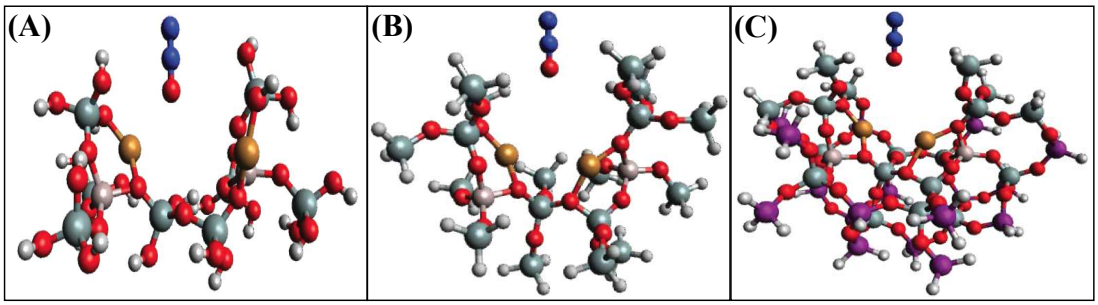
Figure S1. Optimized binuclear Cu^{I} active site model (A) H-capped model (68 atoms) (B) SiH_3 capped model (86 atoms) (C) SiH_3 capped model with additional Si layers (140 atoms). (D) Calculated $[Cu_2O]^{2+}$ DFT models for the other 9 possible pairs. Only the 44 atoms around the active site are shown and hydrogen atoms are omitted for clarity. The Si atoms of SiH_3 capped model are given in grey, Si atoms from the additional layer model are given in purple. To include an additional layer, the terminal SiH_3 groups of 86 atom model were extended to Si-[(O-SiH_xO_y)(O-SiH_xO_y)(O-SiH_xO_y)] (the O and Si positions are obtained from the crystallographic structure), the number of x can be 1, 2, or 3 and y can be 2, 1, 0. The x and y will depend on whether the SiH_xO_y unit of the new O-SiH_xO_y group is terminal or has one or two bridges to nearby Si atoms. Note that the change of the geometric parameters between the 86 atom and 140 atom models includes: the change in the Cu-Olat bond distance is less than 0.06; the change in the Olat-Cu-Olat angle is less than 3 degree; the Cu...Cu distance is slightly shorter in 140 atoms model (3.797 A for 140 atoms model; 4.177 for 86 atoms model). The Si atoms of the three different models are obtained from the crystallographic structure and fixed during the geometry optimization.



(D)

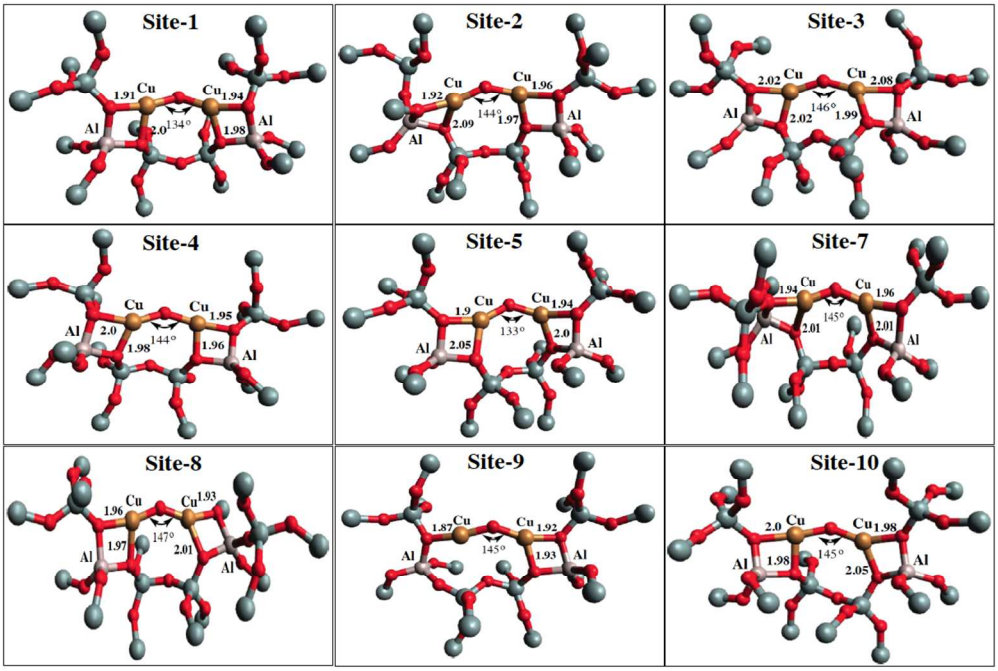


Figure S2. Calculated binuclear Cu^I DFT models for the other 9 possible pairs, labeled with representative Cu^I binding modes. Note that the Si atoms are given in grey and hydrogen atoms are omitted for clarity.

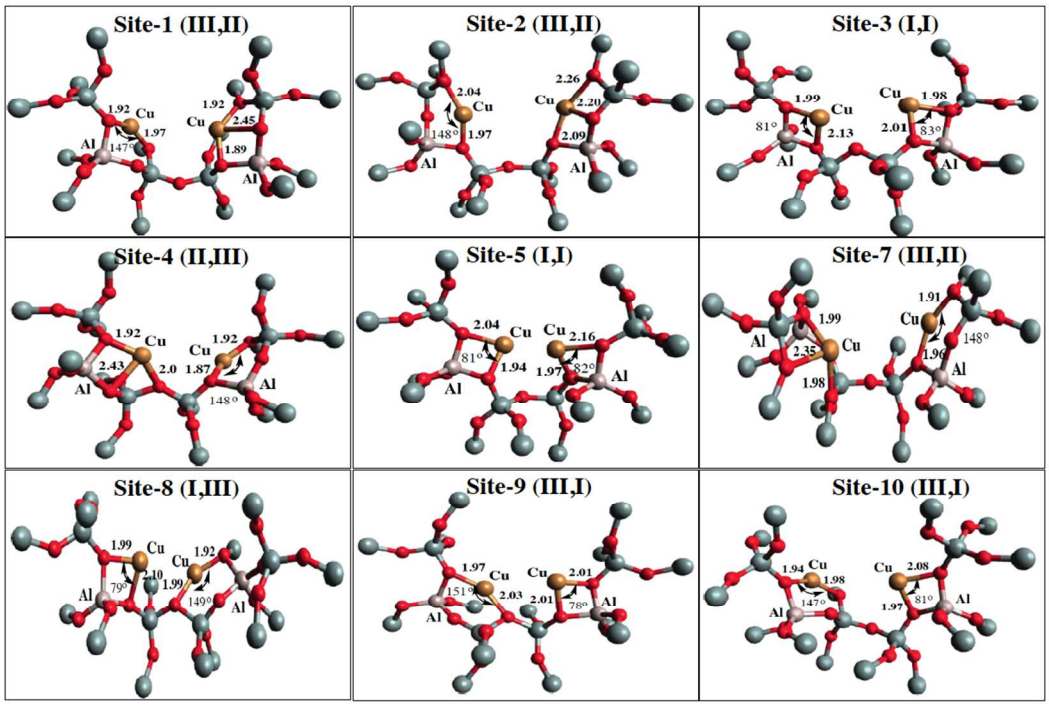


Figure S3. The $\ln(Abs_0 - Abs_f)/Abs_t\text{-}Abs_f)$ vs. time plots with linear fits**.**

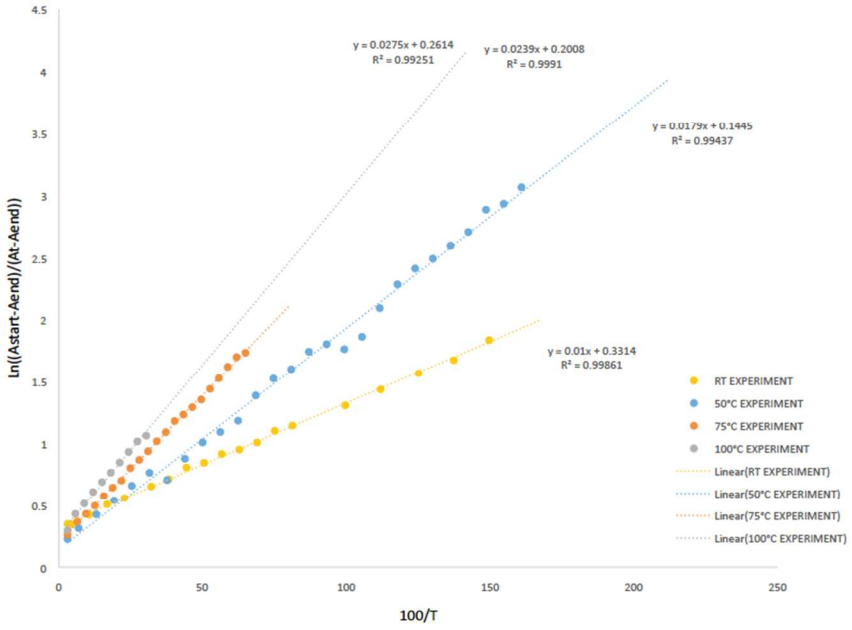


Figure S4. Calculated (A) singlet and triplet PES (B) spin densities (C) Mulliken charges (D) Mayer bond orders for site-6 with a μ-1,3-O N_2O binding mode along the N-O singlet potential energy surface.

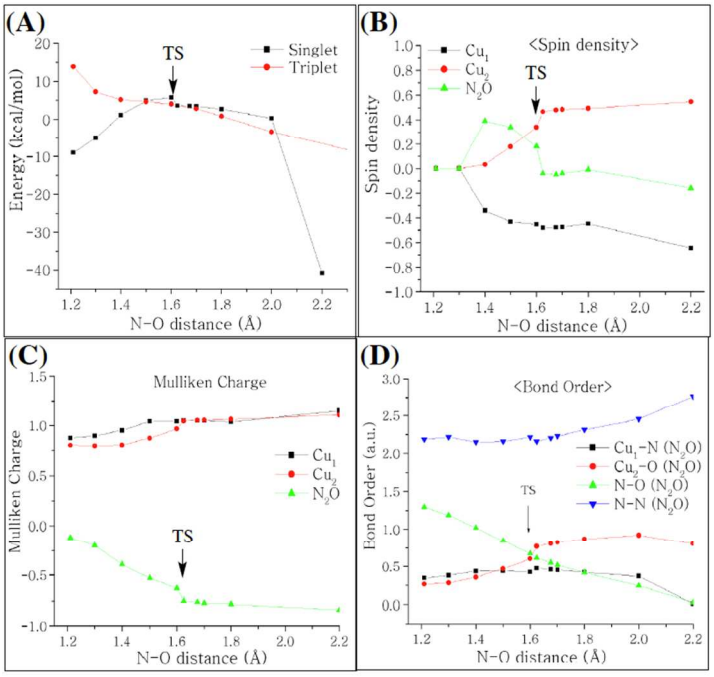


Figure S5. Calculated (A) spin densities (B) Mulliken charges (C) Mayer bond orders for site-6 with a μ-1,1-O N_2O binding mode along the N-O singlet potential energy surface.

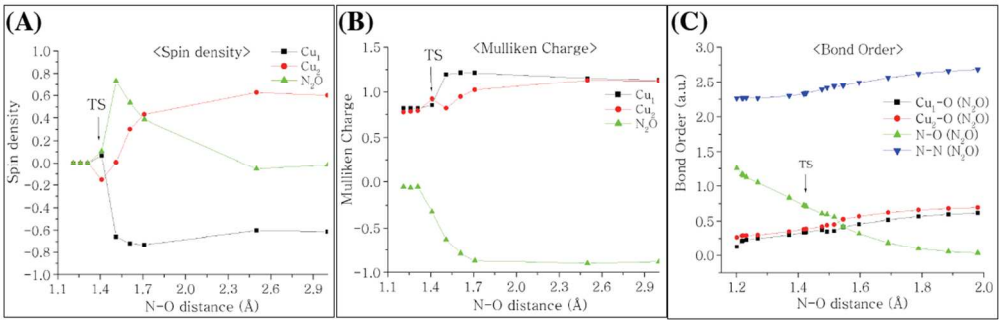


Figure S6. The η^1 N_2O binding modes for site-7 (A) η^1-O (B) η^1-N.

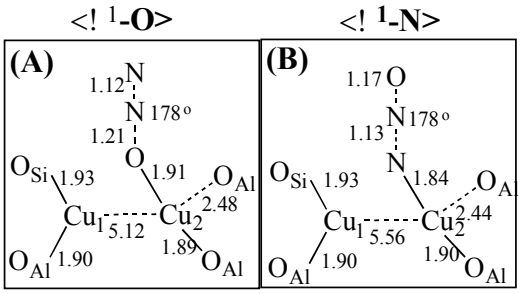


Figure S7. The η^1 N_2O binding modes for site-4 (A) η^1-O (B) η^1-N.

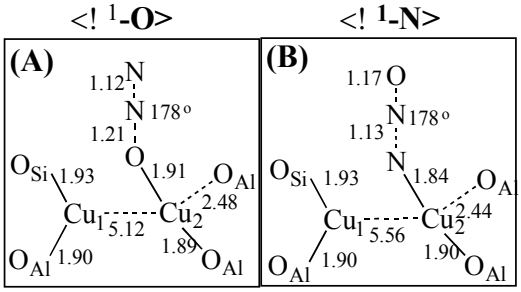


Figure S8. Calculated (A) spin densities (B) Mulliken charges (C) Mayer bond orders for site-7 with a μ-1,1-O N_2O binding mode along the N-O singlet potential energy surface.

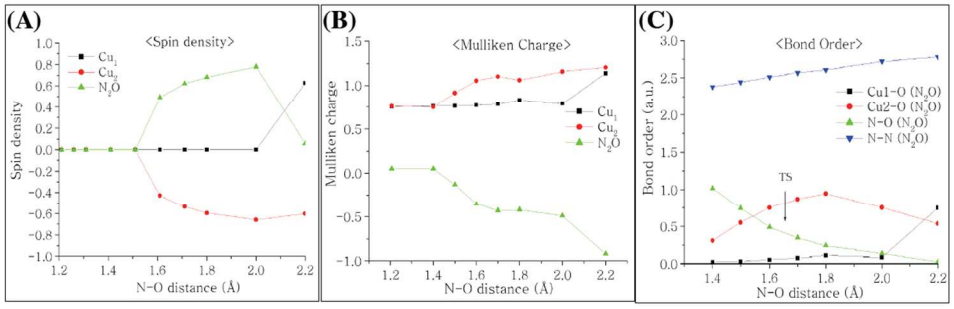
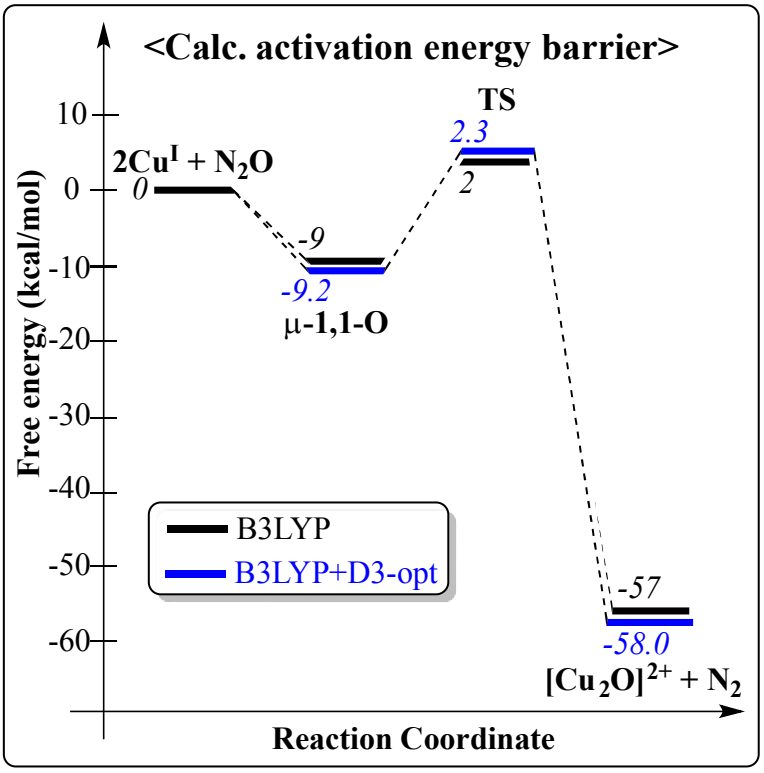


Figure S9. Calculated reaction coordinate for N_2O activation by the binuclear Cu^I site-6 via the μ-1,1-O reactant complex without (black) and with (blue) dispersion correction. Note that the dispersion correction was included by keyword EmpiricalDispersion=GD3 and calculated by Gaussian 09, Revision D.01.



Reference

Gaussian 09, Revision D.01,
M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2013.

Coordinates of $[Cu_2O]^{2+}$ for Site 1 (-10617.8206432 Hartrees)

Al	-4.82174	13.26370	5.88593
Al	1.51837	11.49049	2.39396
Si	3.49753	10.53320	4.60083
Si	4.43616	10.92644	7.43140
Si	2.50246	8.85457	0.63211
Si	5.95823	11.22549	2.88703
Si	3.71284	7.43207	4.41692
Si	2.38100	13.26613	0.24058
Si	-1.44802	10.57939	2.32226
Si	-1.61691	13.27596	10.77014
Si	-1.32003	7.48884	2.51416
Si	-4.55488	16.33812	6.04205
Si	-2.50339	10.88361	-0.63217
Si	-4.08543	11.22528	3.68300
Si	-3.71786	12.30584	8.72137
Si	-7.66090	13.26676	6.33307
Si	-6.13309	13.24778	10.39315
Si	-6.54708	10.53224	1.97152
Si	-4.43630	8.81111	5.71056
Si	-3.49673	9.20626	8.54291
O	-0.19036	11.42658	2.95860
O	2.09778	11.23223	4.09547
O	-3.74462	12.30412	4.84697
O	-3.66004	13.00454	7.24002
H	4.28850	6.68383	3.27593
H	2.37181	6.88871	4.75306
H	4.60064	7.28586	5.60172
H	6.85482	12.39918	3.00641
H	5.31449	11.20004	1.55429
H	6.74062	9.97900	3.09302
H	2.06414	7.60233	1.31671
H	3.99263	8.84768	0.61040
H	2.02406	8.78200	-0.77631
H	2.58071	14.72033	-0.01193
H	1.30699	12.78760	-0.67941
H	3.64225	12.56623	-0.14234
H	-1.74139	10.63542	-1.87827
H	-2.97776	12.28907	-0.59607
H	-3.67282	9.96810	-0.57533
H	-2.64115	6.87649	2.81120
H	-0.27837	6.79938	3.31452
H	-1.02926	7.33733	1.06725
H	-3.59188	7.60061	5.71025
H	-5.85257	8.47423	5.97639

H	-3.96132	9.84278	6.63746
H	-7.35157	11.43116	1.11128
H	-7.43860	9.79232	2.90018
H	-5.80749	9.55909	1.12681
H	-7.50088	14.34627	7.35297
H	-8.74899	12.36873	6.81441
H	-8.11830	13.89954	5.06539
H	-3.08640	16.55680	5.88351
H	-4.85981	16.43818	7.50059
H	-5.26440	17.44479	5.34568
H	-3.23969	8.87680	9.97604
H	-2.55527	8.38830	7.76085
H	-4.91858	8.84036	8.34200
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H	-6.07395	14.65348	9.92630
H	-5.61210	13.16479	11.78231
H	-1.62487	14.61187	11.41358
H	-0.28324	13.03098	10.15982
H	-1.87250	12.22943	11.79536
H	3.87625	10.42063	8.70788
H	4.56795	12.40383	7.49586
H	5.77311	10.32196	7.19854
O	1.99392	13.03391	1.81710
O	1.91133	10.17013	1.38266
O	3.37848	10.48750	6.22793
O	3.59038	9.02549	3.98639
O	4.79748	11.37697	4.09267
O	-5.01896	14.89761	5.42464
O	-6.28214	12.39359	6.15413
O	-1.45786	10.56442	0.66745
O	-5.46532	11.50057	2.83610
O	-4.24551	9.68074	4.28828
O	-2.83278	11.32577	2.67782
O	-3.08333	10.82640	8.44658
O	-2.77278	13.25691	9.61816
O	-5.20417	12.25745	9.39183
O	-1.33580	9.08405	2.95240
Cu	0.34941	11.03880	4.84102
Cu	-2.41503	11.88449	6.25603
O	-1.07065	10.84013	5.83872
N	1.99533	40.30122	-30.78820
N	3.03548	40.43702	-30.47252

Coordinates of $[Cu_2O]^{2+}$ for Site 2 (-10617.8526561Hartrees)

Al	3.65188	10.64155	4.51992
Al	-4.05619	11.25257	3.76739
Si	1.57926	11.27256	2.49435
Si	4.43640	10.92671	7.43180
Si	7.54230	10.88340	7.20310
Si	2.50271	8.85458	0.63208
Si	5.95811	11.22550	2.88729
Si	4.08690	8.51250	9.45830
Si	3.71290	7.43189	4.41700
Si	2.38131	13.26630	0.24049
Si	3.91160	13.24819	9.32029
Si	-1.44851	10.57958	2.32219
Si	-1.31990	7.48860	2.51410
Si	-4.55441	16.33913	6.04271
Si	-4.55441	13.26784	6.04265
Si	-2.50320	10.88350	-0.63209
Si	-3.71260	12.30660	8.72503
Si	-7.66429	13.26591	6.33050
Si	-6.54730	10.53221	1.97130
Si	-4.43589	8.81100	5.71020
O	3.27778	10.88651	6.26210
O	1.98218	11.19646	4.08139
O	-4.61811	12.67693	4.55393
O	-2.32600	11.46628	3.38744
H	-0.94653	6.66663	3.69006
H	-0.39059	7.20694	1.39133
H	-2.70487	7.16016	2.09305
H	-1.24751	11.08350	-1.40144
H	-3.25428	12.16361	-0.58629
H	-3.32405	9.83849	-1.28802
H	2.75148	7.50676	1.19522
H	3.70082	9.31569	-0.11150
H	1.35317	8.77999	-0.31061
H	3.65607	14.01897	0.18247
H	1.24264	14.19348	0.01574
H	2.36821	12.22369	-0.82108
H	4.44687	6.58756	3.43609
H	2.25472	7.13183	4.28305
H	4.11704	6.99384	5.78734
H	6.70515	12.39535	2.34333
H	5.37470	10.49439	1.72578
H	6.95554	10.32378	3.53386
H	-6.51950	10.46436	0.48368
H	-7.29444	11.76120	2.36398
H	-7.31037	9.35261	2.47032

H	-4.24035	7.58761	4.89077
H	-5.88037	9.15384	5.74790
H	-3.94783	8.54693	7.08943
H	3.71421	8.75299	10.87454
H	5.48603	8.01797	9.38986
H	3.17363	7.49525	8.87830
H	8.35559	9.73290	6.74658
H	7.73741	11.08531	8.66335
H	7.93489	12.11461	6.47760
H	-8.44434	13.38265	7.58777
H	-8.01163	11.98548	5.65919
H	-8.01563	14.39415	5.42862
H	-3.41163	17.27240	5.88818
H	-5.26349	16.64152	7.31477
H	-5.50374	16.53132	4.91368
H	-2.44226	11.72998	9.22886
H	-4.84091	11.43805	9.14685
H	-3.90116	13.67107	9.27786
H	4.27568	14.68004	9.19883
H	4.47007	12.70011	10.58395
H	2.42784	13.12161	9.35843
O	-0.02796	11.37731	2.23016
O	2.25594	12.56227	1.75132
O	2.14942	9.88682	1.86391
O	4.03397	9.00708	4.17892
O	4.81465	11.75512	3.93186
O	4.52496	12.45692	8.00375
O	5.92239	10.50867	6.89260
O	3.92823	9.94476	8.63682
O	-3.94979	14.79312	6.05619
O	-3.59980	12.34766	7.04473
O	-6.05372	13.30583	6.73124
O	-2.14927	10.37088	0.89065
O	-5.02012	10.52820	2.56094
O	-3.58180	10.08561	5.08191
O	-1.20791	9.08987	2.98446
Cu	1.37560	11.24340	5.95561
Cu	-1.87750	10.92853	5.35433
O	-0.36259	11.37831	6.11582
N	-6.58965	47.53664	-21.06839
N	-5.62520	47.27058	-21.51452

Coordinates of $[Cu_2O]^{2+}$ for Site 3 (-10617.8455191 Hartrees)

Al	4.26896	10.93475	7.62692
Al	-1.39172	10.49833	2.36991
Si	1.57918	11.27252	2.49417
Si	3.49715	10.53277	4.59978
Si	7.54245	10.88340	7.20307
Si	2.50271	8.85459	0.63211
Si	5.95811	11.22550	2.88728
Si	4.08689	8.51251	9.45828
Si	3.71288	7.43191	4.41699
Si	6.33230	12.30604	10.98810
Si	2.38133	13.26631	0.24053
Si	1.31972	12.24968	10.62779
Si	3.91164	16.35877	9.32030
Si	3.91086	13.24809	9.32035
Si	-1.31989	7.48859	2.51410
Si	-4.55441	13.26786	6.04265
Si	-2.50320	10.88348	-0.63207
Si	-4.08617	11.22512	3.68379
Si	-6.54736	10.53217	1.97128
Si	-4.43592	8.81099	5.71020
O	3.45245	12.56004	7.88131
O	3.20241	10.66797	6.19894
O	-2.46954	11.49174	3.44748
O	-0.01929	11.59647	2.75803
H	4.44350	6.72856	3.33511
H	2.34268	6.87548	4.53896
H	4.43511	7.25038	5.70119
H	2.57924	7.51085	1.24931
H	3.87533	9.34989	0.35554
H	1.74053	8.78464	-0.63721
H	3.52181	14.21304	0.28284
H	1.12330	14.01356	-0.01613
H	2.59328	12.28333	-0.85465
H	6.87849	12.38069	3.00643
H	5.29473	11.25907	1.55883
H	6.71927	9.95637	3.00967
H	8.08636	10.82366	5.81662
H	8.14280	9.75928	7.97608
H	8.01409	12.15857	7.81743
H	2.93029	7.77783	10.04488
H	5.11793	8.65363	10.52952
H	4.67523	7.65494	8.38701
H	5.67413	12.09885	12.30372
H	7.08808	13.58442	11.01907

H	7.24855	11.18122	10.69824
H	4.88672	17.22142	8.61106
H	3.88519	16.71837	10.76131
H	2.55636	16.56702	8.74286
H	0.31822	13.07363	11.34812
H	1.64559	11.04410	11.42336
H	0.75389	11.85326	9.30526
H	-1.00628	6.46111	3.54720
H	-0.39815	7.26051	1.36302
H	-2.70823	7.23844	2.02894
H	-1.60238	10.69342	-1.80506
H	-2.83686	12.33599	-0.55105
H	-3.76605	10.14089	-0.90568
H	-7.04516	11.23724	0.76717
H	-7.46898	10.77351	3.11244
H	-6.46085	9.07454	1.70887
H	-4.09933	7.41895	5.32866
H	-5.83350	8.85684	6.21680
H	-3.52555	9.25897	6.80045
H	-5.29294	14.54567	5.90449
H	-3.12716	13.55796	6.36515
H	-5.13509	12.47290	7.15613
O	2.16234	11.23523	4.00096
O	2.30388	12.49889	1.70527
O	1.72447	9.88508	1.67530
O	3.64771	9.02928	4.02333
O	4.82265	11.35999	4.10825
O	5.91295	10.78675	7.18086
O	3.59793	9.96222	8.88978
O	5.18674	12.34782	9.78317
O	2.66513	13.20502	10.38353
O	4.39142	14.78693	9.12337
O	-4.65032	12.43750	4.62301
O	-1.78071	10.34525	0.72127
O	-5.00942	11.15973	2.32355
O	-4.28307	9.77875	4.39747
O	-1.14836	8.98369	3.17046
Cu	1.87596	12.09797	6.70885
Cu	-0.77179	11.92780	4.56810
O	0.25321	12.25088	5.98478
N	-4.87255	47.90423	-21.00811
N	-3.91562	47.64752	-21.47541

Coordinates of $[Cu_2O]^{2+}$ for Site 4 (-10617.8173630 Hartrees)

Al	1.58718	11.48529	2.41289
Al	3.88945	13.32490	9.27580
Si	3.49710	10.53298	4.59914
Si	4.43636	10.92656	7.43199
Si	7.54227	10.88345	7.20308
Si	2.50247	8.85492	0.63234
Si	1.44812	9.15794	10.81994
Si	5.95802	11.22547	2.88747
Si	4.08691	8.51250	9.45830
Si	3.71295	7.43188	4.41700
Si	6.33201	12.30604	10.98795
Si	2.38125	13.26604	0.24083
Si	1.31954	12.25022	10.62727
Si	3.91159	16.35869	9.32037
Si	-1.44802	10.57894	2.32232
Si	-1.61737	13.27568	10.76997
Si	-1.31994	7.48880	2.51413
Si	2.38073	13.26582	13.38260
Si	-2.50333	10.88369	-0.63227
Si	-4.08627	11.22507	3.68368
O	2.09749	13.24792	9.58448
O	3.61919	12.28114	7.83555
O	-0.09049	11.19500	3.01350
O	2.17052	11.36965	4.12625
H	1.82953	7.69536	1.28688
H	3.96795	8.59121	0.64857
H	2.05756	8.87761	-0.78970
H	2.39089	14.71998	-0.08394
H	1.53443	12.58194	-0.78029
H	3.77523	12.76069	0.08594
H	3.95712	6.63296	3.19408
H	2.52170	6.90140	5.12993
H	4.89459	7.33225	5.31539
H	6.85981	12.39330	3.02418
H	5.33029	11.22002	1.54560
H	6.73800	9.97256	3.07033
H	8.14966	10.76137	5.85404
H	7.64674	9.57835	7.90424
H	8.25750	11.92885	7.97150
H	3.60506	8.90940	10.77720
H	5.32491	7.72440	9.71934
H	3.19577	7.65746	8.65141
H	6.44941	12.32243	12.47230
H	7.25410	13.33575	10.43175
H	6.80318	10.97394	10.51329

H	4.94950	17.37873	9.00774
H	3.69285	16.36430	10.79905
H	2.63298	16.79846	8.68655
H	1.52829	8.16550	9.74553
H	-0.00676	9.23348	11.15720
H	2.10065	8.74631	12.08332
H	1.45914	13.64646	14.48238
H	3.07816	14.47547	12.88141
H	3.37190	12.28603	13.89155
H	-2.59819	13.27938	9.65775
H	-1.23369	14.67343	11.10049
H	-2.22264	12.63812	11.96663
H	-4.82626	12.50801	3.75933
H	-3.83663	10.72278	5.06160
H	-4.90450	10.22541	2.94732
H	-2.46389	6.65590	2.96163
H	-0.09673	7.06845	3.24056
H	-1.12409	7.32249	1.05283
H	-1.84210	10.30934	-1.82573
H	-2.75005	12.33317	-0.82439
H	-3.79389	10.18895	-0.38527
O	1.80319	13.06157	1.76728
O	2.13650	10.25436	1.37121
O	3.55496	10.29209	6.20917
O	3.45212	9.01608	3.95480
O	4.79577	11.35169	4.06984
O	5.95303	11.32551	7.01605
O	4.49379	9.86373	8.63762
O	1.83111	10.71054	10.28740
O	-0.27983	12.40277	10.25674
O	4.77251	12.56534	10.54351
O	1.47143	12.58731	12.19341
O	4.37712	14.88938	8.77815
O	-1.46822	10.64274	0.68657
O	-2.65641	11.51699	2.90756
O	-1.67188	9.06564	2.88305
Cu	1.64894	12.41210	7.81944
Cu	0.36640	11.45434	4.88854
O	0.55858	11.75755	6.60985
N	-4.39869	34.80356	-34.66875
N	-3.34232	34.93206	-34.40884

Coordinates of $[Cu_2O]^{2+}$ for Site 5 (-10617.8183453 Hartrees)

Al	3.75136	10.52826	4.53995
Al	1.39809	12.10134	10.76758
Si	1.57932	11.27245	2.49433
Si	4.43640	10.92672	7.43180
Si	7.54229	10.88340	7.20310
Si	2.50269	8.85463	0.63211
Si	1.44809	9.15819	10.81980
Si	5.95811	11.22550	2.88729
Si	4.08690	8.51249	9.45830
Si	3.71290	7.43190	4.41700
Si	6.33210	12.30610	10.98800
Si	2.38130	13.26632	0.24046
Si	3.91160	16.35879	9.32030
Si	3.91159	13.24821	9.32031
Si	-1.44850	10.57960	2.32219
Si	-1.61732	13.27576	10.76989
Si	-1.61730	16.33121	10.76990
Si	2.38071	13.26591	13.38251
Si	-3.71259	12.30661	8.72501
Si	-2.50320	10.88351	12.50990
O	-0.20942	12.66047	10.12053
O	2.29900	13.24931	9.69801
O	2.14106	11.16470	4.03052
O	3.28861	10.72090	6.25913
H	3.71551	8.74009	10.85533
H	5.44999	7.90520	9.50954
H	3.23075	7.57109	8.71230
H	8.32341	10.79665	5.94848
H	7.96750	9.80860	8.13482
H	7.76528	12.20342	7.84534
H	6.41054	12.24459	12.46592
H	7.20889	13.38960	10.47620
H	6.77161	11.00979	10.41634
H	4.77727	17.23217	8.49188
H	4.05795	16.72927	10.75156
H	2.49127	16.55408	8.91761
H	1.53517	7.98698	9.93025
H	-0.01517	9.24298	11.15042
H	2.10258	8.88841	12.12456
H	1.63270	13.66425	14.60624
H	2.74562	14.51147	12.64397
H	3.64779	12.61049	13.81267
H	-3.76323	10.95142	13.29207
H	-1.41977	10.33146	13.35320

H	-2.71612	10.01541	11.32254
H	-0.92397	17.26034	11.69330
H	-3.07397	16.62175	10.76639
H	-1.08507	16.52091	9.39189
H	-4.35034	13.08077	7.63412
H	-4.75543	11.76740	9.63481
H	-2.93783	11.17669	8.14792
H	4.26225	6.45228	3.44197
H	2.23437	7.23450	4.49329
H	4.27038	7.09968	5.76221
H	6.78750	12.39430	2.47396
H	5.24064	10.74810	1.66874
H	6.89125	10.14643	3.31671
H	2.73067	7.52571	1.24546
H	3.76966	9.38255	0.07238
H	1.51121	8.71231	-0.46800
H	3.62357	14.07259	0.22377
H	1.20849	14.14706	0.00422
H	2.43438	12.23742	-0.83203
H	-2.59796	11.46148	2.63909
H	-1.48613	9.38473	3.20629
H	-1.53533	10.13863	0.90593
O	-0.05360	11.46224	2.58464
O	2.25109	12.54115	1.73214
O	1.88746	9.86801	1.76628
O	4.10095	8.95185	3.97160
O	4.92323	11.69246	4.06564
O	4.22730	12.47445	7.92443
O	5.92680	10.69895	6.81693
O	4.20035	9.94685	8.67900
O	1.84656	10.56728	10.09469
O	4.73919	12.59490	10.57024
O	1.46483	12.26774	12.46441
O	4.37426	14.79119	9.06782
O	-1.31824	14.78856	11.28710
O	-2.70266	13.33750	9.54794
O	-2.12388	12.41658	12.03256
Cu	0.71499	13.15638	8.48478
Cu	1.71662	11.91334	5.72123
O	0.79385	12.97467	6.75939
N	-1.12762	48.17316	-21.79685
N	-0.24657	47.65477	-22.19055

Coordinates of $[Cu_2O]^{2+}$ for Site 6 (-10617.831230 Hartrees)

Al	4.32534	10.82024	7.54214
Al	-1.59137	13.26462	10.79064
Si	1.57928	11.27250	2.49435
Si	3.49726	10.53275	4.59971
Si	7.54247	10.88345	7.20312
Si	1.44807	9.15835	10.81974
Si	5.95807	11.22553	2.88729
Si	4.08691	8.51251	9.45831
Si	3.71287	7.43192	4.41701
Si	6.33253	12.30605	10.98814
Si	1.31984	12.24946	10.62813
Si	3.91166	16.35890	9.32033
Si	3.91037	13.24779	9.31996
Si	-1.61733	16.33126	10.76987
Si	2.38064	13.26590	13.38244
Si	-4.55443	13.26791	6.04256
Si	-3.71246	12.30698	8.72530
Si	-6.13344	13.24812	10.39259
Si	-3.49771	9.20569	8.54226
Si	-2.50319	10.88344	12.50990
O	-2.39821	13.20062	9.15939
O	-0.19258	12.39473	10.02890
O	3.20470	10.86529	6.15346
O	3.89267	12.55840	7.83231
H	1.57472	13.77394	14.51628
H	3.23326	14.35458	12.83860
H	3.25335	12.15579	13.84516
H	6.34635	13.18484	12.18593
H	7.34553	12.78898	10.01878
H	6.62556	10.91139	11.38721
H	1.73465	8.24927	9.70436
H	-0.03376	9.12719	10.96580
H	2.01364	8.69426	12.10541
H	5.08822	17.23234	9.09669
H	3.30593	16.65824	10.64137
H	2.90682	16.58806	8.25003
H	3.87091	8.76156	10.90338
H	5.57129	8.43727	9.31097
H	3.56504	7.16007	9.12341
H	8.19162	10.20291	6.04728
H	8.25997	10.46013	8.43916
H	7.75188	12.35287	7.04474
H	-1.47660	10.79789	13.58911
H	-2.15833	9.85588	11.49583
H	-3.82331	10.52632	13.09915

H	-0.93204	17.37638	11.57836
H	-3.08938	16.48797	10.95949
H	-1.32789	16.61143	9.32949
H	-7.42597	13.68739	9.81126
H	-5.62839	14.28791	11.32118
H	-6.32293	11.96830	11.11987
H	-3.62208	8.23387	9.65133
H	-2.18624	9.04152	7.86391
H	-4.59009	8.99112	7.55922
H	-4.00103	13.06948	4.68049
H	-4.43925	14.70215	6.41479
H	-5.98412	12.86668	6.05707
H	4.60810	7.09773	3.28016
H	2.55448	6.50675	4.42453
H	4.46618	7.31306	5.69013
H	7.21932	11.85365	3.34514
H	5.20974	12.17921	2.02650
H	6.26587	10.00468	2.09779
H	1.11731	12.57740	1.96139
H	0.40170	10.45260	2.87848
H	2.34438	10.55558	1.43952
O	2.53550	11.58227	3.80073
O	3.12124	8.98518	4.22810
O	5.06118	10.82701	4.22877
O	5.96835	10.50059	7.28157
O	3.48366	9.69201	8.52361
O	1.85867	10.72865	10.48620
O	4.82003	12.32344	10.29871
O	1.32097	12.70990	12.20512
O	2.33244	13.24942	9.79901
O	4.45260	14.78057	9.27336
O	-3.65308	12.31317	7.07417
O	-1.08965	14.84874	11.20284
O	-3.60523	10.74816	9.20288
O	-5.08221	13.04479	9.14095
O	-2.57877	12.39411	11.88297
Cu	-0.74453	12.88055	8.18885
Cu	2.16201	12.34247	6.87330
O	0.50957	12.90890	6.95953
N	-2.24703	43.29585	-27.55060
N	-1.28602	42.84105	-27.81443

Coordinates of $[Cu_2O]^{2+}$ for Site 7 (-10617.8170927 Hartrees)

Al	3.87225	13.33922	9.17836
Al	-3.65998	12.14059	8.85691
Si	3.49705	10.53278	4.59956
Si	4.43654	10.92684	7.43199
Si	7.54219	10.88342	7.20306
Si	1.44810	9.15827	10.81979
Si	4.08688	8.51249	9.45834
Si	6.33205	12.30612	10.98799
Si	1.31940	12.24925	10.62783
Si	3.91163	16.35871	9.32028
Si	-1.61729	13.27579	10.76988
Si	-1.61732	16.33123	10.76990
Si	2.38071	13.26596	13.38255
Si	-4.55440	16.33906	6.04267
Si	-4.55435	13.26798	6.04284
Si	-4.08631	11.22499	3.68369
Si	-7.66431	13.26589	6.33049
Si	-6.13348	13.24818	10.39264
Si	-3.49769	9.20583	8.54230
Si	-2.50320	10.88352	12.50989
O	-3.48398	12.62236	7.11009
O	-2.44553	13.39042	9.33285
O	3.55021	12.29044	7.71538
O	2.11075	13.26062	9.60921
H	-3.70482	10.80951	13.37577
H	-1.28500	10.72784	13.34608
H	-2.54519	9.82368	11.48759
H	1.41829	13.55368	14.47543
H	2.93722	14.54130	12.86446
H	3.48093	12.42250	13.91202
H	-0.78040	17.25649	11.56945
H	-3.05276	16.65305	10.96762
H	-1.27662	16.46383	9.32975
H	1.57920	8.14208	9.77471
H	-0.00470	9.16054	11.15957
H	2.12932	8.83440	12.09303
H	-7.49174	13.37144	9.79251
H	-5.52492	14.61151	10.42240
H	-6.29960	12.79067	11.80007
H	-2.45890	8.29552	7.98072
H	-4.54812	9.38788	7.49268
H	-4.13539	8.51195	9.69618
H	-8.35331	14.36933	7.04091
H	-8.21901	11.96009	6.76215
H	-7.86261	13.42385	4.86516

H	-3.60071	17.27663	5.40292
H	-4.60082	16.60006	7.50477
H	-5.91156	16.54208	5.47111
H	-4.18094	11.67150	2.27221
H	-4.93637	10.02395	3.88073
H	-2.67359	10.88044	3.99715
H	6.30980	12.33009	12.47628
H	7.34847	13.29038	10.51941
H	6.78676	10.95237	10.56256
H	4.85873	17.39312	8.82165
H	4.05747	16.27423	10.80434
H	2.52528	16.83386	9.03693
H	3.65757	8.79928	10.82281
H	5.37894	7.77976	9.60330
H	3.21096	7.65385	8.63868
H	8.05541	10.77847	5.81320
H	7.62482	9.55222	7.85608
H	8.35236	11.86966	7.95477
H	3.14585	9.30044	3.85501
H	4.68759	11.17613	3.98788
H	2.35224	11.48436	4.53557
O	3.78815	10.11679	6.17231
O	5.96439	11.41410	7.14716
O	4.38574	9.94505	8.71214
O	1.76476	10.70021	10.22624
O	-0.27264	12.43823	10.37131
O	4.84169	12.63543	10.39772
O	1.58685	12.46089	12.19846
O	4.21089	14.91906	8.59575
O	-4.01079	14.79225	5.74114
O	-4.60823	12.44813	4.65205
O	-6.04171	13.33948	6.70222
O	-1.28951	14.77917	11.30720
O	-2.82369	10.63408	8.96638
O	-5.22226	12.19645	9.53601
O	-2.50901	12.41911	11.82905
Cu	-1.64237	13.17800	7.49896
Cu	1.68312	12.82964	7.69039
O	0.08142	13.38528	7.22994
N	-6.63183	44.58820	-25.83074
N	-5.58033	44.86682	-25.70146

Coordinates of $[Cu_2O]^{2+}$ for Site 8 (-10617.8248218 Hartrees)

Al	1.31957	12.16123	10.67756
Al	-4.60261	13.43020	5.98364
Si	4.43673	10.92762	7.43137
Si	1.44811	9.15372	10.82069
Si	6.33326	12.30704	10.98846
Si	3.91176	16.36086	9.31899
Si	3.90747	13.24425	9.32135
Si	-1.44948	10.57900	2.32378
Si	-1.61865	13.27105	10.77919
Si	-1.61704	16.33351	10.76852
Si	2.38329	13.26767	13.38426
Si	-4.55609	16.33849	6.03970
Si	-4.08140	11.23964	3.67052
Si	-3.71156	12.30656	8.71720
Si	-7.66115	13.26500	6.33320
Si	-6.13429	13.24929	10.39498
Si	-6.55439	10.52797	1.97022
Si	-4.42941	8.80804	5.71830
Si	-3.50320	9.20287	8.54371
Si	-2.50175	10.88523	12.50855
O	-4.56816	12.37836	4.66322
O	-3.43411	12.88963	7.21757
O	-0.22261	12.83435	10.01950
O	2.27904	13.29526	9.63091
H	-2.52830	10.83795	13.98981
H	-1.66203	9.78532	11.98025
H	-3.88519	10.74057	11.98819
H	-7.55474	12.86055	10.24621
H	-5.98134	14.71652	10.23358
H	-5.64271	12.85172	11.73841
H	-1.92821	17.23139	11.90569
H	-2.70077	16.42152	9.75282
H	-0.34523	16.77147	10.13071
H	-3.17361	8.61118	9.87582
H	-2.52935	8.59211	7.62386
H	-4.91435	8.78566	8.34933
H	-3.63421	17.48944	5.83187
H	-5.07672	16.42164	7.42564
H	-5.64506	16.39919	5.03943
H	-8.52451	13.66055	7.47964
H	-7.62422	11.77507	6.27318
H	-8.30128	13.75944	5.08170
H	-3.48864	7.67349	5.78129
H	-5.82350	8.32559	5.88387

H	-4.17784	9.90005	6.67691
H	-7.13895	11.30696	0.85001
H	-7.48173	10.57505	3.13357
H	-6.40075	9.11106	1.54491
H	-0.43447	11.50510	1.76241
H	-2.12364	9.85140	1.21731
H	-0.76782	9.59471	3.20610
H	1.62620	13.61256	14.61839
H	2.84610	14.54566	12.76161
H	3.60013	12.50803	13.79181
H	4.78341	17.22419	8.48737
H	3.97748	16.79490	10.73664
H	2.50220	16.48612	8.84479
H	2.66497	8.31316	10.63345
H	0.28945	8.39845	10.26360
H	1.22268	9.32175	12.28368
H	6.41659	11.07406	11.80361
H	6.78400	13.47707	11.78171
H	7.18446	12.17633	9.77746
H	5.46581	10.95283	6.36173
H	3.19031	10.32812	6.89500
H	4.93367	10.12143	8.57395
O	4.15125	12.49645	7.89644
O	1.62869	10.59088	10.05403
O	4.72461	12.51180	10.53289
O	1.44219	12.40807	12.36384
O	4.41803	14.79063	9.15392
O	-3.63705	14.95680	5.81234
O	-6.15956	13.90285	6.53167
O	-1.45923	14.79541	11.33354
O	-5.07441	11.19943	2.34883
O	-4.21039	9.68825	4.30927
O	-2.53368	11.48788	3.19869
O	-3.18223	10.79459	8.77081
O	-2.83391	13.27124	9.70303
O	-5.26950	12.42895	9.20331
O	-1.88165	12.34208	12.06367
Cu	-2.10794	14.34642	6.82726
Cu	0.71212	13.80740	8.57821
O	-0.44374	14.36255	7.37557
N	-9.01435	45.17813	-25.20177
N	-7.95091	45.40788	-25.07408

Coordinates of $[Cu_2O]^{2+}$ for Site 9 (-10617.8150286 Hartrees)

Al	-1.55775	13.23755	10.76450
Al	-4.18855	11.13646	3.59818
Si	1.57922	11.27252	2.49432
Si	1.44809	9.15818	10.81982
Si	1.31940	12.24948	10.62773
Si	3.91154	13.24821	9.32034
Si	-1.44830	10.57937	2.32207
Si	-1.61732	16.33122	10.76988
Si	-1.31992	7.48871	2.51412
Si	2.38070	13.26591	13.38252
Si	-4.55439	16.33908	6.04273
Si	-4.55451	13.26795	6.04255
Si	-2.50324	10.88354	-0.63208
Si	-3.71227	12.30679	8.72560
Si	-7.66433	13.26589	6.33050
Si	-6.13354	13.24818	10.39255
Si	-6.54733	10.53221	1.97130
Si	-4.43588	8.81097	5.71018
Si	-3.49777	9.20572	8.54219
Si	-2.50323	10.88349	12.50987
O	-2.37492	11.41329	3.41013
O	-4.49388	12.47979	4.65841
O	-0.18737	12.28036	10.04042
O	-2.27840	12.98927	9.12676
H	-2.92041	8.51676	9.73180
H	-2.37932	9.32775	7.58133
H	-4.65526	8.36452	8.17055
H	-6.75143	14.59379	10.32773
H	-5.73058	12.94748	11.78743
H	-7.11506	12.22872	9.93793
H	-8.42056	13.90772	7.43512
H	-8.04691	11.83199	6.24946
H	-8.01003	13.93418	5.04904
H	-3.51398	17.27136	5.54335
H	-4.87886	16.67068	7.45344
H	-5.78166	16.48100	5.21594
H	-3.30685	7.89162	6.00117
H	-5.70262	8.04445	5.87501
H	-4.47901	9.94584	6.66379
H	-7.36188	11.26890	0.96339
H	-7.29878	10.56770	3.26458
H	-6.47377	9.10716	1.53778
H	-1.08646	6.68936	3.74131
H	-0.33049	7.09210	1.47705

H	-2.68915	7.24940	2.00006
H	-1.31204	10.57233	-1.46689
H	-2.76327	12.34308	-0.68898
H	-3.66989	10.12766	-1.14150
H	2.23059	12.54435	2.09964
H	2.14153	10.15098	1.69971
H	1.82623	11.02229	3.93942
H	-2.03285	10.80185	13.92124
H	-1.61867	10.00337	11.69355
H	-3.88421	10.33522	12.44855
H	-0.84518	17.33512	11.55193
H	-3.05292	16.43826	11.16169
H	-1.52013	16.70320	9.32681
H	2.61627	8.29292	10.52369
H	0.31890	8.77440	9.93322
H	1.04624	8.98308	12.23784
H	1.57368	13.56001	14.58791
H	3.11371	14.48048	12.94505
H	3.35778	12.18562	13.67674
H	4.19671	14.60489	8.79602
H	4.26871	12.23372	8.29610
H	4.71286	13.00703	10.54880
O	-0.05606	11.44476	2.21690
O	1.90519	10.72475	10.51955
O	1.32823	12.76293	12.17620
O	2.27542	13.17278	9.66231
O	-3.92910	14.78918	5.92340
O	-3.65530	12.38573	7.09422
O	-6.05827	13.42295	6.66804
O	-2.20761	10.40029	0.91920
O	-1.01852	14.83433	11.03751
O	-5.06439	11.22879	2.11001
O	-4.28618	9.51136	4.24428
O	-3.89733	10.73224	9.11951
O	-4.81381	13.25872	9.40689
O	-1.08829	9.09612	2.91970
O	-2.45831	12.43086	11.97325
Cu	-1.57286	11.99729	4.99301
Cu	-0.70297	12.39409	8.19118
O	-0.62892	12.23261	6.43617
N	-0.86499	43.65907	-26.90139
N	0.20047	43.54395	-26.67442

Coordinates of $[Cu_2O]^{2+}$ for Site 10 (-10617.8094460 Hartrees)

Al	-1.41143	10.52662	2.28000
Al	-3.75971	12.08640	8.89987
Si	1.57928	11.27250	2.49431
Si	3.49711	10.53280	4.59970
Si	2.50271	8.85459	0.63209
Si	2.38131	13.26631	0.24050
Si	1.31940	12.24951	10.62789
Si	-1.61732	13.27574	10.76993
Si	-1.61730	16.33122	10.76989
Si	-1.31990	7.48860	2.51410
Si	-4.55440	16.33907	6.04270
Si	-4.55432	13.26799	6.04266
Si	-2.50318	10.88350	-0.63210
Si	-4.08650	11.22494	3.68378
Si	-7.66430	13.26590	6.33050
Si	-6.13347	13.24813	10.39265
Si	-6.54724	10.53221	1.97131
Si	-4.43588	8.81100	5.71016
Si	-3.49770	9.20589	8.54233
Si	-2.50320	10.88351	12.50990
O	-0.02848	11.59330	2.73256
O	-2.55868	11.62609	3.16091
O	-2.48092	13.31857	9.32185
O	-3.59006	12.45505	7.12121
H	-3.44661	7.85317	6.25005
H	-5.25725	7.95037	4.79404
H	-5.42774	9.35994	6.65262
H	-7.07408	11.58619	1.07118
H	-7.39779	10.44970	3.18757
H	-6.54472	9.22487	1.27478
H	-8.40316	14.19139	7.22151
H	-8.09680	11.86847	6.58280
H	-7.95819	13.61197	4.91379
H	-3.54448	17.27296	5.48991
H	-4.78402	16.65129	7.47673
H	-5.83100	16.48170	5.29709
H	-1.31875	6.51876	3.64612
H	-0.12466	7.18593	1.67229
H	-2.52850	7.21359	1.68298
H	-1.78076	10.77173	-1.93096
H	-2.90853	12.31103	-0.46135
H	-3.75475	10.07837	-0.74240
H	2.89919	7.58908	1.29397
H	3.71544	9.52305	0.08898
H	1.55158	8.58620	-0.47031

H	3.64429	14.04302	0.20303
H	1.22609	14.19252	0.11885
H	2.35742	12.30789	-0.89572
H	3.97912	11.28244	5.78651
H	4.57174	10.50378	3.56995
H	3.18400	9.13657	4.99924
H	-2.53566	8.10414	8.81851
H	-3.19773	9.73998	7.19470
H	-4.87235	8.68009	8.69566
H	-7.52734	13.54942	9.96286
H	-5.41643	14.55089	10.55047
H	-6.20304	12.61732	11.74273
H	-0.80365	17.24827	11.60200
H	-3.05496	16.67580	10.88785
H	-1.20123	16.45774	9.34570
H	-2.18898	11.00869	13.95768
H	-1.48887	10.00554	11.88011
H	-3.86825	10.33788	12.35811
H	1.78243	11.14524	9.75347
H	1.47210	11.85845	12.05381
H	2.14216	13.46006	10.36729
O	2.15313	11.29087	4.02328
O	2.32186	12.46528	1.68142
O	1.78599	9.83868	1.76726
O	-0.25231	12.55140	10.27011
O	-3.93271	14.78627	5.87983
O	-4.63730	12.50323	4.58624
O	-6.05149	13.43940	6.64072
O	-1.54840	10.36750	0.58056
O	-1.33633	14.78278	11.30891
O	-4.99444	10.92199	2.39261
O	-3.85125	9.99340	4.72086
O	-3.17783	10.54045	9.45541
O	-5.40101	12.29092	9.30900
O	-1.30337	9.01545	3.10723
O	-2.44091	12.43056	11.87453
Cu	-1.00284	12.33137	4.28489
Cu	-1.78417	13.20389	7.45031
O	-1.02702	13.15870	5.84596
N	-6.10722	48.87363	-18.93064
N	-5.13593	48.62134	-19.36989

Coordinates of binuclear Cu^{I} model for Site 1 (-10617.7057705 Hartrees)

Al	-4.76129	13.33920	5.93665
Al	1.48653	11.46486	2.40269
Si	3.49667	10.53410	4.59949
Si	4.43640	10.92665	7.43176
Si	2.50227	8.85418	0.63192
Si	5.95847	11.22540	2.88687
Si	3.71282	7.43170	4.41712
Si	2.38254	13.26699	0.24098
Si	-1.44930	10.57782	2.32313
Si	-1.61708	13.27575	10.76977
Si	-1.31992	7.48899	2.51412
Si	-4.55492	16.33813	6.04206
Si	-2.50326	10.88374	-0.63214
Si	-4.08589	11.22506	3.68289
Si	-3.71798	12.30632	8.72213
Si	-7.66050	13.26669	6.33301
Si	-6.13300	13.24764	10.39299
Si	-6.54693	10.53232	1.97150
Si	-4.43606	8.81142	5.71047
Si	-3.49672	9.20619	8.54284
O	-0.25345	11.55711	2.71665
O	2.00398	10.88921	4.05197
O	-3.74149	12.34457	4.81432
O	-3.85956	13.31479	7.48464
H	4.34863	6.62680	3.35050
H	2.25116	7.11493	4.47567
H	4.30762	7.07421	5.73278
H	6.68150	12.51376	2.77337
H	5.43064	10.81374	1.56648
H	6.88428	10.18302	3.40201
H	2.45641	7.60719	1.45831
H	3.93763	9.14253	0.35957
H	1.84432	8.52569	-0.66446
H	2.60407	14.72909	0.06876
H	1.15901	12.89593	-0.53304
H	3.53412	12.55605	-0.38961
H	-1.95813	10.23166	-1.84622
H	-2.33121	12.35433	-0.71375
H	-3.94634	10.55659	-0.50410
H	-2.67479	7.34354	1.93868
H	-1.15515	6.62367	3.70612
H	-0.26718	7.19552	1.52273
H	-4.79573	7.40888	5.38581
H	-5.50466	9.47899	6.46793
H	-3.10577	8.77567	6.35666

H	-7.23215	11.41618	1.00048
H	-7.54396	9.91051	2.88042
H	-5.82244	9.45490	1.24754
H	-7.53824	14.40690	7.29005
H	-8.68946	12.33944	6.88826
H	-8.18588	13.80494	5.04710
H	-3.07659	16.53212	6.12517
H	-5.08792	16.43192	7.43509
H	-5.11857	17.48036	5.26946
H	-3.69520	9.34220	10.00901
H	-2.17800	8.58191	8.30243
H	-4.59178	8.32236	8.09110
H	-7.47145	12.78031	9.96513
H	-5.89758	14.64073	9.94528
H	-6.02790	13.16851	11.87150
H	-0.50217	14.11448	10.26702
H	-1.09026	12.28535	11.74230
H	-2.62328	14.13824	11.44423
H	3.89200	10.34397	8.68373
H	4.58999	12.39388	7.59573
H	5.76678	10.32518	7.14884
O	2.23344	12.90507	1.83605
O	1.73629	10.07056	1.38991
O	3.36738	10.58066	6.22105
O	3.91403	9.02620	4.09302
O	4.69502	11.47357	3.98930
O	-4.95512	14.92885	5.32052
O	-6.24135	12.45758	6.16257
O	-1.64276	10.24655	0.70123
O	-5.47265	11.47172	2.85555
O	-4.16116	9.69252	4.32360
O	-2.85372	11.25577	2.67193
O	-3.49201	10.77614	7.97848
O	-2.30260	12.46767	9.50367
O	-4.97229	12.22726	9.74721
O	-1.12262	9.08588	3.11664
Cu	0.57003	9.61471	3.96636
Cu	-2.95011	11.40488	6.25088
N	-66.75972	-75.87165	-11.44956
N	-67.64554	-76.51374	-11.18195
O	-68.57795	-77.18954	-10.90019

Coordinates of binuclear Cu^{I} model for Site 2 (-10617.7204788 Hartrees)

Al	3.60926	10.44487	4.46091
Al	-4.23572	11.32152	3.57844
Si	1.57921	11.27266	2.49418
Si	4.43694	10.92688	7.43251
Si	7.54190	10.88336	7.20294
Si	2.50269	8.85459	0.63209
Si	5.95823	11.22547	2.88719
Si	4.08687	8.51250	9.45825
Si	3.71290	7.43190	4.41699
Si	2.38130	13.26629	0.24050
Si	3.91152	13.24803	9.32007
Si	-1.44854	10.57966	2.32189
Si	-1.31993	7.48855	2.51420
Si	-4.55440	16.33916	6.04269
Si	-4.55453	13.26779	6.04283
Si	-2.50320	10.88347	-0.63204
Si	-3.71257	12.30663	8.72497
Si	-7.66423	13.26591	6.33049
Si	-6.54717	10.53220	1.97132
Si	-4.43601	8.81093	5.71021
O	3.54401	10.32392	6.24043
O	2.03189	11.28556	4.09322
O	-4.46429	12.80687	4.52209
O	-2.42492	11.29584	3.45196
H	-0.78570	6.67577	3.63385
H	-0.59889	7.13300	1.26303
H	-2.76356	7.18832	2.32886
H	-1.31042	10.63900	-1.48642
H	-2.84265	12.32727	-0.68719
H	-3.63569	10.07066	-1.13427
H	2.49553	7.46482	1.14473
H	3.85753	9.21160	0.14759
H	1.54734	8.95045	-0.50564
H	3.55917	14.16719	0.24394
H	1.15651	14.06150	-0.03905
H	2.54125	12.24537	-0.82964
H	4.06126	6.37255	3.43013
H	2.30960	7.19017	4.86982
H	4.59329	7.23318	5.60950
H	6.80331	12.42863	2.63188
H	5.35622	10.82309	1.58445
H	6.87521	10.13001	3.32140
H	-7.21769	10.94122	0.70410
H	-7.45599	10.90736	3.09636
H	-6.43377	9.04520	1.96143

H	-4.26421	7.47146	5.08331
H	-5.55170	8.72681	6.69466
H	-3.18432	9.08433	6.50116
H	4.34268	8.63492	10.91483
H	4.95474	7.45404	8.88593
H	2.66066	8.16334	9.23483
H	8.34994	11.72429	6.29018
H	7.70132	9.44866	6.85501
H	7.99774	11.09437	8.60285
H	-8.40862	13.40182	7.60643
H	-8.12770	12.06447	5.59839
H	-7.88336	14.47638	5.49669
H	-3.40865	17.26079	6.23910
H	-5.61146	16.65268	7.04072
H	-5.11097	16.51252	4.67678
H	-2.38591	11.95004	9.28232
H	-4.72081	11.29159	9.09798
H	-4.11864	13.65832	9.16659
H	3.53809	14.65617	9.04855
H	5.34279	13.13924	9.68223
H	3.05497	12.69572	10.39686
O	-0.05548	11.45655	2.30831
O	2.27572	12.54605	1.73417
O	2.01857	9.87377	1.82818
O	3.90366	8.90496	3.74815
O	4.83362	11.59080	4.02083
O	3.61966	12.37858	7.84922
O	5.95560	11.34877	7.05679
O	4.44100	9.98788	8.77084
O	-3.99425	14.79101	6.26547
O	-3.50308	12.32004	7.00664
O	-6.04101	13.12535	6.72129
O	-2.16974	10.41727	0.90311
O	-5.08757	11.28069	2.08082
O	-4.68019	9.99333	4.62413
O	-1.08717	9.08383	2.89228
Cu	2.50924	12.23892	5.88832
Cu	-2.46401	11.61486	5.39715
N	-2.82715	-98.64725	1.43893
N	-2.67879	-99.65385	1.92195
O	-2.52261	-100.71339	2.43036

Coordinates of binuclear Cu^{I} model for Site 3 (-10617.6957782 Hartrees)

Al	4.24598	10.91262	7.66070
Al	-1.39497	10.51169	2.32679
Si	1.57912	11.27254	2.49421
Si	3.49716	10.53277	4.59979
Si	7.54245	10.88340	7.20307
Si	2.50272	8.85458	0.63210
Si	5.95812	11.22550	2.88728
Si	4.08689	8.51251	9.45828
Si	3.71288	7.43191	4.41699
Si	6.33230	12.30604	10.98810
Si	2.38134	13.26631	0.24052
Si	1.31972	12.24968	10.62779
Si	3.91164	16.35878	9.32030
Si	3.91087	13.24808	9.32033
Si	-1.31989	7.48856	2.51409
Si	-4.55442	13.26783	6.04261
Si	-2.50321	10.88348	-0.63209
Si	-4.08607	11.22520	3.68387
Si	-6.54740	10.53214	1.97126
Si	-4.43593	8.81099	5.71019
O	3.56343	12.61299	7.83676
O	3.34073	10.49934	6.18896
O	-2.57185	11.57641	3.21612
O	-0.00078	11.61480	2.64341
H	4.17454	6.67226	3.23020
H	2.39400	6.91706	4.86033
H	4.70256	7.28872	5.51268
H	2.53637	7.47144	1.15385
H	3.88186	9.31027	0.32401
H	1.67917	8.91944	-0.59851
H	3.59604	14.11631	0.20934
H	1.17496	14.12412	0.10942
H	2.41835	12.29949	-0.88724
H	6.84327	12.41068	2.97655
H	5.35207	11.16658	1.53292
H	6.74082	9.98553	3.11728
H	7.96832	11.23167	5.81488
H	8.18225	9.58249	7.55215
H	8.11730	11.92255	8.10843
H	2.98893	7.80590	10.17887
H	5.24410	8.60925	10.39737
H	4.51372	7.63920	8.32338
H	5.78470	12.49854	12.35789
H	7.29103	13.40267	10.69874
H	7.02039	10.99840	10.90836

H	4.99002	17.24246	8.81426
H	3.60451	16.70772	10.73099
H	2.68768	16.57038	8.49636
H	0.32832	13.05363	11.38887
H	1.75004	11.09517	11.44990
H	0.67497	11.77639	9.37317
H	-1.06807	6.48735	3.58915
H	-0.32725	7.23617	1.42919
H	-2.67480	7.21851	1.95073
H	-1.69158	10.71179	-1.87151
H	-2.80736	12.33986	-0.49514
H	-3.79741	10.17275	-0.84243
H	-7.00877	11.20744	0.73509
H	-7.51846	10.79416	3.06873
H	-6.46848	9.06657	1.74487
H	-4.00509	7.43442	5.37372
H	-5.89309	8.81445	6.01009
H	-3.70654	9.27865	6.92118
H	-5.25063	14.56677	5.89297
H	-3.09967	13.53273	6.32020
H	-5.11475	12.51571	7.19287
O	2.13307	11.35999	4.08789
O	2.36055	12.46992	1.69889
O	1.82780	9.84448	1.79119
O	3.58476	9.03372	3.95399
O	4.77043	11.40474	4.04679
O	5.92570	10.80190	7.32074
O	3.57155	9.97761	8.95233
O	5.10016	12.30655	9.88871
O	2.58912	13.26538	10.28304
O	4.43534	14.79231	9.19141
O	-4.66187	12.41530	4.64800
O	-1.69351	10.29903	0.65311
O	-5.05043	11.14479	2.36622
O	-4.11483	9.79876	4.44500
O	-1.19283	9.00149	3.14750
Cu	2.65245	12.51353	6.07242
Cu	-1.03705	12.33289	4.20815
N	-32.86190	-94.26573	6.70487
N	-33.34604	-95.16035	7.18841
O	-33.85565	-96.10202	7.69737

Coordinates of binuclear Cu^{I} model for Site 4 (-10617.7155604 Hartrees)

Al	1.69981	11.46010	2.30560
Al	3.93772	13.13157	9.53740
Si	3.49698	10.53499	4.59511
Si	4.43614	10.92779	7.43295
Si	7.54201	10.88330	7.20303
Si	2.50233	8.85453	0.63230
Si	1.44810	9.15789	10.81996
Si	5.95772	11.22551	2.88813
Si	4.08719	8.51167	9.45905
Si	3.71272	7.43029	4.41754
Si	6.33238	12.30589	10.98808
Si	2.38247	13.26689	0.24115
Si	1.31935	12.25001	10.62709
Si	3.91158	16.35891	9.32028
Si	-1.44849	10.57728	2.32330
Si	-1.61728	13.27566	10.76991
Si	-1.31997	7.48914	2.51415
Si	2.38081	13.26588	13.38269
Si	-2.50322	10.88391	-0.63224
Si	-4.08642	11.22515	3.68362
O	2.14774	12.73601	9.29710
O	4.51785	12.39571	8.04798
O	-0.05326	11.32109	2.19030
O	1.99907	10.77947	3.99026
H	2.02219	7.81822	1.60620
H	3.84352	8.41475	0.16238
H	1.55676	8.80151	-0.52067
H	2.18313	14.70545	-0.09193
H	1.37040	12.48797	-0.53767
H	3.73085	12.86920	-0.25321
H	4.31635	6.93692	3.15971
H	2.22865	7.25320	4.35878
H	4.24404	6.66841	5.57282
H	5.93178	12.20745	1.78235
H	5.99669	9.84235	2.35087
H	7.15330	11.45419	3.73620
H	8.35496	10.13780	6.21011
H	7.90634	10.43761	8.56817
H	7.77818	12.33843	7.05530
H	3.88590	9.01763	10.82236
H	5.52724	8.14687	9.34416
H	3.31552	7.28323	9.16751
H	6.78062	12.97321	12.24380
H	6.98221	13.00846	9.84534

H	6.86862	10.91244	11.01215
H	5.16589	17.14876	9.15661
H	3.13511	16.97996	10.43463
H	3.10387	16.54035	8.07418
H	1.72453	8.76354	9.42777
H	-0.02338	8.95358	10.98207
H	2.09664	8.28895	11.82091
H	1.33675	13.72870	14.33636
H	3.51435	14.21774	13.40847
H	2.82758	11.90958	13.78581
H	-2.78172	12.76798	10.00212
H	-1.39178	14.70546	10.43841
H	-1.88731	13.14007	12.22411
H	-4.34892	12.03161	4.89791
H	-4.47294	9.80972	3.92915
H	-4.87853	11.75272	2.54360
H	-2.77036	7.24384	2.34108
H	-0.76456	6.60606	3.56580
H	-0.59606	7.29083	1.24176
H	-3.74514	10.23699	-1.11906
H	-1.37645	10.56870	-1.54116
H	-2.69450	12.35191	-0.53967
O	2.20436	13.04732	1.86705
O	2.57109	10.31272	1.33129
O	3.30064	11.05006	6.17492
O	4.03103	9.01839	4.62341
O	4.58278	11.45172	3.81965
O	5.92454	10.49372	6.87965
O	3.79187	9.72238	8.34746
O	1.77193	10.74519	11.05564
O	-0.29487	12.34414	10.32348
O	4.69013	12.28517	10.86336
O	1.69886	13.25072	11.85974
O	4.24289	14.80595	9.61599
O	-2.18937	10.24363	0.90119
O	-2.45900	11.32598	3.35671
O	-1.08738	9.06600	3.07935
Cu	2.17689	12.03271	7.51064
Cu	0.57272	9.57079	3.89280
N	-66.71286	-52.44429	-56.72476
N	-67.61074	-52.92241	-57.20826
O	-68.55581	-53.42569	-57.71720

Coordinates of binuclear Cu^{I} model for Site 5 (-10617.6610784 Hartrees)

Al	3.61266	10.60086	4.52516
Al	1.27295	12.18651	10.67095
Si	1.57933	11.27244	2.49433
Si	4.43641	10.92669	7.43180
Si	7.54229	10.88340	7.20310
Si	2.50269	8.85463	0.63211
Si	1.44808	9.15818	10.81980
Si	5.95811	11.22550	2.88729
Si	4.08690	8.51251	9.45829
Si	3.71290	7.43191	4.41700
Si	6.33210	12.30610	10.98800
Si	2.38130	13.26632	0.24046
Si	3.91160	16.35879	9.32030
Si	3.91159	13.24821	9.32032
Si	-1.44850	10.57960	2.32219
Si	-1.61731	13.27575	10.76989
Si	-1.61730	16.33121	10.76990
Si	2.38071	13.26591	13.38251
Si	-3.71259	12.30661	8.72501
Si	-2.50320	10.88352	12.50990
O	-0.33333	12.60179	9.96378
O	2.28244	13.16815	9.50235
O	2.00576	11.28629	4.06917
O	3.27374	10.76991	6.29024
H	3.74364	8.73653	10.86244
H	5.49606	8.01595	9.47555
H	3.29383	7.48694	8.75407
H	8.30484	10.79851	5.93708
H	8.02247	9.84634	8.15004
H	7.72305	12.22478	7.81281
H	6.42464	12.22491	12.46385
H	7.20929	13.38999	10.47887
H	6.75239	11.01396	10.39290
H	5.01809	17.23288	8.86122
H	3.62030	16.63123	10.75097
H	2.69138	16.65789	8.51992
H	1.61092	8.02605	9.89330
H	-0.01281	9.11737	11.16458
H	2.13544	8.92180	12.11361
H	1.63618	13.68997	14.59941
H	3.00675	14.48160	12.78251
H	3.48264	12.35876	13.81294
H	-3.85236	10.96913	13.12698
H	-1.54744	10.32025	13.49163
H	-2.57815	10.00055	11.31737

H	-0.77065	17.25893	11.55814
H	-3.05007	16.65080	10.99793
H	-1.31277	16.50751	9.32208
H	-4.72177	13.09184	7.97429
H	-4.38854	11.24580	9.51295
H	-2.78959	11.65721	7.74680
H	4.41627	6.54977	3.44641
H	2.26830	7.05175	4.42184
H	4.24862	7.12716	5.77815
H	6.81139	12.39764	2.53819
H	5.32523	10.74648	1.62387
H	6.86070	10.14549	3.37750
H	2.79458	7.51987	1.20399
H	3.72171	9.41507	-0.00005
H	1.44339	8.71483	-0.40326
H	3.74061	13.83466	0.07931
H	1.37841	14.36140	0.17443
H	2.11161	12.30347	-0.86183
H	-2.59318	11.52393	2.28383
H	-1.58951	9.70304	3.51769
H	-1.46318	9.73402	1.10093
O	-0.05610	11.48127	2.41967
O	2.29667	12.51092	1.71374
O	1.95413	9.84119	1.83486
O	3.93214	8.99509	4.02504
O	4.84400	11.68819	4.00096
O	4.33269	12.48586	7.93101
O	5.92628	10.62156	6.85186
O	4.06954	9.94821	8.65959
O	1.73996	10.60251	10.11389
O	4.72631	12.61220	10.59261
O	1.36429	12.53192	12.33559
O	4.37151	14.79221	9.09567
O	-1.26377	14.78926	11.25346
O	-2.86968	13.34745	9.69950
O	-2.02425	12.40765	12.07898
Cu	0.93373	12.50448	8.22379
Cu	1.84133	12.02779	5.96423
N	-27.06183	-95.67735	15.80428
N	-27.58440	-96.52739	16.32669
O	-28.13444	-97.42215	16.87655

Coordinates of binuclear Cu^{I} model for Site 6 (-10617.7338267 Hartrees)

Al	-0.52698	2.58075	-1.81764
Al	7.06175	2.52802	-2.16551
Si	-0.00001	8.09668	-0.00003
Si	-0.92888	5.29022	-0.56691
Si	-3.12299	1.71416	-3.11232
Si	3.02581	-0.13684	0.24579
Si	-3.58017	6.12656	-1.91035
Si	0.00001	-0.00005	0.00013
Si	-2.09637	4.22588	2.10959
Si	0.09837	-0.68999	-4.62591
Si	4.10447	1.30794	-2.42011
Si	2.59325	3.06286	-6.90788
Si	1.63952	1.92685	-4.13656
Si	7.89842	3.66788	-4.91290
Si	4.78627	-1.08641	-4.31275
Si	7.33132	7.76730	0.03761
Si	7.50980	4.72294	0.03905
Si	10.60125	4.40557	-0.13137
Si	6.37751	3.71150	2.76534
Si	7.63602	0.23008	0.01193
O	7.26285	4.12772	-1.42125
O	5.25024	2.27649	-1.82611
O	0.08783	4.23573	-1.31890
O	0.29234	2.38160	-3.38170
H	6.16084	-1.58401	-4.06003
H	4.54009	-1.01078	-5.77172
H	3.80895	-2.00485	-3.67639
H	0.56859	-1.94706	-5.25632
H	-0.95022	-0.06345	-5.46341
H	-0.41422	-0.96931	-3.26628
H	2.44411	4.49092	-7.27849
H	1.81943	2.21916	-7.85516
H	4.02580	2.67793	-6.96844
H	0.91888	-0.92014	-0.71339
H	-1.36764	-0.54364	-0.25998
H	0.21256	-0.12499	1.46578
H	-4.57356	1.85264	-2.79999
H	-2.79667	0.25788	-3.06460
H	-2.91939	2.16143	-4.52112
H	8.09189	3.04779	-6.25325
H	9.19444	4.28882	-4.50770
H	6.90591	4.77414	-5.06583
H	11.45121	5.58638	0.16165
H	10.52181	4.19161	-1.59571
H	11.16964	3.20865	0.53463

H	6.59733	2.32360	3.22564
H	4.97396	4.10562	3.03598
H	7.32349	4.64789	3.41444
H	6.14002	8.54306	-0.38343
H	8.37566	7.83707	-1.01751
H	7.86972	8.33327	1.30053
H	-0.85061	3.81945	2.81413
H	-3.11483	3.15856	2.25597
H	-2.60326	5.47648	2.73731
H	-3.91761	7.56121	-2.10263
H	-4.36139	5.59298	-0.76682
H	-3.92066	5.38380	-3.14741
H	0.98569	8.62358	0.97716
H	-1.33533	8.67942	0.29389
H	0.41533	8.49289	-1.37093
H	8.92328	-0.08929	0.68591
H	7.02636	-1.03970	-0.47692
H	6.70327	0.76685	1.05634
H	2.06100	0.82710	0.77874
H	4.23819	0.06400	1.10151
H	2.69890	-1.56928	0.34078
O	-0.01356	6.44079	0.16612
O	-1.81815	4.45870	0.50626
O	-1.94020	6.03480	-1.61632
O	-2.23925	2.57753	-2.03806
O	0.12730	1.51779	-0.59054
O	3.47849	0.31534	-1.28855
O	1.47395	0.33332	-4.54166
O	4.64317	0.45047	-3.68091
O	2.85539	2.28187	-2.96983
O	2.01702	2.88020	-5.37702
O	6.85646	6.19477	0.28918
O	7.39419	2.53276	-3.84617
O	6.60434	3.74462	1.10801
O	9.07534	4.70316	0.50525
O	7.84734	1.32514	-1.18011
Cu	5.45131	2.79984	-0.05332
Cu	1.81002	3.59745	-1.91302
N	10.49184	8.91779	-7.85581
N	10.11208	9.66432	-8.60850
O	9.71439	10.44956	-9.40153

Coordinates of binuclear Cu^{I} model for Site 7 (-10617.7147475 Hartrees)

Al	3.84469	13.32060	9.11608
Al	-3.67037	12.07614	8.84372
Si	3.49704	10.53279	4.59955
Si	4.43660	10.92676	7.43201
Si	7.54216	10.88344	7.20306
Si	1.44810	9.15827	10.81979
Si	4.08687	8.51253	9.45832
Si	6.33204	12.30612	10.98798
Si	1.31940	12.24927	10.62785
Si	3.91163	16.35872	9.32029
Si	-1.61729	13.27579	10.76988
Si	-1.61732	16.33123	10.76990
Si	2.38071	13.26595	13.38254
Si	-4.55440	16.33906	6.04267
Si	-4.55435	13.26798	6.04284
Si	-4.08631	11.22499	3.68369
Si	-7.66431	13.26589	6.33049
Si	-6.13348	13.24818	10.39264
Si	-3.49769	9.20583	8.54230
Si	-2.50320	10.88352	12.50989
O	-3.79175	12.34317	7.09646
O	-2.58287	13.40988	9.43916
O	3.57114	12.28201	7.61507
O	2.18740	13.25238	9.74057
H	-2.40762	10.96434	13.99151
H	-1.40214	10.04495	12.00402
H	-3.81632	10.30534	12.14579
H	1.39846	13.54627	14.45974
H	2.84495	14.53899	12.78126
H	3.52937	12.51822	13.94875
H	-0.43657	17.20406	10.95553
H	-2.79054	16.87716	11.49470
H	-1.96830	16.27082	9.30600
H	1.78768	8.18804	9.77803
H	0.01589	8.91150	11.10136
H	2.18108	9.04396	12.09402
H	-7.53552	13.31720	9.88747
H	-5.58112	14.64075	10.32773
H	-6.19224	12.86706	11.83253
H	-2.60406	8.64598	7.48311
H	-4.83388	9.43300	7.91829
H	-3.65612	8.15265	9.58577
H	-8.43124	14.24993	7.12904
H	-7.82798	11.90174	6.88716

H	-8.15254	13.28346	4.92600
H	-3.45211	17.32880	6.02283
H	-5.42894	16.60224	7.20747
H	-5.32036	16.37394	4.77585
H	-4.34378	11.50857	2.25182
H	-4.97948	10.13675	4.15295
H	-2.66840	10.83019	3.87220
H	6.28678	12.86294	12.37202
H	7.44488	12.98752	10.26774
H	6.67841	10.86056	11.10893
H	4.86602	17.40833	8.86379
H	3.95767	16.32660	10.81399
H	2.53829	16.81062	8.93815
H	3.82675	8.95271	10.83136
H	5.55832	8.29462	9.37840
H	3.45072	7.23146	9.09010
H	7.75602	11.79248	6.04728
H	7.72047	9.47786	6.75315
H	8.52406	11.18984	8.26835
H	3.62404	9.32074	3.75392
H	3.85205	11.73404	3.80303
H	2.07864	10.66387	5.05126
O	4.47759	10.37258	5.90104
O	6.01284	11.10666	7.84640
O	3.71415	9.72509	8.35358
O	1.56818	10.67249	10.11706
O	-0.26441	12.48853	10.32805
O	4.87690	12.48871	10.24361
O	1.62546	12.30831	12.23234
O	4.29660	14.91723	8.65162
O	-3.77733	14.81970	6.21362
O	-4.41653	12.64952	4.53193
O	-6.07677	13.73038	6.36353
O	-1.26277	14.79476	11.28094
O	-2.86786	10.57853	9.18005
O	-5.25727	12.20908	9.50705
O	-2.39276	12.44858	11.93252
Cu	-2.88922	14.54485	7.93747
Cu	1.97291	11.30343	8.28017
N	-31.78380	-94.25275	2.82017
N	-32.24800	-95.16764	3.28499
O	-32.73663	-96.13062	3.77425

Coordinates of binuclear Cu^{I} model for Site 8 (-10617.7053528 Hartrees)

Al	1.42664	12.16710	10.73777
Al	-4.56828	13.36914	5.97739
Si	4.43674	10.92762	7.43138
Si	1.44809	9.15375	10.82068
Si	6.33329	12.30703	10.98847
Si	3.91177	16.36086	9.31902
Si	3.90742	13.24426	9.32132
Si	-1.44948	10.57900	2.32378
Si	-1.61866	13.27083	10.77918
Si	-1.61704	16.33359	10.76852
Si	2.38330	13.26769	13.38429
Si	-4.55611	16.33853	6.03969
Si	-4.08141	11.23964	3.67050
Si	-3.71155	12.30652	8.71729
Si	-7.66115	13.26500	6.33320
Si	-6.13427	13.24929	10.39496
Si	-6.55438	10.52797	1.97022
Si	-4.42941	8.80803	5.71830
Si	-3.50320	9.20293	8.54370
Si	-2.50174	10.88531	12.50853
O	-4.60387	12.51435	4.48277
O	-3.71265	12.34849	7.12046
O	-0.05724	13.05819	10.82295
O	2.40399	13.44554	9.90840
H	-1.78764	11.03145	13.80522
H	-1.81129	9.85987	11.69413
H	-3.90074	10.47143	12.76993
H	-6.59065	14.65202	10.54915
H	-5.80499	12.68828	11.72994
H	-7.21554	12.43495	9.78519
H	-2.69818	8.52646	9.60312
H	-2.59435	9.40013	7.40675
H	-4.69190	8.33852	8.39025
H	-3.58997	17.46509	5.88896
H	-5.37220	16.62371	7.24566
H	-5.39902	16.26778	4.82273
H	-8.55257	13.87687	7.36032
H	-7.68141	11.78582	6.54814
H	-8.26955	13.53065	4.99697
H	-3.34490	7.87033	6.06701
H	-5.59102	7.96537	5.30393
H	-4.92591	9.71150	6.76950
H	-7.21293	11.59474	1.17168
H	-7.36829	10.27282	3.19135

H	-6.52318	9.28256	1.15723
H	-0.55600	11.46526	1.53233
H	-2.09886	9.60514	1.40462
H	-0.61272	9.82201	3.29567
H	1.43978	13.40621	14.52153
H	2.23627	14.61025	12.71140
H	3.78492	13.29656	13.87341
H	2.83447	8.67586	11.09511
H	0.77034	8.12798	9.98108
H	0.73060	9.23147	12.12318
H	6.39599	11.08313	11.81888
H	6.75683	13.48240	11.79527
H	7.24390	12.17781	9.82050
H	5.55790	11.05206	6.46672
H	3.27890	10.27874	6.77724
H	4.88136	10.13515	8.60395
H	-2.52613	17.31913	11.39571
H	-1.66288	16.48823	9.27852
H	-0.28131	16.52695	11.20989
H	4.98397	17.36892	9.23615
H	3.37984	16.50945	10.80844
H	2.76976	16.58310	8.50480
O	4.00209	12.46867	7.90801
O	1.46171	10.60001	10.02019
O	4.77560	12.51850	10.48524
O	2.07576	12.06430	12.37076
O	4.49272	14.81727	9.10748
O	-3.63072	14.93966	6.20294
O	-6.15360	13.88414	6.46716
O	-2.05566	14.80534	11.17574
O	-5.01938	10.97798	2.35032
O	-3.97607	9.80969	4.49126
O	-2.55886	11.52658	3.10516
O	-3.85715	10.73125	9.19102
O	-2.21845	13.04402	9.18744
O	-4.80022	13.26554	9.43211
O	-2.53092	12.33869	11.73401
Cu	-2.60164	14.40997	7.75336
Cu	2.62142	15.05539	11.10992
N	-7.57234	-96.83466	-9.67617
N	-7.89260	-97.86832	-9.36384
O	-8.22973	-98.95631	-9.03506

Coordinates of binuclear Cu^{I} model for Site 9 (-10617.6807123 Hartrees)

Al	-1.55155	13.23622	10.78853
Al	-4.18571	11.11880	3.54668
Si	1.57921	11.27252	2.49432
Si	1.44809	9.15818	10.81982
Si	1.31940	12.24948	10.62773
Si	3.91154	13.24821	9.32034
Si	-1.44828	10.57936	2.32205
Si	-1.61732	16.33122	10.76988
Si	-1.31992	7.48871	2.51412
Si	2.38070	13.26591	13.38252
Si	-4.55439	16.33907	6.04273
Si	-4.55453	13.26797	6.04255
Si	-2.50324	10.88354	-0.63207
Si	-3.71226	12.30679	8.72561
Si	-7.66432	13.26589	6.33050
Si	-6.13354	13.24818	10.39255
Si	-6.54733	10.53221	1.97130
Si	-4.43588	8.81097	5.71018
Si	-3.49777	9.20571	8.54219
Si	-2.50323	10.88349	12.50987
O	-2.36027	11.30471	3.49947
O	-4.52783	12.45998	4.65858
O	-0.20001	12.26029	10.10608
O	-2.41307	13.12457	9.20957
H	-2.98365	8.50532	9.75122
H	-2.35285	9.27191	7.60483
H	-4.66363	8.39502	8.13160
H	-6.87967	14.51167	10.18236
H	-5.44331	13.27641	11.70293
H	-7.07749	12.10168	10.35008
H	-8.39573	13.57172	7.58446
H	-8.02651	11.90472	5.86395
H	-8.02971	14.26228	5.29139
H	-3.43951	17.26673	5.73781
H	-5.08580	16.61558	7.40024
H	-5.63994	16.50956	5.04366
H	-3.27804	7.91115	5.93868
H	-5.69126	8.06270	5.98193
H	-4.37373	9.96879	6.64044
H	-7.36454	11.20967	0.92438
H	-7.30776	10.62322	3.25567
H	-6.45118	9.09020	1.60630
H	-0.61951	6.68284	3.54590
H	-0.77765	7.13537	1.17444
H	-2.77076	7.18122	2.54398

H	-1.28414	10.53120	-1.40853
H	-2.74771	12.34186	-0.75570
H	-3.65736	10.12075	-1.16091
H	2.27774	12.44362	1.91158
H	2.14718	10.02041	1.93318
H	1.78418	11.27509	3.97112
H	-2.02553	10.76066	13.91650
H	-1.64032	10.00706	11.66800
H	-3.89057	10.34396	12.45111
H	-0.86308	17.35883	11.53894
H	-3.06008	16.44398	11.13680
H	-1.50731	16.68630	9.31997
H	2.62423	8.28741	10.57018
H	0.35698	8.77545	9.88561
H	0.98747	8.97349	12.21889
H	1.55607	13.63129	14.55730
H	3.19332	14.43410	12.95354
H	3.29806	12.15212	13.74227
H	4.20228	14.62116	8.84044
H	4.29496	12.27155	8.26796
H	4.69041	12.97198	10.55468
O	-0.04523	11.42282	2.13842
O	1.92775	10.72498	10.54568
O	1.35981	12.79498	12.16188
O	2.26476	13.15446	9.61774
O	-3.92791	14.78151	5.96533
O	-3.50888	12.37646	7.02921
O	-6.04730	13.35471	6.66721
O	-2.28533	10.45877	0.95159
O	-1.01061	14.84423	11.06233
O	-5.07690	11.26185	2.07793
O	-4.41526	9.51558	4.23807
O	-3.86208	10.73563	9.08614
O	-5.03107	13.11243	9.16571
O	-1.02622	9.08562	2.85555
O	-2.46159	12.44094	12.00951
Cu	-2.48346	11.67833	5.42805
Cu	-0.67048	12.83451	8.24382
N	-35.04339	-93.30251	12.60665
N	-35.56331	-94.15026	13.13538
O	-36.11058	-95.04262	13.69188

Coordinates of binuclear Cu^{I} model for Site 10 (-10617.6892901 Hartrees)

Al	-1.38626	10.51983	2.25018
Al	-3.79180	12.13599	8.80211
Si	1.57926	11.27251	2.49433
Si	3.49712	10.53280	4.59970
Si	2.50272	8.85458	0.63208
Si	2.38131	13.26631	0.24049
Si	1.31941	12.24950	10.62789
Si	-1.61733	13.27584	10.76992
Si	-1.61729	16.33120	10.76989
Si	-1.31990	7.48860	2.51410
Si	-4.55440	16.33907	6.04270
Si	-4.55434	13.26797	6.04264
Si	-2.50318	10.88350	-0.63210
Si	-4.08650	11.22493	3.68380
Si	-7.66429	13.26590	6.33050
Si	-6.13347	13.24812	10.39265
Si	-6.54724	10.53221	1.97131
Si	-4.43588	8.81101	5.71015
Si	-3.49771	9.20588	8.54233
Si	-2.50320	10.88347	12.50992
O	-0.00529	11.61089	2.61602
O	-2.61160	11.57287	3.07220
O	-2.61951	13.38563	9.45127
O	-3.67200	12.35050	7.03077
H	-3.42159	7.85700	6.20690
H	-5.24601	7.98165	4.75745
H	-5.42699	9.30725	6.68138
H	-7.02604	11.55522	1.00943
H	-7.45202	10.51885	3.15321
H	-6.55738	9.19559	1.33191
H	-8.39658	14.02802	7.36707
H	-7.78790	11.80686	6.56630
H	-8.21874	13.59531	4.99169
H	-3.45034	17.32769	6.02814
H	-5.41522	16.58334	7.22045
H	-5.32581	16.38107	4.78116
H	-1.25174	6.52045	3.64693
H	-0.18179	7.17770	1.60019
H	-2.58094	7.21159	1.76475
H	-1.88779	10.59293	-1.95846
H	-2.65924	12.36684	-0.52632
H	-3.87814	10.30078	-0.64389
H	2.92548	7.56956	1.23976
H	3.69225	9.52346	0.03709
H	1.49968	8.61238	-0.43068

H	3.76378	13.73861	-0.02207
H	1.47714	14.44304	0.33445
H	1.93457	12.40370	-0.88525
H	3.93917	11.23923	5.82958
H	4.59058	10.57765	3.59239
H	3.20832	9.11504	4.93545
H	-2.43505	8.23281	8.92545
H	-3.14484	9.71750	7.20261
H	-4.79717	8.50428	8.62857
H	-2.11358	10.90510	13.94506
H	-1.58823	9.96873	11.78618
H	-3.90933	10.43905	12.40326
H	1.80736	11.14951	9.76138
H	1.46679	11.86444	12.05619
H	2.12832	13.47085	10.37186
H	-0.93977	17.28886	11.67429
H	-3.08278	16.57202	10.77103
H	-1.12220	16.54230	9.37608
H	-7.55557	13.58457	10.10072
H	-5.46802	14.50184	10.86613
H	-6.11808	12.28508	11.53145
O	2.13862	11.30055	4.04156
O	2.38613	12.43029	1.66675
O	1.85948	9.81133	1.82790
O	-0.26564	12.52717	10.25399
O	-3.75726	14.81810	6.19053
O	-4.55047	12.61397	4.52661
O	-6.07011	13.74057	6.38038
O	-1.58391	10.26924	0.56053
O	-1.25707	14.79372	11.26976
O	-5.02546	10.90617	2.43215
O	-3.88249	10.06050	4.79145
O	-3.42548	10.57229	9.46231
O	-5.41799	12.66055	9.05928
O	-1.26438	9.01705	3.10766
O	-2.35691	12.45085	11.95115
Cu	-1.14638	12.12354	4.27928
Cu	-2.90981	14.48949	7.93001
N	-31.71672	-94.31208	12.70044
N	-32.22924	-95.16814	13.22298
O	-32.76872	-96.06923	13.77297

Coordinates of μ-1,1-O N_2O binding mode for site 6 (-10617.7510635 Hartrees)

Al	4.44156	10.86135	7.50901
Al	-1.79887	13.41119	10.88123
Si	1.57926	11.27250	2.49433
Si	3.49728	10.53271	4.59982
Si	7.54246	10.88345	7.20311
Si	1.44796	9.15849	10.81973
Si	5.95809	11.22554	2.88725
Si	4.08689	8.51256	9.45827
Si	3.71286	7.43194	4.41700
Si	6.33253	12.30608	10.98814
Si	1.32007	12.24936	10.62820
Si	3.91168	16.35892	9.32033
Si	3.91030	13.24773	9.31996
Si	-1.61733	16.33128	10.76984
Si	2.38059	13.26588	13.38239
Si	-4.55439	13.26786	6.04257
Si	-3.71262	12.30705	8.72541
Si	-6.13337	13.24807	10.39252
Si	-3.49769	9.20570	8.54222
Si	-2.50315	10.88340	12.50989
O	-2.69728	13.37737	9.33989
O	-0.23057	12.67193	10.39406
O	3.31687	10.46179	6.20359
O	4.21585	12.52978	7.91988
H	1.30316	13.50565	14.37140
H	2.82640	14.55268	12.79472
H	3.51891	12.58067	14.03953
H	6.40668	12.26195	12.47068
H	7.18771	13.40832	10.48052
H	6.81809	11.01200	10.44664
H	5.12671	17.20583	9.22098
H	3.21755	16.65544	10.60207
H	2.99589	16.68269	8.19484
H	3.96697	8.46341	10.92527
H	5.54452	8.41458	9.19116
H	3.46014	7.29739	8.87358
H	8.10514	10.86372	5.82145
H	8.44715	10.07002	8.06423
H	7.59842	12.29299	7.68810
H	-1.02238	17.45120	11.55358
H	-3.03404	16.69900	10.47020
H	-0.89697	16.27082	9.46044
H	-7.40029	13.63286	9.72123
H	-5.39285	14.46165	10.80686
H	-6.43561	12.39303	11.56488

H	-2.78416	8.86678	7.28416
H	-4.96346	9.16222	8.33963
H	-3.06911	8.27198	9.60755
H	-3.68212	13.55065	4.87666
H	-4.93433	14.54251	6.70499
H	-5.78111	12.57040	5.57872
H	4.94117	7.21299	5.22152
H	3.76315	6.59764	3.19123
H	2.53127	7.02556	5.22865
H	6.93451	12.32457	3.07276
H	5.31645	11.35906	1.55358
H	6.65299	9.91499	2.95661
H	0.83947	12.54022	2.27270
H	0.65178	10.13271	2.25953
H	2.70388	11.18389	1.52937
H	-3.80220	10.19203	12.74160
H	-1.70932	10.82675	13.77029
H	-1.75413	10.04909	11.50805
H	1.78520	8.19556	9.76813
H	0.12832	8.69903	11.32801
H	2.35242	9.29247	11.96808
O	2.12161	11.25687	4.05740
O	3.57245	9.01941	3.94307
O	4.81473	11.36274	4.09762
O	6.02678	10.28256	7.22301
O	3.53950	9.90884	8.76597
O	1.20254	10.65222	10.07042
O	4.73292	12.53043	10.56463
O	1.78629	12.25229	12.18305
O	2.29447	13.12847	9.67298
O	4.38039	14.79258	9.26353
O	-3.71125	12.29284	7.08664
O	-1.49847	14.93909	11.60303
O	-3.02264	10.75654	9.02489
O	-5.23968	12.36045	9.28324
O	-2.71957	12.38134	11.94011
Cu	-1.12979	11.14580	9.46723
Cu	1.83183	10.43790	7.83132
N	-0.83067	11.77313	5.21685
N	-0.41688	11.37521	6.17678
O	-0.00594	10.95924	7.23419

Coordinates of μ-1,3-N_2O binding mode for site 6 (-10617.7469651 Hartrees)

Al	4.41377	10.75390	7.57610
Al	-1.59653	13.29272	10.72275
Si	1.57926	11.27250	2.49434
Si	3.49730	10.53281	4.59972
Si	7.54248	10.88345	7.20311
Si	1.44808	9.15834	10.81974
Si	5.95806	11.22552	2.88730
Si	4.08692	8.51255	9.45830
Si	3.71286	7.43189	4.41701
Si	6.33254	12.30606	10.98814
Si	1.31995	12.24957	10.62817
Si	3.91167	16.35893	9.32032
Si	3.91037	13.24769	9.31996
Si	-1.61731	16.33132	10.76976
Si	2.38062	13.26590	13.38243
Si	-4.55445	13.26792	6.04254
Si	-3.71251	12.30700	8.72528
Si	-6.13339	13.24811	10.39255
Si	-3.49776	9.20574	8.54219
Si	-2.50325	10.88321	12.51020
O	-2.61895	13.34537	9.25562
O	-0.22234	12.26937	10.07947
O	3.34527	10.66071	6.18673
O	4.28846	12.53132	7.88552
H	1.53291	13.73309	14.50542
H	3.41437	14.29313	13.09005
H	3.05213	11.99563	13.76125
H	6.37830	12.16657	12.46305
H	7.21214	13.42340	10.56060
H	6.78264	11.04550	10.35329
H	5.11154	17.18757	9.04715
H	3.44839	16.59450	10.71116
H	2.82980	16.74466	8.37412
H	4.58837	8.60517	10.85403
H	5.22863	7.99944	8.64320
H	3.06257	7.44368	9.35965
H	8.10751	10.89225	5.82241
H	8.44742	10.05924	8.05331
H	7.60338	12.28646	7.71167
H	-1.00227	17.36507	11.64976
H	-3.09903	16.41203	10.94635
H	-1.32639	16.72499	9.35633
H	-7.40032	13.59788	9.70270
H	-5.41697	14.48338	10.78751

H	-6.42921	12.41395	11.58085
H	-2.35146	8.32074	8.85279
H	-3.77727	9.15639	7.08622
H	-4.69905	8.81430	9.31450
H	-3.61692	13.66590	4.96052
H	-5.05053	14.48878	6.73191
H	-5.70477	12.54462	5.44291
H	4.64748	7.19104	5.54388
H	4.14843	6.65882	3.22813
H	2.34848	6.99128	4.81354
H	6.78556	12.45599	2.90304
H	5.40108	11.02780	1.52172
H	6.79073	10.05087	3.24423
H	0.40918	12.19131	2.46531
H	1.16385	9.95127	1.95494
H	2.65585	11.82991	1.63619
H	2.49307	8.37149	11.47946
H	1.13115	8.74454	9.43366
H	0.20054	8.93737	11.60312
H	-1.53093	10.70862	13.62766
H	-2.16580	9.85201	11.48636
H	-3.86260	10.55582	13.02830
O	2.06305	11.15021	4.06507
O	3.69911	9.03138	3.99374
O	4.71966	11.45241	3.98991
O	6.02479	10.29170	7.20606
O	3.59318	9.95229	8.87933
O	1.84607	10.74850	10.89128
O	4.74752	12.61819	10.56497
O	1.40080	13.04713	12.05266
O	2.28630	13.03711	9.53046
O	4.31554	14.79173	9.08771
O	-3.75314	12.28700	7.08881
O	-1.01909	14.85777	11.13012
O	-3.00479	10.77112	8.97062
O	-5.21446	12.36051	9.32008
O	-2.48535	12.39765	11.90735
Cu	-1.06139	11.45116	8.49707
Cu	2.92184	12.94469	6.61397
N	-0.26496	11.78494	6.85104
N	0.45184	12.48678	6.33321
O	1.19210	13.28771	5.81440

Coordinates of η^1-N binding mode for site 6 (-10617.7577059 Hartrees)

Al	4.39695	10.79978	7.51559
Al	-1.54913	13.30684	10.65033
Si	1.57926	11.27250	2.49434
Si	3.49731	10.53281	4.59972
Si	7.54248	10.88345	7.20311
Si	1.44808	9.15834	10.81974
Si	5.95806	11.22552	2.88730
Si	4.08692	8.51255	9.45830
Si	3.71286	7.43189	4.41701
Si	6.33254	12.30606	10.98814
Si	1.31994	12.24956	10.62817
Si	3.91167	16.35893	9.32032
Si	3.91037	13.24769	9.31996
Si	-1.61731	16.33132	10.76976
Si	2.38062	13.26590	13.38243
Si	-4.55445	13.26792	6.04254
Si	-3.71252	12.30701	8.72528
Si	-6.13339	13.24811	10.39255
Si	-3.49776	9.20574	8.54219
Si	-2.50324	10.88322	12.51020
O	-2.68932	13.37583	9.31519
O	-0.20819	12.20431	10.06471
O	3.25820	10.66015	6.18096
O	4.11168	12.56008	7.84078
H	1.56234	13.78506	14.50378
H	3.36734	14.29689	12.96775
H	3.11039	12.04870	13.82508
H	6.33347	12.30104	12.47174
H	7.17373	13.42386	10.49185
H	6.86647	11.01641	10.49057
H	5.10501	17.20979	9.09264
H	3.33466	16.65542	10.65556
H	2.89534	16.64562	8.27313
H	3.70324	8.50923	10.90029
H	5.56756	8.34296	9.45853
H	3.49682	7.28926	8.84662
H	8.14137	10.84881	5.83793
H	8.40240	10.04989	8.09019
H	7.62462	12.29256	7.69206
H	-0.91211	17.36993	11.57405
H	-3.06183	16.37393	11.14684
H	-1.52160	16.73960	9.33608
H	-7.48996	13.48516	9.83826
H	-5.49848	14.54393	10.73525

H	-6.24667	12.40839	11.61233
H	-4.00316	8.39290	9.67484
H	-2.23325	8.59388	8.06259
H	-4.49665	9.24369	7.44798
H	-3.72708	13.43824	4.82067
H	-4.81620	14.60086	6.64717
H	-5.84911	12.64418	5.66392
H	4.95540	7.04112	3.70423
H	2.59844	6.55537	3.97829
H	3.91448	7.28511	5.88052
H	7.06613	12.15465	3.21197
H	5.20267	11.75825	1.72096
H	6.51096	9.89406	2.52609
H	1.02688	12.58375	2.06956
H	0.45813	10.30650	2.64290
H	2.51043	10.77259	1.45046
H	1.76462	8.47710	12.08991
H	1.65521	8.35943	9.60643
H	-0.03600	9.26611	10.81325
H	-3.88252	10.62216	12.99672
H	-1.51958	10.55064	13.57615
H	-2.29868	9.82551	11.48667
O	2.34923	11.50062	3.93437
O	3.31082	9.00457	4.03345
O	4.97400	11.11321	4.21046
O	6.01015	10.33431	7.18666
O	3.62559	9.89900	8.77014
O	1.92126	10.72664	10.76197
O	4.75809	12.48045	10.47722
O	1.35342	12.90258	12.12463
O	2.28778	13.12785	9.62042
O	4.39393	14.78697	9.22938
O	-3.72096	12.29132	7.08605
O	-0.94014	14.86620	11.04312
O	-3.15667	10.74750	9.12456
O	-5.25629	12.44261	9.23425
O	-2.33615	12.38512	11.92688
Cu	-1.28570	10.48265	10.22308
Cu	2.38105	12.55819	6.90539
N	0.56577	12.43161	6.64704
N	-0.24789	11.69411	6.91612
O	-1.07022	10.90689	7.21108

Coordinates of transition state for site 6 via μ-1,1-O N_2O binding mode
(-10617.7331357 Hartrees)

Al	4.45582	10.80443	7.45494
Al	-1.64150	13.34897	10.77394
Si	1.57935	11.27244	2.49463
Si	3.49737	10.53242	4.59921
Si	7.54247	10.88345	7.20314
Si	1.44797	9.15849	10.81973
Si	5.95798	11.22552	2.88748
Si	4.08687	8.51262	9.45823
Si	3.71281	7.43218	4.41699
Si	6.33252	12.30607	10.98815
Si	1.32004	12.24938	10.62825
Si	3.91168	16.35890	9.32034
Si	3.91030	13.24782	9.31998
Si	-1.61733	16.33129	10.76985
Si	2.38059	13.26588	13.38238
Si	-4.55443	13.26792	6.04253
Si	-3.71251	12.30694	8.72543
Si	-6.13340	13.24810	10.39254
Si	-3.49770	9.20570	8.54224
Si	-2.50316	10.88341	12.50989
O	-2.64417	13.34315	9.30056
O	-0.22658	12.39205	10.13015
O	3.28750	10.50409	6.18072
O	4.23736	12.42103	7.99442
H	1.51282	13.58680	14.54013
H	3.00785	14.50218	12.85734
H	3.43219	12.30800	13.80818
H	6.43967	12.20022	12.46507
H	7.24137	13.37384	10.49923
H	6.73128	11.00804	10.38635
H	5.04334	17.21949	8.89227
H	3.62423	16.61816	10.75700
H	2.70677	16.70556	8.52191
H	3.84977	8.78797	10.89240
H	5.56045	8.49748	9.29233
H	3.57049	7.16233	9.12000
H	8.16201	10.82765	5.84777
H	8.43281	10.13107	8.13230
H	7.53059	12.30987	7.63620
H	-1.01357	17.41901	11.58881
H	-3.10261	16.43985	10.89555
H	-1.27712	16.59630	9.34067
H	-7.39236	13.59689	9.68875
H	-5.40834	14.48192	10.77519

H	-6.44167	12.43061	11.58927
H	-2.67469	8.27193	9.34226
H	-3.21265	8.99123	7.10243
H	-4.94063	9.03729	8.82333
H	-3.60794	13.72063	4.99478
H	-5.10723	14.44796	6.75889
H	-5.66741	12.51496	5.41030
H	4.99570	7.24331	5.14033
H	3.69686	6.59068	3.19561
H	2.59791	7.00536	5.30981
H	7.06141	12.16705	3.18986
H	5.29993	11.63340	1.61875
H	6.50039	9.85175	2.72373
H	0.79100	12.50936	2.26410
H	0.67876	10.09907	2.32892
H	2.66102	11.18656	1.47916
H	-3.85973	10.50765	12.99961
H	-1.53753	10.69074	13.62941
H	-2.13374	9.88933	11.45951
H	1.76084	8.18525	9.76177
H	-0.03507	9.04588	10.93884
H	2.02998	8.81486	12.13232
O	2.18571	11.33050	4.02291
O	3.50365	9.01336	3.95155
O	4.87512	11.29186	4.15055
O	6.04449	10.23028	7.18019
O	3.48277	9.69034	8.49353
O	1.75548	10.69308	10.30371
O	4.74110	12.64257	10.61961
O	1.41456	12.55171	12.22003
O	2.30102	13.19496	9.72947
O	4.34715	14.79333	9.08046
O	-3.75091	12.28167	7.09441
O	-1.06368	14.88062	11.27799
O	-3.00709	10.76034	8.97176
O	-5.20990	12.33386	9.33892
O	-2.50800	12.40403	11.93548
Cu	-1.07147	11.21538	8.90791
Cu	1.77619	10.13732	7.70395
N	-1.12494	10.65575	5.27434
N	-0.30532	10.45525	6.01986
O	-0.00731	10.55613	7.41028

Coordinates of η^1-O binding mode for site 7 (-10617.7471027 Hartrees)

Al	3.83940	13.30636	9.19867
Al	-3.65646	12.09550	8.83300
Si	3.49707	10.53279	4.59959
Si	4.43649	10.92685	7.43193
Si	7.54218	10.88342	7.20307
Si	1.44807	9.15832	10.81979
Si	4.08688	8.51250	9.45834
Si	6.33203	12.30613	10.98799
Si	1.31959	12.24906	10.62788
Si	3.91163	16.35872	9.32029
Si	-1.61734	13.27593	10.76985
Si	-1.61732	16.33120	10.76990
Si	2.38066	13.26600	13.38253
Si	-4.55440	16.33906	6.04267
Si	-4.55434	13.26795	6.04285
Si	-4.08631	11.22500	3.68369
Si	-7.66431	13.26589	6.33049
Si	-6.13347	13.24817	10.39264
Si	-3.49770	9.20584	8.54229
Si	-2.50320	10.88349	12.50990
O	-3.74477	12.36021	7.07716
O	-2.58758	13.43096	9.43721
O	3.59573	12.30002	7.67122
O	2.12719	13.25826	9.66616
H	-2.82160	11.00298	13.95638
H	-1.20706	10.19599	12.35538
H	-3.58472	10.12579	11.84371
H	1.45603	13.60557	14.49482
H	2.96441	14.51434	12.83040
H	3.46566	12.39932	13.90780
H	-0.44070	17.20744	10.96438
H	-2.80098	16.87801	11.47696
H	-1.95268	16.27087	9.30019
H	1.74353	8.21078	9.73798
H	-0.00680	8.98502	11.06570
H	2.13119	8.84529	12.09468
H	-7.53266	13.30806	9.87966
H	-5.58835	14.64260	10.33674
H	-6.19219	12.85018	11.82694
H	-2.47311	8.33700	7.89281
H	-4.57372	9.45227	7.53682
H	-4.09773	8.42551	9.66077
H	-8.43101	14.24151	7.13855
H	-7.84734	11.89203	6.85627

H	-8.12865	13.31720	4.91906
H	-3.45268	17.32879	6.00969
H	-5.41472	16.59974	7.21844
H	-5.33751	16.37470	4.78609
H	-4.74964	11.33031	2.36285
H	-4.59158	10.04281	4.42138
H	-2.61769	11.11274	3.49385
H	6.37883	12.81268	12.39088
H	7.37579	13.03705	10.21428
H	6.71067	10.86525	11.02794
H	4.86524	17.39470	8.83170
H	3.93757	16.38511	10.81363
H	2.54092	16.79104	8.90254
H	3.79509	8.98297	10.81552
H	5.55990	8.27395	9.43597
H	3.45631	7.22415	9.10371
H	7.77979	11.76163	6.02736
H	7.69099	9.46514	6.78240
H	8.53260	11.19191	8.26012
H	4.02195	9.67040	3.51445
H	3.33926	11.92513	4.10092
H	2.13390	10.05334	4.98456
O	4.51255	10.47342	5.86942
O	6.01544	11.15712	7.84055
O	3.76679	9.68672	8.29890
O	1.70333	10.69509	10.24780
O	-0.28098	12.47009	10.30384
O	4.82466	12.49753	10.36548
O	1.51677	12.45590	12.23127
O	4.30409	14.89521	8.70941
O	-3.77743	14.82077	6.20127
O	-4.43666	12.64463	4.53144
O	-6.07159	13.71217	6.39720
O	-1.26781	14.79587	11.28470
O	-2.81018	10.60072	9.06089
O	-5.24526	12.21681	9.49721
O	-2.42391	12.44428	11.91100
Cu	-2.88613	14.56614	7.93472
Cu	1.69766	12.29608	7.50987
N	-1.26578	10.35610	6.11777
N	-0.70974	11.21668	6.56333
O	-0.14802	12.17732	7.02740

Coordinates of transition state for site 7 via η^1-O binding mode
(-10617.7060927 Hartrees)

Al	3.91251	13.28040	9.21598
Al	-3.68152	12.08838	8.83517
Si	3.49707	10.53279	4.59958
Si	4.43650	10.92684	7.43196
Si	7.54218	10.88342	7.20307
Si	1.44807	9.15831	10.81979
Si	4.08688	8.51251	9.45833
Si	6.33203	12.30613	10.98799
Si	1.31958	12.24911	10.62789
Si	3.91163	16.35872	9.32029
Si	-1.61733	13.27591	10.76984
Si	-1.61732	16.33120	10.76990
Si	2.38066	13.26599	13.38252
Si	-4.55440	16.33906	6.04267
Si	-4.55434	13.26792	6.04285
Si	-4.08631	11.22501	3.68369
Si	-7.66431	13.26589	6.33049
Si	-6.13346	13.24815	10.39264
Si	-3.49771	9.20590	8.54229
Si	-2.50320	10.88349	12.50990
O	-3.76004	12.35070	7.08171
O	-2.59529	13.41625	9.44581
O	3.59676	12.30496	7.70139
O	2.14133	13.23527	9.60490
H	-2.25614	10.93806	13.97585
H	-1.51505	9.99029	11.88593
H	-3.88223	10.39560	12.27730
H	1.45615	13.62602	14.48644
H	3.03821	14.49358	12.86760
H	3.41026	12.32837	13.89627
H	-0.45431	17.21748	11.00454
H	-2.81818	16.85694	11.46368
H	-1.91612	16.28668	9.29552
H	1.73167	8.23637	9.71409
H	-0.00655	9.02046	11.06235
H	2.12631	8.80056	12.08602
H	-7.55899	13.31992	9.95926
H	-5.59962	14.64861	10.36137
H	-6.11745	12.80744	11.81710
H	-2.58930	8.71016	7.46507
H	-4.84408	9.39982	7.92660
H	-3.61553	8.12035	9.55732
H	-8.41597	14.16348	7.23718

H	-7.81585	11.85188	6.74941
H	-8.17741	13.42371	4.94381
H	-3.45443	17.33064	5.99016
H	-5.39411	16.59986	7.23284
H	-5.35450	16.37139	4.79742
H	-5.06323	10.16843	4.04611
H	-2.71028	10.75871	3.98509
H	-4.20143	11.54711	2.24127
H	6.43828	12.80571	12.38896
H	7.30627	13.07096	10.16009
H	6.73832	10.87424	10.99225
H	4.83860	17.39757	8.79355
H	3.93808	16.42518	10.81108
H	2.52876	16.72801	8.88700
H	3.79189	8.99881	10.80941
H	5.55913	8.26807	9.44560
H	3.45077	7.22450	9.11538
H	7.78474	11.77971	6.04293
H	7.67077	9.47004	6.76202
H	8.53697	11.16463	8.26393
H	3.22453	9.14857	4.13828
H	4.07578	11.31939	3.48182
H	2.20349	11.16330	5.00225
O	4.53021	10.52205	5.86137
O	6.01637	11.16708	7.85566
O	3.77626	9.67881	8.28867
O	1.75026	10.70843	10.30166
O	-0.26322	12.49159	10.27534
O	4.78544	12.47432	10.45460
O	1.49904	12.54443	12.20176
O	4.33958	14.88224	8.75581
O	-3.76499	14.81778	6.19132
O	-4.43370	12.64279	4.53230
O	-6.07379	13.72897	6.37657
O	-1.25199	14.79575	11.27459
O	-2.92532	10.58265	9.22244
O	-5.29684	12.25902	9.41799
O	-2.37205	12.45165	11.94289
Cu	-2.76146	14.48115	7.86259
Cu	1.66607	12.85913	7.72412
N	-1.04014	13.32244	4.62299
N	-0.23012	13.10530	5.34511
O	0.16252	13.27323	6.93966

Coordinates of binuclear Cu^{I} model for Site 6 (68 atoms model)
(-8613.77052476 Hartrees)

Al	5.55428	-0.90553	-1.42689
Al	-1.50675	-2.00367	0.15607
Si	5.87729	2.08562	-1.08991
Si	-2.51442	0.93147	-0.46380
Si	8.54535	-1.93176	-1.16975
Si	4.78223	-2.14846	-4.07470
Si	1.37312	-2.77584	-0.76162
Si	4.13722	-2.81660	0.57439
Si	-2.69726	-2.69354	-2.61768
Si	-1.83574	-2.47489	3.10071
Cu	-0.56756	-0.47652	-1.82886
Cu	5.42208	0.16120	0.93540
O	-2.17480	-0.37096	0.42628
O	0.13953	-1.71705	-0.56666
O	5.03144	0.78137	-1.48817
O	5.13384	-1.56207	0.22654
H	-3.73924	-3.08616	4.08769
H	-4.50637	-1.33101	-2.59230
H	-3.45709	-4.77362	-2.62820
H	10.70495	-1.39534	-0.97586
H	6.01586	-3.98822	-4.32307
H	5.44303	-0.78558	-5.72444
H	8.01447	-3.28208	0.51850
H	-0.61551	-2.90353	-3.51445
H	7.84959	-3.09080	-2.94030
H	-0.37268	-2.39470	4.75087
H	-1.93201	-0.32847	2.48409
H	-4.63898	1.08895	0.22530
H	-1.77100	3.03850	-0.33174
H	-2.73295	0.21974	-2.61201
H	6.36541	2.59641	1.13938
H	7.77901	1.11252	-1.64993
H	5.54457	3.91472	-2.31162
H	2.76650	-3.14711	-4.12328
H	2.85067	-2.27310	-2.30371
H	0.25999	-4.39697	0.29542
H	4.24256	-4.93649	-0.14158
H	3.40371	-3.04862	2.66710
O	5.75519	2.01946	0.65401
O	8.43686	-3.23992	-2.17414
O	5.25036	3.55336	-1.46313
O	7.45364	2.03036	-1.53298
O	6.19088	-3.03622	-4.27220
O	-0.93555	-3.07660	4.35703

O	7.30143	-0.91307	-1.52364
O	-1.79814	-0.82925	3.30834
O	4.50774	-1.80649	-2.50984
O	8.55853	-2.49151	0.38901
O	9.90101	-1.00578	-1.34624
O	3.55923	-3.07033	-4.68149
O	1.94413	-2.67445	-2.30368
O	5.02103	-0.71644	-4.85657
O	4.65798	-4.08373	-0.33554
O	0.84245	-4.31225	-0.47976
O	2.58360	-2.36681	0.27614
O	4.23586	-3.16425	2.18670
O	-3.35574	-3.12243	3.20024
O	-2.05519	0.73512	-2.10161
O	-1.26177	-2.88370	1.62990
O	-4.13527	1.23562	-0.58867
O	-1.63618	2.19308	0.12036
O	-2.48810	-2.86577	-1.02741
O	-3.62293	-1.34166	-2.98999
O	-3.35242	-4.05593	-3.27042
O	-1.29355	-2.22200	-3.39198
N	1.55414	3.19273	-0.79671
N	2.23874	4.01951	-1.13067
O	0.83224	2.32086	-0.44452

Coordinates of binuclear Cu^{I} model for Site 6 (140 atoms model)
(-17877.78854934 Hartrees)

Al	-0.10613	3.17509	-0.02381
Al	7.35463	2.12526	-0.45216
Si	2.22941	5.96022	-6.64247
Si	0.86505	6.27482	4.72036
Si	-3.85523	0.69786	-1.99517
Si	-0.33790	4.57764	2.63931
Si	-1.20952	-0.29572	-2.81392
Si	3.17887	9.07384	-3.89529
Si	-2.72144	3.62675	-1.44459
Si	-4.74969	5.39972	0.19109
Si	2.96174	-0.66932	0.11763
Si	-2.72089	6.47047	2.18398
Si	0.00000	0.00005	-0.00005
Si	-1.89274	4.43379	-4.30768
Si	-1.85425	2.35761	4.21021
Si	0.18165	2.15791	-4.13317
Si	-2.04041	0.00442	2.40618
Si	6.36645	5.68100	-3.80206
Si	4.27237	1.79255	-1.23590
Si	3.31781	6.04197	-3.75518
Si	2.04237	3.67391	-2.19243
Si	5.17761	-1.42023	2.16679
Si	2.95766	-2.67202	-2.31596
Si	8.47653	4.48517	-1.84910
Si	2.20631	1.08328	-6.02359
Si	5.99645	3.26397	-5.74341
Si	4.73562	0.92291	-4.19849
Si	9.94451	6.29901	0.16790
Si	8.08373	4.85041	4.48106
Si	6.38160	0.27727	4.24795
Si	7.89684	2.49730	2.67673
Si	10.90101	1.88166	2.32079
Si	10.15300	-1.03442	1.91223
Si	7.58831	-0.87120	0.15277
Si	7.58434	-2.87427	-2.28049
Si	10.80251	5.09701	-3.78592
Si	5.36819	-2.12324	-4.33009
O	0.48114	3.61488	1.59914
O	0.99652	4.09232	-1.03979
O	5.55683	2.17633	-0.33280
O	7.81794	2.74858	1.11055
H	-5.85385	6.16273	-0.42860

H	-5.24964	4.49244	1.25798
H	9.36777	6.91714	1.38831
H	10.19773	7.36178	-0.84119
H	11.23986	5.65984	0.52197
H	11.55030	4.08687	-4.57700
H	11.78593	5.98275	-3.10311
H	9.98800	5.93194	-4.70972
H	7.14876	5.98134	4.69172
H	9.31156	5.33489	3.80086
H	8.45879	4.27023	5.79765
H	5.42142	-2.87317	-5.59135
H	9.81229	-1.04424	3.35677
H	11.16991	-2.06103	1.59804
H	5.81508	1.04715	5.37275
H	7.57955	-0.49597	4.63289
H	7.14909	-4.28086	-2.11793
H	9.03743	-2.77048	-2.53887
H	1.74786	-2.16109	-2.99330
H	2.74933	-4.01388	-1.73298
H	-0.76574	-1.26124	-3.82919
H	-5.13749	0.61261	-2.72862
H	-4.02973	0.32463	-0.57041
H	-3.34373	0.58004	2.00100
H	-2.22622	-1.26023	3.15363
H	-3.28782	2.53649	3.87270
H	-1.66616	2.12236	5.65830
H	1.87258	7.36322	4.66689
H	1.23470	5.32780	5.80557
H	-0.46729	6.86083	5.03609
H	-3.43990	5.94971	3.37443
H	-2.24212	7.85256	2.40244
H	2.61342	10.05148	-2.93596
H	2.49026	9.21147	-5.20561
H	4.62873	9.33883	-4.08490
H	-1.62791	5.79971	-4.80154
H	-3.10799	3.85202	-4.92095
H	6.93754	2.89362	-6.82165
H	4.65985	3.59270	-6.28107
H	11.93712	1.84071	3.37547
H	11.13747	2.95374	1.33739
H	5.40765	-2.86089	2.33848
H	2.42458	2.04332	-7.12749
H	2.30983	-0.31438	-6.50286
H	6.56778	7.00011	-4.42594
H	0.98030	6.67734	-6.27820
H	1.90014	4.56139	-7.00645

H	2.86623	6.63243	-7.80221
O	3.31011	5.98649	-5.38613
O	3.71494	-1.11814	1.50513
O	0.84436	5.52581	3.25823
O	-2.83602	-0.38336	-2.70257
O	-3.29404	2.23324	-2.09197
O	-1.03671	3.74307	3.85646
O	-0.84462	1.24280	-3.26611
O	-1.43409	5.49222	1.86639
O	-0.48503	-0.68700	-1.40826
O	2.93831	7.55104	-3.26395
O	-1.80043	3.36967	-0.16375
O	0.39284	1.52996	-0.20274
O	-1.98791	4.45694	-2.65934
O	-4.03107	4.51910	-0.99125
O	3.41748	-1.61347	-1.12476
O	-3.72199	6.49640	0.88241
O	1.37582	-0.80801	0.43768
O	3.35866	0.89553	-0.19364
O	-1.15346	-0.32650	1.08538
O	7.44133	5.54817	-2.58239
O	-0.56524	3.49872	-4.69021
O	-1.24690	1.08528	3.36829
O	0.70184	1.28624	-5.40663
O	1.46830	2.49386	-3.16056
O	3.31880	1.36263	-4.85354
O	6.64278	4.53665	-4.94316
O	4.61070	0.97764	-2.57328
O	4.81630	5.59112	-3.24619
O	3.40178	3.18108	-1.37793
O	2.28873	4.97569	-3.12163
O	5.19837	-0.67901	3.63425
O	6.28372	-0.70997	1.17918
O	4.18732	-2.77030	-3.39835
O	7.88889	0.48632	-0.60987
O	7.78565	3.05415	-1.80278
O	9.86650	4.32623	-2.68961
O	8.86541	5.16788	-0.40122
O	5.86709	1.97774	-4.69940
O	5.07050	-0.56979	-4.69952
O	7.30194	3.72041	3.56738
O	6.77675	1.29856	3.00723
O	9.43192	2.11496	3.13394
O	10.80021	0.43976	1.52699
O	8.81275	-1.40563	1.07484
O	7.19688	-2.08893	-0.87799

O	6.81250	-2.20562	-3.57048
Cu	5.55908	1.54758	1.47826
Cu	2.29450	3.31439	0.67946
N	4.61896	5.20962	7.46631
N	4.48966	4.65217	6.49647
O	4.35253	4.06411	5.47714