

ELECTRONIC SUPPLEMENTARY INFORMATION

Mechanistic insights into the oxidation of copper(I) species during NH₃-SCR over Cu-CHA zeolites: a DFT study

Chong Liu,*^a Hiroe Kubota,^a Takashi Toyao,^{ab} Zen Maeno^a and Ken-ichi Shimizu*^{ab}

^a Institute for Catalysis, Hokkaido University, N-21, W-10, Sapporo 001-0021, Japan

^b Elements Strategy Initiative for Catalysts and Batteries, Kyoto University, Katsura, Kyoto 615-8520, Japan

Corresponding authors:

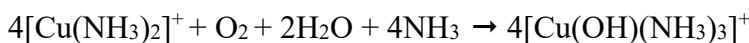
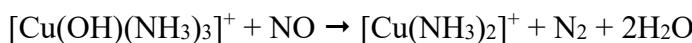
*Chong Liu (chongliu@cat.hokudai.ac.jp)

*Ken-ichi Shimizu (kshimizu@cat.hokudai.ac.jp)

Scheme S1 SCR reaction with exclusive O₂ activation for the oxidation half cycle*Oxidation half cycle*

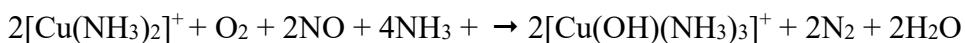
- (1) $2[\text{Cu}(\text{NH}_3)_2]^+ + \text{O}_2 \rightarrow [\text{Cu}_2(\mu\text{-O})_2(\text{NH}_3)_4]^{2+}$
- (2) $2[\text{Cu}(\text{NH}_3)_2]^+ + [\text{Cu}_2(\mu\text{-O})_2(\text{NH}_3)_4]^{2+} \rightarrow [\text{Cu}_4(\mu_3\text{-O})_2(\text{NH}_3)_8]^{4+}$
- (3) $[\text{Cu}_4(\mu_3\text{-O})_2(\text{NH}_3)_8]^{4+} + 2\text{H}_2\text{O} \rightarrow 2[\text{Cu}_2(\mu\text{-OH})(\eta\text{-OH})(\text{NH}_3)_4]^{2+}$
- (4) $2[\text{Cu}_2(\mu\text{-OH})(\eta\text{-OH})(\text{NH}_3)_4]^{2+} + 4\text{NH}_3 \rightarrow 4[\text{Cu}(\text{OH})(\text{NH}_3)_3]^+$

The oxidation half-reaction can be obtained as

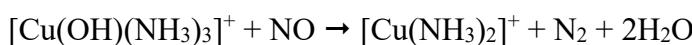
*Reduction half cycle**Overall reaction (Standard SCR mechanism)***Scheme S2** SCR reaction with both O₂ and NO activation for the oxidation half cycle*Oxidation half cycle^a*

- (1) $2[\text{Cu}(\text{NH}_3)_2]^+ + \text{O}_2 \rightarrow [\text{Cu}_2(\mu\text{-O})_2(\text{NH}_3)_4]^{2+}$
- (2) $[\text{Cu}_2(\mu\text{-O})_2(\text{NH}_3)_4]^{2+} + \text{NO} \rightarrow [\text{Cu}_2(\mu\text{-O})(\text{NO}_2)(\text{NH}_3)_4]^{2+}$
- (3) $[\text{Cu}_2(\mu\text{-O})(\text{NO}_2)(\text{NH}_3)_4]^{2+} \rightarrow [\text{Cu}(\text{NH}_3)_2]^+ + [\text{Cu}(\text{NO}_3)(\text{NH}_3)_2]^+$
- (4) $[\text{Cu}(\text{NO}_3)(\text{NH}_3)_2]^+ + \text{NO} \rightarrow [\text{Cu}(\text{NO}_2)(\text{NH}_3)_2]^+ + \text{NO}_2$
- (5) $[\text{Cu}(\text{NH}_3)_2]^+ + \text{NO}_2 \rightarrow [\text{Cu}(\text{NO}_2)(\text{NH}_3)_2]^+$
- (6) $[\text{Cu}(\text{NO}_2)(\text{NH}_3)_2]^+ \rightarrow [\text{Cu}(\text{OH})(\text{NH}_2\text{NO})(\text{NH}_3)]^+ (\Delta E = 164 \text{ kJ/mol})$
- (7) $[\text{Cu}(\text{OH})(\text{NH}_2\text{NO})(\text{NH}_3)]^+ + 2\text{NH}_3 \rightarrow [\text{Cu}(\text{OH})(\text{NH}_3)_3]^+ + \text{N}_2 + \text{H}_2\text{O}$

The oxidation half-reaction can be obtained as



^aThe conversion pathways of Cu nitrite species via nitrosamine (NH₂NO) and ammonium nitrite (NH₄NO₂) intermediates give same stoichiometry of the oxidation half cycle, and only the NH₂NO-involved mechanism is described.

Reduction half cycle*Overall reaction (Standard SCR mechanism)*

Spin states of the transition states and intermediates

During the geometry optimizations of DFT calculations, the electronic configurations with different spin states were evaluated, and the most stable ones were chosen to describe the minimum-energy reaction pathways. The spin-transition reaction was studied using the minimum energy crossing point (MECP) approach for the two potential energy surfaces.

The detailed information of the spin state for the reaction pathways described in the manuscript was summarized in the following Table S1 and additional supporting Fig. S1-S3.

Table S1 Summary of the spin transition information for the optimized structures along the minimum-energy reaction pathways.

Reaction pathways in manuscript	Spin transition	Spin states	Remarks
Fig. 2	Yes	Fig. S1	The spin-transition occurs with O ₂ dissociation.
Fig. 3	No	Singlet	
Fig. 4	No	Singlet	
Fig. 5a	No	Singlet	The “2[Cu(OH)] ⁺ ” intermediate is antiferromagnetic with two unpaired electrons with opposite spin directions. Each Cu center possesses one unpaired electron.
Fig. 5b	No	Doublet	
Fig. 6	No	Singlet	
Fig. 7	Yes	Fig. S2	The change of spin state is due to the release of gaseous NO ₂ .
Fig. 8a	Yes	Fig. S3	The change of spin state is due to the adsorption of gaseous NO. The “[Cu(NO ₂)] ⁺ + NO ₂ ” intermediate is antiferromagnetic with two unpaired electrons with opposite spin directions, which are located on the Cu center and the neutral NO ₂ molecule, respectively.
Fig. 8b	No	Doublet	

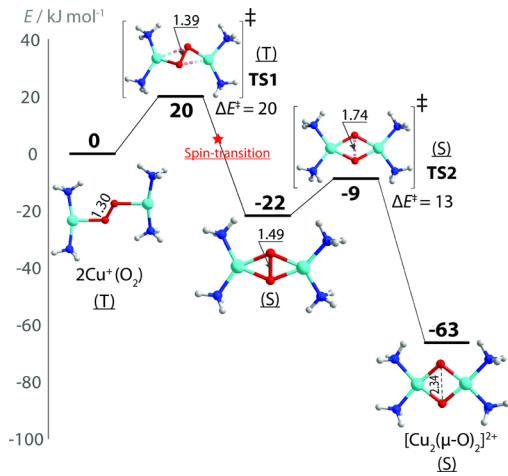


Fig. S1 Spin states of the reaction pathways (Fig. 2 in the main text) for the oxidative activation of Cu(I) into Cu(II) species in CHA zeolite via O₂ dissociation and oxidation of two mononuclear [Cu(NH₃)₂]⁺. The singlet and triplet spin states are denoted by (S) and (T), respectively.

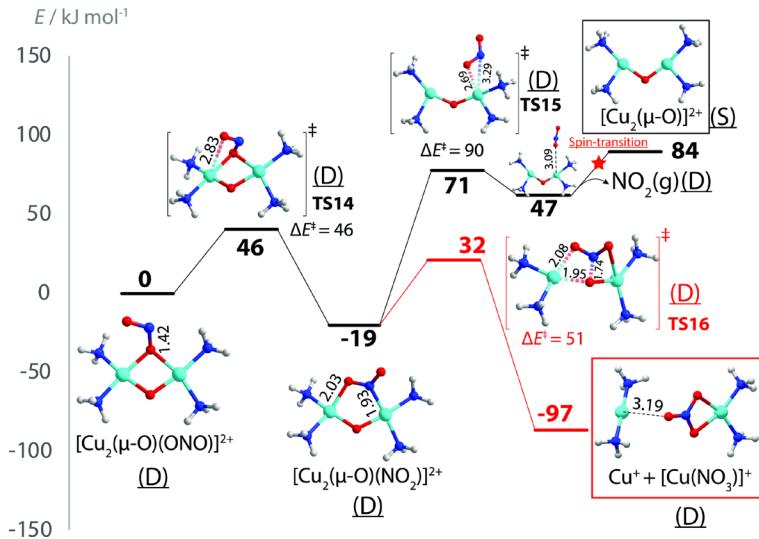


Fig. S2 Spin states of the reaction pathways (Fig. 7 in the main text) for the NO-assisted activation of Cu(I) into Cu(II) species in CHA zeolite. The singlet and doublet spin states are denoted by (S) and (D), respectively.

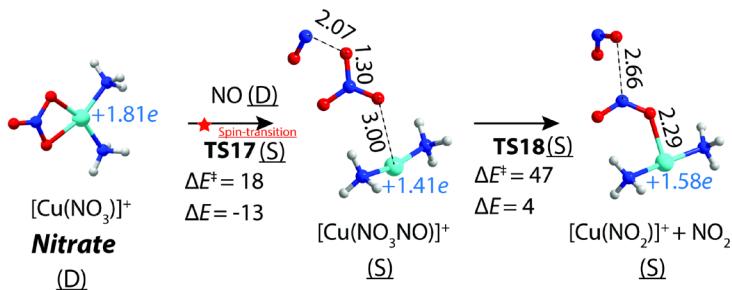


Fig. S3 Spin states of the reaction pathways (Fig. 8a in the main text) for the conversion from Cu nitrate to nitrite species. The singlet and doublet spin states are denoted by (S) and (D), respectively.

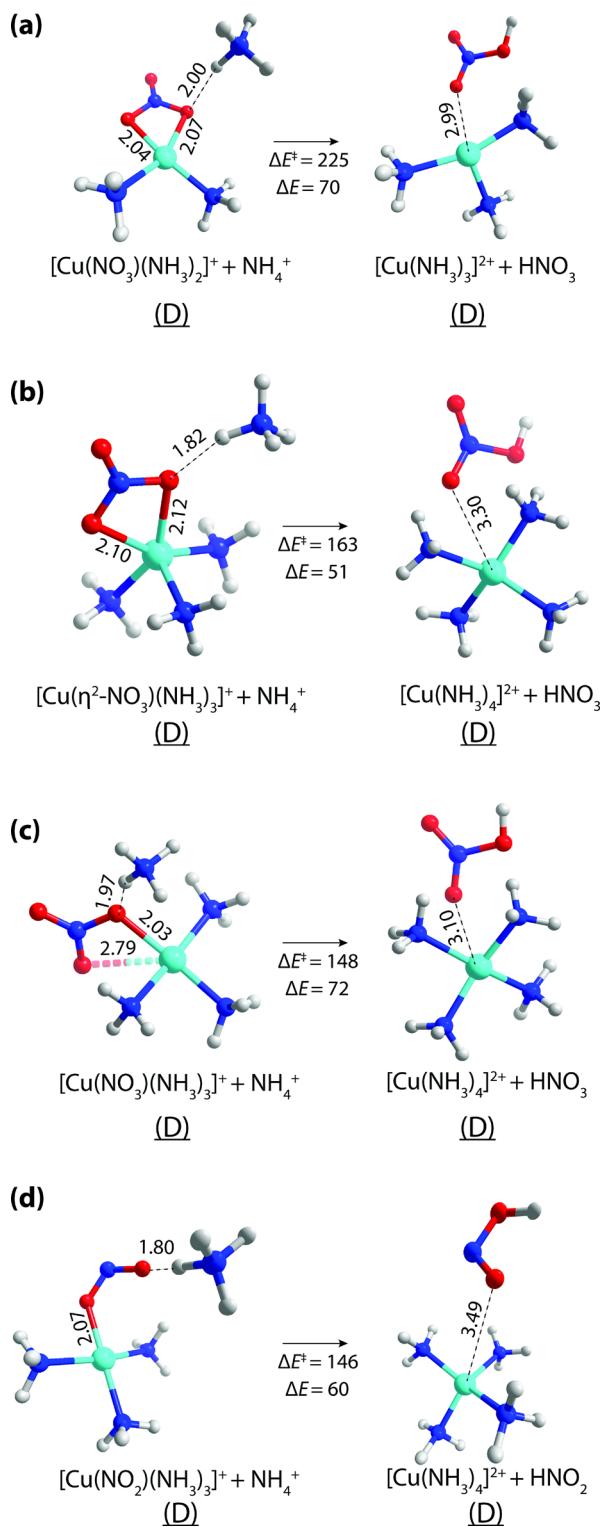


Fig. S4 Reactions of Cu(II) nitrate/nitrate species with Brønsted acid sites (in the form of NH_4^+) to release $\text{HNO}_3/\text{HNO}_2$. Cu nitrate (a) is in bidentate configuration with two NH_3 ligands; (b) and (c) are Cu nitrates with three NH_3 ligands (Ref. C. Negri et al., *ChemCatChem*, 2019, **11**, 3828–3838); Cu nitrite (d) is a structural analog of Cu nitrate (c). Activation and reaction energies (ΔE^\ddagger and ΔE) are in kJ/mol. Zeolite frameworks are omitted for clarity. The doublet spin states are denoted by (D).

Geometric parameters of the transition states and intermediates and their absolute energies

2Cu⁺, Fig. 1, E= -952.241 eV

1.0	13.6750001907	0.0000000000	0.0000000000	0.563171387	0.084455386	0.727400005	0.145417362	0.088203102	0.147139758
	-6.8375000954	11.8428975619	0.0000000000	0.214391783	0.398847103	0.079718463	0.708277524	0.297881395	0.719843090
	0.0000000000	0.0000000000	14.7670001984	0.934554577	0.095266230	0.710102856	0.120749891	0.544186413	0.431455672
H Al Si O N Cu				0.581023335	0.426734835	0.073506773	0.388239861	0.62948295	0.062983707
14 4 32 74 4 2				0.674655974	0.962993801	0.459232509	0.030551830	0.972616792	0.399913251

Direct

0.758640230	0.768444598	0.591197968	0.0291911138	0.329623193	0.459807754	0.008950131	0.310991853	0.721857429
0.746626794	0.668122351	0.660548985	0.731884062	0.660577416	0.789509058	0.674576581	0.642904699	0.087004557
0.747655749	0.649472594	0.548480272	0.032459572	0.969854474	0.125118598	0.330580324	0.975455165	0.371278495
0.353853434	0.521105707	0.576818526	0.683066368	0.331562042	0.474532992	0.918496907	0.111284271	0.479334563
0.377860874	0.513360202	0.685620368	0.402544916	0.003068029	0.150863171	0.230572075	0.786509156	0.145404875
0.392854601	0.630356073	0.644527614	0.793713808	0.475914866	0.610792220	0.907240450	0.424999207	0.489210814
0.210024476	0.401399910	0.210869521	0.488870382	0.794071496	0.937253714	0.564744651	0.728537560	0.791194320
0.181892961	0.350811481	0.317644119	0.887503684	0.750394285	0.386197805	0.250747472	0.066932902	0.125419736
0.239421248	0.487506986	0.298348397	0.131765321	0.637923062	0.271214902	0.919470131	0.755312324	0.157449350
0.498086631	0.333892703	0.275715053	0.597925127	0.788705885	0.086705074	0.574246168	0.443677694	0.806911886
0.557748795	0.449868351	0.215029672	0.542764187	0.935539424	0.603729606	0.802057505	0.891614020	0.780554295
0.571919203	0.456945509	0.326801747	0.152809203	0.127200904	0.250749499	0.789719284	0.504095256	0.790587723
0.284945518	0.163334101	0.469513953	0.879024446	0.592457831	0.273819566	0.795463562	0.541090488	0.105894387
0.736426890	0.853284836	0.382010490	0.089746818	0.235213622	0.591534317	0.443284988	0.844151676	0.097737812
0.243176565	0.533680499	0.044507332	0.727353215	0.552000880	0.944173098	0.133111149	0.216712162	0.423117667
0.704830229	0.767078638	0.286283384	0.389497906	0.853763759	0.269583464	0.497190058	0.879335999	0.776885152
0.130350307	0.107397623	0.364256531	0.536229551	0.214422166	0.605440378	0.144231275	0.179598764	0.078325503
0.801498711	0.983187199	0.500092804	0.226785019	0.295161426	0.928405285	0.810250461	0.546844542	0.444700897
0.251582831	0.321209788	0.821813107	0.884362221	0.892148674	0.261181861	0.612043858	0.111671351	0.493597448
0.695899308	0.544143081	0.050031330	0.078946307	0.4753050320	0.596007168	0.141228810	0.227632970	0.767471910
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0.480343550	0.767005622	0.829267740	0.207205459	0.530112684	0.931495190	0.140825063	0.529109955	0.767753661
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0.578133404	0.206502438	0.708531737	0.238771886	0.415847450	0.277322024	0.469951630	0.207234681	0.096417688
0.911795139	0.875947297	0.364215910	0.516172111	0.416490465	0.275126576	0.280241877	0.448611200	0.794848979
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0.911415040	0.870223403	0.157208845	-6.8375000954	11.8428975619	0.0000000000	0.581060946	0.424227715	0.074826881
0.467749119	0.313036740	0.042432539	0.0000000000	0.0000000000	14.7670001984	0.674887240	0.962755084	0.458965451
0.578517139	0.209763259	0.503744304	H Al Si O N Cu			0.349861532	0.666809678	0.803609431
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0.568186224	0.730914176	0.094566551	0.477984625	0.765656710	0.829671264	0.210314438	0.524433553	0.933769882
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0.916471958	0.755004287	0.158500776	0.580194771</td					

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0.127595171	0.101428233	0.366396219	0.698305011	0.758335412	0.941819787	0.804757178	0.879685163	0.419841856
0.799953818	0.979464829	0.500202537	0.394757688	0.155267209	0.263372123	0.140045896	0.528978288	0.768784225
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0.477224410	0.760040879	0.046142355	0.437357545	0.586657345	0.639870763	0.246500984	0.763042808	0.412492841
0.576535881	0.974277667	0.708688796	0.259868652	0.429322302	0.295798063	0.270254582	0.126043096	0.410214961
0.239715323	0.302252144	0.042822648	0.511617899	0.425883055	0.270517617	0.559537113	0.082675457	0.723825395
0.573390841	0.203080803	0.706470191	0.541160643	0.621431530	0.538686156	0.226414964	0.400422186	0.089242563
0.907184243	0.870633245	0.362681240	0.421953231	0.489063025	0.323105931	0.930509391	0.093018115	0.711880445
0.037324559	0.437340915	0.705398262	0.693903327	0.760264874	0.048376914	0.582989037	0.418867409	0.067239039
1.0						0.674629271	0.961987674	0.459072262
						0.347382218	0.667538285	0.812408566
						0.354085475	0.304289252	0.7911353703
			13.6750001907	0.0000000000	0.0000000000	0.013512568	0.629844666	0.134898007
			-6.8375000954	11.8428975619	0.0000000000	0.033090938	0.330040962	0.464675575
			0.0000000000	0.0000000000	14.7670001984	0.718015075	0.655244112	0.783272803
			H	Al	Si	O	N	Cu
			14	4	32	74	4	2
			Direct					
			0.723051965	0.756927669	0.591273367	0.396006882	0.996191859	0.156969056
			0.693436623	0.649612367	0.658223867	0.790873170	0.473828584	0.610725880
			0.736785591	0.649919748	0.552838802	0.493211985	0.801113834	0.940187395
			0.386257529	0.624783576	0.627686918	0.883807719	0.746824741	0.384090185
			0.390957624	0.519773901	0.676830053	0.134578243	0.628350616	0.273289174
			0.490489841	0.650300920	0.699860692	0.598389089	0.786642194	0.088311777
			0.206432909	0.500313163	0.687166631	0.329543859	0.472862482	
			0.137570173	0.650959611	0.163626119	0.723051965	0.364537143	0.2325663404
			0.036342780	0.440746248	0.497862935	0.238038927	0.478075504	0.307288736
			0.375827879	0.101335436	0.158813000	0.464527875	0.335847855	0.251830667
			0.241242021	0.539372504	0.832983315	0.386257529	0.624783576	0.627686918
			0.798907816	0.439508796	0.504599750	0.390957624	0.519773901	0.676830053
			0.038942341	0.216244623	0.492682343	0.490489841	0.650300920	0.699860692
			0.698864818	0.539479017	0.829529643	0.249645474	0.406999022	0.221525967
			0.364451200	0.865256608	0.166681066	0.205045804	0.346537143	0.323520780
			0.570012748	0.971559227	0.500585675	0.238038927	0.478075504	0.307288736
			0.900717735	0.626701716	0.165335581	0.464527875	0.335847855	0.251830667
			0.129901543	0.651148677	0.379150063	0.511097491	0.451824963	0.191499472
			0.143901139	0.084137551	0.147766024	0.580571592	0.450968087	0.282246470
			0.704900146	0.297960043	0.723523676	0.289632112	0.165109858	0.468466818
			0.120980792	0.543629885	0.433124751	0.736467242	0.825269342	0.151636586
			0.387346625	0.629780412	0.060922612	0.244537488	0.529190340	0.047627412
			0.024902955	0.967324642	0.401384056	0.699645519	0.764946878	0.827226579
			0.709102571	0.013457413	0.720459819	0.130468816	0.104167491	0.366655231
			0.363850353	0.319630295	0.072460651	0.801319897	0.982346654	0.501518167
			0.023764549	0.668969067	0.404142022	0.249445543	0.321045250	0.824226677
			0.004704086	0.307901889	0.724761214	0.693938196	0.540295243	0.046233874
			0.670126975	0.636305809	0.087381952	0.358333088	0.870923162	0.372484595
			0.333971816	0.975605488	0.363945274	0.375356406	0.107969090	0.365255028
			0.916049659	0.107692920	0.479266107	0.898669720	0.636962625	0.373780280
			0.230319723	0.785089791	0.145386875	0.475303739	0.769278586	0.833468437
			0.907267272	0.423919380	0.488774300	0.477135748	0.760991335	0.046103846
			0.558469951	0.727581024	0.790868163	0.578773737	0.961290555	0.708176553
			0.249342978	0.062630609	0.125624761	0.240225449	0.302761912	0.042180702
			0.919447482	0.752759755	0.160969600	0.574679494	0.204835683	0.705452561
			0.571168780	0.437989444	0.043050138	0.911068439	0.873767614	0.364137590
			0.796746790	0.888406336	0.782136679	0.038705464	0.439761549	0.705997884
			0.789319396	0.507412076	0.787133515	0.694623590	0.761526406	0.049192835
			0.797990438	0.541361192	0.100537337	0.807945788	0.597800462	0.707368433
			0.444418073	0.844798803	0.099674903	0.040535726	0.214688241	0.700263083
			0.131555751	0.212409765	0.425159723	0.802996755	0.431329340	0.712171435
			0.492018431	0.878465176	0.778599679	0.470094472	0.312901884	0.826717377
			0.145769164	0.178996622	0.081155792	0.911698878	0.867358863	0.157793432
			0.805745959	0.541892409	0.442826182	0.468790829	0.304681480	0.039328992
			0.605814457	0.105133578	0.490310729	0.580558489	0.209248707	0.501034737
			0.138094068	0.225638494	0.768721700	0.136597842	0.649068832	0.163854331
			0.457491457	0.894673645	0.441330135	0.033844471	0.442142814	0.498481423
			0.487298816	0.219033763	0.771330893	0.375655115	0.101753153	0.157988593
			0.801644623	0.873290658	0.421672851	0.242896169	0.541407168	0.833081901
			0.137951419	0.526104510	0.768725991	0.800318599	0.442558229	0.505989432
			0.814228058	0.857049823	0.090382561	0.041278716	0.218746096	0.492983609
			0.478069812	0.188792944	0.430384576	0.700236559	0.542221189	0.830811918
			0.164968893	0.564858615	0.115502909	0.363891959	0.865016818	0.166620507
			0.468351549	0.201521471	0.095534138	0.574282348	0.976390779	0.499794646
			0.277505606	0.446464062	0.796735781	0.900158763	0.627368331	0.166620508
			0.925277293	0.445715755	0.721899211	0.131512851	0.652164221	0.379080981
			0.243576571	0.762775481	0.412730843	0.144017771	0.086366832	0.147905232
			0.266976297	0.121763386	0.410318762	0.706732512	0.298758626	0.721167684
			0.558797598	0.081457160	0.725551426	0.120971791	0.544649303	0.433649212
			0.225543603	0.399777700	0.089720063	0.386522263	0.630698442</td	

[Cu ₂ (μ-O) ₂] ²⁺ , Fig. 3, E = -1046.176 eV						
1.0						
	13.6750001907	0.0000000000	0.0000000000	0.350688159	0.299992949	0.792115211
	-6.8375000954	11.8428975619	0.0000000000	0.016183143	0.631895125	0.137087777
	0.0000000000	0.0000000000	14.7670001984	0.037339862	0.332190901	0.465752780
H	Al	Si	O	N	Cu	
14	4	32	74	4	2	
Direct						
	0.706835628	0.749177098	0.585726619	0.399940670	0.999159455	0.160120264
	0.677424133	0.639508784	0.651010752	0.789035559	0.471228004	0.609653353
	0.720610797	0.642791450	0.544069171	0.488195360	0.794785261	0.938745975
	0.400389344	0.637224257	0.619720876	0.883414030	0.746565282	0.381187409
	0.392013520	0.523932457	0.666026235	0.141955256	0.629136503	0.272817045
	0.499743104	0.650744081	0.693136513	0.602493882	0.791605890	0.084713317
	0.272170663	0.413190007	0.245002747	0.543411970	0.929627657	0.604147971
	0.226642698	0.350463539	0.347051263	0.154403895	0.126482889	0.252338201
	0.2544424214	0.481179088	0.331060916	0.863826156	0.583162665	0.269633353
	0.460935891	0.357936472	0.259710312	0.092275843	0.234026983	0.598201096
	0.378747463	0.477503836	0.205693245	0.712481737	0.546942711	0.936901391
	0.086413659	0.147930413	0.580975532	0.473284513	0.286439061	0.391082972
	0.219162270	0.493242294	0.287367791	0.160627767	0.470048517	0.538181722
	0.706352413	0.298901260	0.721960664	0.287367791	0.160627767	0.218168676
	0.121235766	0.345549989	0.434033066	0.734748244	0.849929988	0.235316113
	0.387655288	0.631325245	0.061730836	0.249178499	0.531137764	0.050011478
	0.029697699	0.9691156146	0.401646346	0.699670374	0.763103068	0.824510634
	0.711407661	0.015695130	0.722298205	0.130665824	0.104565583	0.365882248
	0.365412235	0.320424080	0.072848216	0.802087605	0.983267546	0.500786483
	0.026399069	0.672512054	0.400999367	0.248985170	0.321116030	0.825164437
	0.005503218	0.309865266	0.723558664	0.693637073	0.540015399	0.045183323
	0.668648243	0.636159897	0.086508378	0.359198051	0.871962488	0.372520477
	0.332266420	0.976204813	0.368214548	0.376877248	0.110697448	0.364668701
	0.918746889	0.110202916	0.482339442	0.897832632	0.636278927	0.370993912
	0.230938002	0.783324897	0.145058766	0.474995494	0.767978489	0.831089616
	0.907630980	0.424852490	0.489464253	0.478374451	0.761886179	0.046181362
	0.563188374	0.733049631	0.792873085	0.579984426	0.976489663	0.708053112
	0.249886423	0.064867891	0.125583053	0.244115502	0.306317776	0.043866508
	0.920573771	0.754354417	0.161079586	0.574047029	0.204990923	0.705544412
	0.570357680	0.439699143	0.807220221	0.909894764	0.873400033	0.361876607
	0.801526785	0.891369939	0.782026529	0.038423870	0.439246684	0.706431925
	0.787971437	0.506949723	0.787823617	0.695824683	0.761643112	0.045645863
	0.798270762	0.542975664	0.100940749	0.807585120	0.976517677	0.706096053
	0.445817322	0.846364677	0.100361668	0.039835330	0.213993832	0.700903356
	0.132614061	0.214386547	0.424631059	0.802422285	0.430826217	0.711603880
	0.493324369	0.880434036	0.777618587	0.468584597	0.310948223	0.825510144
	0.146323204	0.179958537	0.079911128	0.912291706	0.868561625	0.156656489
	0.808850050	0.545399189	0.444565564	0.472210735	0.307293683	0.040539678
	0.610175014	0.109411083	0.493670881	0.580747187	0.209996849	0.500811756
	0.137812093	0.228253081	0.770587862	0.13993720	0.651510239	0.163943172
	0.459950328	0.901271820	0.441241086	0.036573078	0.443842173	0.499562277
	0.489563853	0.221142501	0.771307468	0.376895249	0.103047989	0.158471942
	0.804919243	0.879898906	0.419811577	0.245158494	0.541394830	0.832053542
	0.139782652	0.528383732	0.769446790	0.801519752	0.441559464	0.505111294
	0.813724935	0.857517242	0.093064710	0.043697312	0.220015287	0.494381547
	0.480233848	0.187905818	0.429434627	0.696583271	0.538867414	0.827401280
	0.162036330	0.562507093	0.113775305	0.366246939	0.867111444	0.167290449
	0.469725162	0.202156574	0.095274709	0.573429227	0.970565708	0.500271201
	0.280456960	0.449132562	0.795153201	0.901731253	0.629188836	0.165111125
	0.926513374	0.447550863	0.724501967	0.133067057	0.653333962	0.377687454
	0.246053353	0.763848066	0.412753642	0.146128252	0.087827861	0.14791714
	0.270274222	0.125886634	0.410064548	0.705589056	0.298977313	0.723664284
	0.559779406	0.082866348	0.722485423	0.121882252	0.546698928	0.434180945
	0.228847384	0.401301295	0.090542167	0.390791357	0.632060177	0.065823734
	0.930580914	0.092536971	0.711476505	0.028844453	0.969485104	0.399106652
	0.584373474	0.418371797	0.069362558	0.712240279	0.015842523	0.722896159
	0.674620986	0.962088883	0.459040821	0.368240535	0.323574305	0.074021235
	0.347669601	0.667537451	0.811046898	0.026682321	0.672633529	0.397186190
	0.352827817	0.302787304	0.791358829	0.004058551	0.308670253	0.722634375
	0.014108650	0.630053520	0.135628074	0.668664873	0.636471748	0.086025394
	0.034547541	0.330956747	0.446492257	0.335257888	0.978649735	0.367894511
	0.716721058	0.654022349	0.782087684	0.920673847	0.110742800	0.483318806
	0.031578138	0.969164670	0.124917790	0.232287273	0.785951912	0.146158740
	0.688057959	0.328877807	0.472005367	0.908899486	0.423827022	0.491116904
	0.397056878	0.996887207	0.158508182	0.563153565	0.732592404	0.790281832
	0.790298700	0.473138690	0.610355139	0.249895376	0.063751832	0.126055196
	0.492518574	0.799710274	0.940023482	0.922707015	0.756038189	0.161052853
	0.883164644	0.746469319	0.383149356	0.569215715	0.437296748	0.801781118
	0.137132809	0.629023433	0.273224473	0.801995814	0.890389879	0.780889511
	0.599589255	0.787491679	0.088286400	0.788236856	0.507385790	0.787233651
	0.542210698	0.930599868	0.603884161	0.802284896	0.546689451	0.096456543
	0.152086377	0.123159140	0.252632886	0.446313083	0.847221449	0.099669188
	0.866515875	0.5853759248	0.271615505	0.134471387	0.215122059	0.425362706
	0.090331577	0.233504593	0.597058058	0.494368017	0.881363272	0.778160334
	0.719304860	0.551222801	0.938671350	0.149333864	0.181676611	0.079411887
	0.389662445	0.846179903	0.272461474	0.811264575	0.544914842	0.443747699
	0.537125170	0.216226056	0.601560891	0.607697904	0.108265191	0.493990213
	0.232813478	0.301904351	0.932696581	0.135530680	0.227988258	0.773362458
	0.884090960	0.891938627	0.260765880	0.459410995	0.899715781	0.442081600
	0.079869375	0.475545764	0.601524174	0.487272352	0.218397141	0.771636426
	0.704299808	0.763081551	0.942337215	0.805048645	0.880211771	0.419155091
	0.396163076	0.156308398	0.262579620	0.137991115	0.525963843	0.771902263
	0.790027678	0.921796203	0.605840921	0.815526438	0.857517183	0.089745201
	0.207017660	0.517474473	0.935718715	0.480325311	0.190536320	0.429849207
	0.463637769	0.280323327	0.932610631	0.163779095	0.565452814	0.111702643
	0.410619467	0.528441966	0.459140390	0.469169080	0.201259241	0.093636848
	0.541674972	0.548550606	0.426403373	0.281001478	0.448736847	0.793425679
	0.682449639	0.667661190	0.589393139	0.926244676	0.447311401	0.723549664
	0.443531781	0.599781811	0.645403028	0.245551214	0.765842080	0.412263602
	0.267584741	0.421893477	0.297410995	0.269688189	0.124973215	0.410407871
	0.499319762	0.428689331	0.258906037	0.560451627	0.083100542	0.721331418
	0.527682245	0.593125522	0.541998863	0.231356740	0.403235167	0.093319714
	0.420757800	0.474955946	0.346036077	0.930673838	0.091129079	0.709528983
	0.586878240	0.418360412	0.508824012	0.586878240	0.041836042	0.073149674
	0.675051987	0.962941527	0.458829790	0.650750000	0.365597397	0.859190285
	0.347969860	0.666956484	0.806128919	0.666956484	0.568573773	0.965533018

0.897684813	0.622213483	0.162938446	0.547655940	0.715873361	0.627443314	0.338545889	0.649495900	0.801779091
0.129983768	0.639278531	0.374657273	0.458904475	0.584738731	0.657794714	0.340697199	0.289843976	0.803029656
0.138921916	0.079012632	0.150032088	0.593136072	0.635899246	0.674951077	0.016806807	0.633885682	0.129971638
0.690995097	0.284309745	0.720020533	0.227489710	0.410381794	0.266115338	0.037444934	0.324721217	0.482311457
0.120237130	0.530256748	0.428630561	0.192806602	0.334936470	0.362798810	0.695047319	0.641097963	0.774816215
0.380127043	0.624608755	0.073791720	0.221172184	0.468666673	0.363303512	0.025009133	0.961864054	0.125638664
0.039219953	0.960488021	0.399566472	0.358522743	0.293754786	0.265914351	0.678425372	0.314648420	0.466634274
0.691169620	0.999012172	0.739546537	0.393981189	0.402611703	0.197994947	0.391698360	0.986831307	0.150441110
0.360791981	0.314712256	0.058976047	0.492297351	0.390509093	0.255103201	0.792348385	0.457010210	0.601569712
0.023093766	0.655203044	0.399994284	0.594235063	0.929373264	0.214778468	0.453978896	0.783855259	0.941150784
0.021102108	0.311587632	0.702289402	0.652376771	0.960421562	0.319386959	0.885916829	0.737238407	0.374103040
0.667015672	0.630427122	0.071598738	0.733331800	0.001444019	0.226635367	0.130612046	0.619815707	0.271472812
0.312468916	0.961829007	0.363410681	0.610265315	0.605394781	0.317559183	0.596799254	0.779353261	0.063500471
0.896428466	0.107117236	0.454691410	0.630224764	0.619434416	0.202879280	0.540202314	0.914442301	0.604894519
0.235837221	0.768240035	0.140460491	0.737665057	0.674548209	0.272783667	0.146120772	0.120517008	0.253003091
0.903125584	0.408060193	0.476159692	0.300920695	0.527882338	0.666687667	0.868059397	0.573606670	0.264645249
0.561340928	0.729471803	0.802554011	0.317698985	0.535700083	0.553031540	0.050542235	0.181074679	0.593010306
0.243500695	0.056110308	0.128793210	0.191602483	0.469450384	0.600740731	0.704844415	0.533002138	0.928335369
0.907621980	0.744891644	0.165255919	0.376140386	0.230072111	0.606886863	0.388632327	0.845328808	0.275554717
0.562383115	0.425268620	0.792317033	0.242464453	0.166149735	0.637500703	0.524676085	0.205537573	0.594876826
0.794452786	0.875539124	0.761793613	0.277923495	0.183632493	0.528145194	0.201415554	0.281788170	0.930486381
0.780840158	0.498505473	0.776756644	0.240259230	0.520466328	0.051964097	0.882716715	0.889301717	0.266423076
0.798277915	0.540471494	0.093005270	0.697306931	0.760448098	0.823500574	0.055865668	0.480784118	0.601176143
0.456927776	0.844367683	0.106344067	0.136352670	0.096633390	0.369251788	0.737620711	0.775270045	0.935403228
0.119771935	0.201165855	0.424372464	0.791182697	0.969150305	0.486623049	0.394731194	0.144136220	0.260640919
0.471911758	0.862564862	0.773909390	0.232538402	0.305287391	0.824521780	0.786831558	0.950215518	0.601488769
0.141354442	0.169407949	0.077652194	0.689544559	0.530217109	0.037014805	0.205063030	0.518339276	0.938597739
0.806148291	0.532930315	0.439670146	0.348854780	0.866662323	0.374373972	0.478112608	0.274883538	0.927723944
0.616313219	0.101802282	0.505153596	0.360514849	0.096715830	0.364730358	0.405600071	0.532050788	0.468600046
0.129747838	0.209239095	0.761232853	0.897666216	0.626334548	0.366644472	0.546337724	0.513134778	0.401394576
0.450029135	0.904562831	0.445082068	0.458884209	0.757523060	0.834004521	0.710907042	0.651612997	0.530340627
0.471586972	0.204213902	0.763228416	0.468087494	0.752535045	0.045071770	0.535791576	0.635575891	0.628760040
0.815190434	0.866496682	0.437664092	0.564082265	0.961981475	0.709628582	0.244121000	0.414818615	0.334346384
0.128056765	0.517545521	0.737286939	0.232219368	0.291984260	0.037936430	0.412532866	0.379256040	0.25896297
0.804026961	0.8507611414	0.103468366	0.557695627	0.190981165	0.699188352	0.660104036	0.938448787	0.253962010
0.479667187	0.160251647	0.424151837	0.909132361	0.867889404	0.371779084	0.656982243	0.659507692	0.264274269
0.145297468	0.544083178	0.108030185	0.025262385	0.432374626	0.705891550	0.272637665	0.484705836	0.606984258
0.460389763	0.191733941	0.088486597	0.701100349	0.759928405	0.038013685	0.299086899	0.221366823	0.591313243
0.262590528	0.429458737	0.791647375	0.795231910	0.976306915	0.707759976	0.549974084	0.583188176	0.508895874
0.911059618	0.419470280	0.731263757	0.024871020	0.197354466	0.698293746	0.400127977	0.459664553	0.363442063
0.244252712	0.750291228	0.407719523	0.79007448	0.417100728	0.706885934	0.661223829	0.800130367	0.259855539
0.274714589	0.130347863	0.402184755	0.461354017	0.299733609	0.823241889	0.288714379	0.354880184	0.595916688
0.541001081	0.066172987	0.714355171	0.907046676	0.863025665	0.163482055			
0.224036604	0.391175836	0.088118926	0.469110936	0.297216654	0.034308746			
0.909175336	0.093732886	0.737799274	0.5736764500	0.193311095	0.496838381			
0.580494463	0.410802931	0.69680162	0.133604005	0.639164269	0.161981967			
0.658188820	0.941908836	0.449054003	0.024605719	0.433479607	0.497225136			
0.342828721	0.647712290	0.795973420	0.370802581	0.092640176	0.157666042			
0.341763079	0.288260430	0.794847906	0.231362239	0.529989858	0.833882272			
0.015789701	0.634227574	0.132018133	0.793726623	0.426204979	0.495371491			
0.043026071	0.326039523	0.487458050	0.020591604	0.197015151	0.487363905			
0.704999804	0.642103374	0.777328908	0.685056267	0.529541373	0.818947256			
0.025317276	0.960927010	0.126299143	0.365036070	0.858859544	0.168240517			
0.682445765	0.314893186	0.467233688	0.567658246	0.9654563579	0.502027214			
0.391390741	0.986634851	0.147390381	0.899003983	0.623055577	0.160280496			
0.793282807	0.455710888	0.604088843	0.128954038	0.640874326	0.377881318			
0.458103210	0.777922928	0.937892616	0.139338449	0.078509986	0.150722116			
0.887420475	0.737943888	0.375427246	0.687334955	0.288128316	0.720404411			
0.132431462	0.615211248	0.268655774	0.118681952	0.531264365	0.431334466			
0.597064137	0.778860331	0.0660000819	0.380171716	0.625283837	0.072495259			
0.541309893	0.913642943	0.603256285	0.035731900	0.959069252	0.399172455			
0.144377500	0.122978032	0.251618415	0.692228377	0.999993086	0.738646150			
0.886526569	0.571880221	0.266933143	0.360891968	0.312477112	0.053123833			
0.046196900	0.172104120	0.593833029	0.021352984	0.655724049	0.402957708			
0.705809593	0.530280769	0.929852784	0.013810408	0.309588373	0.707119107			
0.392518640	0.848258018	0.272636294	0.666338742	0.630411267	0.071713187			
0.526285887	0.205162510	0.5950903310	0.308844358	0.960017622	0.364027619			
0.209623680	0.283681035	0.928917408	0.896246970	0.104506873	0.455842495			
0.884404957	0.890897632	0.268040299	0.236076525	0.768289387	0.140678078			
0.006971511	0.487540096	0.601224482	0.898364544	0.406564236	0.471454322			
0.735271513	0.776926637	0.935520113	0.558073580	0.731765684	0.810753286			
0.400639266	0.145184696	0.258632183	0.243149012	0.054944012	0.127585784			
0.786979496	0.954501450	0.601600051	0.908954501	0.745728195	0.162218213			
0.214557230	0.516635418	0.934749186	0.558935463	0.425054938	0.793424606			
0.471344888	0.277894408	0.927159429	0.792789459	0.875220478	0.763065517			
0.395299286	0.552577019	0.459169418	0.778325915	0.504263341	0.772771120			
0.537130892	0.518398643	0.408810347	0.799247384	0.541254163	0.090463132			
0.693585992	0.654797196	0.539932013	0.457890242	0.844104946	0.11287065			
0.511315882	0.679994583	0.606057465	0.118535072	0.201452032	0.422272197			
0.237994984	0.415676236	0.329719454	0.471551806	0.865060091	0.775467753			
0.411435366	0.378944486	0.266794860	0.142351344	0.171068490	0.080705814			
0.660959661	0.936186492	0.252588107	0.803880880	0.515319576	0.435550183			
0.656386435	0.656572044	0.266635478	0.616034329	0.102387890	0.506255746			
0.2788608								

0.372599840	0.094323941	0.157585874	0.0000000000	0.0000000000	14.7670001984	0.250267416	0.751580894	0.409629136				
0.236466333	0.531378508	0.829673350	H	Al	Si	O	N	Cu				
0.795368135	0.428492904	0.496686190	24	4	32	74	8	4				
0.018590696	0.197161138	0.486602366	Direct									
0.688635468	0.528215647	0.822209597	0.740471423	0.731192112	0.495747447	0.918918490	0.088454247	0.741025925				
0.365156919	0.859617114	0.166959047	0.736825228	0.673997939	0.596503139	0.582904518	0.411677092	0.068050548				
0.569316387	0.966724813	0.501884520	0.738804102	0.608905315	0.502102375	0.657715440	0.934778929	0.453802615				
0.898951263	0.623787284	0.161719859	0.522436500	0.648626745	0.678746045	0.341941893	0.657198071	0.97989243				
0.131600052	0.642302215	0.376854151	0.457421571	0.511012971	0.682112932	0.350382358	0.299995661	0.802443624				
0.140156195	0.081807941	0.152348921	0.594740033	0.586368024	0.689307928	0.019655636	0.630701303	0.128472805				
0.690869391	0.289104134	0.721118450	0.218862966	0.413653046	0.267244786	0.030079717	0.320812255	0.463039786				
0.123395398	0.536237061	0.434806734	0.182020530	0.334583014	0.360916078	0.705864251	0.643413663	0.779690206				
0.381055206	0.625854611	0.073660180	0.205728650	0.465692401	0.364909947	0.027910598	0.968367040	0.133584827				
0.038081508	0.959705710	0.398937166	0.330442458	0.301561832	0.259137064	0.688300490	0.316513836	0.460087597				
0.695112586	0.000994210	0.737245023	0.384449482	0.416251034	0.196092889	0.390335232	0.986814797	0.147776052				
0.361458451	0.312271982	0.052747495	0.467982322	0.377753407	0.247711286	0.780227305	0.457258165	0.601356983				
0.023985332	0.657294512	0.400466412	0.571248889	0.849580407	0.234531301	0.466376245	0.782503545	0.939067781				
0.007441330	0.305116564	0.721702874	0.634077549	0.882875264	0.336290807	0.894332469	0.740934491	0.375697821				
0.667248130	0.631006420	0.073760435	0.709666848	0.911322713	0.241904825	0.132209212	0.614414793	0.271309584				
0.312183350	0.962806463	0.362982124	0.619649708	0.540144444	0.316997141	0.599337518	0.780100167	0.071978591				
0.896109283	0.103667580	0.453375250	0.618297637	0.546271086	0.201735094	0.540651679	0.919403374	0.605522275				
0.235724404	0.768010318	0.141631499	0.738753855	0.604780436	0.257377416	0.1532727054	0.136402428	0.254385859				
0.902595818	0.411908209	0.475654036	0.327136934	0.641385019	0.666540027	0.876897454	0.578732967	0.265916497				
0.559654176	0.731089294	0.804970086	0.376645416	0.663215458	0.560506582	0.041793562	0.197109461	0.595131695				
0.244633317	0.058868401	0.130660489	0.240446270	0.608725071	0.579225063	0.714810193	0.532585442	0.931174576				
0.912261069	0.747436285	0.161886781	0.360740870	0.320884764	0.577845752	0.395043671	0.849299312	0.273343533				
0.562974095	0.425571740	0.792737873	0.243873820	0.257915467	0.639620543	0.541666329	0.212419778	0.592955112				
0.792258382	0.871874213	0.761561573	0.236312777	0.268325329	0.528530180	0.203695551	0.287391841	0.925719023				
0.782418132	0.503826976	0.776654065	0.244654298	0.521127641	0.049290188	0.877481639	0.883258045	0.266739637				
0.799701750	0.541628718	0.092487246	0.697696209	0.759419620	0.822467506	0.074680060	0.462457836	0.601153553				
0.456829816	0.845208645	0.108094983	0.143393114	0.101341359	0.370363295	0.726969481	0.775438607	0.935820639				
0.121025734	0.198547140	0.430144250	0.794065654	0.966703832	0.487757146	0.405345827	0.148047656	0.260073543				
0.475575238	0.868002057	0.776572585	0.239413887	0.311453431	0.820830524	0.7963545208	0.955924392	0.602697313				
0.143046528	0.172941521	0.080330171	0.693460941	0.530700266	0.038643535	0.212551446	0.519429445	0.934389591				
0.806626439	0.534774601	0.437896937	0.355025053	0.869965374	0.372249693	0.484629035	0.275549412	0.924830914				
0.619262755	0.103873126	0.505696177	0.367634267	0.100942001	0.364048660	0.391445339	0.505649328	0.488120675				
0.136053428	0.215908975	0.765650465	0.905202448	0.630632460	0.368432730	0.539869487	0.540235937	0.402499586				
0.451666415	0.907349646	0.445277393	0.465782136	0.760687053	0.831099749	0.706731379	0.655084789	0.531531155				
0.470603138	0.204834387	0.762185156	0.472673807	0.753195107	0.04355424	0.525906146	0.579703450	0.654013991				
0.812474430	0.863816917	0.434825778	0.570524931	0.967676461	0.706978289	0.232808679	0.415350795	0.335689843				
0.130117923	0.519889355	0.769511700	0.235154644	0.293412656	0.033458602	0.396666378	0.383538693	0.254956186				
0.806416452	0.852369845	0.102032594	0.566733837	0.196639419	0.698430240	0.635771930	0.853083193	0.272141457				
0.480792731	0.159488395	0.421840221	0.912332594	0.868938804	0.370763630	0.657394528	0.588460267	0.259578824				
0.147430375	0.543425202	0.111534879	0.032049011	0.431098968	0.706717730	0.311510444	0.609210193	0.601500869				
0.462131470	0.191985577	0.089734815	0.701434135	0.759967029	0.040452007	0.281889290	0.310774654	0.585659146				
0.266133606	0.434266696	0.791396618	0.800521255	0.977432489	0.709705570	0.542626679	0.571877658	0.522421837				
0.911858678	0.428460896	0.730164826	0.024865160	0.200226530	0.703769505	0.390467077	0.463372380	0.366481960				
0.246266350	0.752361119	0.410575598	0.794663906	0.421494395	0.704717875	0.641199172	0.717164755	0.273174644				
0.276689589	0.132606849	0.404611975	0.468982249	0.304003090	0.821354330	0.289969355	0.457619756	0.590773523				
0.545712173	0.070357524	0.716294765	0.909561217	0.863666356	0.164774105	0.744690407	0.136750001907	0.00000000000				
0.230092585	0.394429266	0.086282626	0.472137600	0.297611505	0.031006135	-6.8375000954	11.8428975619	0.00000000000				
0.915011108	0.087104060	0.739308894	0.583469152	0.196109802	0.493612587	14.7670001984	H	Al	Si	O	N	Cu
0.580980420	0.411346436	0.071216486	0.136816114	0.637656391	0.161530182	24	4	32	74	8	4	
0.658198595	0.942139566	0.451114208	0.030719010	0.432001412	0.496824324	Direct						
0.342166185	0.652324259	0.796646237	0.373885930	0.095148087	0.158003122	0.743816257	0.614342332	0.503175378				
0.344692230	0.292821944	0.799451411	0.238120315	0.534333646	0.829386950	0.521786630	0.639579058	0.678174138				
0.016921932	0.632783413	0.131847084	0.796229064	0.430377632	0.496657372	0.5458445817	0.501861691	0.675600946				
0.036978472	0.324420482	0.470633566	0.017369293	0.197071493	0.48584076	0.595302284	0.578300476	0.682281137				
0.699457765	0.640379727	0.779220270	0.695755986	0.531651020	0.822605908	0.206640403	0.416890681	0.270760715				
0.027245117	0.964140356	0.126629800	0.367603612	0.860803366	0.166484356	0.181546554	0.337797701	0.363192797				
0.682510674	0.316082865	0.465272486	0.571749866	0.966057718	0.501430631	0.203642294	0.468203515	0.371259153				
0.390099696	0.986565948	0.148656815	0.905499101	0.625971019	0.160661578	0.335147963	0.312692374	0.246656507				
0.789608479	0.457766175	0.602712393	0.134479061	0.642292595	0.377019614	0.341262072	0.417200625	0.187126081				
0.457712829	0.780047357	0.939957380	0.142854705	0.085969947	0.153858721	0.595302284	0.578300476	0.682281137				
0.887785785	0.738234222	0.374415398	0.696186125	0.292098612	0.724052608	0.206640403	0.416890681	0.216478407				
0.133432075	0.616575837	0.721177053	0.125393897	0.536016583	0.435412735	0.181546554	0.337797701	0.363192797				
0.597822666	0.780548394	0.067804433	0.383052617	0.626219332	0.071614303	0.203642294	0.468203515	0.371259153				
0.539296687	0.915731966	0.604749203	0.040124595	0.962542713	0.392707199	0.335169435	0.312692374	0.246656507				
0.145567805	0.124633744	0.254381984	0.699320436	0.0554747497	0.736237586	0.341262072	0.417200625	0.187126081				
0.867490411	0.573736370	0.265631407	0.363666326	0.313540608	0.043667499	0.457019749	0.413396627	0.205824748				
0.044956140	0.190447196	0.594662189	0.028581450	0.658510506	0.403846800	0.591220081	0.744032741	0.216478407				
0.705616141	0.531228244	0.936112255	0.007698770	0.306087822	0.730548406	0.594773889	0.746574998	0.329512209				
0.391625404	0.847976863	0.273956001	0.668860555	0.630268633	0.069946796	0.712837934	0.803032398	0.270831168	</td			

0.954517070	0.423195601	0.706653237	0.630817533	0.593671381	0.278674304	0.472000003	0.216199994	0.754199982
0.469709724	0.305242896	0.821281850	0.295464337	0.461180389	0.584804893	0.811500013	0.867399991	0.432300001
0.0909215748	0.864670575	0.162253097	[Cu₄(μ₃-O)(H₂O)]⁴⁺, Fig. 4, E = -1061.342 eV					
0.471291423	0.297258765	0.030014550	1.0					
0.583469927	0.196704969	0.493746459	13.6750001907	0.000000000	0.0000000000	0.153300002	0.54579971	0.114900000
0.135982126	0.638438880	0.161757767	-6.8375000954	11.8428975619	0.000000000	0.462500006	0.194600001	0.089500003
0.031124517	0.433380604	0.497234523	0.0000000000	0.0000000000	14.7670001984	0.266400009	0.440400004	0.789600015
0.373697251	0.096947923	0.158506513	H Al Si O N Cu			0.915300012	0.433899997	0.721300006
0.238859713	0.535894990	0.892268992	26 4 32 75 8 4			0.252099991	0.757300019	0.407200009
0.797023475	0.432495058	0.499362200	Direct			0.274899989	0.132599995	0.403400004
0.016154258	0.198658645	0.485754400	0.696551561	0.533845127	0.825254679	0.734300017	0.726199985	0.496100008
0.367467761	0.861877739	0.165652156	0.506072936	0.731599987	0.668399990	0.595200002	0.233700007	0.396800011
0.570801616	0.964647227	0.500672936	0.745500028	0.611400008	0.506999997	0.919000030	0.086599998	0.722199976
0.090519273	0.627378106	0.161406055	0.502099991	0.612900019	0.678399980	0.580900013	0.412000000	0.067199998
0.133832887	0.643682539	0.377086669	0.462500006	0.478700012	0.680299997	0.656599998	0.942399979	0.450500011
0.143386409	0.089496568	0.153596550	0.595000029	0.574899971	0.685899973	0.341100007	0.659500003	0.799300015
0.697589993	0.292957634	0.723513305	0.208299994	0.421600014	0.270200004	0.351000011	0.305099994	0.801500022
0.125398263	0.537587643	0.435453624	0.176899999	0.338499993	0.360900015	0.018500000	0.630100012	0.130300000
0.382467657	0.627812624	0.072724253	0.208000004	0.471300006	0.372000009	0.027600000	0.324699998	0.457300007
0.039777864	0.965750873	0.386248827	0.331299990	0.306499988	0.242699996	0.708800018	0.646099985	0.779399991
0.701347709	0.007601016	0.732454181	0.341100007	0.415199995	0.186700001	0.028100001	0.971199989	0.137300000
0.362207621	0.312351465	0.041362666	0.455700010	0.408699989	0.206599995	0.684800029	0.326700002	0.459600002
0.027888076	0.659055471	0.406061441	0.588299990	0.700900018	0.216299994	0.388399988	0.988699973	0.149000004
0.007925801	0.307490468	0.731864989	0.589200020	0.703100026	0.324999988	0.783599973	0.462099999	0.603600025
0.669122458	0.631268144	0.081036493	0.708999991	0.767099977	0.268099993	0.479200006	0.784600019	0.935299993
0.320124090	0.967425346	0.362593919	0.557099998	0.340999991	0.263999999	0.892700016	0.745299995	0.379900004
0.894173980	0.100028709	0.458332628	0.688000023	0.417499989	0.227699995	0.130300000	0.614099979	0.273699999
0.236486390	0.768697500	0.144297436	0.659699976	0.401100010	0.337300003	0.597899973	0.780099988	0.080700003
0.908256471	0.421656609	0.487695903	0.314799994	0.625400007	0.659500003	0.543099999	0.933600008	0.602699995
0.558120787	0.726937413	0.791315019	0.387400001	0.650500000	0.563399971	0.156499997	0.144500002	0.252099991
0.245435104	0.062574401	0.133607656	0.248699993	0.598900020	0.561399996	0.877799988	0.583100021	0.267500013
0.919655919	0.751510322	0.157397255	0.367199987	0.309100002	0.577600002	0.057200000	0.219500005	0.593999982
0.569649994	0.432048053	0.796881318	0.250999987	0.246800005	0.640699983	0.717400014	0.541400015	0.935500026
0.795556843	0.879901767	0.773717284	0.242500007	0.257499993	0.529699981	0.398999989	0.853699982	0.272000015
0.788468063	0.505459666	0.780983329	0.585800023	0.781300008	0.803999990	0.540099978	0.215700001	0.592199981
0.797375202	0.538753450	0.100001892	0.572399974	0.794000030	0.480599999	0.201499999	0.287900001	0.924300015
0.453762352	0.847154319	0.100651219	0.244200006	0.524299979	0.047600001	0.866999984	0.875299990	0.261999995
0.120610639	0.201308563	0.431067586	0.693400025	0.758499980	0.208299983	0.067100003	0.457199991	0.601800025
0.483605951	0.873282313	0.778891206	0.141700000	0.105899997	0.366899997	0.705900013	0.762399971	0.935800016
0.144854620	0.173753262	0.075292282	0.789300025	0.966400027	0.489100009	0.406300008	0.155300006	0.258899987
0.808080256	0.535330951	0.434746454	0.238100007	0.313600004	0.819800019	0.772800028	0.930800021	0.602900028
0.621773601	0.102365822	0.4980007834	0.692200005	0.533200026	0.043000001	0.210199997	0.521300018	0.933899999
0.142946213	0.222510785	0.751477118	0.356599987	0.875500023	0.369300008	0.482300013	0.272300005	0.924300015
0.452247351	0.903311968	0.445510119	0.363590010	0.104800001	0.362399995	0.388500005	0.485799998	0.480899990
0.475489378	0.213353038	0.756145954	0.906499982	0.637099981	0.369100004	0.537299991	0.519200027	0.392899990
0.816282630	0.864642322	0.434977740	0.467999995	0.761399984	0.826600015	0.543200016	0.735800028	0.528900027
0.131357208	0.524871051	0.770988047	0.474599987	0.756500006	0.043499999	0.705200016	0.649800003	0.529299974
0.811734974	0.853069365	0.094142482	0.570999980	0.973500013	0.708599985	0.520699978	0.554199994	0.652400017
0.484968275	0.167571485	0.421737224	0.233899996	0.294299990	0.031300001	0.228499994	0.419600010	0.336800009
0.150673017	0.543578386	0.113119947	0.564700007	0.199900001	0.698099971	0.381099999	0.392800003	0.235200003
0.462107003	0.193582386	0.089299552	0.907500029	0.871500015	0.367000014	0.629599988	0.696200013	0.269199977
0.270224899	0.440772027	0.788904190	0.029800000	0.430200011	0.708199978	0.632399976	0.413700014	0.275900006
0.918709993	0.437454164	0.717026114	0.697499990	0.759000003	0.041900001	0.312099993	0.595399976	0.595200002
0.248953462	0.754547417	0.407281756	0.795300007	0.974500000	0.706300020	0.288500011	0.299100012	0.586499989
0.277632535	0.132951587	0.403279990	0.027300000	0.204899997	0.701200008	0.540300012	0.557699978	0.516300003
0.550419211	0.074999183	0.7200001936	0.794499993	0.423900008	0.707400024	0.385500014	0.455700010	0.358000010
0.233836830	0.395525634	0.084779322	0.468100011	0.306600004	0.822200000	0.629100025	0.554499984	0.282700002
0.920281112	0.089611597	0.737155917	0.908299983	0.864609997	0.160799995	0.293199986	0.444799989	0.587400019
0.580868244	0.411422253	0.069041923	0.470699996	0.297600001	0.029800000	0.772800028	0.930800021	0.602900028
0.132448453	0.931906581	0.455907196	0.583200007	0.203299999	0.492100000	0.352766067	0.413129359	0.194500074
0.350766242	0.6590006119	0.798507512	0.136500001	0.638999999	0.164000005	0.432955176	0.362322986	0.229660021
0.081727252	0.631219923	0.128146008	0.372999996	0.097400002	0.157800004	0.587426543	0.658561110	0.177977622
0.026758673	0.321212411	0.461156487	0.236499995	0.536899984	0.828100013	0.755898535	0.635355561	0.571035743
0.710286915	0.645778716	0.779599786	0.797299981	0.436100006	0.498499990	0.506255627	0.611078739	0.704125345
0.028379843	0.971110165	0.136334017	0.019300001	0.204400003	0.486900002	0.443061948	0.474586278	0.680382788
0.689161181	0.318569598	0.462114066	0.697399974	0.535799980	0.826399982	0.765136242	0.74793291	0.523883820
0.388225555	0.987730384	0.149111614	0.368200004	0.862999976	0.165700004	0.738127708	0.726458490	0.632806599
0.781130493	0.461213559	0.603549421	0.573000014	0.977299988	0.497999996	0.575898535	0.549122155	0.696667492
0.475403756	0.780616879	0.938032329	0.904900014	0.627699971	0.161799997	0.755898535	0.635355561	0.571035743
0.894965529	0.742856681	0.376141608	0.135000005	0.647199988	0.378600001	0.506255627	0.611078739	0.704125345
0.129740268	0.614769101	0.271519780	0.142800003	0.089800000	0.153200001	0.443061948	0.474586278	0.680382788
0.597274125	0.779025793	0.081473552	0.693799973	0.294900000	0.727500013	0.579449534	0.549122155	0.696667492
0.538223803	0.919839084	0.605499804	0.125100002	0.543200016	0.440800011	0.224355191	0.442980945	0.284466922
0.156167358	0.143669680	0.252700269	0.383300006	0.629000008	0.068000004	0.185022071	0.351122051	0.369649976
0.879593968	0.581114173	0.266675860	0.035100002	0.967400014	0.384200007	0.224713787	0.485175699	0.388930321
0.045672413	0.203733906	0.594246089	0.700699985	0.012200000	0.732999980	0.296814620	0.295108527	0.253602803
0.713132858	0.538064718	0.934927940	0.361699998	0.312500000	0.041700002	0.352766067	0.413129359	0.194500074
0.395658582	0.849446127	0.271893978	0.030700000	0.667100012	0.403899997	0.432955176	0.362322986	0.229660021
0.542129099	0.212441936	0.593311906	0.006100000	0.305900007	0.735800028	0.587426543	0.658561110	0.177977622
0.201623589	0.288047969	0.923991382	0.670199990	0.632799983	0.079099998	0.576696277	0.680792987	0.286679626
0.872391164	0.879152060	0.264175624	0.316000015	0.968200028	0.358099997	0.701088548	0.732213318	0.214199523
0.075631507	0.462814182	0.601306260	0.894599974	0.104000002	0.469599992	0.558914840	0.311481059</td	

[Cu ₄ (μ ₃ -O)(μ-OH)(η-OH)] ⁴⁺ , Fig. 4, E = -1060.932 eV						
1.0						
0.364547282	0.102916807	0.363507360	0.410260588	0.507087469	0.485932887	0.919399977
0.899798989	0.635947108	0.373107165	0.544951916	0.501051605	0.384937853	0.751900017
0.462151110	0.756640136	0.827592075	0.586022437	0.698957205	0.423927575	0.572099984
0.469907075	0.752528489	0.043480296	0.721493244	0.686819553	0.570795417	0.426200002
0.570805192	0.966812789	0.706429064	0.512856603	0.550708175	0.666018963	0.775099993
0.230733946	0.292328447	0.031184498	0.241545886	0.433143854	0.350302786	0.858399987
0.561514139	0.194422022	0.698694646	0.368157297	0.374799371	0.248298362	0.507900000
0.902701557	0.869190872	0.367330998	0.621245980	0.662036300	0.240563124	0.773100002
0.027951520	0.425293475	0.709309697	0.632542372	0.386250883	0.268666029	0.141000003
0.703398168	0.769207656	0.031771921	0.313862354	0.606717408	0.595164478	0.168699995
0.799049199	0.977788866	0.701329648	0.284556359	0.308318406	0.579706550	0.057900000
0.024203783	0.195234493	0.702321112	0.556124985	0.598278046	0.537350476	0.773000002
0.792009056	0.417322725	0.707298279	0.393973647	0.455301642	0.367062896	0.142000001
0.466841847	0.301703662	0.822445035	0.622083247	0.523568034	0.271272361	0.204999998
0.905684948	0.862726092	0.161254629	0.297131091	0.457236171	0.581278205	0.429500014
0.467191607	0.298210174	0.031684253				0.774600029
0.578532809	0.199785993	0.495320171				0.515699983
0.133672982	0.637179255	0.165183038				0.773000005
0.029478295	0.436173707	0.500086308	13.6750001907	0.0000000000	0.0000000000	0.438499987
0.372153103	0.096554995	0.158428818	-6.8375000954	11.8428975619	0.0000000000	0.535700023
0.234766647	0.533779025	0.829312921	0.0000000000	14.7670001984		0.101300001
0.794872880	0.432035118	0.498790175	H Al Si O N Cu			0.7465999972
0.019165644	0.203116849	0.484135091	26 4 32 75 8 4			0.021819998
0.700414240	0.530288994	0.827087879				0.447699994
0.364776343	0.860863864	0.166137651	Direct			0.204999998
0.570308387	0.970142782	0.498557836	0.773299992	0.767000020	0.528199971	0.205400005
0.900811732	0.628179908	0.163458169	0.737600029	0.760800004	0.636600018	0.121200003
0.131753564	0.645303786	0.377918363	0.756500006	0.659099996	0.592499971	0.150600001
0.142294005	0.090798065	0.153917834	0.514100015	0.617399991	0.701399982	0.546100020
0.689725161	0.290156096	0.726582050	0.449099988	0.484499991	0.664300025	0.112599999
0.124203205	0.544689536	0.442937434	0.583999991	0.551900029	0.689899981	0.090200000
0.383192420	0.625188589	0.073191836	0.237499997	0.463800013	0.287200004	0.437000006
0.029617343	0.969581366	0.379163861	0.185800001	0.366299987	0.367500007	0.787500024
0.699948728	0.006187763	0.735306799	0.232899994	0.499000013	0.392699987	0.130600005
0.358681351	0.312829405	0.047645073	0.280000001	0.288339994	0.256399988	0.400000006
0.025602473	0.662926674	0.399654031	0.353399992	0.406599998	0.198699996	0.642099977
0.007470089	0.300938755	0.730357051	0.417199999	0.342299998	0.243699998	0.778699998
0.672447205	0.638361752	0.058331672	0.574000001	0.638499975	0.190200001	0.316500008
0.316181660	0.967078924	0.359135896	0.594200015	0.653500021	0.303499997	0.454300002
0.899721146	0.111940823	0.445116311	0.709000018	0.710200012	0.233999997	0.607900012
0.231646135	0.769253790	0.148805290	0.564700007	0.291500002	0.246700004	0.778869998
0.904392719	0.417673051	0.484564602	0.695200026	0.370000005	0.207599998	0.969900012
0.551504672	0.719372511	0.795826554	0.669200003	0.356000003	0.318599999	0.316500008
0.243784726	0.062573567	0.133817688	0.570000004	0.670300007	0.557299972	0.452800002
0.921962082	0.753716588	0.148437902	0.239700004	0.609799981	0.57309971	0.921960001
0.574267566	0.425284207	0.802309513	0.360900015	0.320899993	0.562699974	0.268999994
0.780305147	0.860744357	0.741076767	0.248600006	0.264099985	0.630400002	0.305400005
0.792778432	0.508136690	0.776571333	0.232899994	0.267800003	0.519500017	0.642099996
0.791781369	0.537980199	0.104090907	0.678499997	0.750999987	0.425199986	0.538700021
0.448082209	0.842814624	0.099977426	0.580699980	0.530600011	0.405000001	0.282799989
0.124988787	0.206219509	0.431329310	0.242100000	0.521499991	0.048900001	0.920199990
0.481615454	0.869510651	0.774302185	0.692900002	0.758800030	0.816299975	0.865000010
0.140913561	0.170133293	0.072727703	0.140100002	0.105400003	0.364899993	0.723100007
0.807326615	0.537577689	0.439352721	0.792200029	0.982100010	0.476200014	0.851000011
0.618397474	0.107374877	0.503184736	0.238900006	0.310200006	0.815199971	0.272100002
0.143025920	0.218350112	0.750111818	0.692600012	0.531799972	0.037000000	0.593200001
0.449420989	0.910631478	0.446824163	0.354200006	0.872300029	0.365999998	0.145500004
0.468774378	0.206217229	0.759154975	0.364800006	0.102300003	0.362399995	0.249899994
0.808152437	0.870063484	0.432179630	0.897700012	0.634100020	0.372099996	0.533200026
0.124026269	0.518586814	0.774125457	0.460399985	0.754700005	0.827199996	0.407000004
0.812672853	0.856580496	0.091286123	0.468800008	0.750899971	0.043499999	0.579100013
0.479780346	0.167009383	0.422546446	0.569599986	0.964999974	0.705799997	0.521999988
0.151413769	0.546929955	0.112502493	0.229900002	0.291200012	0.029200001	0.933899999
0.462279737	0.196813077	0.092218235	0.561399996	0.193100005	0.697799981	0.356999987
0.265060574	0.438046753	0.789470315	0.904799988	0.869700015	0.367100000	0.926999986
0.909753919	0.421266079	0.721500027	0.026200000	0.423200011	0.709100008	0.640200019
0.247561023	0.756410956	0.406521410	0.702300012	0.768400013	0.030999999	0.311000006
0.271635205	0.129334420	0.401979119	0.797500014	0.978999972	0.699599981	0.283499998
0.546257317	0.071538724	0.714268267	0.023200000	0.193700001	0.699800014	0.313300014
0.226556823	0.392725259	0.082849309	0.790600002	0.415300012	0.705999970	0.566069999
0.919802248	0.080922924	0.740693688	0.466399997	0.301899999	0.820100009	0.656269997
0.578226030	0.415024072	0.064728931	0.904600024	0.862299979	0.161400005	0.499100000
0.658369660	0.948210895	0.445402384	0.466699988	0.298729992	0.030800000	0.252819990
0.336803883	0.656063735	0.794533312	0.578299993	0.197500005	0.494599998	0.535899997
0.354378462	0.307547468	0.797038555	0.133399993	0.636799991	0.165299997	0.576799989
0.012445392	0.624546230	0.136539459	0.028999999	0.436599999	0.499500006	0.357899994
0.036841951	0.329586148	0.465291560	0.371499985	0.095500000	0.157100007	0.372500002
0.706517398	0.641224086	0.787796319	0.234200001	0.531899989	0.828299998	0.676799983
0.025289887	0.972443819	0.145668671	0.793600023	0.429699987	0.496800005	0.421900004
0.684515893	0.320044130	0.460323513	0.018100001	0.202800006	0.481000006	0.610199988
0.387506783	0.987844467	0.148315370	0.698800027	0.529100001	0.825399995	0.566900015
0.780745506	0.456066842	0.604261816	0.364899993	0.860300004	0.165999994	0.457500011
0.463131666	0.776620209	0.935872972	0.569199979	0.967400014	0.498100013	0.637099981
0.891417682	0.746549428	0.389747473	0.899900019	0.626699984	0.163999994	0.594799995
0.129966229	0.609323382	0.274109244	0.130199999	0.645200014	0.377900004	0.515200019
0.597697675	0.780496240	0.069712795	0.140400007	0.088200003	0.151700005	0.446699997
0.543796360	0.919529617	0.602179050	0.689800024	0.287600011	0.726499975	0.581200004
0.158348680	0.150449485	0.251471519	0.123599999	0.546100002	0.444299996	0.239099994
0.866652608	0.588981032	0.269461334	0.381599993	0.623899996	0.073500000	0.357899994
0.038910173	0.194247514	0.593140125	0.033000000	0.966899991	0.379999995	0.237399995
0.725303233	0.530962825	0.934568942	0.698800027	0.006100000	0.736199975	0.281199992
0.395829737	0.851122737	0.272063434	0.358500004	0.313800007	0.047200002	0.289299995
0.537212431	0.217535824	0.594481051	0.024000000	0.662599981	0.399699986	0.418300003
0.204061791	0.284571260	0.922687411	0.005200000	0.298400015	0.728900015	0.581799984
0.856319606	0.859477341	0.				

TS6, Fig. 4, E = -1075.116 eV									
1.0									
13.6750001907	0.0000000000	0.0000000000	0.0000000000	0.0000000000	0.0000000000	0.0000000000	0.0000000000	0.0000000000	0.0000000000
-6.8375000954	11.8428975619	0.0000000000	0.0000000000	0.0000000000	0.0000000000	0.0000000000	0.0000000000	0.0000000000	0.0000000000
0.0000000000	14.7670001984								
H Al Si O N Cu									
28	4	32	76	8	4				
Direct									
0.791712224	0.768522859	0.533508003	0.245079160	0.752033293	0.409479797				
0.759304047	0.760715902	0.642662108	0.276383549	0.132019326	0.395484477				
0.776288867	0.659105659	0.594755232	0.546823621	0.066935159	0.714264154				
0.519410729	0.624797046	0.704657733	0.214404017	0.382753313	0.075047404				
0.465926200	0.492574930	0.667629540	0.921122313	0.080054842	0.737090588				
0.597849011	0.568040431	0.704656601	0.578001320	0.411347955	0.065161340				
0.189389408	0.420992732	0.243866518	0.657208025	0.940859139	0.442646533				
0.150930718	0.337256819	0.334912717	0.341655821	0.650173903	0.791210711				
0.182901889	0.470997810	0.344924361	0.356615126	0.304699212	0.790280104				
0.257053256	0.265721262	0.243259728	0.012664706	0.621458828	0.131759152				
0.355227232	0.372014403	0.181812719	0.042433374	0.325323045	0.476878971				
0.392255902	0.308835983	0.260328174	0.710938811	0.641452432	0.799325049				
0.571001649	0.643051954	0.194439843	0.023863176	0.959047556	0.122563884				
0.610448360	0.666896522	0.303902179	0.679991722	0.315196753	0.460271001				
0.704455554	0.718993783	0.221421838	0.392148256	0.984168112	0.144118324				
0.561359465	0.296644390	0.249275506	0.795910537	0.447880417	0.601449847				
0.355227232	0.372014403	0.181812719	0.042433374	0.325323045	0.476878971				
0.694960475	0.376382053	0.218577266	0.454736739	0.775420487	0.935883224				
0.598619523	0.359866947	0.327211380	0.890386939	0.740354896	0.383723706				
0.329943925	0.639102221	0.654117763	0.130115510	0.612661421	0.272157103				
0.349957019	0.661181033	0.542914033	0.593578517	0.770207107	0.062670574				
0.220812336	0.594875395	0.585817933	0.544738114	0.915620863	0.600627363				
0.369710714	0.330829978	0.547977805	0.138360262	0.121808097	0.246699095				
0.259956599	0.266983777	0.618184328	0.871269524	0.578275561	0.269843757				
0.658619523	0.359866947	0.327211380	0.890386939	0.740354896	0.383723706				
0.329943925	0.639102221	0.654117763	0.130115510	0.612661421	0.272157103				
0.610448360	0.666896522	0.303902179	0.679991722	0.315196753	0.460271001				
0.704455554	0.718993783	0.221421838	0.392148256	0.984168112	0.144118324				
0.561359465	0.296644390	0.249275506	0.795910537	0.447880417	0.601449847				
0.355227232	0.372014403	0.181812719	0.042433374	0.325323045	0.476878971				
0.694960475	0.376382053	0.218577266	0.454736739	0.775420487	0.935883224				
0.598619523	0.359866947	0.327211380	0.890386939	0.740354896	0.383723706				
0.329943925	0.639102221	0.654117763	0.130115510	0.612661421	0.272157103				
0.610448360	0.666896522	0.303902179	0.679991722	0.315196753	0.460271001				
0.704455554	0.718993783	0.221421838	0.392148256	0.984168112	0.144118324				
0.561359465	0.296644390	0.249275506	0.795910537	0.447880417	0.601449847				
0.355227232	0.372014403	0.181812719	0.042433374	0.325323045	0.476878971				
0.694960475	0.376382053	0.218577266	0.454736739	0.775420487	0.935883224				
0.598619523	0.359866947	0.327211380	0.890386939	0.740354896	0.383723706				
0.329943925	0.639102221	0.654117763	0.130115510	0.612661421	0.272157103				
0.610448360	0.666896522	0.303902179	0.679991722	0.315196753	0.460271001				
0.704455554	0.718993783	0.221421838	0.392148256	0.984168112	0.144118324				
0.561359465	0.296644390	0.249275506	0.795910537	0.447880417	0.601449847				
0.355227232	0.372014403	0.181812719	0.042433374	0.325323045	0.476878971				
0.694960475	0.376382053	0.218577266	0.454736739	0.775420487	0.935883224				
0.598619523	0.359866947	0.327211380	0.890386939	0.740354896	0.383723706				
0.329943925	0.639102221	0.654117763	0.130115510	0.612661421	0.272157103				
0.610448360	0.666896522	0.303902179	0.679991722	0.315196753	0.460271001				
0.704455554	0.718993783	0.221421838	0.392148256	0.984168112	0.144118324				
0.561359465	0.296644390	0.249275506	0.795910537	0.447880417	0.601449847				
0.355227232	0.372014403	0.181812719	0.042433374	0.325323045	0.476878971				
0.694960475	0.376382053	0.218577266	0.454736739	0.775420487	0.935883224				
0.598619523	0.359866947	0.327211380	0.890386939	0.740354896	0.383723706				
0.329943925	0.639102221	0.654117763	0.130115510	0.612661421	0.272157103				
0.610448360	0.666896522	0.303902179	0.679991722	0.315196753	0.460271001				
0.704455554	0.718993783	0.221421838	0.392148256	0.984168112	0.144118324				
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0.355227232	0.372014403	0.181812719	0.042433374	0.325323045	0.476878971				
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0.598619523	0.359866947	0.327211380	0.890386939	0.740354896	0.383723706				
0.329943925	0.639102221	0.654117763	0.130115510	0.612661421	0.272157103				
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0.355227232	0.372014403	0.181812719	0.042433374	0.325323045	0.476878971				
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0.329943925	0.639102221	0.654117763	0.130115510	0.612661421	0.272157103				
0.610448360	0.666896522	0.303902179	0.679991722	0.315196753	0.460271001				
0.704455554	0.718993783	0.221421838	0.392148256	0.984168112	0.144118324				
0.561359465	0.296644390	0.249275506	0.795910537	0.447880417	0.601449847				
0.355227232	0.372014403	0.181812719	0.042433374	0.325323045	0.476878971				
0.694960475	0.376382053	0.218577266	0.454736739	0.775420487	0.935883224				
0.598619523	0.359866947	0.327211380	0.890386939	0.740354896	0.383723706				
0.329943925	0.639102221	0.654117763	0.130115510	0.612661421	0.272157103				
0.610448360	0.666896522	0.303902179	0.679991722	0.315196753	0.460271001				
0.704455554	0.718993783	0.221421838	0.392148256	0.984168112	0.144118324				
0.561359465	0.296644390	0.249275506	0.795910537	0.447880417	0.601449847				
0.355227232	0.372014403	0.181812719	0.042433374	0.325323045	0.476878971				
0.694960475	0.376382053	0.218577266	0.454736739	0.775420487	0.935883224				
0.598619523	0.359866947	0.327211380	0.890386939	0.740354896	0.383723706				
0.329943925	0.639102221	0.654117763	0.130115510	0.612661421	0.272157103				
0.610448360	0.666896522	0.303902179	0.679991722	0.315196753	0.460271001				
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0.561359465	0.296644390	0.249275506	0.795910537	0.447880417	0.601449847				
0.355227232	0.372014403	0.181812719	0.042433374	0.325323045	0.476878971				
0.694960475	0.376382053	0.2185772							

0.776499987	0.761600018	0.644900024	0.277999997	0.132599995	0.392600000	0.930438936	0.882463574	0.375266492
0.795099974	0.662699997	0.592700005	0.550000012	0.066399999	0.715499997	0.038089257	0.437867463	0.713320851
0.524500012	0.629299998	0.703800023	0.212200001	0.380600005	0.071099997	0.707824111	0.767917931	0.043504123
0.485399991	0.498600006	0.672599971	0.922900021	0.080399998	0.733500004	0.810720325	0.985836387	0.709517658
0.612999976	0.584599972	0.716099977	0.579999983	0.407999992	0.064700000	0.034606531	0.208560109	0.706978261
0.162799999	0.398400009	0.211899996	0.658999979	0.939800024	0.441700011	0.809401393	0.431019098	0.713103235
0.127000004	0.327300012	0.310900003	0.347499996	0.647400022	0.790199995	0.474229723	0.307867318	0.824593425
0.157299995	0.461800009	0.307500005	0.358799994	0.303600013	0.788900018	0.915897787	0.868176222	0.166783094
0.240600005	0.252799988	0.239099994	0.013800000	0.619700015	0.128900006	0.473495573	0.306596696	0.038403604
0.351099998	0.351200014	0.197900002	0.043299999	0.322600007	0.478199989	0.589266419	0.206862226	0.499388814
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0.562300026	0.650300026	0.196899995	0.020900000	0.955500007	0.113600001	0.046482809	0.447532803	0.498812050
0.611800015	0.683300018	0.302399993	0.678499997	0.315600008	0.460399985	0.378947765	0.096766189	0.162170589
0.697899997	0.730799973	0.213799998	0.393999994	0.981999993	0.141499996	0.249573022	0.542139530	0.830507994
0.556599975	0.309100002	0.251599997	0.802699983	0.445450000	0.600399971	0.813620627	0.434816599	0.498330861
0.690999985	0.388900012	0.225099996	0.450399995	0.775799990	0.935400009	0.035822581	0.217721432	0.487979293
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0.333099991	0.641900003	0.648100019	0.130799994	0.612399995	0.270399988	0.370611936	0.867244303	0.171947092
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0.374300003	0.336499989	0.544399977	0.132499993	0.109200001	0.245100006	0.137727425	0.651651800	0.380066246
0.264499992	0.264600009	0.612299979	0.875599980	0.573400021	0.269499987	0.142994225	0.092043005	0.158036456
0.244700000	0.275599986	0.503600001	0.046700001	0.168200001	0.582799971	0.708423853	0.302806705	0.732951820
0.698000014	0.735899985	0.425199986	0.730799973	0.508599997	0.933899999	0.142735496	0.562799096	0.450854570
0.516399980	0.537599981	0.378199995	0.391400009	0.844299972	0.272000015	0.384989887	0.628003418	0.067184202
0.435000002	0.579200029	0.464399993	0.533699989	0.204099998	0.592899978	0.063090250	0.966949940	0.387306154
0.400900006	0.642899990	0.338699996	0.206799999	0.271400005	0.915799975	0.708641410	0.007942498	0.745516539
0.239700004	0.516099989	0.040300000	0.893999994	0.887749998	0.266400005	0.373653114	0.333478659	0.063509382
0.709299982	0.764999986	0.826799989	0.044199999	0.470299989	0.597299993	0.031228816	0.668694079	0.401992649
0.139400005	0.094400004	0.363499999	0.760599971	0.812200010	0.934300005	0.012553441	0.311479092	0.733098388
0.794700027	0.973699987	0.474599987	0.407200009	0.140200004	0.255499989	0.675242245	0.636977732	0.066091493
0.242200002	0.303499997	0.810999990	0.798900008	0.964600027	0.590600014	0.343809634	0.988398492	0.395683438
0.695400000	0.523100019	0.035599999	0.210500002	0.518299997	0.926100016	0.908417404	0.135926753	0.456579864
0.352499992	0.865599990	0.370999992	0.471700013	0.268299997	0.924000025	0.240007445	0.766791940	0.161990315
0.365099996	0.094999999	0.359899998	0.450800002	0.554600000	0.524399996	0.922546566	0.424045265	0.469709873
0.902300000	0.627300024	0.371600002	0.479000002	0.477100015	0.331999987	0.572784543	0.748865247	0.814674675
0.465799987	0.753600001	0.828599977	0.629599988	0.660000026	0.426999987	0.249075770	0.069709793	0.160729960
0.466699988	0.743399978	0.038800001	0.356700003	0.576300025	0.376300007	0.930806458	0.758880436	0.156434238
0.573400021	0.961499989	0.704200029	0.767299978	0.715399981	0.585799992	0.578419507	0.432072639	0.801353395
0.229800001	0.285200000	0.024700001	0.551500022	0.579599977	0.672699988	0.798381269	0.872070491	0.751678884
0.562699974	0.187800005	0.697499990	0.176499993	0.404500008	0.280699998	0.795661151	0.523883283	0.769488156
0.917200029	0.868099988	0.363980001	0.320499986	0.323500007	0.243900001	0.805630863	0.546639740	0.101124719
0.027100001	0.420500010	0.700699985	0.626900017	0.662199974	0.238900006	0.457624316	0.811801739	0.229432777
0.707099974	0.762600005	0.030600000	0.629299998	0.382299998	0.268000007	0.131450981	0.204121485	0.435292840
0.801999980	0.974099994	0.667899997	0.290100008	0.599300027	0.591000021	0.486266822	0.880423010	0.779141307
0.031099999	0.187299997	0.689400017	0.294099987	0.319599986	0.558700025	0.156744764	0.178361684	0.077156380
0.798699975	0.409900010	0.706700027	0.602400005	0.630900025	0.550800025	0.815269053	0.540143132	0.445190907
0.470800012	0.299899995	0.818159999	0.333200008	0.449600011	0.311100006	0.605475128	0.098185040	0.497356683
0.909600019	0.856999993	0.161799997	0.619300008	0.518000007	0.258500010	0.148599118	0.229432777	0.758880794
0.466600001	0.295700014	0.029600000	0.295700014	0.461199999	0.575800002	0.455476612	0.886430740	0.453489721
0.577499980	0.191499993	0.493400007	0.134567449	0.353238910	0.174400086	0.487220615	0.213076279	0.768391907
0.135100007	0.634500027	0.160500005	0.049520008	0.094291329	0.242097050	0.2501112206	0.7692353373	0.398814976
0.023600001	0.426899999	0.492500007	0.999925792	0.283406973	0.214937046	0.293180078	0.153453499	0.382186532
0.371699989	0.086400002	0.153400004	0.590593576	0.8029000136	0.248884603	0.218800098	0.392922819	0.083331652
0.238399997	0.527700007	0.821399987	0.136750001907	0.000000000	0.000000000	0.147445541	0.531903863	0.766593277
0.798200011	0.421799988	0.492599994	-6.8375000954	11.8428975619	0.000000000	0.495213032	0.200868487	0.430378586
0.022900000	0.193599999	0.478100002	0.000000000	0.000000000	0.147344734	0.153473347	0.546151876	0.116123043
0.706700027	0.523699999	0.828299999	0.28	0.28	0.2	0.456928909	0.195598960	0.091190875
0.364699990	0.854200006	0.164399996	Direct	0.134567449	0.353238910	0.282792181	0.447229892	0.793483078
0.573000014	0.964900001	0.495200008	0.092624331	0.091719511	0.687119305	0.928655221	0.444618315	0.743443191
0.902400017	0.619099975	0.164700001	0.094291329	0.242097050	0.247327238	0.293180078	0.153453499	0.382186532
0.132100001	0.639299989	0.376800001	0.999925792	0.283406973	0.214937046	0.293180078	0.153453499	0.382186532
0.135399997	0.069200002	0.142900005	0.590593576	0.8029000136	0.248884603	0.218800098	0.392922819	0.083331652
0.690299988	0.285800010	0.722899973	0.729412496	0.862294734	0.267287403	0.930617869	0.093197376	0.743806362
0.118000001	0.529699981	0.431499988	0.644585909	0.750933886	0.335169047	0.592337132	0.4147446732	0.067364015
0.381199986	0.613900006	0.064300001	0.648297429	0.877609909	0.346456856	0.673542619	0.955733538	0.450243473
0.043200001	0.958800018	0.399800009	0.102690026	0.365049154	0.285900861	0.354897439	0.665303886	0.803379774
0.702400029	0.000300000	0.732999980	0.817742825	0.796570241	0.533427835	0.360042572	0.305014133	0.790718734
0.361799985	0.317699999	0.046300001	0.777462775	0.724915958	0.556855559	0.811286867	0.458960682	0.605041397
0.897099972	0.395999998	0.461199999	0.244030237	0.632471323	0.580613792	0.466778785	0.797693193	0.945754051
0.565999985	0.725899994	0.814800024	0.359687567	0.466835499	0.343344480	0.893115819	0.748818159	0.39435262
0.241200000	0.046000000	0.130500004	0.416892976	0.430862010	0.426526368	0.129428700	0.600880325	0.279829174
0.920199990	0.744199991	0.159600005	0.278295940	0.356858313	0.409911990	0.600762367	0.781685412	0.073089920
0.579400003	0.423299998	0.79						

0.347630233	0.437247962	0.408296138	0.156408951	0.179187447	0.076217078	0.811130702	0.998641491	0.488589376
0.527134657	0.416933894	0.525499761	0.814821184	0.540216208	0.444438666	0.255797416	0.325305462	0.817338765
0.298742861	0.406123132	0.594955087	0.606285751	0.100083217	0.497147232	0.700196266	0.540743828	0.045409516
0.611855507	0.675433457	0.522859514	0.150769755	0.229350224	0.757091165	0.367987543	0.889358342	0.378597260
0.345005572	0.537088573	0.509544671	0.455303907	0.888354063	0.455006480	0.388663637	0.125258610	0.367470950
T5, Fig. 5, E = -1055.416 eV								
1.0			0.844336092	0.899822950	0.441290498	0.474419981	0.773913741	0.837684155
13.6750001907	0.0000000000	0.0000000000	0.807111621	0.854699075	0.112863623	0.584535778	0.979168236	0.714549839
-6.8375000954	11.8428975619	0.0000000000	0.495808035	0.203510612	0.429966569	0.245171160	0.307504386	0.034629982
0.0000000000	0.0000000000	14.7670001984	0.154679999	0.549283835	0.115203336	0.582202137	0.210184887	0.706775248
H	Al	Si	O	N	Cu	0.455963761	0.197443202	0.091182075
28	4	32	74	8	2	0.282067746	0.448360384	0.789986014
Direct			0.929776073	0.446123689	0.737126708	0.708952248	0.772168636	0.044164609
0.133440793	0.354538530	0.173720643	0.249103338	0.771727800	0.399069399	0.813596904	0.992767453	0.710749209
0.094229512	0.244389027	0.247427762	0.292641968	0.154288352	0.382038832	0.037908491	0.215425193	0.707650661
0.999185443	0.284646988	0.214986399	0.567439914	0.084895484	0.719436288	0.809646189	0.436759859	0.710693598
0.583760023	0.798739493	0.257563263	0.217227146	0.393500417	0.082162641	0.479586869	0.317945391	0.824092865
0.722823262	0.851073563	0.274522841	0.932238281	0.095513530	0.743187368	0.912380278	0.873652458	0.169450969
0.631564021	0.745073795	0.344107658	0.591757715	0.416297436	0.068059154	0.474215895	0.314864933	0.039272081
0.646165967	0.875038624	0.353172183	0.673101187	0.956493258	0.450995773	0.588747025	0.211177781	0.499495059
0.102320425	0.367468864	0.285306394	0.357386291	0.666296959	0.799803674	0.139153734	0.641992748	0.171132028
0.804381847	0.793022692	0.531965792	0.361800313	0.307950467	0.789200544	0.053358693	0.452473849	0.504305720
0.772264361	0.769014657	0.641726017	0.020167967	0.630234957	0.143268391	0.376493573	0.101430260	0.161932915
0.799228847	0.681251049	0.583076477	0.067118585	0.34872168	0.460029364	0.253342062	0.548930645	0.828550339
0.541198313	0.684772730	0.689241767	0.706850767	0.651528060	0.793528855	0.812994719	0.440266639	0.504240990
0.461647332	0.549699306	0.669286549	0.029807350	0.976690412	0.133359775	0.034251835	0.2211414387	0.488238275
0.594252348	0.604459703	0.699319839	0.705842614	0.318881750	0.469295084	0.709077835	0.544263303	0.829622388
0.357089788	0.659464777	0.639606237	0.380633771	0.985338986	0.134122998	0.372979373	0.874457955	0.169889867
0.387520462	0.728217721	0.540920794	0.806238413	0.463517725	0.605732858	0.575361550	0.970869958	0.503542483
0.256487340	0.632403910	0.565524578	0.464477301	0.795042157	0.943563569	0.908393530	0.640500724	0.166964397
0.350533843	0.457668573	0.326989561	0.892286301	0.748272836	0.395188749	0.139874324	0.656047761	0.378536969
0.447745532	0.454985470	0.390911877	0.129544243	0.601251979	0.280186653	0.142388761	0.098298565	0.158930182
0.312239528	0.352170140	0.400081575	0.601356506	0.783809245	0.071569048	0.711740375	0.307079047	0.730847478
0.697721243	0.652473152	0.399867982	0.559821784	0.928110719	0.609194517	0.141604945	0.567321122	0.451422900
0.460098326	0.641817689	0.361922771	0.130213469	0.144878760	0.254796892	0.383780777	0.633828461	0.081015103
0.526387453	0.3827212692	0.476571769	0.870219231	0.592046738	0.273294359	0.057957556	0.970637262	0.387222230
0.625287414	0.474906683	0.541007698	0.056108277	0.218560532	0.598064363	0.712287664	0.016682360	0.745176256
0.521810889	0.361734301	0.584455252	0.730041027	0.538425386	0.935694218	0.375138193	0.343904793	0.061848067
0.289554417	0.427291751	0.640399277	0.412389129	0.886250615	0.278553903	0.031773698	0.671059132	0.398755819
0.244999602	0.340649307	0.553012669	0.554247439	0.224916905	0.601543725	0.016765041	0.317337811	0.741097391
0.380584806	0.405040681	0.579943359	0.230328590	0.298450172	0.926016152	0.675861740	0.641939938	0.071886167
0.246797874	0.529534936	0.047822084	0.884888411	0.883310914	0.272053421	0.350909884	0.996039152	0.398428559
0.712016761	0.775527596	0.830954492	0.073056691	0.466070950	0.607076883	0.908412576	0.135509163	0.455556571
0.150869071	0.111420766	0.368065953	0.751695275	0.804513693	0.942581832	0.243285790	0.7711655619	0.160734102
0.811377823	0.996799231	0.487816185	0.433167815	0.140936658	0.262602389	0.926469445	0.432152987	0.497545123
0.254349291	0.320731223	0.818748653	0.807762384	0.980474114	0.602414012	0.575143993	0.749446929	0.816095173
0.700638413	0.537195981	0.042292040	0.220365673	0.527213931	0.933109105	0.245485500	0.071157381	0.162232935
0.369649707	0.885440469	0.380489379	0.468815088	0.281362057	0.931267798	0.931701720	0.767399728	0.153021500
0.387328953	0.120792747	0.366963506	0.416898847	0.659325361	0.404749513	0.5855442960	0.440376699	0.796651125
0.904269338	0.638746321	0.376198232	0.626241444	0.642494559	0.409732372	0.800428629	0.879477859	0.754558742
0.474287868	0.774029851	0.838217378	0.081904858	0.313578039	0.231255502	0.804937780	0.524237752	0.781030834
0.474321336	0.758715570	0.049144316	0.644849598	0.817476094	0.305416733	0.808555007	0.552894354	0.100681625
0.583770871	0.975825330	0.713747561	0.762326002	0.730296254	0.579688907	0.460844887	0.852146327	0.113689452
0.244544461	0.303105354	0.035814669	0.540223360	0.616906881	0.657861888	0.131170884	0.206677511	0.438261479
0.581100404	0.206879675	0.706265032	0.338692218	0.615153843	0.571797073	0.492690921	0.885828018	0.782847583
0.927092075	0.880780995	0.376168489	0.365484029	0.437151760	0.390007704	0.159452736	0.183357835	0.075819857
0.040846322	0.439064652	0.713858128	0.539558351	0.423557490	0.537387371	0.817146719	0.538680851	0.440557897
0.708344519	0.769405961	0.043053907	0.310902506	0.451317804	0.576404154	0.600292683	0.099999592	0.494036943
0.812191486	0.988078415	0.7010030973	0.5990949807	0.641121447	0.534813881	0.153075576	0.232431620	0.7555611658
0.036477350	0.211299777	0.707312405	0.357870549	0.541410983	0.487946630	0.456706554	0.886762440	0.451018721
0.809321225	0.432626158	0.712361038	0.289749116	0.630155146	0.594751477	0.491345465	0.220911294	0.770317137
0.474930227	0.310209155	0.824905396	0.829047799	0.357151806	0.173820958	0.842420936	0.898963124	0.443884015
0.914896905	0.868805766	0.167897463	0.0250011861	0.2500011861	0.775700033	0.775700033	0.398097080	
0.472770309	0.308484614	0.038589787	0.094778813	0.248751998	0.248398811	0.292609096	0.157174632	0.382701814
0.589096308	0.208130658	0.499269456	0.997396708	0.286051631	0.216222242	0.567146480	0.087723367	0.720429957
0.138344705	0.637884736	0.172716111	0.172742790	0.522059262	0.742633641	0.313487232	0.216572538	0.396455586
0.370749414	0.869446099	0.172474027	0.653890014	0.811742842	0.260351568	0.934224427	0.099271260	0.743194604
0.576479435	0.968875708	0.503393710	0.631492913	0.730545731	0.357481897	0.592796564	0.419531375	0.074147239
0.138218355	0.652583361	0.380388111	0.636049986	0.860613346	0.361199558	0.672499555	0.957878888	0.453309387
0.142670885	0.094056621	0.158360273	0.101159915	0.371318966	0.285315663	0.358127594	0.696250238	0.795833969
0.709437549	0.303904772	0.732099414	0.791216612	0.791939318	0.535264313	0.366787225	0.317127258	0.789116144
0.142103955	0.563827336	0.452077538	0.763806224	0.776405871	0.645862997	0.023115285	0.640127838	0.144493029
0.386132717	0.629341781	0.070800751	0.805804729	0.696734248	0.597451747	0.062722936	0.350470513	0.457991779
0.059521634	0.967732489	0.387280434	0.528571010	0.664004152	0.695321023	0.715534568	0.656505466	0.792509556
0.710423231	0.010719864	0.745692551	0.448474437	0.526828408	0.682			

0.431923807	0.144197702	0.262244850	0.926727712	0.433245152	0.498434812	0.695936084	0.650936961	0.413358599
0.809013307	0.984306335	0.603292882	0.574115336	0.749410987	0.816492081	0.378322691	0.617788613	0.201303840
0.230497703	0.534995079	0.933969200	0.244553730	0.073731676	0.162223756	0.546976566	0.403621525	0.485632241
0.476712286	0.294567674	0.931249022	0.931162953	0.768854737	0.152579382	0.620493412	0.439647794	0.579429030
0.387442559	0.649378479	0.327029586	0.584618270	0.439724386	0.797197759	0.484134793	0.369623303	0.585300028
0.625224411	0.620658636	0.423296064	0.799241364	0.879455984	0.754753470	0.282672167	0.426609993	0.525876701
0.080605127	0.316680014	0.231770352	0.804392815	0.525147438	0.781475365	0.247962952	0.322645545	0.453534544
0.612158775	0.789308190	0.321084708	0.807320535	0.553950667	0.101510264	0.379674673	0.395192266	0.496009022
0.756493926	0.732940316	0.586727917	0.460405916	0.854912698	0.112740055	0.243930534	0.532673955	0.051875662
0.527827799	0.593180954	0.670393527	0.128686339	0.206276745	0.438807696	0.709130228	0.774612427	0.833795667
0.372152179	0.651539564	0.513110161	0.491930038	0.885853538	0.783460855	0.145745963	0.110630192	0.370242804
0.417444319	0.455710322	0.333285689	0.158291161	0.185408145	0.076636329	0.806880414	0.998573065	0.492559791
0.553548336	0.434040606	0.546587110	0.816340327	0.538222194	0.440521806	0.252662987	0.324523330	0.819962144
0.310116827	0.414936572	0.511348724	0.599200726	0.10006334	0.493677765	0.697481573	0.541189075	0.047470566
0.601609409	0.605699062	0.551353991	0.152164415	0.232348219	0.756639421	0.364097327	0.888115346	0.382563204
0.366969407	0.540424109	0.417682588	0.455691397	0.886347651	0.451146752	0.385267473	0.127729431	0.372427046
[Cu(OH)⁺ + NH₄⁺, Fig. 5, E = -1056.0686 eV]								
1.0			0.841580629	0.900953532	0.444682807	0.469652027	0.770829737	0.839983523
13.6750001907	0.0000000000	0.0000000000	0.139739498	0.536634922	0.779096007	0.469886482	0.759731710	0.053075392
-6.8375000954	11.8428975619	0.0000000000	0.497464389	0.213607743	0.430427670	0.242261693	0.306772560	0.037465699
0.0000000000	0.0000000000	14.7670001984	0.149139360	0.550638378	0.113516003	0.578236461	0.208930567	0.709525764
H Al Si O N Cu	28 4 32 74 8 2		0.450791001	0.200581759	0.090062186	0.918744922	0.880065262	0.379842907
Direct			0.279534602	0.451567441	0.789922595	0.043802980	0.443764031	0.714661717
0.140367150	0.365839779	0.176815838	0.249238387	0.777190268	0.397023618	0.807535357	0.992422760	0.714705288
0.105068043	0.262087107	0.255488604	0.291125894	0.157257140	0.384812117	0.034454528	0.212748036	0.710106313
0.012228928	0.307213366	0.229485229	0.566732585	0.088323355	0.721764028	0.805555284	0.434660405	0.714250386
0.524288356	0.742514193	0.306087852	0.218407109	0.399213403	0.082645379	0.475491792	0.316433549	0.825995207
0.662869275	0.814068377	0.265703827	0.933049202	0.099419393	0.745426774	0.908975542	0.874561548	0.172295272
0.627570152	0.732587874	0.360866249	0.591468215	0.420477450	0.074986733	0.472108513	0.314687282	0.041690309
0.632723451	0.858567059	0.363204330	0.671039879	0.957540274	0.454012990	0.586798668	0.210019484	0.502007186
0.126405016	0.392208370	0.288850933	0.356843740	0.669339895	0.794992745	0.137765959	0.647863746	0.172123417
0.787555754	0.791836321	0.536115646	0.365712076	0.317259699	0.789935112	0.052148476	0.454929024	0.509210646
0.759662867	0.777227759	0.646554291	0.022626815	0.641332828	0.143815041	0.375314116	0.104348943	0.164507896
0.803619683	0.698580027	0.596899033	0.064320408	0.352712810	0.460605424	0.250681788	0.549154937	0.830904245
0.521409094	0.660697043	0.694735467	0.713361204	0.655884326	0.793268025	0.809866428	0.438745290	0.507801771
0.444497555	0.523074269	0.683109045	0.024781764	0.986643076	0.137448922	0.028570404	0.218714461	0.492375195
0.576077282	0.584480524	0.718015353	0.709262013	0.320038050	0.473077178	0.705365956	0.542998016	0.831319392
0.419253767	0.649136782	0.550096810	0.378467500	0.990279436	0.134328544	0.371045649	0.874936998	0.174087957
0.417055488	0.729247391	0.467267007	0.789752185	0.469942808	0.607591033	0.569639802	0.967337906	0.507268786
0.298226267	0.625998616	0.505675375	0.454762161	0.785904944	0.945241511	0.903483987	0.639463127	0.170417681
0.419460922	0.466113031	0.240698189	0.890071571	0.749890447	0.400096744	0.134257481	0.657936990	0.381309658
0.506289601	0.490974605	0.327806026	0.128990337	0.605457485	0.279062808	0.142109871	0.098360844	0.160544306
0.386364758	0.366843253	0.318379313	0.599866450	0.787127473	0.066311307	0.707177579	0.305443674	0.735480130
0.702053010	0.647681653	0.413904577	0.556616545	0.932483733	0.610375524	0.137908503	0.567104101	0.451150090
0.378897876	0.621086597	0.240438998	0.134670049	0.155093640	0.256550729	0.382585895	0.632818282	0.089339271
0.548357970	0.405310780	0.484380454	0.869672060	0.601474941	0.271774828	0.051760741	0.966565490	0.388278842
0.623738408	0.440275520	0.577457666	0.052658718	0.222129777	0.599310100	0.708820105	0.017047929	0.748917639
0.487530708	0.367060572	0.584588660	0.722036898	0.539738357	0.938704789	0.372588307	0.342271775	0.066399261
0.276708186	0.429659635	0.540378749	0.412571490	0.893793583	0.276639432	0.024757680	0.670098364	0.400544792
0.257546723	0.334004194	0.464277625	0.553535354	0.227020383	0.603272050	0.0131318637	0.316300005	0.737794638
0.383140117	0.411223769	0.514616907	0.230352700	0.301794767	0.925058022	0.672688200	0.641544461	0.076543108
0.247665152	0.533737753	0.050408322	0.880323112	0.881452441	0.274741888	0.352239490	0.998415530	0.398050994
0.712872505	0.777270615	0.831614614	0.096648298	0.472274005	0.610108078	0.901674032	0.135973319	0.459987581
0.148862362	0.114482068	0.369074732	0.753735747	0.802506745	0.943506002	0.239484131	0.778831601	0.160417810
0.810244322	0.999954224	0.489016622	0.429966222	0.146417797	0.262916267	0.925109088	0.434154510	0.500957906
0.254789293	0.325618476	0.818047285	0.808703244	0.985759139	0.603820443	0.569684625	0.744964480	0.820676386
0.699015439	0.541642725	0.046131328	0.233549997	0.538278937	0.935208082	0.243374780	0.067077734	0.155250952
0.367826998	0.890731215	0.378720075	0.476483822	0.294628501	0.931629360	0.925782084	0.766240418	0.159437567
0.388261020	0.127054796	0.368556589	0.390811592	0.646503389	0.303565085	0.582593501	0.437927723	0.798472106
0.903612435	0.642352343	0.375822723	0.621514082	0.617732734	0.424889416	0.794916630	0.878107905	0.757851541
0.472983599	0.773374200	0.837715030	0.095702708	0.332495362	0.238610595	0.802262306	0.523405313	0.784089625
0.472238034	0.762078643	0.050781202	0.612881839	0.788762093	0.322317302	0.806670368	0.553497553	0.101408280
0.583720624	0.979557037	0.715400100	0.753050956	0.733232677	0.587848544	0.456369404	0.850288510	0.115656449
0.244909510	0.308789879	0.035105158	0.523298800	0.590772711	0.671318769	0.121525288	0.201522440	0.438209087
0.581029296	0.210313857	0.707467854	0.379954845	0.647672175	0.490805775	0.490319761	0.884832680	0.787224650
0.923468232	0.882038414	0.378438056	0.422545493	0.452245283	0.308520049	0.157053452	0.182045296	0.076979257
0.045622993	0.443487674	0.713355872	0.551255822	0.432484537	0.549453080	0.811120152	0.536835850	0.445021182
0.708155453	0.773073554	0.044425793	0.316013217	0.414438456	0.487878379	0.59319730	0.095861547	0.495683372
0.812746227	0.993196785	0.711389661	0.599870622	0.603240550	0.553313136	0.149179652	0.231031805	0.759417951
0.036907781	0.215327159	0.7088119270	0.372067273	0.537512660	0.392555628	0.451188892	0.881673753	0.454700321
0.808512270	0.437054843	0.7110420774	0.617404481	0.6364338785	0.590064704	0.420515507	0.218600169	0.772063851
0.478365481	0.317593545	0.824456990	0.874908566	0.169839144	0.504813552	0.243848920	0.777573049	0.446428001
0.911520600	0.874908566	0.169839144	0.473320049	0.556549072	0.266282737	0.354319572	0.668703258	0.794880271
0.473740011	0.314979047	0.039556805	0.146913842	0.318701744	0.302314132	0.28		

0.554316163	0.929601371	0.613402069	0.135616094	0.564261258	0.449406415	0.756094038	0.778455079	0.653220773
0.143108651	0.151322678	0.257907331	0.380169719	0.633574307	0.089112468	0.798666239	0.698492825	0.603722394
0.861603677	0.595018208	0.274214178	0.050529182	0.963254690	0.387120634	0.505366206	0.662297606	0.692363620
0.050252996	0.212807372	0.60111531	0.706410766	0.016116397	0.748975694	0.436953753	0.524252892	0.692041039
0.719952524	0.541004956	0.939877868	0.371557862	0.340787590	0.069744751	0.568492055	0.596454739	0.728246987
0.406940967	0.881803155	0.281243861	0.020281777	0.660320342	0.386742592	0.407528073	0.603501618	0.506989241
0.553187490	0.22779850	0.604251027	0.012672196	0.316656023	0.735696554	0.405117184	0.677542210	0.421478331
0.230879962	0.300656617	0.927206933	0.670954883	0.640364707	0.077796727	0.285642505	0.590740919	0.471957624
0.873399772	0.880720973	0.276642740	0.355598450	0.999836028	0.395298898	0.404233277	0.420438439	0.217694581
0.097291149	0.480300516	0.612708032	0.897240341	0.138665140	0.468945742	0.494558960	0.442346841	0.300928324
0.749301612	0.799315214	0.947554170	0.235774353	0.780544877	0.152129844	0.372732580	0.321661621	0.294133753
0.423046559	0.152727142	0.266066700	0.923916459	0.431514025	0.502451897	0.688260078	0.627180815	0.422193140
0.804898262	0.983126462	0.607154727	0.567709804	0.744528353	0.824080110	0.401639491	0.633944809	0.193070531
0.236357039	0.543241203	0.937144935	0.241558433	0.066337898	0.153857291	0.547989130	0.406634182	0.501128733
0.473654032	0.294764638	0.933474779	0.931016743	0.76800484	0.154324830	0.623399854	0.438887894	0.594073832
0.356062949	0.612644372	0.267794073	0.580525237	0.436710924	0.800244033	0.485816717	0.373531044	0.601625025
0.615853488	0.6235666210	0.424830973	0.794050455	0.878541946	0.761300862	0.334533513	0.409177214	0.538248479
0.161076173	0.394852847	0.277865827	0.799474418	0.522295356	0.784699857	0.243424803	0.308576494	0.468512923
0.623395562	0.795894682	0.324955970	0.807033630	0.553837240	0.101490423	0.372985363	0.334165931	0.474907815
0.748982072	0.732785642	0.589743435	0.455261052	0.851060629	0.118436396	0.241789147	0.532025278	0.054232869
0.519077539	0.589053214	0.671681941	0.1113181449	0.195054188	0.438170612	0.707934737	0.776088893	0.838616788
0.375438958	0.632452071	0.461440742	0.487841964	0.883263469	0.788216531	0.143004790	0.108335868	0.374224395
0.419604689	0.433623433	0.291541308	0.154795989	0.182296425	0.078778110	0.803566277	0.996785045	0.494798899
0.549310088	0.433200270	0.549816251	0.810615361	0.533719178	0.445604950	0.249986142	0.324056476	0.824210346
0.313898355	0.403025746	0.472431004	0.589183688	0.093730263	0.497137934	0.694885254	0.539883018	0.048766192
0.596407831	0.603320241	0.553959310	0.145546407	0.229790390	0.766336024	0.359137923	0.882299423	0.385935605
0.361689717	0.514419436	0.370360792	0.449572623	0.879904151	0.454307139	0.382354647	0.126866832	0.375311059
[Cu(H₂O)]²⁺, Fig. 5, E = -1055.9429 eV								
1.0			0.837529123	0.901064336	0.446679175	0.466381013	0.772190213	0.843785048
13.67500001907	0.00000000000	0.00000000000	0.801040351	0.532318175	0.786426902	0.468558937	0.763441563	0.052774094
-6.8375000954	11.8428975619	0.00000000000	0.495201498	0.213749647	0.434775889	0.578266740	0.977535367	0.720855176
H A I Si O N Cu			0.148225367	0.559024155	0.112795874	0.240781620	0.307207972	0.042681471
28 4 32 74 8 2			0.274871701	0.450237006	0.792228162	0.040669478	0.442661881	0.717683733
Direct			0.926189363	0.447162081	0.721591890	0.704517186	0.7711039128	0.048648153
0.189846188	0.396620184	0.220627338	0.237841472	0.779954553	0.413233012	0.8070120919	0.989879966	0.716690481
0.142999470	0.317279041	0.311802447	0.282438010	0.148458496	0.403142959	0.031489920	0.212369710	0.714621902
0.127510771	0.428924322	0.301691294	0.558244050	0.083961323	0.725612462	0.803610146	0.435424596	0.715715528
0.553525686	0.759403408	0.288294792	0.218364790	0.399856716	0.089221545	0.471759081	0.314493120	0.828699350
0.696638107	0.818823099	0.288800806	0.927621186	0.098667718	0.750142038	0.907391667	0.870717585	0.174624532
0.618313372	0.721122682	0.369816154	0.589532375	0.419896632	0.077562995	0.469989330	0.311866999	0.04461370
0.634018600	0.854032159	0.370893478	0.665088117	0.952975035	0.458505690	0.583360434	0.206156239	0.503905118
0.323939830	0.649373751	0.272321224	0.350881696	0.668169916	0.798437893	0.137705952	0.647542715	0.174966544
0.782759428	0.790497124	0.541592002	0.361258626	0.316369474	0.793025970	0.049929236	0.452943444	0.510661066
0.753998578	0.777485847	0.651627362	0.014160450	0.633558273	0.166217953	0.371706009	0.105114885	0.168099716
0.798364341	0.698201060	0.603875101	0.064747378	0.350837618	0.475102693	0.248112291	0.547016799	0.833170652
0.508369505	0.658081234	0.692095399	0.707693934	0.653484881	0.794640362	0.807468891	0.435451984	0.508104384
0.436560452	0.520005405	0.685320079	0.020983305	0.985545156	0.146547288	0.024697075	0.217743099	0.497302607
0.567228317	0.587162614	0.723854959	0.707253158	0.314652354	0.476753557	0.700867236	0.542134345	0.833256602
0.413613407	0.623858035	0.501720071	0.390271604	0.998371363	0.150169119	0.365819782	0.871527255	0.176523697
0.417395949	0.709356248	0.432861239	0.782970667	0.463409156	0.611693740	0.565750122	0.963787138	0.508172631
0.305794448	0.610813535	0.483689070	0.448526770	0.783254921	0.949763238	0.900148153	0.640177310	0.172594979
0.424826771	0.439207673	0.213220045	0.886164129	0.746301651	0.410512149	0.134708941	0.657385945	0.383409292
0.511457682	0.470984042	0.300728500	0.161082834	0.627098382	0.280690730	0.140355483	0.099720560	0.164237618
0.392621070	0.348202342	0.295238443	0.595251024	0.787361263	0.071736842	0.704157948	0.306885332	0.737107635
0.698293388	0.647345543	0.420682788	0.555998807	0.929011345	0.614521265	0.136612386	0.565672994	0.453130394
0.384400576	0.621893883	0.193333894	0.147104889	0.153683588	0.260308862	0.380982608	0.635609806	0.086215645
0.544868290	0.404198319	0.490131468	0.845850407	0.600325854	0.275359482	0.0505094162	0.963356111	0.387432277
0.613491893	0.434346369	0.586004198	0.054728933	0.210985228	0.604212403	0.705391586	0.012881490	0.751108408
0.476360053	0.370068669	0.587715983	0.718916237	0.540669560	0.940871596	0.369540036	0.337146670	0.072184511
0.292506725	0.423984617	0.517607510	0.392038503	0.868688364	0.282463133	0.017738242	0.657131732	0.391048193
0.242496133	0.315420404	0.448005170	0.552624047	0.226946250	0.606501102	0.010033404	0.315513111	0.742675364
0.380889833	0.389252782	0.471624047	0.231320724	0.306177050	0.931451917	0.668600261	0.639727555	0.076626472
0.240939289	0.531325340	0.053863294	0.869205713	0.868110120	0.278951377	0.3563590182	0.998332977	0.391918451
0.707179368	0.774032652	0.378346436	0.096732400	0.485366911	0.614272833	0.895767331	0.137535125	0.468520403
0.143536612	0.107644983	0.372125059	0.748281896	0.798358321	0.947511673	0.234310165	0.779409647	0.154802799
0.804864943	0.997801781	0.494886130	0.417973518	0.158457652	0.268232971	0.923241258	0.432197183	0.499995197
0.2511149863	0.325258882	0.823573291	0.803717911	0.979386628	0.609164298	0.569194138	0.74933024	0.830930233
0.696730316	0.540699840	0.048375916	0.232335091	0.537688136	0.939038217	0.240002856	0.066291124	0.152851939
0.359906137	0.885283887	0.384838551	0.471158355	0.293295115	0.935259879	0.932407796	0.151384085	0.151384085
0.383412510	0.128580704	0.374933422	0.383276016	0.629716754	0.262968540	0.578218281	0.436345994	0.801543593
0.892323256	0.636684239	0.378091305	0.617929041	0.619593799	0.430459440	0.793602586	0.876433611	0.760598838
0.467372339	0.770233393	0.841970325	0.181583330	0.399282873	0.289875388	0.797606289	0.525677025	0.78220899
0.468994468	0.761131346	0.054214317	0.624686480	0.788648784	0.327893734	0.804733634	0.553414464	0.102864631
0.578066289	0.976929426	0.719306231	0.747814417	0.732637167	0.593577325	0.455190897	0.851871789	0.119456902

0.013040436	0.631965280	0.164451793	0.369405329	0.103708841	0.168521374	4	32	75	16	4	2
0.061931212	0.349979758	0.470711857	0.248467967	0.546062946	0.834485829	Direct					
0.703600347	0.653237998	0.797728300	0.807130396	0.434977800	0.508639753	0.246725723	0.521957874	0.051329367			
0.018941198	0.986820459	0.149162576	0.023854898	0.216478944	0.498062789	0.696000993	0.757411599	0.823220253			
0.706082523	0.312710971	0.478752106	0.699761629	0.541340470	0.835188031	0.127553120	0.094510615	0.363047957			
0.388672471	0.996922910	0.156601980	0.364197820	0.870795250	0.176700950	0.807546318	0.968573153	0.502953470			
0.786435425	0.466410905	0.610843301	0.565872610	0.962698936	0.508664846	0.244551614	0.313469350	0.824306846			
0.444136977	0.788031936	0.950074136	0.899884105	0.640256703	0.1731117965	0.692828774	0.532291055	0.043716092			
0.887669504	0.746176422	0.414437920	0.133711889	0.654218137	0.384230375	0.355299890	0.865017653	0.370180905			
0.155130208	0.623403072	0.282755047	0.138345629	0.099383920	0.165321350	0.375419617	0.103318743	0.363055080			
0.595815420	0.786758959	0.066273503	0.703596711	0.307334274	0.737289727	0.895114064	0.627356708	0.369238466			
0.551264703	0.932213187	0.615606189	0.135855198	0.564080715	0.455324173	0.469073534	0.7544456460	0.828407943			
0.150063992	0.155598715	0.262162834	0.380184352	0.635887444	0.089328632	0.473889023	0.748010159	0.047231007			
0.848327339	0.605030477	0.275371939	0.051211059	0.963395000	0.387659639	0.573823929	0.969509900	0.713733077			
0.050773311	0.216531828	0.605791986	0.705504179	0.012403975	0.751824856	0.242075279	0.298232794	0.043028977			
0.717741668	0.537799716	0.941416442	0.367467523	0.333785981	0.072304696	0.569231212	0.198279321	0.705471098			
0.391102105	0.859309196	0.284340054	0.017792467	0.655712366	0.397237955	0.900231540	0.863095641	0.367556393			
0.548687100	0.219944879	0.606832147	0.007941606	0.313697368	0.745514810	0.037054472	0.434957176	0.707374632			
0.231347337	0.305109233	0.932383001	0.667392135	0.638898969	0.076650150	0.694840610	0.754449841	0.045580920			
0.869288445	0.863042831	0.280225545	0.354821950	0.995423231	0.392874688	0.800668001	0.975129008	0.712584078			
0.091453701	0.477316737	0.614853621	0.895226419	0.136583507	0.468783468	0.037790243	0.206007063	0.702108562			
0.754794359	0.800637662	0.949041426	0.232933715	0.776714981	0.157390073	0.798502207	0.423058093	0.710452676			
0.414722681	0.160768494	0.268717945	0.921794593	0.429807454	0.499286622	0.467476696	0.308318585	0.824084222			
0.802380383	0.979499876	0.609332502	0.570439935	0.750908437	0.835018277	0.906307757	0.861225188	0.162111789			
0.230502635	0.535754740	0.939104855	0.238111988	0.066251382	0.153507680	0.471487999	0.302066386	0.039391964			
0.469373524	0.292164743	0.936142266	0.931478262	0.768285692	0.149054334	0.580731273	0.202064499	0.500264466			
0.413150966	0.646778286	0.261048526	0.577190518	0.435938656	0.802892266	0.137032449	0.642334342	0.162855923			
0.611867905	0.611884117	0.435008496	0.793361247	0.875675738	0.762646019	0.038349673	0.438756585	0.501753092			
0.195812881	0.417074174	0.291214406	0.796383739	0.525958657	0.782577038	0.3733374718	0.093396865	0.156109989			
0.631191850	0.785781264	0.329751194	0.803992231	0.552145839	0.104284670	0.241591796	0.534745336	0.830261588			
0.748070300	0.733158588	0.594932079	0.454658526	0.852664351	0.120018646	0.801395535	0.433003306	0.503555894			
0.513948441	0.593600690	0.678157032	0.112907276	0.191887036	0.446148306	0.037068930	0.208622947	0.495685607			
0.361503214	0.599614322	0.451058149	0.485064743	0.881714643	0.787696481	0.696505725	0.535623550	0.824995041			
0.410610676	0.407433212	0.285380006	0.149530098	0.181283489	0.081169285	0.363552541	0.859459758	0.164460018			
0.552572370	0.434685260	0.5666061735	0.805193722	0.529810905	0.443289787	0.563711643	0.965791821	0.505167663			
0.327033669	0.374347568	0.475682974	0.589216232	0.091097087	0.493568301	0.900791705	0.624328971	0.164268866			
0.594687998	0.601549745	0.563958049	0.143927395	0.228927761	0.766786965	0.130513042	0.642990288	0.376608312			
0.345486522	0.477309227	0.366171628	0.446260124	0.875476480	0.458353102	0.1436260700	0.081009895	0.149253324			
Cu²⁺ + H₂O, Fig. 5, E = -1055.966 eV			0.838999274	0.901309133	0.447545379	0.700335324	0.291787386	0.725105166			
1.0			0.135625035	0.5327811959	0.784721076	0.388279766	0.619787872	0.077722214			
13.6750001907	0.0000000000	0.0000000000	0.795806170	0.855442762	0.124739416	0.029723613	0.957567930	0.389952123			
-6.8375000954	11.8428975619	0.0000000000	0.492792040	0.210311979	0.435723245	0.705499709	0.014024346	0.733018577			
H Al Si O N Cu	28	4 32 74 8 2	0.147178113	0.556087792	0.114650160	0.368661284	0.320927948	0.072882481			
Direct			0.925817192	0.448062956	0.727905035	0.667508304	0.628733337	0.083729498			
0.213374987	0.403853238	0.226660684	0.235166088	0.776941359	0.412449926	0.329649389	0.969951451	0.369083494			
0.133363202	0.363367349	0.318911016	0.280281842	0.143020749	0.406759083	0.909114718	0.106580123	0.485399933			
0.201750144	0.497830749	0.289424658	0.563091576	0.086514965	0.731982644	0.231683403	0.776018679	0.145717770			
0.564420104	0.744612217	0.294030309	0.220543534	0.400071800	0.091672435	0.911057332	0.418857545	0.491005599			
0.709848046	0.809841275	0.297998875	0.926788926	0.095339194	0.752358615	0.559399128	0.723577261	0.786696911			
0.629406691	0.713890731	0.379064647	0.586048782	0.418037146	0.080118567	0.244206220	0.051459365	0.128407821			
0.640638471	0.844132245	0.374718070	0.663392901	0.948539797	0.460179031	0.921141088	0.750916302	0.162041962			
0.408852339	0.737618864	0.271971703	0.353405744	0.666232049	0.801460207	0.568535209	0.433914542	0.795938671			
0.781296670	0.789731203	0.544887245	0.358237351	0.312179297	0.794957459	0.797221720	0.888590515	0.785957038			
0.758259237	0.778402448	0.656128168	0.012221246	0.631291986	0.164371833	0.787591636	0.503675699	0.784132695			
0.799704432	0.698356211	0.604996062	0.061734717	0.348713845	0.469774365	0.804428399	0.543557525	0.092503577			
0.504153073	0.666568518	0.691882610	0.701564193	0.652618647	0.801796734	0.444128126	0.837090909	0.097241474			
0.435596287	0.528828800	0.569593336	0.016944738	0.986311793	0.151774824	0.123609729	0.200411052	0.424434781			
0.566682220	0.602056921	0.733032525	0.704478085	0.312594593	0.480418622	0.488179773	0.872118831	0.781953156			
0.407636851	0.598182380	0.499744058	0.384731829	0.994892955	0.156137839	0.149742335	0.171823591	0.075624011			
0.389392436	0.6315158895	0.394816101	0.788333118	0.467239290	0.611620784	0.807397246	0.534262358	0.441855699			
0.282069683	0.578525066	0.467072099	0.442562342	0.787550390	0.951691151	0.609391749	0.099895284	0.497164190			
0.399401188	0.407975723	0.226807818	0.890401423	0.746384978	0.418336868	0.132803873	0.215633601	0.773774862			
0.486630440	0.423935711	0.310598552	0.150672920	0.617897213	0.283492059	0.457508028	0.895005405	0.440258920			
0.371435612	0.300076425	0.292481154	0.595192313	0.786872685	0.066698179	0.482577145	0.213551506	0.770151019			
0.682399750	0.608167291	0.427880764	0.551384687	0.932062626	0.616358638	0.808756709	0.867847681	0.433865130			
0.402121603	0.647037327	0.202837542	0.149256562	0.155876026	0.263209492	0.129647741	0.502045135	0.778293729			
0.545377135	0.404454231	0.511149943	0.849874735	0.607531011	0.276581645	0.813181341	0.850011408	0.089918770			
0.629662037	0.442373306	0.599272966	0.048584118	0.216491580	0.606938779	0.481259763	0.178747416	0.428006023			
0.492974609	0.374772102	0.615181088	0.7								

0.537317336	0.211867779	0.600353241	0.487828016	0.873797596	0.784938753	0.802718580	0.973898649	0.715435386
0.234291837	0.300929815	0.933072150	0.150014564	0.171421960	0.075650074	0.037485436	0.206932619	0.701610863
0.868981481	0.877872705	0.263180673	0.805355132	0.530698597	0.440759003	0.800290644	0.423464924	0.710440159
0.083286017	0.477467746	0.604388952	0.606004298	0.094940595	0.497646630	0.468356162	0.306934804	0.824321628
0.698930562	0.753415585	0.939056575	0.133135617	0.215750888	0.773872674	0.906391501	0.858198404	0.165343046
0.397008687	0.146723002	0.260132670	0.456261396	0.888025045	0.442708671	0.471214801	0.300354987	0.040698573
0.775791764	0.921384811	0.611639857	0.483218580	0.213297382	0.770322978	0.579289615	0.198197365	0.501428783
0.223689392	0.521131814	0.936232626	0.809169590	0.865832686	0.435230821	0.137209624	0.640825868	0.164101154
0.468746454	0.285858691	0.931340158	0.130853161	0.5207676510	0.778754354	0.041466381	0.438262254	0.502558410
0.43239432	0.686648965	0.528500140	0.814461768	0.850119412	0.090399288	0.373921067	0.092002951	0.157563135
0.381550968	0.468970835	0.478441954	0.481054485	0.178730235	0.429224193	0.245377675	0.534273267	0.830626845
0.555863976	0.555688381	0.406575978	0.159122795	0.554804742	0.110065207	0.801510811	0.427543461	0.504184365
0.641981721	0.892980814	0.409246385	0.462368548	0.191513702	0.090078570	0.035296530	0.206265971	0.495720565
0.292030513	0.168627799	0.462388843	0.270761251	0.437805623	0.790234625	0.699762527	0.535191715	0.825387359
0.397680074	0.712148130	0.573169410	0.921309233	0.436744124	0.722245991	0.366502583	0.858390927	0.167944208
0.374341935	0.610383987	0.510255456	0.242286563	0.755731463	0.409537017	0.559859514	0.956824899	0.509143233
0.715008259	0.721972406	0.532999337	0.270014107	0.119472422	0.407072625	0.904856964	0.620569289	0.164745882
0.701084077	0.647407949	0.626981497	0.550955296	0.073566578	0.721264720	0.128617257	0.640731514	0.377370387
0.726001441	0.607289732	0.526187420	0.225167677	0.391896516	0.093273081	0.143412322	0.078750983	0.150974244
0.390095592	0.492029458	0.656859457	0.923890352	0.090462446	0.715557933	0.704172423	0.291858763	0.727282271
0.504271090	0.490403801	0.691174448	0.585810334	0.409811318	0.073970184	0.125433028	0.537900865	0.434208333
0.505388021	0.611145437	0.685861349	0.667213082	0.945415199	0.459143251	0.388174385	0.618751228	0.082510196
0.243764967	0.396023929	0.250853688	0.346111417	0.656873941	0.797564864	0.031125216	0.948806107	0.389074564
0.211545929	0.337979794	0.354985565	0.350658983	0.298193306	0.790914297	0.705031276	0.007958452	0.740722299
0.224737808	0.463212162	0.336693555	0.016081693	0.626932859	0.136155397	0.367621750	0.318335354	0.072812423
0.454744011	0.438494474	0.201353729	0.038225088	0.325092018	0.470927238	0.019647220	0.654367626	0.398813933
0.445214689	0.552968323	0.190911427	0.714011133	0.649246633	0.778648555	0.009936567	0.307582438	0.722021639
0.559960186	0.560774088	0.236590236	0.026215775	0.966893313	0.134815112	0.669438243	0.627444148	0.084735334
0.683587134	0.641617358	0.558547199	0.692551851	0.312658876	0.470157743	0.343025446	0.973411977	0.378265977
0.476521969	0.534331343	0.652587712	0.397830379	0.898912255	0.153822139	0.905956507	0.105018772	0.489376068
0.257714838	0.412841260	0.319226503	0.783689022	0.459010988	0.607141316	0.233277604	0.774236381	0.148506075
0.473628998	0.512455046	0.233784944	0.474507779	0.768694162	0.940306902	0.914692760	0.420119882	0.495073378
0.524456978	0.551833451	0.526660383	0.881207824	0.734352529	0.380632341	0.567509353	0.735837579	0.791410446
0.415529937	0.486429632	0.357806712	0.138233557	0.616674449	0.272002323	0.245071605	0.051161900	0.129664494
TS10, Fig. 6, E = -977.351 eV								
1.0								
13.6750001907	0.0000000000	0.0000000000	0.862987459	0.573067248	0.267198622	0.788340867	0.504961550	0.782766461
-6.8375000954	11.8428975619	0.0000000000	0.087177061	0.218048111	0.598836303	0.804825187	0.540404558	0.092218399
0.0000000000	0.0000000000	14.7670001984	0.707474589	0.537476718	0.934657335	0.446989626	0.836551189	0.102098688
Al Si O H N Cu	4 32 75 16 4 2		0.393420786	0.843486547	0.272333354	0.116698921	0.190563262	0.424951881
Direct			0.234634414	0.301094800	0.933116734	0.148106515	0.168833956	0.076833494
0.247940794	0.522321582	0.051878858	0.868055701	0.875878274	0.263940752	0.803060472	0.524755657	0.439570487
0.699627757	0.760384202	0.824261189	0.083261907	0.476749569	0.604604065	0.594871640	0.087810785	0.496531457
0.127329543	0.093550421	0.363179505	0.700045168	0.754817486	0.939094630	0.132728830	0.216165587	0.772956789
0.807674468	0.967034042	0.504062831	0.397001922	0.145636782	0.261284828	0.454045922	0.876147926	0.446203530
0.245192841	0.313152075	0.824246168	0.775306046	0.920499861	0.612918139	0.485043168	0.212577000	0.771337330
0.693077087	0.532167852	0.043707911	0.226203889	0.522174656	0.936662257	0.811512458	0.865803242	0.437511981
0.355866075	0.862494648	0.371957123	0.469130218	0.286036432	0.931549966	0.133666337	0.520358622	0.778485853
0.375838071	0.101756699	0.364112437	0.431783676	0.669175744	0.521353841	0.814946175	0.849903139	0.092481546
0.894126952	0.624950111	0.369191140	0.357156128	0.475856721	0.472775161	0.482521623	0.186722159	0.430401236
0.470139921	0.756589770	0.830559254	0.543691278	0.581311405	0.407599121	0.158646211	0.5537354866	0.110304952
0.474689212	0.748299778	0.049284000	0.640008271	0.885853946	0.413278282	0.462699741	0.190244108	0.090505950
0.574618220	0.968897402	0.715392470	0.288566619	0.160627738	0.464984506	0.274331808	0.437502831	0.791427076
0.242443725	0.297840357	0.042958841	0.407966614	0.687794149	0.577932596	0.924682677	0.440690309	0.720194638
0.569955707	0.197873071	0.705851376	0.361546814	0.554792881	0.489691892	0.239629462	0.756849170	0.409019144
0.900178611	0.861322880	0.368065298	0.723976791	0.71986422	0.523109972	0.270215929	0.118560977	0.409183532
0.037705548	0.435550521	0.707824886	0.704047680	0.648606302	0.620436072	0.554142892	0.074193336	0.722076595
0.695871830	0.754857838	0.046392664	0.710935652	0.592897474	0.520905852	0.224009067	0.389436185	0.090088639
0.802169442	0.975237548	0.713526666	0.396524221	0.510468841	0.666879833	0.922942102	0.090763748	0.716314673
0.038552012	0.206876576	0.701997399	0.512582064	0.505810797	0.687725425	0.587585628	0.408747107	0.074272051
0.798692644	0.422966719	0.710385442	0.514305234	0.626957515	0.697574079	0.666589916	0.943951309	0.462002844
0.467975855	0.308152825	0.824066043	0.242057681	0.395435274	0.239884034	0.349584669	0.655662835	0.797255397
0.906381912	0.860728443	0.163040668	0.209096217	0.337156266	0.344608307	0.350782335	0.295832276	0.790219724
0.471789867	0.301959783	0.040223822	0.212703899	0.457459658	0.324188650	0.016529184	0.626893401	0.135913789
0.580370486	0.199117929	0.500768185	0.460078001	0.449055851	0.204959869	0.038254336	0.324405670	0.470821261
0.137395382	0.641909838	0.163416877	0.447939366	0.561737120	0.188583165	0.712749124	0.648387134	0.77860198
0.038666132	0.437933147	0.501912296	0.560771644	0.573205059	0.242119640	0.026190680	0.963024676	0.136174619
0.373587191	0.093232609	0.156965554	0.682817698	0.640495733	0.552819729	0.696323281	0.307206631	0.471524328
0.243056893	0.535036981	0.830559611	0.482535935	0.553734899	0.658003986	0.397829644	0.153753653	0.772076595
0.800936878	0.430465430	0.503177524	0.251804018	0.412055999	0.308647394	0.781904042	0.457045972	0.607214451
0.037166547	0.207929000	0.495745867	0.475066245	0.523144662	0.234929606	0.473532498	0.767513037	0.942752182
0.696294188	0.535846651	0.824900866	0.520502930	0.580523968	0.530161262	0.875783263	0.728545308	0.380970210
0.365859270	0.859306157	0.165981263	0.406425178	0.497765243	0.354042453	0.135685280	0.614329278	0.272215865
0.562744021	0.96131367	0.507682830	0.470850676	0.757874846	0.833030581	0.522669471	0.596496642	0.414018661
0.901176214	0.623769999	0.164114609						

0.408806890	0.510976195	0.680009782	0.925947666	0.091875426	0.718299389	0.900477409	0.625165522	0.165068105
0.534596324	0.523983657	0.690608501	0.586829245	0.412553221	0.076782376	0.126659438	0.641236484	0.376135707
0.520185649	0.635647893	0.709203362	0.663680136	0.943155885	0.468386859	0.141150922	0.080878280	0.153730199
0.251104027	0.395272166	0.222098231	0.350899011	0.657285690	0.796679676	0.707889438	0.291344821	0.725710034
0.213991493	0.328765661	0.324154258	0.352460742	0.296397090	0.791748345	0.127433002	0.541906536	0.435274899
0.210186303	0.445264965	0.307859898	0.017099310	0.631274462	0.134213060	0.380689979	0.619301379	0.077634975
0.482616633	0.479076803	0.204842120	0.038430337	0.324193060	0.470815003	0.042590961	0.942600608	0.386958838
0.457392484	0.585367977	0.193117961	0.716872573	0.650280893	0.781361341	0.705142438	0.079748597	0.725478768
0.567287624	0.600649655	0.255214483	0.025498381	0.963094950	0.137277350	0.368348330	0.324282646	0.070812568
0.675081670	0.634875774	0.544057488	0.695247650	0.307462513	0.472928852	0.016251866	0.651437044	0.399502158
0.493156344	0.564329803	0.667135239	0.397818685	0.991200089	0.1480830443	0.010705765	0.309196174	0.731420040
0.254993111	0.405751586	0.291871637	0.783335090	0.045870574	0.607740104	0.667743027	0.628243625	0.083306082
0.484658033	0.545218587	0.239461929	0.473372847	0.768113077	0.943201900	0.343779548	0.978179336	0.382115483
0.517504334	0.598187625	0.538778543	0.878647745	0.2792792407	0.381306976	0.901635051	0.110569812	0.493637115
0.400378615	0.495203584	0.353697211	0.133161634	0.611488938	0.270724431	0.233235586	0.7711722019	0.146977156
[Cu₂(μ-O)(η-OH)₂]²⁺ + ads(H₂O), Fig. 6, E = -992.532 eV								
1.0			0.530371458	0.914425552	0.612296224	0.570267916	0.733842194	0.797659397
13.6750001907	0.00000000000	0.00000000000	0.156769440	0.127265587	0.252277462	0.241229251	0.050620709	0.135036781
-6.8375000954	11.8428975619	0.00000000000	0.085822903	0.2172636772	0.598357377	0.570846450	0.437009424	0.796812236
Al Si O H N Cu	4 32 76 18 4 2		0.394637704	0.855548799	0.274921328	0.788688838	0.503922045	0.781049669
Direct			0.232502505	0.296672732	0.932474017	0.805319250	0.544125855	0.092499904
0.246349797	0.521353602	0.051479004	0.869687796	0.876872659	0.271199822	0.447352141	0.839175463	0.102495186
0.702521026	0.759936929	0.829239428	0.089702368	0.477239251	0.604058981	0.111718357	0.180002913	0.431231648
0.126906574	0.088165775	0.364461929	0.710508585	0.764257014	0.944160402	0.150091559	0.1711037078	0.077725030
0.796420991	0.967372298	0.492664397	0.396983743	0.142916337	0.263039142	0.800043523	0.518692076	0.437695622
0.247453198	0.312491328	0.824290454	0.787694454	0.918257833	0.613102317	0.582667470	0.081359223	0.495181829
0.693149865	0.532884002	0.045221981	0.228880897	0.523659468	0.935865700	0.136817396	0.216779634	0.770180821
0.353804111	0.866167963	0.376810521	0.472503811	0.289049864	0.933388770	0.447172046	0.870179752	0.446648061
0.376686543	0.106389143	0.367964596	0.391512185	0.603870511	0.529326677	0.491901547	0.217417523	0.772633195
0.892145514	0.618742108	0.369004488	0.330426754	0.406868845	0.455098361	0.832441092	0.874582887	0.450884908
0.472136974	0.758420169	0.833804727	0.529570878	0.583147466	0.413635126	0.139507964	0.528018475	0.770874560
0.472979635	0.746864378	0.052263875	0.417755812	0.674201608	0.323435128	0.807063231	0.851181686	0.104452781
0.571053743	0.966645300	0.713975191	0.812003613	0.862346828	0.615454078	0.485291094	0.194166154	0.430031091
0.239542469	0.294778079	0.042517066	0.297349900	0.191159919	0.451446325	0.149958715	0.548864901	0.109312885
0.574472010	0.199901015	0.707455873	0.375607491	0.627354264	0.587418199	0.457164645	0.190884933	0.089923434
0.905356407	0.857968271	0.373075992	0.322263360	0.463780314	0.491168618	0.274023145	0.438340455	0.790973127
0.041083872	0.437506109	0.706060863	0.718565285	0.700079083	0.506207168	0.928119838	0.444135606	0.719363272
0.697823346	0.757512033	0.050649341	0.707397401	0.631980658	0.604533315	0.235121876	0.760151148	0.404768288
0.805957556	0.978997111	0.719254196	0.687270641	0.567540944	0.504593968	0.273671180	0.124431796	0.409147978
0.040924888	0.209745884	0.701464593	0.408349246	0.512914777	0.679658771	0.555803239	0.075358495	0.722873211
0.801682174	0.424270362	0.710616887	0.530902684	0.519519508	0.692272473	0.219356269	0.389972717	0.084882736
0.47075726	0.308928281	0.825671852	0.522049010	0.634718060	0.707839496	0.926106393	0.093099743	0.719037771
0.905805945	0.860199094	0.169566974	0.248326361	0.391227543	0.223957211	0.587861896	0.409680307	0.074356474
0.471369833	0.303627998	0.042159237	0.206113935	0.328036159	0.327116728	0.665304840	0.945401371	0.467626512
0.578359425	0.197541177	0.502384186	0.219791576	0.453614593	0.308478147	0.353343189	0.657364368	0.796180427
0.136368858	0.641629815	0.162572205	0.484224737	0.470206469	0.201055780	0.354387641	0.298983723	0.789165914
0.041595638	0.438274592	0.501754999	0.447659880	0.569066644	0.195233613	0.016752049	0.632324987	0.134356303
0.373580843	0.094197899	0.157998711	0.562911226	0.594111323	0.251490712	0.042115312	0.325067967	0.461298674
0.246741518	0.5353650373	0.830112100	0.474323899	0.693883886	0.371015161	0.719653368	0.651791215	0.781087899
0.801164687	0.426914573	0.504495680	0.430207672	0.744988024	0.296781152	0.022235999	0.967312320	0.137740657
0.032574862	0.204845935	0.495637536	0.674273551	0.624225378	0.540742898	0.698303232	0.301931381	0.472708851
0.698102832	0.535466373	0.826343417	0.493249565	0.562720239	0.666781306	0.394415408	0.988757789	0.149320468
0.365694433	0.862079799	0.167059273	0.253557682	0.403292694	0.293421149	0.784225106	0.456407756	0.605277181
0.562066919	0.956441700	0.506720543	0.481796175	0.533120513	0.237003103	0.470656455	0.770606339	0.942443490
0.900522172	0.622566640	0.164970368	0.517435014	0.588617921	0.537461996	0.873500049	0.725632131	0.386045545
0.128696961	0.639235973	0.375389695	0.400887519	0.483781934	0.352407217	0.13016225	0.611997843	0.271362573
0.142746031	0.079221442	0.151327044	0.307858378	0.722027779	0.594231129	0.774040818	0.084520116	
0.706195951	0.292615414	0.727750957	0.136750001907	0.000000000	0.000000000	0.531806231	0.912671387	0.610887468
0.125939935	0.537578166	0.433765322	-6.8375000954	11.8428975619	0.000000000	0.153638005	0.130127236	0.255195558
0.387015045	0.618374348	0.081126228	13.6750001907	0.000000000	0.000000000	0.861932635	0.570653200	0.266665399
0.037820302	0.947547555	0.388884097	-6.8375000954	11.8428975619	0.000000000	0.083077557	0.225000575	0.599495232
0.705031455	0.007564721	0.728050292	0.000000000	0.000000000	0.14.7670001984	0.709618330	0.536651015	0.935321748
0.363574734	0.320327640	0.072409779	Al Si O H N Cu	4 32 76 18 4 2		0.392537624	0.851315975	0.274128675
0.018442683	0.650038719	0.398817182	0.240242683	0.298817182	0.541864395	0.213990927	0.602281809	
0.010295251	0.307858378	0.722027779	0.240262583	0.521510780	0.047988426	0.232326419	0.293960750	0.930185139
0.669631660	0.630557549	0.084606320	0.705575526	0.761567831	0.830586791	0.087503143	0.466411293	0.602253258
0.332905501	0.974198163	0.380708665	0.127487421	0.084951408	0.366567075	0.717340708	0.766858518	0.945307672
0.902872562	0.104853712	0.493367672	0.798340678	0.971575916	0.492232174	0.399609089	0.144419059	0.262454867
0.232861191	0.775370240	0.149182439	0.248043314	0.312688857	0.8222175086	0.797041563	0.921072602	0.612456262
0.914585233	0.419768870	0.495137602	0.693297207	0.531685650	0.044493571	0.221618205	0.523888588	0.932851562
0.244658649	0.052293949	0.129604325	0.355517358	0.864886820	0.375265896	0.470084071	0.287574708	0.931795716
0.915908456	0.474245014	0.167639941	0.381182820	0.108241059	0.367387742	0.421081662	0.630946338	0.530385256
0.570098996	0.435321629	0.796322763	0.889053881	0.618047237	0.369953513	0.300084247	0.450553447	0.434669673
0.805943191	0.886877000	0.783585548	0.473380506	0.759137094	0.833738575	0.55433517		

0.535413027	0.598166049	0.546182096	0.873104095	0.726596177	0.387731016	0.910042644	0.113719530	0.481043905
0.375864893	0.498028964	0.329925716	0.132101938	0.613936901	0.270879626	0.236674041	0.071212161	0.142607525
2 Cu(OH)2]+, Fig. 6, E = -992.643 eV								
1.0								
13.6750001907	0.0000000000	0.0000000000	0.533690214	0.912427306	0.608446300	0.560142696	0.726323426	0.790599346
-6.8375000954	11.8428975619	0.0000000000	0.083075583	0.228817612	0.598546863	0.574864209	0.437455714	0.803945959
0.0000000000	14.7670001984	0.712026060	0.536746085	0.935461819	0.795882761	0.888282835	0.784104229	
Al Si O H N Cu	4 32 76 18 4 2	0.391047180	0.847448826	0.272534162	0.791762888	0.506252170	0.784100354	
Direct		0.542158544	0.214837193	0.601263583	0.801917672	0.539588332	0.100081153	
0.235897809	0.522082984	0.044317298	0.8682278921	0.876025856	0.274864197	0.128829315	0.203894675	0.428420097
0.706258297	0.762879848	0.831342816	0.087193273	0.462290436	0.600402057	0.489132524	0.875254154	0.780368447
0.127372071	0.084471688	0.365918517	0.717347085	0.767038584	0.949530481	0.149707302	0.175884292	0.076252840
0.799541295	0.974005759	0.491515815	0.397315919	0.143725350	0.262200624	0.805912614	0.531408727	0.438264132
0.248317689	0.312894583	0.820372105	0.788904607	0.920493841	0.611446023	0.595530629	0.093644738	0.489249259
0.693291247	0.530450344	0.044546459	0.213906184	0.521471381	0.929852366	0.139041469	0.222359106	0.768490314
0.356188953	0.862725616	0.374047339	0.467979759	0.285918742	0.931023002	0.457287550	0.877800941	0.442220688
0.380156487	0.106124766	0.366737187	0.439794989	0.635830700	0.528998017	0.484509509	0.217978209	0.768384159
0.889166176	0.619756043	0.370361686	0.293019176	0.461995721	0.426257709	0.812007666	0.875126362	0.433717787
0.474348217	0.761157990	0.832496285	0.613402486	0.638709398	0.446486086	0.131381512	0.526417375	0.773551285
0.4711166521	0.751659930	0.0479117895	0.456732810	0.646335006	0.343591541	0.81083216	0.852047622	0.091706134
0.571946263	0.966901064	0.709189594	0.823738158	0.873363495	0.607087135	0.483549953	0.193547502	0.427994430
0.240255326	0.296884507	0.037987974	0.294546396	0.176473618	0.458156437	0.151596916	0.546082914	0.118874311
0.575551569	0.199907556	0.704861164	0.4213882874	0.668512106	0.580509901	0.459125400	0.191101283	0.089480892
0.909857869	0.859090805	0.375027895	0.339725018	0.524843872	0.468726814	0.271198392	0.444263309	0.792041659
0.041381899	0.436339289	0.703957677	0.749950111	0.674492598	0.538710356	0.922573984	0.440248311	0.715762198
0.695286036	0.754184425	0.051570021	0.725051224	0.648425758	0.653912246	0.242809370	0.764115453	0.409453362
0.806730390	0.979992986	0.717153668	0.697754920	0.545921504	0.579869330	0.269801527	0.118901089	0.407708824
0.039966654	0.212830573	0.702435315	0.405873626	0.515832126	0.673791409	0.550499380	0.076037847	0.721002221
0.802188933	0.422928602	0.704735906	0.516697109	0.505816460	0.705900550	0.225938216	0.395928413	0.086688302
0.471255600	0.309519619	0.823720634	0.517403066	0.626168609	0.722570002	0.927415729	0.091449142	0.721144497
0.902731836	0.862133384	0.172276360	0.19779727	0.382037550	0.205393702	0.587711632	0.409008384	0.69791637
0.469254911	0.301825047	0.039758962	0.207978934	0.295418739	0.278870642	0.670314670	0.952694416	0.457580864
0.577672422	0.195805430	0.500093043	0.153905168	0.373027503	0.315117121	0.343298376	0.662542343	0.803263247
0.133427337	0.639397085	0.162601784	0.424631119	0.449647442	0.174849913	0.355812490	0.307480603	0.788632810
0.042735122	0.435286731	0.496500462	0.417845875	0.565896749	0.155717209	0.018200602	0.633097708	0.131530628
0.368261814	0.091182709	0.158534572	0.519839883	0.572190762	0.221608102	0.043762293	0.332363844	0.462309599
0.244593039	0.537104905	0.825830936	0.559984280	0.648576915	0.405975491	0.722653687	0.653642118	0.78487784
0.801743686	0.423176885	0.501160145	0.435265332	0.665956914	0.401664466	0.023720855	0.971407592	0.135155484
0.031164743	0.207082331	0.494836837	0.698242009	0.620711565	0.588353693	0.696907520	0.313513279	0.471109003
0.700579941	0.535726011	0.826595247	0.492289662	0.558752298	0.677008808	0.392844707	0.989450216	0.154948071
0.364856392	0.859436810	0.166309565	0.213313714	0.373022616	0.272713035	0.782416403	0.462843657	0.606376231
0.561256051	0.952686191	0.502268136	0.436352825	0.525238960	0.2047404316	0.480134398	0.781330466	0.939017117
0.900599003	0.626750588	0.165195882	0.556981087	0.612488925	0.559550941	0.880556226	0.738620102	0.384030819
0.126564339	0.642425776	0.375701576	0.351381719	0.501724958	0.314671874	0.131903753	0.623207927	0.274074256
0.133990922	0.082908355	0.154143021				0.594250858	0.773794711	0.086980216
0.707893074	0.291066259	0.725339890				0.546720445	0.925657451	0.607454479
0.124905460	0.542401016	0.434806943				0.155946299	0.136872306	0.252075374
0.376506358	0.623146474	0.069688905				13.6750001907	0.0000000000	0.0000000000
0.045843881	0.940943480	0.380738705				-6.8375000954	11.8428975619	0.0000000000
0.705768645	0.008876793	0.724523842				0.0000000000	0.0000000000	14.7670001984
0.368326366	0.325822771	0.069549106						
0.017116670	0.654335380	0.398598194						
0.010470086	0.309447408	0.732842922						
0.666261137	0.626072049	0.082759298						
0.344506061	0.976406932	0.379710853						
0.898876607	0.114465587	0.495493025						
0.233935699	0.769695103	0.143200964						
0.914982796	0.415857226	0.493800104						
0.570660055	0.734018505	0.797746062						
0.237658277	0.049871370	0.136109173						
0.919068813	0.752896130	0.165189773						
0.571382701	0.437237442	0.79765357						
0.806797028	0.889020324	0.783047020						
0.788773537	0.503660202	0.780120790						
0.805297375	0.544131577	0.093216635						
0.450028360	0.84330264	0.101332076						
0.107857801	0.174901083	0.433223635						
0.492605120	0.876344800	0.784157753						
0.149869010	0.173743173	0.078008845						
0.801406611	0.519018114	0.437246650						
0.582617283	0.081295237	0.494346857						
0.137497276	0.216953069	0.768020332						
0.448597887	0.869700193	0.445141673						
0.492186844	0.217570141	0.771880686						
0.844227612	0.884863913	0.452893138						
0.140006199	0.529301882	0.767059147						
0.804641783	0.489571168	0.105288938						
0.483880341	0.192473739	0.429523647						
0.145548686	0.545700371	0.108988382						
0.453460634	0.189340100	0.089644171						
0.273377568	0.438600808	0.790571928						
0.928365827	0.444831997	0.715817511						
0.235984519	0.759761751	0.104594160						
0.272523046	0.121965244	0.408753037						
0.555138469	0.075030454	0.720233798						
0.219022572	0.392170966	0.080459736						
0.926472843	0.093418591	0.717251778						
0.587875009	0.407598555	0.072366863						
0.666908324	0.946811199	0.464380473						
0.3533728950	0.657714367	0.798102379						
0.355293185	0.300178111	0.786918044						
0.016383549	0.633817732	0.134595841						
0.042105373	0.325058192	0.456960022						
0.720989466	0.652581334	0.783825755						
0.019082235	0.970603585	0.139837667						
0.697684526	0.301658571	0.471266389						
0.391313881	0.987633169	0.149992853						
0.781856596	0.455447048	0.604424834						
0.476647705	0.780443370	0.940475106						

$[Cu_2(\mu-OH)_2]^{2+}$, Fig. 6, $E = -973.560$ eV							
0.358560562	0.865055919	0.373456508	0.458891213	0.277640492	0.929901898	0.810689807	0.851634324
0.379322082	0.108195074	0.364609092	0.387733608	0.507392287	0.441675454	0.482200265	0.194001868
0.893035531	0.628539026	0.370400488	0.559619665	0.608309269	0.340273261	0.149555549	0.544834852
0.469782948	0.760101616	0.831448317	0.650587380	0.903808117	0.404831588	0.460391909	0.191896424
0.474474251	0.754997194	0.046886344	0.285496026	0.157704920	0.465473890	0.267499655	0.441300273
0.575412810	0.972292066	0.713326156	0.309677988	0.449516296	0.454369634	0.920336187	0.437687248
0.242296323	0.299284488	0.041800514	0.234404847	0.404537141	0.221143961	0.24048303	0.763752520
0.568931043	0.199946240	0.704646885	0.211724311	0.343033344	0.323095143	0.268405974	0.117213033
0.899681747	0.862997115	0.367083758	0.207692012	0.461009324	0.311170250	0.550005078	0.075659268
0.036028631	0.434938818	0.706126988	0.427309632	0.447699219	0.163404882	0.225429833	0.395485252
0.693273187	0.752501547	0.046089400	0.427648276	0.568885744	0.153685674	0.924190104	0.089308642
0.801813841	0.977087975	0.713372350	0.541864693	0.568263352	0.194125310	0.586888373	0.409469306
0.037511602	0.208960593	0.704331338	0.563491106	0.610531449	0.406499624	0.669886827	0.954102278
0.797988653	0.424692750	0.707145154	0.718498170	0.578786082	0.582770348	0.341465652	0.661113143
0.467644155	0.310478359	0.823479116	0.700913489	0.648143232	0.639648855	0.351956457	0.305546343
0.904361904	0.861644030	0.160993680	0.713922858	0.651581407	0.527048111	0.017760549	0.632919431
0.469605535	0.300483555	0.037607383	0.306826204	0.502988219	0.597889602	0.050329678	0.333306581
0.578088284	0.202560246	0.498410881	0.369854867	0.554836988	0.695072234	0.712289333	0.648923755
0.134896591	0.641750693	0.164859489	0.356954902	0.637018621	0.620540142	0.023898561	0.968829811
0.040911056	0.440774858	0.499300480	0.249091014	0.419712663	0.290241480	0.695662260	0.310426176
0.370592088	0.093786158	0.156985238	0.455256909	0.524762690	0.194141656	0.392778873	0.989188612
0.235328600	0.538202405	0.834796071	0.678737462	0.671641648	0.579910278	0.783529162	0.460622847
0.801578820	0.431014240	0.501049519	0.373179793	0.571950555	0.627075791	0.481128335	0.782280564
0.039138678	0.213095337	0.495777993	0.409951299	0.512837291	0.318401098	0.869340718	0.731916368
0.700492501	0.538335562	0.825747311	0.519164145	0.611268520	0.584054589	0.131935385	0.624830425
0.366717666	0.860475540	0.165829152				0.593870938	0.773031890
0.561462402	0.962609291	0.503622174				0.544753188	0.923354268
0.902577639	0.626475632	0.162886456				0.155036449	0.130818427
0.127601460	0.650098264	0.380293220	13.6750001907	0.0000000000	0.0000000000	0.870513737	0.580905378
0.140970290	0.082926035	0.150462255	-6.8375000954	11.8428975619	0.0000000000	0.087227300	0.224925712
0.700084150	0.293628871	0.273830521	0.0000000000	0.0000000000	14.7670001984	0.719654858	0.544809997
0.125742033	0.546350181	0.435673058	Al Si O H N Cu			0.391891927	0.843898118
0.377926677	0.627461433	0.070233889	4 32 74 16 4 2			0.536744118	0.212500200
0.031661140	0.953336120	0.386873394	Direct			0.233661428	0.300559729
0.707414031	0.017330268	0.732923627	0.238553032	0.522742927	0.049760744	0.866159856	0.874243200
0.367860407	0.322505653	0.072358109	0.693486333	0.750700234	0.823235691	0.085681953	0.473793834
0.020463403	0.665142953	0.404812753	0.126417771	0.091466025	0.363068461	0.695884526	0.753427148
0.007164765	0.307172388	0.727177441	0.809719682	0.975203693	0.502296925	0.393539190	0.146280304
0.670088351	0.627938926	0.083274998	0.245079756	0.316668123	0.823361754	0.775605261	0.922342002
0.350159764	0.979891598	0.377577364	0.695257366	0.532056690	0.041957341	0.208343476	0.519844115
0.908774853	0.116118411	0.487242907	0.358538866	0.864646733	0.371982604	0.457213759	0.276189595
0.236317575	0.770685613	0.141637996	0.378759056	0.107746445	0.363992423	0.362843156	0.506555080
0.913114965	0.418812007	0.490654409	0.892626464	0.628282607	0.369726151	0.543072939	0.598920405
0.556458175	0.724717855	0.791162848	0.468896180	0.759886920	0.830339670	0.651632905	0.910311759
0.241652071	0.053522840	0.130294859	0.474453479	0.754597306	0.046663441	0.286006570	0.159609511
0.919521630	0.751618922	0.157310143	0.574735284	0.720574762	0.712815762	0.286671579	0.465930700
0.572879434	0.4346494529	0.803682923	0.241316929	0.299376190	0.041369446	0.225570738	0.401604772
0.794458032	0.887344658	0.784911931	0.568635285	0.200095192	0.704236567	0.197397381	0.341176987
0.790150225	0.506925523	0.780562341	0.898924947	0.862641275	0.365851632	0.192926720	0.457890749
0.803100348	0.539072216	0.096138783	0.036170851	0.435528010	0.705316901	0.431643009	0.450959802
0.454040867	0.847055495	0.101859458	0.693187714	0.752963722	0.045390464	0.432994723	0.570541859
0.124399498	0.195557803	0.430246741	0.800665796	0.975977182	0.711951911	0.546543241	0.570000112
0.487483501	0.874557674	0.780023813	0.036926776	0.208532602	0.703294814	0.618780196	0.641058922
0.149256617	0.174877599	0.076863989	0.797752321	0.424610049	0.707038581	0.693783820	0.755922377
0.803894699	0.527234674	0.435935915	0.465674043	0.308721542	0.823446810	0.669593811	0.637752354
0.592456758	0.091676183	0.488565564	0.904662013	0.861596525	0.159591585	0.718563795	0.667258382
0.136301979	0.221141309	0.772666860	0.468281984	0.300332248	0.037547678	0.382702410	0.503286362
0.456169993	0.875533104	0.442600459	0.577614188	0.203011811	0.498205215	0.482577443	0.632579148
0.481073043	0.215854824	0.767845571	0.134874865	0.614567349	0.163033530	0.371850908	0.610537112
0.814275563	0.878800035	0.432043731	0.040698145	0.440839827	0.499103457	0.236135751	0.417278677
0.130365223	0.525479138	0.773360074	0.370447129	0.093895279	0.156264305	0.460454762	0.528253436
0.809936881	0.851267457	0.090495877	0.237104461	0.537256837	0.831591249	0.662996598	0.671078980
0.482389510	0.194351122	0.427847266	0.801457405	0.430869937	0.500781238	0.428509951	0.583054245
0.150354981	0.544290841	0.121999212	0.038663346	0.212120086	0.496432841	0.398832440	0.510907471
0.459703982	0.191248089	0.089867912	0.698381126	0.537264228	0.825254083	0.505333900	0.593091547
0.269223124	0.444223255	0.797187269	0.367107660	0.860617399	0.164722458		0.521390319
0.920596778	0.437705040	0.716559768	0.560207190	0.962537289	0.503624022		
0.240961626	0.764413178	0.411455929	0.902093470	0.626169443	0.161902800		
0.268884301	0.117982790	0.4075667680	0.127355695	0.649433313	0.378508091		
0.550022960	0.075568385	0.720716715	0.141494751	0.083332695	0.149629042		
0.227744853	0.396020293	0.090143643	0.699778080	0.293458670	0.723736882		
0.926308453	0.893497911	0.719137669	0.124335296	0.545375824	0.434083819		
0.588114202	0.409058183	0.065802075	0.378792226	0.627911329	0.071666218		
0.670319319	0.952889025	0.457985401	0.030920139	0.951436222	0.384732425		
0.340629816	0.661619902	0.808534920	0.706482708	0.160954526	0.732334793		
0.353977233	0.307923526	0.788918138	0.367436290	0.321967363	0.071997657		
0.018186308	0.632840991	0.131155550	0.020395849	0.665362060	0.402975291		
0.050938215	0.334057510	0.464291006	0.007198532	0.307372451	0.724963546		
0.716519237	0.650871456	0.779417336	0.670224667	0.628568649	0.083096452		
0.023299729	0.969049990	0.132416621	0.349931896	0.979387820	0.376194000		
0.695865631	0.310438544	0.470003784	0.907848716	0.115283616	0.489763081		
0.392926961	0.989146888	0.154775515	0.236677036	0.770687521	0.140785962		
0.783357745	0.460928768	0.604125679	0.912784696	0.418631703	0.490468481		
0.481211662	0.785165012	0.939934969	0.557070434	0.726263583	0.788321317		
0.873097777	0.733676910	0.383681178	0.241989806	0.504074357	0.128003150		
0.132268876	0.625840783	0.274833053	0.919221342	0.751350522	0.156209216		
0.592592359	0.770682812	0.086351402	0.570659041	0.433344722	0.803768754		
0.545							

TS13, Fig. 6, E = -1013.324 eV							
0.237768650	0.538803816	0.834144890	0.506112754	0.391479015	0.494392604	0.351339221	0.664903224
0.802551985	0.431583464	0.500822544	0.399327010	0.684383810	0.376796842	0.357851446	0.312216610
0.037268791	0.215139836	0.495026529	0.450859040	0.72475374	0.273653269	0.019342378	0.632332206
0.699898779	0.539138675	0.824829280	0.314389348	0.644870698	0.288304538	0.054251350	0.338050395
0.364419222	0.866675615	0.163269714	0.235832050	0.398910642	0.293354601	0.723980665	0.658399761
0.560329139	0.964173079	0.502115190	0.463566959	0.509625196	0.207462236	0.030300815	0.973535538
0.901738048	0.627322555	0.161805734	0.665682316	0.682089269	0.571004391	0.697078586	0.320275038
0.126098484	0.652647376	0.379241556	0.429191411	0.588640571	0.638711572	0.396283954	0.995561302
0.139934570	0.086247295	0.148460120	0.511471570	0.416851908	0.560190678	0.793395698	0.469883680
0.700813472	0.294692695	0.723864496	0.391076684	0.659172952	0.310817450	0.491244227	0.795322239
0.124695018	0.549988925	0.435129672	0.399521679	0.498830497	0.330770016	0.875145078	0.737544954
0.382524192	0.625779867	0.068242304	0.506369352	0.578204334	0.526814044	0.135535583	0.630853236
0.032916144	0.951293111	0.384012550				0.599251747	0.781917632
0.706543028	0.016056268	0.736833453				0.549397707	0.930634797
0.365649074	0.320616573	0.070041873	1.0	13.6750001907	0.0000000000	0.0000000000	0.157723933
0.019178065	0.668585241	0.402314693		-6.8375000954	11.8428975619	0.0000000000	0.087548361
0.008737548	0.310119361	0.725844145		0.0000000000	0.0000000000	14.7670001984	0.23946530
0.672339380	0.631574452	0.082505837	Al	Si	O	H	N
0.344434381	0.984750450	0.395229697	4	32	74	22	6
0.905408502	0.121464252	0.487437636	Cu				
0.233302787	0.776140571	0.143147022	Direct				
0.913799942	0.419459969	0.490726948	0.244171470	0.529382586	0.048470374	0.233561695	0.298981696
0.559238791	0.730608404	0.792108297	0.703655064	0.767009437	0.828560650	0.875808060	0.881415784
0.243689984	0.061714031	0.128363281	0.131962970	0.095489854	0.367045671	0.085039869	0.473362386
0.920493066	0.752989352	0.154937267	0.813858330	0.981091440	0.504426420	0.087220088	0.601205111
0.572900414	0.434431374	0.802726686	0.248531252	0.320304573	0.824474037	0.718404233	0.546839833
0.798887134	0.887562752	0.780384600	0.696763694	0.538398395	0.047540583	0.395066351	0.939406574
0.790344477	0.508531511	0.779575792	0.358919442	0.873116016	0.373954684	0.854377270	0.273826301
0.802533090	0.540075421	0.094998114	0.382965595	0.113510720	0.364275992	0.538280547	0.600284398
0.451061577	0.840814471	0.109095295	0.898037851	0.636936048	0.372155339	0.154115140	0.225181730
0.117681555	0.191669092	0.429201901	0.477037221	0.767261386	0.832953036	0.260912687	0.613007784
0.486431569	0.875393569	0.779629767	0.479962319	0.760577381	0.047481265	0.207058967	0.932213724
0.144301280	0.175655976	0.074300081	0.578372598	0.976873636	0.715673923	0.209772408	0.464634860
0.803989394	0.527405024	0.435742676	0.242425452	0.302737505	0.041782983	0.198774502	0.226392671
0.588629544	0.091717802	0.483269989	0.573776186	0.205328822	0.705968618	0.208554864	0.292234272
0.136388466	0.221290439	0.770142078	0.908509374	0.869131804	0.369189084	0.155387953	0.390186608
0.454399765	0.876314700	0.441411823	0.042429280	0.442485482	0.707951128	0.419536680	0.444348454
0.481526941	0.216704696	0.765883505	0.698712587	0.760905802	0.050691679	0.433359027	0.567555010
0.817578256	0.885837018	0.429621756	0.806096852	0.983034790	0.715221226	0.531890094	0.559798241
0.132581621	0.528075517	0.773812830	0.041591700	0.215850517	0.705521643	0.686496377	0.667360246
0.812179804	0.854678631	0.089166857	0.804144025	0.430661261	0.711079538	0.728691578	0.766255736
0.484024882	0.202211082	0.426595449	0.472635111	0.317530483	0.825097024	0.710243702	0.659326315
0.157252772	0.5525216580	0.120490544	0.911342919	0.867025197	0.162888229	0.760934949	0.552046895
0.464340419	0.198276609	0.091817096	0.472637349	0.307340205	0.039630607	0.463404477	0.495240837
0.269389153	0.443994015	0.794561863	0.584987879	0.206070378	0.506072758	0.505930245	0.630040407
0.921880722	0.439731985	0.717832446	0.139111367	0.648402469	0.165292293	0.385653672	0.544219315
0.239350110	0.766973019	0.410019964	0.042723928	0.443496376	0.499030103	0.467805952	0.338432074
0.270289689	0.128681675	0.404253364	0.376515388	0.101781629	0.156831563	0.414186895	0.396261841
0.551343501	0.076941669	0.721926093	0.242320791	0.543299775	0.832891464	0.534383118	0.397573620
0.225081548	0.395650148	0.088361613	0.806910336	0.43771887	0.504536092	0.440246761	0.715440154
0.925442040	0.092321148	0.717590749	0.039323155	0.216517761	0.497190803	0.542701364	0.683277113
0.586915433	0.413111657	0.064583033	0.703560174	0.543196917	0.830703357	0.492783040	0.742210686
0.669571459	0.955660582	0.455777559	0.368229687	0.868692040	0.166305155	0.216631994	0.394579291
0.343141913	0.663060129	0.810776889	0.567406461	0.969566584	0.505946696	0.446501374	0.522693098
0.354044646	0.307843059	0.786720514	0.905956864	0.630316019	0.163916454	0.703601122	0.681553185
0.016670721	0.631720603	0.131104991	0.131588581	0.653961539	0.380504817	0.467168361	0.561994255
0.054597490	0.338618487	0.464514464	0.145394132	0.089833491	0.152611449	0.485256433	0.400171936
0.713025570	0.650412202	0.778918564	0.705413342	0.29878445	0.723227203	0.474291503	0.690775037
0.025016241	0.969387233	0.131339886	0.126163334	0.549207032	0.435760319	0.370261699	0.523102045
0.696788371	0.311097771	0.469771862	0.386828661	0.631031351	0.0654649891	0.545727193	0.584810615
0.391674131	0.991885126	0.135715172	0.041755214	0.954277158	0.387235790		
0.783374965	0.460681379	0.604059279	0.709037364	0.018675169	0.757290680		
0.483688772	0.791021228	0.494282736	0.3674604089	0.322497398	0.071981952		
0.866980851	0.732875884	0.384108365	0.026038138	0.671949625	0.405036539		
0.133036301	0.628220141	0.273998290	0.016538929	0.316535354	0.732505620		
0.596047878	0.775873661	0.087005079	0.674602866	0.636563540	0.088362463		
0.549145460	0.929657042	0.606523097	0.339263350	0.981133103	0.375827014		
0.149947450	0.132237613	0.250554174	0.907391489	0.122392990	0.490707159		
0.869350910	0.583041012	0.266582698	0.236368680	0.780006886	0.144913554		
0.084443487	0.2261152614	0.598958969	0.914040200	0.419370562	0.490775943		
0.720764748	0.546665847	0.933797777	0.568358362	0.737369061	0.792039573		
0.389774889	0.870344968	0.272724509	0.248237446	0.664492710	0.130703121		
0.537849844	0.208870158	0.598478734	0.925334215	0.756436646	0.157181188		
0.233394355	0.300315112	0.930199835	0.575081229	0.443498403	0.803374588		
0.867706478	0.875382304	0.261085361	0.805094481	0.895699859	0.786566496		
0.086661227	0.476548046	0.603016138	0.791731000	0.509135842	0.785833180		
0.697938383	0.757576108	0.939042985	0.803938091	0.543036163	0.099109180		
0.394179821	0.135383219	0.260922313	0.453174114	0.847460926	0.104329057		
0.775637627	0.931301475	0.609208524	0.121061049	0.192164242	0.434090946		
0.205079749	0.518494964	0.938023686	0.489136755	0.879164457	0.781426370		
0.459218264	0.278084794	0.939075420	0.148225251	0.180504844	0.080611542		
0.361955106	0.491836190	0.459596843	0.810218573	0.533826888	0.438243133		
0.546127498	0.572315991	0.398066700	0.610524058	0.102221332	0.493779451		
0.653593361	0.915729702	0.398067504	0.139796406	0.221832201	0.7711443784		
0.286882252	0.176455423	0.457768947	0.459471494	0.892153382	0.443528175		
0.285511255	0.452086091	0.484134078	0.487913102	0.224583775	0.768125554		
0.225528911	0.390052885	0.224074900	0.825341940	0.888149500	0.434147179		
0.198520496	0.319976002	0.321506351	0.140740126	0.536850989	0.770197809		
0.189896464	0.434494704	0.315663874	0.816180825	0.858833909	0.094395854		
0.434522539	0.433184206	0.176187873	0.490540445	0.190915301	0.426		

0.571850061	0.974926114	0.506220341	0.448569715	0.529546499	0.211979300	0.275448084	0.450271457	0.791889608
0.907867253	0.632723391	0.168050528	0.747900069	0.701565325	0.597975314	0.925986946	0.446887285	0.726795256
0.135214865	0.656552017	0.380164653	0.505467653	0.561389565	0.661922812	0.249288604	0.774080575	0.410438955
0.147653013	0.088992678	0.152428403	0.490752578	0.426945925	0.503739417	0.268003851	0.124417193	0.409553438
0.710529804	0.297943592	0.725949109	0.464083105	0.669914663	0.366325349	0.563775659	0.089961670	0.726421952
0.125691175	0.550323784	0.435200930	0.358368397	0.510102868	0.325696617	0.236873686	0.411510050	0.090198800
0.386258274	0.633752108	0.067241907	0.596802533	0.586032987	0.548247993	0.931615055	0.100135893	0.711355925
0.045019526	0.957782388	0.395760089				0.589997888	0.422961563	0.072558865
0.712408304	0.020024810	0.739422441				0.681858599	0.975443363	0.461985797
0.37070924	0.325940102	0.074561535	1.0			0.351366073	0.669443071	0.805598795
0.033048566	0.679891586	0.404792875	13.6750001907	0.0000000000	0.0000000000	0.357861578	0.312863171	0.791888416
0.020031339	0.318955272	0.730447769	-6.8375000954	11.8428975619	0.0000000000	0.016240133	0.635289907	0.141359136
0.676243007	0.637947261	0.088440083	0.0000000000	0.0000000000	14.7670001984	0.046812400	0.342365026	0.464244813
0.342921168	0.982618034	0.375981003	H Al Si O N Cu			0.720322132	0.660347581	0.779717863
0.908664346	0.124508880	0.488853008	14 4 32 75 5 2			0.030202305	0.98024311	0.125072986
0.241754249	0.783244908	0.146237031	Direct			0.688657582	0.336415917	0.471201509
0.914652646	0.418976873	0.491230637	0.727990806	0.746568263	0.574913383	0.395604968	0.002210841	0.159300029
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0.252164751	0.065601088	0.131950542	0.743390262	0.638589501	0.539369941	0.491604596	0.802059591	0.935831428
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0.494270742	0.226285636	0.771946847	0.131409615	0.109473914	0.365690559	0.705696982	0.766471744	0.940358460
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0.302363604	0.188410595	0.458936870	0.567489684	0.738711357	0.789567351			
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0.199065819	0.307372034	0.284148842	0.575388551	0.445575267	0.800417900			
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0.030998832	0.977866888	0.400450110	0.736337423	0.858693957	0.385824412	0.231662586	0.306554347	0.931992829
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0.142379954	0.224419191	0.426783949	0.810036540	0.983527184	0.706597865			
0.491996437	0.880742550	0.769650638	0.044336174	0.219564781	0.701475739			
0.149744093	0.191013023	0.080775067	0.804949522	0.434859246	0.713555932			
0.815809131	0.554175258	0.447315186	0.473525196	0.318191677	0.285690389			
0.608404458	0.116762973	0.485928923	0.912795961	0.874690056	0.158473253			
0.141653791	0.226087034	0.769606650	0.474632472	0.312505692	0.040548600			
0.466817945	0.905062258	0.437269688	0.579575241	0.215345770	0.498766512			
0.486934096	0.223840073	0.769330680	0.138978079	0.653372824	0.165625721			
0.806486309	0.885577261	0.422547609	0.039952055	0.451078355	0.499478370			
0.141797081	0.538312674	0.768968344	0.375355065	0.108383127	0.158363372			
0.813408256	0.866249094	0.095349886	0.244922340	0.546361685	0.831150055			
0.480751932	0.201069310	0.429825842	0.804754615	0.445991307	0.505878091			
0.160504133	0.567494750	0.111792356	0.048414353	0.228426799	0.493282855			
0.468876004	0.207698777	0.093814462	0.702561140	0.545930326	0.829010069			
0.274990588	0.449253201	0.791612566	0.366133541	0.871752262	0.166166380			
0.274991810	0.444370121	0.728870690	0.573624611	0.979768455	0.497178853			
0.249986485	0.774455547	0.410262942	0.902008772	0.635846615	0.167062595			
0.270079941	0.127684399	0.410347551	0.134330228	0.661067128	0.379059970			
0.559489906	0.086467668	0.723235369	0.145050392	0.095842621	0.148952901			
0.235121652	0.412419856	0.088884883	0.704591453	0.304687172	0.724753439			
0.931557775	0.100825258	0.711480677	0.126948312	0.558488905	0.439062059			
0.587836862	0.426119149	0.075207233	0.387415171	0.641899288	0.064194843			
0.683564544	0.977741599	0.454454869	0.029767551	0.974817336	0.401263624			
0.353347629	0.667373240	0.805708647	0.712048829	0.019038023	0.723870635			
0.358157337	0.312678337	0.793983400	0.367652774	0.325330526	0.069896050			
0.016583411	0.638382077	0.139261395	0.024911787	0.675528204	0.398298353			
0.045081396	0.341916263	0.464310348	0.016828911	0.318294019	0.729226351			
0.719557881	0.658593535	0.780583918	0.669740856	0.642780900	0.085819751			
0.030560855	0.981283009	0.127728385	0.354202360	0.992050588	0.373114765			
0.689429641	0.337473989	0.471018583	0.924678266	0.120503552	0.481085420			
0.396557629	0.004290337	0.157931864	0.232855901	0.786574244	0.144989401			
0.795662463	0.475385010	0.611002088	0.912246823	0.430024236	0.487077683			
0.490934670	0.806776047	0.934338748	0.568076253	0.738769293	0.793237209			
0.887358963	0.754945338	0.387051880	0.249650583	0.073761851	0.125734642			
0.143075556	0.633524239	0.273262084	0.925605834	0.76316840	0.159751371			
0.600914538	0.796272039	0.079743572	0.575405955	0.444008052	0.799793243			
0.551754296	0.944093943	0.599806845	0.806465387	0.897461772	0.780655682			
0.155003239	0.135950729	0.252342103	0.793975770	0.514411390	0.788334844			
0.865516186	0.594002903	0.271933496	0.802670598	0.552851021	0.098685987			
0.094338007	0.239752144	0.597797036	0.449748009	0.857789576	0.098079808			
0.716024310	0.552256346	0.938256085	0.140414676	0.221429989	0.427237779			
0.393898159	0.853817642	0.269305557	0.493028790	0.882840931	0.774041593			
0.540873766	0.221655544	0.601198196	0.147596225	0.190215454	0.081415720			
0.231764913	0.307514787	0.931844056	0.809950113	0.548635960	0.445716143			
0.474641857	0.294012338	0.932652590	0.180505092	0.482293308	0.912495628			
0.371213108	0.488743722	0.519084334	0.482083917	0.208629340	0.429571360			
0.554665983	0.564346969	0.430918097	0.159008056	0.564609826	0.113127492			
0.394805729	0.651198566	0.467395753	0.469668806	0.205869928	0.094013952			
0.687830210	0.657001376	0.5779447974	0.274532050	0.449510336	0.792163134			
0.485758781	0.557290018	0.677527666	0.925294399	0.444608897	0.727961719			
0.282233089	0.441856652	0.287884086	0.243096381	0.779080987	0.409791172			
0.505416036	0.442748696	0.275572777	0.269062430	0.124927625	0.410633087			
0.348969012	0.548896730	0.460170686	0.560807228	0.087768525	0.725790918			
0.526125789	0.569354177	0.551146485	0.237191573	0.411867676	0.089539289			
0.424939543	0.498912603	0.357572615	0.931457043	0.100149848	0.711500943			
			0.586726367	0.424448669	0.076620974			
			0.693281114	0.331161350	0.473719686			
			0.351692945	0.669059098	0.806746066			
			0.357629418	0.312432915	0.794284880			
			0.015145187	0.635052145	0.141038030			
			0.045439404	0.342453837	0.463844895			
			0.720156193	0.658911109	0.781922638			
			0.030839028	0.979515016	0.126723394			
			0.693281114	0.331161350	0.473719686			
			0.394100577	0.02012548	0.159375653			
			0.285010785	0.158967525	0.474222232			
			0.70375001907	0.118428975619	0.521913239			
			-6.8375000954	0.000000000000	0.042440347			
			0.000000000000	0.000000000000	0.147670001984			
	H	Al	Si	O	N	Cu		
	14	4	32	75	5	2		
	Direct							
0.730992496	0.747985303	0.572073638	0.394100577	0.02012548	0.159375653	0.233785169	0.786474705	0.143053025
0.711036980	0.647906601	0.644318104	0.795493066	0.476365355	0.610912681	0.910126746	0.426212758	0.484328419
0.741675854	0.637735797	0.535232007	0.490290850	0.803977489	0.936845422	0.568735659	0.736829877	0.787813723
0.396015972	0.517605364	0.677150190	0.883362353	0.752018809	0.387670785	0.250366986	0.073890634	0.124592066
0.507366002	0.508432269	0.705477595	0.141509695	0.632537007	0.274732798	0.924831092	0.762652814	0.160002440

0.574100137	0.440537333	0.800872386	0.246348083	0.310551465	0.041255064	0.289662480	0.444980234	0.329784095
0.807380140	0.894106328	0.775661528	0.574664414	0.205210820	0.704560399	0.510403991	0.453908861	0.270552129
0.793102741	0.511999428	0.785791993	0.909670591	0.876187205	0.362159252	0.340363413	0.694607377	0.595201790
0.803920805	0.553175807	0.095146559	0.040007293	0.441087872	0.707076609	0.547364950	0.582176864	0.538489103
0.450025707	0.857916236	0.092588454	0.696852624	0.765451372	0.043601770	0.447244585	0.507127166	0.369588077
0.141687319	0.220893323	0.426312268	0.809508324	0.980609715	0.703357816			
0.491958112	0.879135549	0.768561900	0.043769721	0.216189027	0.700682282			
0.147623152	0.189332098	0.079564631	0.804311216	0.430362314	0.711600780			
0.815273166	0.550667048	0.444360971	0.472259820	0.314255625	0.823994637			
0.595548511	0.108138420	0.482153893	0.912557006	0.873001397	0.155977264			
0.140024424	0.223669842	0.769024134	0.474941075	0.311721683	0.039484370			
0.465653658	0.892504930	0.434988558	0.577663779	0.213452056	0.498417884			
0.489413381	0.220485553	0.771127343	0.139652774	0.649715066	0.161974207			
0.805251002	0.883874059	0.418816328	0.038596749	0.447479278	0.497010648			
0.142771587	0.534844339	0.767128170	0.375576317	0.105731986	0.156216905			
0.815905213	0.864099205	0.089731634	0.245872155	0.540497479	0.827896595			
0.480056018	0.205627277	0.429431528	0.804600537	0.442283690	0.503070712			
0.158640414	0.565419078	0.105264984	0.049896833	0.226171881	0.492617369			
0.471877515	0.208362922	0.096503891	0.700041533	0.542463183	0.824746490			
0.276458889	0.445495129	0.788676679	0.367519081	0.869463027	0.161932021			
0.927547395	0.446267247	0.725224733	0.573688984	0.977184057	0.494906247			
0.247993916	0.771639287	0.403825790	0.901502609	0.634457052	0.164781258			
0.267398030	0.122188903	0.410222739	0.135317296	0.656756103	0.3722662157			
0.562352538	0.085368149	0.720854640	0.145533904	0.093367405	0.146628425			
0.237180963	0.411853164	0.089183606	0.706003189	0.299196482	0.722870708			
0.931307971	0.097694747	0.707842827	0.125025272	0.555493295	0.436437666			
0.587076902	0.426294059	0.072407313	0.386044741	0.638862789	0.064746693			
0.683901130	0.979206502	0.453719497	0.028074356	0.973937273	0.396868558			
0.352907985	0.665212274	0.803712308	0.712026834	0.016486039	0.721378386			
0.356440663	0.305476576	0.794565022	0.370640963	0.328014493	0.071162350			
0.016697578	0.637032926	0.138382778	0.027835701	0.675654173	0.386404753			
0.044645991	0.339576393	0.461647809	0.014740149	0.314325035	0.726719558			
0.718648434	0.655659974	0.777663946	0.668878019	0.639589012	0.082054190			
0.031898100	0.978063941	0.124669790	0.355269521	0.987972975	0.369936973			
0.691298366	0.331850529	0.470507056	0.926146150	0.119200170	0.478896081			
0.394844323	0.002126079	0.154950887	0.234048530	0.783052623	0.142738387			
0.794530094	0.474149346	0.608842423	0.909793973	0.422150135	0.483831182			
0.492603809	0.804227650	0.932032347	0.567388415	0.733966589	0.786641181			
0.884837985	0.751154065	0.382714778	0.248842701	0.608687290	0.125126362			
0.143223211	0.626242757	0.269332141	0.926178694	0.762570322	0.159644902			
0.601875484	0.795372784	0.078823209	0.572048485	0.441003054	0.796721697			
0.548091352	0.939447820	0.597940624	0.806073070	0.893296182	0.776088655			
0.152385488	0.131944925	0.251798630	0.790478706	0.509118974	0.785372019			
0.861890554	0.587777376	0.268470168	0.806386630	0.554579616	0.092330329			
0.094761916	0.239945412	0.596642911	0.450449824	0.856522560	0.092370845			
0.715882063	0.551380098	0.935712636	0.142262325	0.219547614	0.426843077			
0.395954996	0.855155706	0.266742170	0.493469596	0.879040539	0.771993876			
0.540709674	0.220922843	0.600874543	0.150163621	0.187103242	0.077564754			
0.232184052	0.305883139	0.931364894	0.815876365	0.548072278	0.444163531			
0.881447256	0.894292891	0.258942336	0.592046142	0.104738034	0.484629393			
0.078650922	0.474440203	0.600110233	0.138632521	0.221738771	0.770426631			
0.711522877	0.769068301	0.937317669	0.464091420	0.888450801	0.436116815			
0.394026846	0.159160525	0.262785196	0.489544988	0.219893605	0.771800578			
0.791866779	0.928969324	0.600760520	0.805241406	0.883585215	0.419281453			
0.212086409	0.519006371	0.930896819	0.141251311	0.532657325	0.768403590			
0.475523978	0.288654208	0.933426440	0.814410210	0.806080401	0.090143114			
0.336049378	0.542028129	0.512087047	0.479791462	0.204525188	0.428758240			
0.562928319	0.569029748	0.425715178	0.154954612	0.561569452	0.104944743			
0.339701921	0.700075030	0.554780304	0.469115257	0.204178229	0.092136666			
0.704194129	0.677635908	0.576404170	0.274976724	0.444101602	0.788224392			
0.486915201	0.546331048	0.667805195	0.925994515	0.443907529	0.728530645			
0.286262095	0.452119619	0.303507268	0.246831596	0.772425234	0.403766721			
0.509356916	0.449148327	0.274614602	0.267736584	0.119270541	0.407502800			
0.320189476	0.604576051	0.563014090	0.560279667	0.083051100	0.719648838			
0.544105589	0.575042069	0.543943703	0.233345374	0.407730013	0.088982277			
0.436496913	0.507994354	0.359828591	0.930746078	0.096635491	0.708256006			
			0.590993822	0.421291113	0.072219163			
			0.683066487	0.978619516	0.455637991			
			0.351740205	0.663881955	0.480216154			
			0.355180562	0.304091841	0.789808035			
			0.015920322	0.634420931	0.143462285			
			0.049813695	0.314614589	0.462621480			
			0.719427538	0.655716360	0.776674390			
			0.030544050	0.9776670670	0.124796262			
			0.690974891	0.328995556	0.471118152			
			0.394414991	0.999310374	0.156134188			
			0.795930684	0.471153140	0.608599544			
			0.488765091	0.795645893	0.933429293			
			0.884674728	0.750345886	0.384968132			
			0.146820188	0.624701381	0.270094544			
			0.600893795	0.792560220	0.079776488			
			0.545648515	0.934074058	0.599424929			
			0.153018981	0.131484299	0.250985116			
			0.855297267	0.587448180	0.267960012			
			0.094347157	0.238105297	0.597431958			
			0.712206960	0.549273014	0.934160650			
			0.395942718	0.850372732	0.266634613			
			0.538792431	0.219828919	0.601089060			
			0.237853140	0.306478411	0.930984259			
			0.881718755	0.892863512	0.259256244			
			0.076062903	0.475930691	0.601650953			
			0.357065588	0.641218781	0.536916852			
			0.580623686	0.581017494	0.423172727			
			0.276288152	0.730525613	0.601143062			
			0.704072297	0.681678772	0.580166101			
			0.479640633	0.548748612	0.658445537			
			0.289662480	0.444980234	0.329784095			
			0.136750001907	0.00000000000	0.00000000000			
			-6.8375000954	11.8428975619	0.00000000000			
			0.00000000000	14.7670001984	0.00000000000			
			H Al Si O N Cu					
			14 4 32 75 5 2					
			Direct					
			0.727758229	0.766670942	0.581490934			
			0.714506269	0.660710096	0.465368525			
			0.755961955	0.670588315	0.536598682			
			0.393235087	0.507367611	0.661121309			
			0.503428280	0.499847531	0.694857359			
			0.507645071	0.621180987	0.598019087			
			0.279970735	0.260684133				

0.246651158	0.772387862	0.404484272	0.704929709	0.303348392	0.726895869	0.561649561	0.441986322	0.210160807
0.267720580	0.119182803	0.407570541	0.125114560	0.554606378	0.435643286	0.597049952	0.494328648	0.313850313
0.559951127	0.083106600	0.719628155	0.386543065	0.642375708	0.058768298	0.285924971	0.171121433	0.465849310
0.233370617	0.407796264	0.089014105	0.029776601	0.974781692	0.403378010	0.725210309	0.824840724	0.405098110
0.930692434	0.096464664	0.708271384	0.711176257	0.018777056	0.728236318	0.241527438	0.534745753	0.045106694
0.590926945	0.421189427	0.072437607	0.365865022	0.328403205	0.066358320	0.706002891	0.773462176	0.828605592
0.683148086	0.978619516	0.455663711	0.028790506	0.678585231	0.399696916	0.126628816	0.105211467	0.367389441
0.351747930	0.663808465	0.801948011	0.017016886	0.318158001	0.728504121	0.802524626	0.991517067	0.496594161
0.355037183	0.303863794	0.789676845	0.670217037	0.645755470	0.083475843	0.245938271	0.321446002	0.822816670
0.015935114	0.634470224	0.143742889	0.345992930	0.987520814	0.375066131	0.690814793	0.544148147	0.046925236
0.049879774	0.341684699	0.462412685	0.925685108	0.119013965	0.478748530	0.361589462	0.876562774	0.372494042
0.719394863	0.655662835	0.776609004	0.232694909	0.789703488	0.144589931	0.376734823	0.116846837	0.366349757
0.030467289	0.977763176	0.124318667	0.909274638	0.426322460	0.483999461	0.895753980	0.639696419	0.371683955
0.691357613	0.328912675	0.470975101	0.568638742	0.73849872	0.795239270	0.474805802	0.771849453	0.830278218
0.394491017	0.999245942	0.156042635	0.247658268	0.073332004	0.129838914	0.472764224	0.764647901	0.044222444
0.795898795	0.471261173	0.608362377	0.922709823	0.763941169	0.159729242	0.579852283	0.980049551	0.706886590
0.488914669	0.795446098	0.933287621	0.574503243	0.44333122	0.802472532	0.234843940	0.306038588	0.039383203
0.885014474	0.750312567	0.385069758	0.807764351	0.895838499	0.777335227	0.571214318	0.207996070	0.705877483
0.146918267	0.624550462	0.270175248	0.793272972	0.514435053	0.787210643	0.910049736	0.878186285	0.367140800
0.600807428	0.792329490	0.079713278	0.800056517	0.552523613	0.100701764	0.038438547	0.442330509	0.706301868
0.545548439	0.934214652	0.599498868	0.448451310	0.857267273	0.097526632	0.6967363515	0.770642698	0.048804790
0.153334765	0.131626353	0.251016021	0.141552672	0.222724065	0.427828848	0.809259713	0.983528674	0.704608381
0.855060935	0.587330520	0.267999709	0.490407228	0.878752291	0.768697619	0.043023691	0.218945503	0.698477924
0.094394684	0.238068655	0.597351253	0.146675244	0.190717310	0.082653672	0.803175986	0.435242981	0.712501287
0.711893616	0.549131602	0.934133112	0.812259853	0.550046694	0.446067512	0.472341239	0.316591591	0.826348841
0.395481795	0.850254059	0.266822994	0.600649714	0.112478808	0.481545627	0.911276877	0.873938799	0.159443870
0.538997769	0.220155016	0.600819230	0.141365409	0.224870324	0.768417537	0.469247788	0.313909411	0.040889934
0.237726614	0.306536674	0.931005299	0.464308828	0.897037208	0.439667374	0.574939489	0.215112388	0.500548840
0.881743729	0.892818987	0.259299010	0.486133516	0.223793969	0.769307971	0.136062443	0.654512584	0.163281426
0.075932458	0.475825071	0.601629555	0.805216849	0.884191871	0.422906369	0.035704117	0.448425591	0.496161968
0.710351169	0.767500818	0.937430024	0.141388774	0.538018584	0.768064320	0.373896360	0.107683815	0.157777473
0.396087915	0.160006791	0.260378718	0.811823070	0.867101610	0.097788580	0.242548168	0.545349896	0.828338444
0.791924000	0.92858052	0.600956857	0.478297532	0.204838395	0.432611108	0.801616013	0.446015984	0.504603565
0.214784309	0.519993544	0.931516945	0.159891322	0.567841113	0.112196863	0.043297067	0.226355299	0.489424858
0.473805487	0.293032974	0.931321263	0.468190223	0.210726663	0.098102614	0.700389802	0.543736875	0.829258978
0.581395268	0.581252396	0.423058063	0.272714198	0.447604865	0.792217731	0.364956562	0.872307301	0.165403828
0.704331398	0.681782961	0.580315530	0.925208092	0.444254637	0.728769061	0.570699811	0.978949070	0.498108536
0.478848070	0.549530447	0.657781601	0.247414736	0.773778439	0.411066592	0.897875249	0.632713199	0.165741220
0.289772749	0.444897443	0.330417961	0.267096976	0.124875850	0.412009388	0.131834462	0.658193409	0.376944363
0.510393202	0.454696625	0.270522773	0.559515655	0.086038776	0.727267265	0.140490487	0.088740043	0.147423416
0.547679543	0.581895331	0.538193941	0.233058825	0.412116289	0.089251645	0.700956889	0.305926293	0.724155605
0.447635531	0.507652164	0.370034426	0.931085944	0.099865628	0.7111443305	0.124704204	0.555382371	0.436209202
Ts16, Fig. 7, E = -976.520 eV			0.586236560	0.978092611	0.454133838	0.026825404	0.972897887	0.409174711
1.0			0.352092057	0.666433394	0.805936098	0.711454391	0.018413180	0.724307239
13.6750001907	0.0000000000	0.0000000000	0.356592327	0.311223596	0.795157673	0.360993803	0.326297134	0.065236270
-6.8375000954	11.8428975619	0.0000000000	0.015645161	0.638763249	0.138040766	0.023890516	0.6744881995	0.398426980
0.0000000000	0.0000000000	14.7670001984	0.043868400	0.340467900	0.463001102	0.014528911	0.316378772	0.728777587
H	Al	Si	O	N	Cu	0.670997739	0.644534230	0.083276644
14	4	32	75	5	2	0.346834868	0.988808334	0.376522309
Direct			0.689181209	0.334573627	0.471407950	0.920645118	0.11768182	0.476520956
0.733686388	0.747494400	0.567996442	0.395318240	0.004624906	0.156219199	0.230723456	0.788125575	0.145796126
0.709593713	0.651868939	0.645912886	0.794942439	0.473709196	0.610555887	0.908728600	0.429999590	0.484109789
0.736797452	0.631259263	0.538898766	0.487869650	0.807876110	0.934583724	0.568321884	0.739921808	0.797033787
0.393893749	0.514006436	0.682438314	0.885193348	0.752223134	0.387861699	0.247823283	0.070877299	0.125306845
0.507224560	0.505889058	0.706197083	0.140833497	0.634176254	0.273084372	0.915012062	0.757948160	0.160755306
0.512348950	0.628027618	0.714047372	0.599971473	0.796852410	0.078517474	0.574787855	0.441303641	0.797007322
0.273592085	0.418601364	0.217817828	0.552758336	0.946976542	0.600544512	0.805799246	0.894594550	0.775750041
0.221665606	0.350503206	0.315919727	0.149594426	0.133922905	0.254944831	0.794316769	0.516627550	0.787161648
0.244839221	0.479361473	0.301096261	0.865965962	0.593204260	0.271950752	0.796998441	0.5472397716	0.099251829
0.480460852	0.344965458	0.277987540	0.093069926	0.240162417	0.597604990	0.444851190	0.852393031	0.098355524
0.530593872	0.454759061	0.210640073	0.717027247	0.552415013	0.938396692	0.134990066	0.220039502	0.423219532
0.593474090	0.464034677	0.307766259	0.392599046	0.856608450	0.270535755	0.492646694	0.883292377	0.774999030
0.284119636	0.162957266	0.470669776	0.541563988	0.219177216	0.602367103	0.142752588	0.184972927	0.082373299
0.734324157	0.851529479	0.388775140	0.225114973	0.304958731	0.932126224	0.805969954	0.547899425	0.443484247
0.246041790	0.538330317	0.046411770	0.883164287	0.895310319	0.263887227	0.590081811	0.106940016	0.487936586
0.706641376	0.771913826	0.825539768	0.075527593	0.477966189	0.601790667	0.142072573	0.225339070	0.763745368
0.130467370	0.109370954	0.368424773	0.719778001	0.775157679	0.940842986	0.458895057	0.891643047	0.441342473
0.0805917919	0.993669033	0.499211133	0.395591766	0.161746204	0.263535766	0.483721107	0.219076529	0.773183644
0.247152790	0.322677583	0.824579895	0.789736987	0.932749033	0.603874505	0.803145528	0.881953835	0.422355205
0.694408178	0.547992289	0.046162438	0.207429122	0.523789346	0.933403076	0.139150932	0.536604404	0.766790688
0.363953328	0.876946430	0.372654766	0.476019830	0.289721906	0.933715999	0.808325231	0.865416646	0.102097027
0.377831459	0.116248660	0.368206173	0.380169034	0.571569800	0.500384986	0.479302883	0.207657412	0.428741753
0.900400817	0.643065095	0.374002606	0.545110464	0.607584119	0.418047637	0.156539336	0.566918790	0.109785184
0.476572663	0.772148669	0.828460157	0.40121917	0.668039799	0.3731110265	0.466589987	0.209183246	0.095433064
0.477172613	0.771619797	0.041220706	0					

0.708168983	0.543935835	0.938861787	0.146774143	0.186577588	0.078457564	0.908540606	0.870660782	0.157634571
0.392458022	0.857252061	0.270923018	0.812208831	0.550376654	0.445523113	0.469726026	0.311623871	0.041310035
0.533689857	0.221076742	0.602529109	0.592757285	0.108215012	0.482607335	0.573429346	0.211885899	0.500336111
0.220131174	0.298087806	0.929714799	0.141432479	0.227201715	0.767488480	0.136066943	0.648334086	0.166398808
0.894159555	0.903271973	0.263526171	0.459904075	0.891161859	0.441367626	0.033238448	0.446048081	0.498702377
0.074361637	0.474518448	0.600755572	0.483984947	0.221435785	0.771235704	0.371481836	0.104101025	0.158540443
0.719501019	0.780893949	0.943475068	0.802840769	0.882957280	0.421579927	0.239320740	0.546144783	0.830303133
0.393755883	0.158552721	0.262698859	0.139124200	0.537472785	0.768310010	0.799691916	0.443415701	0.504360914
0.791453302	0.931925833	0.602057159	0.812851429	0.861071646	0.091246583	0.040419362	0.224332571	0.490545750
0.207368702	0.526360393	0.931556642	0.477874994	0.206827432	0.430417180	0.700221837	0.545475960	0.827865124
0.477985898	0.296720356	0.933701277	0.153476700	0.556791246	0.113200405	0.364711046	0.869273782	0.166657656
0.416674644	0.601870000	0.491479248	0.464173734	0.203726739	0.092457585	0.567602754	0.977152705	0.499743998
0.585181296	0.694813848	0.434432060	0.273890108	0.450015426	0.791855812	0.899315894	0.632497668	0.16508132
0.437439382	0.665278971	0.350171751	0.923327506	0.443840265	0.727525949	0.130353242	0.655505180	0.377766252
0.716636777	0.694202304	0.596414328	0.243795291	0.774118066	0.406901926	0.140100539	0.090761371	0.148196205
0.484967619	0.560361803	0.676716208	0.266290396	0.125434086	0.408784926	0.699592352	0.306836605	0.724961817
0.249844566	0.415767908	0.281699479	0.564102709	0.090173393	0.727039456	0.121851340	0.554859519	0.440460563
0.534159184	0.431163758	0.276470304	0.223673299	0.404467613	0.087370709	0.381972849	0.633314133	0.061636101
0.476248235	0.655159593	0.421548218	0.931232035	0.099424899	0.712075055	0.024476215	0.972985506	0.399738252
0.557261050	0.633825898	0.563590288	0.588105917	0.420598626	0.073536023	0.70990677	0.017996583	0.720557928
0.392510146	0.425383985	0.280221760	0.678661942	0.976908088	0.460979134	0.366470665	0.331641048	0.070984602
[Cu(NO₃)⁺ + ads(NO), Fig. 8, E = -970.402 eV								
1.0			0.357084876	0.313024193	0.791851103	0.011546172	0.315391988	0.731768012
13.6750001907	0.00000000000	0.00000000000	0.015173377	0.638827269	0.142477736	0.668387413	0.638426125	0.083369106
-6.8375000954	11.8428975619	0.00000000000	0.717739463	0.658767462	0.783051133	0.917372048	0.117726423	0.473448277
H Al Si O N Cu	12 4 32 76 5 1		0.688628495	0.331787437	0.474285334	0.905808389	0.424675077	0.485357285
Direct			0.391373456	0.998619258	0.153557688	0.559401691	0.732968390	0.793516219
0.286226124	0.168725982	0.465127051	0.490069675	0.802748680	0.937172055	0.243943825	0.066864990	0.128961772
0.724189401	0.825981975	0.404702365	0.881415129	0.750579536	0.383490562	0.922971070	0.760355771	0.159498319
0.172936663	0.388318300	0.191311434	0.140993461	0.621420383	0.274159700	0.799009681	0.892556727	0.77773023
0.047923584	0.337566555	0.247096539	0.597451508	0.789451003	0.084372979	0.794149399	0.519159555	0.784512162
0.152221173	0.466316611	0.271928638	0.541908443	0.941819370	0.603389978	0.803031683	0.549507439	0.095000811
0.157108337	0.350179136	0.306299844	0.145747215	0.131304920	0.251178712	0.445381433	0.849901915	0.099812217
0.763352394	0.782139122	0.592068136	0.858569980	0.586940169	0.269600903	0.133416846	0.219713822	0.424550474
0.734797776	0.671414554	0.656204998	0.089487396	0.240821570	0.596043110	0.492387936	0.883782208	0.777662873
0.768861592	0.670250566	0.546661258	0.714264572	0.548489809	0.937705457	0.146241441	0.185138255	0.078290001
0.399342775	0.516906738	0.663630605	0.393733948	0.856289208	0.271081686	0.807460725	0.545840502	0.442733586
0.507127821	0.503691733	0.698081434	0.535751989	0.217519060	0.602295876	0.590952456	0.105804443	0.482123882
0.507641971	0.622749865	0.717682421	0.231326059	0.306844890	0.930681705	0.141741991	0.228529558	0.766599298
0.243755817	0.534940064	0.045010254	0.880951166	0.894051194	0.259697527	0.456411868	0.888275266	0.442956865
0.702060223	0.770562291	0.825634837	0.074967220	0.474481910	0.602281034	0.481186569	0.220090926	0.772018075
0.129072845	0.108521409	0.365263313	0.705883563	0.768763661	0.940757632	0.801688910	0.879549205	0.423117548
0.803871819	0.991247058	0.498235554	0.394120812	0.157021821	0.261646688	0.136310622	0.536806881	0.768196881
0.249054417	0.324847440	0.822401047	0.795844197	0.932542562	0.603507757	0.809663177	0.859054029	0.093224250
0.693986654	0.542565107	0.046026248	0.206049144	0.523205757	0.932653487	0.475014269	0.204615310	0.432248026
0.363196254	0.877194405	0.372416317	0.470228165	0.292355984	0.932684779	0.154063433	0.557381690	0.114523396
0.378568590	0.117672965	0.365473390	0.424136847	0.594325125	0.483309358	0.462094277	0.203698069	0.093996719
0.895530641	0.640537322	0.370293677	0.591655910	0.695760369	0.426306933	0.271158993	0.450656652	0.793448567
0.475895077	0.772503793	0.829896569	0.440845549	0.658647060	0.343426257	0.920535207	0.442109913	0.727213204
0.476806879	0.766789496	0.044008881	0.479578823	0.446457833	0.284479916	0.241089180	0.7711874666	0.405933678
0.579767704	0.981985211	0.707966447	0.133635268	0.385471284	0.255045235	0.264024764	0.124233924	0.409057558
0.242323548	0.308828592	0.040051330	0.726332188	0.694723666	0.591242194	0.563080549	0.089624166	0.731244504
0.572571576	0.208858669	0.706303349	0.4854819780	0.558653235	0.669642150	0.220188111	0.402229160	0.088036701
0.906382084	0.877103746	0.363209784	0.482288480	0.650320470	0.413804710	0.930189610	0.098170333	0.717379630
0.038598955	0.442891926	0.707929492	0.416270137	0.464132845	0.245744750	0.566276193	0.557843328	0.345013380
0.694393635	0.764494359	0.046987321	0.562289480	0.65032107377	0.557843328	0.673926771	0.9711005082	0.463690788
0.809579730	0.983675480	0.705797136	0.480513378	0.562103169	0.405238558	0.345013380	0.670040488	0.807872117
0.042930223	0.219357520	0.700731814	0.105301417	0.157504424	0.448151214	0.357027680	0.315651029	0.791419268
0.803808331	0.436116397	0.712680578	0.283709701	0.825709701	0.013998079	0.632855535	0.141446903	0.458903963
0.471691936	0.317418903	0.825709701	0.157504424	0.723439455	0.815769017	0.409872323	0.880643308	0.748638928
0.910462379	0.871984959	0.156954482	0.170640856	0.387319207	0.191939771	0.136741921	0.618023875	0.274800688
0.472135961	0.312444270	0.040739056	0.047006052	0.336480558	0.249828443	0.594794512	0.786537468	0.085015304
0.701536894	0.545667794	0.828671634	0.150542125	0.466657102	0.271827191	0.537419438	0.942272425	0.605291128
0.366065979	0.870166540	0.165449753	0.158005372	0.352364451	0.307715088	0.143856257	0.130982429	0.251539379
0.571082354	0.980082929	0.498256773	0.792491853	0.796283960	0.590799391	0.858017862	0.585763633	0.268545270
0.900463760	0.633541882	0.166000679	0.777292669	0.685888469	0.648780942	0.088221949	0.237015858	0.596123517
0.133048862	0.658348203	0.376974881	0.797124684	0.690092921	0.536561131	0.714958666	0.549455822	0.936988083
0.141797259	0.092092201	0.147607535	0.393038392	0.527578712	0.643009424	0.393593907	0.856436431	0.272078484
0.702251554	0.306866765	0.724643111	0.472172064	0.485805899	0.696538150	0.533316612	0.213357106	0.603431642
0.122687049	0.556299686	0.438969582	0.488489509	0.611306489	0.719661295	0.231068924	0.306693047	0.930913448
0.382630676	0.638333738	0.061301690	0.241601720	0.533161163	0.045238558	0.880284190	0.892908990	0.260551691
0.025358675	0.974708796	0.399420440	0.697486699	0.767798066	0.825194061	0.072192076	0.470788270	0.602801025
0.711491227	0.018858882	0.722007334	0.126794368	0.107303470	0.365628749	0.704590857	0.769846499	0.940719843
0.367375731	0.330314398	0.069427647	0.801893353	0.989288867	0.496837258	0.393077731		

-6.8375000954	11.8428975619	0.0000000000	0.704503715	0.653290510	0.781183958	0.913515925	0.117544055	0.470600426
0.0000000000	0.0000000000	14.7670001984	0.024448993	0.973865986	0.124178834	0.228626549	0.780061126	0.151121035
H Al Si O N Cu	12 4 32 76 5 1		0.683342516	0.325407773	0.475690693	0.903962135	0.422483772	0.482656658
Direct			0.390226960	0.997049332	0.153495952	0.554309249	0.731081843	0.795441806
0.281352997	0.169259936	0.463505447	0.794613421	0.474869431	0.607787490	0.241844758	0.063590952	0.132067233
0.717662930	0.813167095	0.401656300	0.480747223	0.797325432	0.940024018	0.919737160	0.758063674	0.153869942
0.166449592	0.384526163	0.191741705	0.878875911	0.746475637	0.386351287	0.574929833	0.436813593	0.804131269
0.043877717	0.331716329	0.251750261	0.132666752	0.614903867	0.275301456	0.794665873	0.888676584	0.776915073
0.145086974	0.464264810	0.270186216	0.592809916	0.784317315	0.084808387	0.795019269	0.524488980	0.781263828
0.158061119	0.353810459	0.307993293	0.532607615	0.940519571	0.607421458	0.798994899	0.545153499	0.095627345
0.811586916	0.802436531	0.598776162	0.139631480	0.130505846	0.251664251	0.442573220	0.847343624	0.101920605
0.842214704	0.708067715	0.642103314	0.856314421	0.586356103	0.267835468	0.131606713	0.217769399	0.426528215
0.811458111	0.702528298	0.532803535	0.074120425	0.230211049	0.596742094	0.492382884	0.885313272	0.780029833
0.432574153	0.555125475	0.609799325	0.716850758	0.552098632	0.935741305	0.144442752	0.182927728	0.076884791
0.446819514	0.475142568	0.687784970	0.592948717	0.856400788	0.273737341	0.804772079	0.542706251	0.441453427
0.478918612	0.605670810	0.713516712	0.531216621	0.212361649	0.604399204	0.589341462	0.103201956	0.482551783
0.239695519	0.531727970	0.045564227	0.230264157	0.306237251	0.930596471	0.142111674	0.230693504	0.765693784
0.691529214	0.766319931	0.825601459	0.458101744	0.888577998	0.260802180	0.452668577	0.885782599	0.445084125
0.123548858	0.105097041	0.365854293	0.704660714	0.770251632	0.940477490	0.475000054	0.217148885	0.770764470
0.798457563	0.985085607	0.495878547	0.393492967	0.154801413	0.263970286	0.131681561	0.534769475	0.769166052
0.246679872	0.326889753	0.822329879	0.803880095	0.937505484	0.602998853	0.807094395	0.860788882	0.095364705
0.692175031	0.540842235	0.043392450	0.200034082	0.524471223	0.934136987	0.473779887	0.202844188	0.433314472
0.358254343	0.874102831	0.374672979	0.485101744	0.284748673	0.933165371	0.153159067	0.557154953	0.115278706
0.373858541	0.114430018	0.367711365	0.517550170	0.674993336	0.484943673	0.459307641	0.203235999	0.099417604
0.890646756	0.635610878	0.369742453	0.610335350	0.716944098	0.354838639	0.270491183	0.453357875	0.794346750
0.467805892	0.769882381	0.832219064	0.42816213	0.593860507	0.359225988	0.916259468	0.439223588	0.729744375
0.471368223	0.760605097	0.045953896	0.535394371	0.5399481878	0.232325703	0.238384619	0.769841194	0.406295508
0.575950980	0.980851114	0.710694075	0.129547909	0.383587927	0.256191194	0.263852298	0.125724599	0.409143865
0.238226548	0.306105137	0.040175252	0.792594552	0.718861818	0.596004784	0.564120114	0.091063462	0.732464015
0.566873610	0.206359565	0.709324777	0.481508613	0.555229664	0.662230372	0.215602994	0.399807215	0.087066069
0.902331471	0.872873425	0.365274101	0.520316303	0.663350707	0.401390433	0.929165363	0.095839895	0.723950326
0.031102695	0.438113898	0.709437490	0.446162790	0.524464786	0.240211189	0.584247530	0.418803573	0.066310853
0.692074597	0.763539493	0.046673715	0.638808727	0.629747272	0.633782983	0.669835329	0.965446949	0.465909421
0.806693852	0.981415689	0.705976069	0.134107507	0.826512337	0.000000000	0.038166158	0.338057935	0.459150434
0.036521740	0.215161845	0.703340650	0.906870782	0.868944347	0.157060891	0.6387500954	0.706966221	0.782827377
0.799093544	0.435297608	0.711861610	0.40720508	0.000000000	14.7670001984	0.024487097	0.974483788	0.124558903
0.465951294	0.314107507	0.826512337	0.794310129	0.129547909	0.383587927	0.684458911	0.325841576	0.476042539
0.697712958	0.543828249	0.827312171	0.144918472	0.463904053	0.268807113	0.389478355	0.997108996	0.152836487
0.363134325	0.868118818	0.168301806	0.158154353	0.353669643	0.306418985	0.140464425	0.131574944	0.251499176
0.563416958	0.974154830	0.501753032	0.809231937	0.801119151	0.598360062	0.858667318	0.587620735	0.267922994
0.896859944	0.630469203	0.163755313	0.823659602	0.702914536	0.642942548	0.074702181	0.231080562	0.596972167
0.127542943	0.652792335	0.378381371	0.813087046	0.703651071	0.532012939	0.718439397	0.552993238	0.936392069
0.138020664	0.089332029	0.148953274	0.421748012	0.547969162	0.616743803	0.392203361	0.857596099	0.273797810
0.694310129	0.308921993	0.272848828	0.451387018	0.476823230	0.691682875	0.531257510	0.210938856	0.603821236
0.120634504	0.553120017	0.441525340	0.482921392	0.607716024	0.714816511	0.229551494	0.306986094	0.930127859
0.380791873	0.630321920	0.062588371	0.239853173	0.532133520	0.045536902	0.880446449	0.888487816	0.261385918
0.022123409	0.970553696	0.400528848	0.692274392	0.766354680	0.826333523	0.067058165	0.468294173	0.603715479
0.707604766	0.015485571	0.719823182	0.126320183	0.107355244	0.365732998	0.704127014	0.771399438	0.941483855
0.363788784	0.330921352	0.071586989	0.800526798	0.989015400	0.497817963	0.393250644	0.153763264	0.263770044
0.019437272	0.669724405	0.393735468	0.247678101	0.328447968	0.822143197	0.804793775	0.939079106	0.603762209
0.007609888	0.312632293	0.732266044	0.691816330	0.541073143	0.043774337	0.200026199	0.524502933	0.934119940
0.669134617	0.638783574	0.081759192	0.358105044	0.874744475	0.375001371	0.456891984	0.283062518	0.932639301
0.342904896	0.985763252	0.378308386	0.375041217	0.114991464	0.367639214	0.056859234	0.648043811	0.473906875
0.913309038	0.114119619	0.470228821	0.891037166	0.635802911	0.369832158	0.603494585	0.727543414	0.348403186
0.228913337	0.780213773	0.151513726	0.468651414	0.770561512	0.832640707	0.414973773	0.568859875	0.331355485
0.903317451	0.421617806	0.824124286	0.471622929	0.761496425	0.046119299	0.523369610	0.517760873	0.252237874
0.553389930	0.730969727	0.794984281	0.576987565	0.981729984	0.710873306	0.129531294	0.383359730	0.254715562
0.241823956	0.064638123	0.132411107	0.238265216	0.306683689	0.039735042	0.78819263	0.717312753	0.593246485
0.919257104	0.757409205	0.154325217	0.567111790	0.206642732	0.709107220	0.480189590	0.554777563	0.663135350
0.574041545	0.436211377	0.803539336	0.907021761	0.874553859	0.365012318	0.521788239	0.663182259	0.393484503
0.794441521	0.887868702	0.776117996	0.031507313	0.438659877	0.709713936	0.432419002	0.506244004	0.263049364
0.794552803	0.524371564	0.780759513	0.691437960	0.763523877	0.047656942	0.632972717	0.628313065	0.624303102
0.799499333	0.545235455	0.094990075	0.807626009	0.982503295	0.707092583	0.132331112	0.457080096	0.568859875
0.442546099	0.846554220	0.101675436	0.037280239	0.216035694	0.703678668	0.288221359	0.183233112	0.457080096
0.131259635	0.216976359	0.426303923	0.799259484	0.435857624	0.712058127	0.726431966	0.809456050	0.422165006
0.491353601	0.8848441919	0.780286968	0.466594398	0.314723253	0.826467097	0.841220856	0.709611893	0.648231149
0.144876242	0.182428747	0.072799755	0.906992793	0.869260907	0.156911984	0.163898930	0.383588761	0.189167008
0.804381669	0.542291641	0.441487491	0.465784072	0.310084666	0.040136278	0.039891243	0.331100583	0.247481570
0.585783541	0.102311313	0.482942343	0.571690798	0.202987539	0.501082182	0.142439723	0.463196516	0.267029494
0.140788466	0.2291185194	0.766208887	0.133708179	0.647185862	0.166829526	0.153457403	0.352198064	0.305002636
0.451875716	0.885829394	0.445345670	0.031142540	0.444385737	0.498897433	0.818261147	0.808307886	0.602927625
0.474940628	0.216488019	0.771705329	0.370260984	0.103519872	0.159213960	0.692164898	0.769442439	0.826496780
0.797366202	0.875661612	0.422155827	0.236456454	0.547264874	0.830783129	0.125917032	0.108748026	0.364508331
0.131399736	0.534236133	0.768855810						

[Cu(NO ₂) ⁺ (Nitrite), Fig. 8, E = -994.652 eV]						
1.0						
13.6750001907	0.0000000000	0.0000000000	0.808706880	0.895575225	0.412252009	
-6.8375000954	11.8428975619	0.0000000000	0.132282645	0.536697924	0.771506429	
0.0000000000	0.0000000000	14.7670001984	0.806741416	0.859483242	0.096446522	
H	Al	Si	O	N	Cu	
18	4	32	74	6	1	
Direct						
0.164682448	0.374404013	0.192701265	0.010052480	0.623819888	0.148598179	
0.038686968	0.323827565	0.245547205	0.045047347	0.345087141	0.466591448	
0.146090925	0.445652425	0.280308664	0.054507221	0.779451132		
0.141590357	0.3212949487	0.303800792	0.022186752	0.980228841	0.129676551	
0.815513790	0.810075402	0.606175661	0.692214310	0.320675373	0.476813793	
0.849793494	0.715090096	0.644150615	0.388734519	0.995868325	0.149637774	
0.817213118	0.716468751	0.535163224	0.800717652	0.479526073	0.603374243	
0.426854759	0.546762824	0.630032599	0.487799287	0.805592954	0.944651961	
0.464404434	0.490481466	0.712495148	0.883720338	0.752129316	0.405893952	
0.0911464311	0.147488251	0.489783049	0.142806605	0.619704247	0.277929634	
0.615816176	0.800209701	0.621992111	0.592609406	0.781503618	0.091158547	
0.690524578	0.383923961	0.344216257	0.535158038	0.930722058	0.609354973	
0.562939644	0.720587254	0.336659163	0.143934667	0.145409569	0.247764274	
0.571345806	0.846565425	0.330146909	0.856451273	0.613192141	0.265689613	
0.294720948	0.205477175	0.500244796	0.087694995	0.232128382	0.594628930	
0.232204616	0.247213766	0.580201805	0.723041415	0.559578121	0.933491588	
0.345488340	0.233671874	0.609489918	0.392301261	0.860300362	0.276338398	
0.362940437	0.339168996	0.541016996	0.529586563	0.223652989	0.600287676	
0.239487290	0.529588163	0.046550393	0.234621748	0.311409324	0.927959323	
0.692600489	0.727233927	0.826804578	0.874036491	0.856055260	0.259716541	
0.117232554	0.467701346	0.135869280	0.068430901	0.481969297	0.605169356	
0.227682859	0.7979855132	0.150741756	0.700836360	0.770414829	0.942040265	
0.019216128	0.669781268	0.393754452	0.402204871	0.156753540	0.261055201	
0.008969092	0.316204011	0.732203901	0.798934162	0.935729742	0.602407098	
0.670075357	0.640629530	0.083295271	0.199164808	0.521504045	0.934918582	
0.340568274	0.986679912	0.380360007	0.453200400	0.281316191	0.929808686	
0.912628829	0.117232554	0.467701346	0.443445683	0.496440887	0.482320845	
0.362139851	0.3299498857	0.068147637	0.601218462	0.655881584	0.501772761	
0.019216128	0.669781268	0.393754452	0.124092035	0.366489828	0.256430835	
0.008969092	0.316204011	0.732203901	0.798934162	0.727313459	0.600554407	
0.670075357	0.640629530	0.083295271	0.199164808	0.563460648	0.677536786	
0.574447751	0.436693609	0.804118514	0.443445683	0.590696216	0.453699321	
0.797923625	0.889935738	0.776544213	0.610162793	0.801618516	0.311713874	
0.794814527	0.529264867	0.779342890	0.377333492	0.309083283	0.559017181	
0.798014939	0.544684052	0.094813712	0.641027072	0.637605220	0.637605220	
0.442281753	0.847451746	0.102752492	0.181072061	0.801618516	0.311713874	
0.131037891	0.218567058	0.426003784	0.568103313	0.703193188	0.309083283	
0.488028586	0.888026595	0.780166328	0.904936969	0.875047483	0.641249180	
0.142842606	0.183387950	0.075678751	0.032336261	0.709455132	0.633736193	
0.803602219	0.543196082	0.440520734	0.692161381	0.761915803	0.048700146	
0.589498341	0.104227677	0.482427269	0.8067799623	0.784226777	0.704595559	
0.142655894	0.232220501	0.763697863	0.039402314	0.218816057	0.699412644	
0.450727016	0.887521148	0.446113527	0.800962090	0.440542489	0.708196700	
0.474165976	0.217253625	0.769056082	0.466566741	0.314284652	0.824532926	
0.801076353	0.878596246	0.424588650	0.909675419	0.865170181	0.154236034	
0.132735357	0.537942946	0.768596411	0.466474921	0.308533731	0.037644107	
0.807267487	0.862498283	0.094451509	0.570832729	0.211667746	0.498611093	
0.474232107	0.204048485	0.432047814	0.135430291	0.645587444	0.169938296	
0.151999801	0.557044327	0.114388488	0.037123736	0.452939481	0.499895543	
0.460393995	0.204280391	0.093273222	0.371021360	0.103695214	0.1592225345	
0.270460755	0.454784125	0.793049216	0.237825960	0.550038517	0.832496285	
0.916409671	0.442124844	0.730393291	0.801257133	0.441636323	0.498579443	
0.237504736	0.770272732	0.405750930	0.034681343	0.222933054	0.490342945	
0.264960855	0.130047277	0.406420469	0.697896898	0.547571003	0.825784564	
0.567627072	0.094842359	0.731198251	0.361321539	0.868569610	0.169979730	
0.215708315	0.400401682	0.086269606	0.561863363	0.972064078	0.501469822	
0.927946866	0.099016026	0.726131260	0.899949491	0.636238217	0.160245314	
0.583176196	0.420311213	0.063389547	0.130177453	0.657687724	0.379102856	
0.669026434	0.966494143	0.466350734	0.140035987	0.094122738	0.149021000	
0.343114346	0.673505247	0.809420347	0.694653392	0.314609349	0.724154294	
0.357978106	0.322297305	0.789851487	0.129952937	0.561878204	0.443830907	
0.010630759	0.630483925	0.140467733	0.380771905	0.630477548	0.059457239	
0.036921650	0.338353574	0.459465146	0.031791802	0.972839594	0.386696130	
0.699939072	0.654015243	0.779708564	0.708859384	0.018973924	0.724294424	
0.024484182	0.974871218	0.124789625	0.367352277	0.333618164	0.069088787	
0.685184299	0.326945543	0.474996626	0.016696658	0.665520966	0.390425086	
0.387901723	0.996757209	0.150458604	0.009629129	0.316856742	0.723422647	
0.795294881	0.478020787	0.607171476	0.669216990	0.636804938	0.081736282	
0.483066708	0.803221345	0.940527439	0.351136465	0.995598733	0.382046044	
0.880712569	0.748551965	0.390011132	0.906221867	0.124866776	0.485378861	
0.132539824	0.615921140	0.274735063	0.228159492	0.779038668	0.150988087	
0.592578351	0.785957469	0.085203357	0.911219299	0.430242211	0.477842599	
0.534308672	0.942101777	0.607631385	0.556623280	0.743454594	0.795488477	
0.140290961	0.132698134	0.250274390	0.240747899	0.063821167	0.135894328	
0.856754839	0.591360509	0.267341197	0.931360245	0.761934946	0.128624931	
0.071167573	0.229723006	0.596173286	0.574705780	0.437145442	0.804290771	
0.718566239	0.557579167	0.935191989	0.798205197	0.892641425	0.776424825	
0.391747981	0.859380007	0.273802341	0.794025779	0.531355500	0.774206161	
0.532788515	0.213318288	0.602710009	0.800388038	0.544151127	0.095464744	
0.227962717	0.307568818	0.928754449	0.443992972	0.843729436	0.109427899	
0.878040409	0.884446800	0.260892093	0.119467124	0.213808253	0.419354647	
0.066333697	0.470502585	0.603618503	0.491881520	0.895014584	0.785722789	
0.703983903	0.770840943	0.941211998	0.148682714	0.180685014	0.069532178	
0.394535214	0.153485164	0.262477160	0.800269604	0.537384331	0.434051245	
0.806198299	0.942924023	0.604344368	0.578964770	0.098629601	0.493162692	
0.199125633	0.524158180	0.933581114	0.142852694	0.235121280	0.764584661	
0.456228048	0.281269699	0.931348383	0.450450748	0.883139789	0.446149558	
0.383102417	0.549885571	0.304602861	0.474496001	0.217841983	0.767798185	

0.465334088	0.308249712	0.039350905	H	Al	Si	O	N	Cu	0.343948781	0.672597945	0.807856143
0.571534097	0.211961463	0.499059469	18	4	32	74	6	1	0.355632639	0.318100959	0.788101375
0.134678438	0.647686839	0.167416811	Direct						0.006846699	0.624400914	0.157536253
0.034026645	0.448775977	0.499487817	0.165143937	0.376494557	0.194384426	0.043961097	0.345562786	0.466755569			
0.370144337	0.103912435	0.161577240	0.040622015	0.326676071	0.249413520	0.712575138	0.660008907	0.789209783			
0.237705052	0.547223747	0.832439721	0.148323819	0.449921787	0.281255007	0.018016869	0.981124580	0.128662767	0.05467724	0.157536253	
0.799242735	0.440267414	0.500694752	0.145425409	0.326573133	0.306436986	0.690967083	0.320705026	0.479701340			
0.0353349518	0.219568082	0.490679592	0.763600111	0.796975315	0.592935622	0.382155955	0.993403463	0.150467724			
0.699855626	0.545858681	0.828713477	0.762859344	0.688109876	0.646849334	0.796540916	0.479320437	0.606332779			
0.364309847	0.869691491	0.169369519	0.784793615	0.703770459	0.533052266	0.479333669	0.798192382	0.944377184			
0.566238284	0.974904180	0.502703190	0.399632335	0.526069045	0.675514042	0.885425351	0.752891113	0.413329780			
0.8996654625	0.632546425	0.162738830	0.500495732	0.506016314	0.716436803	0.144803569	0.616463721	0.278744161			
0.129649743	0.655447423	0.379323304	0.507834613	0.629123330	0.730410635	0.590314150	0.781761825	0.090062924			
0.138694137	0.090387985	0.149573731	0.630748034	0.824102104	0.226883054	0.536540866	0.929888070	0.607575476			
0.695629537	0.307117343	0.729208589	0.701512277	0.854916513	0.331676424	0.137917817	0.142735809	0.250851721			
0.125709638	0.554455221	0.439506203	0.573178232	0.741255999	0.318475395	0.850309968	0.617585301	0.268465221			
0.379893392	0.633044243	0.059341315	0.587028801	0.869192481	0.317178696	0.088192619	0.233988479	0.595647931			
0.027481817	0.971123219	0.379579581	0.292855054	0.203074917	0.500526786	0.712893486	0.543832302	0.938174427			
0.709171295	0.021287965	0.726151645	0.230151787	0.243600428	0.581794739	0.390612274	0.858874738	0.275558482			
0.364416689	0.331376374	0.068704829	0.348428696	0.236774698	0.608362377	0.525000215	0.220645994	0.601373374			
0.022342760	0.671945155	0.399358690	0.356573403	0.337262332	0.538071334	0.230009809	0.309629947	0.929238856			
0.011957223	0.316129118	0.721504331	0.237088114	0.530364275	0.048757069	0.884769976	0.585542621	0.265859842			
0.669030607	0.637148380	0.083404176	0.699753702	0.773341715	0.830911577	0.070704363	0.479908109	0.607284248			
0.348743469	0.989412665	0.376701117	0.135245144	0.111136809	0.365556901	0.713113725	0.783357084	0.946424127			
0.908770323	0.118584618	0.482415199	0.797154605	0.987319648	0.491029024	0.400517553	0.157210037	0.260539830			
0.230912089	0.780600727	0.152163044	0.246727332	0.328051567	0.821522892	0.788082719	0.934041440	0.600685239			
0.907388270	0.425492048	0.479389280	0.690726161	0.537080467	0.046515267	0.206945792	0.524901927	0.953126428			
0.555977166	0.735406220	0.794748008	0.356343031	0.880760372	0.376476228	0.462590754	0.292455524	0.931824327			
0.241444573	0.063838206	0.132750571	0.372767657	0.123165253	0.366609663	0.417245984	0.47719204	0.456455618			
0.921955228	0.758475552	0.146250337	0.888600171	0.643504977	0.373805791	0.567596972	0.644346952	0.447989792			
0.574880421	0.437951773	0.804307044	0.470061034	0.773677588	0.836006463	0.126292452	0.370125234	0.258751243			
0.796654403	0.893313169	0.779703081	0.468782872	0.760486186	0.050244808	0.741925120	0.711797118	0.587016881			
0.973774605	0.523643017	0.779536843	0.575959802	0.981192350	0.709595740	0.485298961	0.563284039	0.683481634			
0.798448145	0.543021381	0.098526858	0.237860054	0.306951374	0.039233748	0.476587743	0.562965572	0.411363720			
0.445562065	0.848904371	0.103624113	0.564780474	0.208365634	0.704004747	0.623617053	0.822932839	0.296819597			
0.123937085	0.214978546	0.421010107	0.908113480	0.876261878	0.374177694	0.307261944	0.254921049	0.558842123			
0.491554976	0.888007998	0.781615674	0.031497255	0.441271454	0.711047709	0.578592360	0.625334382	0.577134192			
0.145509422	0.181877509	0.075469881	0.692608893	0.763476670	0.051527567						
0.051520342	0.542066455	0.434969041	0.804092109	0.983747900	0.703310847						
0.584945917	0.102018550	0.492766500	0.038576744	0.216795281	0.700182557						
0.142808884	0.231607333	0.764791310	0.798348069	0.435934424	0.709727407						
0.455575436	0.886498213	0.444152385	0.467559427	0.317857146	0.825440168						
0.474919558	0.218178347	0.768040061	0.909668386	0.865319550	0.158640265						
0.801371217	0.883631229	0.418663621	0.464954734	0.309679240	0.040729593						
0.133643702	0.535126626	0.770142376	0.569605809	0.211462423	0.499870092						
0.050757084	0.859898984	0.097367935	0.132132180	0.642795146	0.171399400						
0.474680424	0.204054385	0.431539476	0.3036486205	0.452953160	0.502203822						
0.155266091	0.557193279	0.117474765	0.365890563	0.101991825	0.159443155						
0.457570285	0.201070011	0.092973329	0.238517076	0.547858953	0.831427813						
0.273335516	0.454875469	0.793466747	0.799756289	0.441969991	0.501758933						
0.916688740	0.438498914	0.732226372	0.035200585	0.224351719	0.491467148						
0.241546452	0.771612108	0.405737936	0.698810160	0.545716822	0.82944587						
0.261025876	0.121315747	0.409557879	0.358793318	0.867369056	0.169442952						
0.557766378	0.088759899	0.721322417	0.561141968	0.972256958	0.502565503						
0.216429248	0.399080276	0.087668508	0.896849990	0.637356818	0.163992375						
0.929354846	0.097301997	0.717453003	0.129332364	0.656557679	0.378695667						
0.583812535	0.417512596	0.065832071	0.135423332	0.094135217	0.151185587						
0.671750844	0.973035157	0.459118247	0.693715632	0.307843775	0.721744835						
0.341593981	0.674282908	0.815022409	0.128160015	0.563032448	0.446453641						
0.356927216	0.318774879	0.7879715051	0.376442760	0.632014930	0.068832852						
0.013580435	0.631522655	0.137720077	0.033245573	0.975196064	0.397023320						
0.041532606	0.339990503	0.468704049	0.708935857	0.022362554	0.723101854						
0.709284902	0.657427907	0.786953688	0.363424122	0.332083255	0.069166332						
0.024211377	0.975334585	0.124316841	0.014796677	0.662899613	0.386286467						
0.688063860	0.324082673	0.471367955	0.008746154	0.314164668	0.726220489						
0.391217202	0.997924924	0.155098051	0.667435765	0.636653125	0.080962926						
0.794659913	0.470388174	0.606631935	0.351519429	0.996204853	0.381032321						
0.490494370	0.804981768	0.942166567	0.906762803	0.125886217	0.485547125						
0.881240070	0.749146163	0.391777337	0.226480052	0.775009274	0.150225282						
0.131505981	0.617942691	0.275815815	0.909988105	0.430289209	0.482924312						
0.592188120	0.782711089	0.092495218	0.560190141	0.737720847	0.802272394						
0.539786750	0.932570755	0.607244611	0.235357887	0.063115440	0.137643307						
0.140001401	0.133867726	0.250879914	0.930519879	0.762732625	0.128948495						
0.865239501	0.596231878	0.268716127	0.493674714	0.888703227	0.783378482						
0.087959424	0.228686020	0.595129788	0.796352625	0.892866492	0.774646819						
0.591799197	0.551071882	0.937366247	0.791020453	0.521212181	0.780837655						
0.396618873	0.834564243	0.274424940	0.798603535	0.098382987	0.493729770						
0.534680247	0.224720955	0.601796210	0.444747955	0.848573506	0.107565656						
0.229837418	0.307646185	0.929466426	0.121751569	0.216363835	0.421949655						
0.878376722	0.881307662	0.261219293	0.493674714	0.888703227	0.783378482						
0.069085270	0.482280105	0.603825808	0.144576937	0.182064250	0.072976619						
0.698707402	0.770943820	0.943410575	0.799531579	0.536773993	0.435418755						
0.394563079	0.156210363	0.264061689	0.576967418	0.098382987	0.493729770						
0.792419553	0.935086548	0.604746163	0.140149608	0.229462862	0.766048133						
0.197625756	0.518541873	0.934689820	0.449360669	0.882993221	0.445240408						
0.456342131	0.281788141	0.931386828	0.476573634	0.219706789	0.771049500						
0.633064568	0.355434343	0.272639394	0.808								

Cu ²⁺ + NH ₄ NO ₂ , Fig. 8, E = -992.319 eV						
1.0						
13.6750001907						0.0000000000
-6.8375000954						0.0000000000
0.0000000000						14.7670001984
H	Al	Si	O	N	Cu	
18	4	32	74	6	1	
Direct						
0.156795621		0.372668803		0.190034077		
0.030992547		0.321534663		0.243919626		
0.138812765		0.444654912		0.277453423		
0.135854825		0.320787936		0.300563782		
0.821990430		0.823290229		0.603348494		
0.868497483		0.737836063		0.643085897		
0.826370060		0.727399170		0.535583436		
0.452930313		0.570033431		0.614922106		
0.467924983		0.496378988		0.698857844		
0.496979088		0.627618730		0.718077064		
0.533411894		0.455635875		0.277998775		
0.644486833		0.586256623		0.286441058		
0.422930866		0.684396744		0.305913270		
0.544135571		0.557746232		0.210925639		
0.288984325		0.198088199		0.498240590		
0.223408058		0.235550433		0.581204951		
0.337152302		0.220947459		0.609471142		
0.354309589		0.328514129		0.545465529		
0.237094924		0.530808926		0.048847828		
0.693725705		0.775515139		0.830350697		
0.135947838		0.111492850		0.361221761		
0.796712637		0.984794021		0.493767053		
0.248579234		0.333231807		0.819745123		
0.694104791		0.540730834		0.042212013		
0.355213225		0.880145490		0.376385659		
0.372918069		0.123207532		0.365754694		
0.889263809		0.641159356		0.370694965		
0.465784818		0.775200486		0.834690034		
0.466801375		0.759499729		0.050746508		
0.574202836		0.983145773		0.710659564		
0.241179943		0.309115052		0.037893623		
0.372918069		0.123207532		0.365754694		
0.889263809		0.641159356		0.370694965		
0.465784818		0.775200486		0.834690034		
0.466801375		0.759499729		0.050746508		
0.574202836		0.983145773		0.710659564		
0.241179943		0.309115052		0.037893623		
0.372918069		0.123207532		0.365754694		
0.889263809		0.641159356		0.370694965		
0.465784818		0.775200486		0.834690034		
0.466801375		0.759499729		0.050746508		
0.574202836		0.983145773		0.710659564		
0.241179943		0.309115052		0.037893623		
0.372918069		0.123207532		0.365754694		
0.889263809		0.641159356		0.370694965		
0.465784818		0.775200486		0.834690034		
0.466801375		0.759499729		0.050746508		
0.574202836		0.983145773		0.710659564		
0.241179943		0.309115052		0.037893623		
0.372918069		0.123207532		0.365754694		
0.889263809		0.641159356		0.370694965		
0.465784818		0.775200486		0.834690034		
0.466801375		0.759499729		0.050746508		
0.574202836		0.983145773		0.710659564		
0.241179943		0.309115052		0.037893623		
0.372918069		0.123207532		0.365754694		
0.889263809		0.641159356		0.370694965		
0.465784818		0.775200486		0.834690034		
0.466801375		0.759499729		0.050746508		
0.574202836		0.983145773		0.710659564		
0.241179943		0.309115052		0.037893623		
0.372918069		0.123207532		0.365754694		
0.889263809		0.641159356		0.370694965		
0.465784818		0.775200486		0.834690034		
0.466801375		0.759499729		0.050746508		
0.574202836		0.983145773		0.710659564		
0.241179943		0.309115052		0.037893623		
0.372918069		0.123207532		0.365754694		
0.889263809		0.641159356		0.370694965		
0.465784818		0.775200486		0.834690034		
0.466801375		0.759499729		0.050746508		
0.574202836		0.983145773		0.710659564		
0.241179943		0.309115052		0.037893623		
0.372918069		0.123207532		0.365754694		
0.889263809		0.641159356		0.370694965		
0.465784818		0.775200486		0.834690034		
0.466801375		0.759499729		0.050746508		
0.574202836		0.983145773		0.710659564		
0.241179943		0.309115052		0.037893623		
0.372918069		0.123207532		0.365754694		
0.889263809		0.641159356		0.370694965		
0.465784818		0.775200486		0.834690034		
0.466801375		0.759499729		0.050746508		
0.574202836		0.983145773		0.710659564		
0.241179943		0.309115052		0.037893623		
0.372918069		0.123207532		0.365754694		
0.889263809		0.641159356		0.370694965		
0.465784818		0.775200486		0.834690034		
0.466801375		0.759499729		0.050746508		
0.574202836		0.983145773		0.710659564		
0.241179943		0.309115052		0.037893623		
0.372918069		0.123207532		0.365754694		
0.889263809		0.641159356		0.370694965		
0.465784818		0.775200486		0.834690034		
0.466801375		0.759499729		0.050746508		
0.574202836		0.983145773		0.710659564		
0.241179943		0.309115052		0.037893623		
0.372918069		0.123207532		0.365754694		
0.889263809		0.641159356		0.370694965		
0.465784818		0.775200486		0.834690034		
0.466801375		0.759499729		0.050746508		
0.574202836		0.983145773		0.710659564		
0.241179943		0.309115052		0.037893623		
0.372918069		0.123207532		0.365754694		
0.889263809		0.641159356		0.370694965		
0.465784818		0.775200486		0.834690034		
0.466801375		0.759499729		0.050746508		
0.574202836		0.983145773		0.710659564		
0.241179943		0.309115052		0.037893623		
0.372918069		0.123207532		0.365754694		
0.889263809		0.641159356		0.370694965		
0.465784818		0.775200486		0.834690034		
0.466801375		0.759499729		0.050746508		
0.574202836		0.983145773		0.710659564		
0.241179943		0.309115052		0.037893623		
0.372918069		0.123207532		0.365754694		
0.889263809		0.641159356		0.370694965		
0.465784818		0.775200486		0.834690034		
0.466801375		0.759499729		0.050746508		
0.574202836		0.983145773		0.710659564		
0.241179943		0.309115052		0.037893623		
0.372918069		0.123207532		0.365754694		
0.889263809		0.641159356		0.370694965		
0.465784818		0.775200486		0.834690034		
0.466801375		0.759499729		0.050746508		
0.574202836		0.983145773		0.710659564		
0.241179943		0.309115052		0.037893623		
0.372918069		0.123207532		0.365754694		
0.889263809		0.641159356		0.370694965		
0.465784818		0.775200486		0.834690034		
0.466801375		0.759499729		0.050746508		
0.574202836		0.983145773		0.710659564		
0.241179943		0.309115052		0.037893623		
0.372918069		0.123207532		0.365754694		
0.889263809		0.641159356		0.370694965		
0.465784818		0.775200486		0.834690034		
0.466801375		0.759499729		0.050746508		
0.574202836		0.983145773		0.710659564		
0.241179943		0.309115052		0.037893623		
0.372918069		0.123207532		0.365754694		
0.889263809		0.641159356		0.370694965		
0.465784818		0.775200486		0.834690034		
0.466801375		0.759499729		0.050746508		
0.574202836		0.983145773		0.710659564		
0.241179943		0.309115052		0.037893623		
0.372918069		0.123207532		0.365754694		
0.889263809		0.641159356		0.370694965		
0.465784818		0.775200486		0.834690034		
0.466801375		0.759499729		0.050746508		
0.574202836		0.983145773		0.710659564		
0.241179943		0.309115052		0.037893623		
0.372918069		0.123207532		0.365754694		
0.8						

0.573789123	0.441323459	0.804512739	0.467353880	0.777099729	0.832172096	0.125563368	0.370284855	0.253180355
0.795566663	0.895569444	0.778812110	0.471343189	0.763449750	0.044972256	0.834235907	0.750790358	0.615704119
0.793068290	0.529916525	0.774285376	0.575134158	0.982735574	0.709137499	0.510467112	0.580959141	0.666666925
0.801028848	0.546803355	0.095649235	0.239205182	0.307465076	0.036733333	0.295006573	0.226004273	0.567524195
0.443553603	0.849588694	0.105484046	0.567018628	0.211108282	0.702838480	0.649772882	0.657024264	0.492547840
0.117479242	0.210904047	0.422269613	0.902098656	0.876026630	0.368535697	0.535110474	0.617202520	0.469837546
0.492725044	0.893819988	0.786849976	0.031819206	0.445414096	0.705058813	0.671926677	0.657103419	0.636103630
0.149279997	0.181837678	0.068204723	0.691122890	0.762935400	0.046411358			
0.800207200	0.536541164	0.434495424	0.803653777	0.986154795	0.708561659			
0.577146888	0.097894348	0.493490428	0.037874613	0.218043700	0.698431194			
0.140589252	0.231961146	0.767589808	0.799177766	0.437883139	0.708205581			
0.446118593	0.883558631	0.44747481334	0.464231461	0.315358073	0.822818160			
0.473656833	0.221135274	0.766694427	0.904038668	0.870655835	0.163109139			
0.820528090	0.895031929	0.427278555	0.465646654	0.309829652	0.036868822			
0.127019227	0.535136580	0.776567400	0.570793092	0.210689366	0.496687949			
0.803221524	0.857116342	0.101306982	0.133584842	0.648903489	0.163533956			
0.481403023	0.212020174	0.426270634	0.032447066	0.449440092	0.496717095			
0.141483411	0.550743043	0.111295126	0.368475497	0.104234599	0.15835975			
0.451938510	0.198459849	0.088071883	0.237748161	0.547972858	0.828510106			
0.269786209	0.456536859	0.788203180	0.798138499	0.441146851	0.497189462			
0.912735224	0.437785536	0.732287824	0.032427981	0.218164694	0.490519044			
0.231056392	0.777878603	0.405321538	0.695790946	0.546948612	0.823396478			
0.268669397	0.136346892	0.402312279	0.361991614	0.870515227	0.167032763			
0.558518946	0.093094915	0.720843732	0.564876556	0.973347843	0.500416279			
0.213202566	0.397479594	0.087251812	0.899229109	0.634967148	0.162829518			
0.927409410	0.100147821	0.719604850	0.128788933	0.653144658	0.375894070			
0.587502301	0.415797561	0.059446283	0.137728870	0.095558479	0.148840621			
0.667221606	0.969984353	0.464955568	0.693875134	0.312106311	0.726448774			
0.340783030	0.676145852	0.802722454	0.125468493	0.550713539	0.434268624			
0.357917517	0.325243920	0.782986939	0.380744755	0.632721841	0.056567188			
0.006684371	0.624637306	0.160679772	0.030202968	0.972725928	0.385983437			
0.047996677	0.346233517	0.470825732	0.706241131	0.020419532	0.730038583			
0.703792095	0.659266233	0.781653225	0.365256131	0.333418816	0.066692941			
0.017368734	0.983771503	0.133097306	0.018308302	0.664030790	0.398487806			
0.691848695	0.320314705	0.476890087	0.009322230	0.317963302	0.715495288			
0.382402509	0.994086206	0.150844514	0.662049949	0.635711133	0.078743190			
0.798993766	0.479106873	0.603672206	0.342234462	0.988586426	0.379590273			
0.470884323	0.791188240	0.943629622	0.905522346	0.117296025	0.484868318			
0.891411331	0.752618253	0.409608185	0.228464141	0.781707704	0.148568645			
0.150989398	0.617234886	0.276500612	0.906455815	0.427804619	0.474493980			
0.589436233	0.781536281	0.085021108	0.557946086	0.743564367	0.793249249			
0.532031119	0.930536926	0.609763622	0.239076227	0.066637695	0.133123621			
0.144802645	0.151951611	0.247686744	0.924143255	0.763283908	0.159800351			
0.844491243	0.613237739	0.266522020	0.571032643	0.439915061	0.800031066			
0.087353103	0.229968649	0.596864522	0.800486803	0.895497918	0.778945982			
0.723391652	0.559188306	0.934137285	0.791655004	0.530077398	0.772394896			
0.386426121	0.855682909	0.275233150	0.801266968	0.553801239	0.092177227			
0.528450131	0.224251360	0.599634886	0.442159295	0.847508013	0.102121845			
0.237682760	0.316868991	0.927877605	0.119375348	0.214012116	0.419323832			
0.873490930	0.855331004	0.264759213	0.486090481	0.890088797	0.779347003			
0.069539964	0.485849261	0.607200563	0.144827679	0.181690082	0.069177948			
0.707955182	0.771653354	0.940464796	0.800116837	0.543515980	0.438468844			
0.401937515	0.159296945	0.260002017	0.588360667	0.103130125	0.492024928			
0.792697251	0.936922491	0.605569780	0.138898611	0.233028024	0.765541017			
0.212783009	0.529655874	0.934529722	0.450337172	0.887915492	0.445854187			
0.451661259	0.283614427	0.928712428	0.473906487	0.219120890	0.765925884			
0.399830192	0.638748464	0.361780196	0.810958028	0.877316296	0.437151879			
0.491849363	0.617887914	0.471280277	0.132057801	0.535290897	0.768010139			
0.116551772	0.365115464	0.253971964	0.807021916	0.856956422	0.094472140			
0.811001599	0.741729021	0.601249278	0.475189418	0.203271106	0.428428024			
0.501313448	0.574434249	0.669342697	0.153855070	0.559153736	0.111982860			
0.504499078	0.664515257	0.399937183	0.456371963	0.202040136	0.089938998			
0.559905350	0.539239287	0.274320006	0.273488492	0.456115991	0.788549840			
0.300885289	0.245183125	0.560044706	0.915438712	0.441915661	0.731889665			
0.661144018	0.649914742	0.645855784	0.237937987	0.770276606	0.404417485			
0.212783009	0.529655874	0.280867262	0.263013005	0.128944427	0.404152006			
0.559292669	0.777709958	0.092597298	0.719781995	0.215856748	0.399728626	0.084624238		
0.0	13.6750001907	0.0000000000	0.0000000000	0.927095652	0.099924669	0.718290448		
-6.837500954	11.8428975619	0.0000000000	0.0000000000	0.587309182	0.417659193	0.059035946		
0.0000000000	14.7670001984			0.668371439	0.965898573	0.458446625		
H	Al	Si	O	N	Cu			
18	4	32	74	6	1			
direct								
0.165579349	0.378908098	0.188752890	0.037318297	0.338124245	0.470901728			
0.040010318	0.324271411	0.243528932	0.701117456	0.657751560	0.776052415			
0.145094514	0.448945612	0.276619166	0.019874087	0.979936957	0.133014828			
0.146755859	0.327612966	0.299988627	0.686919808	0.324494898	0.470628291			
0.843075991	0.830893695	0.611794174	0.387244314	0.997598866	0.147977874			
0.876950443	0.746139169	0.670772195	0.795955658	0.474280894	0.603069365			
0.865999877	0.735386089	0.557935119	0.483152092	0.804638386	0.939294040			
0.454816580	0.571672082	0.616714895	0.8861117578	0.749817729	0.385957927			
0.482856631	0.504742265	0.698059916	0.130630448	0.618510425	0.271730244			
0.509648263	0.636010528	0.715937436	0.594091415	0.788326979	0.081416458			
0.655481100	0.796038628	0.280867262	0.541263819	0.934356451	0.606399655			
0.593600452	0.818934679	0.356331795	0.143969268	0.148599684	0.247424647			
0.283093601	0.183087766	0.503592491	0.861652315	0.587524772	0.266810030			
0.221754596	0.228731468	0.583295584	0.086347088	0.226401404	0.594459236			
0.314480722	0.187702566	0.618495286	0.718381464	0.557737887	0.931059420			
0.361645520	0.306284547	0.560049772	0.391906828	0.861155510	0.272859991			
0.701337032	0.741395354	0.470337629	0.532521784	0.224286735	0.599195421			
0.677689672	0.604223967	0.467893064	0.233151451	0.311456233	0.926640034			
0.239967734	0.532131732	0.043582290	0.863221049	0.881550431	0.264518559			
0.693700612	0.774868906	0.826629281	0.064952485	0.487520933	0.600971401			
0.1338767905	0.110448472	0.361080974	0.706676960	0.769516766	0.939854443			
0.795272708	0.979951262	0.495765418	0.396997899	0.154841587	0.261265010			
0.247903258	0.331052393	0.819122851	0.787728190	0.933758318	0.607659042			
0.691750407	0.542869210	0.039907037	0.200523809	0.519993424	0.931136966			
0.357051611	0.878225088	0.374190688	0.454918116	0.284207046	0.928300560			
0.367468089	0.116905652	0.366399109	0.588514745	0.757961333	0.318337709			
0.893386424	0.637788355	0.368692726	0.482755542	0.515981019	0.455193877			