

Supporting Information for

Informing our Understanding of the Copper-Cuprizone Reaction with Computational Chemistry

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Table S1. Thermodynamic parameters for all geometry-optimized structures.

Name	$E_{(g)}$ (<i>har</i>)	ZPE^{sc} (<i>kJ/mol</i>)	H^{corr} (<i>har</i>)	$H^{298}_{(g)}$ (<i>har</i>)	$S_{(g)}$ (<i>J/mol * K</i>)	$\Delta G_{(solv)}(1M)$ (<i>kJ/mol</i>)	$G^{298}_{(aq)}$ (<i>har</i>)
H^+ ^a	0	0	0	0.00236	82.3	-1112.5	-0.430708
H2O	-76.42325	55.9	0.02542	-76.39818	162.0	-16.4 ^b	-76.422838
OH-	-75.78672	22.8	0.01212	-75.77474	145.6	-1533.8 ^b	-76.375468
CuII_OH2_5	-2021.96984	324.7	0.14126	-2021.83060	461.5	-978.5	-2022.255684
CuI_OH2_2	-1793.05390	124.7	0.05513	-1792.99953	288.9	-328.0	-1793.157255
CPZ (Fig 1) [1]	-915.85673	928.6	0.37962	-915.48286	600.7	-138.0	-915.603637
CPZ_step2c (CPZ + OH ⁻ , Fig 3)	-991.72422	966.8	0.39488	-991.33533	591.0	-310.6	-991.520754
CPZ_step1 (CPZ + H ⁺ , Fig 3)	-916.22828	961.3	0.39258	-915.84166	599.8	-372.2	-916.051536
CPZ_step4b (CPZmh, Fig 1) [2]	-682.50816	604.4	0.24906	-682.26285	480.8	-151.4	-682.375115
CPZ_step4a (C ₆ H ₁₀ O, Fig 3)	-309.77256	387.7	0.15753	-309.61744	307.2	-39.3	-309.667290
CuII_CPZ_OH2_4_Geom1 (Fig 4) [3]	-2861.50487	1191.4	0.49484	-2861.01740	850.0	-877.0	-2861.447977
CuII_CPZ_OH2_5_Geom2b (Fig 4)	-2937.94278	1257.6	0.52265	-2937.42792	904.5	-864.2	-2937.859787
CuII_CPZ_OH2_3_Step2c (Fig 4)	-2861.22932	1169.1	0.48418	-2860.75239	818.8	-383.6	-2860.991472
CuII_CPZmh_OH2_4_Geom1 (Fig 4) [4]	-2628.12273	869.6	0.36449	-2627.76362	731.0	-967.6	-2628.215181
CuII_CPZmh-H_OH2_3_Geom3 (Fig 5)	-2551.43921	776.5	0.32439	-2551.11963	649.8	-372.3	-2551.335235
CuII_CPZmh-2H_OH2_3_Geom3 (Fig 5)	-2551.01096	740.0	0.31027	-2550.70527	671.2	-230.9	-2550.869460
CuII_CPZmh-2H_OH2_2_Geom7 (Fig 5)	-2474.59202	678.8	0.28246	-2474.31377	563.9	-170.6	-2474.442760
CuII_CPZmh-2H_OH2_2_CuIIW2_cis (Fig 5) [6]	-4267.35235	796.7	0.33955	-4267.01773	812.2	-818.2	-4267.421583
sCuIII_CPZmh2-4H_GeomX2 (Fig 6) [7]	-3003.12401	1095.0	0.45165	-3002.67914	719.9	-349.2	-3002.893885
CuII_CPZmh2-4H_GeomX1 (Fig 7, Fig S1)	-3003.11136	1092.1	0.45079	-3002.66733	736.5	-834.8	-3003.068923
sCuIII_CPZmh2-4H_GeomX1_CuIW (Fig 7, Fig S1)	-4719.92361	1164.7	0.48353	-4719.44729	831.3	-274.0	-4719.646040
CuII_CPZmh2-4H_GeomX1_CuIIW2 (Fig 7)	-4796.37635	1234.9	0.51258	-4795.87141	870.0	-270.5	-4796.073245
CuII_CPZ_3_CPZ (Fig 8)	-8581.07770 ^c	–	–	–	–	–	–

^a – Parameters are based on electron convention with Boltzmann statistics and $\Delta G_{(solv)}$ from reference 15.

^b – The $\Delta G_{(solv)}(H_2O)$ is derived from experimental values in reference 16 and $\Delta G_{(solv)}(HO^-)$ is derived from our assumed value of $\Delta G_{(solv)}(H^+)$ from footnote a (above) and the value for $\Delta G^{298}_{hyd}K(H^+) + \Delta G^{298}_{hyd}K(HO^-) \approx -1534.1$ kJ/mol, consistent with experimental data from references 17 and 18.

^c – Further parameters not calculated.

Figure S1. Relative stabilities of alternative structures for geometry optimized Cu(CPZ)₂ complexes: Cu(II), singlet Cu(III), and triplet Cu(III) complexes. The blue complex, **7**, corresponds to the experimentally-observed Cu(III) complex, containing two singly hydrolyzed CPZ ligands which have tautomerized once. The second complex is the analogous (*hypothetical*) complex where the CPZ ligands have not undergone hydrolysis. Steric repulsion of the C₆H₁₀ moieties in the hypothetical complex do not allow the CPZ ligands to lie in the same plane, forcing a greater distortion toward D_{2d}-type symmetry for the Cu coordination sphere. This distortion can be accommodated by Cu(II), but is unfavourable for Cu(III), despite the analogous 4 N⁻ donor environment observed in **7**. Energies (E_g) are listed in kJ/mol relative to the stability of the Cu(II) complex. The N···N···N···N torsion angle about the Cu centre is shown in degrees below each position on the energy scale. Dashed lines indicate energy divisions of 25 kJ/mol. Note that the two complexes are on separate energy scales.

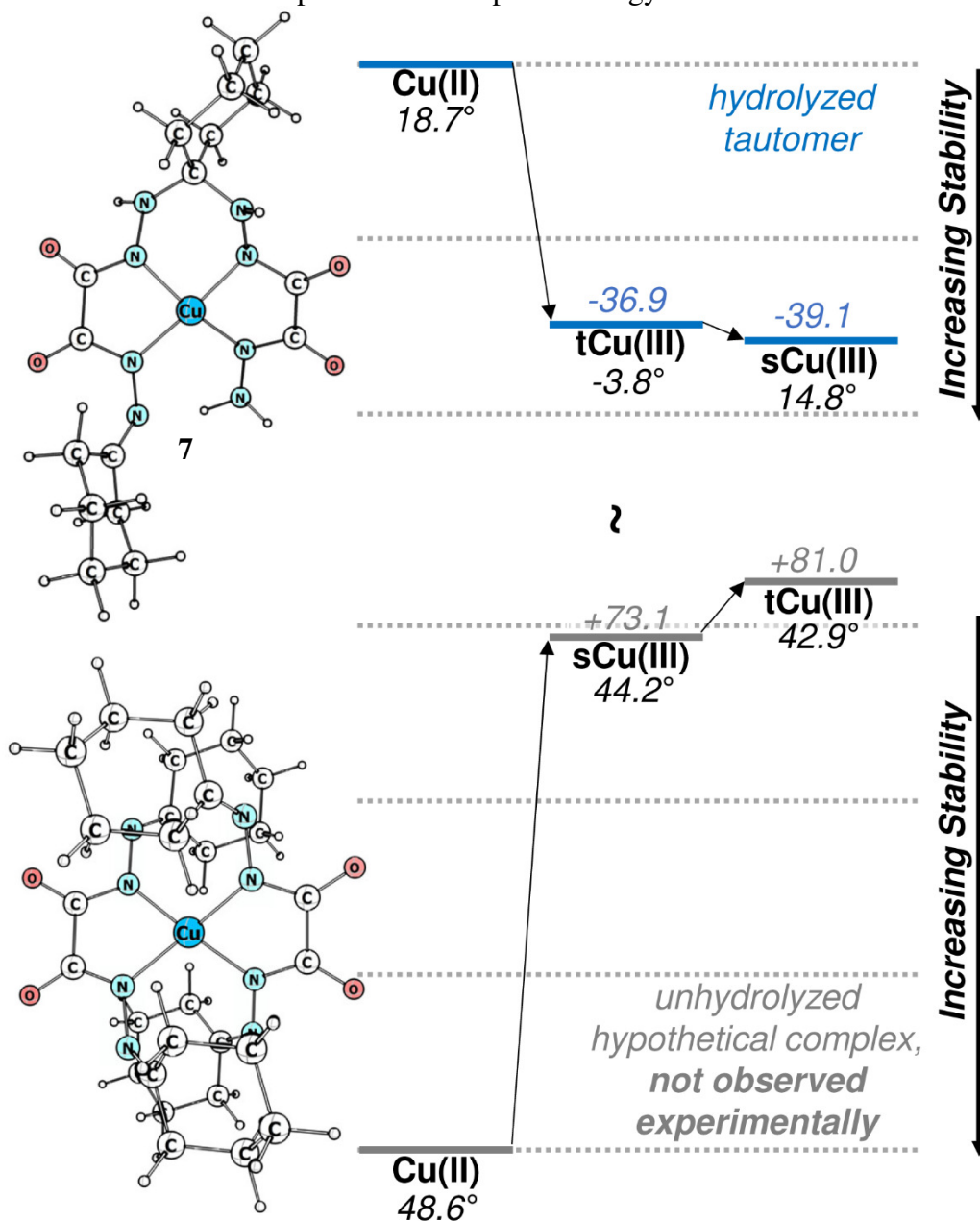


Figure S2. Gaussian output from geometry optimizations:

Structures from Figure 1.

CPZ [1]

8	0.202034000	1.752950000	0.302983000
8	-0.197514000	-1.703945000	-0.149801000
7	1.757199000	0.106001000	-0.155412000
7	-1.760802000	-0.054136000	0.263141000
7	2.846367000	0.925383000	-0.162525000
7	-2.840073000	-0.885781000	0.301990000
6	0.517692000	0.595330000	0.085931000
6	-0.516156000	-0.544026000	0.050486000
1	1.807806000	-0.900322000	-0.314315000
1	-1.817490000	0.952450000	0.418072000
6	-4.005460000	-0.371120000	0.456501000
6	-4.381149000	1.081535000	0.567850000
6	-5.441336000	1.436517000	-0.484056000
6	-6.642872000	0.502404000	-0.403419000
6	-6.212748000	-0.951794000	-0.554731000
6	-5.163061000	-1.323274000	0.495922000
1	-3.528382000	1.763426000	0.481126000
1	-4.808138000	1.243317000	1.570951000
1	-5.747763000	2.481791000	-0.354049000
1	-4.988771000	1.362285000	-1.484626000
1	-7.379974000	0.768303000	-1.171625000
1	-7.143017000	0.635965000	0.570055000
1	-7.075254000	-1.625027000	-0.474909000
1	-5.784725000	-1.104147000	-1.557574000
1	-4.786550000	-2.342208000	0.359059000
1	-5.628237000	-1.269539000	1.494680000
6	3.994510000	0.412902000	-0.419955000
6	5.169336000	1.344345000	-0.406167000
6	6.257287000	0.838279000	0.545007000
6	6.648951000	-0.596019000	0.210210000
6	5.433557000	-1.514576000	0.241800000
6	4.334957000	-1.023689000	-0.710705000
1	4.822110000	2.347257000	-0.137144000
1	5.588303000	1.398129000	-1.425217000
1	7.129727000	1.501993000	0.501044000
1	5.879082000	0.882297000	1.578075000
1	7.414343000	-0.959301000	0.907710000
1	7.101702000	-0.626427000	-0.794569000
1	5.712421000	-2.542363000	-0.021697000
1	5.029527000	-1.550576000	1.264941000
1	3.472868000	-1.697929000	-0.669439000
1	4.714348000	-1.072562000	-1.744394000

CPZmh [2]

8	-1.978518000	1.934039000	0.214646000
8	-2.579806000	-1.503810000	-0.188382000
7	-0.509804000	0.195858000	-0.194878000
7	-4.044840000	0.203084000	0.190385000
7	0.620863000	0.957373000	-0.219820000
7	-5.197874000	-0.580546000	0.221265000
6	-1.723668000	0.760115000	0.020909000
6	-2.819428000	-0.314982000	-0.006964000
1	-0.508581000	-0.813714000	-0.337291000
1	-4.141052000	1.200193000	0.345166000
6	1.745930000	0.372881000	-0.419299000
6	2.967178000	1.242163000	-0.434273000
6	4.004874000	0.744011000	0.575415000
6	4.326764000	-0.727711000	0.344513000
6	3.063608000	-1.577781000	0.403132000
6	2.016200000	-1.095265000	-0.609747000
1	2.667370000	2.276876000	-0.238744000
1	3.410828000	1.207534000	-1.443538000
1	4.912158000	1.357255000	0.510890000
1	3.606348000	0.876480000	1.593097000
1	5.055591000	-1.083404000	1.083743000
1	4.800054000	-0.847448000	-0.644040000
1	3.293108000	-2.633949000	0.215324000
1	2.633335000	-1.523016000	1.414714000
1	1.118297000	-1.719722000	-0.546909000
1	2.417292000	-1.232692000	-1.627072000
1	-5.071470000	-1.308608000	0.921802000
1	-5.293845000	-1.048591000	-0.678038000

Structures from Figure 3.

CPZ_step2c

8	-0.847919000	2.743824000	0.215045000
8	0.561115000	-0.485935000	-0.211137000
7	-1.750631000	0.614464000	0.200017000
7	1.598874000	1.631740000	-0.215282000
7	-3.021743000	0.990793000	0.426549000
7	2.921683000	1.556062000	-0.460002000
6	-0.714807000	1.525621000	0.114553000
6	0.559814000	0.791173000	-0.124833000
1	-1.443620000	-0.354311000	0.090450000
1	1.284126000	2.598389000	-0.142698000
6	3.513096000	0.242632000	-0.369278000
6	3.430334000	-0.338463000	1.060132000
6	4.267014000	-1.603191000	1.225387000
6	5.721193000	-1.361729000	0.833991000

6	5.814889000	-0.816881000	-0.587815000
6	4.981452000	0.447903000	-0.745857000
1	2.378935000	-0.542826000	1.298556000
1	3.785279000	0.440235000	1.755463000
1	4.204809000	-1.966958000	2.262607000
1	3.846549000	-2.391944000	0.583494000
1	6.309968000	-2.286545000	0.934950000
1	6.163701000	-0.627935000	1.531304000
1	6.864252000	-0.613572000	-0.851235000
1	5.447231000	-1.577869000	-1.292111000
1	5.003109000	0.817408000	-1.779533000
1	5.380331000	1.249132000	-0.104939000
6	-3.945904000	0.099703000	0.476347000
6	-5.344809000	0.572201000	0.748790000
6	-6.323345000	0.058213000	-0.308689000
6	-6.231061000	-1.458147000	-0.440789000
6	-4.806543000	-1.891102000	-0.768771000
6	-3.808000000	-1.388365000	0.280053000
1	-5.338651000	1.666376000	0.803932000
1	-5.670311000	0.192921000	1.734810000
1	-7.349117000	0.363985000	-0.059703000
1	-6.079086000	0.522105000	-1.277282000
1	-6.927298000	-1.823410000	-1.208485000
1	-6.541109000	-1.923656000	0.510622000
1	-4.741797000	-2.984552000	-0.850201000
1	-4.522070000	-1.484883000	-1.751647000
1	-2.792843000	-1.687145000	-0.001552000
1	-4.022201000	-1.887197000	1.241272000
8	3.008651000	-0.716973000	-1.302622000
1	2.067820000	-0.853899000	-1.056656000

CPZ_step1

8	-0.333877000	1.840482000	-0.374721000
8	0.406024000	-1.539283000	0.162865000
7	-1.826868000	0.158644000	0.197984000
7	1.708768000	0.282876000	-0.203279000
7	-2.948106000	0.948225000	0.152259000
7	2.773762000	-0.552895000	-0.361079000
6	-0.627151000	0.693447000	-0.078299000
6	0.493050000	-0.340130000	-0.009981000
1	-1.866252000	-0.837485000	0.414340000
1	1.708459000	1.242310000	-0.551818000
6	4.026874000	-0.231762000	-0.450254000
6	4.508064000	1.167626000	-0.364526000
6	5.666924000	1.261617000	0.649885000

6	6.743403000	0.224053000	0.369108000
6	6.161977000	-1.182400000	0.392363000
6	5.022276000	-1.319809000	-0.631480000
1	3.708539000	1.870443000	-0.111991000
1	4.885906000	1.441735000	-1.362697000
1	6.069402000	2.278622000	0.609366000
1	5.265578000	1.123156000	1.663641000
1	7.543089000	0.310797000	1.112509000
1	7.207491000	0.420069000	-0.609719000
1	6.923356000	-1.935159000	0.164953000
1	5.778759000	-1.415856000	1.395894000
1	4.544270000	-2.305712000	-0.587470000
1	5.440625000	-1.206945000	-1.644583000
6	-4.078965000	0.398678000	0.426012000
6	-5.284115000	1.282287000	0.351159000
6	-6.328361000	0.691720000	-0.602689000
6	-6.669946000	-0.742629000	-0.219869000
6	-5.418304000	-1.609968000	-0.186532000
6	-4.365999000	-1.033718000	0.774020000
1	-4.972825000	2.287889000	0.051746000
1	-5.723384000	1.353508000	1.359519000
1	-7.224343000	1.322831000	-0.599756000
1	-5.931434000	0.715013000	-1.628976000
1	-7.399108000	-1.163293000	-0.922382000
1	-7.149182000	-0.755276000	0.771972000
1	-5.657536000	-2.636118000	0.115902000
1	-4.986259000	-1.671190000	-1.196887000
1	-3.479297000	-1.678621000	0.790656000
1	-4.773332000	-1.047801000	1.797185000
1	2.459049000	-1.534527000	-0.351243000

Cyclohexanone (CPZ_step4a)

6	0.155478000	0.495524000	1.276224000
6	-0.412471000	1.072867000	0.000000000
6	0.155478000	0.495524000	-1.276224000
6	0.155478000	-1.036094000	-1.254740000
6	0.834937000	-1.571786000	0.000000000
6	0.155478000	-1.036094000	1.254740000
1	-0.404602000	0.904147000	2.123657000
1	1.195918000	0.850744000	1.360522000
1	-0.404602000	0.904147000	-2.123657000
1	1.195918000	0.850744000	-1.360522000
1	0.643899000	-1.418975000	-2.159305000
1	-0.883776000	-1.397704000	-1.286533000
1	0.822889000	-2.669015000	0.000000000

1	1.895360000	-1.270236000	0.000000000
1	0.643899000	-1.418975000	2.159305000
1	-0.883776000	-1.397704000	1.286533000
8	-1.260925000	1.942898000	0.000000000

Structures from Figure 4.

CuII_CPZ_OH2_4_Geom1 [3]

29	1.722557000	1.566445000	-0.048428000
8	-1.297374000	-2.201028000	-1.137780000
8	-0.119151000	0.923164000	-0.044461000
7	-2.586980000	-0.397846000	-0.467319000
7	0.909942000	-0.995240000	-0.624584000
7	-3.782536000	-1.011983000	-0.757616000
7	2.136517000	-0.418203000	-0.335617000
6	-1.452440000	-1.067885000	-0.717545000
6	-0.184008000	-0.274259000	-0.423208000
1	-2.537520000	0.550315000	-0.095387000
8	0.904680000	3.406797000	0.263679000
1	1.343201000	4.223471000	-0.010485000
1	-0.051799000	3.525252000	0.186663000
8	1.771534000	1.837809000	-2.454143000
1	1.272010000	2.506059000	-2.941245000
1	1.945041000	1.139441000	-3.098565000
8	3.452037000	2.607733000	-0.325595000
1	3.853261000	2.657123000	-1.204414000
1	4.125235000	2.754087000	0.352817000
6	-4.870035000	-0.405347000	-0.422603000
6	-6.145431000	-1.100757000	-0.772663000
6	-7.023316000	-1.282744000	0.471710000
6	-7.244808000	0.045390000	1.182179000
6	-5.916679000	0.692703000	1.552469000
6	-5.028051000	0.892894000	0.311638000
1	-5.913689000	-2.052657000	-1.259848000
1	-6.686589000	-0.474795000	-1.500658000
1	-7.976389000	-1.735106000	0.177577000
1	-6.537130000	-1.994462000	1.155555000
1	-7.851791000	-0.098637000	2.083180000
1	-7.814773000	0.724856000	0.529335000
1	-6.071657000	1.662118000	2.039780000
1	-5.385199000	0.055101000	2.274938000
1	-4.077031000	1.357022000	0.606061000
1	-5.525851000	1.600583000	-0.369697000
6	3.190789000	-1.176844000	-0.321891000

6	4.496030000	-0.591266000	0.091705000
6	5.024670000	-1.341966000	1.330585000
6	5.103649000	-2.839529000	1.076316000
6	3.752587000	-3.388753000	0.645568000
6	3.220387000	-2.643504000	-0.597926000
1	4.395297000	0.478917000	0.289006000
1	5.212248000	-0.721823000	-0.733360000
1	6.002907000	-0.928847000	1.598082000
1	4.355664000	-1.145191000	2.183413000
1	5.447693000	-3.355951000	1.978767000
1	5.854278000	-3.044513000	0.298569000
1	3.811874000	-4.454613000	0.403617000
1	3.023041000	-3.293978000	1.463337000
1	2.266968000	-3.068984000	-0.921348000
1	3.928570000	-2.797290000	-1.426533000
1	0.776190000	-1.963303000	-0.931968000
8	2.313823000	1.656286000	2.158289000
1	2.465686000	0.920575000	2.764552000
1	1.913045000	2.356339000	2.690681000

CuII_CPZ_OH2_5_Geom2b

29	-0.919108000	2.359327000	-0.050189000
8	0.751518000	-2.781291000	-0.034235000
8	0.059052000	0.651801000	-0.172557000
7	2.236544000	-1.031643000	-0.268167000
7	-1.273318000	-1.237244000	0.085838000
7	3.337965000	-1.849384000	-0.367036000
7	-2.522731000	-0.653539000	0.094296000
6	1.028461000	-1.599106000	-0.124459000
6	-0.132089000	-0.587902000	-0.071089000
1	2.301191000	-0.017881000	-0.330292000
8	-2.519443000	1.756104000	-0.979978000
1	-2.443217000	1.740175000	-1.944390000
1	-2.654163000	0.804644000	-0.646359000
8	-1.641166000	1.983105000	2.125981000
1	-1.786111000	1.142361000	2.577455000
1	-2.257101000	2.610153000	2.527118000
8	-1.825757000	4.180795000	0.129905000
1	-2.668642000	4.389031000	-0.294537000
1	-1.359163000	5.002280000	0.333401000
6	4.495836000	-1.295810000	-0.468818000
6	4.838702000	0.166144000	-0.452707000
6	5.880591000	0.453376000	0.642073000
6	7.100893000	-0.446423000	0.490663000
6	6.700446000	-1.915300000	0.512238000

6	5.665974000	-2.219905000	-0.577544000
1	3.967164000	0.824681000	-0.324964000
1	5.275533000	0.415352000	-1.432482000
1	6.165143000	1.511509000	0.600011000
1	5.421577000	0.284178000	1.628264000
1	7.820994000	-0.233025000	1.288700000
1	7.610724000	-0.214708000	-0.457553000
1	7.573904000	-2.561196000	0.373234000
1	6.276068000	-2.170971000	1.494668000
1	5.310541000	-3.253784000	-0.534038000
1	6.132686000	-2.068319000	-1.564377000
6	-3.529262000	-1.395617000	0.445288000
6	-4.886714000	-0.786201000	0.350900000
6	-5.743052000	-1.600790000	-0.637542000
6	-5.773602000	-3.072133000	-0.247700000
6	-4.366705000	-3.644288000	-0.146798000
6	-3.505496000	-2.832197000	0.845470000
1	-4.823154000	0.269037000	0.060208000
1	-5.357221000	-0.832062000	1.344810000
1	-6.751640000	-1.175338000	-0.665432000
1	-5.326086000	-1.490315000	-1.650154000
1	-6.356383000	-3.642455000	-0.979116000
1	-6.290056000	-3.189035000	0.717045000
1	-4.382547000	-4.687549000	0.184428000
1	-3.883211000	-3.636704000	-1.134954000
1	-2.503885000	-3.262543000	0.942875000
1	-3.968036000	-2.899436000	1.841929000
1	-1.138325000	-2.257830000	0.119808000
8	0.150886000	2.976181000	-2.024603000
1	0.138473000	3.810170000	-2.511528000
1	0.651646000	2.357247000	-2.571038000
8	0.610275000	3.223471000	0.941330000
1	0.691948000	2.934379000	1.862462000
1	1.489465000	3.215729000	0.539188000

CuII_CPZ-OH_OH2_3_Step2c

29	-2.286898000	1.554364000	-0.183928000
8	1.350030000	-2.124748000	0.898665000
8	0.356488000	1.129924000	0.045660000
7	2.692894000	-0.290368000	0.468509000
7	-0.826845000	-0.791265000	0.465394000
7	3.878448000	-0.950558000	0.664903000
7	-2.029025000	-0.291079000	0.190122000
6	1.530080000	-0.953255000	0.603809000
6	0.320551000	-0.060014000	0.334581000

1	2.648627000	0.691620000	0.199741000
8	-1.294448000	3.394651000	0.472814000
1	-1.628729000	3.617594000	1.351100000
1	-0.381140000	3.091838000	0.579948000
8	-3.724388000	2.138205000	1.481123000
1	-3.897404000	1.263429000	1.875217000
1	-4.579352000	2.564315000	1.353321000
8	-3.001500000	2.787583000	-1.676359000
1	-3.029447000	2.546079000	-2.609081000
1	-2.551406000	3.641162000	-1.609635000
6	4.970009000	-0.291620000	0.500806000
6	6.245812000	-1.048751000	0.701057000
6	7.125978000	-0.959832000	-0.550433000
6	7.358978000	0.490399000	-0.954821000
6	6.035699000	1.214825000	-1.170961000
6	5.147905000	1.139872000	0.080880000
1	6.009621000	-2.084152000	0.965619000
1	6.786901000	-0.599532000	1.549741000
1	8.077330000	-1.472148000	-0.366607000
1	6.633414000	-1.498158000	-1.374462000
1	7.968418000	0.541906000	-1.864854000
1	7.931084000	1.004636000	-0.166120000
1	6.201018000	2.266199000	-1.434406000
1	5.500928000	0.755837000	-2.016354000
1	4.206059000	1.673834000	-0.094044000
1	5.652048000	1.666873000	0.906183000
6	-3.187671000	-1.140841000	0.580769000
6	-4.306875000	-0.846689000	-0.406930000
6	-4.005581000	-1.410469000	-1.791344000
6	-3.743498000	-2.910911000	-1.729073000
6	-2.612729000	-3.229366000	-0.756816000
6	-2.903427000	-2.637844000	0.622018000
1	-4.477621000	0.239708000	-0.445399000
1	-5.220975000	-1.298641000	0.002372000
1	-4.843746000	-1.190900000	-2.462346000
1	-3.124382000	-0.900206000	-2.213794000
1	-3.505652000	-3.300296000	-2.725308000
1	-4.659913000	-3.426480000	-1.402703000
1	-2.475002000	-4.311740000	-0.660028000
1	-1.664670000	-2.837794000	-1.156796000
1	-2.113671000	-2.880352000	1.350966000
1	-3.816459000	-3.095147000	1.028652000
1	-0.671640000	-1.776143000	0.706972000
8	-3.613639000	-0.669861000	1.853901000
1	-3.094249000	-1.086061000	2.555828000

CuII_CPZmh_OH2_4_Geom1 [4]

29	2.955977000	-0.408285000	-0.058247000
8	-0.828156000	2.774387000	0.468945000
8	1.031177000	-0.129964000	-0.194838000
7	-1.682840000	0.711880000	-0.152495000
7	1.586985000	1.936542000	0.526799000
7	-2.985315000	1.149786000	-0.167972000
7	2.938497000	1.556877000	0.546169000
6	-0.728886000	1.599926000	0.165887000
6	0.689484000	1.033340000	0.142467000
1	-1.427308000	-0.250820000	-0.373394000
8	2.684028000	-2.322626000	-0.621844000
1	3.322432000	-2.811598000	-1.160369000
1	1.797887000	-2.572195000	-0.922832000
8	3.047217000	-1.290691000	2.134235000
1	2.766630000	-2.214450000	2.192612000
1	2.952294000	-0.943191000	3.031459000
8	4.946134000	-0.620626000	0.196415000
1	5.212078000	-1.067302000	1.014844000
1	5.677843000	-0.657447000	-0.434038000
6	-3.912125000	0.290613000	-0.429344000
6	-3.778640000	-1.178834000	-0.693826000
6	-4.665904000	-1.974965000	0.280851000
6	-6.106285000	-1.480170000	0.244904000
6	-6.179503000	0.009056000	0.551042000
6	-5.310463000	0.814625000	-0.423920000
1	-2.745198000	-1.549424000	-0.649936000
1	-4.130363000	-1.360160000	-1.721319000
1	-4.607514000	-3.039489000	0.026811000
1	-4.264268000	-1.868312000	1.299985000
1	-6.711472000	-2.048385000	0.960221000
1	-6.536778000	-1.676012000	-0.749475000
1	-7.211395000	0.371542000	0.496851000
1	-5.835887000	0.196159000	1.579306000
1	-5.295109000	1.881370000	-0.181748000
1	-5.722794000	0.706468000	-1.440136000
1	1.258522000	2.879438000	0.763120000
8	3.287870000	0.436321000	-2.239436000
1	4.051729000	0.653245000	-2.790939000
1	2.537492000	0.429226000	-2.849251000
1	3.329166000	1.716026000	1.478033000
1	3.465179000	2.124025000	-0.124320000

Structures in Figure 5.

CuII_CPZmh-H_OH2_3_Geom3

29	-2.656671000	-0.496348000	-0.092521000
8	-0.702457000	-0.761642000	-0.148958000
8	-0.394557000	2.741587000	-0.202870000
7	1.189955000	0.529295000	-0.233657000
7	-2.205611000	1.343259000	0.187979000
7	2.047534000	-0.536826000	-0.374887000
7	-3.169954000	2.358272000	0.094277000
6	-0.113576000	0.349268000	-0.141931000
6	-0.916375000	1.645086000	-0.049254000
1	1.492435000	1.507641000	-0.248672000
8	-2.858925000	-2.409067000	-0.822522000
1	-3.488639000	-2.587692000	-1.532965000
1	-1.997243000	-2.751374000	-1.101998000
8	-4.569849000	0.048661000	-0.439229000
1	-4.486798000	1.032063000	-0.340373000
1	-5.213145000	-0.260206000	0.212219000
6	3.305549000	-0.271218000	-0.461713000
6	3.988533000	1.063209000	-0.395257000
6	5.087449000	1.045456000	0.680342000
6	6.053805000	-0.112019000	0.467723000
6	5.311467000	-1.441559000	0.449555000
6	4.218460000	-1.444557000	-0.625298000
1	3.309872000	1.905811000	-0.221779000
1	4.456076000	1.239253000	-1.376847000
1	5.612636000	2.007090000	0.667465000
1	4.617815000	0.955952000	1.671463000
1	6.818374000	-0.110995000	1.253156000
1	6.586077000	0.025718000	-0.486697000
1	6.000362000	-2.274548000	0.269999000
1	4.850793000	-1.620672000	1.432928000
1	3.626869000	-2.365343000	-0.612264000
1	4.695221000	-1.367215000	-1.616042000
8	-3.254160000	-1.406004000	1.902514000
1	-2.929979000	-1.033653000	2.731017000
1	-3.177770000	-2.364280000	1.985974000
1	-3.272965000	2.820070000	0.997873000
1	-2.862287000	3.068178000	-0.573820000

CuII_CPZmh-2H_OH2_3_Geom3

29	-2.506724000	-0.536537000	-0.286112000
8	-0.613352000	-0.657287000	-0.102268000
8	-0.696372000	2.862622000	0.046421000
7	1.169634000	0.727042000	0.470229000

7	-2.304058000	1.250152000	0.365972000
7	1.952584000	-0.402354000	0.580864000
7	-3.327050000	2.194983000	0.116178000
6	-0.066263000	0.502600000	0.197340000
6	-1.013128000	1.691993000	0.199444000
8	-2.267289000	-2.478008000	-1.032010000
1	-2.539481000	-2.673860000	-1.935466000
1	-1.294180000	-2.430411000	-1.020226000
8	-4.455385000	-0.145752000	-0.774359000
1	-4.408361000	0.826734000	-0.561939000
1	-5.024801000	-0.551903000	-0.108722000
6	3.100275000	-0.353657000	0.008079000
6	3.626536000	0.777460000	-0.829708000
6	5.022660000	1.197910000	-0.359722000
6	5.971291000	0.008143000	-0.269673000
6	5.408979000	-1.063548000	0.657489000
6	4.025978000	-1.520788000	0.188307000
1	2.922307000	1.614895000	-0.803644000
1	3.691173000	0.431834000	-1.875608000
1	5.423924000	1.966436000	-1.033077000
1	4.935780000	1.666426000	0.632722000
1	6.961810000	0.333421000	0.075408000
1	6.115517000	-0.421085000	-1.275704000
1	6.088722000	-1.923711000	0.718917000
1	5.325250000	-0.653297000	1.676097000
1	3.569010000	-2.232360000	0.885488000
1	4.139689000	-2.033871000	-0.782576000
8	-3.227193000	-1.428307000	1.791856000
1	-2.747030000	-0.741053000	2.273365000
1	-2.745451000	-2.247583000	1.954873000
1	-3.607175000	2.616430000	1.001341000
1	-2.930702000	2.956936000	-0.443144000

CuII_CPZmh-2H_OH2_2_Geom7

8	0.815671000	1.852053000	-0.811072000
8	-1.726106000	3.006160000	0.113296000
7	-0.100262000	-0.049292000	0.162653000
7	-2.482133000	0.890037000	-0.386251000
7	0.969659000	-0.890184000	-0.121027000
7	-3.809200000	1.246629000	-0.039176000
6	-0.116719000	1.229356000	-0.326619000
6	-1.524976000	1.834052000	-0.175325000
29	-1.843694000	-0.866896000	0.021006000
6	2.151337000	-0.614047000	0.304311000
6	3.264652000	-1.533867000	-0.095760000

6	4.357041000	-0.729193000	-0.810051000
6	4.847430000	0.417482000	0.067205000
6	3.696392000	1.330823000	0.474759000
6	2.573720000	0.540886000	1.158270000
1	2.873270000	-2.337633000	-0.729914000
1	3.695811000	-1.992582000	0.809535000
1	5.185042000	-1.393235000	-1.088961000
1	3.941917000	-0.321920000	-1.744741000
1	5.619000000	0.993807000	-0.459264000
1	5.328414000	0.001936000	0.968836000
1	4.047865000	2.121393000	1.148974000
1	3.271302000	1.826890000	-0.408265000
1	1.731731000	1.186812000	1.413804000
1	2.965318000	0.108659000	2.095616000
8	-0.966746000	-2.695195000	-0.158857000
1	-1.212813000	-3.248818000	-0.907321000
1	-0.037870000	-2.348725000	-0.301920000
8	-3.779715000	-1.408529000	0.403696000
1	-4.011317000	-1.857000000	1.223345000
1	-4.155417000	-0.482631000	0.416079000
1	-3.768144000	2.068962000	0.571080000
1	-4.291516000	1.544894000	-0.886691000

CuII_CPZmh-2H_OH2_2_CuIIW2_cis [6]

29	3.455920000	-1.411677000	-0.645445000
8	1.545924000	-1.286994000	-0.965566000
8	2.799155000	0.948199000	0.162423000
7	-0.395472000	-0.049825000	-0.756920000
7	0.793368000	2.096212000	0.087602000
7	-1.185354000	-1.085633000	-1.196400000
7	1.144127000	2.856636000	1.042806000
6	0.903561000	-0.242593000	-0.682678000
6	1.619192000	0.943358000	-0.107844000
8	5.382991000	-1.527326000	-0.935301000
1	5.675483000	-1.463010000	-1.875087000
1	5.775995000	-2.366525000	-0.594425000
8	3.490452000	-2.264271000	1.433161000
1	4.124058000	-1.822293000	2.039961000
1	2.620848000	-2.195020000	1.884446000
6	-2.142618000	-1.496951000	-0.439171000
6	-2.453681000	-1.028541000	0.949401000
6	-3.916508000	-0.580014000	1.070045000
6	-4.868441000	-1.643870000	0.536631000
6	-4.516014000	-2.021119000	-0.897461000
6	-3.071384000	-2.529929000	-0.989403000

1	-1.760021000	-0.242853000	1.289675000
1	-2.290041000	-1.899657000	1.612913000
1	-4.131855000	-0.349755000	2.124114000
1	-4.054532000	0.355291000	0.501103000
1	-5.904171000	-1.282887000	0.592477000
1	-4.810307000	-2.542056000	1.173833000
1	-5.199198000	-2.792035000	-1.283535000
1	-4.627365000	-1.134391000	-1.547714000
1	-2.787232000	-2.777479000	-2.022057000
1	-2.974469000	-3.445419000	-0.376722000
1	1.826223000	2.521922000	1.806408000
1	0.716185000	3.832938000	1.086012000
29	-1.113876000	1.654454000	-0.176952000
1	-2.761029000	1.217540000	-2.166190000
8	-2.840605000	1.704164000	-1.311170000
1	-3.141956000	2.612246000	-1.553773000
1	-2.900223000	2.919928000	1.172559000
1	-1.592610000	2.880152000	2.046342000
8	-1.914338000	2.974541000	1.115647000

Structures in Figure 7.

sCuIII_CPZmh2-4H_GeomX1_CuIW

29	-0.028715000	-0.573696000	-0.654027000
7	-0.717229000	-2.028522000	-1.683502000
6	-0.159261000	-3.188129000	-1.197772000
6	1.147701000	-2.912612000	-0.504357000
8	-0.708299000	-4.283353000	-1.210199000
8	1.686567000	-3.694893000	0.259659000
7	1.624830000	-1.609815000	-0.745470000
7	2.563613000	-1.268451000	0.138646000
6	3.208200000	0.043650000	0.083361000
6	4.419498000	-0.021488000	-0.850339000
6	5.512558000	-0.937288000	-0.314609000
6	5.933228000	-0.538417000	1.096012000
6	4.736714000	-0.526357000	2.041372000
6	3.642408000	0.393892000	1.509213000
1	4.075678000	-0.363308000	-1.837741000
1	4.805469000	1.004175000	-0.964868000
1	6.372886000	-0.913520000	-0.994641000
1	5.144873000	-1.973723000	-0.310364000
1	6.381788000	0.468422000	1.071522000
1	6.709062000	-1.218665000	1.468855000
1	5.036266000	-0.190314000	3.041975000
1	4.363060000	-1.554532000	2.168882000
1	4.015908000	1.425961000	1.471875000

1	2.755684000	0.402766000	2.159438000
6	-4.028435000	-3.338234000	1.670660000
6	-2.571278000	-2.892968000	1.664619000
6	-2.456541000	-1.364540000	1.698805000
6	-3.275774000	-0.725814000	0.614030000
6	-4.698075000	-1.190676000	0.525911000
6	-4.795734000	-2.719094000	0.508446000
7	-2.892056000	0.174663000	-0.222765000
7	-1.553725000	0.530087000	-0.151170000
6	-1.256708000	1.815044000	-0.044682000
6	0.252739000	2.082846000	-0.142579000
8	-2.030153000	2.784136000	0.126941000
8	0.670108000	3.270479000	-0.249736000
7	0.995421000	0.989438000	-0.132700000
1	-4.500682000	-3.033786000	2.619660000
1	-4.088731000	-4.432507000	1.626628000
1	-2.030123000	-3.316730000	2.519084000
1	-2.070608000	-3.288243000	0.766643000
1	-1.412289000	-1.036334000	1.651904000
1	-2.857952000	-1.001211000	2.660018000
1	-5.170532000	-0.733730000	-0.351052000
1	-5.230342000	-0.817740000	1.417104000
1	-4.387873000	-3.101928000	-0.440361000
1	-5.850362000	-3.020541000	0.530795000
7	2.340697000	1.105597000	-0.429798000
1	2.464092000	1.230128000	-1.435274000
1	2.503337000	-1.750695000	1.039449000
7	-1.997978000	-2.193243000	-2.091648000
1	-2.516799000	-1.323599000	-2.142847000
1	-2.473242000	-2.980513000	-1.645173000
29	-0.728786000	4.549680000	-0.097658000
8	-2.247648000	5.775368000	0.052215000
1	-2.260322000	6.453497000	0.737001000
1	-2.987792000	5.172058000	0.219640000

CuII_CPZmh2-4H_GeomX1_CuIIW2

29	0.631851000	0.484467000	-0.629385000
7	-0.706436000	-0.792246000	-1.191407000
6	-0.574814000	-1.958604000	-0.568251000
6	0.783105000	-2.105746000	0.116665000
8	-1.458075000	-2.834495000	-0.460503000
8	0.979289000	-2.990534000	0.935512000
7	1.658033000	-1.118512000	-0.260590000
7	2.760526000	-1.033306000	0.536796000
6	3.833238000	-0.146431000	0.123547000

6	4.688864000	-0.825358000	-0.950840000
6	5.428698000	-2.043191000	-0.409579000
6	6.259004000	-1.693679000	0.821586000
6	5.393085000	-1.063295000	1.909002000
6	4.672678000	0.166900000	1.365700000
1	4.038048000	-1.104588000	-1.791982000
1	5.413763000	-0.082038000	-1.323096000
1	6.067928000	-2.459942000	-1.199352000
1	4.694997000	-2.820701000	-0.150576000
1	7.053074000	-0.981972000	0.537371000
1	6.763951000	-2.589953000	1.204321000
1	6.004912000	-0.771439000	2.772420000
1	4.670349000	-1.807491000	2.277972000
1	5.409346000	0.926410000	1.066464000
1	4.026957000	0.642967000	2.119362000
6	-4.111234000	1.638143000	2.365545000
6	-2.597489000	1.758782000	2.500641000
6	-2.028345000	2.835000000	1.563444000
6	-2.454809000	2.497572000	0.170329000
6	-3.935592000	2.393873000	-0.038912000
6	-4.512709000	1.348178000	0.923918000
7	-1.695524000	2.131478000	-0.801477000
7	-0.327287000	2.103975000	-0.581286000
6	0.395291000	3.243435000	-0.499115000
6	1.883622000	2.886206000	-0.530096000
8	-0.012779000	4.392518000	-0.438334000
8	2.749061000	3.651429000	-0.896790000
7	2.129720000	1.571622000	-0.096090000
1	-4.580646000	2.581249000	2.688823000
1	-4.493874000	0.855253000	3.033658000
1	-2.314205000	1.982334000	3.536243000
1	-2.127712000	0.792126000	2.247775000
1	-0.940787000	2.894379000	1.645704000
1	-2.431220000	3.822480000	1.833468000
1	-4.143833000	2.137436000	-1.084938000
1	-4.401388000	3.370474000	0.163876000
1	-4.122350000	0.353431000	0.631403000
1	-5.604489000	1.302399000	0.816973000
7	3.339649000	1.109182000	-0.450561000
1	3.610415000	1.306137000	-1.416813000
1	2.526585000	-0.973772000	1.529249000
7	-2.001040000	-0.523171000	-1.738708000
1	-1.955155000	-0.716223000	-2.740567000
1	-2.125181000	0.503097000	-1.639110000
29	-3.332967000	-1.620362000	-0.853708000
8	-4.667461000	-2.716341000	-0.007543000

1	-4.161065000	-3.435189000	0.485454000
1	-5.268741000	-2.299022000	0.608817000
8	-2.972036000	-4.368918000	1.151470000
1	-2.151147000	-3.974420000	0.791572000
1	-2.909209000	-5.315615000	0.996462000

Structure in Figure 8.

CuII_CPZ_3_CPZgreen

8	0.044855000	-6.443178000	0.532004000
8	1.966763000	-3.497605000	0.416796000
7	-0.406381000	-4.272086000	1.141811000
7	2.393194000	-5.476014000	-0.634167000
7	-1.595830000	-4.783343000	1.656626000
7	3.537391000	-4.980958000	-1.228992000
6	0.348625000	-5.216691000	0.617969000
6	1.658496000	-4.681393000	0.116160000
6	4.284959000	-5.832898000	-1.856457000
6	5.497114000	-5.274656000	-2.523143000
6	6.763662000	-5.999163000	-2.041594000
6	6.628190000	-7.504736000	-2.216867000
6	5.399020000	-8.027732000	-1.487244000
6	4.118150000	-7.315842000	-1.968229000
1	5.544666000	-4.194581000	-2.348492000
1	5.390106000	-5.435246000	-3.607996000
1	7.626720000	-5.613860000	-2.594439000
1	6.936060000	-5.760374000	-0.981506000
1	7.524471000	-8.012755000	-1.844840000
1	6.556459000	-7.750654000	-3.287255000
1	5.277494000	-9.105701000	-1.638234000
1	5.512660000	-7.870211000	-0.404418000
1	3.248121000	-7.712363000	-1.429030000
1	3.965605000	-7.549194000	-3.033583000
6	-2.656100000	-4.026983000	1.686289000
6	-2.788611000	-2.697563000	1.028772000
6	-3.880754000	-2.811007000	-0.059924000
6	-5.194713000	-3.324209000	0.509065000
6	-4.999187000	-4.662662000	1.203818000
6	-3.907596000	-4.562462000	2.286479000
1	-1.849016000	-2.350511000	0.588945000
1	-3.098971000	-1.965967000	1.788575000
1	-4.004820000	-1.825600000	-0.521683000
1	-3.525765000	-3.486405000	-0.853550000
1	-5.937718000	-3.416110000	-0.290550000
1	-5.600519000	-2.593377000	1.224389000
1	-5.926664000	-5.012347000	1.668668000

1	-4.706956000	-5.430679000	0.468504000
1	-3.733166000	-5.517636000	2.788987000
1	-4.234108000	-3.842800000	3.052700000
29	-1.566335000	-6.781180000	1.635539000
8	-2.378491000	-7.256106000	3.352683000
8	-3.631563000	-10.372512000	4.397162000
7	-2.517418000	-9.262999000	2.338688000
7	-3.404666000	-8.463122000	5.682558000
7	-2.038307000	-8.675324000	1.182498000
7	-4.278540000	-8.765604000	6.729778000
6	-2.687343000	-8.477759000	3.393716000
6	-3.299113000	-9.208110000	4.575266000
6	-4.053453000	-9.841800000	7.408878000
6	-2.875815000	-10.756196000	7.302528000
6	-2.301237000	-11.090489000	8.686688000
6	-3.379390000	-11.576378000	9.644281000
6	-4.474014000	-10.528978000	9.787280000
6	-5.090520000	-10.191454000	8.426670000
1	-2.103868000	-10.332540000	6.650633000
1	-3.231511000	-11.679858000	6.818601000
1	-1.510765000	-11.839914000	8.566607000
1	-1.820581000	-10.192615000	9.104160000
1	-2.938971000	-11.804565000	10.621275000
1	-3.811648000	-12.517791000	9.270945000
1	-5.265385000	-10.871939000	10.462085000
1	-4.055987000	-9.615358000	10.235987000
1	-5.827578000	-9.384369000	8.485701000
1	-5.615029000	-11.082635000	8.044280000
6	-1.993069000	-9.367943000	0.084196000
6	-1.466959000	-8.722421000	-1.148773000
6	-0.201085000	-9.472000000	-1.605192000
6	-0.486802000	-10.956937000	-1.788071000
6	-1.063109000	-11.565889000	-0.518314000
6	-2.332454000	-10.811655000	-0.056189000
1	-1.273817000	-7.657212000	-0.989918000
1	-2.236747000	-8.816095000	-1.929178000
1	0.159033000	-9.020604000	-2.536821000
1	0.585516000	-9.329735000	-0.846076000
1	0.428720000	-11.487596000	-2.071267000
1	-1.192433000	-11.096048000	-2.620310000
1	-1.329506000	-12.617232000	-0.666368000
1	-0.316731000	-11.542474000	0.289278000
1	-2.749963000	-11.274738000	0.841740000
1	-3.099859000	-10.896832000	-0.839628000
8	4.465130000	2.127183000	0.700023000
8	5.937243000	5.318058000	0.775811000

7	4.719826000	3.639797000	2.344964000
7	6.028577000	3.776556000	-0.948506000
7	4.048403000	2.779029000	3.195979000
7	6.362883000	4.604736000	-2.025225000
6	4.921462000	3.231331000	1.102488000
6	5.698818000	4.231886000	0.265924000
6	7.486248000	5.239176000	-1.974862000
6	7.754554000	6.184480000	-3.099104000
6	8.047078000	7.584066000	-2.537964000
6	9.181215000	7.539276000	-1.523164000
6	8.860321000	6.573826000	-0.389160000
6	8.548113000	5.166352000	-0.927070000
1	6.909270000	6.184496000	-3.793847000
1	8.642814000	5.825980000	-3.642384000
1	8.284280000	8.258468000	-3.367528000
1	7.136259000	7.978186000	-2.062426000
1	9.367807000	8.540442000	-1.118730000
1	10.112050000	7.229120000	-2.022851000
1	9.694972000	6.504231000	0.317410000
1	7.989642000	6.935881000	0.175823000
1	8.289382000	4.472971000	-0.120837000
1	9.450169000	4.773995000	-1.422999000
6	3.969681000	3.084505000	4.456575000
6	4.433982000	4.358709000	5.076373000
6	3.192618000	5.086698000	5.644106000
6	2.438040000	4.204927000	6.628001000
6	2.048978000	2.874436000	5.995481000
6	3.274499000	2.161207000	5.394605000
1	4.996177000	5.020058000	4.412453000
1	5.107698000	4.102795000	5.906677000
1	3.530124000	6.012982000	6.119903000
1	2.536129000	5.383308000	4.812720000
1	1.545340000	4.728536000	6.987979000
1	3.064493000	4.019355000	7.512806000
1	1.591394000	2.212204000	6.740978000
1	1.305590000	3.038042000	5.195633000
1	3.000211000	1.222755000	4.907178000
1	3.981275000	1.928318000	6.204839000
29	3.318655000	1.282173000	2.030446000
8	1.715959000	0.875507000	3.063701000
8	-0.548088000	-1.806171000	2.805148000
7	1.468171000	-0.783449000	1.490415000
7	-0.654687000	0.009191000	4.188475000
7	2.658895000	-0.302267000	0.937776000
7	-1.901226000	-0.327872000	4.691244000
6	1.116500000	-0.129912000	2.574992000

6	-0.109674000	-0.701095000	3.224478000
6	-2.193713000	0.164995000	5.852403000
6	-1.327736000	0.995749000	6.742484000
6	-1.955671000	2.394129000	6.898772000
6	-3.393388000	2.282586000	7.393580000
6	-4.227704000	1.391226000	6.482133000
6	-3.595296000	-0.006204000	6.324770000
1	-0.283274000	1.046966000	6.411194000
1	-1.310091000	0.506413000	7.727741000
1	-1.344509000	2.985967000	7.590562000
1	-1.933284000	2.914647000	5.927057000
1	-3.844228000	3.278525000	7.461894000
1	-3.394534000	1.873411000	8.415102000
1	-5.245375000	1.278995000	6.870110000
1	-4.321158000	1.853905000	5.488006000
1	-4.156232000	-0.628224000	5.620399000
1	-3.587281000	-0.508360000	7.303603000
6	2.915379000	-0.601089000	-0.308222000
6	1.930850000	-1.147919000	-1.286017000
6	1.884693000	-0.217096000	-2.516897000
6	3.261130000	-0.061174000	-3.143375000
6	4.242659000	0.499267000	-2.125769000
6	4.277230000	-0.361868000	-0.854418000
1	0.932138000	-1.254747000	-0.849746000
1	2.280735000	-2.140865000	-1.603028000
1	1.166325000	-0.635496000	-3.230180000
1	1.492237000	0.766973000	-2.220487000
1	3.205307000	0.596917000	-4.017111000
1	3.616580000	-1.036851000	-3.508818000
1	5.254681000	0.562456000	-2.541638000
1	3.932927000	1.520038000	-1.852562000
1	4.948302000	0.041132000	-0.092807000
1	4.648272000	-1.368156000	-1.117183000
29	0.583762000	-2.570401000	1.418994000
1	5.084877000	4.558243000	2.610342000
1	-2.830243000	-10.234969000	2.414235000
1	-0.197538000	0.890686000	4.433534000
1	2.062418000	-6.431948000	-0.784384000
1	5.619465000	2.895157000	-1.242506000
1	-3.206206000	-7.470701000	5.603386000

Additional Structures

CuII_CPZmh2-4H_GeomX1 (Fig 7, Fig S1)

7	1.066555000	1.863404000	-0.998266000
6	0.562588000	2.639110000	-0.034899000

6	-0.552783000	1.916230000	0.747513000
8	0.994679000	3.767028000	0.285440000
8	-0.740608000	2.163990000	1.944965000
7	-1.159985000	0.960939000	-0.005104000
7	-1.930379000	0.050767000	0.753106000
6	-2.772092000	-0.830405000	-0.051081000
6	-4.041005000	-0.061365000	-0.434394000
6	-4.865098000	0.330358000	0.785001000
6	-5.213722000	-0.888519000	1.635413000
6	-3.956431000	-1.648844000	2.051250000
6	-3.137969000	-2.033425000	0.823044000
1	-3.734686000	0.836790000	-0.991174000
1	-4.635158000	-0.696365000	-1.113402000
1	-5.782841000	0.850457000	0.469716000
1	-4.274250000	1.036913000	1.385211000
1	-5.860486000	-1.565152000	1.047406000
1	-5.794361000	-0.586608000	2.520966000
1	-4.227113000	-2.550662000	2.622162000
1	-3.354674000	-1.012374000	2.716594000
1	-3.710290000	-2.723518000	0.185554000
1	-2.212991000	-2.566102000	1.090915000
29	0.277961000	0.095975000	-1.115199000
6	4.277004000	0.828272000	2.026924000
6	2.831062000	0.399368000	1.805989000
6	2.747769000	-0.884198000	0.972526000
6	3.514035000	-0.734428000	-0.314316000
6	4.935868000	-0.279427000	-0.139684000
6	4.997171000	1.004564000	0.693448000
7	3.071205000	-0.884256000	-1.509179000
7	1.715342000	-1.186748000	-1.639279000
6	1.343087000	-2.479413000	-1.553179000
6	-0.207702000	-2.642905000	-1.627296000
8	2.078181000	-3.464154000	-1.396969000
8	-0.727501000	-3.708278000	-1.962063000
7	-0.796641000	-1.493444000	-1.241655000
1	4.804539000	0.060218000	2.622411000
1	4.310471000	1.762050000	2.605700000
1	2.310386000	0.261703000	2.763178000
1	2.292017000	1.203859000	1.281657000
1	1.704394000	-1.155200000	0.772571000
1	3.195147000	-1.722758000	1.534423000
1	5.384405000	-0.145459000	-1.132483000
1	5.504872000	-1.068549000	0.384227000
1	4.505358000	1.817564000	0.134307000
1	6.043873000	1.308852000	0.849299000
7	-2.197602000	-1.348398000	-1.312506000

1	-2.367131000	-0.641018000	-2.028087000
1	-1.300640000	-0.505809000	1.336226000
7	2.141261000	2.423418000	-1.727109000
1	2.811099000	1.668581000	-1.876907000
1	2.555040000	3.146473000	-1.128829000

sCuIII_CPZmh2-4H_GeomX1 (Fig6, Fig S1) [7]

7	0.316532000	1.484504000	-0.588426000
6	-0.276230000	1.783751000	0.610638000
6	-1.459167000	0.862481000	0.910212000
8	0.145609000	2.611610000	1.411300000
8	-1.984274000	0.828671000	2.018017000
7	-1.745796000	0.021242000	-0.138694000
7	-2.514128000	-1.056819000	0.239718000
6	-2.860408000	-2.078168000	-0.760107000
6	-4.278045000	-1.805089000	-1.278313000
6	-5.333106000	-1.970944000	-0.192718000
6	-5.261668000	-3.352083000	0.450997000
6	-3.870756000	-3.617024000	1.018519000
6	-2.808840000	-3.446624000	-0.064414000
1	-4.284776000	-0.788750000	-1.692813000
1	-4.483688000	-2.499247000	-2.111500000
1	-6.332261000	-1.794646000	-0.613872000
1	-5.169599000	-1.201174000	0.575514000
1	-5.490924000	-4.120205000	-0.307829000
1	-6.022570000	-3.450345000	1.237672000
1	-3.810263000	-4.630276000	1.439426000
1	-3.684766000	-2.926074000	1.855427000
1	-2.972921000	-4.206722000	-0.844987000
1	-1.792337000	-3.608676000	0.320516000
29	-0.078941000	-0.306116000	-1.020785000
6	3.912974000	2.140791000	-4.306393000
6	2.600213000	1.367142000	-4.367598000
6	1.693861000	1.744861000	-3.202657000
6	2.374081000	1.515921000	-1.855281000
6	3.707338000	2.260934000	-1.802655000
6	4.618616000	1.910859000	-2.973944000
7	2.684797000	0.082615000	-1.680202000
7	1.586749000	-0.751540000	-1.760167000
6	1.583592000	-1.821388000	-2.608761000
6	0.170980000	-2.449659000	-2.645461000
8	2.506965000	-2.235995000	-3.289841000
8	-0.186361000	-3.223350000	-3.534266000
7	-0.624934000	-1.983669000	-1.653701000
1	3.706136000	3.218801000	-4.425974000

1	4.570614000	1.851831000	-5.137516000
1	2.080676000	1.567944000	-5.313854000
1	2.804996000	0.287149000	-4.337128000
1	0.749906000	1.189810000	-3.245687000
1	1.432136000	2.812936000	-3.244641000
1	4.206488000	2.041333000	-0.844339000
1	3.481125000	3.337819000	-1.800361000
1	4.913145000	0.854825000	-2.901525000
1	5.537719000	2.510270000	-2.913669000
7	-1.992887000	-2.009262000	-1.923658000
1	-2.190423000	-2.724106000	-2.624660000
1	-2.202781000	-1.437284000	1.134221000
7	1.547451000	2.058582000	-0.776115000
1	2.042960000	2.172905000	0.114861000
1	3.136400000	-0.037049000	-0.771016000

tCuIII_CPZmh2-4H_GeomX1 (Fig S1)

7	0.366109000	2.316101000	-0.263947000
6	-0.661853000	3.244463000	-0.217537000
6	-2.011674000	2.598379000	-0.377870000
8	-0.462429000	4.448250000	-0.076910000
8	-3.081058000	3.219449000	-0.360413000
7	-1.893469000	1.259796000	-0.560779000
7	-3.045065000	0.590439000	-0.823792000
6	-3.126054000	-0.798620000	-0.295691000
6	-4.533264000	-1.300852000	-0.629555000
6	-5.639276000	-0.588097000	0.143531000
6	-5.377337000	-0.626002000	1.645804000
6	-3.992813000	-0.077020000	1.975383000
6	-2.908850000	-0.837583000	1.223073000
1	-4.691291000	-1.208942000	-1.713914000
1	-4.546079000	-2.373258000	-0.388371000
1	-6.604555000	-1.057744000	-0.090377000
1	-5.732282000	0.459059000	-0.184960000
1	-5.437622000	-1.671760000	1.992033000
1	-6.156834000	-0.069186000	2.183711000
1	-3.804716000	-0.139659000	3.055356000
1	-3.944907000	0.993691000	1.717290000
1	-2.906482000	-1.897592000	1.518496000
1	-1.915235000	-0.445403000	1.465824000
29	-0.138122000	0.404120000	-0.534798000
6	5.928790000	-0.928371000	1.898821000
6	4.562161000	-1.586207000	2.040892000
6	3.830222000	-1.703737000	0.700146000
6	3.797337000	-0.389769000	-0.021102000

6	5.094861000	0.366225000	-0.082008000
6	5.787346000	0.455601000	1.277008000
7	2.771437000	0.172087000	-0.557745000
7	1.567941000	-0.502351000	-0.607009000
6	1.487810000	-1.692614000	-1.272220000
6	0.019627000	-2.155317000	-1.447528000
8	2.424040000	-2.337181000	-1.735295000
8	-0.275693000	-3.085658000	-2.197124000
7	-0.842707000	-1.398587000	-0.729398000
1	6.570002000	-1.552806000	1.253820000
1	6.429730000	-0.864492000	2.875006000
1	4.654616000	-2.582491000	2.493649000
1	3.949822000	-0.985024000	2.732228000
1	2.809161000	-2.068092000	0.849096000
1	4.325032000	-2.444446000	0.052917000
1	4.909724000	1.357433000	-0.515356000
1	5.762010000	-0.166853000	-0.781154000
1	5.188542000	1.092495000	1.947955000
1	6.767284000	0.941373000	1.170378000
7	-2.194591000	-1.691047000	-0.946142000
1	-2.385504000	-1.785422000	-1.946684000
1	-3.846165000	1.196257000	-0.625481000
7	1.584029000	2.812895000	-0.145344000
1	2.328589000	2.146127000	-0.377626000
1	1.660934000	3.827049000	-0.192201000

CuII_CPZ-2H_2_Geom1 (Fig S1)

6	5.611714000	3.912467000	-0.073787000
6	4.279385000	3.992521000	0.687770000
6	3.659481000	2.596860000	0.893074000
6	3.538897000	1.874590000	-0.428744000
6	4.836796000	1.765375000	-1.196146000
6	5.456207000	3.162609000	-1.405997000
7	2.486533000	1.385488000	-0.963797000
7	1.264901000	1.540666000	-0.306048000
6	0.725134000	2.775539000	-0.271810000
6	-0.725544000	2.775524000	0.271646000
8	1.264512000	3.835899000	-0.625608000
8	-1.264984000	3.835890000	0.625296000
7	-1.265225000	1.540569000	0.306193000
7	-2.486845000	1.385522000	0.963907000
6	-3.539173000	1.874644000	0.428816000
6	-3.659720000	2.596818000	-0.893058000
6	-4.279672000	3.992479000	-0.687934000
6	-5.612018000	3.912467000	0.073588000

6	-5.456542000	3.162737000	1.405873000
6	-4.837114000	1.765468000	1.196151000
1	6.356683000	3.390336000	0.545380000
1	6.006913000	4.920762000	-0.253836000
1	4.429428000	4.482241000	1.658114000
1	3.556133000	4.591387000	0.126167000
1	2.687931000	2.666749000	1.377087000
1	4.316082000	1.997322000	1.542434000
1	4.644017000	1.267636000	-2.149078000
1	5.547693000	1.146456000	-0.627155000
1	4.799447000	3.739167000	-2.067896000
1	6.427506000	3.073693000	-1.910411000
1	-2.688143000	2.666680000	-1.377030000
1	-4.316274000	1.997197000	-1.542404000
1	-4.429702000	4.482054000	-1.658351000
1	-3.556458000	4.591427000	-0.126381000
1	-6.356946000	3.390259000	-0.545562000
1	-6.007262000	4.920767000	0.253528000
1	-6.427854000	3.073868000	1.910264000
1	-4.799778000	3.739335000	2.067734000
1	-5.548013000	1.146527000	0.627180000
1	-4.644406000	1.267826000	2.149140000
29	0.000001000	-0.000143000	0.000126000
6	5.612176000	-3.911724000	0.073089000
6	4.279752000	-3.991740000	-0.688303000
6	3.659591000	-2.596096000	-0.893018000
6	3.539047000	-1.874357000	0.429090000
6	4.837069000	-1.765156000	1.196308000
6	5.456759000	-3.162358000	1.405585000
7	2.486677000	-1.385633000	0.964460000
7	1.265056000	-1.540782000	0.306663000
6	0.725483000	-2.775751000	0.272140000
6	-0.725100000	-2.775863000	-0.271636000
8	1.265011000	-3.836084000	0.625760000
8	-1.264533000	-3.836315000	-0.625077000
7	-1.264855000	-1.541000000	-0.306119000
7	-2.486429000	-1.385942000	-0.964001000
6	-3.538897000	-1.874752000	-0.428911000
6	-3.659698000	-2.596682000	0.893076000
6	-4.279482000	-3.992430000	0.687946000
6	-5.611687000	-3.912595000	-0.073852000
6	-5.456022000	-3.162983000	-1.406180000
6	-4.836708000	-1.765672000	-1.196491000
1	6.356955000	-3.389246000	-0.546012000
1	6.007570000	-4.920016000	0.252718000
1	4.429753000	-4.481087000	-1.658845000

1	3.556679000	-4.590917000	-0.126810000
1	2.687997000	-2.665924000	-1.376966000
1	4.316037000	-1.996178000	-1.542175000
1	4.644387000	-1.267763000	2.149438000
1	5.547774000	-1.145944000	0.627390000
1	4.800207000	-3.739257000	2.067391000
1	6.428126000	-3.073439000	1.909870000
1	-2.688224000	-2.666390000	1.377281000
1	-4.316468000	-1.997049000	1.542174000
1	-4.429665000	-4.481963000	1.658364000
1	-3.556092000	-4.591350000	0.126581000
1	-6.356782000	-3.390398000	0.545101000
1	-6.006784000	-4.920954000	-0.253775000
1	-6.427256000	-3.074242000	-1.910752000
1	-4.799114000	-3.739619000	-2.067861000
1	-5.547691000	-1.146700000	-0.627676000
1	-4.643838000	-1.268083000	-2.149478000

sCuIII_CPZ-2H_2_Geom1 (Fig S1)

6	-5.620434000	3.796108000	0.117312000
6	-4.320388000	3.895470000	-0.692774000
6	-3.698336000	2.506266000	-0.939183000
6	-3.538168000	1.748931000	0.355509000
6	-4.799892000	1.633612000	1.175968000
6	-5.405906000	3.030165000	1.430880000
7	-2.470713000	1.228206000	0.835555000
7	-1.282087000	1.449397000	0.139448000
6	-0.730295000	2.688705000	0.221020000
6	0.730302000	2.688745000	-0.221087000
8	-1.301792000	3.714428000	0.577062000
8	1.301696000	3.714474000	-0.577283000
7	1.282158000	1.449475000	-0.139488000
7	2.470843000	1.228371000	-0.835551000
6	3.538270000	1.749114000	-0.355457000
6	3.698437000	2.506298000	0.939326000
6	4.320318000	3.895608000	0.693063000
6	5.620318000	3.796506000	-0.117128000
6	5.405778000	3.030726000	-1.430787000
6	4.799951000	1.634064000	-1.176020000
1	-6.387636000	3.281826000	-0.478814000
1	-6.009593000	4.798719000	0.328136000
1	-4.507772000	4.387946000	-1.653178000
1	-3.587155000	4.501323000	-0.153504000
1	-2.748574000	2.586721000	-1.463031000
1	-4.376476000	1.915362000	-1.572215000

1	-4.575365000	1.117704000	2.111293000
1	-5.532471000	1.030620000	0.620759000
1	-4.724258000	3.597638000	2.074382000
1	-6.351419000	2.927764000	1.975327000
1	2.748704000	2.586575000	1.463250000
1	4.376685000	1.915388000	1.572235000
1	4.507714000	4.387977000	1.653519000
1	3.586979000	4.501449000	0.153926000
1	6.387619000	3.282224000	0.478870000
1	6.009350000	4.799189000	-0.327840000
1	6.351261000	2.928515000	-1.975321000
1	4.724012000	3.598208000	-2.074156000
1	5.532639000	1.031088000	-0.620943000
1	4.575422000	1.118259000	-2.111401000
29	0.000084000	-0.000002000	0.000016000
6	-5.620464000	-3.796081000	-0.117333000
6	-4.320422000	-3.895463000	0.692756000
6	-3.698355000	-2.506267000	0.939178000
6	-3.538177000	-1.748920000	-0.355506000
6	-4.799897000	-1.633585000	-1.175968000
6	-5.405924000	-3.030130000	-1.430894000
7	-2.470719000	-1.228202000	-0.835554000
7	-1.282082000	-1.449400000	-0.139468000
6	-0.730301000	-2.688710000	-0.221024000
6	0.730289000	-2.688754000	0.221108000
8	-1.301799000	-3.714436000	-0.577061000
8	1.301682000	-3.714492000	0.577278000
7	1.282153000	-1.449485000	0.139521000
7	2.470825000	-1.228391000	0.835604000
6	3.538255000	-1.749114000	0.355496000
6	3.698427000	-2.506226000	-0.939328000
6	4.320290000	-3.895557000	-0.693140000
6	5.620284000	-3.796515000	0.117067000
6	5.405740000	-3.030810000	1.430770000
6	4.799929000	-1.634127000	1.176082000
1	-6.387662000	-3.281794000	0.478794000
1	-6.009634000	-4.798686000	-0.328165000
1	-4.507814000	-4.387944000	1.653156000
1	-3.587193000	-4.501318000	0.153484000
1	-2.748596000	-2.586736000	1.463029000
1	-4.376490000	-1.915362000	1.572215000
1	-4.575362000	-1.117673000	-2.111288000
1	-5.532472000	-1.030591000	-0.620756000
1	-4.724278000	-3.597605000	-2.074397000
1	-6.351433000	-2.927717000	-1.975344000
1	2.748697000	-2.586463000	-1.463267000

1	4.376688000	-1.915285000	-1.572196000
1	4.507689000	-4.387874000	-1.653623000
1	3.586938000	-4.501420000	-0.154044000
1	6.387596000	-3.282206000	-0.478894000
1	6.009303000	-4.799215000	0.327723000
1	6.351220000	-2.928643000	1.975318000
1	4.723962000	-3.598324000	2.074099000
1	5.532629000	-1.031126000	0.621049000
1	4.575395000	-1.118377000	2.111491000

tCuIII_CPZ-2H_2_Geom1 (Fig S1)

29	0.237079000	0.210673000	0.272023000
8	1.248389000	3.924230000	-0.785770000
8	3.529287000	2.216229000	-0.776706000
7	0.170886000	2.163342000	0.263273000
7	1.996262000	0.498827000	-0.526148000
7	-1.001695000	2.888380000	0.354829000
7	3.000901000	-0.449899000	-0.539058000
6	1.199668000	2.762890000	-0.397912000
6	2.394647000	1.800089000	-0.574336000
6	2.836473000	-1.452093000	-1.324297000
6	3.805811000	-2.593089000	-1.251033000
6	3.055288000	-3.900560000	-0.967345000
6	1.949090000	-4.137207000	-1.991431000
6	0.978839000	-2.960479000	-2.032529000
6	1.721844000	-1.650223000	-2.312053000
1	4.561424000	-2.379771000	-0.484984000
1	4.328246000	-2.682861000	-2.219323000
1	3.760567000	-4.743223000	-0.957460000
1	2.601475000	-3.836655000	0.034154000
1	1.408689000	-5.063599000	-1.756491000
1	2.397145000	-4.273476000	-2.991518000
1	0.202089000	-3.118947000	-2.793461000
1	0.460469000	-2.886509000	-1.064363000
1	1.053940000	-0.782764000	-2.308667000
1	2.175308000	-1.708523000	-3.316396000
6	-1.581763000	2.904160000	1.499892000
6	-2.945204000	3.517220000	1.610026000
6	-3.937823000	2.487174000	2.165441000
6	-3.448270000	1.907460000	3.489518000
6	-2.061198000	1.290277000	3.339097000
6	-1.065488000	2.311779000	2.780428000
1	-3.254099000	3.895910000	0.627899000
1	-2.898516000	4.377340000	2.300301000
1	-4.927521000	2.948893000	2.287638000
1	-4.042729000	1.667277000	1.436707000

1	-4.157658000	1.154731000	3.857698000
1	-3.408865000	2.708183000	4.248997000
1	-1.698328000	0.901134000	4.300534000
1	-2.122184000	0.430918000	2.654537000
1	-0.069761000	1.883305000	2.625998000
1	-0.957733000	3.134704000	3.507616000
8	-3.137345000	-1.974092000	0.944355000
8	-0.843086000	-3.447768000	1.709687000
7	-1.653598000	-0.386114000	0.137758000
7	0.356940000	-1.521273000	1.236861000
7	-2.677448000	0.381794000	-0.290988000
7	1.507289000	-2.123920000	1.608493000
6	-2.004968000	-1.545172000	0.791919000
6	-0.773493000	-2.304359000	1.288478000
6	2.296943000	-1.524970000	2.425961000
6	3.667789000	-2.079600000	2.651085000
6	4.722167000	-0.993452000	2.398638000
6	4.440609000	0.254416000	3.229524000
6	3.045688000	0.795673000	2.937798000
6	1.979478000	-0.275127000	3.192055000
1	3.816796000	-2.955556000	2.008350000
1	3.741840000	-2.417130000	3.699258000
1	5.721566000	-1.392655000	2.618705000
1	4.693845000	-0.719512000	1.332882000
1	5.192038000	1.024906000	3.015109000
1	4.525568000	0.012983000	4.304065000
1	2.827487000	1.681313000	3.549394000
1	2.995262000	1.115217000	1.887231000
1	0.971887000	0.078067000	2.945724000
1	1.979375000	-0.535332000	4.264224000
6	-2.667235000	0.838502000	-1.491631000
6	-3.667858000	1.878931000	-1.883367000
6	-2.948839000	3.102692000	-2.467351000
6	-2.024521000	2.705165000	-3.613808000
6	-1.008308000	1.665805000	-3.154539000
6	-1.708828000	0.433877000	-2.571746000
1	-4.283527000	2.138714000	-1.013868000
1	-4.335832000	1.452410000	-2.651392000
1	-3.690782000	3.840716000	-2.801147000
1	-2.344554000	3.565496000	-1.671949000
1	-1.503149000	3.590721000	-3.998830000
1	-2.620972000	2.295017000	-4.448186000
1	-0.353596000	1.357803000	-3.980623000
1	-0.361124000	2.111209000	-2.386049000
1	-0.995730000	-0.305659000	-2.190499000
1	-2.294143000	-0.057878000	-3.367108000