

Supporting Information

for

Complete σ^* Intramolecular Aromatic Hydroxylation Mechanism through O₂ Activation by a Macrocyclic Dinuclear Copper(I) Complex.

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Table S1. xyz coordinate data sets, Lewis and 3D representation for DFT (B3LYP/6-31G(d) method using Gaussian03) optimized complexes.

Table S2. Multiplicity states, $\langle S^2 \rangle$ values for all species involved in this reaction mechanism.

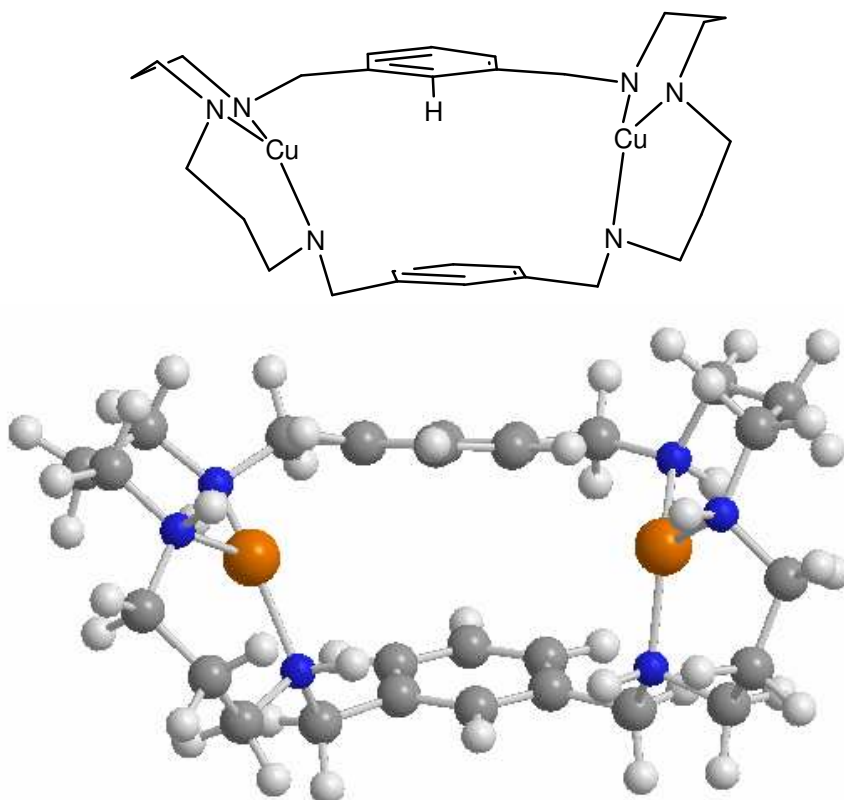
Table S3. Free energies, ZPE, and thermal corrections, *i. e.* sum of electronic and thermal free energies, (in a.u.) for all species involved in this reaction mechanism.

Table S4. Comparison between the X-ray data of complex I and the corresponding B3LYP/6-31G(d) geometry (Distances in Å and angles in degrees).

Table S1. xyz coordinate data sets, Lewis and 3D representation for DFT (B3LYP/6-31G(d) method using Gaussian03) optimized complexes.

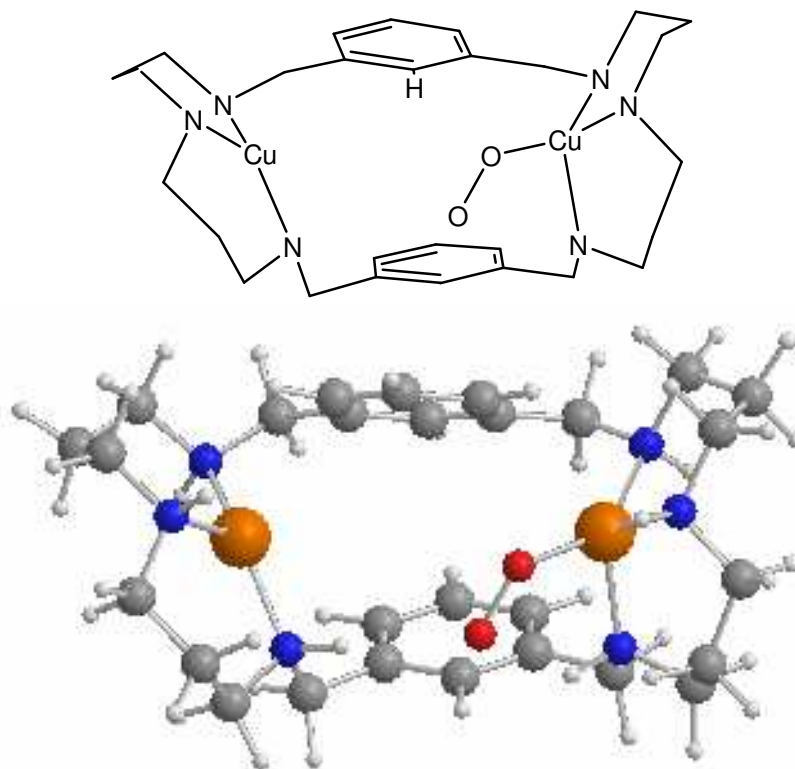
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H	-1.82907400	3.82204300	-0.74800900
C	-0.01752100	2.46674600	3.03656400
H	-2.10944900	2.67219500	2.56592500
C	1.28011200	2.40235400	2.52824800
C	-1.10132300	2.59307800	2.16692100
C	1.51217400	2.46617700	1.14689000
C	-0.89708800	2.66251300	0.78298500
H	3.63002800	2.37642400	1.46130000
C	0.41343700	2.60460700	0.29062800
H	-2.96301400	3.13205800	0.41313800
C	2.93524200	2.51835600	0.62858100
C	-2.05322200	2.92197000	-0.15467600
H	0.57684500	2.72753900	-0.78011200
H	-2.50634700	3.10054200	-2.76170600
H	4.60447300	2.80392100	-1.40579900
H	2.59509600	1.59573300	-1.15663600
H	-1.45507200	1.47520600	-1.45486700
H	5.34218300	1.78774000	-0.17329300
N	3.26994100	1.47756900	-0.39519100
H	-3.99573500	2.86110800	-1.85459400
N	-2.36062900	1.78732300	-1.09268600
C	4.61297000	1.78586600	-0.99201100
C	-3.12015900	2.33983200	-2.25887500
H	1.86918600	-0.41557100	3.19008600
H	-2.89401300	-0.36827700	3.07143300
H	-3.88437600	1.84810100	-4.17686500
H	5.90204400	1.24916300	-2.59901200
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H	4.26405300	0.69490500	-2.83878700
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H	3.84838400	-1.68451600	-2.06004200
C	3.86012600	-2.69666000	1.80445400
H	4.14090400	-3.02942000	2.81200200
C	-5.24325400	-1.38700400	1.09003600
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H	5.78802900	-1.93885900	1.13398800
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C	5.08750800	-2.74790800	0.88253600
C	-5.52515800	-1.47972000	-1.47919100
C	-6.09219100	-1.01724600	-0.13206200
C	4.79660500	-2.77693100	-0.62770800
H	-5.20943400	-2.52612700	-1.39417100
H	4.00389200	-3.50923700	-0.82162500
H	-6.31344500	-1.44788600	-2.24304100
H	5.68974500	-3.12766800	-1.16237000
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H	-0.59728600	-0.85008100	3.31039200



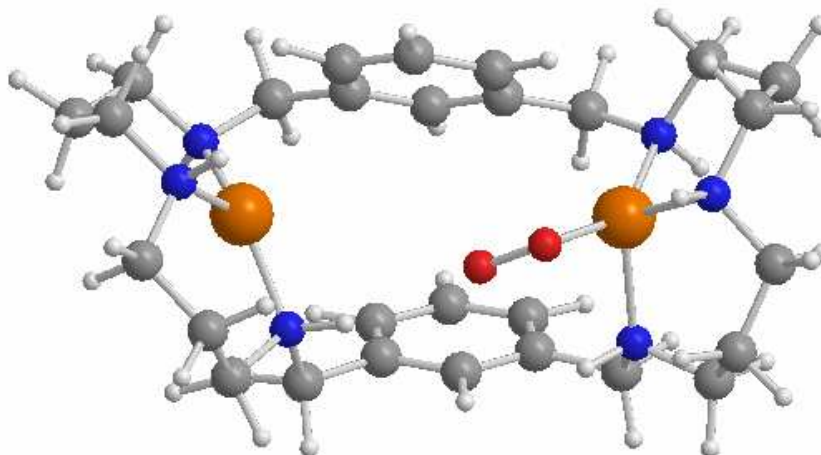
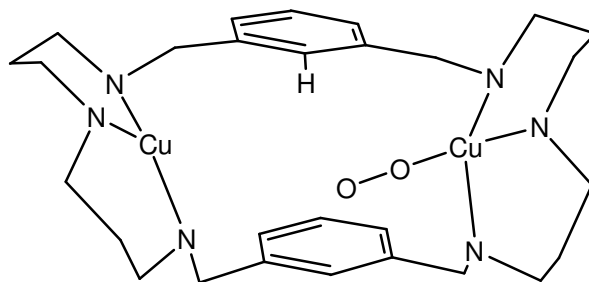
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H	-2.07102800	3.76874600	-0.09471800
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H	-2.29115100	2.21242100	3.06807000
C	1.11042100	2.10315800	3.02019700
C	-1.28031200	2.23515400	2.66825800
C	1.33899600	2.36848600	1.66275300
C	-1.07605000	2.50187700	1.30921200
H	3.47095700	2.16401000	1.88976400
C	0.23632400	2.58851200	0.82874100
H	-3.16903900	2.84432900	0.93096000
C	2.75358400	2.52348900	1.14447200
C	-2.22911600	2.78652100	0.37606800
H	0.39172300	2.85681600	-0.21310600
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H	2.28932900	2.07596500	-0.80162000
H	-1.47313400	1.57568100	-1.08874200
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N	3.01633700	1.79669300	-0.13225300
H	-4.14036100	2.73561500	-1.36966000
N	-2.40531500	1.75809300	-0.70392400
C	4.32873100	2.22508300	-0.70757300
C	-3.20797500	2.36527100	-1.81133600
H	2.00911300	-0.52565800	2.74396700
H	-2.67352500	-0.61940400	3.03833500
H	-3.87908500	2.02178300	-3.79736300
H	5.48456300	2.15127800	-2.48840700
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C	4.70143700	1.53615600	-2.03056800
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H	3.85814800	1.56628500	-2.73318500
C	2.12240300	-1.44085500	2.15691500
H	2.32625800	-2.25461400	2.86702800
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C	0.82224600	-1.70628800	1.41854100
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C	-1.65894100	-2.23895800	0.21137600
H	-2.60181100	-2.52940300	-0.23665400
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Cu	2.83448200	-0.22688100	-0.40835400
C	-0.47336400	-2.54202900	-0.45395600
H	-0.50437800	-3.01177400	-1.43244900
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N	-3.97600800	-0.82632100	1.39175800
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H	5.83435700	-0.12415000	-2.83971300
H	-5.04604300	-0.00077500	-3.61368100
H	-3.47262400	-1.27688200	-2.45699800
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H	-5.68128000	-1.98082000	1.94460300
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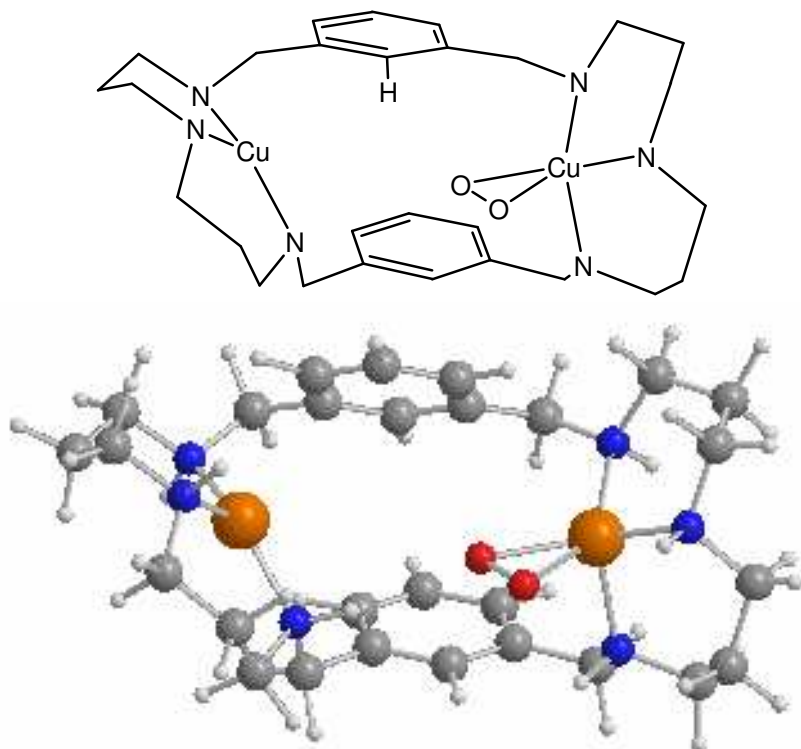
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C	-0.15080500	2.23471000	3.38869000
H	-2.25028400	2.38646400	2.92984400
C	1.15016200	2.26526200	2.88271600
C	-1.23959400	2.39190100	2.52926200
C	1.37951100	2.47901400	1.51606100
C	-1.03613300	2.60547700	1.16068800
H	3.50467300	2.26237100	1.76265800
C	0.27646000	2.67385700	0.67713200
H	-3.12779400	2.95102800	0.77346100
C	2.79803800	2.60253900	0.99851100
C	-2.19229100	2.84505400	0.21848800
H	0.42974400	2.90383600	-0.37519200
H	-2.63930600	3.15970100	-2.36982200
H	4.38745100	3.30487600	-1.03066200
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H	-1.46133000	1.52580700	-1.16231100
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H	-4.11473000	2.69902600	-1.52724200
N	-2.38950100	1.75256300	-0.79386000
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H	1.91424600	-0.36967600	2.68252500
H	-2.71475500	-0.46115100	3.04808700
H	-3.82158400	1.86317000	-3.91487000
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H	4.82985600	1.45699600	-2.06359600
H	-2.57333500	0.77135200	-3.35445300
H	4.01650200	1.43426300	-2.80169800
C	2.04169600	-1.33081900	2.17804600
H	2.25615300	-2.07616700	2.95733300
C	-2.96083800	-1.23702300	2.31846200
H	-3.34386900	-2.09769400	2.88447000
C	-0.45261900	-1.30354400	2.10121500
C	0.74387500	-1.67650300	1.47165800
C	-1.70201000	-1.61400800	1.55929700
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C	0.67280400	-2.38028500	0.26522200
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C	-1.74816700	-2.33685700	0.35481800
H	-2.69613300	-2.66591600	-0.05550100
H	-4.47833100	0.06013400	1.91265300
Cu	-3.21992500	0.05339200	-0.22414200
Cu	2.86157200	-0.26061700	-0.46435700
C	-0.56814600	-2.70926200	-0.28573100
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N	3.24633800	-1.20502900	1.29288900
N	-4.02596000	-0.70557900	1.41395500
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H	-4.99615300	-0.14812000	-3.64441700
H	-3.44929400	-1.36059100	-2.38092900
H	3.88901000	-1.13453600	-2.53963800
C	3.98624300	-2.50458700	1.16763000
H	4.28788700	-2.82869800	2.17177600
C	-5.11341500	-1.69960800	1.13100100
H	-5.78184000	-1.76352400	1.99929400
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C	5.21835400	-2.42229700	0.26481500
C	-5.22826300	-1.74200300	-1.45337700
C	-5.91553200	-1.36830400	-0.13257200
C	4.92488500	-2.31353100	-1.23476000
H	-4.81531100	-2.75381500	-1.36986500
H	4.20886100	-3.09011300	-1.52548300
H	-5.97227600	-1.77073600	-2.26082200
H	5.84538100	-2.49318400	-1.80539900
H	5.79433100	-3.34201700	0.41878800
H	-6.85435500	-1.93216200	-0.08253000
H	-0.40663300	-0.74398400	3.03172200
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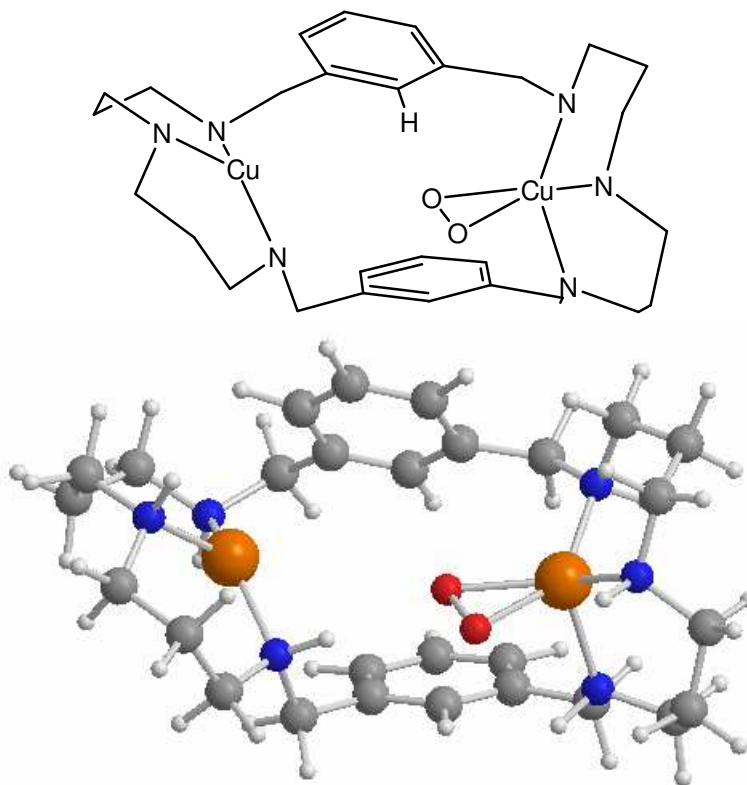
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H	-1.61339300	3.62470700	-0.89793800
C	-0.05017500	2.52961100	3.12825700
H	-2.11484600	2.66185500	2.52558800
C	1.27914800	2.48853700	2.70396900
C	-1.08188900	2.61073100	2.19078600
C	1.59606000	2.56017300	1.33908900
C	-0.79216900	2.67059400	0.82329300
H	3.68773800	2.29842500	1.73936600
C	0.54939300	2.67370200	0.41741700
H	-2.83218300	3.07411600	0.25155600
C	3.04890000	2.62640000	0.91276800
C	-1.88091300	2.80522100	-0.21474700
H	0.76748300	2.79074000	-0.64232000
H	-1.96377300	2.60361000	-2.87539200
H	4.93653600	3.13126500	-0.89568000
H	2.82970900	2.13776300	-1.05241300
H	-1.18095700	1.16228700	-1.21290200
H	5.43834900	1.86506700	0.21870900
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H	-3.56201300	2.58518300	-2.13831300
N	-2.10755200	1.55891000	-1.02726500
C	4.81612000	2.06439300	-0.66200500
C	-2.68433700	1.96267000	-2.34765600
H	1.67364200	-0.31165100	2.57973800
H	-2.87768200	0.00637700	3.07092100
H	-3.24744800	1.22132600	-4.25632400
H	6.25398900	1.68513800	-2.18262700
C	-3.09689800	0.80155600	-3.25469200
C	5.31845800	1.22677400	-1.84216600
H	-2.27409700	0.07883000	-3.35537500
H	4.62896100	1.30246500	-2.69533900
C	1.74615400	-1.32248600	2.17030500
H	1.93489900	-1.99795900	3.01788400
C	-3.21895500	-0.79444200	2.40972100
H	-3.71450100	-1.54331200	3.04196900
C	-0.72627300	-1.09258800	2.12487100
C	0.40922200	-1.67119500	1.53926500
C	-2.02178900	-1.39329100	1.69447200
H	1.06836200	-3.04745900	-0.00504400
C	0.22566600	-2.57235500	0.48451200
H	3.64869300	-0.78096200	1.81816000
C	-2.18084800	-2.32244500	0.65123900
H	-3.16959300	-2.65512600	0.35439600
H	-4.50674700	0.67595700	1.81163300
Cu	-3.20953200	0.10082900	-0.26357000
Cu	2.85739500	-0.31409100	-0.46035800
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H	-1.18775500	-3.62382400	-0.74736300
N	2.96729000	-1.33554800	1.29378700
N	-4.19333400	-0.21660000	1.43260900
H	6.14727400	-0.31464100	-0.56990900
H	-5.13555000	0.81660000	-2.53269800
C	5.62791700	-0.24129800	-1.53088800
C	-4.38985500	0.08224200	-2.85819000
N	-4.18668100	-0.88268800	-1.74550400
N	4.41057700	-1.10585300	-1.46533800
H	6.30443300	-0.64953200	-2.29255700
H	-4.81453700	-0.43574100	-3.72968000
H	-3.61332200	-1.63507700	-2.12880000
H	4.04163800	-1.14034200	-2.41842000
C	3.59200900	-2.69742200	1.21452400
H	3.77905600	-3.05212700	2.23641000
C	-5.43237800	-1.03783300	1.24381300
H	-6.13105000	-0.84145500	2.06706600
H	5.61468700	-2.00510400	0.84002500
H	2.86932800	-3.38364500	0.76903200
H	-5.15203200	-2.09325600	1.31669600
H	-6.19806800	0.29660500	-0.29302500
C	4.89651700	-2.72188400	0.41875500
C	-5.47634300	-1.49653000	-1.30248200
C	-6.11759300	-0.78300600	-0.10467400
C	4.74034500	-2.51389400	-1.08941800
H	-5.27824800	-2.54039000	-1.03369100
H	3.93171700	-3.14930000	-1.46731400
H	-6.18373300	-1.51641300	-2.14226700
H	5.66005700	-2.81825400	-1.60482700
H	5.34856900	-3.70877900	0.57063500
H	-7.14865500	-1.14683700	-0.02367300
H	-0.59649100	-0.37979000	2.93472500
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O	0.93196000	0.03653100	-1.01577400



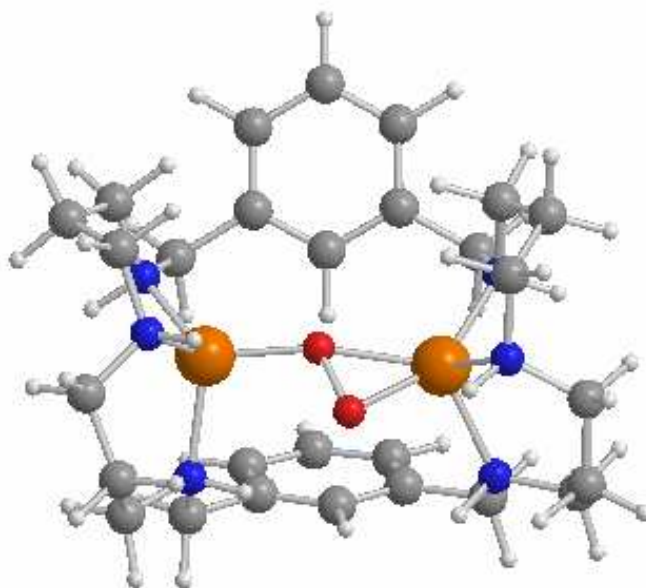
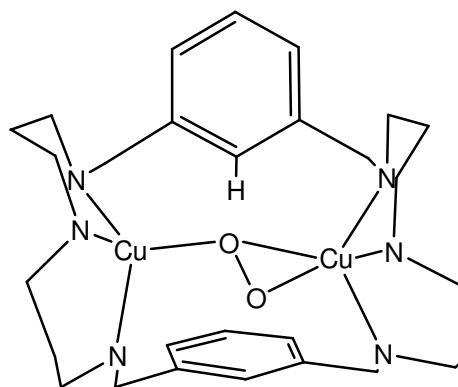
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H	2.16590000	-3.72356600	1.85416300
C	0.24362300	-0.54311700	4.25138600
H	2.33662100	-0.95656200	3.94634200
C	-1.05886600	-0.75392800	3.79569400
C	1.32490800	-1.12862800	3.58827500
C	-1.29745000	-1.58062900	2.68858300
C	1.10978400	-1.95987800	2.48280600
H	-3.39154500	-1.07979200	2.61563400
C	-0.20651700	-2.19963600	2.06932400
H	3.21268000	-2.34013400	2.18800700
C	-2.71284000	-1.83848500	2.21346400
C	2.25261000	-2.62994300	1.75433900
H	-0.37365600	-2.90008100	1.25247200
H	3.01579200	-4.21316100	-0.15426000
H	-4.43569200	-3.21210500	0.75573000
H	-2.19272000	-2.53146900	0.37355800
H	1.34235800	-2.47027000	-0.05948100
H	-4.92128600	-1.52259200	0.66689700
N	-2.83476700	-1.81777500	0.72348900
H	4.22921900	-2.93633100	-0.13817300
N	2.27891100	-2.27007600	0.30169600
C	-4.19729300	-2.25088700	0.28185700
C	3.20480500	-3.17126000	-0.44888900
H	-1.98536700	1.27738100	2.17620200
H	2.80752000	1.30322100	2.30173300
H	3.60344300	-3.88746000	-2.41529600
H	-5.21775700	-3.02180600	-1.42034400
C	3.06231200	-3.04554100	-1.96864200
C	-4.33876300	-2.39177300	-1.24343800
H	2.00865400	-3.18334800	-2.25517900
H	-3.48929200	-2.95739300	-1.65327800
C	-2.13558600	2.10227700	1.47761800
H	-2.77551000	2.84725000	1.96719500
C	2.94660000	2.00892600	1.47876200
H	3.67529300	2.76446500	1.80400200
C	0.40299200	2.05402800	1.31364200
C	-0.80606900	2.74708900	1.14517300
C	1.63789000	2.70572100	1.16496900
H	-1.68678000	4.67619400	0.72161100
C	-0.76360300	4.10915600	0.80573100
H	-3.83423000	1.30876800	0.72493800
C	1.64619600	4.06351500	0.81830700
H	2.59265100	4.59111600	0.73353400
H	4.42451400	0.86825200	0.72208900
Cu	2.70853000	-0.43393700	-0.23121900
Cu	-2.27212800	-0.21665300	-0.45509400
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N	3.54118800	1.22338400	0.34337800
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H	4.63452800	-1.59583700	-2.25203500
C	-4.55730600	-1.10025300	-2.04464300
C	3.60769900	-1.76208400	-2.59791800
N	2.80398400	-0.56365200	-2.25321900
N	-3.33119600	-0.26282400	-2.19481500
H	-4.94795800	-1.34830000	-3.04004300
H	3.65924100	-1.88208700	-3.68987000
H	1.86133800	-0.70738400	-2.62207600
H	-2.69977300	-0.74996900	-2.83416300
C	-3.20560100	2.55925100	-0.73855300
H	-3.61708100	3.45286500	-0.25181000
C	3.92166800	2.10976400	-0.79993800
H	4.67928000	2.83076100	-0.46183900
H	-5.11073100	1.72129600	-1.36258000
H	-2.24926200	2.84367000	-1.18538900
H	3.03205600	2.68048700	-1.08051800
H	5.20570000	0.61343500	-1.71945800
C	-4.18056400	2.08598000	-1.81968800
C	3.35543500	0.66935500	-2.87438200
C	4.43965000	1.34190800	-2.02030900
C	-3.61605900	1.06461100	-2.81026100
H	2.52353700	1.36842300	-3.01533800
H	-2.66884000	1.43376900	-3.21712300
H	3.76067500	0.44248200	-3.87098900
H	-4.31094300	0.94109000	-3.65140400
H	-4.47249800	2.97049400	-2.39762500
H	4.96107300	2.06469800	-2.65851500
H	0.38760000	1.01488300	1.63517500
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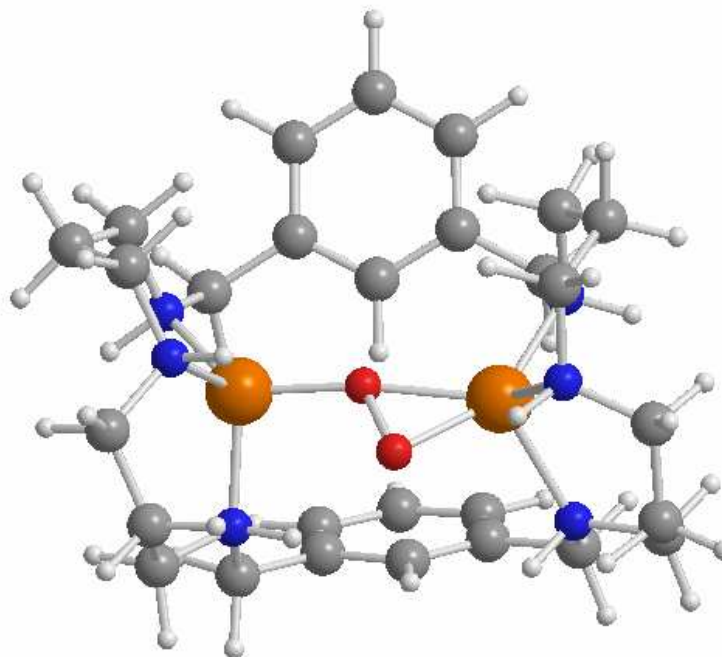
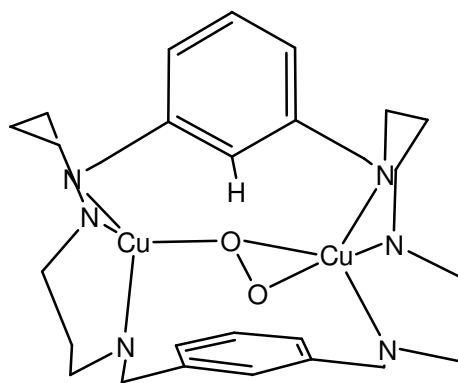
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H	2.02972700	-3.36050300	2.40551400
C	0.08435000	0.06680100	4.30085800
H	2.16610500	-0.43702600	4.06813800
C	-1.21839900	-0.15109200	3.85137600
C	1.15377300	-0.61282300	3.71186000
C	-1.47032300	-1.08009100	2.83192500
C	0.92308900	-1.53903500	2.68724800
H	-3.51919500	-0.47631700	2.58645500
C	-0.39405300	-1.78691300	2.28853000
H	3.02322900	-1.90832500	2.40515100
C	-2.88651000	-1.34165600	2.36245200
C	2.06406000	-2.31367900	2.06795100
H	-0.57369700	-2.53369500	1.52194200
H	2.82284900	-4.28844400	0.46436500
H	-4.78282100	-2.67896900	1.17713100
H	-2.43667600	-2.44916600	0.71679700
H	1.15420100	-2.62069200	0.24304000
H	-4.97751800	-1.01157200	0.64599700
N	-2.97290000	-1.59861900	0.89687900
H	4.04482500	-3.02449100	0.56071400
N	2.07573400	-2.30610100	0.56700800
C	-4.37320800	-1.91578800	0.50040500
C	3.08987700	-3.29040200	0.09192000
H	-2.40086200	1.78258100	1.74702500
H	2.41391200	1.35016400	2.21105900
H	3.89056600	-4.21238200	-1.64919700
H	-5.49377600	-2.86214100	-1.04777000
C	3.26205600	-3.34297900	-1.42551300
C	-4.50038600	-2.41059600	-0.94538500
H	2.29765800	-3.53777400	-1.91682400
H	-3.78747800	-3.22829300	-1.12923300
C	-2.33235500	2.40851400	0.85238000
H	-3.07975500	3.20655700	0.94099600
C	2.66556800	2.00920900	1.37578300
H	3.48112100	2.66909900	1.69973300
C	0.18048600	2.27557100	1.07030700
C	-0.95627700	3.02106800	0.74150500
C	1.46059900	2.83372700	0.99157200
H	-1.67552700	4.96525700	0.13104100
C	-0.80111900	4.35965500	0.35553200
H	-3.72239700	1.35076500	-0.16524800
C	1.59455800	4.17415200	0.60304400
H	2.57878100	4.63483200	0.57179100
H	3.97563200	0.63351700	0.69572400
Cu	2.01899700	-0.49224300	-0.38380700
Cu	-1.90669400	-0.31042100	-0.48792200
C	0.46832900	4.93425700	0.28772300
H	0.57779000	5.97698400	0.00631800
N	-2.72613800	1.53028500	-0.31418800
N	3.18115800	1.12170500	0.27221000
H	-5.03401200	-0.50156100	-1.79198600
H	4.81762300	-1.83405900	-1.46388900
C	-4.37723300	-1.34311000	-2.03581800
C	3.93224400	-2.11540400	-2.04373000
N	3.01405000	-0.94374100	-2.09356900
N	-2.99481700	-0.82055100	-2.19952200
H	-4.73062900	-1.75112400	-2.99312000
H	4.27184300	-2.34740800	-3.06169300
H	2.22804400	-1.23877900	-2.67954800
H	-2.41804800	-1.59531800	-2.53246700
C	-2.63373100	2.26419600	-1.61668800
H	-3.00717100	3.28662600	-1.47620000
C	3.76840900	1.93119900	-0.83635800
H	4.45949500	2.67260000	-0.41167300
H	-4.48839500	1.54100600	-2.47228800
H	-1.57398800	2.34013200	-1.87591200
H	2.95256800	2.48554200	-1.31016200
H	5.28100300	0.47175900	-1.39019600
C	-3.42706700	1.60573700	-2.74758500
C	3.61949300	0.23887100	-2.77887200
C	4.51239600	1.08984400	-1.87480200
C	-2.90628500	0.24956200	-3.23055900
H	2.79238200	0.85243300	-3.15307000
H	-1.84930800	0.34151200	-3.50474900
H	4.19032100	-0.10663900	-3.65035100
H	-3.45544800	-0.05044800	-4.13390900
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H	0.06614600	1.25421800	1.41761500
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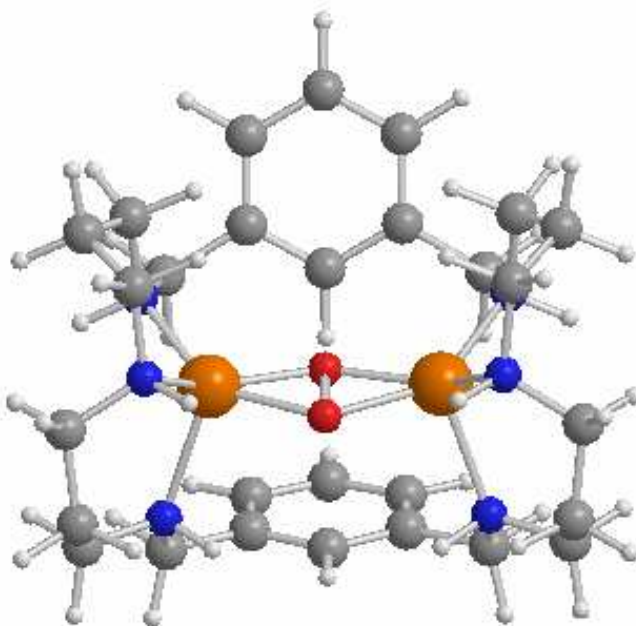
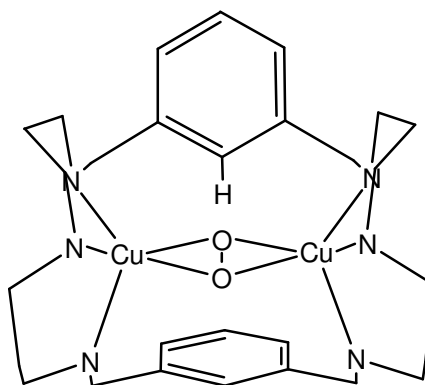
TS-de

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H	1.721278	-3.298091	2.602257
C	-0.019943	0.324565	4.355286
H	2.029084	-0.322263	4.184019
C	-1.326619	0.175174	3.889500
C	1.013559	-0.447004	3.815676
C	-1.621941	-0.774214	2.900088
C	0.737780	-1.395685	2.824736
H	-3.604967	-0.028410	2.529745
C	-0.585195	-1.568012	2.405705
H	2.813133	-1.917954	2.559372
C	-3.041383	-0.959067	2.404169
C	1.826168	-2.265328	2.237778
H	-0.799090	-2.326201	1.659790
H	2.445457	-4.312353	0.718666
H	-5.004147	-2.252254	1.265341
H	-2.644140	-2.243232	0.876720
H	0.867979	-2.522500	0.420575
H	-5.054594	-0.616670	0.616856
N	-3.108487	-1.337648	0.964083
H	3.743501	-3.129463	0.600965
N	1.818036	-2.294037	0.739938
C	-4.519912	-1.572603	0.550023
C	2.733090	-3.364677	0.244470
H	-2.128540	1.955370	1.632008
H	2.662395	1.296493	2.189690
H	3.204629	-4.512663	-1.482456
H	-5.672470	-2.542749	-0.959447
C	2.736551	-3.543171	-1.277238
C	-4.652029	-2.154846	-0.862158
H	1.706084	-3.621861	-1.651343
H	-3.994947	-3.029951	-0.975139
C	-2.031288	2.538480	0.712045
H	-2.712283	3.395431	0.782847
C	2.942256	1.873501	1.303597
H	3.802349	2.502523	1.567089
O	0.142095	-0.351104	-0.526568
C	0.474131	2.255335	0.950929
C	-0.614675	3.043371	0.559524
C	1.785316	2.737653	0.860128
H	-1.211111	4.983110	-0.182331
C	-0.375990	4.342972	0.090491
H	-3.531328	1.574011	-0.239603
O	-0.557489	-1.565126	-0.865417
C	2.001024	4.039407	0.386956
H	3.010897	4.439151	0.341736
H	4.128102	0.342094	0.708390
Cu	1.977402	-0.567821	-0.263059
Cu	-1.894070	-0.259810	-0.499754
C	0.924733	4.839195	0.003618
H	1.097255	5.853120	-0.343645
N	-2.525519	1.651955	-0.410790
N	3.374578	0.873078	0.261930
H	-5.032341	-0.271935	-1.838192
H	4.491169	-2.324431	-1.608581
C	-4.434277	-1.171693	-2.015220
C	3.510154	-2.485940	-2.069149
N	2.801607	-1.179118	-2.121685
N	-3.015032	-0.759396	-2.184553
H	-4.799582	-1.614054	-2.952335
H	3.695011	-2.848228	-3.089856
H	1.952329	-1.338773	-2.667196
H	-2.492365	-1.587955	-2.474814
C	-2.392587	2.316108	-1.746847
H	-2.685310	3.369349	-1.650031
C	4.009602	1.551289	-0.912206
H	4.798552	2.222345	-0.546115
H	-4.307516	1.697217	-2.550630
H	-1.333667	2.298293	-2.019231
H	3.245441	2.178464	-1.381149
H	5.269455	-0.138288	-1.444539
C	-3.247946	1.668243	-2.838316
C	3.589482	-0.134519	-2.834787
C	4.605079	0.583618	-1.940029
C	-2.837888	0.254844	-3.260299
H	2.878009	0.598695	-3.231404
H	-1.776883	0.248437	-3.534106
H	4.106303	-0.580163	-3.695743
H	-3.408736	-0.039710	-4.151683
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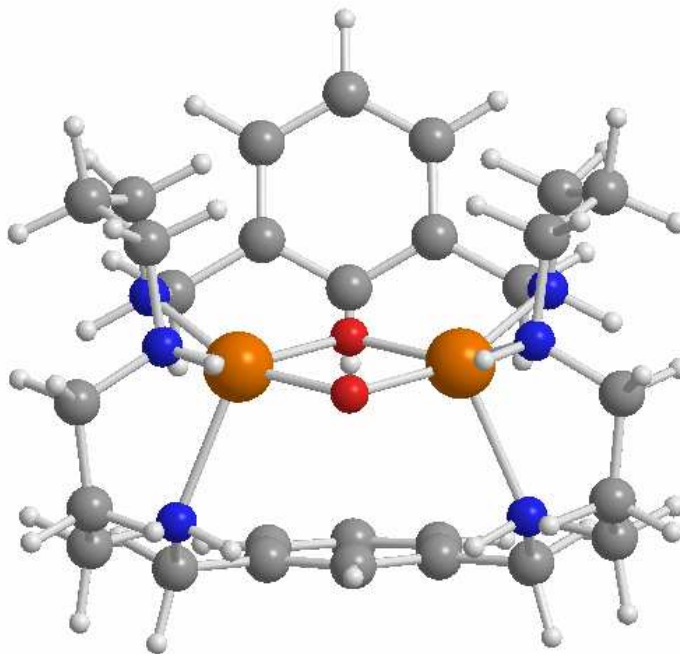
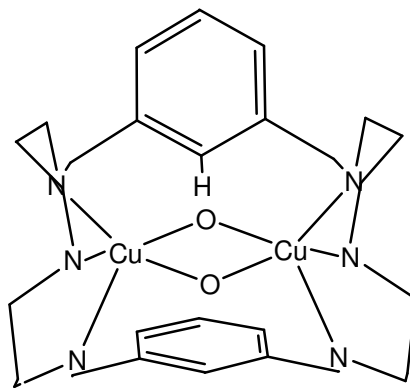
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H	2.752086	-3.278467	2.286776
C	0.000449	-0.554980	4.301422
H	2.148693	-0.630082	4.172770
C	-1.209482	-0.955121	3.731352
C	1.209962	-0.955937	3.731034
C	-1.220407	-1.793838	2.609162
C	1.220026	-1.794642	2.608828
H	-3.347381	-1.622748	2.371145
C	-0.000408	-2.234236	2.089392
H	3.347098	-1.625230	2.370481
C	-2.526915	-2.240037	1.991264
C	2.526042	-2.241674	1.990502
H	-0.000728	-2.923531	1.247928
H	3.956245	-3.726475	0.379907
H	-3.959159	-3.723908	0.381858
H	-1.791431	-2.744682	0.159818
H	1.789612	-2.744741	0.158982
H	-4.634527	-2.098804	0.359774
N	-2.541273	-2.139377	0.500306
H	4.633458	-2.102127	0.358958
N	2.540180	-2.140397	0.499582
C	-3.810308	-2.712829	-0.024054
C	3.808520	-2.714934	-0.025269
H	-2.444238	1.223764	2.146569
H	2.443501	1.222519	2.147224
H	4.744649	-3.392330	-1.815406
H	-4.747098	-3.390646	-1.813704
C	3.877752	-2.775103	-1.553380
C	-3.879624	-2.774041	-1.552119
H	3.004832	-3.309978	-1.956953
H	-3.007205	-3.310036	-1.955290
C	-2.508614	2.014127	1.393651
C	-3.340358	2.676991	1.663253
C	2.508626	2.013082	1.394584
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O	-0.000001	0.087405	-0.074733
C	0.000014	2.140241	1.521746
C	-1.218755	2.798300	1.337641
C	1.219120	2.797807	1.338118
H	-2.145467	4.721369	0.989451
C	-1.209037	4.178014	1.088718
H	-3.818724	0.963812	0.260238
O	-0.000037	-0.953691	-1.134834
C	1.210052	4.177533	1.089222
H	2.146736	4.720523	0.990356
H	3.818846	0.962480	0.261542
Cu	1.810943	-0.294184	-0.538434
Cu	-1.810959	-0.294039	-0.538443
C	0.000667	4.867656	0.987604
H	0.000915	5.940616	0.822707
N	-2.877701	1.328318	0.088480
N	2.878100	1.327517	0.089390
H	-4.832497	-0.847336	-1.767434
H	4.832160	-0.848955	-1.767093
C	-4.049214	-1.430081	-2.262518
C	4.048578	-1.430774	-2.262793
N	2.800707	-0.616448	-2.276388
N	-2.800740	-0.616681	-2.276338
H	-4.377576	-1.593732	-3.297640
H	4.377083	-1.593952	-3.297943
H	2.106633	-1.162984	-2.790747
H	-2.106980	-1.163974	-2.790316
C	-3.020172	2.311928	-1.028294
H	-3.583710	3.182610	-0.668465
C	3.021713	2.311479	-1.026930
H	3.585736	3.181600	-0.666504
H	-4.732015	1.384218	-1.986547
H	-2.016855	2.660622	-1.287917
H	2.018749	2.661010	-1.286788
H	4.733226	1.382904	-1.984951
C	-3.729013	1.739657	-2.257615
C	2.960934	0.664899	-3.026778
C	3.730594	1.739227	-2.256226
C	-2.959899	0.664399	-3.027419
H	1.952756	1.028644	-3.255079
H	-1.951409	1.027319	-3.255646
H	3.464391	0.466524	-3.982208
H	-3.463251	0.465891	-3.982876
H	-3.896839	2.573178	-2.949493
H	3.899299	2.572936	-2.947666
H	-0.000244	1.092057	1.794510



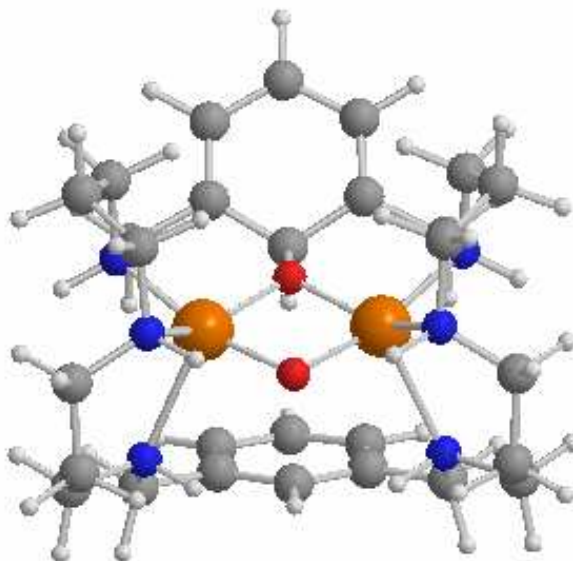
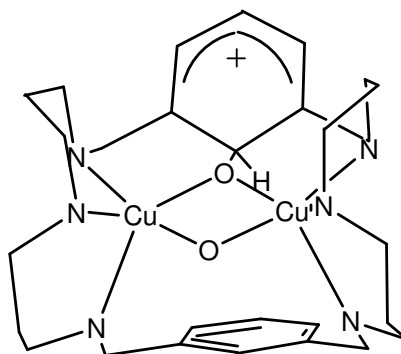
TS-eg

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H	-2.14929900	-0.08621300	4.38401600
H	2.80391200	-2.77254500	2.75938000
C	-0.00015500	-0.00426500	4.50379000
H	2.14899900	-0.08603200	4.38414700
C	-1.21146900	-0.43161400	3.95529100
C	1.21122500	-0.43151300	3.95536400
C	-1.22160300	-1.31850400	2.87046000
C	1.22150600	-1.31839200	2.87052400
H	-3.33376500	-1.11443900	2.52838600
C	-0.00001200	-1.77054900	2.36601700
H	3.33362700	-1.11398300	2.52846000
C	-2.52712900	-1.81563800	2.28666800
C	2.52713000	-1.81536500	2.28680800
H	0.00003000	-2.48273900	1.54646400
H	3.89234600	-3.57732400	0.90875600
H	-3.89237900	-3.57736200	0.90855400
H	-1.72529100	-2.61289100	0.59127400
H	1.72536400	-2.61282900	0.59148900
H	-4.57774200	-1.99275500	0.57071700
N	-2.49177600	-1.97416300	0.80763000
H	4.57783000	-1.99272100	0.57114500
N	2.49182600	-1.97405700	0.80779400
C	-3.72784000	-2.64869600	0.34141000
C	3.72792300	-2.64860000	0.34167400
H	-2.44852900	1.36293300	1.94166000
H	2.44822000	1.36310400	1.94188300
H	4.55344300	-3.64787700	-1.35267800
H	-4.55313300	-3.64815600	-1.35295700
C	3.71337500	-2.97268700	-1.15378300
C	-3.71311600	-2.97291300	-1.15402100
H	2.80913800	-3.54302400	-1.41356200
H	-2.80882700	-3.54323400	-1.41365200
C	-2.51029700	2.06533000	1.10658800
H	-3.35501300	2.74236500	1.28643600
C	2.51000800	2.06550300	1.10681400
H	3.35466000	2.74259900	1.28673100
O	-0.00002100	0.52442100	-0.08438200
C	-0.00016100	2.23861100	1.31606900
C	-1.22415600	2.84808900	0.97791600
C	1.22382400	2.84817200	0.97802900
H	-2.14657300	4.65793900	0.24939300
C	-1.21158600	4.14915600	0.46825200
H	-3.73270300	0.80532300	0.08161100
O	0.00008600	-1.11429600	-1.15384600
C	1.21121200	4.14923800	0.46836300
H	2.14618500	4.65808500	0.24959100
H	3.73260800	0.80560700	0.08192400
Cu	1.57616800	-0.27945700	-0.60293000
Cu	-1.57613000	-0.27954800	-0.60309600
C	-0.00019900	4.81173600	0.24856700
H	-0.00021700	5.83437800	-0.11569600
N	-2.83163000	1.24257500	-0.12578200
N	2.83150800	1.24277200	-0.12553100
H	-4.68319800	-1.13445000	-1.72154100
H	4.68337300	-1.13407700	-1.72098100
C	-3.87153600	-1.77163800	-2.08601600
C	3.87183700	-1.77131700	-2.08565000
N	2.64309600	-0.93652200	-2.20629000
N	-2.64286300	-0.93672200	-2.20653000
H	-4.16133600	-2.11218500	-3.08937000
H	4.16184200	-2.11174600	-3.08898300
H	1.92184300	-1.52493700	-2.62982300
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C	-3.03606100	2.09721000	-1.33425700
H	-3.67157500	2.95188200	-1.06669500
C	3.03594000	2.09742900	-1.33399100
H	3.67134300	2.95216800	-1.06637700
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H	-2.05875700	2.49477200	-1.62076400
H	2.05861600	2.49488800	-1.62057000
H	4.67412600	0.99024500	-2.22435600
C	-3.67776700	1.35360800	-2.50676000
C	2.84057400	0.22759200	-3.12038900
C	3.67781000	1.35389700	-2.50644800
C	-2.84038000	0.22738100	-3.12063800
H	1.84457400	0.60503000	-3.37798800
H	-1.84439600	0.60491100	-3.37816400
H	3.31452600	-0.11361900	-4.05013800
H	-3.31423500	-0.11387000	-4.05042200
H	-3.85463800	2.09289300	-3.29651400
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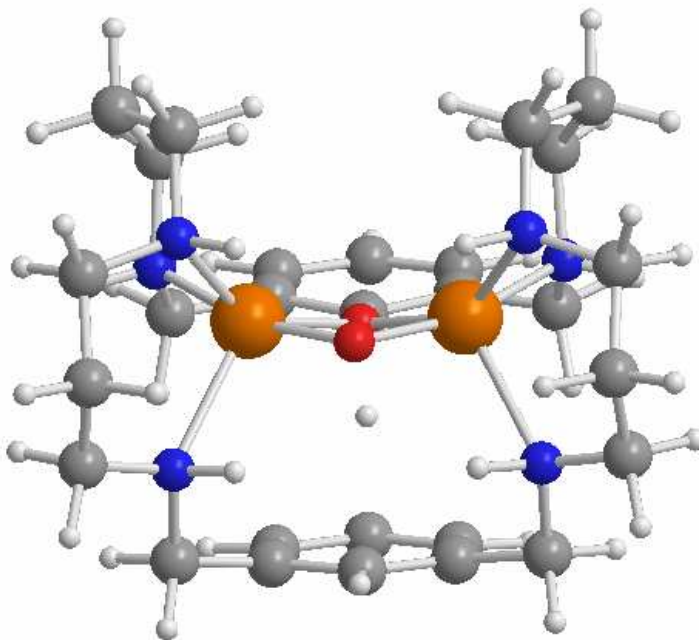
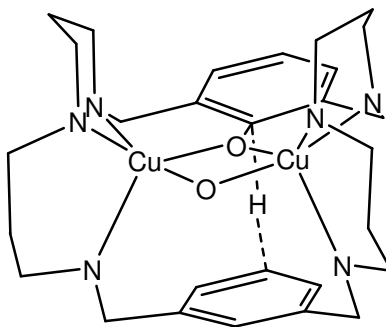
g

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H	1.278973	3.684623	2.800200
H	-1.871187	4.030127	2.150814
H	1.276253	3.683500	-2.800890
C	-1.990715	4.110422	0.000824
H	-1.872848	4.028410	-2.149190
C	-1.371772	3.796099	1.213643
C	-1.372739	3.795062	-1.212222
C	-0.104802	3.198115	1.222688
C	-0.105714	3.197198	-1.221799
H	-0.123024	2.768887	3.332211
C	0.520666	2.945155	0.000301
H	-0.125371	2.766051	-3.330914
C	0.603943	2.859760	2.517215
C	0.602217	2.858260	-2.516624
H	1.520603	2.524837	0.000061
H	2.784949	2.327854	-3.844573
H	2.787170	2.327936	3.843990
H	2.013182	1.657600	1.653127
H	2.013539	1.658370	-1.652907
H	1.547870	1.272859	4.511604
N	1.367908	1.585834	2.440177
H	1.545943	1.271481	-4.510677
N	1.367523	1.585171	-2.439217
C	2.210516	1.411515	3.647014
C	2.209225	1.411031	-3.646723
H	-1.893014	1.116281	2.597893
H	-1.892713	1.115930	-2.598466
H	3.889289	0.309232	-4.364936
H	3.889903	0.308251	4.364450
C	3.178123	0.231873	-3.534657
C	3.178337	0.231517	3.534456
H	3.779912	0.318687	-2.618565
H	3.779835	0.317868	2.618136
C	-2.193083	0.062312	2.567127
H	-2.887173	-0.118059	3.397117
C	-2.192664	0.061922	-2.567642
H	-2.886773	-0.118543	-3.397599
O	-0.809790	-0.362599	-0.000071
C	-2.154414	0.170913	-0.000173
C	-2.863764	-0.254395	1.261188
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H	-4.595719	-1.113677	2.153704
C	-4.095563	-0.856214	1.222858
H	-0.581186	-0.431054	3.716363
O	1.597057	-0.402736	0.000357
C	-4.095244	-0.856481	-1.223447
H	-4.595205	-1.114090	-2.154356
H	-0.580718	-0.431350	-3.716819
Cu	0.473373	-0.401990	-1.452008
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C	-4.744190	-1.146135	-0.000348
H	-5.725816	-1.606945	-0.000426
N	-0.941435	-0.737338	2.810177
N	-0.940924	-0.737591	-2.810606
H	1.823918	-1.176765	4.447588
H	1.824829	-1.177416	-4.447693
C	2.539679	-1.154761	3.619793
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N	1.834248	-1.575483	2.377243
H	3.308369	-1.906336	3.846219
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H	2.513557	-1.589375	-1.612241
H	2.512759	-1.589188	1.612080
C	-1.205873	-2.204719	2.896559
H	-2.053042	-2.377756	3.572975
C	-1.205164	-2.205004	-2.896911
H	-2.052296	-2.378266	-3.573324
H	0.255931	-2.714022	4.414973
H	-1.511253	-2.532897	1.899122
H	-1.510485	-2.533192	-1.899456
H	0.256860	-2.714030	-4.415195
C	0.004138	-3.002607	3.386678
C	1.244543	-2.940322	-2.488089
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H	0.984562	-3.258605	-1.472343
H	0.983877	-3.258515	1.472144
H	2.005071	-3.635310	-2.868002
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H	-0.302016	-4.053120	3.448996
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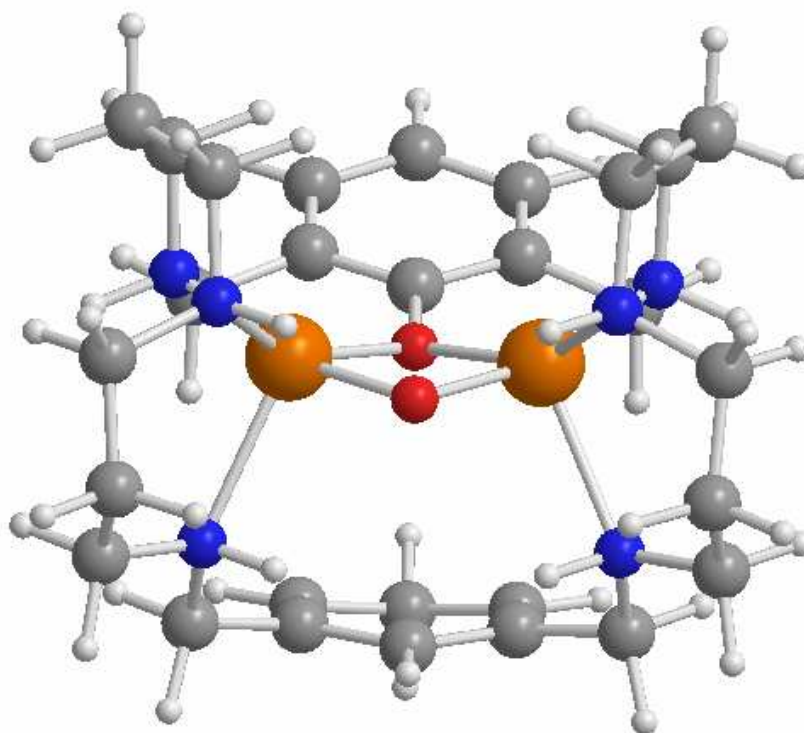
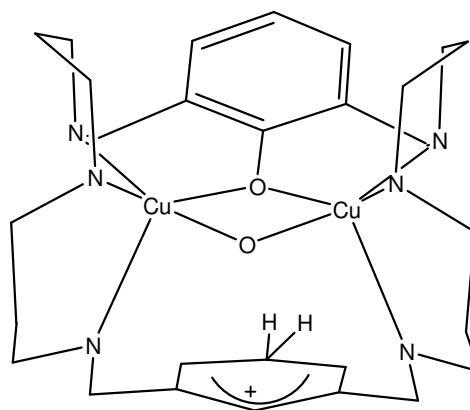
TS-gh

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O	1.65368900	0.10683700	0.00000000
H	-2.41745300	2.77733100	2.16018100
H	-2.89551700	-0.75317500	-3.36510200
H	-4.79013000	-1.06114200	-2.14558600
H	-1.72084100	-2.84937600	-3.23639000
H	0.57323400	-2.77089300	-4.23066500
H	-0.57862400	-0.71345800	-3.67989800
H	1.47075000	1.48937900	4.52586800
H	-2.11192900	0.70929600	-2.76439500
H	-0.30261500	2.90747700	-3.37676900
C	-2.22961200	-0.36574200	-2.58267800
H	-2.41745300	2.77733100	2.16018100
H	2.00179200	-0.97184800	-4.40951800
C	-4.25699700	-0.89891100	-1.21278800
H	0.29946400	-4.14780800	-3.19498600
C	-0.87636600	-2.44975600	-2.65770900
H	-5.98469800	-1.32980700	0.00000000
N	-0.87447500	-0.96000300	-2.73356500
C	0.42788500	-3.05932900	-3.18086600
C	2.09554100	1.68762600	-3.64487900
H	2.58762900	2.65689600	-3.82114300
H	3.87760200	0.75353200	-4.34499900
C	-2.90660600	-0.56641900	-1.24789800
C	-4.93294600	-1.06156500	0.00000000
C	0.34150000	2.96759800	-2.49305300
H	0.93950200	3.88734200	-2.59529200
C	-1.86759900	2.81495700	-1.22381400
C	2.70342300	-0.84866200	-3.57616800
H	3.56363100	-1.49895900	-3.79149400
H	-1.03826100	-2.72429700	-1.60900900
H	-3.66049800	2.73171300	0.00000000
C	3.17665400	0.60810000	-3.51500900
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C	-0.48875200	3.00798600	-1.22937300
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H	2.52353900	-3.34517900	-2.74519000
C	1.68445400	-2.75037000	-2.35730700
N	2.04344200	-1.31124000	-2.33008900
Cu	0.54548500	-0.20988900	-1.45387300
C	-4.25699700	-0.89891100	-1.21278800
H	3.76075000	0.77249100	-2.59849400
H	1.80231300	1.81861800	-1.62709100
H	1.51986700	-3.05671100	-1.31745700
H	-4.79013000	-1.06114200	-2.14558600
H	2.68010200	-1.15269900	-1.54393000
C	-2.90660600	-0.56641900	-1.24789800
C	0.16826600	3.14772200	0.00000000
C	-1.86759900	2.81495700	-1.22381400
H	1.23796200	3.34414100	0.00000000
C	-0.48875200	3.00798600	-1.22937300
H	-2.11192900	0.70929600	-2.76439500
C	-2.22961200	-0.36574200	-2.58267800
H	-1.03826100	-2.72429700	-1.60900900
H	-2.89551700	-0.75317500	-3.36510200
Cu	0.54548500	-0.20988900	-1.45387300
C	0.34150000	2.96759800	-2.49305300
N	-0.87447500	-0.96000300	-2.73356500
C	-0.87636600	-2.44975600	-2.65770900
H	-1.72084100	-2.84937600	-3.23639000
H	1.80231300	1.81861800	-1.62709100
H	0.93950200	3.88734200	-2.59529200
H	-0.30261500	2.90747700	-3.37676900
H	1.51986700	-3.05671100	-1.31745700
N	1.21043500	1.76466500	-2.46131000
H	-0.57862400	-0.71345800	-3.67989800
H	2.68010200	-1.15269900	-1.54393000
N	2.04344200	-1.31124000	-2.33008900
C	1.68445400	-2.75037000	-2.35730700
C	0.42788500	-3.05932900	-3.18086600
H	0.29946400	-4.14780800	-3.19498600
H	2.52353900	-3.34517900	-2.74519000
C	2.09554100	1.68762600	-3.64487900
H	3.76075000	0.77249100	-2.59849400
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H	0.57323400	-2.77089300	-4.23066500
H	1.47075000	1.48937900	4.52586800
C	3.17665400	0.60810000	-3.51500900
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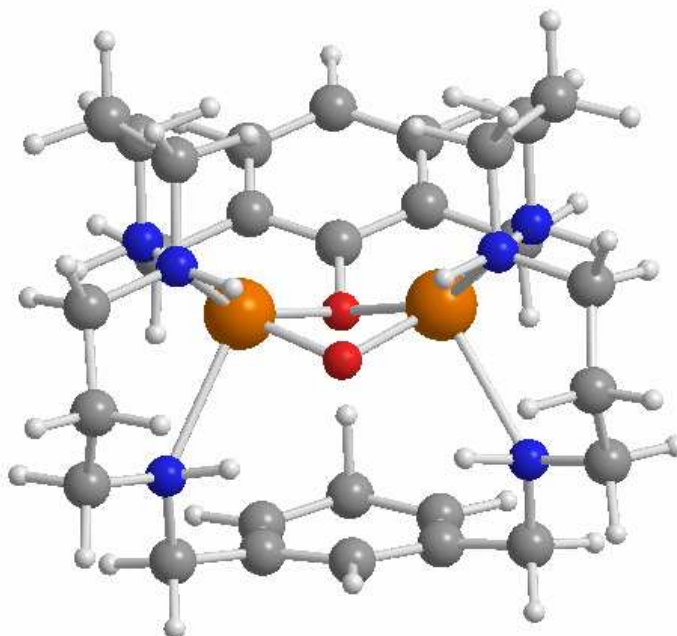
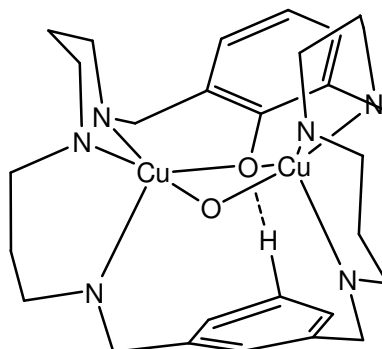
h

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O	1.624728	0.199739	0.000000
H	-3.059626	2.671734	2.198182
H	-2.647801	-1.150482	-3.353082
H	-4.272932	-2.223731	-2.142573
H	-1.089101	-3.014857	-3.503306
H	1.211278	-2.548975	-4.326416
H	-0.382327	-0.695162	-3.695857
H	1.143623	1.774327	-4.455651
H	-2.116071	0.344725	-2.564395
H	-0.962355	2.620800	-3.357903
C	-2.047811	-0.747987	-2.528457
H	-3.059626	2.671734	-2.198182
H	2.118774	-0.503623	-4.363203
C	-3.794494	-1.971374	-1.199656
H	1.137295	-3.985702	-3.340319
C	-0.356976	-2.551610	-2.829585
H	-5.330057	-2.895508	0.000000
N	-0.607522	-1.081086	-2.776637
C	1.058144	-2.893625	-3.295888
C	1.695897	2.078336	-3.556796
H	1.972463	3.132907	-3.706220
H	3.645166	1.546038	-4.237919
C	-2.588919	-1.260722	-1.219403
C	-4.397694	-2.341392	0.000000
C	-0.344567	2.912941	-2.502307
H	0.052045	3.916776	-2.726005
C	-2.531063	2.792730	-1.255005
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H	3.755456	-0.743981	-3.760129
H	-0.546763	-2.948416	-1.827295
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C	2.973398	1.246322	-3.425519
N	0.787988	1.945612	-2.393644
C	-1.172244	2.949849	-1.238394
C	-3.354296	2.851260	0.000000
H	3.143613	-2.774429	-2.736921
C	2.178945	-2.386809	-2.384173
N	2.253852	-0.900748	-2.294185
Cu	0.571347	-0.199694	-1.448129
C	-3.794494	-1.971374	1.199656
H	3.501316	1.499431	-2.494864
H	1.326487	2.207463	-1.565859
H	2.026835	-2.759763	-1.364697
H	-4.272932	-2.223731	2.142573
H	2.877894	-0.664536	-1.519138
C	-2.588919	-1.260722	1.219403
C	-0.498974	3.137903	0.000000
C	-2.531063	2.792730	1.255005
H	0.556238	3.401071	0.000000
C	-1.172244	2.949849	1.238394
H	-2.116071	0.344725	2.564395
C	-2.047811	-0.747987	2.528457
H	-0.546763	-2.948416	1.827295
H	-2.647801	-1.150482	3.353082
Cu	0.571347	-0.199694	1.448129
C	-0.344567	2.912941	2.502307
N	-0.607522	-1.081086	2.776637
C	-0.356976	-2.551610	2.829585
H	-1.089101	-3.014857	3.503306
H	1.326487	2.207463	1.565859
H	0.052045	3.916776	2.726005
H	-0.962355	2.620800	3.357903
H	2.026835	-2.759763	1.364697
N	0.787988	1.945612	2.393644
H	-0.382327	-0.695162	3.695857
H	2.877894	-0.664536	1.519138
N	2.253852	-0.900748	2.294185
C	2.178945	-2.386809	2.384173
C	1.058144	-2.893625	3.295888
H	1.137295	-3.985702	3.340319
H	3.143613	-2.774429	2.736921
C	1.695897	2.078336	3.556796
H	3.501316	1.499431	2.494864
H	1.972463	3.132907	3.706220
H	1.211278	-2.548975	4.326416
H	1.143623	1.774327	4.455651
C	2.973398	1.246322	3.425519
C	2.791645	-0.268547	3.532753
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H	3.755456	-0.743981	3.760129
H	3.645166	1.546038	4.237919



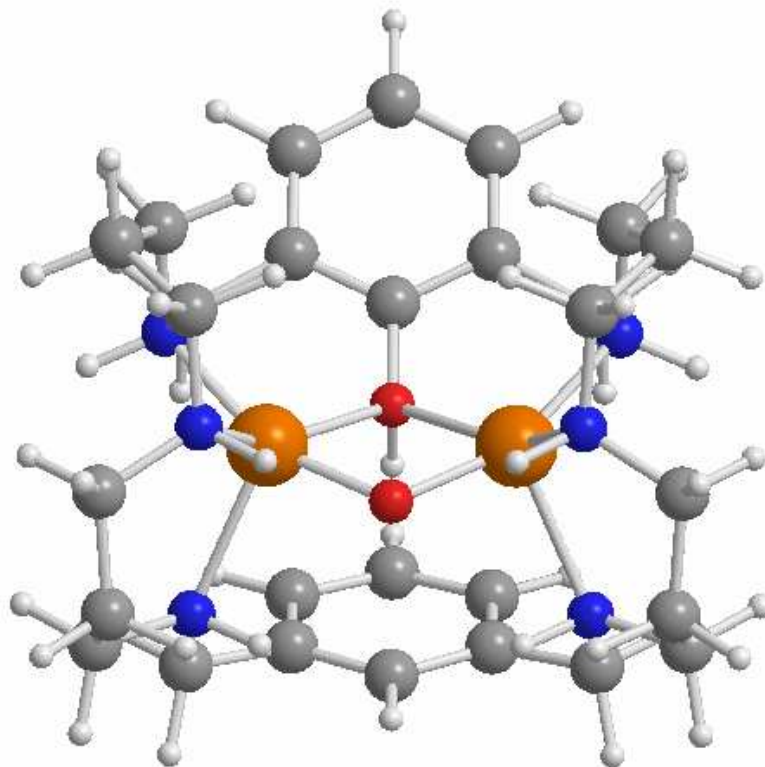
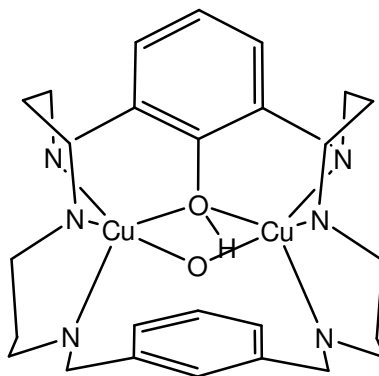
TS-hi

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O	-0.00015000	0.85920100	0.87613500
H	-0.00004700	0.49675900	2.69620200
O	0.00024700	-1.29859400	-0.60506800
H	-2.18129600	-0.32980200	3.71982600
H	3.35519000	2.89906800	1.17580200
H	2.14258700	4.84688700	1.35504700
H	3.38664900	3.12604900	-1.22530600
H	4.16306300	1.20820200	-2.61042800
H	3.65614300	0.97859000	-0.12643700
H	4.58322100	-2.41525700	0.24384800
H	2.61229200	1.46852000	1.89549900
H	3.39092200	-2.14262200	2.56831600
C	2.53133100	2.18293000	1.06787000
H	2.18142700	-0.32909700	3.71985200
H	4.32370700	-0.89539300	-1.78107700
C	1.19971900	4.31094700	1.27941200
H	3.11183400	2.28938700	-3.48814000
C	2.71502600	2.27424700	-1.39629100
H	-0.00147700	6.08778100	1.50692900
N	2.72275400	1.39149100	-0.18959500
C	3.12278400	1.55027700	-2.67886800
C	3.64167100	-2.89892200	-0.04661400
H	3.71437200	-3.94902200	0.27997400
H	4.31656000	-3.46124100	-1.98477000
C	1.21785900	2.92225400	1.10542600
C	-0.00120500	5.01189400	1.36840500
C	2.49949400	-2.55108500	2.08095100
H	2.51466300	-3.64187500	2.24351000
C	1.24793100	-0.80511400	3.43123300
C	3.52546400	-1.49772300	-2.22857400
H	3.77888600	-1.61830200	-3.29151900
H	1.70305500	2.67962800	-1.49258100
H	-0.00009300	0.62253600	4.51344400
C	3.48874800	-2.87697900	-1.56728700
N	2.53478900	-2.21070700	0.64480700
C	1.24748900	-1.95267300	2.67116300
C	0.00003000	-0.10527500	3.70051600
H	2.47374100	0.05126100	-4.09310100
C	2.20411800	0.39555500	-3.08508500
N	2.24511600	-0.74383900	-2.13273200
Cu	1.41047400	-0.13328300	-0.33655300
C	-1.20177300	4.31031100	1.27963300
H	2.57206000	-3.40868700	-1.86137800
H	1.64556200	-2.49234800	0.21986100
H	1.16667100	0.74877000	-3.12639500
H	-2.14490900	4.84575500	1.35544700
H	1.47897400	-1.38188100	-2.36027400
C	-1.21921500	2.92161000	1.10564600
C	0.00042800	-2.50301000	2.30752600
C	-1.24764400	-0.80550800	3.43119900
H	0.00058800	-3.41652300	1.71685000
C	-1.24682600	-1.95302200	2.67106600
H	-2.61269000	1.46705400	1.89588600
C	-2.53230400	2.18159000	1.06831300
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H	-3.35652400	2.89727200	1.17650800
Cu	-1.41047900	-0.13388300	-0.33643300
C	-2.49860600	-2.55180100	2.08073800
N	-2.72357400	1.39016900	-0.18918800
C	-2.71663900	2.27307700	-1.39577800
H	-3.38874800	3.12444600	-1.22454200
H	-1.64370200	-2.49290400	0.22003600
H	-2.51373400	-3.64252000	2.24378800
H	-3.39020500	-2.14318600	2.56766300
H	-1.16761300	0.74905900	-3.12648400
N	-2.53347600	-2.21208600	0.64441200
H	-3.65671200	0.97672400	-0.12586300
H	-1.47815500	-1.38193100	-2.36048300
N	-2.24475000	-0.74448900	-2.13279500
C	-2.20478700	0.39505600	-3.08498600
C	-3.12421900	1.54902300	-2.67835800
H	-3.11407100	2.28827200	-3.48751100
H	-2.47439000	0.05072200	-4.09299500
C	-3.63918800	-2.90185100	-0.04730900
H	-2.56898600	-3.40945200	-1.86233100
H	-3.71012900	-3.95221800	0.27882300
H	-4.16421000	1.20611900	-2.60966900
H	-4.58154200	-2.41988500	0.24336100
C	-3.48628800	-2.87896400	-1.56796400
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H	-4.32306700	-0.89795700	-1.78026400
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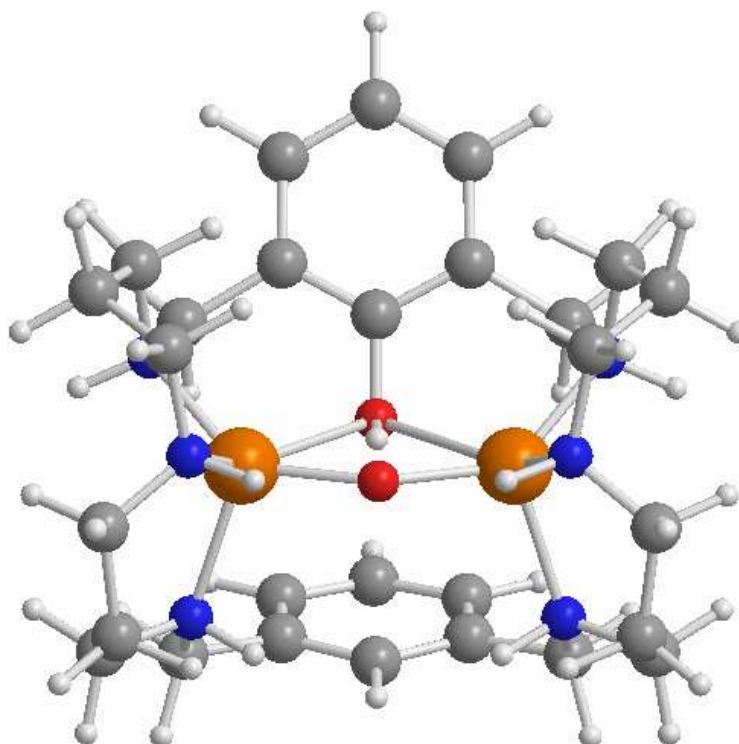
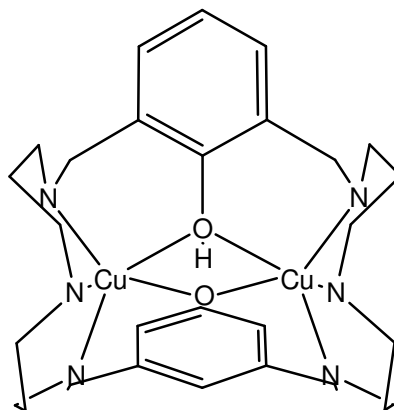
i

C	-0.000276	2.341542	0.547223
O	-0.000473	0.937415	0.685640
H	-0.001345	0.698083	1.637370
O	-0.000082	-1.389265	-0.665606
H	-2.149733	0.718638	4.057218
H	3.358035	2.975270	0.598809
H	2.147025	4.936811	0.240625
H	3.451833	2.738764	-1.769462
H	4.362530	0.575663	-2.648028
H	3.702632	0.852889	-0.263303
H	4.484647	-1.984126	0.714278
H	2.571901	1.730335	1.575440
H	3.357402	-0.964442	2.786676
C	2.533772	2.252090	0.613107
H	2.154015	0.715787	4.056564
H	4.405635	-1.454775	-1.724044
C	1.208294	4.392801	0.298045
H	3.438699	1.487500	-3.813096
C	2.817650	1.842870	-1.809051
H	0.000483	6.163098	0.091409
N	2.766049	1.219378	-0.449471
C	3.342866	0.900925	-2.892097
C	3.596091	-2.624138	0.639081
H	3.771914	-3.481860	1.305578
H	4.237849	-3.876192	-0.959126
C	1.228140	3.001981	0.466669
C	0.000269	5.085261	0.217148
C	2.500079	-1.614792	2.584959
H	2.693480	-2.564639	3.108763
C	1.215570	0.234264	3.792990
C	3.546209	-2.106901	-1.913853
H	3.741440	-2.617406	-2.867399
H	1.804225	2.176779	-2.053876
H	0.002923	1.755898	4.724015
C	3.438167	-3.145068	-0.793777
N	2.424014	-1.847979	1.114858
C	1.224365	-0.983565	3.097073
C	0.002234	0.825544	4.164114
H	2.822515	-0.821986	-4.090588
C	2.446682	-0.302366	-3.198584
N	2.336446	-1.255576	-2.065867
Cu	1.517445	-0.400125	-0.407372
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H	2.497923	-3.706585	-0.888801
H	1.597783	-2.423945	0.937796
H	1.431887	0.045859	-3.424360
H	-2.146553	4.937480	0.239057
H	1.529352	-1.862506	-2.232349
C	-1.228429	3.002368	0.465786
C	0.000421	-1.598902	2.814044
C	-1.212010	0.235860	3.793372
H	-0.000265	-2.566495	2.318776
C	-1.222651	-0.982083	3.097619
H	-2.573670	1.731602	1.573824
C	-2.534413	2.252905	0.611276
H	-1.802084	2.175394	-2.055315
H	-3.358473	2.976294	0.595844
Cu	-1.517351	-0.399708	-0.407361
C	-2.499471	-1.611936	2.586554
N	-2.765870	1.219747	-0.451011
C	-2.815940	1.842386	-1.811036
H	-3.449508	2.738766	-1.772591
H	-1.599440	-2.423370	0.939297
H	-2.693799	-2.561189	3.111098
H	-3.355814	-0.960338	2.788417
H	-1.430709	0.042065	-3.423772
N	-2.424731	-1.846133	1.116553
H	-3.702686	0.853489	-0.265585
H	-1.531482	-1.865145	-2.230090
N	-2.337574	-1.256689	-2.064327
C	-2.446059	-0.304674	-3.198232
C	-3.341063	0.900026	-2.893789
H	-3.435169	1.485848	-3.815447
H	-2.821963	-0.824921	-4.089840
C	-3.598240	-2.620955	0.642138
H	-2.502900	-3.706592	-0.885520
H	-3.774914	-3.477904	1.309407
H	-4.361403	0.576267	-2.650553
H	-4.485809	-1.979584	0.717407
C	-3.442053	-3.143252	-0.790408
C	-3.548768	-2.105743	-1.911223
H	-4.406979	-1.451975	-1.721529
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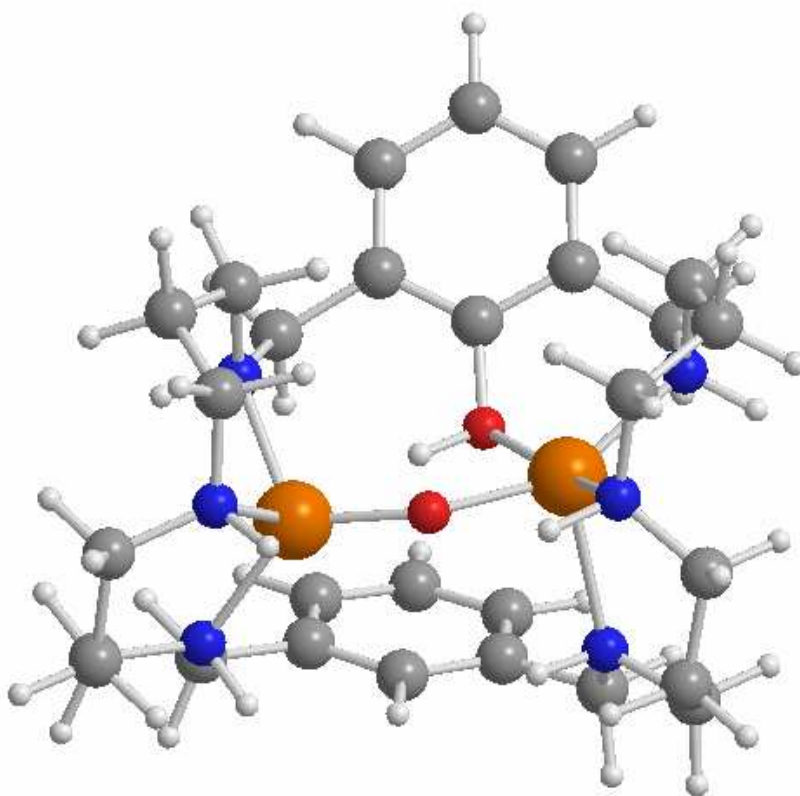
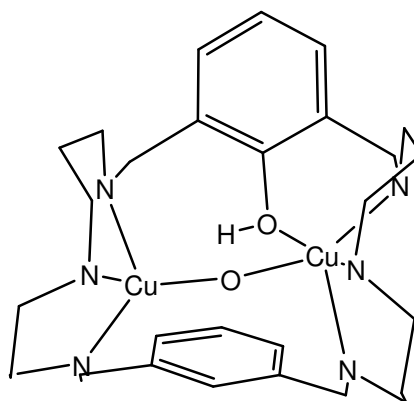
TS-ij

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H	1.29258900	-2.06694000	4.67849500
H	0.90343000	0.31910300	3.89160300
H	-2.07546400	-0.08615300	4.48473000
H	1.10258200	2.15677600	2.43244500
H	-1.78744200	2.24260300	3.33461600
C	1.91605600	1.43186000	2.52195100
H	-1.08775500	4.23418200	2.14852900
H	-0.88506200	-2.27103900	4.52873900
C	4.09144200	1.41260800	1.20719500
H	2.67541300	-2.85968100	3.97028500
C	2.33268700	-0.92777600	3.14981900
H	5.87410500	1.48906100	0.00000000
N	1.28464500	0.12486400	2.96212400
C	1.80432200	-2.24194500	3.72298500
C	-2.67144300	-0.35843600	3.60499500
H	-3.69540300	-0.01023500	3.79944100
H	-3.37554400	-2.28873200	4.17654000
C	2.69140000	1.35842100	1.22595000
C	4.79040100	1.43426900	0.00000000
C	-2.38984200	1.83577700	2.51642100
H	-3.44445400	1.98639500	2.79549100
C	-1.37662200	3.76568700	1.21077500
C	-1.35803500	-2.61111500	3.60229800
H	-1.54093200	-3.68815500	3.71680000
H	2.79276100	-1.10104600	2.17282600
H	-0.53545400	5.33437500	0.00000000
C	-2.69219600	-1.88221800	3.42217300
N	-2.11924300	0.36612000	2.42635400
C	-2.07102300	2.55106300	1.22060800
C	-1.05858700	4.38294200	0.00000000
H	0.76122600	-4.05744400	3.17195600
C	0.92462000	-3.05012100	2.76602400
N	-0.38741000	-2.40336100	2.49038900
Cu	-0.24438400	-0.49673900	1.77911000
C	4.09144200	1.41260800	-1.20719500
H	-3.14165300	-2.13955100	2.45161100
C	2.00849300	1.31939100	0.00000000
H	-2.65157200	0.03105300	1.62213200
H	1.43702200	3.16113400	1.80420800
H	4.63899800	1.46189400	-2.14502700
H	-0.77134900	-2.83332500	1.64668700
O	0.63696300	1.34747900	0.00000000
C	2.69140000	1.35842100	-1.22595000
C	-2.45996600	1.99387700	0.00000000
C	-1.37662200	3.76568700	-1.21077500
H	-3.06387400	1.08823700	0.00000000
H	-1.08775500	4.23418200	-2.14852900
C	-2.07102300	2.55106300	-1.22060800
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H	1.10258200	2.15677600	-2.43244500
C	1.91605600	1.43186000	-2.52195100
H	0.24442200	0.41013300	0.00000000
H	2.79276100	-1.10104600	-2.17282600
H	2.58679400	1.76564200	-3.32237400
Cu	-0.24438400	-0.49673900	-1.77911000
C	-2.38984200	1.83577700	-2.51642100
N	1.28464500	0.12486400	-2.96212400
C	2.33268700	-0.92777600	-3.14981900
H	3.11475300	-0.52928400	-3.80924400
H	-2.65157200	0.03105300	-1.62213200
H	-3.44445400	1.98639500	-2.79549100
H	-1.78744200	2.24260300	-3.33461600
H	1.43702200	-3.16113400	-1.80420800
N	-2.11924300	0.36612000	-2.42635400
H	0.90343000	0.31910300	-3.89160300
H	-0.77134900	-2.83332500	-1.64668700
N	-0.38741000	-2.40336100	-2.49038900
C	0.92462000	-3.05012100	-2.76602400
C	1.80432200	-2.24194500	-3.72298500
H	2.67541300	-2.85968100	-3.97028500
H	0.76122600	-4.05744400	-3.17195600
C	-2.67144300	-0.35843600	-3.60499500
H	-3.14165300	-2.13955100	-2.45161100
H	-3.69540300	-0.01023500	-3.79944100
H	1.29258900	-2.06694000	-4.67849500
H	-2.07546400	-0.08615300	-4.48473000
C	-2.69219600	-1.88221800	-3.42217300
C	-1.35803500	-2.61111500	-3.60229800
H	-0.88506200	-2.27103900	-4.52873900
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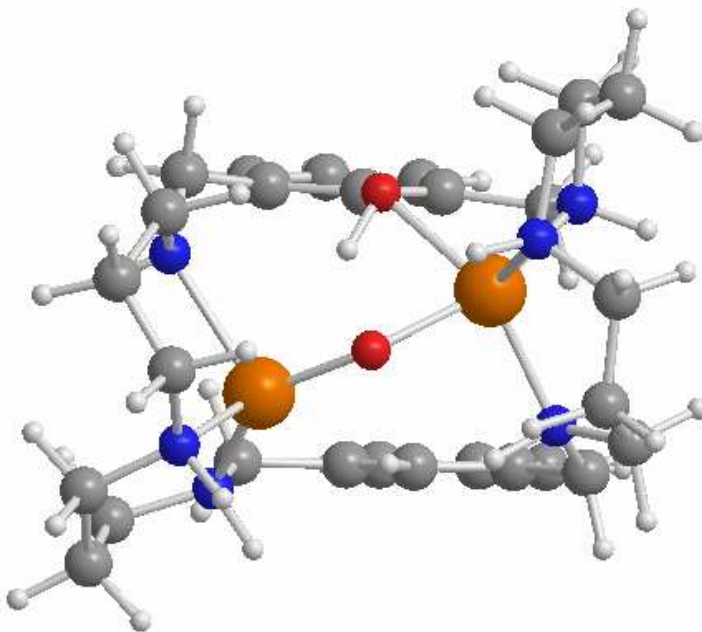
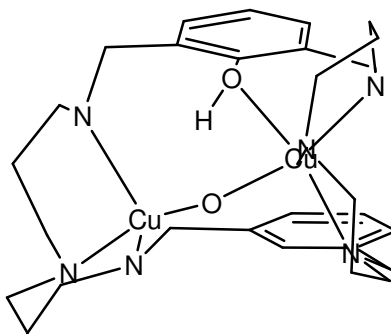
j

H	1.983876	3.695693	0.617883
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H	3.657240	1.909445	-2.696218
H	3.005358	1.952067	-0.331343
H	5.099614	-0.095613	-0.014259
H	1.561078	2.253219	1.551612
H	3.918571	0.418645	2.091046
C	1.407834	2.763002	0.594249
H	2.640254	1.247555	3.972675
H	4.699264	0.006791	-2.462703
C	-0.433591	4.455344	0.182235
H	2.444500	2.420446	-3.836278
C	1.727759	2.412305	-1.839157
H	-2.046787	5.863490	-0.043272
N	1.995860	1.866175	-0.472786
C	2.592618	1.799641	-2.944682
C	4.709983	-1.117295	0.067771
H	5.379749	-1.660990	0.746680
H	5.736032	-2.068995	-1.544439
C	-0.052353	3.127743	0.428034
C	-1.776074	4.828829	0.138708
C	3.436861	-0.564234	2.104420
H	4.106621	-1.234151	2.663449
C	1.849329	0.544125	3.723108
C	4.165068	-0.948563	-2.451386
H	4.377990	-1.439198	-3.411117
H	0.668441	2.247270	-2.054697
H	0.443955	1.410971	5.103627
C	4.701109	-1.802428	-1.301853
N	3.352555	-1.040100	0.687396
C	2.083600	-0.465986	2.779172
C	0.612051	0.637464	4.360474
H	2.728038	0.137677	-4.318124
C	2.269443	0.355833	-3.343702
N	2.710864	-0.658802	-2.344241
Cu	1.828726	-0.275391	-0.461397
C	-2.769821	3.869569	0.339625
H	4.157622	-2.757555	-1.243366
C	-1.075455	2.192353	0.616405
H	3.031664	-2.010570	0.738114
H	1.186580	0.242456	-3.454646
H	-3.816693	4.160019	0.316777
H	2.210276	-1.520063	-2.569945
O	-0.789859	0.871538	0.908061
C	-2.431224	2.535233	0.583329
C	1.059559	-1.379690	2.503883
C	-0.416685	-0.246237	4.029956
H	1.241867	-2.203725	1.817945
H	-1.386161	-0.147424	4.511278
C	-0.208058	-1.258648	3.087917
O	0.153593	-0.843816	-0.794185
H	-3.309141	0.999305	1.814184
C	-3.467833	1.468143	0.837209
H	0.077148	0.588940	0.532454
H	-3.022312	1.552423	-1.862423
H	-4.467261	1.919030	0.839868
Cu	-1.643640	-0.639107	-0.251657
C	-1.323095	-2.217310	2.723256
N	-3.429154	0.361208	-0.182579
C	-3.809508	0.864459	-1.538509
H	-4.735392	1.449313	-1.456540
H	-0.589963	-2.640688	0.864735
H	-1.133508	-3.199594	3.186615
H	-2.270513	-1.857360	3.136398
H	-1.938659	-0.330982	-3.212613
N	-1.501354	-2.390571	1.252648
H	-4.159284	-0.296571	0.100937
H	-1.250880	-2.123251	-2.038097
N	-2.199590	-1.833448	-1.787602
C	-2.732085	-1.027724	-2.919767
C	-4.001005	-0.247249	-2.569053
H	-4.364804	0.222758	-3.490003
H	-2.929872	-1.684537	-3.777502
C	-2.410693	-3.530249	0.974789
H	-1.349858	-4.233159	-0.782841
H	-2.148551	-4.387119	1.613729
H	-4.803287	-0.926561	-2.253186
H	-3.428633	-3.232290	1.256674
C	-2.380908	-3.989764	-0.485533
C	-3.012097	-3.047422	-1.512003
H	-3.999999	-2.730576	-1.161338
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H	-2.932388	-4.935393	-0.539093



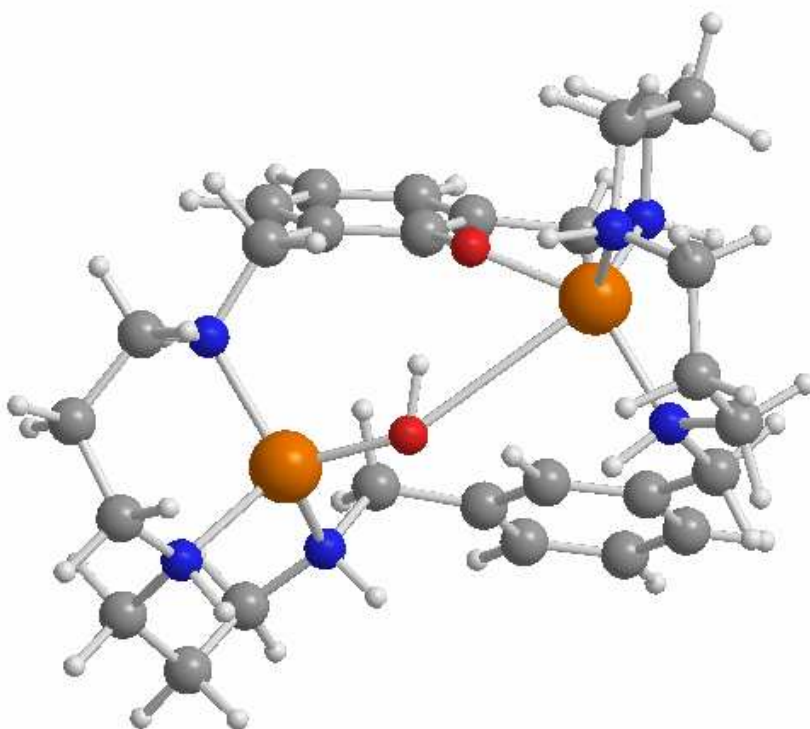
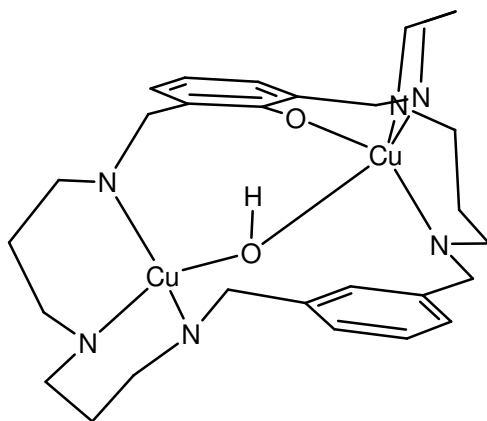
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O	-0.07229400	-1.25102800	-0.42379800
H	2.15743200	3.91014700	-2.51052800
H	-1.24843500	-0.49502100	3.75367800
H	-2.10045900	2.76835900	3.44114400
H	-2.17117300	-2.38873000	3.34977700
H	-3.90391400	-3.06904500	1.69972900
H	-3.26680100	-0.71816400	1.91190800
H	-4.74687900	0.55197500	-0.01383800
H	-2.63171800	0.55101500	3.49845700
H	-2.67754100	2.23032400	0.37572100
C	-1.75959300	0.11601000	3.00112800
H	-1.71655900	4.74572500	-0.85015600
H	-4.79771100	-1.96753900	0.10734000
C	-1.15216400	2.56013100	2.95168300
H	-2.64730100	-4.23706600	1.97417800
C	-1.98545400	-2.24363000	2.27725900
H	-0.47989100	4.60792700	3.04241600
N	-2.25097300	-0.81586700	1.91401700
C	-2.83882000	-3.26008000	1.51406900
C	-4.44540300	0.52244600	-1.06723800
H	-4.98242400	1.33188900	-1.57779300
H	-5.90589600	-0.84200000	-1.82330700
C	-0.83977300	1.24562700	2.59199600
C	-0.24033400	3.59477400	2.73610300
C	-2.64828100	2.19017200	-0.71886000
H	-3.43274300	2.86370200	-1.08828200
C	-0.99041800	4.02470200	-1.21654500
C	-4.41079100	-2.05564600	-0.91185900
H	-4.87062200	-2.95080100	-1.35108800
H	-0.92268400	-2.43985900	2.10635200
H	0.48550400	5.52412700	-1.66333500
C	-4.81638400	-0.81691200	-1.70900300
N	-2.97926200	0.79060700	-1.13774600
C	-1.30125700	2.65969700	-1.23727400
C	0.25203500	4.46382900	-1.67281900
H	-3.10430800	-4.31480000	-0.34610400
C	-2.56122700	-3.43260300	0.01820200
N	-2.93600700	-2.25392800	-0.82912600
Cu	-1.78663900	-0.65732100	-0.33296500
C	0.98533500	3.31674500	2.14116100
H	-4.41311600	-0.86691600	-2.73155500
H	-2.74676600	0.74773200	-2.13506600
H	-1.49268300	-3.59599300	-0.14464200
H	1.69332900	4.12448400	1.97246100
H	-2.61473500	-2.48398000	-1.77234200
C	1.32886700	2.01605000	1.73955900
C	-0.35401300	1.76031100	-1.73092000
C	1.19692600	3.55075500	-2.14887100
H	-0.57404000	0.70138300	-1.72469600
C	0.90050700	2.18327700	-2.18118900
H	2.51687000	2.37453300	0.01181500
C	2.64563900	1.88327900	0.98168900
H	2.98438200	-0.26404600	2.63477000
H	3.42072300	2.44437600	1.52151300
Cu	1.70709400	-0.60468700	-0.15556400
C	1.90288300	1.20505000	-2.75756400
N	3.16082000	0.51346400	0.68896700
C	3.77457100	-0.13307100	1.89239800
H	4.51515400	0.55955000	2.31324000
H	0.93035500	-0.56825700	-2.37097600
H	1.75923900	1.13369500	-3.84722200
H	2.91932200	1.58690900	-2.61362300
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N	1.85677100	-0.17438200	-2.18746100
H	3.92247900	0.64740300	0.02131100
H	1.93474300	-3.10295500	0.05072000
N	2.73708700	-2.47230800	0.01738800
C	3.49982200	-2.64013400	1.28342900
C	4.44843100	-1.47298600	1.58359100
H	5.03424800	-1.74941600	2.46798500
H	4.07303400	-3.57771300	1.25901700
C	2.83831200	-1.03886300	-2.91125100
H	1.78487900	-2.89194900	-2.48027900
H	2.64239900	-0.96391800	-3.98967300
H	5.18465700	-1.34787500	0.77732800
H	3.83718900	-0.61783100	-2.74487500
C	2.81712500	-2.51598500	-2.49791500
C	3.52779400	-2.85007200	-1.18202200
H	4.48350700	-2.31692600	-1.14194600
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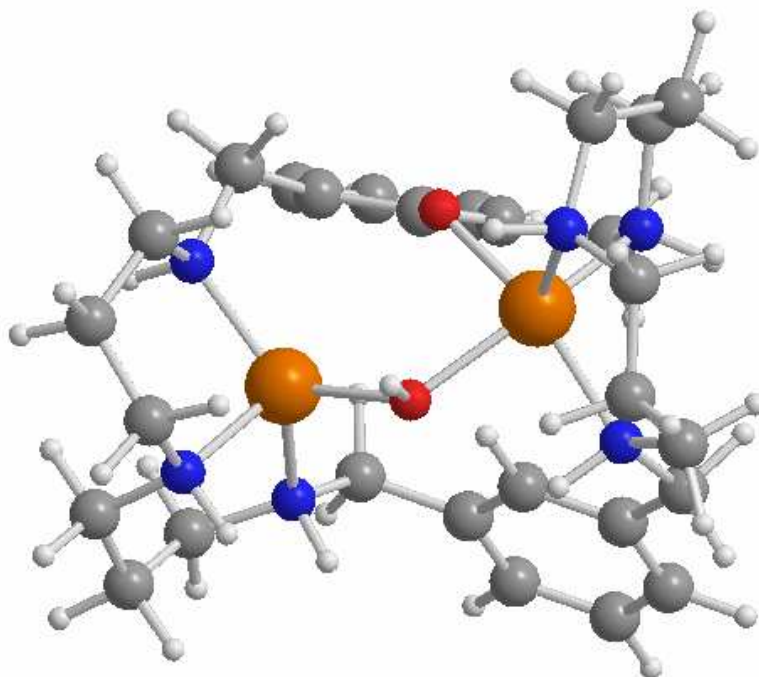
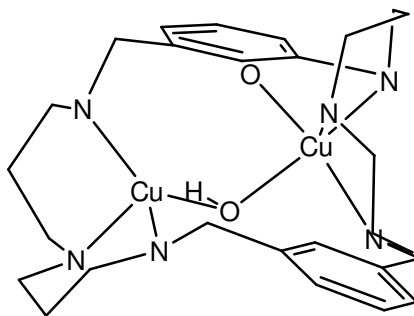
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O	-0.76639800	-0.43437000	-1.21235600
H	2.81180900	4.75933300	-0.73856700
H	-0.75659500	-2.81050600	0.53341900
H	-2.22634300	-1.51910000	3.72456200
H	-3.55411200	-3.87859300	0.85988600
H	-5.40122000	-2.21572500	0.30885000
H	-3.25472300	-1.58975200	1.44089100
H	-4.27146600	1.90371800	0.94409600
H	-1.68572500	-3.33171600	1.94079900
H	-1.33793100	1.23708400	1.37711600
C	-1.41410800	-2.46046400	1.32929900
H	-0.93172300	4.72877800	1.36497500
H	-5.69065500	0.11610200	-0.06553100
C	-1.29239400	-1.05592300	3.40904700
H	-5.33449200	-3.64644200	-0.69042000
C	-3.43040100	-3.10189200	0.09347300
H	-1.11446800	0.14648700	5.19476000
N	-2.67693300	-1.95334100	0.67744000
C	-4.80088600	-2.71641900	-0.46318800
C	-3.94527500	2.26727900	-0.03730500
H	-3.87704300	3.36070900	0.03249800
H	-5.87552500	2.49405200	-0.91022400
C	-0.71826800	-1.43461800	2.19115900
C	-0.67221400	-0.12822100	4.24303100
C	-1.64007800	2.13246500	0.82862500
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C	-0.20403800	4.21474800	0.74240000
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H	-2.80641300	-3.52882800	-0.69997300
H	1.12499600	5.91061100	0.65171800
C	-4.98145800	1.88718900	-1.09303200
N	-2.58267300	1.70748300	-0.28469900
C	-0.42128700	2.89113500	0.35235800
C	0.96018700	4.88207800	0.34568700
H	-5.75267400	-1.88158700	-2.21990000
C	-4.76203800	-1.88946000	-1.74816200
N	-4.30943200	-0.47728700	-1.54569100
Cu	-2.50336900	-0.33457100	-0.62034500
C	0.54448100	0.41930700	3.84491800
H	-4.63204600	2.17129500	-2.09702300
H	-2.22707800	2.13909200	-1.14052300
H	-4.06618200	-2.35087700	-2.45779700
H	1.03946100	1.13948800	4.49284100
H	-4.06255100	-0.13424700	-2.47868600
C	1.15945300	0.06868600	2.63549700
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C	1.91019600	4.23130600	-0.43665100
H	0.31818300	1.22092200	-0.74832500
C	1.70302700	2.90260200	-0.84186200
H	2.15558400	1.81432600	1.86396800
C	2.42491200	0.83833800	2.28326500
H	3.28143100	-1.58115100	2.40153700
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Cu	2.32552100	-0.41499700	-0.35904800
C	2.75116800	2.24283000	-1.71692500
N	3.32607000	0.19465800	1.28534400
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H	1.56842000	0.70119300	-2.34456500
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H	3.74529100	2.33908300	-1.26456700
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N	2.52176800	0.79055000	-1.97319000
H	4.04194500	0.88500000	1.05332200
H	2.21498800	-2.73991400	-1.30943900
N	3.04643900	-2.17629500	-1.12603400
C	3.78325900	-2.84176700	-0.00025000
C	4.70462500	-1.89958100	0.79658800
H	5.41157000	-2.53710000	1.34014400
H	4.37400600	-3.67240000	-0.40641500
C	3.43746300	0.31420700	-3.05700200
H	2.20440800	-1.39181800	-3.59846800
H	3.26729400	0.92919800	-3.94949400
H	5.32605100	-1.29473900	0.12079100
H	4.46443100	0.50695600	-2.72647400
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C	3.84541100	-2.13131400	-2.37896100
H	4.86218700	-1.81854900	-2.11809000
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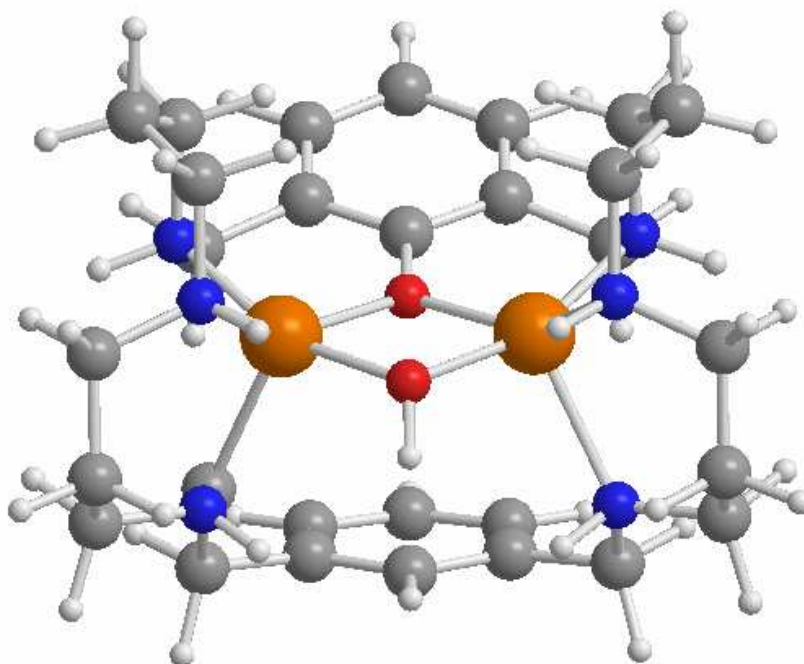
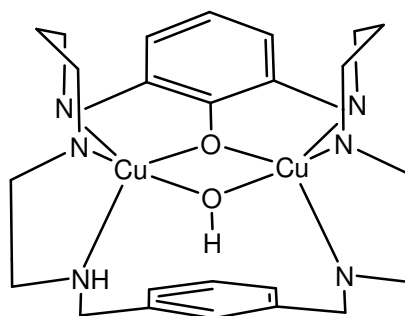


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O	-0.10874900	-0.71058900	-1.24277000
H	2.54857700	4.68056500	-1.94093100
H	-1.01531300	-2.58545300	2.27940000
H	-2.68633300	0.18291800	3.98912200
H	-2.96149500	-3.91975600	1.32520300
H	-4.56957600	-3.18029300	-0.42332700
H	-3.50458400	-1.57050000	1.26041400
H	-4.34345000	1.29337200	0.43446800
H	-2.48272300	-2.11089600	3.15461800
H	-1.65128000	2.14725800	1.33041600
C	-1.79387900	-1.82412400	2.35277000
H	-1.29070300	5.26512700	-0.10125000
H	-4.95443700	-0.96671500	-0.64986000
C	-1.71790300	0.40606000	3.54626600
H	-3.53298600	-4.46998900	-0.97132400
C	-2.61823600	-3.25475400	0.52242600
H	-1.45879300	2.24585900	4.64586800
N	-2.54730200	-1.85696800	1.04359400
C	-3.53090200	-3.41039600	-0.69112400
C	-3.97277900	1.65617000	-0.53165600
H	-4.25965400	2.71291900	-0.60556000
H	-5.68808500	1.16819700	-1.70624200
C	-1.15464800	-0.49299500	2.63299000
C	-1.02930400	1.55497900	3.92801900
C	-1.87238000	2.60465600	0.36273100
H	-2.61498100	3.39088900	0.53818200
C	-0.50382500	4.59233600	-0.43169800
C	-4.54606300	-0.62310900	-1.60511000
H	-5.15750000	-1.07222200	-2.39862400
H	-1.59322700	-3.54983400	0.27280800
H	0.75341400	6.18481000	-1.15735400
C	-4.62643900	0.89748600	-1.68588400
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C	-0.64016600	3.21221600	-0.26535100
C	0.65077600	5.11194200	-1.02690700
H	-3.73414600	-2.88033600	-2.77713800
C	-3.09891700	-2.61490200	-1.92269400
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Cu	-1.87020200	-0.50095400	-0.29408000
C	0.24771800	1.78402100	3.40619100
H	-4.21502400	1.24790500	-2.64464900
H	-2.18419400	1.80237700	-1.47810900
H	2.06784400	-2.87069600	-2.19116000
H	0.79692100	2.66709000	3.72703200
H	-2.76047000	-0.72015000	-2.58019100
C	0.85117800	0.90842400	2.50132500
C	0.38923300	2.37177500	-0.70492000
C	1.66333200	4.26228500	-1.46818000
H	0.27699800	1.30715000	-0.56749000
C	1.54112500	2.87321900	-1.30779000
H	2.15380600	2.16290100	1.34196600
C	2.23457300	1.28686400	1.99450100
H	2.71337100	-1.22056600	2.70469600
H	2.85880800	1.58509300	2.84896200
Cu	1.66448100	-0.53185300	-0.19838800
C	2.66960900	1.97094000	-1.76670500
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C	3.53221500	-0.80702000	2.11334800
H	4.22707400	-0.31164200	2.80483000
H	1.42929900	0.45717900	-2.37371100
H	3.03267700	2.32667900	-2.74100000
H	3.52666100	2.05146600	-1.08457800
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N	2.32250700	0.52393500	-1.87722000
H	3.73320700	0.69862000	0.75874100
H	1.93425900	-3.07382400	-0.75348500
N	2.71767600	-2.44658200	-0.56761700
C	3.36519500	-2.95805100	0.67447000
C	4.26322600	-1.92765000	1.36925300
H	4.86088800	-2.46732900	2.11322500
H	3.95300900	-3.85800000	0.44478100
C	3.35335900	-0.15310900	-2.72146400
H	2.10466500	-1.87770900	-3.17188900
H	3.37481800	0.33947100	-3.70259600
H	4.99259300	-1.50382000	0.66428800
H	4.32953500	0.03098600	-2.25724900
C	3.15180700	-1.66004900	-2.91516900
C	3.61753600	-2.52963100	-1.74572900
H	4.61354800	-2.19877800	-1.43377700
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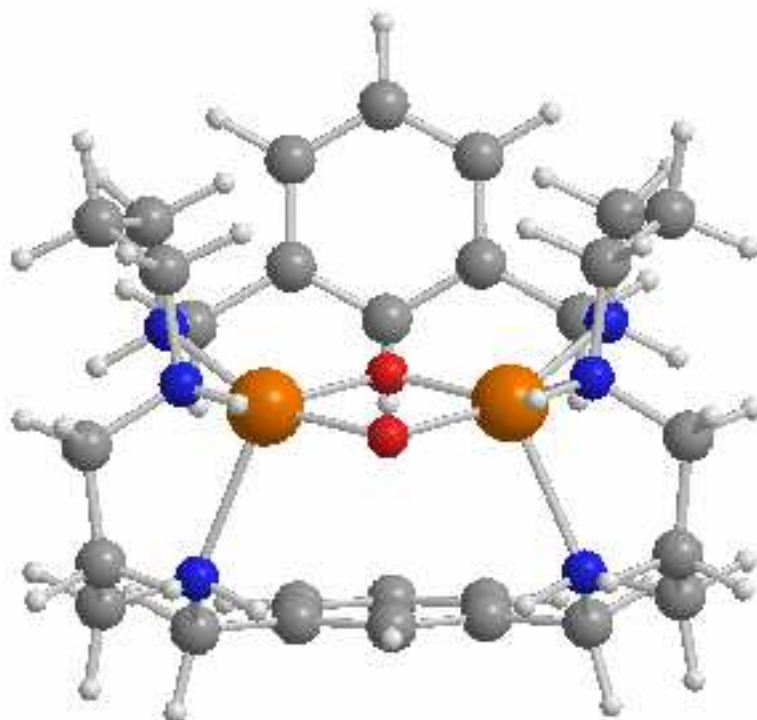
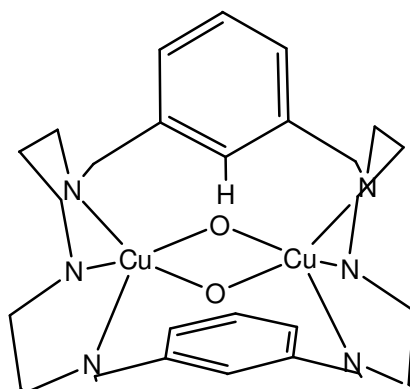


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H	2.140220	4.212940	-2.270845
H	3.346300	1.025984	-3.127844
H	4.374830	-1.181793	-2.631133
H	3.748993	0.378529	-0.802520
H	4.576923	-0.733166	1.599676
H	2.603622	2.108026	0.266989
H	3.340277	1.144172	2.552275
C	2.539905	2.009852	-0.823162
H	2.146926	3.189084	2.663452
H	4.589462	-1.965935	-0.546940
C	1.195619	3.735985	-2.021294
H	3.289957	-1.250866	-3.993670
C	2.764880	0.267497	-2.588111
H	0.000070	5.278573	-2.941468
N	2.798945	0.569673	-1.127306
C	3.313599	-1.123425	-2.905376
C	3.829764	-1.402298	2.045013
H	4.137061	-1.560816	3.088998
H	4.744163	-3.279501	1.610508
C	1.214877	2.525944	-1.317942
C	0.000057	4.344196	-2.390797
C	2.529599	0.491711	2.892009
H	2.786559	0.184011	3.917776
C	1.208611	2.643165	2.724583
C	3.831467	-2.683584	-0.216182
H	4.122574	-3.660038	-0.627472
H	1.725644	0.364460	-2.916184
H	-0.000032	4.419540	2.580262
C	3.832421	-2.748720	1.313661
N	2.515394	-0.707613	1.999691
C	1.220545	1.250335	2.867774
C	-0.000034	3.338202	2.676006
H	2.940335	-3.237101	-2.654666
C	2.530265	-2.285784	-2.289669
N	2.521469	-2.283250	-0.797161
Cu	1.542235	-0.591206	-0.101135
C	-1.195521	3.735980	-2.021358
H	3.002224	-3.377885	1.669712
C	0.000025	1.878370	-0.992397
H	1.848318	-1.358434	2.417777
H	1.483273	-2.234176	-2.610979
H	-2.140111	4.212931	-2.270958
H	1.832879	-2.981629	-0.512646
O	0.000016	0.667260	-0.387251
C	-1.214813	2.525938	-1.318005
C	-0.000040	0.578060	2.984373
C	-1.208682	2.643168	2.724560
H	-0.000044	-0.497253	3.157801
H	-2.146995	3.189088	2.663409
C	-1.220621	1.250338	2.867756
O	-0.000010	-1.746200	0.305384
H	-2.603643	2.108032	0.266853
C	-2.539867	2.009848	-0.823293
H	-0.000028	-2.187067	1.168063
H	-1.725497	0.364451	-2.916260
H	-3.345921	2.614449	-1.255877
Cu	-1.542213	-0.591194	-0.101195
C	-2.529678	0.491718	2.891986
N	-2.798882	0.569664	-1.127433
C	-2.764746	0.267469	-2.588231
H	-3.346158	1.025937	-3.128000
H	-1.848389	-1.358418	2.417732
H	-2.786634	0.184019	3.917753
H	-3.340353	1.144185	2.552256
H	-1.483143	-2.234249	-2.610888
N	-2.515483	-0.707603	1.999664
H	-3.748941	0.378515	-0.802684
H	-1.833044	-2.981664	-0.512551
N	-2.521515	-2.283209	-0.797167
C	-2.530167	-2.285812	-2.289674
C	-3.313422	-1.123467	-2.905513
H	-3.289634	-1.250941	-3.993801
H	-2.940231	-3.237134	-2.654663
C	-3.829850	-1.402294	2.045040
H	-3.002420	-3.377889	1.669543
H	-4.137056	-1.560911	3.089037
H	-4.374689	-1.181832	-2.631408
H	-4.577045	-0.733117	1.599832
C	-3.832585	-2.748643	1.313558
C	-3.831612	-2.683335	-0.216278
H	-4.589449	-1.965481	-0.546958
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H	-4.744356	-3.279402	1.610356



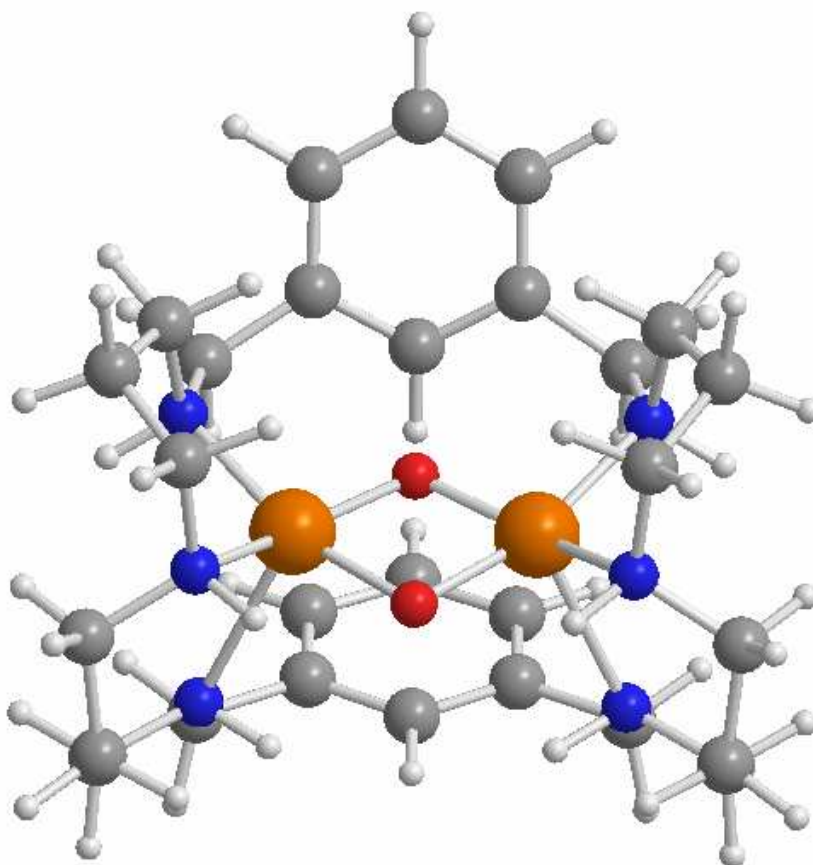
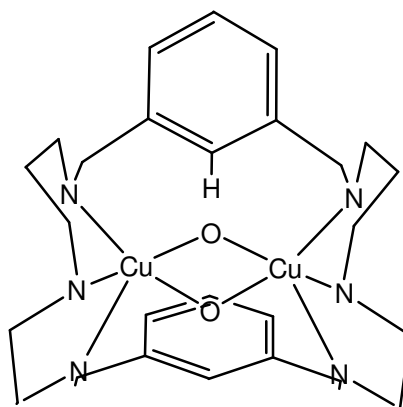
TS-ef

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H	2.77832000	-3.27629400	2.25127200
C	-0.00001300	-0.71323800	4.38358100
H	2.14904200	-0.77700200	4.25138200
C	-1.21085800	-1.07261800	3.78770200
C	1.21084500	-1.07259200	3.78771300
C	-1.22123600	-1.83073800	2.60952600
C	1.22124900	-1.83071200	2.60953700
H	-3.34066600	-1.61321100	2.33367000
C	0.00001300	-2.23037300	2.06172700
H	3.34067500	-1.61313100	2.33369000
C	-2.52535000	-2.24294600	1.96147800
C	2.52537800	-2.24289300	1.96150200
H	0.00002300	-2.86130000	1.17674200
H	3.90008200	-3.73060900	0.29594500
H	-3.89998000	-3.73069400	0.29588300
H	-1.73963400	-2.71465100	0.14270700
H	1.73969500	-2.71465200	0.14273200
H	-4.59394500	-2.11391200	0.26857700
N	-2.50604500	-2.12770500	0.47602500
H	4.59398100	-2.11379900	0.26860500
N	2.50608100	-2.12767200	0.47604700
C	-3.74647400	-2.71184900	-0.09057700
C	3.74653500	-2.71177900	-0.09053800
H	-2.43844400	1.07959900	2.17327200
H	2.43846400	1.07964100	2.17325400
H	4.60716400	-3.36921500	-1.92763600
H	-4.60707800	-3.36927200	-1.92769100
C	3.75585300	-2.75130000	-1.62005200
C	-3.75578700	-2.75133600	-1.62009200
H	2.86325200	-3.27268100	-1.99722700
H	-2.86316900	-3.27267900	-1.99727800
C	-2.50059500	1.89988200	1.45349800
H	-3.35266400	2.53527400	1.72680500
C	2.50059100	1.89991800	1.45347200
H	3.35265500	2.53532500	1.72676300
O	0.00000100	0.32564900	0.04478500
C	-0.00000200	2.05403500	1.68210900
C	-1.22045600	2.70275600	1.45387600
C	1.22044100	2.70277300	1.45386300
H	-2.14622800	4.61440400	1.05192900
C	-1.21055500	4.07548500	1.17693800
H	-3.72820900	0.82065800	0.24969000
O	0.00000000	-0.88783600	-1.24917600
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H	2.14618200	4.61443400	1.05190300
H	3.72820800	0.82070800	0.24965400
Cu	1.61768400	-0.20930600	-0.61276300
Cu	-1.61768300	-0.20931100	-0.61276100
C	-0.00002400	4.76554700	1.07370400
H	-0.00003200	5.83572800	0.89160900
N	-2.81761600	1.26567400	0.10985900
N	2.81760300	1.26570300	0.10983400
H	-4.69888300	-0.82153400	-1.81356500
H	4.69889600	-0.82147700	-1.81357500
C	-3.91061800	-1.39586200	-2.30953000
C	3.91064200	-1.39583700	-2.30952100
N	2.66451300	-0.57713300	-2.30484200
N	-2.66451000	-0.57712700	-2.30484400
H	-4.22821000	-1.53964600	-3.35109000
H	4.22822800	-1.53963500	-3.35108000
H	1.96568900	-1.10518900	-2.83262300
H	-1.96567500	-1.10515700	-2.83263700
C	-3.00844800	2.29517800	-0.95667500
H	-3.63169900	3.10823300	-0.56172100
C	3.00839300	2.29519800	-0.95671600
H	3.63162700	3.10827600	-0.56178200
H	-4.66190900	1.35945400	-2.00392700
H	-2.02610400	2.72013700	-1.18073900
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H	4.66186800	1.35950600	-2.00397300
C	-3.66118400	1.75000000	-2.22876400
C	2.84141700	0.72437100	-3.01644500
C	3.66113000	1.75002100	-2.22880500
C	-2.84145000	0.72438400	-3.01642500
H	1.83877600	1.12189100	-3.21045000
H	-1.83882000	1.12193300	-3.21042900
H	3.31908400	0.54558800	-3.98875400
H	-3.31911800	0.54560400	-3.98873500
H	-3.82968500	2.60553500	-2.89299700
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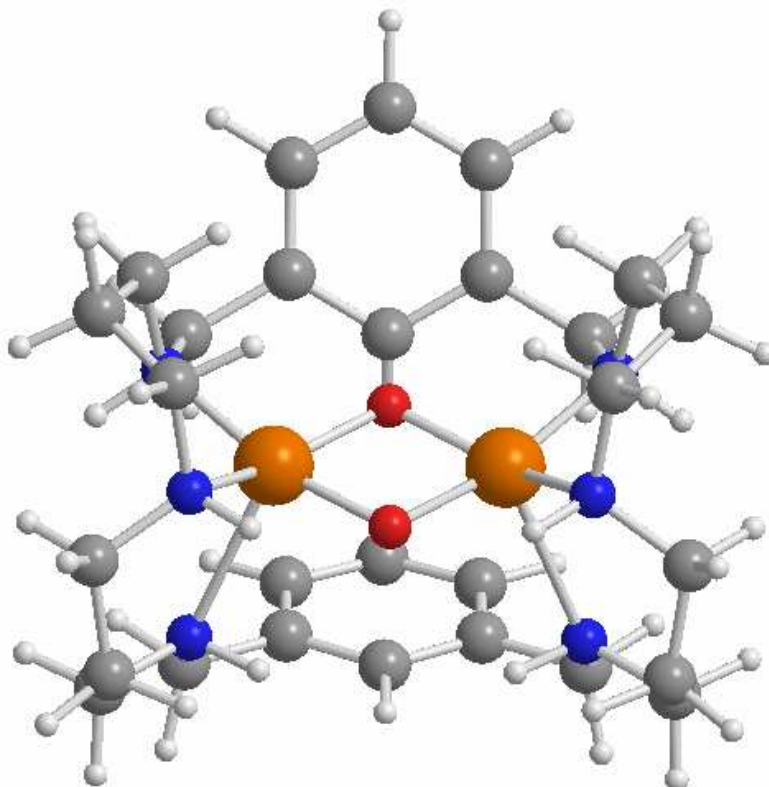
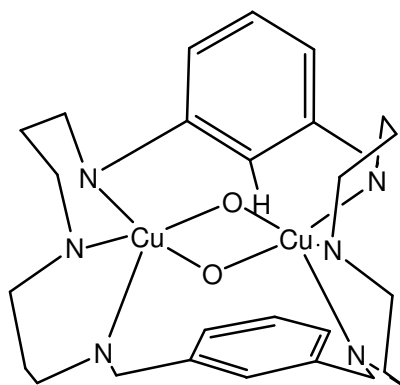
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H	3.60910400	1.82033800	2.73996900
H	1.34132200	4.15360900	2.15005400
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C	1.29569100	4.29314300	0.00000000
H	1.34132200	4.15360900	-2.15005400
C	1.58175200	3.65922000	1.21174700
C	1.58175200	3.65922000	-1.21174700
C	2.20038700	2.40235900	1.22171200
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H	1.99456400	2.15766500	3.34895200
C	2.53710700	1.81555400	0.00000000
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C	2.53598000	1.69544900	2.51624300
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H	3.07957200	0.87252600	0.00000000
H	3.84082700	-0.24379900	-3.74664300
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H	2.64173900	-0.15725800	1.67079500
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H	2.30299000	-0.00208700	4.56630500
N	2.18674400	0.24965900	2.48897900
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C	2.75927200	-0.43547900	3.66687900
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H	-0.70126800	2.24167300	2.40780400
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H	3.08617600	-2.37962700	-4.48193100
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C	2.52182200	-1.94520900	-3.64914000
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H	2.94790300	-2.39139000	-2.73835800
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C	-1.62811500	1.66685300	2.47244100
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H	-2.17891000	1.99175100	-3.36405200
O	-0.51389400	0.22392500	0.00000000
C	-1.78714100	2.04492900	0.00000000
C	-2.45389200	1.85073300	1.22049600
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H	-4.39394700	1.62702600	2.14630100
C	-3.84599600	1.71688400	1.21172200
H	-0.68444800	0.25034700	3.58899700
O	0.74092600	-1.59415700	0.00000000
C	-3.84599600	1.71688400	-1.21172200
H	-4.39394700	1.62702600	-2.14630100
H	-0.68444800	0.25034700	-3.58899700
Cu	0.03094800	-0.70977600	-1.42291400
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H	-5.62919700	1.64070000	0.00000000
N	-1.21292100	0.21984000	2.71378100
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H	0.57297900	-1.74011100	4.56036100
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C	1.06340300	-2.37525300	3.81651800
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N	0.26681000	-2.32808400	-2.55423700
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H	0.75534600	-2.90334800	-1.86259400
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C	-2.39322300	-0.67102000	2.93348000
H	-3.10559800	-0.16041600	3.59406400
C	-2.39322300	-0.67102000	-2.93348000
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H	-1.64050500	-1.88929900	4.56324100
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H	-1.64050500	-1.88929900	-4.56324100
C	-2.03675500	-2.02562000	3.54944900
C	-1.10085900	-2.90741400	-2.71894500
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H	-1.01847500	-3.89683100	-3.18587800
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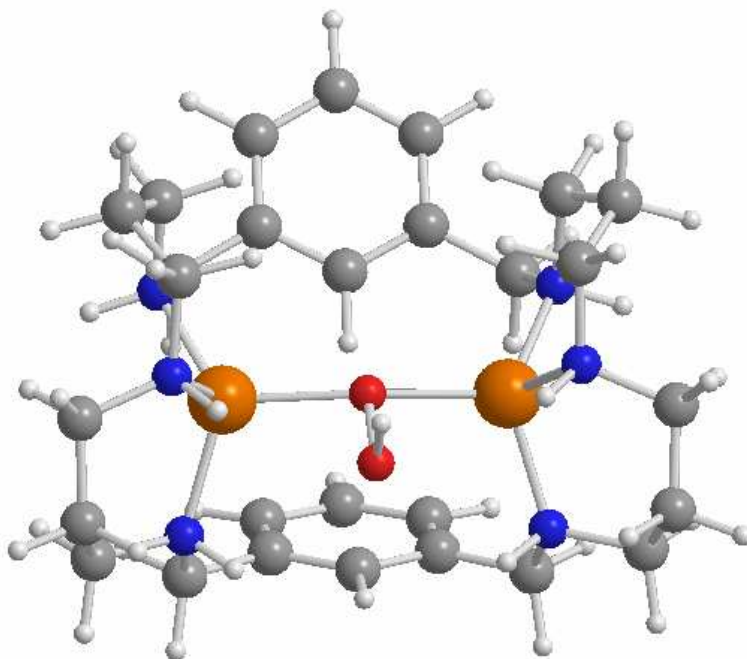
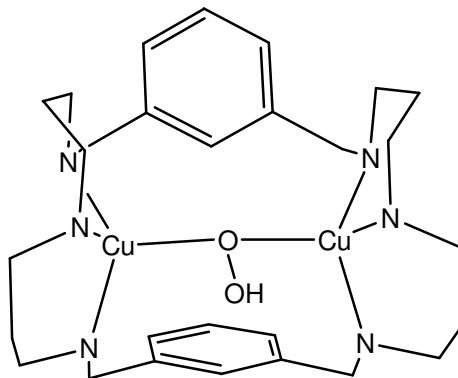
TS-fg

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H	2.71831300	-3.66210300	1.68106700
C	-0.00009400	-1.41889000	4.26114100
H	2.15091800	-1.45845700	4.12068300
C	-1.21299700	-1.68494600	3.61903400
C	1.21289900	-1.68471700	3.61911900
C	-1.22259900	-2.26797100	2.34507900
C	1.22270200	-2.26774300	2.34515900
H	-3.35363300	-2.07604200	2.09406900
C	0.00010200	-2.58977800	1.75216500
H	3.35365600	-2.07498700	2.09411300
C	-2.50887700	-2.58138200	1.61293600
C	2.50912100	-2.58083800	1.61310400
H	0.00015600	-3.11503400	0.79975400
H	3.62750400	-3.84560200	-0.40335500
H	-3.62751000	-3.84568100	-0.40355200
H	-1.60697800	-2.53491800	-0.21781400
H	1.60700300	-2.53503800	-0.21751300
H	-4.52223600	-2.34948200	-0.16709400
N	-2.46366500	-2.15781500	0.18833800
H	4.52223900	-2.34931600	-0.16738800
N	2.46368800	-2.15768300	0.18839600
C	-3.58426300	-2.75707500	-0.56631600
C	3.58419800	-2.75703100	-0.56632900
H	-2.47610800	0.57864400	2.23432500
H	2.47794800	0.57813300	2.23409500
H	4.27926500	-3.08399300	-2.55571300
H	-4.27978200	-3.08366700	-2.55557700
C	3.50160500	-2.48492800	-2.06868800
C	-3.50198400	-2.48470900	-2.06864000
H	2.54685100	-2.85288200	-2.47226900
H	-2.54733600	-2.85267200	-2.47247700
C	-2.52658400	1.52663600	1.69111600
C	-3.37324700	2.10637800	2.08031200
C	2.52663300	1.52618800	1.69101700
H	3.37341000	2.10571300	2.08029200
O	-0.00001200	0.75771200	0.26100300
C	0.00003700	1.55312600	1.87084400
C	-1.23514800	2.29101500	1.84760600
C	1.23534600	2.29080000	1.84757400
H	-2.14800500	4.23397700	1.88415500
C	-1.21368900	3.67849700	1.87805000
H	-3.65857700	0.60636900	0.26869400
O	-0.00016900	-0.64039300	-1.51215800
C	1.21412600	3.67828600	1.87802400
H	2.14853800	4.23360600	1.88411200
H	3.65840300	0.60574000	0.26855100
Cu	1.44767100	0.05931200	-0.66945000
Cu	-1.44781900	0.05932900	-0.66918400
C	0.00028000	4.37832500	1.93066700
H	0.00037600	5.46145400	1.99796100
N	-2.81423800	1.18246900	0.25089600
N	2.81424800	1.18211100	0.25077400
H	-4.52771300	-0.59508000	-1.87689600
H	4.52743400	-0.59531400	-1.87735800
C	-3.72547600	-1.02902700	-2.48157400
C	3.72510400	-1.02930800	-2.48187900
N	2.51634900	-0.16621900	-2.35181400
N	-2.51661000	-0.16610300	-2.35152800
H	-4.05714200	-0.98369000	-3.52791500
H	4.05668400	-0.98413200	-3.52825200
H	1.77332300	-0.58316500	-2.91805000
H	-1.77364300	-0.58320100	-2.91773300
C	-3.10138900	2.39028600	-0.57952000
H	-3.81942100	3.02734700	-0.04590000
C	3.10179100	2.38991400	-0.57952500
H	3.82007300	3.02666000	-0.04586400
H	-4.64905200	1.59164600	-1.87345800
H	-2.16771300	2.95174300	-0.66911000
H	2.16831300	2.95171700	-0.66900800
H	4.64917300	1.59101100	-1.87363900
C	-3.66012500	2.05715000	-1.96479400
C	2.74753300	1.21659900	-2.86442300
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C	-2.74754600	1.21669600	-2.86428800
H	1.76489000	1.69306400	-2.95426900
H	-1.76480900	1.69294500	-2.95425500
H	3.18094900	1.16200000	-3.87140900
H	-3.18104000	1.16205400	-3.87123800
H	-3.83596000	3.00965500	-2.47761800
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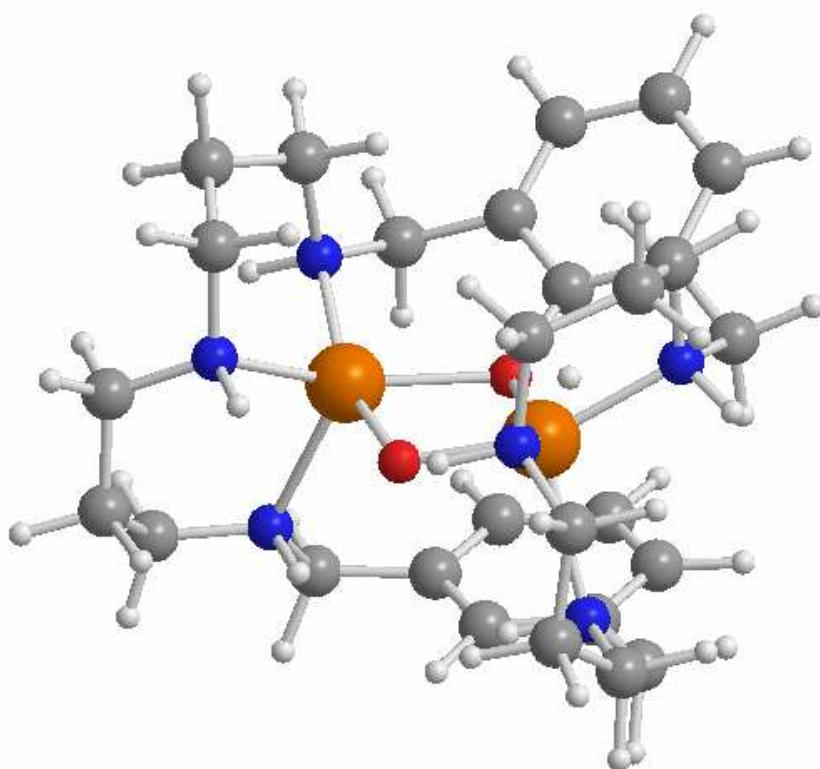
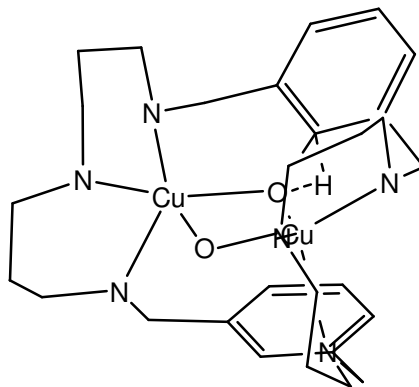
d+H

H	-0.132361	0.916595	4.879734
H	-3.133701	-2.684327	2.540774
H	-2.331202	0.260369	3.948586
H	2.164569	-3.290250	2.806243
C	-0.190116	0.137690	4.125994
H	1.929841	-0.229921	4.129778
C	-1.427497	-0.229468	3.593861
C	0.971505	-0.506453	3.696787
C	-1.515496	-1.259949	2.645637
C	0.902151	-1.541115	2.751595
H	-3.636943	-1.002170	2.447065
C	-0.348019	-1.923385	2.254869
H	3.036712	-1.765665	2.722174
C	-2.861937	-1.703961	2.126615
C	2.150972	-2.289913	2.352581
H	-0.417584	-2.765301	1.569220
H	3.643391	-4.083952	1.149569
H	-4.616305	-3.091353	0.745577
H	-2.346872	-2.578511	0.338373
H	1.585686	-3.088087	0.545414
H	-5.000244	-1.374559	0.657403
N	-2.939225	-1.793971	0.622750
H	4.413921	-2.503215	1.046158
N	2.318645	-2.448325	0.862654
C	-4.348290	-2.153061	0.245510
C	3.631728	-3.131928	0.605726
H	-2.318943	1.859085	1.860816
H	2.629285	1.255220	1.977605
H	4.850901	-3.973569	-0.920856
H	-5.606192	-2.651352	-1.395199
C	3.932777	-3.377743	-0.869436
C	-4.583777	-2.282796	-1.255641
H	3.152996	-4.001143	-1.331330
H	-3.932544	-3.054632	-1.691631
C	-2.251657	2.543136	1.008711
H	-2.967552	3.355431	1.177335
C	2.757991	1.912646	1.111025
H	3.648361	2.525563	1.290880
C	0.260193	2.278236	1.009646
C	-0.859691	3.107905	0.883542
C	1.555154	2.802997	0.930142
H	-1.531475	5.145919	0.625352
C	-0.671945	4.484217	0.692657
H	-3.721322	1.640867	-0.052066
C	1.722985	4.181445	0.737368
H	2.721928	4.608304	0.704661
H	3.986767	0.645649	0.120325
Cu	1.993638	-0.722100	-0.194904
Cu	-2.129528	-0.180636	-0.348209
C	0.614010	5.019664	0.621802
H	0.751602	6.088507	0.492881
N	-2.715914	1.767532	-0.209841
N	3.050191	1.014189	-0.075606
H	-5.048544	-0.185661	-1.560099
H	4.889338	-1.459369	-1.203166
C	-4.451524	-0.973608	-2.029076
C	4.154293	-2.108717	-1.688532
N	2.880147	-1.342642	-1.866599
N	-3.026664	-0.516771	-2.096968
H	-4.822700	-1.099561	-3.053295
H	4.547005	-2.361971	-2.680673
H	2.212576	-2.026770	-2.233151
H	-2.512622	-1.322388	-2.464291
C	-2.619171	2.585319	-1.461433
H	-3.032506	3.582455	-1.267750
C	3.193937	1.788257	-1.350317
H	3.824904	2.666152	-1.166334
H	-4.436658	1.877739	-2.421577
H	-1.558611	2.710927	-1.693424
H	2.201275	2.150835	-1.629596
H	4.828691	0.642860	-2.211253
C	-3.361801	1.947029	-2.632355
C	2.969743	-0.255005	-2.898038
C	3.806779	0.948397	-2.469849
C	-2.803860	0.597418	-3.079712
H	1.943620	0.064393	-3.113711
H	-1.721355	0.675123	-3.233711
H	3.382361	-0.689060	-3.816627
H	-3.254627	0.303928	-4.035128
H	-3.280872	2.630038	-3.485594
H	3.914982	1.596078	-3.347211
H	0.121312	1.220395	1.222980
O	-0.231864	-1.969739	-1.096853
O	-0.073516	-0.573487	-0.597208
H	-0.189393	-1.838321	-2.062188



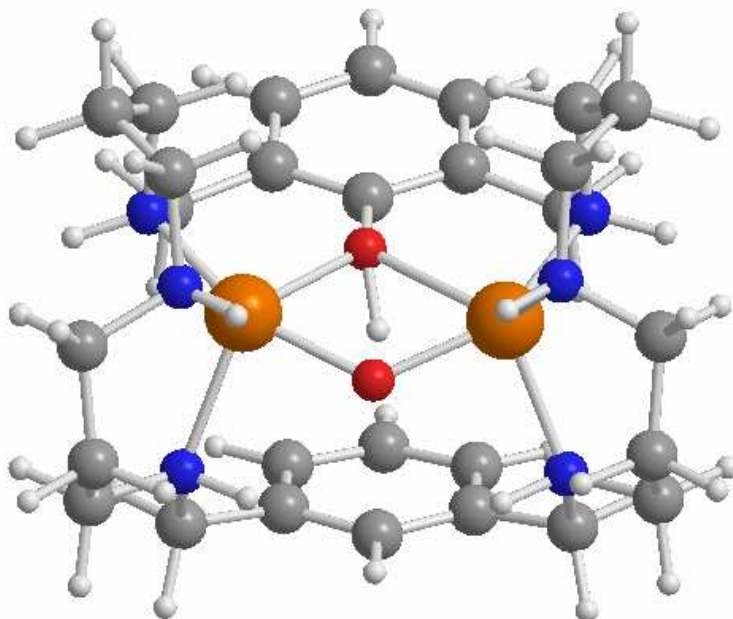
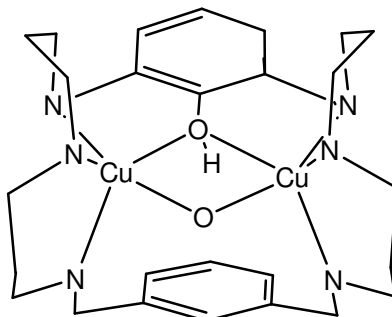
TS-gi

C	-2.326066	0.277285	0.000000
O	-0.859020	0.359557	0.000000
H	-1.788531	1.401712	0.000000
O	1.431251	-0.494603	0.000000
H	-1.407357	3.749285	2.152913
H	-3.006875	0.141208	-3.374144
H	-4.902736	-0.364533	-2.147156
H	-2.404364	-2.172187	-3.471469
H	-0.130994	-2.731382	-4.331995
H	-0.767208	-0.393356	-3.702225
H	1.871950	1.039459	-4.490528
H	-1.908389	1.300728	-2.611538
H	0.497643	2.866545	-3.356847
C	-2.289630	0.275035	-2.554585
H	-1.407357	3.749285	-2.152913
H	1.686943	-1.440515	-4.392041
C	-4.363630	-0.239625	-1.212137
H	-0.842647	-4.002074	-3.373719
C	-1.528716	-2.065482	-2.816076
H	-6.105188	-0.621168	0.000000
N	-1.119803	-0.629513	-2.772086
C	-0.416609	-2.994498	-3.305393
C	2.514254	1.057532	-3.600368
H	3.256970	1.852745	-3.767891
H	3.980532	-0.336893	-4.272289
C	-3.005369	0.064447	-1.242465
C	-5.045604	-0.387475	0.000000
C	1.171087	2.784204	-2.497223
H	2.008834	3.475518	-2.683744
C	-0.885469	3.578660	-1.214157
C	2.379239	-1.535529	-3.548721
H	3.014779	-2.407956	-3.757688
H	-1.843048	-2.346565	-1.805910
H	-2.566958	4.178123	0.000000
C	3.248448	-0.279059	-3.458730
N	1.667871	1.381255	-2.428897
C	0.449038	3.156142	-1.221824
C	-1.544711	3.810572	0.000000
H	1.471728	-3.886156	-2.753986
C	0.817295	-3.077072	-2.401079
N	1.588115	-1.809956	-2.320077
Cu	0.426556	-0.362931	-1.500440
C	-4.363630	-0.239625	1.212137
H	3.836064	-0.291841	-2.529268
H	2.264083	1.310622	-1.602190
H	0.507859	-3.326881	-1.379679
H	-4.902736	-0.364533	2.147156
H	2.232968	-1.885865	-1.530654
C	-3.005369	0.064447	1.242465
C	1.109850	3.009150	0.000000
C	-0.885469	3.578660	1.214157
H	2.162496	2.732653	0.000000
C	0.449038	3.156142	1.221824
H	-1.908389	1.300728	2.611538
C	-2.289630	0.275035	2.554585
H	-1.843048	-2.346565	1.805910
H	-3.006875	0.141208	3.374144
Cu	0.426556	-0.362931	1.500440
C	1.171087	2.784204	2.497223
N	-1.119803	-0.629513	2.772086
C	-1.528716	-2.065482	2.816076
H	-2.404364	-2.172187	3.471469
H	2.264083	1.310622	1.602190
H	2.008834	3.475518	2.683744
H	0.497643	2.866545	3.356847
H	0.507859	-3.326881	1.379679
N	1.667871	1.381255	2.428897
H	-0.767208	-0.393356	3.702225
H	2.232968	-1.885865	1.530654
N	1.588115	-1.809956	2.320077
C	0.817295	-3.077072	2.401079
C	-0.416609	-2.994498	3.305393
H	-0.842647	-4.002074	3.373719
H	1.471728	-3.886156	2.753986
C	2.514254	1.057532	3.600368
H	3.836064	-0.291841	2.529268
H	3.256970	1.852745	3.767891
H	-0.130994	-2.731382	4.331995
H	1.871950	1.039459	4.490528
C	3.248448	-0.279059	3.458730
C	2.379239	-1.535529	3.548721
H	1.686943	-1.440515	4.392041
H	3.014779	-2.407956	3.757688
H	3.980532	-0.336893	4.272289



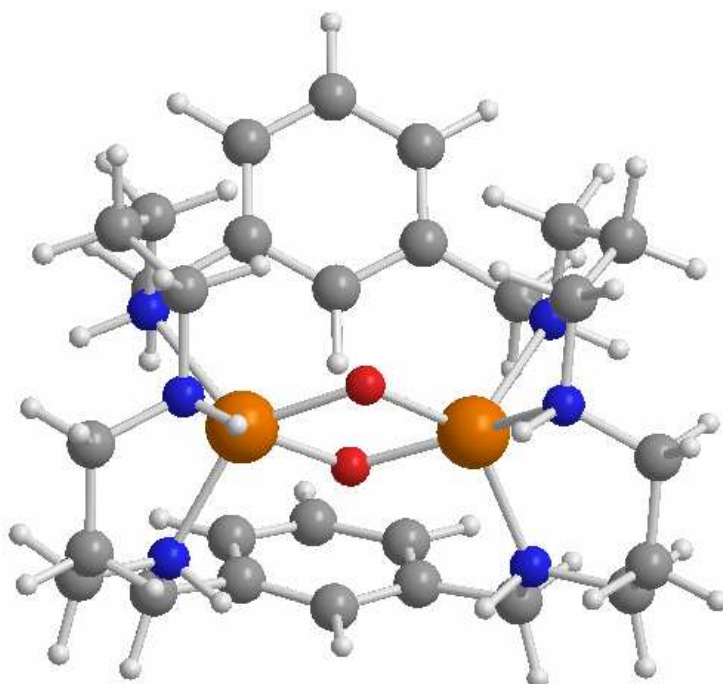
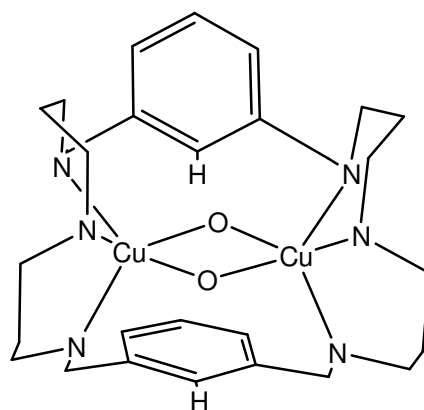
TS-ii

H	3.576509	2.619678	-1.041595
H	2.447735	4.549169	-1.579259
H	3.477160	1.160706	-3.001684
H	4.421411	-1.126333	-2.540652
H	3.873720	0.368457	-0.730252
H	4.411516	-1.375844	1.836257
H	2.859805	2.056543	0.467615
H	3.269387	0.699342	2.789270
C	2.745485	2.039263	-0.622545
H	2.107421	2.812621	2.840124
H	4.408737	-2.240589	-0.529828
C	1.486993	4.064017	-1.428347
H	3.468059	-1.016758	-3.995970
C	2.875498	0.390112	-2.502271
H	0.355813	5.805179	-2.000022
N	2.923666	0.601723	-1.026687
C	3.392678	-0.995778	-2.902720
C	3.491342	-1.931775	2.056711
H	3.578028	-2.278080	3.097302
H	4.181174	-3.853659	1.456435
C	1.447129	2.731691	-0.998994
C	0.310758	4.775961	-1.659628
C	2.399661	0.063422	2.984012
H	2.564928	-0.409415	3.964965
C	1.155979	2.287566	2.880472
C	3.570829	-2.925381	-0.360210
H	3.829389	-3.871886	-0.854256
H	1.837646	0.530304	-2.821067
H	-0.009798	4.095974	2.766868
C	3.390742	-3.161633	1.144293
N	2.348004	-0.995844	1.929569
C	1.132059	0.892253	3.001615
C	-0.037025	3.012762	2.832924
H	2.938714	-3.106481	-2.924708
C	2.519360	-2.188102	-2.491457
N	2.360752	-2.352703	-1.017600
Cu	1.626645	-0.665132	-0.130616
C	-0.924240	4.161784	-1.457001
H	2.445223	-3.692120	1.329574
C	0.190288	2.135565	-0.818481
H	1.486988	-1.526279	2.086630
H	1.513103	-2.060236	-2.907512
H	-1.836785	4.725352	-1.632910
H	1.598912	-3.015760	-0.864425
O	0.145739	0.782935	-0.574956
C	-1.010455	2.828832	-1.032507
C	-0.107524	0.252433	3.104436
C	-1.264405	2.345969	2.840801
H	-0.135435	-0.822841	3.257921
H	-2.188327	2.915848	2.774582
C	-1.310305	0.950356	2.957898
O	-0.089900	-1.252228	0.520351
H	-2.527779	2.274674	0.381382
C	-2.379934	2.259844	-0.703954
H	-0.064985	0.224553	0.332317
H	-1.499933	0.665344	-2.851791
H	-3.131185	2.928774	-1.140675
Cu	-1.738810	-0.625178	-0.141510
C	-2.614410	0.183773	2.884036
N	-2.704922	0.853341	-1.142516
C	-2.568969	0.660699	-2.617408
H	-3.019784	1.517349	-3.134970
H	-1.775872	-1.476238	2.048304
H	-2.843342	-0.293253	3.849244
H	-3.444924	0.859832	2.657944
H	-1.510352	-1.928620	-3.030870
N	-2.568968	-0.870655	1.820257
H	-3.701726	0.759624	-0.934527
H	-1.865059	-2.931985	-1.038160
N	-2.514773	-2.164264	-1.216109
C	-2.551431	-1.939868	-2.688071
C	-3.232806	-0.631280	-3.107294
H	-3.226775	-0.606854	-4.203133
H	-3.052309	-2.784271	-3.180779
C	-3.799190	-1.705024	1.835366
H	-2.890977	-3.528525	1.071480
H	-3.972345	-2.091751	2.849898
H	-4.294595	-0.636371	-2.826587
H	-4.649002	-1.053291	1.598242
C	-3.763967	-2.893536	0.861390
C	-3.830978	-2.572221	-0.640156
H	-4.546493	-1.761061	-0.813157
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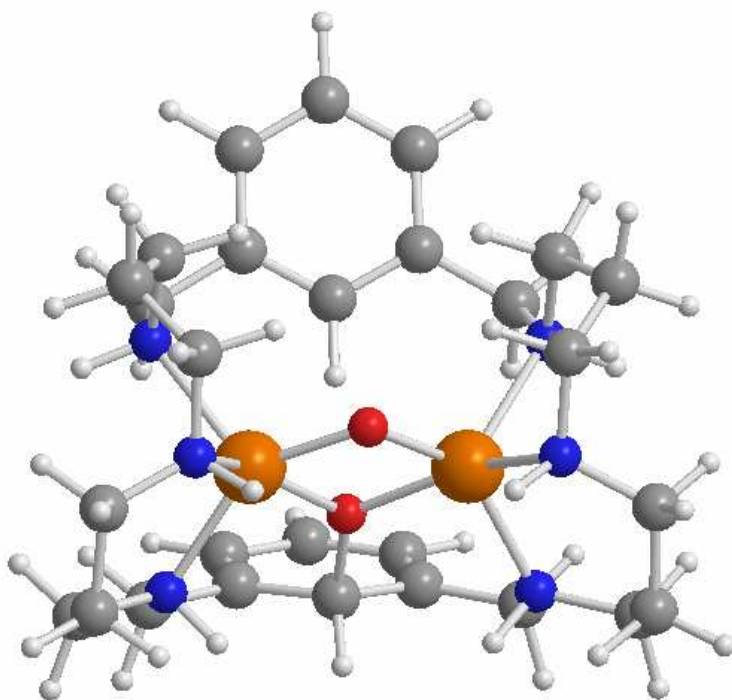
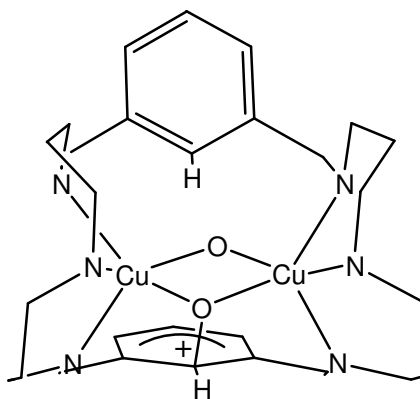
TS-em

H	-1.679503	4.777405	0.000000
H	2.406305	3.061747	2.824519
H	-0.696005	4.032290	2.146654
H	2.406306	3.061746	-2.824518
C	-0.782908	4.165737	0.000000
H	-0.696005	4.032290	-2.146654
C	-0.221676	3.751646	1.209714
C	-0.221676	3.751646	-1.209715
C	0.949441	2.986733	1.222593
C	0.949442	2.986733	-1.222593
H	0.780529	2.607812	3.326718
C	1.566372	2.683395	0.000000
H	0.780529	2.607812	-3.326719
C	1.519346	2.480269	2.530488
C	1.519346	2.480269	-2.530488
H	2.529591	2.179827	0.000000
H	3.306273	1.344223	-4.067816
H	3.306272	1.344224	4.067817
H	2.657269	0.944139	1.826989
H	2.657268	0.944139	-1.826989
H	1.716317	0.792677	4.588490
N	1.901125	1.024013	2.510257
H	1.716318	0.792677	-4.588490
N	1.901125	1.024013	-2.510257
C	2.491329	0.648352	3.826834
C	2.491330	0.648351	-3.826834
H	-1.796840	1.730425	2.508817
H	-1.796840	1.730425	-2.508817
H	3.622630	-0.878607	-4.788859
H	3.622630	-0.878606	4.788860
C	3.018207	-0.787182	-3.879402
C	3.018207	-0.787181	3.879403
H	3.712873	-0.973283	-3.046186
H	3.712873	-0.973282	3.046186
C	-2.336029	0.777617	2.518559
H	-3.054256	0.809515	3.349597
C	-2.336029	0.777617	-2.518558
H	-3.054256	0.809515	-3.349596
O	0.697526	0.449781	0.000000
C	-2.426351	0.773796	0.000000
C	-3.085691	0.590277	1.218512
C	-3.085691	0.590277	-1.218512
H	-4.980055	0.124154	2.147391
C	-4.444950	0.250524	1.209515
H	-0.976619	-0.089636	3.731776
O	0.536432	-1.359497	0.000000
C	-4.444950	0.250524	-1.209514
H	-4.980055	0.124154	-2.147391
H	-0.976620	-0.089636	-3.731776
Cu	0.661846	-0.425605	-1.604200
Cu	0.661846	-0.425605	1.604200
C	-5.122884	0.089277	0.000000
H	-6.179328	-0.161081	0.000000
N	-1.316246	-0.292783	2.788110
N	-1.316246	-0.292782	-2.788110
H	1.201286	-1.614791	4.695522
H	1.201286	-1.614791	-4.695522
C	1.942332	-1.872498	3.933677
C	1.942332	-1.872498	-3.933677
N	1.234514	-2.053609	-2.637639
N	1.234514	-2.053609	2.637639
H	2.390096	-2.829516	4.232574
H	2.390095	-2.829516	-4.232574
H	1.926006	-2.414567	-1.975880
H	1.926007	-2.414566	1.975880
C	-1.965573	-1.629905	2.865203
H	-2.896621	-1.563339	3.447368
C	-1.965574	-1.629904	-2.865203
H	-2.896621	-1.563339	-3.447368
H	-0.809848	-2.420847	4.524117
H	-2.246699	-1.921096	1.848810
H	-2.246699	-1.921096	-1.848810
H	-0.809849	-2.420846	-4.524117
C	-1.076585	-2.702440	3.496758
C	0.164608	-3.100425	-2.697660
C	-1.076585	-2.702439	-3.496759
C	0.164609	-3.100425	2.697660
H	-0.116579	-3.311911	-1.661344
H	-0.116579	-3.311911	1.661344
H	0.597128	-4.015988	-3.122380
H	0.597129	-4.015988	3.122379
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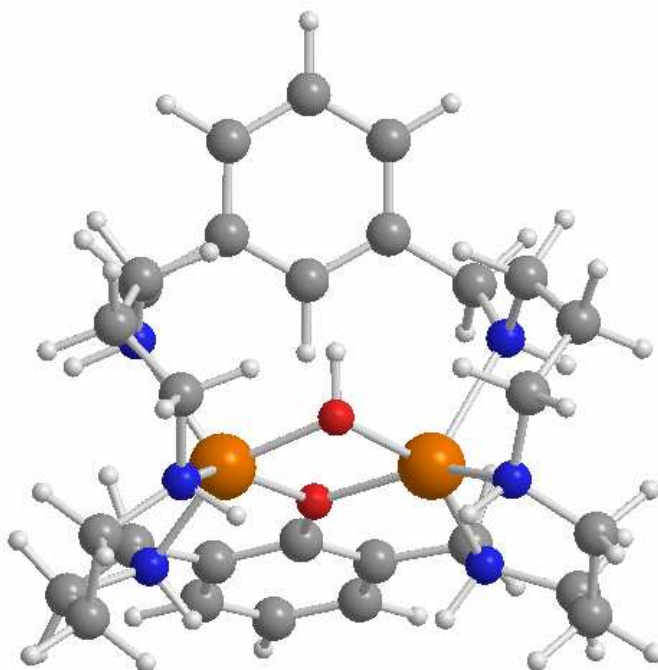
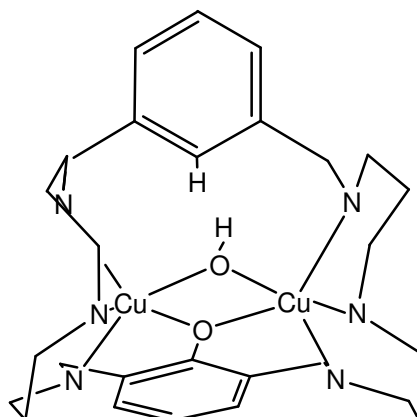
m

H	-2.317805	4.842398	0.000000
H	1.527693	3.438763	2.902530
H	-1.350775	4.132743	2.154196
H	1.527666	3.438729	-2.902530
C	-1.435478	4.208860	0.000001
H	-1.350807	4.132690	-2.154192
C	-0.885164	3.800587	1.230195
C	-0.885182	3.800557	-1.230189
C	0.233518	3.001529	1.262378
C	0.233505	3.001504	-1.262368
H	0.087640	2.533935	3.347795
C	0.829736	2.475748	0.000007
H	0.087610	2.533896	-3.347780
C	0.862883	2.617957	2.579057
C	0.862860	2.617922	-2.579048
H	1.928477	2.602077	0.000001
H	2.831659	1.930800	-4.195370
H	2.831700	1.930834	4.195361
H	2.398904	1.467319	1.904371
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H	1.425561	0.946016	4.606375
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H	-2.501900	-2.202720	-3.264290
H	-0.281686	-2.581621	4.378991
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C	-0.469924	-2.895966	3.342801
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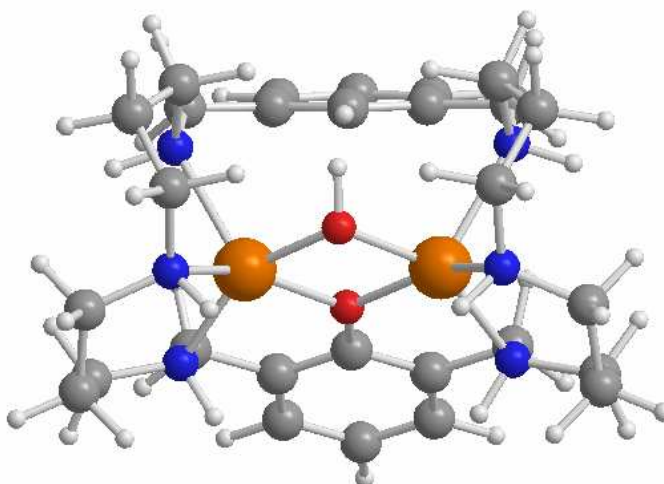
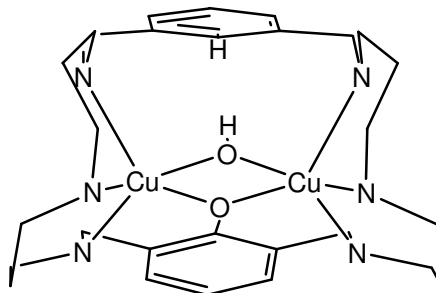
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C	-1.196993	-4.429476	2.133777
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TS-nl

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C	2.574275	0.658906	2.541159
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H	3.633024	-0.465248	1.257687
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C	-1.206326	2.630833	3.207920
H	-2.144266	3.149337	3.392279
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H	3.189831	-3.835166	2.111247
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de											
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H	-3.270919	-2.439211	2.761873	H	-3.560705	-1.717880	3.010498	H	-3.560705	-1.717880	3.010498
H	-2.097020	0.280015	4.220183	H	-2.120763	0.789219	4.307348	H	-2.120763	0.789219	4.307348
H	2.059712	-3.473641	2.404252	H	1.721278	-3.298091	2.602257	H	1.721278	-3.298091	2.602257
C	0.035015	-0.017553	4.265132	C	-0.019943	0.324565	4.355286	C	-0.019943	0.324565	4.355286
H	2.129192	-0.489795	4.073699	H	2.029084	-0.322263	4.184019	H	2.029084	-0.322263	4.184019
C	-1.257053	-0.267510	3.799258	C	-1.326619	0.175174	3.889500	C	-1.326619	0.175174	3.889500
C	1.123866	-0.699810	3.716398	C	1.013559	-0.447004	3.815676	C	1.013559	-0.447004	3.815676
C	-1.478897	-1.237029	2.811170	C	-1.621941	-0.774214	2.900088	C	-1.621941	-0.774214	2.900088
C	0.922209	-1.669750	2.727379	C	0.737780	-1.395685	2.824736	C	0.737780	-1.395685	2.824736
H	-3.551985	-0.712425	2.583967	H	-3.604967	-0.028410	2.529745	H	-3.604967	-0.028410	2.529745
C	-0.384981	-1.956144	2.324287	C	-0.585195	-1.568012	2.405705	C	-0.585195	-1.568012	2.405705
H	3.030860	-2.002980	2.446545	H	2.813133	-1.917954	2.559372	H	2.813133	-1.917954	2.559372
C	-2.873553	-1.522670	2.297327	C	-3.041383	-0.959067	2.404169	C	-3.041383	-0.959067	2.404169
C	2.077911	-2.415274	2.101178	C	1.826168	-2.265328	2.237778	C	1.826168	-2.265328	2.237778
H	-0.547245	-2.747342	1.596356	H	-0.799090	-2.326201	1.659790	H	-0.799090	-2.326201	1.659790
H	2.947133	-4.263219	0.450668	H	2.445457	-4.312353	0.718666	H	2.445457	-4.312353	0.718666
H	-4.633826	-2.921595	0.970482	H	-5.004147	-2.252254	1.265341	H	-5.004147	-2.252254	1.265341
H	-2.317469	-2.437831	0.565848	H	-2.644140	-2.243232	0.876720	H	-2.644140	-2.243232	0.876720
H	1.152969	-2.687172	0.298308	H	0.867979	-2.522500	0.420575	H	0.867979	-2.522500	0.420575
H	-4.978392	-1.229893	0.631693	H	-5.054594	-0.616670	0.616856	H	-5.054594	-0.616670	0.616856
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H	4.073407	-2.911498	0.401139	H	3.743501	-3.129463	0.600965	H	3.743501	-3.129463	0.600965
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C	3.095567	-3.254119	0.041192	C	2.733090	-3.364677	0.244470	C	2.733090	-3.364677	0.244470
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H	2.631881	1.388578	2.198333	H	2.662395	1.296493	2.189690	H	2.662395	1.296493	2.189690
H	3.718966	-4.193372	-1.762163	H	3.204629	-4.512663	-1.482456	H	3.204629	-4.512663	-1.482456
H	-5.380595	-2.857509	-1.264454	H	-5.672470	-2.542749	-0.959447	H	-5.672470	-2.542749	-0.959447
C	3.100995	-3.330338	-1.489120	C	2.736551	-3.543171	-1.277238	C	2.736551	-3.543171	-1.277238
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H	2.091699	-3.559618	-1.861944	H	1.706084	-3.621861	-1.651343	H	1.706084	-3.621861	-1.651343
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C	-2.224488	2.328592	1.007374	C	-2.031288	2.538480	0.712045	C	-2.031288	2.538480	0.712045
H	-2.995901	3.087624	1.184994	H	-2.712283	3.395431	0.782847	H	-2.712283	3.395431	0.782847
C	2.791395	2.037911	1.332545	C	2.942256	1.873501	1.303597	C	2.942256	1.873501	1.303597
H	3.634443	2.704283	1.558934	H	3.802349	2.502523	1.567089	H	3.802349	2.502523	1.567089
O	0.132621	-0.290179	-0.301151	O	0.142095	-0.351104	-0.526568	O	0.142095	-0.351104	-0.526568
C	0.290817	2.259979	1.156861	C	0.474131	2.255335	0.950929	C	0.474131	2.255335	0.950929
C	-0.873660	2.990856	0.901471	C	-0.614675	3.043371	0.559524	C	-0.614675	3.043371	0.559524
C	1.552433	2.855955	1.061723	C	1.785316	2.737653	0.860128	C	1.785316	2.737653	0.860128
H	-1.664109	4.946151	0.423545	H	-1.211111	4.983110	-0.182331	H	-1.211111	4.983110	-0.182331
C	-0.767410	4.353292	0.586141	C	-0.375990	4.342972	0.090491	C	-0.375990	4.342972	0.090491
H	-3.625678	1.323335	-0.055197	H	-3.531328	1.574011	-0.239603	H	-3.531328	1.574011	-0.239603
O	-0.445312	-1.391572	-0.944988	O	-0.557489	-1.565126	-0.865417	O	-0.557489	-1.565126	-0.865417
C	1.639443	4.216815	0.740306	C	2.001024	4.039407	0.386956	C	2.001024	4.039407	0.386956
H	2.611381	4.701101	0.691500	H	3.010897	4.439151	0.341736	H	3.010897	4.439151	0.341736
H	4.035476	0.681541	0.517312	H	4.128102	0.342094	0.708390	H	4.128102	0.342094	0.708390
Cu	2.051535	-0.502590	-0.303390	Cu	1.977402	-0.567821	-0.263059	Cu	1.977402	-0.567821	-0.263059
Cu	-1.823835	-0.228556	-0.561022	Cu	-1.894070	-0.259810	-0.499754	Cu	-1.894070	-0.259810	-0.499754
C	0.483797	4.964461	0.509794	C	0.924733	4.839195	0.003618	C	0.924733	4.839195	0.003618
H	0.558010	6.023449	0.282957	H	1.097255	5.853120	-0.343645	H	1.097255	5.853120	-0.343645
N	-2.640380	1.544282	-0.222836	N	-2.525519	1.651955	-0.410790	N	-2.525519	1.651955	-0.410790
N	3.177775	1.137345	0.190368	N	3.374578	0.873078	0.261930	N	3.374578	0.873078	0.261930
H	-4.945278	-0.388882	-1.705722	H	-5.032341	-0.271935	-1.838192	H	-5.032341	-0.271935	-1.838192
H	4.608908	-1.804230	-1.751731	H	4.491169	-2.324431	-1.608581	H	4.491169	-2.324431	-1.608581
C	-4.308308	-1.203305	-2.065241	C	-4.434277	-1.171693	-2.015220	C	-4.434277	-1.171693	-2.015220
C	3.669840	-2.112852	-2.224528	C	3.510154	-2.485940	-2.069149	C	3.510154	-2.485940	-2.069149
N	2.743639	-0.949146	-2.218692	N	2.801607	-1.179118	-2.121685	N	2.801607	-1.179118	-2.121685
N	-2.922433	-0.678393	-2.223156	N	-3.015032	-0.759396	-2.184553	N	-3.015032	-0.759396	-2.184553
H	-4.689527	-1.492393	-3.054063	H	-4.799582	-1.614054	-2.952335	H	-4.799582	-1.614054	-2.952335
H	3.912234	-2.388313	-3.260725	H	3.695011	-2.848228	-3.089856	H	3.695011	-2.848228	-3.089856
H	1.915003	-1.245205	-2.736874	H	1.952329	-1.338773	-2.667196	H	1.952329	-1.338773	-2.667196
H	-2.364005	-1.436362	-2.620373	H	-2.492365	-1.587955	-2.474814	H	-2.492365	-1.587955	-2.474814
C	-2.609245	2.384584	-1.462199	C	-2.392587	2.316108	-1.746847	C	-2.392587	2.316108	-1.746847
H	-3.032777	3.369880	-1.231029	H	-2.685310	3.369349	-1.650031	H	-2.685310	3.369349	-1.650031
C	3.593065	1.929023	-1.007264	C	4.009602	1.551289	-0.912206	C	4.009602	1.551289	-0.912206
H	4.296229	2.712517	-0.691353	H	4.798552	2.222345	-0.546115	H	4.798552	2.222345	-0.546115
H	-4.448454	1.674059	-2.364321	H	-4.307516	1.697217	-2.550630	H	-4.307516	1.697217	-2.550630
H	-1.559984	2.538778	-1.727520	H	-1.333667	2.298293	-2.019231	H	-1.333667	2.298293	-2.019231
H	2.703152	2.432724	-1.396322	H	3.245441	2.178464	-1.381149	H	3.245441	2.178464	-1.381149
H	5.058282	0.472498	-1.677493	H	5.269455	-0.138288	-1.444539	H	5.269455	-0.138288	-1.444539
C	-3.387990	1.775237	-2.629575	C	-3.247946	1.668243	-2.838316	C	-3.247946	1.668243	-2.838316
C	3.304060	0.223729	-2.946443	C	3.589482	-0.134519	-2.834787	C	3.589482	-0.134519	-2.834787
C	4.250604	1.084382	-2.103388	C	4.605079	0.583618	-1.940029	C	4.605079	0.583618	-1.940029
C	-2.839154	0.458973	-3.184991	C	-2.837888	0.254844	-3.260299	C	-2.837888	0.254844	-3.260299
H	2.457545	0.838782	-3.273002	H	2.878009	0.598695	-3.231404	H	2.878009	0.598695	-3.231404
H	-1.781497	0.580012	-3.444925	H	-1.776883	0.248437	-3.534106	H	-1.776883	0.248437	-3.534106
H	3.827140	-0.113987	-3.852270	H	4.106303	-0.580163	-3.695743	H	4.106303	-0.580163	-3.695743
H	-3.377337	0.199194	-4.106256	H	-3.408736	-0.039710	-4.151683	H	-3.408736	-0.039710	-4.151683
H	-3.365147	2.505620	-3.446561	H	-3.174145	2.307806	-3.725617	H	-3.174145	2.307806	-3.725617
H	4.748547	1.780180	-2.788750	H	5.257020	1.173169	-2.595114	H	5.257020	1.173169	-2.595114
H	0.214671	1.221778	1.461996	H	0.294580	1.268940	1.367158	H	0.294580	1.268940	1.367158

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H	0.000700	0.165134	5.183817	H	0.000777	0.080251	5.181909	H	-0.127014	5.182395	0.000000	
H	-2.759492	-3.230776	2.346503	H	-2.753777	-3.276515	2.288016	H	3.249403	2.321911	2.759492	
H	-2.147959	-0.558048	4.185277	H	-2.147875	-0.628615	4.173324	H	0.589319	4.178930	2.147959	
H	2.758397	-3.232239	2.345524	H	2.752086	-3.278467	2.286776	H	3.249403	2.321911	-2.759492	
C	0.000433	-0.483585	4.313202	C	0.000449	-0.554980	4.301422	C	0.515733	4.307361	0.000000	
H	2.148764	-0.559184	4.184836	H	2.148693	-0.630082	4.172770	H	0.589319	4.178930	-2.147959	
C	-1.209516	-0.892060	3.749083	C	-1.209482	-0.955121	3.731352	C	0.920338	3.740461	1.209516	
C	1.210056	-0.892687	3.748820	C	1.209962	-0.955937	3.731034	C	0.920338	3.740461	-1.209516	
C	-1.220618	-1.748331	2.640225	C	-1.220407	-1.793838	2.609162	C	1.769002	2.625770	1.220618	
C	1.220480	-1.748939	2.639946	C	1.220026	-1.794642	2.608828	C	1.769002	2.625770	-1.220618	
H	-3.345781	-1.573005	2.393088	H	-3.347381	-1.622748	2.371145	H	1.591989	2.379838	3.345781	
C	-0.000242	-2.197549	2.128468	C	-0.000408	-2.234236	2.089392	C	2.214708	2.110951	0.000000	
H	3.345712	-1.574834	2.392449	H	3.347098	-1.625230	2.370481	H	1.591989	2.379838	-3.345781	
C	-2.527367	-2.201793	2.027856	C	-2.526915	-2.240037	1.991264	C	2.218263	2.010312	2.527367	
C	2.526842	-2.203027	2.027205	C	2.526042	-2.241674	1.990502	C	2.218263	2.010312	-2.527367	
H	-0.000500	-2.902356	1.299564	H	-0.000728	-2.923531	1.247928	H	2.913827	1.277244	0.000000	
H	3.964787	-3.709056	0.446239	H	3.956245	-3.726475	0.379907	H	3.714669	0.418419	-3.964787	
H	-3.966921	-3.707096	0.447825	H	-3.959159	-3.723908	0.381858	H	3.714669	0.418419	3.964787	
H	-1.792428	-2.750943	0.211663	H	-1.791431	-2.744482	0.159818	H	2.754973	0.190404	1.792428	
H	1.791014	-2.751028	0.211017	H	1.789612	-2.744741	0.158982	H	2.754973	0.190404	-1.792428	
H	-4.628697	-2.077507	0.382714	H	-4.634527	-2.098804	0.359774	H	2.082723	0.366059	4.628697	
N	-2.536755	-2.130468	0.535884	N	-2.541273	-2.093773	0.500306	N	2.136731	0.518863	2.536755	
H	4.627884	-2.079986	0.381644	H	4.633458	-2.102127	0.358958	H	2.082723	0.366059	-4.628697	
N	2.535940	-2.131285	0.535259	N	2.540180	-2.140397	0.499582	N	2.136731	0.518863	-2.536755	
C	-3.806741	-2.706894	0.019346	C	-3.810308	-2.712829	-0.024054	C	2.709609	-0.001607	3.806741	
C	3.805325	-2.708546	0.018210	C	3.808520	-2.714934	-0.025269	C	2.709609	-0.001607	-3.806741	
H	-2.447429	1.268248	2.136724	H	-2.444238	1.223764	2.146569	H	-1.250951	2.142921	2.447429	
H	2.446642	1.266927	2.137247	H	2.443501	1.222519	2.147224	H	-1.250951	2.142921	-2.447429	
H	4.733485	-3.422497	-1.762442	H	4.744649	-3.392330	-1.815406	H	3.413004	-1.788250	-4.733485	
H	-4.735906	-3.420851	-1.760775	H	-4.747098	-3.390646	-1.813704	H	3.413004	-1.788250	4.733485	
C	3.864607	-2.804728	-1.508319	C	3.877752	-2.775103	-1.553380	C	2.796988	-1.529906	-3.864607	
C	-3.866459	-2.803693	-1.507128	C	-3.879624	-2.774041	-1.552119	C	2.796988	-1.529906	3.864607	
H	2.992253	-3.354623	-1.892806	H	3.004832	-3.309978	-1.956953	H	3.344240	-1.918146	-2.992253	
H	-2.994649	-3.354491	-1.891563	H	-3.007205	-3.310036	-1.955290	H	3.344240	-1.918146	2.992253	
C	-2.506345	2.041251	1.365693	C	-2.508614	2.014127	1.393651	C	-2.029212	1.377198	2.506345	
H	-3.342786	2.707863	1.611549	H	-3.340358	2.676991	1.663253	H	-2.694126	1.627609	3.342786	
C	2.506373	2.040133	1.366489	C	2.508626	2.013082	1.394584	C	-2.029212	1.377198	-2.506345	
H	3.343038	2.706221	1.612935	H	3.340518	2.675505	1.664815	H	-2.694126	1.627609	-3.342786	
O	-0.000068	0.080522	-0.054296	O	-0.000001	0.087405	-0.074733	O	-0.078245	-0.056174	0.000000	
C	0.000054	2.174576	1.505290	C	0.000014	2.140241	1.521746	C	-2.161579	1.517704	0.000000	
C	-1.218577	2.827347	1.303531	C	-1.218755	2.798300	1.337641	C	-2.815715	1.320416	1.218577	
C	1.219021	2.826848	1.303927	C	1.219120	2.797807	1.338118	C	-2.815715	1.320416	-1.218577	
H	-2.145468	4.741431	0.910451	H	-2.145467	4.721369	0.989451	H	-4.732444	0.940442	2.145468	
C	-1.208951	4.201126	1.023807	C	-1.209037	4.178014	1.088718	C	-4.191376	1.050098	1.208951	
H	-3.795884	0.956463	0.244644	H	-3.818724	0.963812	0.260238	H	-0.952120	0.248752	3.795884	
O	-0.000019	-0.932344	-1.082863	O	-0.000037	-0.953691	-1.134834	O	0.827537	-0.988675	0.000000	
C	1.210077	4.400629	1.024207	C	1.210052	4.177533	1.089222	C	-4.191376	1.050098	-1.208951	
H	2.146858	4.740535	0.911147	H	2.146736	4.720523	0.990356	H	-4.732444	0.940442	-2.145468	
H	3.795886	0.954981	0.245777	H	3.818846	0.962480	0.261542	H	-0.952120	0.248752	-3.795884	
Cu	1.796939	-0.299796	-0.543349	Cu	1.810943	-0.294184	-0.538434	Cu	0.298718	-0.547818	-1.796939	
Cu	-1.797096	-0.299744	-0.543307	Cu	-1.810959	-0.294039	-0.538443	Cu	0.298718	-0.547818	1.796939	
C	0.000724	4.888671	0.909108	C	0.000667	4.867656	0.987604	C	-4.879690	0.940107	0.000000	
H	0.000968	5.995776	0.720814	H	0.000915	5.940616	0.822707	H	-5.950058	0.759132	0.000000	
N	-2.856669	1.325325	0.072796	N	-2.877701	1.328318	0.088480	N	-1.322150	0.079432	2.856669	
N	2.856964	1.324414	0.073531	N	2.878100	1.327517	0.089390	N	-1.322150	0.079432	-2.856669	
H	-4.803630	-0.876671	-1.768099	H	-4.832497	-0.847336	-1.767434	H	0.867199	-1.776487	4.803630	
H	4.803237	-0.878313	-1.768557	H	4.832160	-0.848955	-1.767093	H	0.867199	-1.776487	-4.803630	
C	-4.023446	-1.475223	-2.248808	C	-4.049214	-1.430081	-2.262518	C	1.462447	-2.261280	4.023446	
C	4.022545	-1.476061	-2.249441	C	4.048578	-1.430774	-2.262793	C	1.462447	-2.261280	-4.023446	
N	2.770221	-0.669107	-2.279602	N	2.800707	-0.616448	-2.276388	N	0.656140	-2.286558	-2.770221	
N	-2.770492	-0.669280	-2.279397	N	-2.800740	-0.616681	-2.276338	N	0.656140	-2.286558	2.770221	
H	-4.351994	-1.659698	-3.280621	H	-4.377576	-1.593732	-3.297640	H	1.639858	-3.294331	4.351994	
H	4.350848	-1.660351	-3.281367	H	4.377083	-1.593952	-3.297943	H	1.639858	-3.294331	-4.351994	
H	2.086514	-1.225086	-2.796785	H	2.106633	-1.162984	-2.790747	H	1.208567	-2.807533	-2.086514	
H	-2.087231	-1.226055	-2.796316	H	-2.106980	-1.163974	-2.790316	H	1.208567	-2.807533	2.086514	
C	-2.998224	2.283944	-1.064843	C	-3.020172	2.311928	-1.028294	C	-2.288530	-1.051621	2.998224	
H	-3.566055	3.160583	-0.725981	H	-3.583710	3.182610	-0.668465	H	-3.162830	-0.706768	3.566055	
C	2.999699	2.283409	-1.063663	C	3.021713	2.311479	-1.026930	C	-2.288530	-1.051621	-2.998224	
H	3.568093	3.159439	-0.724183	H	3.585736	3.181600	-0.666504	H	-3.162830	-0.706768	-3.566055	
H	-4.704417	1.333745	-2.009845	H	-4.732015	1.384218	-1.986547	H	-1.344820	-2.003102	4.704417	
H	-1.995593	2.631694	-1.328640	H	-2.016855	2.660622	-1.287917	H	-2.638077	-1.313032	1.995593	
H	1.997429	2.632067	-1.327645	H	2.018749	2.661010	-1.286788	H	-2.638077	-1.313032	-1.995593	
H	4.705473	1.332336	-2.008562	H	4.733226	1.382904	-1.984951	H	-1.344820	-2.003102	-4.704417	
C	-3.702301	1.687678	-2.285782	C	-3.729013	1.739657	-2.257615	C	-1.700633	-2.276611	3.702301	
C	2.932775	0.604066	-3.042473	C	2.960934	0.664899	-3.026778	C	-0.622223	-3.040699	-2.932775	
C	3.703712	1.687158	-2.284636	C	3.730594	1.739227	-2.256226	C	-1.700633	-2.276611	-3.702301	
C	-2.931993	0.603654	-3.042918	C	-2.959899	0.664399	-3.027419	C	-0.622223	-3.040699	2.932775	
H	1.925751	0.967225	-3.276966	H	1.952756	1.028644	-3.255079	H	-0.986978	-3.272702	-1.925751	
H	-1.924651	0.965948	-3.277380	H	-1.951409	1.027319	-3.255646	H	-0.986978	-3.272702	1.925751	
H	3.438167	0.396100	-3.995186	H	3.464391	0.466524	-3.982208	H	-0.420781	-3.994813	-3.438167	
H	-3.437348	0.395589	-3.995631	H	-3.463251	0.465891	-3.982876	H	-0.420781	-3.994813	3.438167	
H	-3.872901	2.510073	-2.990232	H	-3.896839	2.573178	-2.949493	H	-2.527828	-2.975417	3.872901	
H	3.875135	2.509753	-2.988654	H	3.899299	2.572936	-2.947666	H	-2.527828	-2.975417	-3.872901	
H	-0.000197	1.134373	1.807353	H	-0.000244	1.092057	1.794510	H	-1.119333	1.812642	0.000000	

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H	0.000045	-0.303952	5.368111	H	-2.965542	4.588812	0.001011	H	-3.427567	4.185941	0.000000
H	-2.728683	-3.366479	2.137932	H	1.278973	3.684623	2.800200	H	0.961338	3.838670	2.780836
H	-2.148529	-0.904324	4.289120	H	-1.871187	4.030127	2.150814	H	-2.267554	3.778319	2.150563
H	2.750756	-3.351757	2.141655	H	1.276253	3.683500	-2.800890	H	0.961338	3.838670	-2.780836
C	0.002204	-0.845602	4.426772	C	-1.990715	4.110422	0.000824	C	-2.394426	3.850669	0.000000
H	2.153431	-0.893318	4.292622	H	-1.872848	4.028410	-2.149190	H	-2.267554	3.778319	-2.150563
C	-1.209565	-1.186648	3.818712	C	-1.371772	3.796099	1.213643	C	-1.737838	3.623941	1.213381
C	1.216685	-1.180743	3.820873	C	-1.372739	3.795062	-1.212222	C	-1.737838	3.623941	-1.213381
C	-1.216139	-1.913582	2.620921	C	-0.104802	3.198115	1.222688	C	-0.395667	3.220396	1.224861
C	1.228895	-1.907509	2.622988	C	-0.105714	3.197198	-1.221799	C	-0.395667	3.220396	-1.224861
H	-3.341560	-1.728879	2.324200	H	-0.123024	2.768887	3.332211	H	-0.365617	2.831752	3.344834
C	0.007815	-2.300772	2.071790	C	0.520666	2.945155	0.000301	C	0.265194	3.075949	0.000000
H	3.353541	-1.710630	2.329790	H	-0.125371	2.766051	-3.330914	H	-0.365617	2.831752	-3.344834
C	-2.501055	-2.308123	1.925479	C	0.603943	2.859760	2.517215	C	0.345744	2.960846	2.521217
C	2.517119	-2.294686	1.929438	C	0.602217	2.858260	-2.516624	C	0.345744	2.960846	-2.521217
H	0.009952	-2.926830	1.183102	H	1.520603	2.524837	0.000061	H	1.324082	2.835587	0.000000
H	3.675929	-3.783682	0.117247	H	2.784949	2.327854	-3.844573	H	2.615264	2.630078	-3.780997
H	-3.661212	-3.796726	0.112947	H	2.787170	2.327936	3.843990	H	2.615264	2.630078	3.780997
H	-1.589668	-2.536958	0.111323	H	2.013182	1.657600	1.653127	H	1.807805	1.839834	1.643368
H	1.604943	-2.519726	0.115409	H	2.013539	1.658370	-1.652907	H	1.807805	1.839834	-1.643368
H	-4.497418	-2.248998	0.082966	H	1.547870	1.272859	4.511604	H	1.468873	1.522372	4.527370
N	-2.436838	-2.085600	0.456644	N	1.367908	1.585834	2.440177	N	1.200320	1.744752	2.456962
H	4.513425	-2.236867	0.081201	H	1.545943	1.271481	-4.510677	H	1.468873	1.522372	-4.527370
N	2.453719	-2.071252	0.460588	N	1.367523	1.585171	-2.439217	N	1.200320	1.744752	-2.456962
C	-3.570131	-2.751664	-0.222437	C	2.210516	1.411151	3.647014	C	2.092755	1.671643	3.636069
C	3.584805	-2.739395	-0.220434	C	2.209225	1.411031	-3.646723	C	2.092755	1.671643	-3.636069
H	-2.538043	0.853909	2.108673	H	-1.893014	1.116281	2.597893	H	-2.018067	0.872158	2.598741
H	2.545199	0.867579	2.102331	H	-1.892713	1.115930	-2.598466	H	-2.018067	0.872158	-2.598741
H	4.234537	-3.383129	-2.146891	H	3.889289	0.309232	-4.364936	H	3.851482	0.703382	-4.355068
H	-4.221404	-3.395336	-2.148499	H	3.889903	0.308251	4.364450	H	3.851482	0.703382	4.355068
C	3.458650	-2.721510	-1.745341	C	3.178123	0.231873	-3.534657	C	3.137225	0.554061	-3.537418
C	-3.448242	-2.730207	-1.747488	C	3.178337	0.231517	3.534456	C	3.137225	0.554061	3.537418
H	2.500914	-3.163997	-2.055251	H	3.779912	0.318687	-2.618565	H	3.718765	0.658965	-2.610108
H	-2.488696	-3.166131	-2.061083	H	3.779835	0.317868	2.618136	H	3.718765	0.658965	2.610108
C	-2.561172	1.720797	1.440352	C	-2.193083	0.062312	2.567127	C	-2.206502	-0.206617	2.576519
H	-3.866129	2.374400	1.751907	H	-2.887173	-0.118059	3.397117	H	-2.887914	-0.450160	3.401863
C	2.559800	1.732548	1.431276	C	-2.192664	0.061922	-2.567642	C	-2.206502	-0.206617	-2.576519
C	3.382281	2.392054	1.736884	H	-2.886773	-0.118543	-3.397599	H	-2.887914	-0.450160	-3.401863
O	-0.001262	0.858109	0.220120	O	-0.809790	-0.362599	-0.000071	O	-0.772182	-0.395505	0.000000
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H	-2.156538	4.402139	1.516200	H	-4.595719	-1.113677	2.153704	H	-4.485542	-1.607514	2.154116
H	-1.223872	3.843782	1.513124	C	-4.095563	-0.856214	1.222858	H	-4.010498	-1.301559	1.225026
H	-3.708787	0.645085	0.146184	H	-0.581186	-0.431054	3.716363	H	-0.562495	-0.497762	3.737072
O	-0.000979	-0.850419	-1.353731	O	1.597057	-0.402736	0.000357	O	1.640277	-0.264765	0.000000
C	1.212619	3.849208	1.509239	C	-4.095244	-0.856481	-1.223447	C	-4.010498	-1.301559	-1.225026
H	2.142742	4.411794	1.509160	H	-4.595205	-1.114090	-2.154356	H	-4.485542	-1.607514	-2.154116
H	3.706806	0.658793	0.135021	H	-0.580718	-0.431350	-3.716819	H	-0.562495	-0.497762	-3.737072
Cu	1.465057	-0.045881	-0.629963	Cu	0.473373	-0.401990	-1.452008	Cu	0.493011	-0.389493	-1.466025
Cu	-1.467510	-0.048637	-0.628071	Cu	0.472943	-0.402136	1.451793	Cu	0.493011	-0.389493	1.466025
C	-0.007147	4.547944	1.543595	C	-4.744190	-1.146135	-0.000348	C	-4.621583	-1.643394	0.000000
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N	-2.853231	1.197778	0.065448	N	-0.941435	-0.737338	2.810177	N	-0.883172	-0.863383	2.838738
N	2.848557	1.207568	0.056387	N	-0.940924	-0.737591	-2.810606	N	-0.883172	-0.863383	-2.838738
H	-4.488180	-0.849687	-1.925576	H	1.823918	-1.176765	4.447588	H	1.868825	-0.920972	4.474309
H	4.487636	-0.835325	-1.933005	H	1.824829	-1.177416	-4.447693	H	1.868825	-0.920972	-4.474309
C	-3.646906	-1.362919	-2.401931	C	2.539679	-1.154761	3.619793	C	2.603392	-0.875481	3.663272
C	3.647569	-1.354836	-2.404635	C	2.540507	-1.154878	-3.619841	C	2.603392	-0.875481	-3.663272
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H	1.672867	-0.952182	-2.796891	H	2.513557	-1.589375	-1.612241	H	2.645894	-1.341529	-1.659781
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C	-3.098660	2.286045	-0.926471	C	-1.205873	-2.204719	2.896559	C	-0.989520	-2.348052	2.966865
H	-3.825656	2.994879	-0.506814	H	-2.053042	-2.377756	3.572975	H	-1.804920	-2.594183	3.661483
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H	3.811321	3.007556	-0.523336	H	-2.052296	-2.378266	-3.573324	H	-1.804920	-2.594183	-3.661483
H	-4.604955	1.315617	-2.147583	H	0.255931	-2.714022	4.414973	H	0.529079	-2.663214	4.479970
H	-2.155419	2.822026	-1.059995	H	-1.511253	-2.532897	1.899122	H	-1.272889	-2.733801	1.983001
H	2.139857	2.826415	-1.070065	H	-1.510485	-2.533192	-1.899456	H	-1.272889	-2.733801	-1.983001
H	4.592771	1.329819	-2.163533	H	0.256860	-2.714030	-4.415195	H	0.529079	-2.663214	-4.479970
C	-3.614982	1.771668	-2.271828	C	0.004138	-3.002607	3.386678	C	0.306824	-2.996990	3.459037
C	2.659435	0.827571	-3.032590	C	1.244543	-2.940322	-2.488089	C	1.529468	-2.811991	-2.553383
C	3.599725	1.779880	-2.284950	C	0.005001	-3.002727	-3.386947	C	0.306824	-2.996990	-3.459037
C	-2.672287	0.826446	-3.025430	C	1.243743	-2.940238	2.487917	C	1.529468	-2.811991	2.553383
H	1.672923	1.290006	-3.148996	H	0.984562	-3.258605	-1.472343	H	1.302096	-3.169674	-1.542728
H	-1.688587	1.294362	-3.143903	H	0.983877	-3.258515	1.472144	H	1.302096	-3.169674	1.542728
C	3.057833	0.641474	-4.038762	H	2.005071	-3.635310	-2.868002	H	2.362357	-3.416123	-2.938940
H	-3.073117	0.641074	-4.030770	H	2.004262	-3.635184	2.867910	H	2.362357	-3.416123	2.938940
H	-3.778364	2.647490	-2.910043	H	-0.302016	-4.053120	3.448996	H	0.119635	-4.073885	3.540383
H	3.755599	2.655000	-2.925997	H	-0.301034	-4.053270	-3.449386	H	0.119635	-4.073885	-3.540383
H	0.002220	0.902093	2.292701	H	-2.061581	1.271816	-0.000286	H	-2.274866	1.008493	0.000000

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S				SO				T			
C	-1.063938	0.824319	1.130000	C	-2.19954100	-0.29691000	0.00000000	C	-2.193938	-0.305681	0.000000
O	0.254477	0.961352	1.130000	O	-0.88119200	-0.16074000	0.00000000	O	-0.875523	-0.168648	0.000000
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O	2.804957	1.265441	1.130000	O	1.65368900	0.10683700	0.00000000	O	1.674957	0.135441	0.000000
H	-1.300279	3.894973	3.290185	H	-2.41745300	2.77733100	2.16018100	H	-2.430279	2.764973	2.160185
H	-1.758778	0.360911	-2.235211	H	-2.89551700	-0.75317500	-3.36510200	H	-2.888778	-0.769089	-3.365211
H	-3.651988	0.054663	-1.015697	H	-4.79013000	-1.06114200	-2.14558600	H	-4.781988	-1.075337	-2.145697
H	-0.575577	-1.732134	-2.104479	H	-1.72084100	-2.84937600	-3.23639000	H	-1.705577	-2.862134	-3.234479
H	1.719426	-1.646732	-3.095161	H	0.57323400	-2.77089300	-4.23066500	H	0.589426	-2.776732	-4.225161
H	0.563029	0.409443	-2.546946	H	-0.57862400	-0.71345800	-3.67989800	H	-0.566971	-0.720557	-3.676946
H	2.590405	2.625063	-3.396030	H	1.47075000	1.48937900	-4.52586800	H	1.460405	1.495063	-4.526030
H	-0.978867	1.826655	-1.637648	H	-2.11192900	0.70929600	-2.76439500	H	-2.108867	0.696655	-2.767648
H	0.813128	4.042401	-2.246979	H	-0.30261500	2.90747700	-3.37676900	H	-0.316872	2.912401	-3.376979
C	-1.093039	0.751459	-1.454097	C	-2.22961200	-0.36574200	-2.58267800	C	-2.223039	-0.378541	-2.584097
H	-1.300279	3.894973	-1.030185	H	-2.41745300	2.77733100	-2.16018100	H	-2.430279	2.764973	-2.160185
H	3.124786	0.166113	-3.271787	H	2.00179200	-0.97184800	-4.40951800	H	1.994786	-0.963887	-4.401787
C	-3.119255	0.218160	-0.082895	C	-4.25699700	-0.89891100	-1.21278800	C	-4.249255	-0.911840	-1.212895
H	1.450385	-3.022588	-2.056835	H	0.29944600	-4.14780800	-3.19498600	H	0.320385	-4.152588	-3.186835
C	0.266457	-1.328202	-1.525122	C	-0.87636600	-2.44975600	-2.65770900	C	-0.863543	-2.458202	-2.655122
H	-4.846518	-0.213912	1.130000	H	-5.98469800	-1.32980700	0.00000000	H	-5.976518	-1.343912	0.000000
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C	1.573911	-1.933526	-2.044977	C	0.42788500	-3.05932900	-3.18086600	C	0.443911	-3.063526	-3.174977
C	3.213707	2.826120	-2.514588	C	2.09554100	1.68762600	-3.64487900	C	2.083707	1.696120	-3.644588
H	3.703457	3.796457	-2.691732	H	2.58762900	2.65689600	-3.82114300	H	2.573457	2.666457	-3.821732
H	4.998575	1.896004	-3.212395	H	3.87760200	0.75353200	-4.34499900	H	3.868575	0.766004	-4.342395
C	-1.769072	0.551264	-0.118338	C	-2.90660600	-0.56641900	-1.24789800	C	-2.899072	-0.578736	-1.248338
C	-3.795011	0.055373	1.130000	C	-4.93294600	-1.06156500	0.00000000	C	-4.925011	-1.074627	0.000000
C	1.457101	4.103013	-1.363166	C	0.34150000	2.96759800	-2.49305300	C	0.327101	2.973013	-2.493166
H	2.052942	5.024305	-1.464334	H	0.93950200	3.88734200	-2.59529200	H	0.922942	3.894305	-2.594334
C	-0.750745	3.937363	-0.093832	C	-1.86759900	2.81495700	-1.22381400	C	-1.880745	2.807363	-1.223832
C	3.829396	0.291461	-2.441275	C	2.70342300	-0.84866200	-3.57616800	C	2.699396	-0.838539	-3.571275
H	4.691026	-0.355517	-2.660947	H	3.56363100	-1.49895900	-3.79149400	H	3.561026	-1.485517	-3.790947
H	0.103735	-1.602505	-0.476319	H	-1.03826100	-2.72429700	-1.60900900	H	-1.026265	-2.732505	-1.606319
H	-2.542745	3.840121	1.130000	H	-3.66049800	2.73171300	0.00000000	H	-3.672745	2.710121	0.000000
C	4.297875	1.749927	-2.382319	C	3.17665400	0.60810000	-3.51500900	C	3.167875	0.619927	-3.512319
N	2.327842	2.901714	-1.331881	N	1.21043500	1.76466500	-2.46131000	N	1.197842	1.771714	-2.461881
C	0.626776	4.140137	-0.099451	C	-0.48875200	3.00798600	-1.22937300	C	-0.503224	3.010137	-1.229451
C	-1.454919	3.776281	1.130000	C	-2.57329300	2.65787400	0.00000000	C	-2.584919	2.646281	0.000000
H	3.670967	-2.206141	-1.608413	H	2.52353900	-3.34517900	-2.74519000	H	2.540967	-3.336141	-2.738413
C	2.828007	-1.616733	-1.220515	C	1.68445400	-2.75037000	-2.35730700	C	1.698007	-2.746733	-2.350515
N	3.176563	-0.175174	-1.192760	N	2.04344200	-1.31124000	-2.33008900	N	2.046563	-1.305174	-2.322760
Cu	1.673633	0.922661	-0.307152	Cu	0.54548500	-0.20988900	-1.45387300	Cu	0.543633	-0.207339	-1.437152
C	-3.119255	0.218160	2.342895	C	-4.25699700	-0.89891100	-1.21278800	C	-4.249255	-0.911840	-1.212895
H	4.881168	1.917783	-1.465963	H	3.76075000	0.77249100	-2.59849400	H	3.751168	0.787783	-2.595963
H	2.918929	2.954913	-0.497033	H	1.80231300	1.81861800	-1.62709100	H	1.788929	1.824913	-1.627033
H	2.664924	-1.925237	-0.180977	H	1.51986700	-3.05671100	-1.31745700	H	1.534924	-3.055237	-1.310977
H	-3.651988	0.054663	3.275697	H	-4.79013000	-1.06114200	-2.14558600	H	-4.781988	-1.075337	2.145697
H	3.814829	-0.011047	-0.409180	H	2.68010200	-1.15269900	-1.54393000	H	2.684829	-1.141047	-1.539180
C	-1.769072	0.551264	2.378338	C	-2.90660600	-0.56641900	1.24789800	C	-2.899072	-0.578736	1.248338
C	1.282812	4.284691	1.130000	C	0.16826600	3.14772200	0.00000000	C	0.152812	3.154691	0.000000
C	-0.750745	3.937363	2.353832	C	-1.86759900	2.81495700	1.22381400	C	-1.880745	2.807363	1.223832
H	2.351189	4.488100	1.130000	H	1.23796200	3.34414100	0.00000000	H	1.221189	3.358100	0.000000
C	0.626776	4.140137	2.359451	C	-0.48875200	3.00798600	1.22937300	C	-0.503224	3.010137	1.229451
H	-0.978867	1.826655	3.897648	H	-2.11192900	0.70929600	2.76439500	H	-2.108867	0.696655	2.767648
C	-1.093039	0.751459	3.714097	C	-2.22961200	-0.36574200	2.58267800	C	-2.223039	-0.378541	2.584097
H	0.103735	-1.602505	2.736319	H	-1.03826100	-2.72429700	1.60900900	H	-1.026265	-2.732505	1.606319
H	-1.758778	0.360911	4.495211	H	-2.89551700	-0.75317500	3.36510200	H	-2.888778	-0.769089	3.365211
Cu	1.673633	0.922661	2.567152	Cu	0.54548500	-0.20988900	1.45387300	Cu	0.543633	-0.207339	1.437152
C	1.457101	4.103013	3.623166	C	0.34150000	2.96759800	2.49305300	C	0.327101	2.973013	2.493166
N	0.263333	0.161094	3.862433	N	-0.87447500	-0.96003000	2.73356500	N	-0.866667	-0.968906	2.732433
C	0.266457	-1.328202	3.785122	C	-0.87636600	-2.44975600	2.65770900	C	-0.863543	-2.458202	2.655122
H	-0.575577	-1.732134	4.364479	H	-1.72084100	-2.84937600	3.23639000	H	-1.705577	-2.862134	3.234479
H	2.918929	2.954913	2.757033	H	1.80231300	1.81861800	1.62709100	H	1.788929	1.824913	1.627033
H	2.052942	5.024305	3.724334	H	0.93950200	3.88734200	2.59529200	H	0.922942	3.894305	2.594334
H	0.813128	4.042401	4.506979	H	-0.30261500	2.90747700	3.37676900	H	-0.316872	2.912401	3.376979
H	2.664924	-1.925237	2.440977	H	1.51986700	-3.05671100	1.31745700	H	1.534924	-3.055237	1.310977
N	2.327842	2.901714	3.591881	N	1.21043500	1.76466500	2.46131000	N	1.197842	1.771714	2.461881
H	0.563029	0.409443	4.806946	H	-0.57862400	-0.71345800	3.67989800	H	-0.566971	-0.720557	3.676946
H	3.814829	-0.011047	2.669180	H	2.68010200	-1.15269900	1.54393000	H	2.684829	-1.141047	1.539180
N	3.176563	-0.175174	3.452760	N	2.04344200	-1.31124000	2.33008900	N	2.046563	-1.305174	2.322760
C	2.828007	-1.616733	3.480515	C	1.68445400	-2.75037000	2.35730700	C	1.698007	-2.746733	2.350515
C	1.573911	-1.933526	4.304977	C	0.42788500	-3.05932900	3.18086600	C	0.443911	-3.063526	3.174977
H	1.450385	-3.022588	4.316835	H	0.29944600	-4.14780800	3.19498600	H	0.320385	-4.152588	3.186835
H	3.670967	-2.206141	3.868413	H	2.52353900	-3.34517900	2.74519000	H	2.540967	-3.336141	2.738413

h												
S				SO				T				
C	-0.236351	2.245650	0.000000	C	-1.958077	-0.932441	0.000000	C	-1.957588	-0.932933	0.000000	
O	0.084979	0.940503	0.000000	O	-0.766017	-0.290005	0.000000	O	-0.765997	-0.289418	0.000000	
H	5.066738	2.342167	0.000000	H	-4.105500	2.044936	0.000000	H	-4.106232	2.041855	0.000000	
O	-0.285109	-1.510246	0.000000	O	1.624728	0.199739	0.000000	O	1.624471	0.200771	0.000000	
H	4.878642	1.034084	2.189259	H	-3.059626	2.671734	2.198182	H	-3.061098	2.670010	2.198170	
H	-0.330660	2.975664	-3.351814	H	-2.647801	-1.150482	-3.353082	H	-2.647127	-1.152272	-3.353081	
H	-0.891318	4.825545	-2.142649	H	-4.272932	-2.223731	-2.142573	H	-4.271222	-2.226481	-2.142555	
H	-2.621861	2.100587	-3.361921	H	-1.089101	-3.014857	-3.503306	H	-1.087447	-3.015272	-3.503202	
H	-2.929121	-0.218784	-4.230391	H	1.211278	-2.548975	-4.326416	H	1.212773	-2.548007	-4.326252	
H	-0.664637	0.707583	-3.707270	H	-0.382327	-0.695162	-3.695857	H	-0.381823	-0.695225	-3.695890	
H	1.004530	-1.390066	-4.483371	H	1.143623	1.774327	-4.455651	H	1.142061	1.773228	-4.455270	
H	0.939616	1.995294	-2.607194	H	-2.116071	0.344725	-2.564395	H	-2.116455	0.343582	-2.564808	
H	2.523241	0.280275	-3.241528	H	-0.962355	2.620800	-3.357903	H	-0.964476	2.618547	-3.357495	
C	-0.118536	2.274185	-2.535088	C	-2.047811	-0.747987	-2.528457	C	-2.047439	-0.749053	-2.528578	
H	4.878642	1.034084	-2.189259	H	-3.059626	2.671734	-2.198182	H	-3.061098	2.670010	-2.198170	
H	-1.432728	-1.834156	-4.371819	H	2.118774	-0.503623	-4.363203	H	2.120736	-0.503270	-4.363124	
C	-0.764622	4.298816	-1.200013	C	-3.794494	-1.971374	-1.199656	C	-3.793038	-1.973643	-1.199641	
H	-4.228987	0.303659	-3.192937	H	1.137295	-3.985702	-3.340319	H	1.139414	-3.984929	-3.340382	
C	-2.370727	1.239856	-2.727212	C	-0.356976	-2.551610	-2.829585	C	-0.355554	-2.551603	-2.829513	
H	-1.233748	6.029693	0.000000	H	-5.330057	-2.895508	0.000000	H	-5.327797	-2.899116	0.000000	
N	-0.896791	1.013302	-2.759795	N	-0.607522	-1.081086	-2.776637	N	-0.606862	-1.081213	-2.776659	
C	-3.170505	0.019015	-3.186237	C	1.058144	-2.893625	-3.295888	C	1.059742	-2.892896	-3.295787	
C	1.234447	-2.114764	-3.690817	C	1.695897	2.078336	-3.556796	C	1.694276	2.078554	-3.556818	
H	2.138686	-2.652911	-4.014537	H	1.972463	3.132907	-3.706220	H	1.969691	3.133286	-3.707217	
H	0.136728	-3.804092	-4.395892	H	3.645166	1.546038	-4.237919	H	3.644047	1.548129	-4.237826	
C	-0.403544	2.948272	-1.219553	C	-2.588919	-1.260722	-1.219403	C	-2.588094	-1.261907	-1.219415	
C	-0.952217	4.982182	0.000000	C	-4.397694	-2.341392	0.000000	C	-4.395928	-2.344168	0.000000	
C	2.734402	-0.558954	-2.567384	C	-0.344567	2.912941	-2.502307	C	-0.346577	2.912205	-2.502487	
H	3.533502	-1.143772	-3.052633	H	0.052045	3.916776	-2.726005	H	0.048912	3.916198	-2.727436	
C	4.405007	0.750918	-1.251665	C	-2.531063	2.792730	-1.255005	C	-2.532654	2.791287	-1.254964	
C	-1.324834	-2.526844	-3.530754	C	2.791645	-0.268547	-3.532753	C	2.792596	-0.267144	-3.532146	
H	-2.060426	-3.328972	-3.686287	H	3.755456	-0.743981	-3.760129	H	3.757151	-0.741558	-3.758512	
H	-2.633552	1.511342	-1.700300	H	-0.546763	-2.948416	-1.827295	H	-0.545119	-2.948454	-1.827200	
H	6.109583	0.977524	0.000000	H	-3.968735	3.773850	0.000000	H	-3.971430	3.770947	0.000000	
C	0.085981	-3.118668	-3.542210	C	2.973398	1.246322	-3.425519	C	2.972659	1.247954	-3.425279	
N	1.506860	-1.364260	-2.442119	N	0.787988	1.945612	-2.393644	N	0.786792	1.945978	-2.393337	
C	3.280457	-0.031464	-1.246499	C	-1.172244	2.949849	-1.238394	C	-1.173910	2.949210	-1.238337	
C	5.032278	1.233617	0.000000	C	-3.354296	2.851260	0.000000	C	-3.355954	2.849057	0.000000	
H	-3.751806	-1.989681	-2.636830	H	3.143613	-2.774429	-2.736921	H	3.145073	-2.772859	-2.736608	
C	-3.035540	-1.226097	-2.302805	C	2.178945	-2.386809	-2.384173	C	2.180211	-2.385666	-2.383915	
N	-1.664731	-1.800661	-2.280640	N	2.253852	-0.900748	-2.294185	N	2.254512	-0.899574	-2.293824	
Cu	-0.385656	-0.447771	-1.485947	Cu	0.571347	-0.199694	-1.448129	Cu	0.571401	-0.199185	-1.448093	
C	-0.764622	4.298816	1.200013	C	-3.794494	-1.971374	1.199656	C	-3.793038	-1.973643	1.199641	
H	0.244723	-3.741229	-2.650183	H	3.501316	1.499431	-2.494864	H	3.500405	1.501900	-2.494756	
H	1.649356	-2.062156	-1.709878	H	1.326487	2.207463	-1.565859	H	1.325270	2.208811	-1.565860	
H	-3.287748	-0.969113	-1.267749	H	2.026835	-2.759763	-1.364697	H	2.028180	-2.758764	-1.364478	
H	-0.891318	4.825545	2.142649	H	-4.272932	-2.223731	2.142573	H	-4.271222	-2.226481	2.142555	
H	-1.605641	-2.453489	-1.495648	H	2.877894	-0.664536	-1.519138	H	2.878242	-0.663210	-1.518584	
C	-0.403544	2.948272	1.219553	C	-2.588919	-1.260722	1.219403	C	-2.588094	-1.261907	1.219415	
C	2.688256	-0.378875	0.000000	C	-0.498974	3.137903	0.000000	C	-0.500721	3.137996	0.000000	
C	4.405007	0.750918	1.251665	C	-2.531063	2.792730	1.255005	C	-2.532654	2.791287	1.254964	
H	1.755041	-0.936019	0.000000	H	0.556238	3.401071	0.000000	H	0.554414	3.401470	0.000000	
C	3.280457	-0.031464	1.246499	C	-1.172244	2.949849	1.238394	C	-1.173910	2.949210	1.238337	
H	0.939616	1.995294	2.607194	H	-2.116071	0.344725	2.564395	H	-2.116455	0.343582	2.564808	
C	-0.118536	2.274185	2.535088	C	-2.047811	-0.747987	2.528457	C	-2.047439	-0.749053	2.528578	
H	-2.633552	1.511342	1.700300	H	-0.546763	-2.948416	1.827295	H	-0.545119	-2.948454	1.827200	
H	-0.330660	2.975664	3.351814	H	-2.647801	-1.150482	3.353082	H	-2.647127	-1.152272	3.353081	
Cu	-0.385656	-0.447771	1.485947	Cu	0.571347	-0.199694	1.448129	Cu	0.571401	-0.199185	1.448093	
C	2.734402	-0.558954	2.567384	C	-0.344567	2.912941	2.502307	C	-0.346577	2.912205	2.502487	
N	-0.896791	1.013302	2.759795	N	-0.607522	-1.081086	2.776637	N	-0.606862	-1.081213	2.776659	
C	-2.370727	1.239856	2.727212	C	-0.356976	-2.551610	2.829585	C	-0.355554	-2.551603	2.829513	
H	-2.621861	2.100587	3.361921	H	-1.089101	-3.014857	3.503306	H	-1.087447	-3.015272	3.503202	
H	1.649356	-2.062156	1.709878	H	1.326487	2.207463	1.565859	H	1.325270	2.208811	1.565860	
H	3.533502	-1.143772	3.052633	H	0.052045	3.916776	2.726005	H	0.048912	3.916198	2.727436	
H	2.523241	0.280275	3.241528	H	-0.962355	2.620800	3.357903	H	-0.964476	2.618547	3.357495	
H	-3.287748	-0.969113	1.267749	H	2.026835	-2.759763	1.364697	H	2.028180	-2.758764	1.364478	
N	1.506860	-1.364260	2.442119	N	0.787988	1.945612	2.393644	N	0.786792	1.945978	2.393337	
H	-0.664637	0.707583	3.707270	H	-0.382327	-0.695162	3.695857	H	-0.381823	-0.695225	3.695890	
H	-1.605641	-2.453489	1.495648	H	2.877894	-0.664536	1.519138	H	2.878242	-0.663210	1.518584	
N	-1.664731	-1.800661	2.280640	N	2.253852	-0.900748	2.294185	N	2.254512	-0.899574	2.293824	
C	-3.035540	-1.226097	2.302805	C	2.178945	-2.386809	2.384173	C	2.180211	-2.385666	2.383915	
C	-3.170505	0.019015	3.186237	C	1.058144	-2.893625	3.295888	C	1.059742	-2.892896	3.295787	
H	-4.228987	0.303659	3.192937	H	1.137295	-3.985702	3.340319	H	1.139414	-3.984929	3.340382	
H	-3.751806	-1.989681	2.636830	H	3.143613	-2.774429	2.736921	H	3.145073	-2.772859	2.736608	
C	1.234447	-2.114764	3.690817	C	1.695897	2.078336	3.556796	C	1.694276	2.078554	3.556818	
H	0.244723	-3.741229	2.650183	H	3.501316	1.499431	2.494864	H	3.500405	1.501900	2.494756	
H	2.138686	-2.652911	4.014537	H	1.972463	3.132907	3.706220	H	1.969691	3.133286	3.707217	
H	-2.929121	-0.218784	4.230391	H	1.211278	-2.548975	4.326416	H	1.212773	-2.548007	4.326252	
H	1.004530	-1.390066	4.483371	H	1.143623	1.774327	4.455651	H	1.142061	1.773228	4.455270	
C	0.085981	-3.118668	3.542210	C	2.973398	1.246322	3.425519	C	2.972659	1.247954	3.425279	
C	-1.324834	-2.526844	3.530754	C	2.791645	-0.268547	3.532753	C	2.792596	-0.267144	3.532146	
H	-1.432728	-1.834156	4.371819	H	2.118774	-0.503623	4.363203	H	2.120736	-0.503270	4.363124	
H	-2.060426	-3.328972	3.686287	H	3.755456	-0.743981	3.760129	H	3.757151	-0.741558	3.758512	
H	0.136728	-3.804092	4.395892	H	3.645166	1.546038	4.237919	H	3.644047	1.548129	4.237826	

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S			SO						T		
C	-0.001478	2.371690	0.609422	C	-0.000276	2.341542	0.547223	C	-0.000274	2.334201	0.519611
O	-0.001309	0.979859	0.777465	O	-0.000473	0.937415	0.685640	O	-0.000484	0.927582	0.666995
H	-0.002229	0.760817	1.733765	H	-0.001345	0.698083	1.637370	H	-0.001614	0.692176	1.620150
O	0.000217	-1.326689	-0.629585	O	-0.000082	-1.389265	-0.665606	O	-0.000241	-1.448718	-0.622530
H	-2.149941	0.616055	4.115984	H	-2.149733	0.718638	4.057218	H	-2.148622	0.770142	4.042072
H	3.355446	2.983177	0.650085	H	3.358035	2.975270	0.598809	H	3.358598	2.972210	0.565408
H	2.145844	4.957459	0.217284	H	2.147025	4.936811	0.240625	H	2.147082	4.928153	0.211021
H	3.462094	2.756568	-1.716300	H	3.451833	2.738764	-1.769462	H	3.456321	2.716352	-1.801500
H	4.324821	0.581519	-2.625464	H	4.362530	0.575663	-2.648028	H	4.352198	0.541231	-2.663244
H	3.697396	0.879128	-0.224902	H	3.702632	0.852889	-0.263303	H	3.692900	0.833873	-0.282959
H	4.431928	-1.978376	0.605450	H	4.484647	-1.984126	0.714278	H	4.478498	-1.974372	0.719017
H	2.550562	1.739436	1.614831	H	2.571901	1.730335	1.575440	H	2.578100	1.731916	1.551987
H	3.343589	-0.969819	2.713035	H	3.357402	-0.964442	2.786676	H	3.359126	-0.938922	2.802734
C	2.523443	2.268026	0.656437	C	2.533772	2.252090	0.613107	C	2.535589	2.247846	0.586585
H	2.153431	0.615193	4.115251	H	2.154015	0.715787	4.056564	H	2.155375	0.766198	4.041026
H	4.338109	-1.480422	-1.828074	H	4.405635	-1.454775	-1.724044	H	4.386410	-1.481464	-1.729952
C	1.207548	4.414741	0.292797	C	1.208294	4.392801	0.298045	C	1.208016	4.384860	0.268995
H	3.427274	1.541769	-3.771441	H	3.438699	1.487500	-3.813096	H	3.433158	1.447730	-3.836489
C	2.811816	1.872061	-1.762291	C	2.817650	1.842870	-1.809051	C	2.816150	1.824445	-1.834488
H	-0.001671	6.177765	0.035358	H	0.000483	6.163098	0.091409	H	0.000601	6.155008	0.059062
N	2.756454	1.234917	-0.410805	N	2.766049	1.219378	-0.449471	N	2.760716	1.210331	-0.470900
C	3.314376	0.938726	-2.863087	C	3.342866	0.900925	-2.892097	C	3.334455	0.870362	-2.910006
C	3.551546	-2.631658	0.553824	C	3.596091	-2.624138	0.639081	C	3.587057	-2.612255	0.696647
H	3.758263	-3.487535	1.213439	H	3.771914	-3.481860	1.305578	H	3.767210	-3.463026	1.333988
H	4.144052	-3.890607	-1.059497	H	4.237849	-3.876192	-0.959126	H	4.207814	-3.887587	-0.928646
C	1.226035	3.029821	0.503385	C	1.228140	3.001981	0.466669	C	1.228272	2.994362	0.439896
C	-0.001622	5.104057	0.192558	C	0.000269	5.085261	0.217148	C	0.000357	5.077399	0.186724
C	2.498585	-1.643154	2.536966	C	2.500079	-1.614792	2.584959	C	2.499832	-1.587735	2.604168
H	2.736631	-2.590789	3.045897	H	2.693480	-2.564639	3.108763	H	2.689410	-2.534867	3.134361
C	1.215462	0.139687	3.839524	C	1.215570	0.234264	3.792990	C	1.216732	0.280948	3.785033
C	3.457340	-2.109186	-1.994446	C	3.546209	-2.106901	-1.913853	C	3.519039	-2.128291	-1.901196
H	3.609056	-2.618574	-2.956863	H	3.741440	-2.617406	-2.867399	H	3.700743	-2.655255	-2.848475
H	1.803272	2.226155	-1.996902	H	1.804225	2.176779	-2.053876	H	1.804890	2.163639	-2.081694
H	0.002072	1.618367	4.836532	H	0.002923	1.755898	4.724015	H	0.004483	1.818189	4.690901
C	3.357905	-3.149215	-0.875977	C	3.438167	-3.145068	-0.793777	C	3.413786	-3.149795	-0.765568
N	2.381590	-1.873599	1.066927	N	2.424014	-1.847979	1.114858	N	2.421539	-1.828293	1.136166
C	1.223915	-1.047278	3.093138	C	1.224365	-0.983565	3.097073	C	1.225299	-0.948876	3.110206
C	0.001796	0.712019	4.238522	C	0.002234	0.825544	4.164114	C	0.003509	0.878895	4.146110
H	2.739020	-0.728983	-4.113362	H	2.822515	-0.821986	-4.090588	H	2.803932	-0.863154	-4.088654
C	2.386602	-0.232118	-3.198724	C	2.446682	-0.302366	-3.198584	C	2.431022	-0.331271	-3.202594
N	2.265981	-1.225118	-2.102327	N	2.336446	-1.255576	-2.065867	N	2.316083	-1.267869	-2.057229
Cu	1.533560	-0.409977	-0.388779	Cu	1.517445	-0.400125	-0.407372	Cu	1.492477	-0.393690	-0.398361
C	-1.210731	4.414488	0.291830	C	-1.208033	4.393179	0.297168	C	-1.207622	4.385310	0.268114
H	2.408788	-3.698870	-0.952633	H	2.497923	-3.706585	-0.888801	H	2.469459	-3.706562	-0.845249
H	1.562338	-2.465417	0.917727	H	1.597783	-2.423945	0.937796	H	1.589132	-2.395780	0.959514
H	1.377913	0.147959	-3.398775	H	1.431887	0.045859	-3.424360	H	1.418582	0.020932	-3.433765
H	-2.149091	4.956985	0.215511	H	-2.146553	4.937480	0.239057	H	-2.146441	4.928954	0.209444
H	1.450738	-1.811195	-2.292408	H	1.529352	-1.862506	-2.232349	H	1.501772	-1.870124	-2.206199
C	-1.229052	3.029578	0.502432	C	-1.228429	3.002368	0.465786	C	-1.228522	2.994821	0.439017
C	0.001076	-1.655005	2.793958	C	0.000421	-1.598902	2.814044	C	0.000945	-1.568702	2.837673
C	-1.212257	0.140158	3.839955	C	-1.212010	0.235860	3.793372	C	-1.210999	0.283155	3.785635
H	0.000810	-2.604781	2.265790	H	-0.000265	-2.566495	2.318776	H	-0.000012	-2.543930	2.357717
C	-1.221456	-1.046960	3.093760	C	-1.222651	-0.982083	3.097619	C	-1.222184	-0.946841	3.111069
H	-2.554512	1.739394	1.613088	H	-2.573670	1.731602	1.573824	H	-2.579962	1.733527	1.550518
C	-2.526381	2.267452	0.654409	C	-2.534413	2.252905	0.611276	C	-2.536261	2.248867	0.584834
H	-1.803176	2.224086	-1.998374	H	-1.802084	2.175394	-2.055315	H	-1.803036	2.161804	-2.083238
H	-3.358642	2.982288	0.646676	H	-3.358473	2.976294	0.595844	H	-3.358990	2.973516	0.562451
Cu	-1.533175	-0.411006	-0.388649	Cu	-1.517351	-0.399708	-0.407361	Cu	-1.492655	-0.393240	-0.398110
C	-2.496652	-1.642681	2.538612	C	-2.499471	-1.611936	2.586554	C	-2.498312	-1.583825	2.606640
N	-2.757633	1.233666	-0.412511	N	-2.765870	1.219747	-0.451011	N	-2.760725	1.210763	-0.472168
C	-2.811848	1.869884	-1.764461	C	-2.815940	1.842386	-1.811036	C	-2.814746	1.823728	-1.836326
H	-3.462419	2.754240	-1.719734	H	-3.449508	2.738766	-1.772591	H	-3.454157	2.716228	-1.804601
H	-1.561699	-2.465409	0.918824	H	-1.599440	-2.423370	0.939297	H	-1.590653	-2.394836	0.961794
H	-2.734556	-2.590082	3.048054	H	-2.693799	-2.561189	3.111098	H	-2.689118	-2.530104	3.137924
H	-3.341355	-0.969080	2.715114	H	-3.355814	-0.960338	2.788417	H	-3.356231	-0.933264	2.805453
H	-1.376357	0.143814	-3.398024	H	-1.430709	0.042065	-3.423772	H	-1.418371	0.016196	-3.432902
N	-2.380842	-1.873584	1.068571	N	-2.424731	-1.846133	1.116553	N	-2.421962	-1.825876	1.138799
H	-3.698501	0.877285	-0.227400	H	-3.702686	0.853489	-0.265585	H	-3.693143	0.834618	-0.284789
H	-1.450773	-1.814318	-2.289696	H	-1.531482	-1.865145	-2.230090	H	-1.504824	-1.873255	-2.203136
N	-2.265768	-1.227523	-2.100712	N	-2.337574	-1.256689	-2.064327	N	-2.318049	-1.269359	-2.054861
C	-2.385300	-0.235800	-3.198391	C	-2.446059	-0.304674	-3.198232	C	-2.431384	-0.334258	-3.201617
C	-3.313183	0.935602	-2.865020	C	-3.341063	0.900026	-2.893789	C	-3.333336	0.869031	-2.911198
H	-3.424770	1.537786	-3.774105	H	-3.435169	1.485848	-3.815447	H	-3.430411	1.445417	-3.838466
H	-2.737047	-0.733724	-4.112710	H	-2.821963	-0.824921	-4.089840	H	-2.804705	-0.866933	-4.087030
C	-3.551245	-2.631718	0.556659	C	-3.598240	-2.620955	0.642138	C	-3.589262	-2.608394	0.664275
H	-2.409958	-3.700540	-0.949763	H	-2.502900	-3.706592	-0.885520	H	-2.475270	-3.706622	-0.840455
H	-3.757718	-3.487200	1.216865	H	-3.774914	-3.477904	1.309407	H	-3.770216	-3.458120	1.339718
H	-4.324014	0.578864	-2.628356	H	-4.361403	0.576267	-2.650553	H	-4.351771	0.541648	-2.664967
H	-4.431482	-1.978254	0.608468	H	-4.485809	-1.979584	0.717407	H	-4.479565	-1.968938	0.723820
C	-3.358626	-3.150124	-0.872959	C	-3.442053	-3.143252	-0.7904				

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S				SO				T			
H	2.158593	3.595224	1.107832	H	1.983876	3.695693	0.617883	H	2.192526	3.452975	1.139016
H	0.590514	5.204252	0.623318	H	0.336943	5.209264	0.044774	H	0.660142	5.111135	0.672837
H	2.532992	3.680926	-1.264051	H	1.889908	3.498874	-1.827974	H	2.244801	3.629671	-1.289040
H	4.044629	1.881090	-2.246281	H	3.657240	1.909445	-2.696218	H	3.918471	2.062816	-2.352397
H	3.203362	1.857902	0.105020	H	3.005358	1.952067	-0.331343	H	3.171308	1.805378	-0.015452
H	4.922183	-0.918409	0.184992	H	5.099614	-0.095613	-0.014259	H	5.026780	-0.356932	0.070006
H	1.645618	2.075351	1.849591	H	1.561078	2.253219	1.551612	H	1.670799	1.916268	1.839625
H	3.796665	-0.353058	2.340492	H	3.918571	0.418645	2.091046	H	3.826962	-0.093068	2.222037
C	1.569085	2.685133	0.942531	C	1.407834	2.763002	0.594249	C	1.574552	2.564915	0.961968
H	2.500092	0.717618	4.085640	H	2.640254	1.247555	3.972675	H	2.564904	0.534225	4.180750
H	4.636441	-0.257046	-2.170249	H	4.699264	0.006791	-2.462703	H	4.800204	0.060668	-2.363807
C	-0.204624	4.463894	0.607261	C	-0.433591	4.455344	0.182235	C	-0.156655	4.394891	0.701391
H	3.074484	2.790906	-3.374200	H	2.444500	2.420446	-3.836278	H	2.789146	2.833144	-3.433011
C	2.179448	2.657412	-1.451336	C	1.727759	2.412305	-1.839157	C	1.999155	2.576454	-1.481417
H	-1.761448	5.940980	0.436811	H	-2.046787	5.863490	-0.043272	H	-1.676225	5.916414	0.598263
N	2.217579	1.890773	-0.167764	N	1.995860	1.866175	-0.472786	N	2.166505	1.805859	-0.207897
C	3.009844	2.039396	-2.578703	C	2.592618	1.799641	-2.944682	C	2.859251	2.074904	-2.644060
C	4.255206	-1.784860	0.096342	C	4.709983	-1.117295	0.067771	C	4.581976	-1.357575	0.011513
H	4.729742	-2.607351	0.650566	H	5.379749	-1.660990	0.746680	H	5.198922	-2.017777	0.635145
H	5.028494	-2.703966	-1.666971	H	5.736032	-2.068995	-1.544439	H	5.612667	-2.188779	-1.663085
C	0.129353	3.104739	0.710506	C	-0.052353	3.127743	0.428034	C	0.140473	3.026768	0.801182
C	-1.530803	4.883407	0.509090	C	-1.776074	4.828829	0.138708	C	-1.472573	4.853026	0.666376
C	3.122720	-1.205401	2.206574	C	3.436861	-0.564234	2.104420	C	3.283227	-1.032140	2.076701
H	3.621209	-2.076851	2.659264	H	4.106621	-1.234151	2.663449	H	3.894835	-1.820940	2.539345
C	1.641055	0.114691	3.800041	C	1.849329	0.544125	3.723108	C	1.737249	-0.075101	3.825208
C	3.901776	-1.043551	-2.372423	C	4.165068	-0.948563	-2.451386	C	4.185582	-0.836672	-2.490682
H	4.096886	-1.403606	-3.392540	H	4.377990	-1.439198	-3.411117	H	4.405910	-1.227290	-3.494248
H	1.130776	2.731876	-1.754831	H	0.668441	2.247270	-2.054697	H	0.939630	2.537465	-1.749251
H	0.283491	1.166887	5.100229	H	0.443955	1.410971	5.103627	H	0.364121	0.664536	5.308908
C	4.105819	-2.188754	-1.376064	C	4.701109	-1.802428	-1.301853	C	4.590698	-1.865897	-1.434214
N	2.959839	-1.432870	0.738839	N	3.352555	-1.040100	0.687396	N	3.211250	-1.282384	0.602962
C	1.794589	-0.930403	2.879038	C	2.083600	-0.465986	2.779172	C	1.925062	-0.947518	2.743820
C	0.391153	0.370522	4.369905	C	0.612051	0.637464	4.360474	C	0.497934	-0.001112	4.461689
H	2.937782	0.564626	-4.159183	H	2.728038	0.137677	-4.318124	H	2.930614	0.621021	-4.241117
C	2.436780	0.761924	-3.201153	C	2.269443	0.355833	-3.343702	C	2.447076	0.733937	-3.260361
N	2.546471	-0.428071	-2.317987	N	2.710864	-0.658802	-2.344241	N	2.760426	-0.434357	-2.395771
Cu	1.771490	-0.118784	-0.433805	Cu	1.828726	-0.275391	-0.461397	Cu	1.791354	-0.234275	-0.461579
C	-2.560123	3.941218	0.514765	C	-2.769821	3.869569	0.339625	C	-2.526286	3.940249	0.732131
H	3.305363	-2.935778	-1.482791	H	4.157622	-2.757555	-1.243366	H	3.970693	-2.771245	-1.519059
C	-0.931771	2.191073	0.704304	C	-1.075455	2.192353	0.616405	C	-0.942308	2.140684	0.854203
H	2.363278	-2.255627	0.637827	H	3.031664	-2.010570	0.738114	H	2.823422	-2.222950	0.495239
H	1.372136	0.911199	-3.415476	H	1.186580	0.242456	-3.454646	H	1.364514	0.729650	-3.427588
H	-3.594712	4.266941	0.450643	H	-3.816693	4.160019	0.316777	H	-3.553271	4.294996	0.717545
H	1.880749	-1.124537	-2.655428	H	2.210276	-1.520063	-2.569945	H	2.199503	-1.214004	-2.742659
O	-0.705186	0.829897	0.834483	O	-0.789859	0.871538	0.908061	O	-0.751877	0.778986	0.998348
C	-2.272906	2.576851	0.617606	C	-2.431224	2.535233	0.583329	C	-2.273777	2.568921	0.829709
C	0.681247	-1.717690	2.572276	C	1.059559	-1.379690	2.503883	C	0.853092	-1.746333	2.329619
C	-0.725571	-0.374255	3.984109	C	-0.416685	-0.246237	4.029956	C	-0.575720	-0.763381	3.998621
H	0.803658	-2.570133	1.908906	H	1.241867	-2.203725	1.817945	H	0.998425	-2.460335	1.523200
H	-1.700943	-0.140451	4.403352	H	-1.386161	-0.147424	4.511278	H	-1.544661	-0.678341	4.483764
C	-0.592539	-1.421575	3.065762	C	-0.208058	-1.258648	3.087917	C	-0.412822	-1.637907	2.919022
O	0.228139	-1.077352	-0.683070	O	0.153593	-0.843816	-0.794185	O	0.138616	-0.801965	-0.879161
H	-3.303800	0.968575	1.617822	H	-3.309141	0.999305	1.814184	H	-3.275323	0.960223	1.855457
C	-3.352537	1.522796	0.674348	C	-3.467833	1.468143	0.837209	C	-3.378881	1.545860	0.935777
H	0.227640	0.586908	0.622951	H	0.077148	0.588940	0.532454	H	0.121291	0.491398	0.645346
H	-2.548506	1.799614	-1.922929	H	-3.022312	1.552423	-1.862423	H	-2.827663	1.908804	-1.718511
H	-4.336116	2.004161	0.617452	H	-4.467261	1.919030	0.839868	H	-4.348941	2.056011	0.970576
Cu	-1.508041	-0.585714	-0.379345	Cu	-1.643640	-0.639107	-0.251657	Cu	-1.658110	-0.560204	-0.335381
C	-1.785854	-2.219697	2.581613	C	-1.323095	-2.217310	2.723256	C	-1.578256	-2.465216	2.415469
N	-3.238622	0.502372	-0.426843	N	-3.429154	0.361208	-0.182579	N	-3.376866	0.563456	-0.204589
C	-3.404984	1.134959	-1.770620	C	-3.809508	0.864459	-1.538509	C	-3.672587	1.248110	-1.500822
H	-4.303171	1.766728	-1.761532	H	-4.735392	1.449313	-1.456540	H	-4.558002	1.885653	-1.375943
H	-0.862613	-2.645054	0.812140	H	-0.589963	-2.640688	0.864735	H	-0.808821	-2.761246	0.550962
H	-1.779625	-3.223171	3.038397	H	-1.133508	-3.199594	3.186615	H	-1.479167	-3.503857	2.771602
H	-2.718263	-1.739302	2.895783	H	-2.270513	-1.857360	3.136398	H	-2.513306	-2.081685	2.835861
H	-1.381498	-0.077193	-3.282023	H	-1.938659	-0.330982	-3.212613	H	-1.829650	0.137236	-3.257013
N	-1.796970	-2.347952	1.096308	N	-1.501354	-2.390571	1.252648	N	-1.708822	-2.462529	0.930091
H	-4.025142	-0.136883	-0.292620	H	-4.159284	-0.296571	0.100937	H	-4.159983	-0.068530	-0.021613
H	-0.991141	-1.997192	-2.136549	H	-1.250880	-2.123251	-2.038097	H	-1.299835	-1.824280	-2.296451
N	-1.937086	-1.628526	-2.003479	N	-2.199590	-1.833448	-1.787602	N	-2.237703	-1.507958	-2.037621
C	-2.254531	-0.724373	-3.141224	C	-2.732085	-1.027724	-2.919767	C	-2.676255	-0.534026	-3.073799
C	-3.506406	0.127728	-2.915209	C	-4.001005	-0.247249	-2.569053	C	-3.902649	0.282550	-2.662211
H	-3.686468	0.696905	-3.834340	H	-4.364804	0.222758	-3.490003	H	-4.205967	0.882465	-3.527994
H	-2.377887	-1.321724	-4.054365	H	-2.929872	-1.684537	-3.777502	H	-2.886347	-1.064731	-4.012248
C	-2.737503	-3.398258	0.644040	C	-2.410693	-3.530249	0.974789	C	-2.703393	-3.474447	0.492511
H	-1.475976	-4.122137	-0.966788	H	-1.349858	-4.233159	-0.782841	H	-1.603557	-4.075312	-1.277926
H	-2.636283	-4.297978	1.269817	H	-2.148551	-4.387119	1.613729	H	-2.555722	-4.412007	1.048920
H	-4.392688	-0.506531	-2.789206	H	-4.803287	-0.926561	-2.253186	H	-4.757096	-0.372863	-2.449949
H	-3.763336	-3.034677	0.787418	H	-3.428633	-3.232290	1.256674	H	-3.703759	-3.109092	0.757160
C	-2.516424	-3.798796	-0.818279	C	-2.380908	-3.989764	-0.485533	C	-2.628837	-3.782974	-1.005750
C	-2.897674	-2.760559	-1.876341	C	-3.012097	-3.047422	-1.512003	C	-3.131794	-2.693142	-1.954204
H	-3.887483	-2.351398	-1.650399	H	-3.999999	-2.730576	-1.161338	H	-4.123506	-2.357432	-1.633304
H	-2.973478	-3.248851	-2.857691	H	-3.168656	-3.589322	-2.455098	H	-3.251968	-3.115917	-2.961398
H	-3.131270	-4.685185	-1.011873	H	-2.932388	-4.935393	-0.539093	H	-3.244575	-4.671402	-1.186714

I											
S				SO				T			
H	3.341918	2.708791	-1.085235	H	3.345979	2.614461	-1.255696	H	3.346289	2.564290	-1.341978
H	2.137032	4.375451	-1.968274	H	2.140220	4.212940	-2.270845	H	2.140472	4.128076	-2.416139
H	3.373959	1.239083	-3.043822	H	3.346300	1.025984	-3.127844	H	3.353031	0.913568	-3.157792
H	4.398045	-0.992720	-2.676449	H	4.374830	-1.181793	-2.631133	H	4.380906	-1.274263	-2.581362
H	3.752427	0.453872	-0.761749	H	3.748993	0.378529	-0.802520	H	3.746278	0.344090	-0.810318
H	4.590774	-0.885834	1.622102	H	4.576923	-0.733166	1.599676	H	4.572757	-0.678885	1.624611
H	2.601211	2.105242	0.402885	H	2.603622	2.108026	0.266989	H	2.599983	2.110862	0.195170
H	3.343462	0.958107	2.634149	H	3.340277	1.144172	2.552275	H	3.337907	1.245323	2.479747
C	2.538205	2.074621	-0.690959	C	2.539905	2.009852	-0.823162	C	2.538697	1.975221	-0.891144
H	2.147072	2.992129	2.853089	H	2.146926	3.189084	2.663452	H	2.147170	3.301076	2.580005
H	4.590413	-1.900073	-0.634422	H	4.589462	-1.965935	-0.546940	H	4.591508	-1.998271	-0.472491
C	1.192792	3.879332	-1.759025	C	1.195619	3.735985	-2.021294	C	1.195856	3.659834	-2.150529
H	3.328076	-0.974848	-4.051902	H	3.289957	-1.250866	-3.993670	H	3.301553	-1.392646	-3.945027
C	2.785115	0.449254	-2.558826	C	2.764880	0.267497	-2.588111	C	2.769729	0.173590	-2.594879
H	-0.002237	5.488752	-2.556906	H	0.000070	5.278573	-2.941468	H	0.000032	5.169022	-3.124173
N	2.804363	0.660515	-1.083401	N	2.798945	0.569673	-1.127306	N	2.797824	0.524936	-1.145349
C	3.339616	-0.918403	-2.957427	C	3.313599	-1.123425	-2.905376	C	3.320718	-1.226973	-2.861812
C	3.816261	-1.573249	1.985411	C	3.829764	-1.402298	2.045013	C	3.821081	-1.327377	2.092268
H	4.086888	-1.827229	3.021023	H	4.137061	-1.560816	3.088998	H	4.123541	-1.446140	3.142898
H	4.724182	-3.413786	1.405830	H	4.744163	-3.279501	1.610508	H	4.730206	-3.222631	1.736099
C	1.213800	2.617815	-1.153048	C	1.214877	2.525944	-1.317942	C	1.214926	2.474790	-1.405946
C	-0.001949	4.514070	-2.081346	C	0.000057	4.344196	-2.390797	C	0.000020	4.254432	-2.541215
C	2.530171	0.285133	2.924368	C	2.529599	0.491711	2.892009	C	2.530777	0.607856	2.854608
H	2.779746	-0.089070	3.930176	H	2.786559	0.184011	3.917776	H	2.797868	0.345420	3.890359
C	1.208773	2.443321	2.881242	C	1.208611	2.643165	2.724583	C	1.209023	2.755906	2.649653
C	3.842858	-2.657314	-0.376820	C	3.831467	-2.683584	-0.216182	C	3.827855	-2.697639	-0.116518
H	4.158108	-3.590163	-0.865133	H	4.122574	-3.660038	-0.627472	H	4.114378	-3.691367	-0.487699
H	1.749943	0.567219	-2.892028	H	1.725644	0.364460	-2.916184	H	1.731789	0.259136	-2.930194
H	-0.000252	4.224958	2.841418	H	-0.000032	4.419540	2.580262	H	0.000023	4.529468	2.477891
C	3.820808	-2.852175	1.141769	C	3.832421	-2.748720	1.313661	C	3.822831	-2.701909	1.414639
N	2.519421	-0.850306	1.953734	N	2.515394	-0.707613	1.999691	N	2.509528	-0.628984	2.016227
C	1.221222	1.044445	2.942394	C	1.220545	1.250335	2.867774	C	1.220863	1.365183	2.812053
C	-0.000039	3.139820	2.872914	C	-0.000034	3.338202	2.670060	C	0.000016	3.449744	2.590537
H	2.970428	-3.043228	-2.862682	H	2.940335	-3.237101	-2.654666	H	2.947055	-3.331050	-2.538213
C	2.553857	-2.122517	-2.431464	C	2.530265	-2.285784	-2.289669	C	2.536091	-2.367482	-2.207979
N	2.533348	-2.235412	-0.943743	N	2.521469	-2.283250	-0.797161	N	2.522548	-2.311889	-0.716407
Cu	1.581659	-0.584980	-0.158464	Cu	1.542235	-0.591206	-0.101135	Cu	1.534011	-0.598834	-0.080758
C	-1.196309	3.878391	-1.759547	C	-1.195521	3.735980	-2.021358	C	-1.195832	3.659823	-2.150594
H	2.981021	-3.503124	1.430309	H	3.002224	-3.377885	1.669712	H	2.989591	-3.314398	1.791974
C	-0.001196	1.941081	-0.882631	C	0.000025	1.878370	-0.992397	C	-0.000009	1.839395	-1.059022
H	1.823887	-1.510505	2.304537	H	1.848318	-1.358434	2.417777	H	1.839699	-1.257336	2.463252
H	1.509420	-2.049914	-2.756086	H	1.483273	-2.234176	-2.610979	H	1.489896	-2.327366	-2.533457
H	-2.140854	4.373756	-1.969209	H	-2.140111	4.212931	-2.270958	H	-2.140438	4.128055	-2.416259
H	1.860202	-2.970122	-0.725425	H	1.832879	-2.981629	-0.512646	H	1.828445	-2.995517	-0.409805
O	-0.000494	0.680443	-0.386066	O	0.000016	0.667260	-0.387251	O	-0.000025	0.649666	-0.414593
C	-1.216619	2.616851	-1.153535	C	-1.214813	2.525938	-1.318005	C	-1.214934	2.474778	-1.406013
C	0.000561	0.366613	3.019621	C	-0.000040	0.578060	2.984373	C	-0.000003	0.694689	2.934429
C	-1.208552	2.442829	2.881522	C	-1.208682	2.643168	2.724560	C	-1.209001	2.755921	2.649635
H	0.000781	-0.716956	3.128306	H	-0.000044	-0.497253	3.157801	H	-0.000012	-0.379513	3.111998
H	-2.147099	2.991220	2.853596	H	-2.146995	3.189088	2.663409	H	-2.147139	3.301103	2.579971
C	-1.220394	1.043951	2.942891	C	-1.220621	1.250338	2.867756	C	-1.220860	1.365200	2.812041
O	0.000389	-1.651382	0.183232	O	-0.000010	-1.746200	0.305384	O	0.000003	-1.758419	0.362557
H	-2.604610	2.103662	0.401789	H	-2.603643	2.108032	0.266853	H	-2.600139	2.110913	0.195000
C	-2.540887	2.072766	-0.692025	C	-2.539867	2.009848	-0.823293	C	-2.538739	1.975201	-0.891299
H	-0.000282	-2.316059	0.894092	H	-0.000028	-2.187067	1.168063	H	0.000053	-2.179118	1.234767
H	-1.751776	0.566570	-2.893226	H	-1.725497	0.364451	-2.916260	H	-1.731647	0.259055	-2.930203
H	-3.344889	2.706141	-1.086984	H	-3.345921	2.614449	-1.255877	H	-3.346300	2.564222	-1.342251
Cu	-1.580408	-0.584680	-0.159532	Cu	-1.542213	-0.591194	-0.101195	Cu	-1.534064	-0.598828	-0.080688
C	-2.528985	0.284060	2.925929	C	-2.529678	0.491718	2.891986	C	-2.530782	0.607890	2.854594
N	-2.805562	0.658319	-1.084149	N	-2.798882	0.569664	-1.127433	N	-2.797816	0.524896	-1.145443
C	-2.786559	0.446652	-2.559514	C	-2.764746	0.267469	-2.588231	C	-2.769608	0.173492	-2.594958
H	-3.377180	1.235196	-3.044439	H	-3.346158	1.025937	-3.128000	H	-3.352889	0.913436	-3.157938
H	-1.823012	-1.510930	2.303989	H	-1.848389	-1.358418	2.417732	H	-1.839757	-1.257320	2.463235
H	-2.776872	-0.091157	3.931777	H	-2.786634	0.184019	3.917753	H	-2.797870	0.345442	3.890340
H	-3.343061	0.956841	2.637484	H	-3.340353	1.144185	2.552256	H	-3.337904	1.245372	2.479741
H	-1.507100	-2.051227	-2.753584	H	-1.483143	-2.234249	-2.610888	H	-1.489725	-2.327429	-2.533335
N	-2.519003	-0.850583	1.954345	N	-2.515483	-0.707603	1.999664	N	-2.509559	-0.628946	2.016199
H	-3.753092	0.450338	-0.761838	H	-3.748941	0.378515	-0.802684	H	-3.746294	0.344053	-0.810481
H	-1.859263	-2.970791	-0.722422	H	-1.833044	-2.981664	-0.512551	H	-1.828494	-2.995544	-0.409679
N	-2.532220	-2.236244	-0.941845	N	-2.521515	-2.283209	-0.797167	N	-2.522532	-2.311896	-0.716380
C	-2.551708	-2.124773	-2.429726	C	-2.530167	-2.285812	-2.289674	C	-2.535947	-2.367558	-2.207946
C	-3.338589	-0.922198	-2.957542	C	-3.313422	-1.123467	-2.905513	C	-3.320542	-1.227092	-2.861891
H	-3.325560	-0.979525	-4.051957	H	-3.289634	-1.250941	-3.993801	H	-3.301271	-1.392803	-3.945098
H	-2.966811	-3.046428	-2.860329	H	-2.940231	-3.237134	-2.654663	H	-2.946859	-3.331151	-2.538175
C	-3.815670	-1.573772	1.986958	C	-3.829850	-1.402294	2.045040	C	-3.821136	-1.327305	2.092240
H	-2.981259	-3.504025	1.431875	H	-3.002420	-3.377889	1.669543	H	-2.989779	-3.314383	1.791949
H	-4.085474	-1.827965	3.022738	H	-4.137056	-1.560911	3.089037	H	-4.123574	-1.446083	3.142874
H	-4.397252	-0.997845	-2.677855	H	-4.374689	-1.181832	-2.631408	H	-4.380756	-1.274397	-2.581539
H	-4.590611	-0.886491	1.624311	H	-4.577045	-0.733117	1.599832	H	-4.572800	-0.678776	1.624616
C	-3.820605	-2.852574	1.143191	C	-3.832585	-2.748643	1.313558	C	-3.822954	-2.701825	1.414585
C	-3.842134	-2.657417	-0.375354	C	-3.831612	-2.683335	-0.216278	C	-3.827911	-2.697525	-0.116574
H	-4.589217	-1.899715	-0.632970	H	-4.589449	-1.965481	-0.546958	H	-4.591470	-1.998062	-0.472561
H	-4.157807	-3.589957	-0.863990	H	-4.122923	-3.659674	-0.627697	H	-4.114529	-3.691211	-0.487792
H	-4.724377	-3.413715	1.406900	H	-4.744356	-3.279402	1.610356	H	-4.732205	-3.222480	1.735995

d+H				gi				il			
SO				SO				SO			
H	-0.132361	0.916595	4.879734	H	-0.000170	-0.990629	5.259157	H	3.576509	2.619678	-1.041595
H	-3.133701	-2.684327	2.540774	H	-2.717611	-3.662756	1.680601	H	2.447735	4.549169	-1.579259
H	-2.331202	0.260369	3.948586	H	-2.151093	-1.458861	4.120535	H	3.477160	1.160706	-3.001684
H	2.164569	-3.290250	2.806243	H	2.718313	-3.662103	1.681067	H	4.421411	-1.126333	-2.540652
C	-0.190116	0.137690	4.125994	C	-0.000094	-1.418890	4.261141	H	3.873720	0.368457	-0.730252
H	1.929841	-0.229921	4.129778	H	2.150918	-1.458457	4.120683	H	4.411516	-1.375844	1.836257
C	-1.427497	-0.229468	3.593861	C	-1.212997	-1.684946	3.619034	H	2.859805	2.056543	0.467615
C	0.971505	-0.506453	3.696787	C	1.212899	-1.684717	3.619119	H	3.269387	0.699342	2.789270
C	-1.515496	-1.259949	2.645637	C	-1.222599	-2.267971	2.345079	C	2.745485	2.039263	-0.622545
C	0.902151	-1.541115	2.751595	C	1.222702	-2.267743	2.345159	H	2.107421	2.812621	2.840124
H	-3.636943	-1.002170	2.447065	H	-3.353633	-2.076042	2.094069	H	4.408737	-2.240589	-0.529828
C	-0.348019	-1.923385	2.254869	C	0.000102	-2.589778	1.752165	C	1.486993	4.064017	-1.428347
H	3.036712	-1.765665	2.722174	H	3.353656	-2.074987	2.094113	C	3.468059	-1.016758	-3.995970
C	-2.861937	-1.703961	2.126615	C	-2.508877	-2.581382	1.612936	C	2.875498	0.390112	-2.502271
C	2.150972	-2.289913	2.352581	C	2.509121	-2.580838	1.613104	H	0.355813	5.805179	-2.000022
H	-0.417584	-2.765301	1.569220	H	0.000156	-3.115034	0.799754	N	2.923666	0.601723	-1.026687
H	3.643391	-4.083952	1.149569	H	3.627504	-3.845602	-0.403355	C	3.392678	-0.995778	-2.902720
H	-4.616305	-3.091353	0.745577	H	-3.627510	-3.845681	-0.403552	C	3.491342	-1.931775	2.056711
H	-2.346872	-2.578511	0.338373	H	-1.606978	-2.534918	-0.217814	H	3.578028	-2.278080	3.097302
H	1.585686	-3.088087	0.545414	H	1.607003	-2.535038	-0.217513	H	4.181174	-3.853659	1.456435
H	-5.000244	-1.374559	0.657403	H	-4.522236	-2.349482	-0.167094	C	1.447129	2.731691	-0.998994
N	-2.939225	-1.793971	0.622750	N	-2.463665	-2.157815	0.188338	C	0.310758	4.775961	-1.659628
H	4.413921	-2.503215	1.046158	H	4.522239	-2.349316	-0.167388	C	2.399661	0.063422	2.984012
N	2.318645	-2.448325	0.862654	N	2.463688	-2.157683	0.188396	H	2.564928	-0.409415	3.964965
C	-4.348290	-2.153061	0.245510	C	-3.584263	-2.757075	-0.566316	C	1.155979	2.287566	2.880472
C	3.631728	-3.131928	0.605726	C	3.584198	-2.757031	-0.566329	C	3.570829	-2.925381	-0.360210
H	-2.318943	1.859085	1.860816	H	-2.478108	0.578644	2.234325	H	3.829389	-3.871886	-0.854256
H	2.629285	1.255220	1.977605	H	2.477948	0.578133	2.234095	H	1.837646	0.530304	-2.821067
H	4.850901	-3.973569	-0.920856	H	4.279265	-3.083993	-2.555713	H	-0.009798	4.095974	2.766868
H	-5.606192	-2.651352	-1.395199	H	-4.279782	-3.083667	-2.555577	C	3.390742	-3.161633	1.144293
C	3.932777	-3.377743	-0.869436	C	3.501605	-2.484928	-2.068688	N	2.348004	-0.995844	1.929569
C	-4.583777	-2.282796	-1.255641	C	-3.501984	-2.484709	-2.068640	C	1.132059	0.892253	3.001615
H	3.152996	-4.001143	-1.331330	H	2.546851	-2.852882	-2.472269	C	-0.037025	3.012762	2.832924
C	-3.932544	-3.054632	-1.691631	H	-2.547336	-2.852672	-2.472477	H	2.938714	-3.106481	-2.924708
C	-2.251657	2.543136	1.008711	C	-2.526584	1.526636	1.691116	N	2.519360	-2.188102	-2.491457
H	-2.967552	3.355431	1.177335	H	-3.373247	2.106378	2.080312	N	2.360752	-2.352703	-1.017600
C	2.757991	1.912646	1.111025	C	2.526633	1.526188	1.691017	Cu	1.626645	-0.665132	-0.130616
H	3.648361	2.525563	1.290880	H	3.373410	2.105713	2.080292	C	-0.924240	4.161784	-1.457001
C	0.260193	2.278236	1.009646	O	-0.000012	0.757712	0.261003	H	2.445223	-3.692120	1.329574
C	-0.859691	3.107905	0.883542	C	0.000037	1.553126	1.870844	C	0.190288	2.135565	-0.818481
C	1.555154	2.802997	0.930142	C	-1.235148	2.291015	1.847606	H	1.486988	-1.526279	2.086630
H	-1.531475	5.145919	0.625352	C	1.235346	2.290800	1.847574	H	1.513103	-2.060236	-2.907512
C	-0.671945	4.484217	0.692657	H	-2.148005	4.233977	1.884155	H	-1.836785	4.725352	-1.632910
H	-3.721322	1.640867	-0.052066	C	-1.213689	3.678497	1.878050	H	1.598912	-3.015760	-0.864425
C	1.722985	4.181445	0.737368	H	-3.658577	0.606369	0.268694	O	0.145739	0.782935	-0.574956
H	2.721928	4.608304	0.704661	O	-0.000169	-0.640393	-1.512158	C	-1.010455	2.828832	-1.032507
H	3.986767	0.645649	0.120325	C	1.214126	3.678286	1.878024	C	-0.107524	0.252433	3.104436
Cu	1.993638	-0.722100	-0.194904	H	2.148538	4.233606	1.884112	C	1.264405	2.345969	2.840801
Cu	-2.129528	-0.180636	-0.348209	H	3.658403	0.605740	0.268551	H	-0.135435	-0.822841	3.257921
C	0.614010	5.019664	0.621802	Cu	1.447671	0.059312	-0.669450	H	-2.188327	2.915848	2.774582
H	0.751602	6.088507	0.492881	Cu	-1.447819	0.059329	-0.669184	C	-1.310305	0.950356	2.957898
N	-2.715914	1.767532	-0.209841	C	0.000280	4.378325	1.930667	O	-0.089900	-1.252228	0.520351
N	3.050191	1.014189	-0.075606	H	0.000376	5.461454	1.997961	H	-2.527779	2.274674	0.381382
H	-5.048544	-0.185661	-1.560099	N	-2.814238	1.182469	0.250896	C	-2.379934	2.259844	-0.703954
H	4.889338	-1.459369	-1.203166	N	2.814248	1.182111	0.250774	H	-0.064985	0.224553	0.332317
C	-4.451524	-0.973608	-2.029076	H	-4.527713	-0.595080	-1.876896	H	-1.499933	0.665344	-2.851791
C	4.154293	-2.108717	-1.688532	H	4.527434	-0.595317	-1.877358	H	-3.131185	2.928774	-1.140675
N	2.880147	-1.342642	-1.866599	C	-3.725476	-1.029027	-2.481574	Cu	-1.738810	-0.625178	-0.141510
N	-3.026664	-0.516771	-2.096968	C	3.725104	-1.029308	-2.481879	C	-2.614410	0.183773	2.884036
H	-4.822700	-1.099561	-3.053295	N	2.516349	-0.166219	-2.351814	N	-2.704922	0.853341	-1.142516
H	4.547005	-2.361971	-2.680673	N	-2.516610	-0.166103	-2.351528	C	-2.568969	0.660699	-2.617408
H	2.212576	-2.026770	-2.233151	H	-4.057142	-0.983690	-3.527915	H	-3.019784	1.517349	-3.134970
H	-2.512622	-1.322388	-2.464291	H	4.056684	-0.984132	-3.528252	H	-1.775872	-1.476238	2.048304
C	-2.619171	2.585319	-1.461433	H	1.773323	-0.583165	-2.918050	H	-2.843342	-0.293253	3.849244
H	-3.032506	3.582455	-1.267750	H	-1.773643	-0.583201	-2.917733	H	-3.444924	0.859832	2.657944
C	3.193937	1.788257	-1.350317	C	-3.101389	2.390286	-0.579520	H	-1.510352	-1.928620	-3.030870
H	3.824904	2.666152	-1.166334	H	-3.819421	3.027347	-0.045900	N	-2.568968	-0.870655	1.820257
H	-4.436658	1.877739	-2.421577	C	3.101791	2.389914	-0.579525	H	-3.701726	0.759624	-0.934527
H	-1.558611	2.710927	-1.693424	H	3.820073	3.026660	-0.045864	H	-1.865059	-2.931985	-1.038160
H	2.201275	2.150835	-1.629596	H	-4.649052	1.591646	-1.873458	N	-2.514773	2.164264	-1.216109
H	4.828691	0.642860	-2.211253	H	-2.167713	2.951743	-0.669110	C	-2.551431	-1.939868	-2.688071
C	-3.361801	1.947029	-2.632355	H	2.168313	2.951717	-0.669008	C	-3.232806	-0.631280	-3.107294
C	2.969743	-0.255005	-2.898038	H	4.649173	1.591011	-1.873639	H	-3.226775	-0.606854	-4.203133
C	3.806779	0.948397	-2.469849	C	-3.660125	2.057150	-1.964794	H	-3.052309	-2.784271	-3.180779
C	-2.803860	0.597418	-3.079712	C	2.747533	1.216599	-2.864423	C	-3.799190	-1.705024	1.835366
H	1.943620	0.064393	-3.113711	C	3.660353	2.056756	-1.964875	H	-2.890977	-3.528525	1.071480
H	-1.721355	0.675123	-3.233711	C	-2.747546	1.216696	-2.864288	H	-3.972345	-2.091751	2.849898
H	3.382361	-0.689060	-3.816627	H	1.764890	1.693064	-2.954269	H	-4.294595	-0.636371	-2.826587
H	-3.254627	0.303928	-4.035128	H	-1.764809	1.692945	-2.954255	H	-4.649002	-1.053291	1.598242
H	-3.280872	2.630038	-3.485594	H	3.180949	1.162000	-3.871409	C	-3.763967	-2.893536	0.861390
H	3.914982	1.596078	-3.347211	H	-3.181040	1.162054	-3.871238	C	-3.830978	-2.572221	-0.640156
H	0.121312	1.220395	1.222980	H	-3.835960	3.009655	-2.477618	H	-4.546493	-1.761061	-0.813157
O	-0.231864	-1.969739	-1.096853	H	3.836389	3.009267	-2.477618	H	-4.205060	-3.446582	-1.189634
O	-0.073516	-0.573487	-0.597208	H	-0.000050	0.589525	2.373353	H	-4.637745	-3.512345	1.094690
H	-0.189393	-1.838321	-2.062188								

em			m			n					
SO			SO			SO					
H	-1.679503	4.777405	0.000000	H	-2.317805	4.842398	0.000000	H	0.000191	-5.899584	3.160657
H	2.406305	3.061747	2.824519	H	1.527693	3.438763	2.902530	H	-3.308934	-3.510627	1.007032
H	-0.696005	4.032290	2.146654	H	-1.350775	4.132743	2.154196	H	-2.139886	-4.887975	2.420718
H	2.406306	3.061746	-2.824518	H	1.527666	3.438729	-2.902530	H	3.309082	-3.510813	1.006467
C	-0.782908	4.165737	0.000000	C	-1.435478	4.208860	0.000001	C	0.000164	-5.003805	2.549298
H	-0.696005	4.032290	-2.146654	H	-1.350807	4.132690	-2.154192	H	2.140198	-4.888058	2.420411
C	-0.221676	3.751646	1.209714	C	-0.885164	3.800587	1.230195	C	-1.196993	-4.429476	2.133777
C	-0.221676	3.751646	-1.209715	C	-0.885182	3.800557	-1.230189	C	1.197282	-4.429522	2.133605
C	0.949441	2.986733	1.222593	C	0.233518	3.001529	1.262378	C	-1.217942	-3.274086	1.344379
C	0.949442	2.986733	-1.222593	C	0.233505	3.001504	-1.262368	C	1.218166	-3.274134	1.344200
H	0.780529	2.607812	3.326718	H	0.087640	2.533935	3.347795	H	-2.890009	-1.892044	1.550816
C	1.566372	2.683395	0.000000	C	0.829736	2.475748	0.000007	C	0.000096	-2.664507	0.959910
H	0.780529	2.607812	-3.326719	H	0.087610	2.533896	-3.347780	H	2.890387	-1.892249	1.550477
C	1.519346	2.480269	2.530488	C	0.862883	2.617957	2.579057	C	-2.554415	-2.720044	0.915748
C	1.519346	2.480269	-2.530488	C	0.862860	2.617922	-2.579048	C	2.554612	-2.720159	0.915385
H	2.529591	2.179827	0.000000	H	1.928477	2.602077	0.000001	H	-0.000044	1.428825	-0.370864
H	3.306273	1.344223	-4.067816	H	2.831659	1.930800	-4.195370	H	4.203153	-3.348201	-1.124749
H	3.306272	1.344224	4.067817	H	2.831700	1.930834	4.195361	H	-4.203306	-3.348219	-1.124039
H	2.657269	0.944139	1.826989	H	2.398904	1.467319	1.904371	H	-1.905030	-2.852514	-1.004196
H	2.657268	0.944139	-1.826989	H	2.398889	1.467288	-1.904368	H	1.904923	-2.852425	-1.004465
H	1.716317	0.792677	4.588490	H	1.425561	0.946016	4.606375	H	-4.566467	-1.710273	-0.578209
N	1.901125	1.024013	2.510257	N	1.618271	1.339599	2.552065	N	-2.529186	-2.224044	-0.492822
H	1.716318	0.792677	-4.588490	H	1.425524	0.945967	-4.606362	H	4.566472	-1.710338	-0.578772
N	1.901125	1.024013	-2.510257	N	1.618252	1.339567	-2.552058	N	2.529182	-2.224028	-0.493128
C	2.491329	0.648352	3.826834	C	2.236842	1.062830	3.878337	C	-3.853565	-2.308163	-1.158527
C	2.491330	0.648351	-3.826834	C	2.236812	1.062793	-3.878333	C	3.853453	-2.308124	-1.159053
H	-1.796840	1.730425	2.508817	H	-2.168571	1.301631	2.552871	H	-2.512583	-0.117703	2.712233
H	-1.796840	1.730425	-2.508817	H	-2.168430	1.301763	-2.552826	H	2.512198	-0.118084	2.712245
H	3.622630	-0.878607	-4.788859	H	3.715001	-0.187356	-4.775429	H	4.696018	-2.167497	-3.123196
H	3.622630	-0.878606	4.788860	H	3.715027	-0.187329	4.775425	H	-4.696453	-2.167717	-3.122541
C	3.018207	-0.787182	-3.879402	C	3.115580	-0.189211	-3.858065	C	3.793354	-1.821444	-2.607445
C	3.018207	-0.787181	3.879403	C	3.115598	-0.189182	3.858067	C	-3.793673	-1.821670	-2.606990
H	3.712873	-0.973283	-3.046186	H	3.840606	-0.131905	-3.032138	H	2.950980	-2.297981	-3.130697
H	3.712873	-0.973282	3.046186	H	3.840617	-0.131886	3.032134	H	-2.951429	-2.298344	-3.130325
C	-2.336029	0.777617	2.518559	C	-2.476826	0.249978	2.520119	C	-2.522015	0.920811	2.364888
C	-3.054256	0.809515	3.349597	H	-3.171582	0.085285	3.355698	H	-3.350678	1.430447	2.875627
C	-2.336029	0.777617	-2.518558	C	-2.476709	0.250114	-2.520138	C	2.521843	0.920475	2.365042
C	-3.054256	0.809515	-3.349596	H	-3.171436	0.085478	-3.355752	C	3.350528	1.429910	2.875943
O	0.697526	0.449781	0.000000	O	0.507432	1.043451	0.000013	O	0.000052	-1.527538	0.206412
C	-2.426351	0.773796	0.000000	C	-2.573170	0.249433	-0.000011	C	-0.000083	0.981822	2.423628
C	-3.085691	0.590277	1.218512	C	-3.188993	-0.047715	1.218563	C	-1.219213	1.599462	2.722657
C	-3.085691	0.590277	-1.218512	C	-3.188938	-0.047643	-1.218631	C	1.219109	1.599294	2.722745
H	-4.980055	0.124151	2.147391	H	-4.969579	-0.844591	2.147561	H	-2.147016	3.326764	3.627798
C	-4.444950	0.250524	1.209515	C	-4.467982	-0.618907	1.209827	C	-1.208916	2.843531	3.367112
H	-0.976619	-0.089636	3.731776	H	-0.937466	-0.355449	3.681493	H	-3.718686	0.479172	0.795032
O	0.536432	-1.359497	0.000000	O	0.819333	-1.318600	0.000023	O	-0.000024	0.611699	-0.898288
C	-4.444950	0.250524	-1.209514	C	-4.467926	-0.618837	-1.209986	C	1.208936	2.843361	3.367207
H	-4.980055	0.124151	-2.147391	H	-4.969478	-0.844470	-2.147757	H	2.147084	3.326461	3.627968
H	-0.976620	-0.089636	-3.731776	H	-0.937380	-0.355370	-3.681513	H	3.718643	0.478899	0.795262
Cu	0.661846	-0.425605	-1.604200	Cu	0.695983	-0.263794	-1.508868	Cu	1.579887	-0.463345	-0.535733
Cu	0.661846	-0.425605	1.604200	Cu	0.695990	-0.263769	1.508886	Cu	-1.579875	-0.463393	-0.535702
C	-5.122884	0.089277	0.000000	C	-5.107948	-0.893171	-0.000102	C	0.000041	3.458205	3.695724
H	-6.179328	-0.161081	0.000000	H	-6.103318	-1.326790	-0.000137	H	0.000088	4.414544	4.209590
N	-1.316246	-0.292783	2.788110	N	-1.239164	-0.572189	2.728367	N	-2.787276	0.893201	0.885923
N	-1.316246	-0.292782	-2.788110	N	-1.239064	-0.572072	-2.728374	N	2.787267	0.893017	0.886101
H	1.201286	-1.614791	4.695522	H	1.596621	-1.516658	4.606359	H	-4.585755	0.131708	-2.214800
H	1.201286	-1.614791	-4.695522	H	1.596610	-1.516703	-4.606340	H	4.585658	0.131815	-2.215128
C	1.942332	-1.872498	3.933677	C	2.348742	-1.511344	3.811682	C	-3.738400	-0.303245	-2.751575
C	1.942332	-1.872498	-3.933677	C	2.348737	-1.511380	-3.811668	C	3.738178	-0.302997	-2.751818
N	1.234514	-2.053609	-2.637639	N	1.657817	-1.760543	-2.520950	N	2.494257	0.320065	-2.216691
N	1.234514	-2.053609	2.637639	N	1.657809	-1.760515	2.520972	N	-2.494342	0.319792	-2.216741
H	2.390096	-2.829516	4.232574	H	3.034842	-2.343328	4.020779	H	-3.854228	-0.021729	-3.806831
H	2.390095	-2.829516	-4.232574	H	3.034842	-2.343360	-4.020768	H	3.853847	-0.021346	-3.807055
H	1.926006	-2.414567	-1.975880	H	2.368230	-1.926980	-1.805803	H	1.749668	0.120261	-2.886854
H	1.926007	-2.414566	1.975880	H	2.368214	-1.926956	1.805819	H	-1.749872	0.119779	-2.886976
C	-1.965573	-1.629905	2.865203	C	-1.563016	-2.026321	2.719015	C	-2.905996	2.279149	0.355610
H	-2.896621	-1.563339	3.447368	H	-2.501930	-2.202875	3.264353	H	-3.532833	2.884247	1.027238
C	-1.965574	-1.629904	-2.865203	C	-1.562969	-2.026198	-2.718969	C	2.906200	2.279014	0.355967
H	-2.896621	-1.563339	-3.447368	H	-2.501900	-2.202720	-3.264290	H	3.533126	2.883933	1.027673
H	-0.809848	-2.420847	4.524117	H	-0.281686	-2.581621	4.378991	H	-4.490740	1.901197	-1.072214
H	-2.246699	-1.921096	1.848810	H	-1.731678	-2.320586	1.679379	H	-1.909158	2.731913	0.374696
H	-2.246699	-1.921096	-1.848810	H	-1.731638	-2.320422	-1.679322	H	1.909428	2.731922	0.375104
H	-0.809849	-2.420846	-4.524117	H	-0.281699	-2.581629	-4.378948	H	4.490863	1.900970	-1.071929
C	-1.076585	-2.702440	3.496758	C	-0.469924	-2.895966	3.342801	C	-3.491936	2.357175	-1.054896
C	0.164608	-3.100425	-2.697660	C	0.833768	-3.008746	-2.550242	C	2.618814	1.812234	-2.188006
C	-1.076585	-2.702439	3.496759	C	-0.469937	-2.895928	-3.342744	C	3.492143	2.357126	-1.054531
C	0.164609	-3.100425	2.697660	C	0.833777	-3.008736	2.550284	C	-2.618731	1.811981	-2.188321
H	-0.116579	-3.311911	-1.661344	H	0.611768	-3.241008	-1.506295	H	1.604549	2.208622	-2.099982
H	-0.116579	-3.311911	1.661344	H	0.611773	-3.241019	1.506342	H	-1.604415	2.208264	-2.100422
H	0.597128	-4.015988	-3.122380	H	1.443068	-3.823509	-2.964809	H	3.027251	2.149302	-3.150568
H	0										

nl		
SO		
H	0.000015	5.752411
H	3.335894	2.651391
H	2.140569	4.544454
H	-3.335860	2.651416
C	0.000017	4.712004
H	-2.140534	4.544467
C	1.196021	4.028235
C	-1.195984	4.028243
C	1.214690	2.684144
C	-1.214643	2.684153
H	2.772541	1.932078
C	0.000025	1.988260
H	-2.772414	1.932027
C	2.548819	2.026205
C	-2.548760	2.026209
H	0.000000	-2.144484
H	-4.413870	1.020435
H	4.413882	1.020335
H	2.098827	0.687566
H	-2.098810	0.687640
H	4.635633	0.372613
N	2.629161	0.653175
H	-4.635590	0.372610
N	-2.629129	0.653208
C	4.025032	0.286384
C	-4.025006	0.286439
H	3.273716	1.423795
H	-3.273915	1.423537
H	-5.112632	-1.231722
H	5.112641	-1.231839
C	-4.126232	-1.122785
C	4.126251	-1.122877
H	-3.398178	-1.252644
H	3.398179	-1.252790
C	2.574275	0.658906
H	2.958894	0.333296
C	-2.574387	0.658695
H	-2.958938	0.332987
O	0.000023	0.672997
C	-0.000058	0.663791
C	1.218797	1.314369
C	-1.218965	1.314275
H	2.143956	3.149502
C	1.206056	2.630925
H	3.633024	-0.465248
O	0.000016	-1.706573
C	-1.206326	2.630833
H	-2.144266	3.149337
H	-3.633049	-0.465439
Cu	-1.550178	-0.570232
Cu	1.550217	-0.570216
C	-0.000160	3.283504
H	-0.000199	4.304828
N	2.665414	-0.487015
N	-2.665447	-0.487178
H	4.697461	-2.061100
H	-4.697401	-2.061131
C	3.980481	-2.231349
C	-3.980434	-2.231324
N	-2.619668	-2.313202
N	2.619726	-2.313199
H	4.233416	-3.201439
H	-4.233371	-3.201387
H	-1.993913	-2.654934
H	1.993960	-2.654985
C	2.521524	-1.812639
H	2.961372	-1.773610
C	-2.521510	-1.812833
H	-2.961373	-1.773882
H	4.267818	-2.704630
H	1.455906	-2.027775
H	-1.455885	-2.027933
H	-4.267758	-2.704856
C	3.203310	-2.944462
C	-2.577803	-3.358859
C	-3.203238	-2.944643
C	2.577892	-3.358787
H	-1.527853	-3.622565
H	1.527951	-3.622521
H	-3.089148	-4.259676
H	3.089266	-4.259611
H	3.189831	-3.835166
H	-3.189716	-3.835385
H	-0.000021	-0.349021

Table S2. Multiplicity states, $\langle S^2 \rangle$ values for all species involved in this reaction mechanism.

	Multiplicity State	$\langle S^2 \rangle$
a	S	0.0000
b	T	2.0083
TS-bc	T	2.0092
c	T	2.0097
TS-cd	T	2.0089
d	T	2.0104
TS-de	T	2.0080
e	SO	0.7005
TS-eg	SO	0.5489
g	SO	1.0661
TS-gh	SO	0.9664
h	SO	1.0383
TS-hi	SO	0.9879
i	SO	0.9205
TS-ij	SO	0.8547
j	SO	0.9672
TS-jk	SO	0.9037
k	SO	1.0036
TS-kl	SO	0.9714
l	SO	0.9763

TS-ef	S	0.0000
f	S	0.0000
TS-fg	S	0.0000
d+H	SO	1.0034
TS-gi	SO	0.9879
TS-il	SO	0.9201
TS-em	SO	0.4687
m	SO	0.9546
n	SO	0.9546
TS-nl	SO	0.9700

Table S3. Free energies in solvent (B3LYP/6-31G(d,p)), ZPE, and thermal corrections, *i. e.* sum of electronic and thermal free energies, (in a.u.) in gas (B3LYP/6-31G(d)) for all species involved in this reaction mechanism.

	Free energies	ZPE ¹	Thermal corrections ¹
a	-4854.7524	0.7419	0.6534
b	-4854.7651	0.7435	0.6724
TS-bc	-4854.7637	0.7433	0.6728
c	-4854.7640	0.7431	0.6729
TS-cd	-4854.7624	0.7438	0.6742
d	-4854.7832	0.7446	0.6761
TS-de	-4854.7785	0.7444	0.6770
e	-4854.7920	0.7443	0.6786
TS-eg	-4854.7701	0.7440	0.6776
g	-4854.7818	0.7452	0.6790
TS-gh	-4854.7795	0.7383	0.6753
h	-4854.7989	0.7399	0.6767
TS-hi	-4854.7985	0.7425	0.6782
i	-4854.8549	0.7460	0.6798
TS-ij	-4854.8372	0.7443	0.6774
j	-4854.8519	0.7449	0.6788
TS-jk	-4854.8455	0.7458	0.6793
k	-4854.8852	0.7467	0.6797
TS-kl	-4854.8851	0.7456	0.6810
l	-4854.9288	0.7459	0.6811

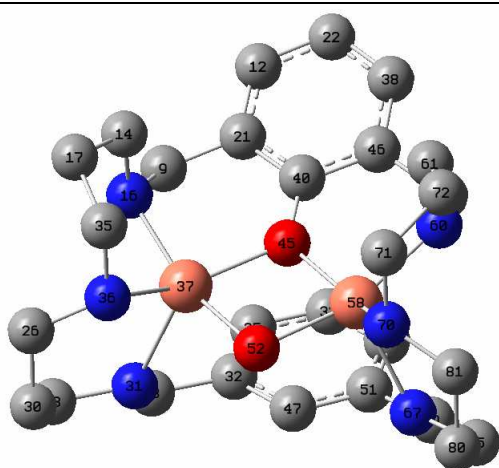
TS-ef	-4854.7622	0.7439	0.6772
f	-4854.7657	0.7452	0.6798
TS-fg	-4854.7590	0.7451	0.6800
TS-gi	-4854.7619	0.7425	0.6782
TS-il	-4854.8294	0.7416	0.6757
TS-em	-4854.7449	0.7498	0.6794
m	-4854.7687	0.7436	0.6776
n	-4854.9534	0.7470	0.6838
TS-nl	-4854.7598	0.7462	0.6851

¹ Calculated with the 6-31G(d) basis set.

Table S4. Comparison between the X-ray data of complex **I** and the corresponding B3LYP/6-31G(d) geometry (Distances in Å and angles in degrees).

Distances	dist(RX)	dist(opt)
Cu37-O45	2.032	2.011
Cu37-O52	1.918	1.969
Cu58-O45	2.022	2.011
Cu58-O52	1.920	1.969
O45-O52	2.464	2.511
Cu37-N16	1.981	1.995
Cu37-N36	2.053	2.075
Cu37-N31	2.321	2.318
Cu58-N60	1.968	1.995
Cu58-N70	2.059	2.075
Cu58-N67	2.339	2.318
N16-C9	1.458	1.495
N60-C54	1.497	1.495
C9-C21	1.527	1.506
C54-C46	1.518	1.506
N16-C14	1.464	1.492
C14-C17	1.563	1.529
C17-C35	1.510	1.531
N36-C35	1.455	1.493
N60-C61	1.450	1.492
C61-C72	1.562	1.529
C72-C71	1.466	1.531
N70-C71	1.529	1.493
N36-C26	1.460	1.488
C26-C30	1.528	1.531
N31-C18	1.493	1.532
N31-C23	1.447	1.487
C23-C32	1.471	1.495
N70-C81	1.477	1.513
C81-C80	1.458	1.488
C80-C75	1.507	1.531
N67-C75	1.500	1.532
N67-C59	1.456	1.487
C59-C51	1.483	1.495
O45-C40	1.487	1.513

Angles	ang(RX)	ang(opt)
Cu37-O45-Cu58	97.4	100.2
Cu37-O51-Cu58	105.0	103.1
N16-Cu37-N36	91.6	90.3
N36-Cu37-N31	91.5	93.7
N31-Cu37-N16	100.2	103.4
N60-Cu58-N70	91.7	90.3
N70-Cu58-N67	92.0	93.7
N16-Cu37-O45	92.9	92.6
C51-C48-C43	119.7	120.4
C32-C25-C33	121.4	120.4
C235-C33-C48	119.5	120.1
C40-C21-C12	120.9	120.0
C21-C12-C22	121.9	121.5
C12-C22-C38	118.2	118.5
C22-C38-C46	121.9	121.5
C38-C46-C40	120.0	120.0
C46-C40-C21	116.9	118.4
N60-Cu58-O45	93.9	92.6
N60-Cu58-O45	93.9	92.6
N60-Cu58-O45	93.9	92.6
Cu37-O45-C40	126.9	128.6
Cu58-O45-C41	126.8	128.6
O45-Cu37-O52	77.1	78.2
O45-Cu58-O52	77.3	78.2
N16-C9-C21	115.7	114.6
N60-C54-C46	113.6	114.6
N31-C23-C32	111.5	112.6
N67-C59-C51	110.2	112.6
N16-C14-C17	111.1	112.3
N60-C61-C72	112.0	112.3
N36-C35-C17	115.3	113.8
N70-C71-C72	114.1	113.8
N31-C18-C30	112.7	113.4
N67-C75-C80	113.7	113.4
N36-C26-C30	112.2	113.7



Standard deviations for the distances and for the angles,

$$s_{n-1} = \sqrt{\frac{\sum_{i=1}^N (CV - EV)^2}{N - 1}}$$
, where CV means calculated value, EV experimental value (X-ray data), and N is the number of distances or angles taken into account.

	BP86
Distances	0.032
Angles	1.399

Complete ref 18:

Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Montgomery, J. A., Jr.; Vreven, T.; Kudin, K. N.; Burant, J. C.; Millam, J. M.; Iyengar, S. S.; Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, G.; Rega, N.; Petersson, G. A.; Nakatsuji, H.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Klene, M.; Li, X.; Knox, J. E.; Hratchian, H. P.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Ayala, P. Y.; Morokuma, K.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Zakrzewski, V. G.; Dapprich, S.; Daniels, A. D.; Strain, M. C.; Farkas, O.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Ortiz, J. V.; Cui, Q.; Baboul, A. G.; Clifford, S.; Cioslowski, J.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; Gonzalez, C.; Pople, J. A. *Gaussian 03*, revision C.02; Gaussian, Inc.: Wallingford, CT, 2004.