

## Supplementary Material

### Theoretical Investigation of Catalytic Oxidation of Benzylalcohol by Au, Cu and Au-Cu nanoclusters

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### Single point reaction energy profiles with SDD basis set :

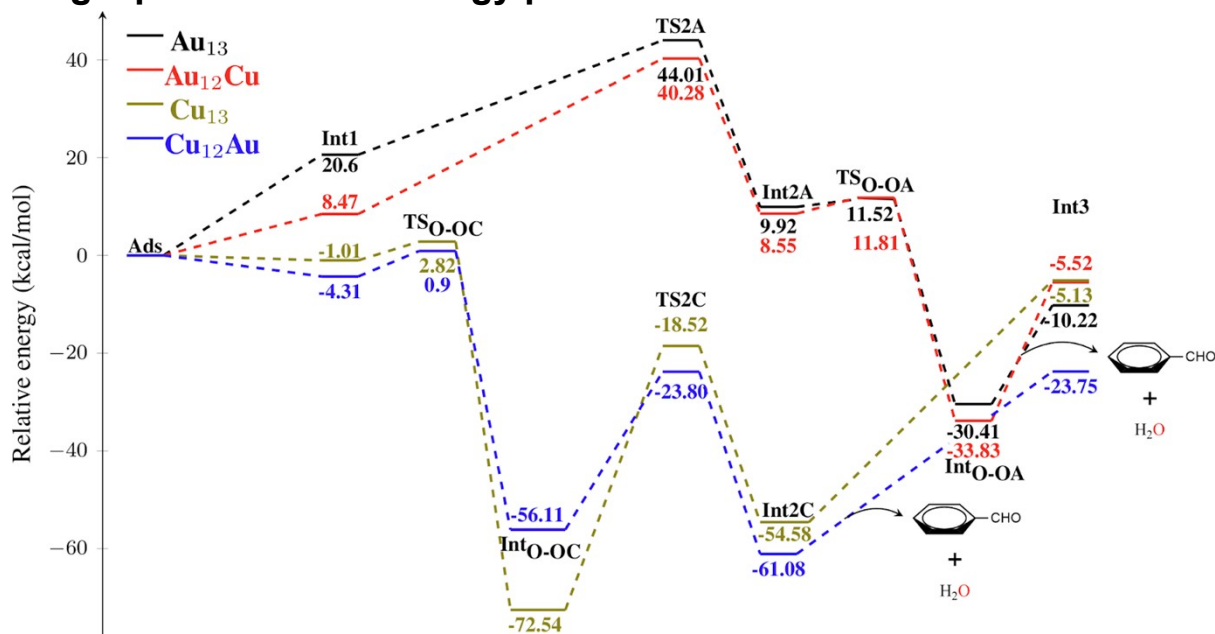


Fig S1 : Reaction energy profile of first benzyl alcohol oxidation to benzaldehyde.

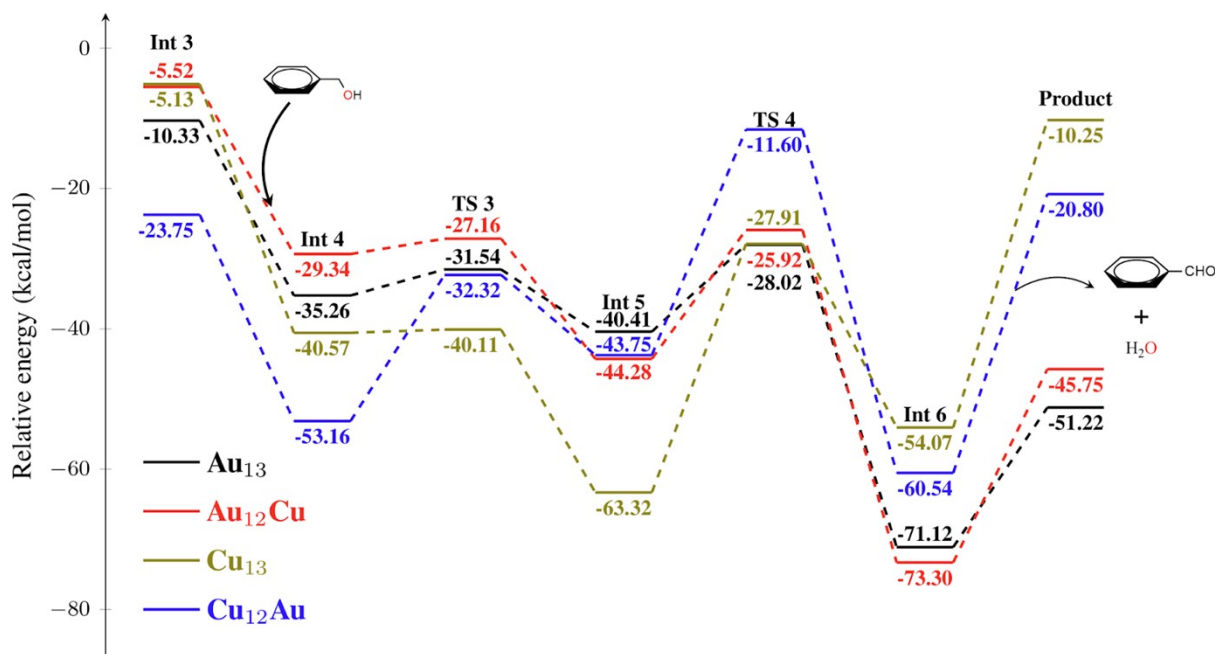


Fig S2 : Reaction energy profile of second benzyl alcohol oxidation to benzaldehyde.



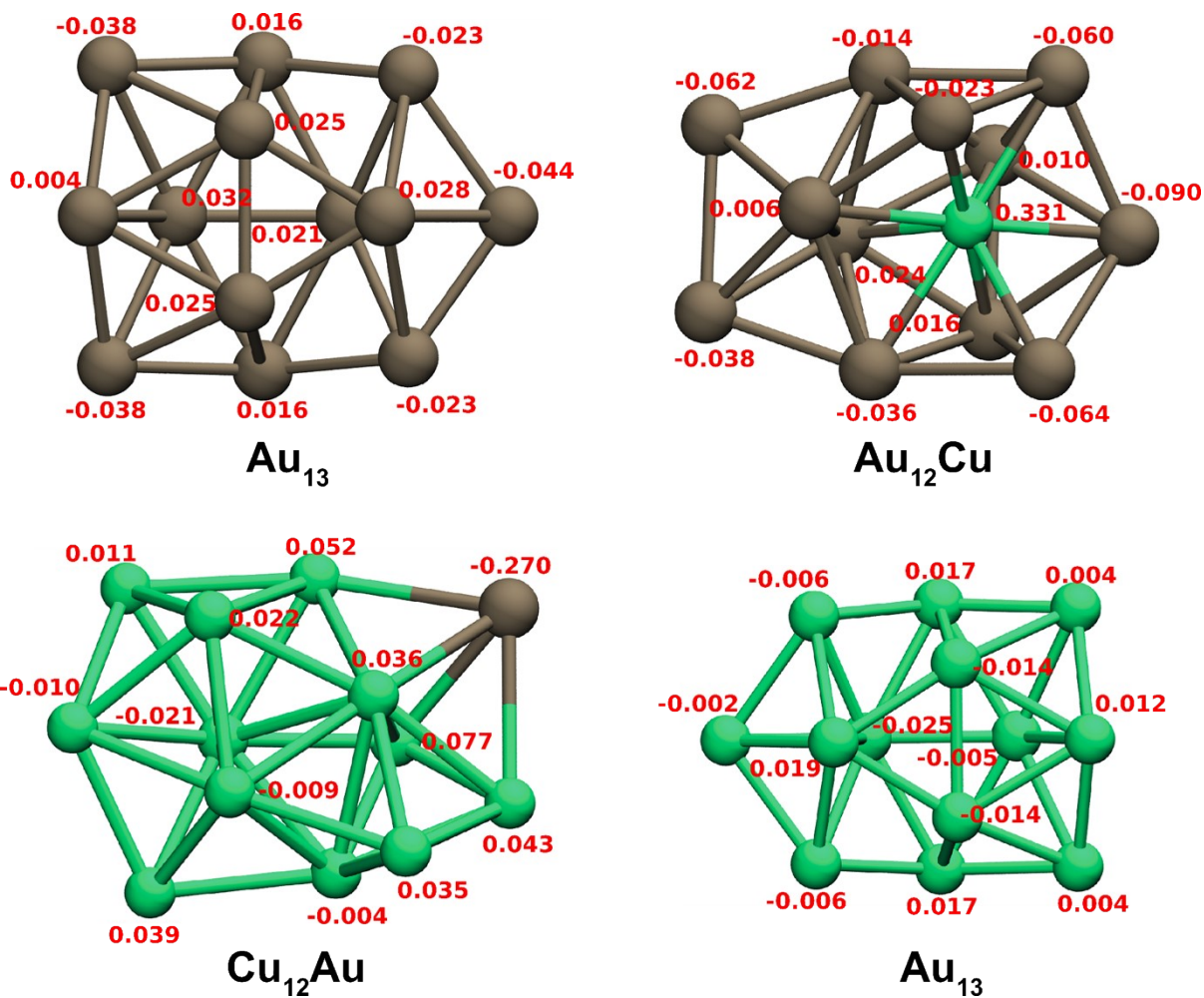


Fig S5 : Hirshfeld charge analysis of the 4 catalysts indicate higher negative charge transfer to Au atom(s) from Cu atom(s).

## Hirshfeld Charges of the O<sub>2</sub>-adsorbed clusters

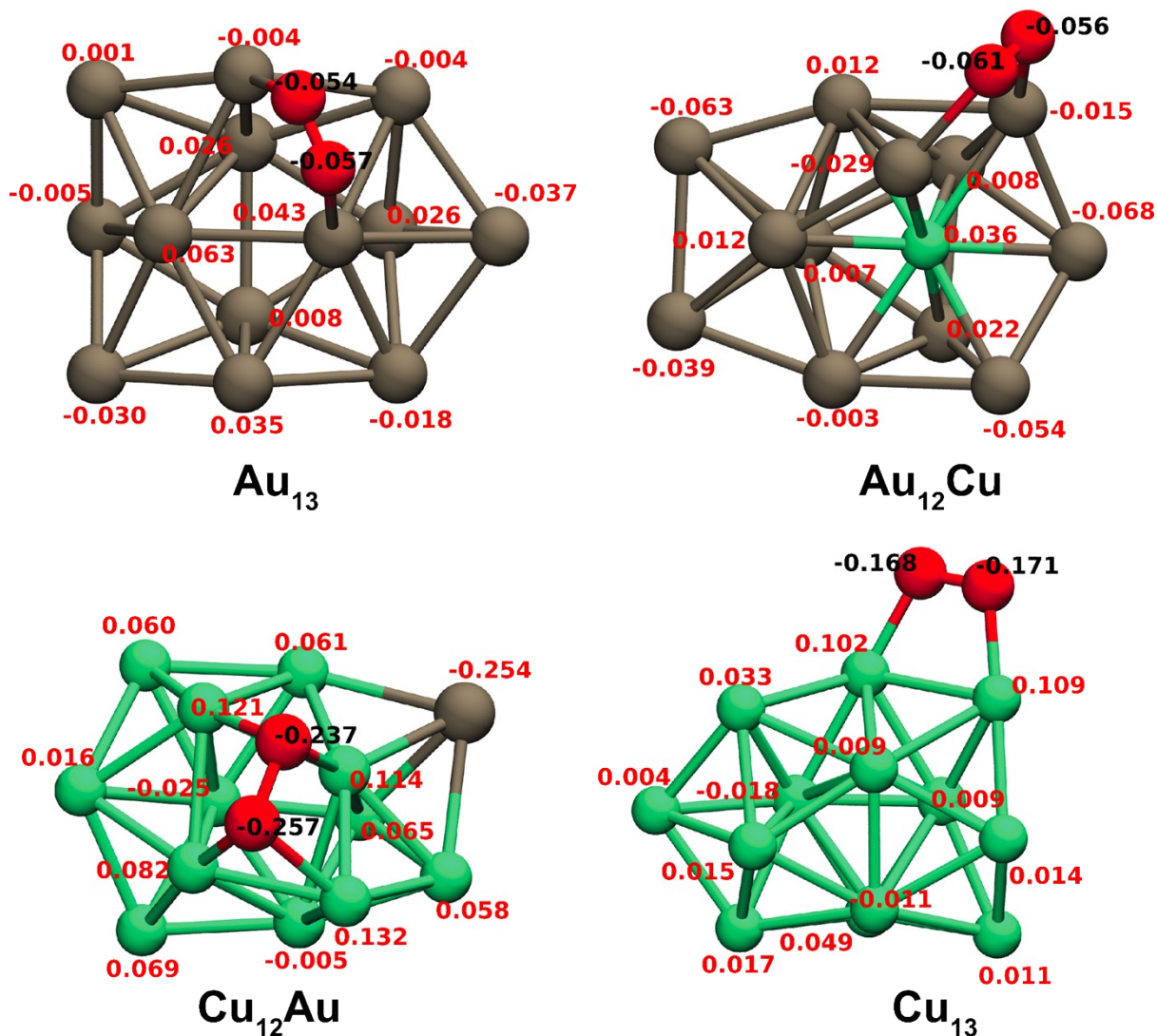
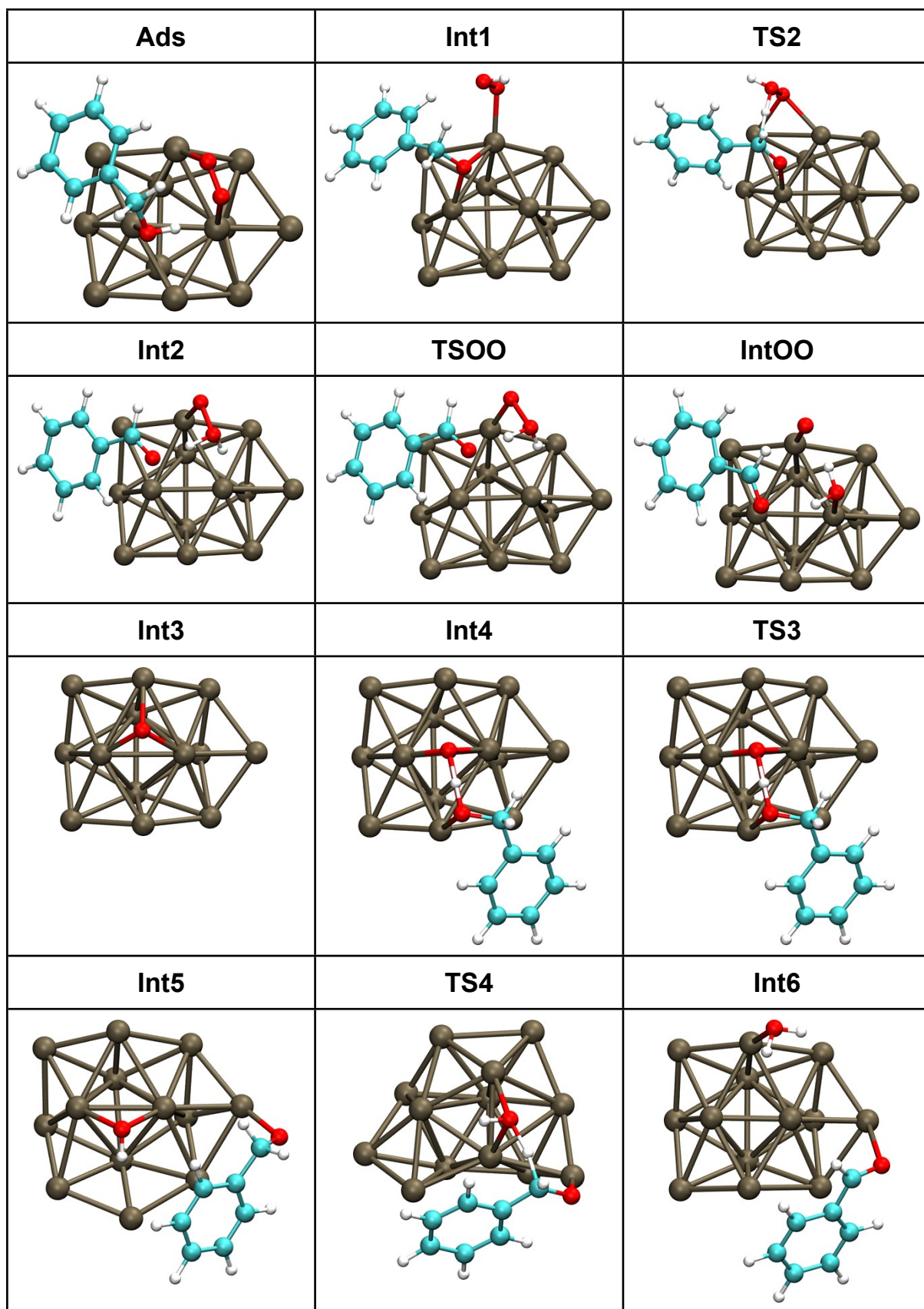


Fig S6 : Hirshfeld charge analysis of the O<sub>2</sub> adsorbed catalysts indicate higher activation of O<sub>2</sub> over Cu-rich clusters due to enhanced charge metal to oxygen charge transfer.

Table S1 : Structures of all steps in the reaction with Au<sub>13</sub> as the catalyst



**Cartesian Coordinates of all , reactants intermediates and products of all clusters :**

## Au<sub>13</sub> cluster

### Cluster

Au	1.19691900	0.00001900	-1.17009800
Au	-2.73140100	2.46469300	-0.15152900
Au	-1.58009000	0.00003700	-1.22973600
Au	-0.16931000	2.53596900	-1.34180700
Au	-2.73142600	-2.46469200	-0.15153100
Au	-3.04798800	-0.00000100	1.16421600
Au	-0.46658500	1.42124900	1.23019400
Au	-0.16937500	-2.53582100	-1.34192700
Au	2.22562600	-2.32379700	0.11395400
Au	3.87021600	-0.00005500	-0.22952100
Au	2.22571100	2.32373800	0.11398000
Au	1.84431100	-0.00004100	1.76362600
Au	-0.46660800	-1.42129700	1.23017800

## Au<sub>13</sub>-O<sub>2</sub>

Au	1.26224100	0.00415300	1.15830900
Au	-2.80588000	-2.36679300	0.34358200
Au	-1.57682300	0.07147600	1.16111700
Au	-0.21797500	-2.37208100	1.55179800
Au	-2.79985900	2.34176600	0.03896900
Au	-2.98282100	-0.11217900	-1.33925400
Au	-0.50165600	-1.56378300	-1.17837900
Au	-0.21427300	2.71559300	1.10066100
Au	2.21840300	2.21693300	-0.34932700
Au	3.89134600	-0.08057700	0.06483800
Au	2.15370100	-2.38878900	-0.08072500
Au	1.79618100	-0.18494300	-1.82220900
Au	-0.46559400	1.31645900	-1.30717800
O	1.44628000	1.40727300	3.28410600
O	0.95342900	2.57003400	3.21166500

## Ads.

Au	-1.22376800	-0.39202700	1.16386100
Au	1.89369400	3.09859700	0.21200600
Au	1.55344900	0.33536900	0.81498400
Au	-0.39769200	2.27512800	1.71104900
Au	3.04255300	-1.42950500	-0.87997800
Au	2.41775300	1.15473200	-1.76644800
Au	-0.32107900	1.82881900	-1.10023600
Au	0.84578800	-2.57722600	0.53275300
Au	-1.80706700	-2.59244300	-0.53361900
Au	-3.93422900	-0.92385100	0.41559200
Au	-2.90450400	1.73687000	0.46186000
Au	-2.25547600	-0.02496000	-1.70332300
Au	0.37103900	-0.89823100	-1.64492000
O	-0.45306300	-1.81418700	3.14895800
O	0.29524900	-2.81987900	2.84799700
C	5.17224100	-2.41629200	0.74868600

C	4.34128100	-3.30092800	1.44292100
C	3.52578400	-2.83048200	2.47063900
C	3.53322900	-1.47676800	2.82433500
C	4.37742500	-0.59704400	2.13424100
C	5.19107300	-1.05920800	1.10124300
H	5.82314300	-2.78226100	-0.04070700
H	4.32172100	-4.35261200	1.17283100
H	2.86628700	-3.51345900	3.00187800
H	4.38674900	0.45732700	2.40493900
H	5.84249500	-0.36932500	0.57238200
C	2.64837200	-0.95687800	3.92131200
H	3.25689600	-0.48030600	4.69947600
H	2.09628800	-1.78132700	4.38430100
O	1.74008500	0.04581900	3.44400700
H	0.85532700	-0.35701500	3.41389000

### Int1

Au	-1.20673000	-0.37258000	1.01994700
Au	1.66007200	3.25006600	0.19557600
Au	1.58884300	0.56987100	1.00053100
Au	-0.64635600	2.31402000	1.72951100
Au	3.05001900	-1.32093000	-0.89238200
Au	2.34712100	1.22703800	-1.64417000
Au	-0.45993000	1.80801800	-1.05378000
Au	0.77465100	-2.39312500	0.89680100
Au	-1.66457800	-2.66095800	-0.50423800
Au	-3.92601800	-1.13904600	0.35220000
Au	-3.10379600	1.56541200	0.58719400
Au	-2.30270300	-0.11362400	-1.76319900
Au	0.39953400	-0.88381700	-1.53068200
O	2.00610600	-4.38335100	2.77912800
O	1.35032400	-4.41636200	1.54856000
C	5.99376600	-1.24534800	0.01369100
C	5.20147500	-2.38777600	0.21370000
C	4.27375700	-2.42173400	1.26948600
C	4.11603900	-1.30785400	2.11126000
C	4.91843900	-0.18475400	1.89769800
C	5.85380300	-0.15130300	0.86194400
H	6.71498600	-1.22427400	-0.79747100
H	5.34415100	-3.26718700	-0.40872800
H	3.67195200	-3.31274100	1.43927900
H	4.79609700	0.68037700	2.54736000
H	6.46503300	0.73357900	0.71178800
C	3.01967800	-1.28684200	3.14018600
H	3.26721300	-0.55254600	3.92588700
H	2.95308400	-2.27676100	3.62381700
O	1.75810000	-0.99825500	2.60252000
H	1.30928800	-4.66035900	3.39714200

### TS2<sub>A</sub>

Au	1.27807800	-0.37278400	-1.16243200
Au	-1.72649200	3.14870600	0.00958000

Au	-1.44881700	0.47024200	-0.88240800
Au	0.54175000	2.35078500	-1.65347700
Au	-2.90474900	-1.49070200	0.84488500
Au	-2.35661900	0.99719100	1.75984500
Au	0.47110900	1.72732700	1.11562000
Au	-0.62392700	-2.37597100	-0.97055900
Au	1.89703600	-2.65323600	0.31684900
Au	4.04103600	-1.00269100	-0.55990900
Au	3.06357900	1.65393800	-0.59081600
Au	2.43726000	-0.13451300	1.64706900
Au	-0.21867300	-0.98495300	1.54839400
O	-3.50618000	-3.78568300	-1.52428500
O	-2.60642800	-3.56248600	-0.33712000
C	-7.19045100	-0.20352900	-0.63730000
C	-7.20511800	-1.29279400	-1.51352800
C	-6.05490300	-1.64990700	-2.20057500
C	-4.85276400	-0.92997000	-2.03178700
C	-4.86318800	0.17899500	-1.16539700
C	-6.01730500	0.53295700	-0.47667600
H	-8.09039500	0.07523500	-0.09769500
H	-8.12101200	-1.85819200	-1.66194200
H	-6.07301300	-2.49076400	-2.89586500
H	-3.96447100	0.78291100	-1.05543100
H	-5.99903400	1.39637400	0.18356500
C	-3.64821400	-1.40757700	-2.71059800
H	-3.84286500	-1.95214100	-3.65667300
H	-3.57677600	-2.75968900	-2.02135700
O	-2.45838600	-0.89851100	-2.59809900
H	-4.36793000	-3.92304500	-1.09192100

## Int2<sub>A</sub>

Au	-1.22488800	-0.31633800	1.13384100
Au	2.08473000	2.95142000	0.19534800
Au	1.47348600	0.18794400	0.81621600
Au	-0.24546100	2.32974500	1.67581400
Au	2.86037000	-1.77430700	-0.91987000
Au	2.53379400	0.91954700	-1.70072500
Au	-0.18542900	1.80672000	-1.13578000
Au	0.62897800	-2.64326600	0.58118200
Au	-2.05393000	-2.46968600	-0.53485500
Au	-3.95162700	-0.60771200	0.55282700
Au	-2.76373800	2.00335800	0.41633000
Au	-2.29469800	0.12418100	-1.68083900
Au	0.24717000	-1.00630000	-1.64256700
O	-0.40421800	-2.71495100	3.42301600
O	0.22017700	-3.73933900	2.50980400
C	5.74491300	-0.26128400	0.97576400
C	5.65273200	-1.65438300	0.99595600
C	4.67265800	-2.26873100	1.76781900
C	3.78584500	-1.48946800	2.52401300
C	3.89525000	-0.08670900	2.51337700
C	4.87306900	0.52168100	1.73576300

H	6.49774400	0.21915400	0.35773600
H	6.33454300	-2.25407800	0.40106100
H	4.56515600	-3.35165700	1.77083900
H	3.20701600	0.49906600	3.11898600
H	4.94644900	1.60506000	1.70653700
C	2.67677500	-2.14172200	3.19940100
H	2.62108900	-3.24271400	3.11087800
H	0.43758700	-2.20165500	3.73289700
O	1.79397800	-1.52202900	3.80774700
H	-0.88842300	-2.09808000	2.80708100

### Int3<sub>A</sub>

Au	1.29735100	-0.04342400	1.23098400
Au	-2.77275600	-2.42578900	0.16265300
Au	-1.72263100	-0.05687500	1.22309900
Au	-0.18514900	-2.58623400	1.30789400
Au	-2.73539500	2.42048600	0.06823600
Au	-2.97783900	-0.00999700	-1.28799600
Au	-0.44689600	-1.43324600	-1.23556900
Au	-0.18357600	2.68217000	1.34203100
Au	2.19244000	2.29132100	-0.16789000
Au	3.90193100	0.00704100	0.16368300
Au	2.23449600	-2.31653100	-0.07811700
Au	1.85478600	-0.02473900	-1.78666100
Au	-0.43467200	1.41368700	-1.20422000
O	-0.21813900	0.81105700	2.58600800

### TS<sub>O-OA</sub>

Au	-1.22164500	-0.34487700	1.09967000
Au	2.04431900	2.98319400	0.25270200
Au	1.47476600	0.19485600	0.82543600
Au	-0.27714200	2.27725300	1.74539900
Au	2.90578500	-1.68347500	-0.93426100
Au	2.51687700	1.00808800	-1.69178400
Au	-0.21538400	1.84097500	-1.09133900
Au	0.69091800	-2.64189400	0.55729100
Au	-2.00813400	-2.47973900	-0.59082500
Au	-3.94736500	-0.67076000	0.52105100
Au	-2.79683400	1.97295800	0.43962800
Au	-2.27250500	0.13659900	-1.69812200
Au	0.28230200	-0.96197000	-1.64236100
O	-0.50799700	-2.93136900	3.36766500
O	0.28229300	-3.90181100	2.26759200
C	5.62353200	-0.33863500	0.94475300
C	5.53581900	-1.73250700	0.93503200
C	4.58392300	-2.36933700	1.72562900
C	3.71533300	-1.61311600	2.52348800
C	3.81707300	-0.21007100	2.53893300
C	4.77346800	0.42146500	1.75134800
H	6.35652600	0.15882500	0.31593700
H	6.20163200	-2.31621200	0.30647000
H	4.48129200	-3.45268600	1.70798700

H	3.14655700	0.35892200	3.17944000
H	4.84440500	1.50558100	1.74855500
C	2.62454100	-2.28918800	3.21628200
H	2.59814200	-3.39177600	3.12548400
H	0.30771300	-2.43865500	3.70774500
O	1.73631500	-1.69220100	3.83052300
H	-0.96390000	-2.29805900	2.76300000

### Int<sub>o</sub>-oA

Au	1.26111200	0.37884800	1.14707100
Au	-2.15060200	-2.91002800	0.24547200
Au	-1.53506700	-0.21902000	0.78439600
Au	0.17593000	-2.22581500	1.78353600
Au	-2.95253200	1.58556300	-0.89084300
Au	-2.43893300	-1.03285800	-1.84277100
Au	0.19735600	-1.88840700	-1.09685400
Au	-0.68007600	2.61617400	0.60258900
Au	2.00713000	2.46467100	-0.66542600
Au	4.02285500	0.66763200	0.37470100
Au	2.74354200	-1.90917300	0.53067000
Au	2.22913700	-0.16303900	-1.66860400
Au	-0.30232900	0.95408200	-1.61746200
O	1.14624700	1.68764400	3.22949500
O	-0.47106900	3.73691100	2.30119400
C	-5.50796400	1.53585700	0.99554600
C	-4.92157000	2.77727900	1.26700400
C	-3.84642700	2.85665100	2.14953400
C	-3.34894200	1.69283300	2.74434600
C	-3.94790800	0.44970700	2.47941200
C	-5.02970500	0.37445500	1.61034700
H	-6.34772900	1.47572100	0.30841700
H	-5.30467900	3.67481200	0.79025500
H	-3.34860900	3.80511900	2.34459600
H	-3.54459200	-0.43636600	2.96579700
H	-5.48685000	-0.58607900	1.39061900
C	-2.12285300	1.76597200	3.55006200
H	-1.74822300	2.79559700	3.74812700
H	0.47682000	1.21353700	3.74983200
O	-1.50512500	0.78213900	3.93601500
H	0.67147500	2.51578900	2.95953100

### Int4

Au	-1.21564500	-0.42180600	1.00745000
Au	1.76174000	3.16251700	-0.43673200
Au	1.55617200	0.79394300	1.10991100
Au	-0.77023300	2.52063700	0.67832300
Au	3.59114000	-1.21693200	0.64438600
Au	3.01128700	0.75649200	-1.27578700
Au	0.13142400	1.07904600	-1.54555200
Au	1.13211800	-2.08579600	1.83980500
Au	-0.87702700	-3.18169300	0.13216600

Au	-3.39767600	-1.72420300	-0.10464000
Au	-2.74210300	0.98016600	-0.90321900
Au	-1.27252600	-1.25232700	-1.92580500
Au	1.28523300	-1.54493700	-0.97155800
O	0.20687900	-0.06676700	2.64233600
C	-2.48321100	3.85108800	1.96348900
C	-3.12133500	4.45951700	0.87122200
C	-4.24248900	3.86467900	0.29920100
C	-4.74537700	2.67776800	0.83884100
C	-4.11856900	2.07312500	1.92903300
C	-2.97413700	2.63727500	2.49411200
H	-1.65134100	4.34361700	2.46369700
H	-2.73464500	5.39526300	0.47844600
H	-4.73016600	4.32449100	-0.55486100
H	-5.62122800	2.20959300	0.39676600
H	-4.49256100	1.12596800	2.31274800
C	-2.23144800	1.96658600	3.62038800
H	-2.42300900	0.88374700	3.58325700
H	-2.62712300	2.32701300	4.58263700
O	-0.85087500	2.24877000	3.56600200
H	-0.38702100	1.41066600	3.32185800

### TS3

Au	-1.06176000	-0.78356000	1.12158000
Au	1.43343600	3.38545900	-0.37433100
Au	1.46342600	0.86752600	1.18239700
Au	-0.93547300	2.53592000	0.78895600
Au	3.71721700	-0.82736400	0.66213000
Au	2.91890300	1.14293300	-1.17355900
Au	-0.01242900	1.21706500	-1.48337000
Au	1.46195600	-2.21037700	1.58987900
Au	-0.47928800	-3.33278800	-0.09834100
Au	-3.14612100	-2.13646600	-0.06743800
Au	-2.81479500	0.70630500	-0.60778500
Au	-1.20063300	-1.21430400	-1.88883600
Au	1.42920800	-1.29907300	-1.07730700
O	0.01730400	0.22819100	2.67458300
C	-3.45879000	3.65708800	1.69715600
C	-4.17654100	4.28814300	0.68054900
C	-5.14118900	3.58583700	-0.03673900
C	-5.40350100	2.25263900	0.27917700
C	-4.69408700	1.62176600	1.30694600
C	-3.70202700	2.31305600	2.01893900
H	-2.70931800	4.20391600	2.26583700
H	-3.97561900	5.32953800	0.44657500
H	-5.69000400	4.07232100	-0.83731500
H	-6.15871600	1.69719400	-0.27028700
H	-4.90374500	0.58318800	1.55769000
C	-2.85788600	1.61878900	3.05271000
H	-2.90222000	0.52902200	2.87027600
H	-3.28252800	1.78809100	4.05611500
O	-1.52927800	2.08619900	3.02799000

H	-0.79600500	1.20696300	2.95425500
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## Int5

Au	-0.86457000	-0.72241000	1.04352600
Au	1.33703400	3.29677400	0.21937800
Au	1.78596000	0.60000700	1.38013500
Au	-1.43946400	3.15984200	0.27044300
Au	3.89810500	-0.87602200	0.43468700
Au	2.89908100	1.35873100	-1.08886900
Au	0.00880700	1.30181400	-1.22753500
Au	1.70429300	-2.39809400	1.36159500
Au	-0.53260400	-3.22899500	-0.14270200
Au	-3.09890100	-2.04662700	-0.02699400
Au	-2.75935200	0.85269500	-0.66801800
Au	-1.21290400	-1.11631000	-1.92669300
Au	1.45703900	-1.13537500	-1.12335400
O	-0.12018100	0.73903400	2.53975200
C	-3.62545000	1.40759900	2.78052800
C	-3.44272300	2.77964500	2.60827400
C	-4.05202400	3.44569600	1.53725100
C	-4.82972000	2.72143800	0.62821400
C	-4.99993500	1.34252000	0.79481400
C	-4.41602300	0.67570400	1.89022900
H	-3.14304000	0.89514900	3.61063000
H	-2.82938400	3.33661800	3.31239100
H	-3.93897100	4.52104900	1.42574800
H	-5.30232300	3.22778400	-0.20862100
H	-5.62815600	0.76501900	0.11943100
C	-4.68203400	-0.79501100	2.10722700
H	-5.59915000	-0.86095100	2.72683600
H	-3.88070100	-1.20797300	2.74884700
O	-4.91888100	-1.53366300	0.96350500
H	-0.49780700	1.57847400	2.21707600

## TS4

Au	-1.63911900	-0.16956400	1.44580000
Au	3.99421800	-0.53422000	-0.36996300
Au	1.51570500	-0.29225200	1.26683500
Au	2.88912300	1.95576900	0.31019700
Au	0.04818900	-2.59448300	1.59876100
Au	2.07658600	-2.51711400	-0.43578600
Au	1.60231500	0.19571600	-1.70647600
Au	-2.67600000	-2.64369400	0.51919000
Au	-3.26908300	-0.33009600	-0.95472200
Au	-2.77004500	2.23904000	-0.27996800
Au	0.09145600	1.89125400	0.20431200
Au	-1.04885100	0.96607700	-2.21557000
Au	-0.53776000	-1.42638600	-0.91428200
O	-1.71859300	1.26181100	3.11449000
C	0.39360500	4.10958600	2.86095100
C	1.71253300	4.42838200	2.56392300
C	2.06758300	4.82965600	1.27059500

C	1.08592100	4.92067300	0.28225300
C	-0.24140500	4.59214300	0.57738600
C	-0.60517300	4.18097900	1.87565300
H	0.12116400	3.80293300	3.86972600
H	2.47212600	4.36400300	3.33787800
H	3.09589000	5.10047200	1.04535200
H	1.34788400	5.24940700	-0.71968100
H	-1.02228600	4.70323500	-0.17181700
C	-2.01848100	3.80466900	2.20599900
H	-2.37496600	4.32336600	3.11634000
H	-1.93683000	2.67302000	2.62597900
O	-2.92497700	3.84121900	1.22400400
H	-0.78396900	1.29909900	3.36988300

### Int6

Au	-1.02505200	-0.50463500	0.93597600
Au	1.70112600	3.25182500	-0.00354900
Au	1.52302300	0.57666900	1.20813300
Au	-0.70792100	2.30413300	1.14572800
Au	3.66508000	-1.16509000	0.54522100
Au	3.05448800	1.04046900	-1.13815600
Au	0.18386000	1.32131600	-1.42218700
Au	1.26803600	-2.35477900	1.44493700
Au	-0.93108300	-3.10927900	-0.19833500
Au	-3.37264500	-1.58119300	-0.17792500
Au	-2.67204600	1.16469900	-0.85618100
Au	-1.28984900	-0.94937500	-2.02572400
Au	1.31583500	-1.32141800	-1.12356500
O	0.33394900	-3.04658100	3.68739800
C	-3.00345500	2.82021500	2.62754700
C	-2.69803600	4.03949100	2.00542200
C	-3.35048000	4.39343800	0.81747400
C	-4.27509900	3.52505700	0.23821500
C	-4.56584100	2.29899500	0.84681400
C	-3.94331800	1.95070100	2.05669100
H	-2.53131300	2.55014300	3.57094100
H	-1.99701300	4.72693400	2.46990000
H	-3.12038500	5.33995600	0.33895300
H	-4.77548000	3.80080700	-0.68524600
H	-5.30348300	1.61674500	0.43126200
C	-4.18934700	0.63859700	2.66626200
H	-3.65631900	0.47062600	3.63261700
O	-4.88723700	-0.22932700	2.17159800
H	0.17752500	-2.16542500	4.04737200
H	-0.52896400	-3.32539000	3.35641700

### Au<sub>12</sub>Cu Cluster

Au	-1.73383900	0.25243300	1.45042400
Au	-0.71305600	-2.36660600	0.70349500
Au	-1.17892100	-0.41101100	-1.45922900

Au	-3.32251700	-1.53752400	0.06381800
Au	2.03943200	-2.27906900	1.27191500
Au	3.37407000	-0.25437000	-0.17051500
Au	1.22534700	-1.88369700	-1.41883100
Au	1.29474800	0.83081700	-2.04998700
Au	-3.23917300	1.36707900	-0.71079100
Au	0.34067000	1.74870900	2.35162800
Au	2.21936600	2.29207800	0.18471400
Au	-0.59828800	2.25387100	-0.38821800
Cu	0.79588500	-0.03462800	0.46740300

### **Au<sub>12</sub>Cu-O<sub>2</sub>**

Au	-1.66754400	0.52069400	1.42180000
Au	-0.95386200	-2.17763600	0.99855600
Au	-1.31438000	-0.49713400	-1.44795600
Au	-3.50868900	-1.19568100	0.29080100
Au	1.86534100	-2.33974900	1.43838400
Au	3.27669600	-0.66735400	-0.32076600
Au	0.87157600	-2.24294700	-1.20202100
Au	1.29996000	0.38615300	-2.17535900
Au	-3.19514900	1.49705500	-0.85929600
Au	0.54261400	1.88017700	2.16402400
Au	2.47095200	1.98705700	-0.21142600
Au	-0.46817600	2.15059700	-0.61844100
Cu	0.75994600	-0.11124500	0.41276500
O	2.16633400	3.56499600	2.38337500
O	2.78790700	3.73860000	1.27213600

### **Ads**

Au	1.67334200	-0.56317000	1.52593500
Au	1.92432700	2.04055600	0.45766400
Au	1.36694000	-0.21916400	-1.47640700
Au	3.86902800	0.08461700	-0.02214300
Au	-0.54419500	3.35629300	0.87593000
Au	-2.67429800	1.97692400	-0.34738100
Au	-0.00566700	2.20164400	-1.65075200
Au	-1.46686300	-0.20489900	-1.88560800
Au	2.54563400	-2.53510700	-0.42640700
Au	-0.75493200	-0.90092300	2.66150800
Au	-2.90643000	-0.61019300	0.53113200
Au	-0.22524800	-2.09666500	0.09172900
Cu	-0.48118200	0.66880200	0.48158100
O	-2.77267700	-1.71228000	3.46714300
O	-3.61646700	-1.70939300	2.47560400
C	-1.45735100	-2.90429500	-3.44882500
C	-2.72890300	-2.37789100	-3.19004500
C	-3.40572900	-2.70339700	-2.00853500
C	-2.81532800	-3.55054500	-1.06760600
C	-1.53971800	-4.08020800	-1.33796800
C	-0.86926600	-3.76418500	-2.52315700
H	-0.93582000	-2.64722100	-4.36557200

H	-3.20823000	-1.73193200	-3.92188000
H	-4.38566600	-2.28739300	-1.79771100
H	-1.08823700	-4.77815500	-0.63271600
H	0.12150400	-4.17042300	-2.70395100
C	-3.51306500	-3.89776800	0.21922500
H	-2.81576800	-3.73392700	1.05753500
H	-3.75805800	-4.97356400	0.21995700
O	-4.68115200	-3.12294200	0.37325600
H	-4.76624800	-2.90905800	1.31120700

## Int1

Au	1.52932700	-0.66954700	1.53242600
Au	1.87182200	2.01890000	0.68554400
Au	1.47377100	-0.10467700	-1.44851500
Au	3.84439800	0.11828900	0.21927800
Au	-0.60720300	3.33999300	0.98448600
Au	-2.66261900	1.98793100	-0.39013500
Au	0.10551900	2.32509100	-1.53814200
Au	-1.31710300	-0.06999000	-2.02512700
Au	2.65425300	-2.45896600	-0.50109100
Au	-1.01753000	-1.12463700	2.40070900
Au	-2.98996400	-0.62018000	0.22852000
Au	-0.17339800	-2.11990900	-0.15953000
Cu	-0.52432200	0.64065100	0.44786800
O	-2.58732800	-1.80552400	3.92318000
O	-3.77762800	-2.24825600	3.54398500
C	-1.69828400	-3.26186200	-3.41168200
C	-2.95048600	-2.75429900	-3.05061000
C	-3.43292300	-2.91799700	-1.75361500
C	-2.67025500	-3.58269400	-0.78524900
C	-1.42882600	-4.12928200	-1.16773100
C	-0.94731500	-3.96852800	-2.47720900
H	-1.31998700	-3.11896700	-4.41920600
H	-3.55216900	-2.22452500	-3.78465100
H	-4.39616600	-2.50404100	-1.46570500
H	-0.87054500	-4.73695900	-0.45487400
H	0.02096800	-4.38125800	-2.74540200
C	-3.14113200	-3.65526600	0.64652700
H	-2.26133000	-3.88565600	1.28195700
H	-3.82814400	-4.51399600	0.75340800
O	-3.80851600	-2.49835300	1.06277300
H	-3.77465800	-2.33847800	2.51891200

## TS2

Au	-1.37146000	0.95188000	1.38993500
Au	-1.85931600	-1.82718600	1.12188900
Au	-1.61555400	-0.19656800	-1.40365300
Au	-3.82478700	0.02686500	0.44563600
Au	0.70719800	-3.03241400	1.49519700
Au	2.59901900	-2.07253500	-0.33345700
Au	-0.29617200	-2.66994900	-1.11864400
Au	1.05307500	-0.46396900	-2.27453000

Au	-2.59607700	2.34960900	-0.87285500
Au	1.27213500	1.25856200	2.02518700
Au	3.02948600	0.61227400	-0.58975300
Au	0.27063400	1.94412400	-0.67166200
Cu	0.53136200	-0.59585800	0.33870500
O	2.97498500	1.73226700	3.30162000
O	4.21538600	1.76141000	2.50141000
C	0.30420100	5.23277900	-0.05932700
C	0.84756500	4.50955000	-1.12873000
C	2.08382300	3.85802500	-0.98252400
C	2.80637200	3.96340300	0.23083100
C	2.25361800	4.71776700	1.27750600
C	1.01366000	5.33273200	1.13670200
H	-0.66051800	5.71794700	-0.17049500
H	0.34180300	4.49620600	-2.09115400
H	2.55690300	3.36257700	-1.82772100
H	2.79631600	4.79743600	2.21747400
H	0.59631200	5.89494100	1.96671000
C	4.09581400	3.28329500	0.37640100
H	4.07037500	2.51889800	1.61813200
H	4.91337200	3.90375200	0.78853100
O	4.46263800	2.34873700	-0.47026000
H	4.23529900	0.88881300	2.05892200

## Int2

Au	1.67532800	-0.25588300	1.30078500
Au	0.28534500	2.22336100	1.08761000
Au	1.22652700	1.00602200	-1.47915100
Au	3.01164400	2.14371500	0.35448500
Au	-2.49136600	1.69433200	1.23170600
Au	-3.31517800	-0.15955600	-0.71543800
Au	-1.38353800	2.07799300	-1.34747200
Au	-0.96184400	-0.44981200	-2.53679000
Au	3.50055500	-0.56068400	-0.79532400
Au	-0.64926100	-0.26703500	2.65408300
Au	-1.70916100	-2.47540400	-0.69239300
Au	1.05086900	-1.91865800	-1.01067900
Cu	-0.74757000	-0.09411300	0.06422600
O	-2.64861400	-0.80341600	3.54544600
O	-3.40256300	-1.53304700	2.47469800
C	3.07169000	-4.34091000	1.07106700
C	1.92245700	-4.73197200	0.38181200
C	0.66525100	-4.43153300	0.89932400
C	0.55977500	-3.73675500	2.11532000
C	1.72291800	-3.35659600	2.80539300
C	2.97350000	-3.65485200	2.28374700
H	4.04997800	-4.56667200	0.65684500
H	2.00700800	-5.26868200	-0.55843700
H	-0.24293500	-4.73616000	0.38434300
H	1.62739500	-2.79810600	3.73512400
H	3.87159100	-3.34493700	2.80856800
C	-0.72917900	-3.33101300	2.63620400

H	-2.83875000	-2.38130700	2.31299500
H	-0.73474600	-2.87478900	3.64359100
O	-1.80073400	-3.46907300	2.01462500
H	-3.31697500	-0.96688600	1.65667600

### TS<sub>0-OA</sub>

Au	-1.66502000	0.44672100	1.27160800
Au	-0.36779200	-2.09417100	1.30065600
Au	-1.26245700	-1.14017100	-1.38263200
Au	-3.09507900	-1.97952100	0.58711800
Au	2.42463600	-1.60108500	1.42203000
Au	3.30957900	-0.06575800	-0.76276100
Au	1.31899200	-2.28513400	-1.11931000
Au	1.00605300	0.15146800	-2.56604200
Au	-3.50093700	0.55988000	-0.86242300
Au	0.69311900	0.67581400	2.56003700
Au	1.78011000	2.30149000	-0.83102700
Au	-1.00259700	1.78241500	-1.23026300
Cu	0.73433800	0.02752700	0.04125200
O	2.48495900	1.40243600	3.49745200
O	3.56964400	1.79260400	2.26492900
C	-2.97157500	4.28689200	0.75545200
C	-1.90110800	4.62400400	-0.07620300
C	-0.59396400	4.48411400	0.38140000
C	-0.35691100	4.01141000	1.68191700
C	-1.44022200	3.69377300	2.51633000
C	-2.74259200	3.82310500	2.05196500
H	-3.98897700	4.37870000	0.38636600
H	-2.08794600	4.99280900	-1.08065900
H	0.25382000	4.74605300	-0.24767400
H	-1.24224100	3.30545400	3.51418100
H	-3.57842900	3.55326300	2.68998600
C	0.99043900	3.74258000	2.15135600
H	3.10057500	2.61618400	1.92884000
H	1.10194100	3.48042300	3.21878100
O	1.99664300	3.76046200	1.41870900
H	3.38098300	1.08563100	1.59965100

### Int<sub>0-OA</sub>

Au	-1.54567500	-0.14679800	1.59561500
Au	-0.82390200	-2.24546000	-0.18100800
Au	-1.73798500	0.21915000	-1.47075000
Au	-3.54029700	-1.44273300	-0.03889100
Au	2.18017900	-2.19466900	-0.33456600
Au	3.00465300	0.29903600	-1.29894500
Au	0.66808800	-1.09654600	-2.37966400
Au	0.56085800	1.78519900	-1.97982800
Au	-3.54551900	1.43338000	0.47780100
Au	0.65523200	-1.62683700	2.22561300
Au	2.00993900	2.34333200	0.31781300
Au	-0.88426600	2.32298200	0.43896300

Cu	0.64584300	0.03137900	0.04701300
O	2.07680700	-2.58392200	3.36577200
O	3.56614100	-3.28689000	1.21384200
C	1.85922300	3.29698900	3.45639200
C	2.97285400	3.27174800	2.60012900
C	3.63740100	2.05984800	2.35544500
C	3.18935400	0.88417900	2.98553100
C	2.09943000	0.93311200	3.86193300
C	1.42808900	2.13327900	4.08632500
H	1.34086200	4.23544500	3.63022400
H	3.35106300	4.19566000	2.17012600
H	4.52213000	2.01376500	1.72571900
H	1.77750800	0.01255300	4.34786500
H	0.56710600	2.15860300	4.74675200
C	3.79414200	-0.41455700	2.67075300
H	4.26580800	-2.61837200	1.31048700
H	3.41659200	-1.26547000	3.29463700
O	4.60814500	-0.60269400	1.77745000
H	3.03477400	-3.19448900	2.05525900

### Int3

Au	-1.72941100	0.24063500	1.45158300
Au	-0.70064600	-2.31459700	0.80871800
Au	-1.20087800	-0.37863200	-1.48576100
Au	-3.31178900	-1.57574700	0.12886900
Au	2.09898300	-2.24786300	1.27574500
Au	3.39634800	-0.26521000	-0.30848500
Au	1.10283700	-1.98121000	-1.36936300
Au	1.30899200	0.73116800	-2.08468000
Au	-3.28863100	1.30869900	-0.82388900
Au	0.36800100	1.70683000	2.39438200
Au	2.30803800	2.17918300	0.11956200
Au	-0.71579800	2.27115000	-0.36630400
Cu	0.78744200	-0.05714500	0.44274700
O	0.73958200	3.42239500	0.95881400

### Int4

Au	-1.51552500	0.62284300	1.58271300
Au	-1.08404000	-2.09209600	1.10681000
Au	-1.84958900	-0.42300400	-1.29843000
Au	-3.65033000	-1.03588500	0.92599000
Au	1.75787600	-1.87775400	1.22162100
Au	2.88330700	-0.92972600	-1.28942300
Au	0.27997000	-2.38695000	-1.33393500
Au	0.52877700	0.12241800	-2.70258500
Au	-3.28762500	1.76494700	-0.41105300
Au	1.14986500	0.97949100	2.09878800
Au	2.27282800	1.69876100	-1.03409500
Au	-0.59017400	2.38733100	-0.48597700
Cu	0.48214100	-0.08508900	-0.12235000
O	1.25519400	3.39835200	-0.35109500

C	4.93801600	-0.40331200	1.53132500
C	4.67353600	0.94358200	1.29177300
C	3.93056700	1.69888500	2.20244700
C	3.47362700	1.07745200	3.38229500
C	3.73830900	-0.27551700	3.62183600
C	4.46191600	-1.02010000	2.68983100
H	5.49486000	-0.98090600	0.79794900
H	5.01901500	1.41022200	0.37057600
H	2.95080100	1.67434600	4.12828300
H	3.38141100	-0.74060000	4.53632900
H	4.67058800	-2.07038700	2.87452800
C	3.56075500	3.13450200	1.93252500
H	3.86181400	3.40703200	0.91048500
H	4.10272800	3.79617000	2.62237000
O	2.16773900	3.34893700	2.11878600
H	1.76118800	3.46079000	1.20042800

### TS3

Au	-1.57787800	0.62924100	1.56078400
Au	-1.09798100	-2.06705000	1.14418100
Au	-1.84290200	-0.47252200	-1.30895000
Au	-3.68991000	-1.04895300	0.85613000
Au	1.72581100	-1.74533600	1.35369200
Au	2.87652700	-0.99507200	-1.25764100
Au	0.29909200	-2.42715000	-1.24462800
Au	0.53348900	0.04340300	-2.70005300
Au	-3.20765300	1.79811700	-0.48762800
Au	1.04009700	1.19027400	2.04401200
Au	2.31195200	1.63818200	-1.07838300
Au	-0.51363300	2.42047900	-0.45572500
Cu	0.46739000	-0.07309900	-0.11724500
O	1.41866600	3.40188900	-0.33318100
C	4.92346400	-0.62586300	1.48498200
C	4.72660500	0.73565600	1.26124000
C	4.00685900	1.51535700	2.16986500
C	3.51488400	0.90584900	3.33723600
C	3.69912200	-0.46009100	3.56127600
C	4.39543000	-1.23406100	2.62674400
H	5.46781400	-1.21964600	0.75512000
H	5.10938100	1.19590200	0.35169200
H	2.99654900	1.51482900	4.07655700
H	3.31180600	-0.91727300	4.46766400
H	4.55559300	-2.29419800	2.80570000
C	3.67203900	2.95841800	1.88833400
H	4.06425800	3.23114000	0.89489800
H	4.17195900	3.60770500	2.62294700
O	2.27708800	3.19149300	1.94863200
H	1.86806600	3.35740900	0.88635900

### Int5

Au	-1.52666100	0.03434300	1.65662500
Au	-0.91707300	-2.41247500	0.38403800

Au	-1.75756400	-0.20245200	-1.40140800
Au	-3.57173600	-1.54247800	0.37943500
Au	1.86536400	-2.17575400	0.66172700
Au	3.02134900	-0.04351000	-1.08416800
Au	0.65014900	-1.78930100	-1.87042400
Au	0.50053900	0.97105800	-2.47552800
Au	-3.52949300	1.35844300	0.14064900
Au	0.91020500	1.10878300	2.32155000
Au	2.00795700	2.35324500	-0.47026200
Au	-0.87080900	2.34464500	0.20664300
Cu	0.55088700	0.03295600	-0.00617500
O	0.64879600	4.05123000	-0.05767000
C	5.32735700	-1.78350800	0.91728000
C	5.09724000	-0.45488300	1.27424300
C	4.12037500	-0.11038400	2.21898800
C	3.38745800	-1.13236000	2.82344400
C	3.59547000	-2.47837000	2.45773000
C	4.57328500	-2.80315900	1.49776500
H	6.08605100	-2.02352600	0.17798900
H	5.67936000	0.33803900	0.80595300
H	2.64750400	-0.86626400	3.57419100
H	3.07526700	-3.27103700	2.99126100
H	4.74590700	-3.84108300	1.23002100
C	3.84201500	1.33993800	2.54819600
H	3.84990600	1.89275300	1.57741800
H	4.71750100	1.73302100	3.10136200
O	2.71736000	1.56836500	3.30467100
H	0.83848600	4.30281200	0.85774500

## TS4

Au	-1.15049000	-1.59478400	1.40987700
Au	-0.86606400	-1.68057600	-1.45654100
Au	-2.60761100	0.35944000	-0.24298000
Au	-3.35569600	-2.28390100	-0.26758300
Au	1.63939500	-0.44392500	-2.08683400
Au	0.81899400	2.76841000	0.18998900
Au	-0.58902700	1.19879500	-2.13832500
Au	-1.87368300	3.07577700	-0.19752500
Au	-1.00867700	1.22974800	2.03987000
Au	1.25501700	-2.48004300	0.18706300
Au	2.85253300	1.06148500	0.27166600
Au	1.21105400	-0.33415400	2.47394300
Cu	0.28721700	0.16491300	0.06507800
O	3.25583600	-1.02751100	2.91634100
C	5.35533000	0.71009300	-1.07558300
C	5.08433300	-0.18046800	-0.01887600
C	4.42388600	-1.40544200	-0.25833500
C	4.00149700	-1.68607100	-1.57726700
C	4.27050600	-0.78846900	-2.62455100
C	4.95218200	0.41007400	-2.37397200
H	5.88764500	1.63399600	-0.86844800
H	5.46166600	0.02971500	0.98150400

H	3.55006300	-2.65661700	-1.77129500
H	4.01845200	-1.06517300	-3.64637200
H	5.16367300	1.09785000	-3.18586500
C	4.15762400	-2.37046900	0.83828600
H	3.71836500	-1.68172200	1.83269000
H	5.08693700	-2.70982900	1.33649700
O	3.29711600	-3.35104300	0.58507500
H	3.15419700	-1.76308900	3.53744000

## Int6

Au	-1.55354200	0.11375600	1.67903700
Au	-0.80205200	-2.40614500	0.49786200
Au	-1.76912200	-0.25834600	-1.36221600
Au	-3.46528700	-1.54051300	0.60150600
Au	1.98745500	-2.42735300	0.25996800
Au	2.97988400	-0.16310300	-1.14175100
Au	0.53856400	-1.72071200	-2.03402100
Au	0.54030900	1.07596500	-2.35136300
Au	-3.55886000	1.40271800	0.06000700
Au	0.74157600	1.41293800	2.24637400
Au	1.97953200	2.35153800	-0.35386200
Au	-0.88957800	2.26055000	-0.13262500
Cu	0.62210300	-0.06638300	0.06399200
O	3.11475300	4.09951600	0.96598800
C	4.62113900	-2.53774600	2.03488500
C	4.81364200	-1.16627600	1.95771800
C	3.92226600	-0.29146300	2.59783700
C	2.85916600	-0.80617100	3.36296600
C	2.65001800	-2.17493200	3.41728800
C	3.51776600	-3.04090600	2.73666900
H	5.29698900	-3.21735500	1.52596600
H	5.63065100	-0.75438200	1.36875800
H	2.20224300	-0.11914300	3.89171800
H	1.80699500	-2.57663200	3.97112200
H	3.35130500	-4.11361600	2.78179000
C	4.06564400	1.13211300	2.37772200
H	4.93628000	1.42866500	1.75296100
O	3.28585400	2.00049600	2.79142600
H	3.26708900	3.55778800	1.76557500
H	3.98334600	4.22977300	0.57215800

## Cu<sub>12</sub>Au Cluster

Au	2.87007600	-0.86407600	-0.14755100
Cu	0.64598100	0.26296900	-0.90807600
Cu	-1.28618200	-1.17410500	-1.51612800
Cu	0.45809500	-2.06098100	0.09753100
Cu	-2.03927500	-2.65125200	0.30516600
Cu	2.19784500	1.74261400	0.32750200
Cu	-2.79387600	1.49183500	1.05622300
Cu	-1.25518200	-0.43171200	0.96033900

Cu	-0.27614700	1.86598700	1.00283400
Cu	1.10072200	-0.10088800	1.61847900
Cu	-3.36622600	-0.55774000	-0.30702900
Cu	0.43983000	2.72590000	-1.15552600
Cu	-1.64406800	1.24123600	-1.07936400

### **Cu<sub>12</sub>Au-O<sub>2</sub>**

Au	-3.01386200	-0.70659900	0.08122100
Cu	-0.75076900	0.26276400	0.87666700
Cu	1.28432300	-1.03480800	1.57422000
Cu	-0.67462300	-2.06093200	0.02466400
Cu	1.75598900	-2.78634900	0.00419800
Cu	-2.05568500	1.87079900	-0.40138500
Cu	2.75529800	1.06348400	-1.59347200
Cu	1.11788100	-0.64312900	-1.01208800
Cu	0.32215000	1.72567800	-1.17424300
Cu	-1.18918700	-0.18268000	-1.67517000
Cu	3.33751500	-0.81471300	0.04584100
Cu	-0.14912300	2.64111000	1.08150900
Cu	2.02459300	1.27884700	0.67211200
O	0.40556700	0.42692300	2.54527300
O	1.15976200	1.76548300	2.36983200

### **Ads**

Au	2.51580500	1.78145000	-0.24592600
Cu	0.82866200	0.06397900	0.76616400
Cu	-1.66452300	0.16712500	0.92974400
Cu	-0.13851300	1.62386000	-0.86865900
Cu	-2.62974400	0.91200300	-1.17258100
Cu	3.02175100	-0.90263400	0.24032400
Cu	-1.17768000	-3.14712300	-1.29000700
Cu	-0.78188900	-0.74442500	-1.32060400
Cu	1.08326600	-2.25568700	-0.56347300
Cu	1.54579000	-0.11327500	-1.73015800
Cu	-2.94325100	-1.50545900	-0.51160300
Cu	1.46390900	-2.00149400	1.89890900
Cu	-0.94924600	-2.24665000	0.95849800
O	-0.38117300	-0.08773400	2.44976000
O	-0.34197700	-1.59703400	2.76510900
C	-3.46732600	2.67102300	0.48824600
C	-2.38711800	2.71530700	1.39237700
C	-1.16569800	3.24199300	0.95701200
C	-1.00480600	3.68749200	-0.36733900
C	-2.07392500	3.59458100	-1.27580200
C	-3.31888000	3.10999800	-0.83565300
H	-4.43092300	2.29540400	0.82666600
H	-0.34270100	3.28793700	1.66609700
H	-0.06848300	4.15134200	-0.67263000
H	-1.95514700	3.94433300	-2.29676900
H	-4.17323600	3.11152800	-1.50859800
C	-2.55664300	2.22726100	2.81913700

H	-3.24139400	2.91408200	3.33831200
H	-3.07829500	1.24998800	2.79195200
O	-1.37084800	2.16950800	3.54363500
H	-0.95752600	1.29057100	3.38719100

## TS1

Au	2.43510400	1.79784100	-0.25328100
Cu	0.81459500	-0.03549700	0.76103200
Cu	-1.77169300	0.20070100	1.07758200
Cu	-0.28966900	1.68051100	-0.65509400
Cu	-2.78728200	0.95562600	-1.03153100
Cu	3.00163500	-0.88313300	-0.13590000
Cu	-1.35031700	-3.05143900	-1.27635400
Cu	-0.95073200	-0.65526600	-1.22442900
Cu	0.98840300	-2.20935100	-0.85023600
Cu	1.29471000	0.06358200	-1.80210900
Cu	-3.03450700	-1.46552100	-0.28947900
Cu	1.75104700	-2.25110800	1.49038900
Cu	-0.85043800	-2.14634100	0.97776800
O	0.59290800	-0.50121800	2.76037100
O	0.14692100	-1.94442300	2.69493000
C	-2.89336500	2.64913000	1.33577400
C	-1.52258200	2.84789700	1.55504600
C	-0.77660400	3.54985900	0.58424400
C	-1.36653500	3.91781100	-0.63463900
C	-2.73442000	3.67341000	-0.85639100
C	-3.50566500	3.09069300	0.15288800
H	-3.47227200	2.12317500	2.09111700
H	0.27112900	3.77726800	0.77574500
H	-0.77337200	4.42576900	-1.39015200
H	-3.19379700	3.98475300	-1.78991700
H	-4.57477800	2.95345700	0.01441000
C	-0.85312600	2.22503200	2.75648600
H	0.23326700	2.18068500	2.56468900
H	-1.00425700	2.84534000	3.65244700
O	-1.37636900	0.92658100	2.98059800
H	-0.50981800	0.22946900	3.03567500

## Int1

Au	2.10928700	2.15997500	-0.18660700
Cu	0.83387300	0.05415900	0.77044100
Cu	-1.75339400	-0.10294700	1.15345900
Cu	-0.55528300	1.62211600	-0.58542000
Cu	-2.92296400	0.52869600	-0.92595000
Cu	3.10511400	-0.37615500	-0.21696400
Cu	-0.85079100	-3.20817900	-1.28871200
Cu	-0.85381600	-0.77007800	-1.19967500
Cu	1.31542300	-1.98558400	-0.94801600
Cu	1.23126400	0.33340400	-1.81344900
Cu	-2.75022400	-1.92565700	-0.24329100
Cu	2.16688400	-2.01316100	1.35919600
Cu	-0.44127100	-2.26083300	0.95837000

O	0.75573400	-0.49654300	2.86044300
O	0.61293600	-1.98866800	2.69718700
C	-3.35297700	2.14442900	1.24193500
C	-2.04253200	2.59606300	1.46677700
C	-1.43757500	3.41338600	0.48794700
C	-2.07033200	3.63018300	-0.74875000
C	-3.36395000	3.12939000	-0.97600000
C	-4.02982600	2.44313700	0.04955000
H	-3.82039600	1.52885900	2.00652600
H	-0.45804700	3.84825300	0.68575800
H	-1.57030600	4.21468300	-1.51614300
H	-3.86172700	3.32418600	-1.92127300
H	-5.06040200	2.12397200	-0.08523700
C	-1.27875700	2.07357800	2.67179100
H	-0.19783400	2.24183100	2.46625300
H	-1.52135900	2.68768800	3.55876200
O	-1.58553900	0.73738200	2.90656400
H	-0.17260100	-0.18342300	3.09452600

### TS<sub>o-oc</sub>

Au	2.04371300	2.22848500	-0.19758100
Cu	0.85970600	0.08067800	0.79694700
Cu	-1.71389300	-0.16404600	1.22354600
Cu	-0.59783100	1.60028800	-0.56380800
Cu	-2.94079700	0.43475100	-0.82897100
Cu	3.13614600	-0.30472200	-0.23766800
Cu	-0.77468300	-3.23359600	-1.31249900
Cu	-0.84546800	-0.80347200	-1.17434300
Cu	1.36967500	-1.97385800	-0.94919000
Cu	1.21710100	0.34268000	-1.76873300
Cu	-2.68549100	-2.02017600	-0.18201800
Cu	2.22988800	-1.95766300	1.35286900
Cu	-0.38443200	-2.32135800	0.95170100
O	0.86459100	-0.23920200	2.84051000
O	0.67608800	-1.97109200	2.55513400
C	-3.45058600	2.07761600	1.13714900
C	-2.16450700	2.60317900	1.35509400
C	-1.59163800	3.41125500	0.35067200
C	-2.21989700	3.54699200	-0.89977800
C	-3.48198600	2.97363700	-1.12015000
C	-4.12825500	2.29535300	-0.07274100
H	-3.89447900	1.47232500	1.92371800
H	-0.63811700	3.90365400	0.54099400
H	-1.73770600	4.11870700	-1.68767600
H	-3.97723800	3.10244100	-2.07773200
H	-5.14455100	1.93078300	-0.20190200
C	-1.38870500	2.17297700	2.58731600
H	-0.31672500	2.39260000	2.38525400
H	-1.67550100	2.81622800	3.44092800
O	-1.62509500	0.83874100	2.88321600
H	-0.06794500	-0.00633400	3.10186400

## Intro-oc

Au	1.98944500	2.21231400	-0.39145600
Cu	0.73535500	-0.01697000	0.81713000
Cu	-1.75006000	-0.03487900	1.28592000
Cu	-0.58617100	1.62369300	-0.64500800
Cu	-2.93149900	0.74694900	-0.74119100
Cu	2.98950700	-0.20930900	-0.15084000
Cu	-1.26462100	-3.16206500	-1.26960900
Cu	-1.05446600	-0.75070700	-1.18179400
Cu	1.03018800	-2.10059000	-0.77402400
Cu	1.12359600	0.13416100	-1.79033400
Cu	-2.93281400	-1.77624600	0.01541000
Cu	2.31452700	-2.11756600	1.38857700
Cu	-0.73097700	-2.31258100	1.06822900
O	3.90011500	-1.07313900	1.38687800
O	0.93893100	-3.22397800	0.89060200
C	-2.80727400	2.22336100	1.84305800
C	-1.51099000	2.72251400	1.63259300
C	-1.28899400	3.56222100	0.52420300
C	-2.31977000	3.82250500	-0.39284500
C	-3.59135000	3.27515400	-0.19790100
C	-3.84523700	2.49841300	0.94250000
H	-3.00038500	1.61355100	2.72578200
H	-0.30894000	4.02043400	0.39415300
H	-2.12539100	4.44977100	-1.25761300
H	-4.39009300	3.49047900	-0.90154600
H	-4.84562200	2.12224400	1.13690600
C	-0.37781500	2.21624400	2.49524200
H	0.55359100	2.72977400	2.19612200
H	-0.57092400	2.47019000	3.55096100
O	-0.25570800	0.81867700	2.37545800
H	3.96910400	-0.45693100	2.12414600

## TS2

Au	3.41571800	-0.51842000	0.20142700
Cu	1.46442300	0.96133400	-0.62269700
Cu	-2.48042700	1.22838500	0.69535800
Cu	-0.01309100	0.04211600	-2.53513600
Cu	-0.77582500	2.01726400	-1.17231500
Cu	1.10997900	-0.57389500	1.45039500
Cu	-1.18878500	-2.00883900	-1.77741200
Cu	-0.68597100	-0.17269600	-0.14790500
Cu	-0.62814000	-2.54244800	0.63082600
Cu	1.20080200	-1.60031900	-0.85710200
Cu	-2.50826000	0.18674500	-1.73013300
Cu	-1.36741700	-0.82265100	2.36169200
Cu	-2.87494800	-1.28612400	0.25877200
O	0.03299700	0.43418300	3.05459300
O	-2.23613900	-2.36370800	1.74085300
C	-0.77389500	3.82919900	0.17584200
C	-0.13751500	3.25392400	1.30867700
C	1.24635400	3.02203900	1.24142900

C	1.97679600	3.30513700	0.07854200
C	1.33842300	3.86069900	-1.03972800
C	-0.03559900	4.15375600	-0.97827800
H	-1.82912100	4.08003600	0.25400000
H	1.75565100	2.56839800	2.09051200
H	3.04540400	3.10530000	0.05281100
H	1.90218100	4.07732600	-1.94101000
H	-0.52081100	4.66127000	-1.80847000
C	-0.96233700	2.77072000	2.43095400
H	-0.37555600	1.52709300	2.78364100
H	-0.74417900	3.23563600	3.40961900
O	-2.23974700	2.51378300	2.18785500
H	0.23660900	0.41597700	3.99913500

## Int2

Au	1.62387500	2.60320700	0.23984700
Cu	0.98472000	0.19569300	0.88078400
Cu	-1.19118900	-0.79666500	1.51435000
Cu	-0.83919500	1.45711800	-0.21261100
Cu	-2.77957900	-0.26915800	-0.32348500
Cu	3.25643900	0.38694600	-0.11291800
Cu	0.10674600	-3.19661700	-1.63886700
Cu	-0.50565000	-0.86825800	-1.09008600
Cu	1.93835100	-1.51625000	-1.06617200
Cu	1.20680900	0.79817800	-1.61061100
Cu	-1.97304500	-2.60119100	-0.20532500
Cu	2.61308300	-1.50766800	1.36783200
Cu	0.37466200	-2.58407800	0.67100500
O	-2.38640400	0.02004400	3.00869000
O	0.72314900	-1.40587500	2.16478500
C	-4.17276000	1.80326300	-1.46212900
C	-3.99872300	1.55227300	-0.07346400
C	-2.94939900	2.24975300	0.61482400
C	-2.18956900	3.22098300	-0.06660800
C	-2.35730600	3.40820400	-1.44645400
C	-3.34978600	2.68703300	-2.13597600
H	-4.96223000	1.27178600	-1.99010300
H	-2.84958900	2.12510300	1.68939500
H	-1.48536500	3.83693400	0.48831300
H	-1.73570300	4.12747800	-1.97006900
H	-3.48248100	2.84154300	-3.20223200
C	-4.86917900	0.62361100	0.63096700
H	-5.69417600	0.20502800	0.02130100
O	-4.78409800	0.33969400	1.84466700
H	-2.43812600	-0.54561800	3.78529800
H	-3.31169800	0.13931900	2.67517600

## Int3

Au	3.40708900	0.06642800	-0.10909900
Cu	1.37409200	-1.37033200	-0.73284900
Cu	-2.64347100	-0.44296800	-1.65183900
Cu	-0.12196900	-2.01380200	1.18322300

Cu	-0.99864100	-2.30075000	-1.20351700
Cu	1.22772300	1.19376500	-1.04464100
Cu	-1.14234400	0.05292000	2.15542000
Cu	-0.66233000	-0.11490800	-0.30720200
Cu	-0.42945700	2.11857100	0.92240400
Cu	1.25224300	0.27274900	1.36096600
Cu	-2.59433400	-1.39404800	0.67537900
Cu	-1.19515700	1.92830100	-1.49284500
Cu	-2.79074100	1.11140000	0.42735200
O	-2.01910400	2.82077000	0.01938700

#### Int4

Au	-1.59718700	-2.49304300	0.31355200
Cu	-0.55538400	-0.13259700	0.52270800
Cu	1.67549100	0.12751300	1.78780600
Cu	1.05680100	-2.11643700	0.68663100
Cu	3.44642200	-1.23294500	0.94807900
Cu	-2.12858600	-0.40994500	-1.37333400
Cu	2.29668400	1.89725800	-1.82234800
Cu	1.96787100	-0.35117700	-0.83811600
Cu	0.02996800	0.78365600	-1.94963600
Cu	0.03533200	-1.66111200	-1.56782100
Cu	3.41086600	1.23699400	0.33433600
Cu	-1.61385500	1.93025300	-0.56547200
Cu	0.89765000	1.97965100	0.14553500
O	0.12162900	1.23220100	1.78065700
C	-4.01976200	0.53722300	0.96332800
C	-3.15061000	1.31082500	1.73289300
C	-2.83051900	2.62248500	1.35288700
C	-3.36596200	3.12464200	0.14293900
C	-4.23899200	2.33832700	-0.62969600
C	-4.57158700	1.04750500	-0.21556100
H	-4.25062700	-0.47832000	1.27483700
H	-2.69730600	0.91787400	2.63841200
H	-3.15704200	4.15291400	-0.14956400
H	-4.64758100	2.74044200	-1.55195600
H	-5.24804800	0.44172400	-0.81180200
C	-1.93185700	3.48732400	2.21334500
H	-1.18227300	3.96222600	1.54834400
H	-2.53752800	4.30868000	2.62211500
O	-1.34692800	2.82104800	3.27939100
H	-0.70223300	2.18658500	2.87512500

#### TS3

O	1.17137600	3.05797200	-1.39521900
C	3.22965200	-2.87515400	-1.28369600
C	2.68575500	-1.80926500	-2.02071900
C	3.24690600	-0.52496300	-1.95274400
C	4.37026600	-0.32823000	-1.13553000
C	4.91410600	-1.37701300	-0.39908100
C	4.34136800	-2.65379000	-0.45447800
H	2.80819600	-3.87282200	-1.38224600

H	1.81250400	-1.97938300	-2.64808900
H	4.78764200	0.67389000	-1.08047500
H	5.77984200	-1.20307500	0.23372400
H	4.77133400	-3.47623400	0.10960300
C	2.63083000	0.62231400	-2.71682400
H	1.51909900	0.51552200	-2.63341700
H	2.85827200	0.49612600	-3.79137800
O	3.04846200	1.86117300	-2.25251300
H	2.13033700	2.52784400	-2.11054100
Au	-3.12955800	-1.36749300	-0.24885300
Cu	-1.39762000	0.18269900	0.93287500
Cu	0.55210400	-0.88509400	2.10373100
Cu	-0.56334600	-2.04401300	0.21002800
Cu	2.04772200	-2.12389600	0.56460200
Cu	-2.78918600	1.29239400	-0.79979600
Cu	2.24049100	2.06133300	-0.09639700
Cu	0.96030200	-0.09764100	-0.28583800
Cu	-0.31878800	2.00899400	-0.97009200
Cu	-1.10206900	-0.32640200	-1.59453300
Cu	2.71967600	0.21053800	1.49873300
Cu	-1.70947700	2.57126200	1.02465200
Cu	0.54970400	1.58684300	1.61625800

## Int5

Au	-0.52215700	-3.01619200	0.01423300
Cu	-0.41960500	-0.43856400	0.85957500
Cu	1.92487000	0.29419500	1.76428300
Cu	1.71382800	-1.75271700	0.27378200
Cu	3.77504800	-0.28513400	0.38462900
Cu	-2.07941900	-0.83877900	-0.90438200
Cu	1.43319800	2.73930000	-1.47059100
Cu	1.84860200	0.39048000	-0.97268100
Cu	-0.45543000	1.04539500	-1.52785700
Cu	0.24228900	-1.28268300	-1.76023300
Cu	2.98260300	2.12980500	0.34633000
Cu	-2.02835000	1.52172100	0.23891300
Cu	0.37167100	2.11430700	0.62666900
O	0.18956100	0.97046100	2.36378900
C	-5.12264200	1.69985200	-0.81764100
C	-4.72381800	0.59276400	-0.07589000
C	-4.02982400	0.74388900	1.13949500
C	-3.72187200	2.05040600	1.57614400
C	-4.10387800	3.16650700	0.80688600
C	-4.80635100	2.99002200	-0.38118500
H	-5.66965600	1.56099900	-1.74572700
H	-4.94689800	-0.41564600	-0.42230700
H	-3.22269500	2.18651600	2.53455500
H	-3.84999600	4.16528600	1.14977100
H	-5.10017000	3.85257300	-0.97084000
C	-3.49671000	-0.47556000	1.84948600
H	-3.12596500	-0.17260300	2.84584200
H	-4.32379500	-1.18703200	2.02231000

O	-2.48970000	-1.08351500	1.09823500
H	-0.04856300	1.10370100	3.28735000

#### TS4

Au	1.94493900	1.93270800	-0.31200700
Cu	0.37998800	-0.00163200	0.37224200
Cu	-1.56951000	0.57572300	1.80356100
Cu	-0.67630300	2.27345800	-0.04079300
Cu	-3.17863900	1.88781500	0.56082400
Cu	2.05794700	-0.70265300	-1.31851700
Cu	-2.89135100	-1.86073800	-1.22916100
Cu	-1.96016700	0.31622800	-0.85121300
Cu	-0.35057600	-1.51856900	-1.55285400
Cu	0.24328300	0.87277400	-1.97156400
Cu	-3.62128200	-0.54686300	0.80981200
Cu	1.00495500	-2.38097900	0.40917700
Cu	-1.42524000	-1.80930300	0.74484600
O	0.38073800	0.17111600	2.53458100
C	4.08989400	-1.95465700	-0.40319900
C	3.92204300	-0.79678100	0.36961300
C	3.26696300	-0.84275900	1.62018800
C	2.78100400	-2.08863800	2.06195700
C	2.93571500	-3.25153000	1.28410900
C	3.59301800	-3.18456800	0.04299700
H	4.63843000	-1.90273400	-1.34087000
H	4.33591300	0.15927400	0.05688800
H	2.30261800	-2.16103000	3.03835900
H	2.60108700	-4.21002900	1.67349400
H	3.71698600	-4.07938300	-0.55809100
C	3.00691300	0.41610200	2.36868600
H	1.67952400	0.37821900	2.52336100
H	3.21394700	0.33670200	3.45676800
O	3.32068700	1.54576200	1.79399200
H	0.29653400	-0.77554700	2.74943300

#### Int6

Au	-3.16280400	0.49311300	0.61637600
Cu	-0.57096000	0.46949200	0.60668700
Cu	0.66248600	-1.58188600	1.40902800
Cu	-1.68902700	-1.74720500	0.37046200
Cu	0.12139200	-3.52629500	-0.06002500
Cu	-1.63372600	2.25211900	-0.75190000
Cu	2.21148100	-0.58534600	-2.26184600
Cu	0.19481400	-1.36223500	-1.16400500
Cu	0.29778600	1.04201800	-1.80007300
Cu	-1.89809000	-0.11353000	-1.61834800
Cu	2.31833600	-2.30499500	-0.39007200
Cu	0.66566000	2.56471300	0.16867300
Cu	1.88445300	0.20222800	0.05050800
O	0.93920200	-1.91743600	3.45378300
C	2.32226800	3.80750700	1.07223400
C	2.27758900	2.68310800	1.90351800

C	3.04974400	1.52385200	1.59528700
C	3.81264500	1.52279900	0.39494600
C	3.80944500	2.63756300	-0.45005500
C	3.08972700	3.78653400	-0.11535800
H	1.79821700	4.71424100	1.36465400
H	1.70777700	2.68301100	2.82844600
H	4.44324800	0.66419700	0.16868400
H	4.39361600	2.61266000	-1.36527900
H	3.10484900	4.65387400	-0.76631400
C	3.01150100	0.35945100	2.46564500
H	3.62764500	-0.50151700	2.12709800
O	2.37938200	0.32130000	3.53905900
H	1.52281300	-1.15445000	3.69499200
H	0.10362700	-1.74700300	3.90037700

### **Cu<sub>13</sub> cluster**

#### **Cluster**

Cu	3.39584100	0.00002700	-0.27008200
Cu	1.93285400	-2.04919600	0.11728800
Cu	1.68803100	0.00001000	1.50982600
Cu	1.93277600	2.04921800	0.11728500
Cu	1.03352000	-0.00001900	-0.95545100
Cu	-0.18560300	-2.19444100	-1.20985100
Cu	-2.41746500	-2.13839400	-0.12614100
Cu	-2.57438200	0.00001900	1.12571400
Cu	-2.41747600	2.13833300	-0.12617400
Cu	-0.18564500	2.19425700	-1.21006000
Cu	-0.37362700	1.27369100	1.03414300
Cu	-0.37366900	-1.27348100	1.03413600
Cu	-1.45515500	-0.00002400	-1.04063200

### **Cu<sub>13</sub>-O<sub>2</sub>**

Cu	3.32308600	-1.05169100	-0.28048900
Cu	1.29362400	-2.39190600	0.39991800
Cu	1.81523700	-0.25598600	1.53179200
Cu	2.63971000	1.34944500	-0.17411400
Cu	1.03949600	-0.33321800	-0.91295700
Cu	-0.81156100	-1.99281400	-1.02494200
Cu	-2.89726100	-1.06397000	0.20945100
Cu	-2.27138100	1.09729900	1.23937700
Cu	-1.49451000	2.92510400	-0.27338600
Cu	0.55706400	2.07156500	-1.44457100
Cu	0.25085200	1.59010800	0.94188400
Cu	-0.57479500	-0.78463900	1.19307700
Cu	-1.31573800	0.53539800	-0.92119400
O	-2.27974700	-3.30855700	-1.20170900
O	-3.35286100	-2.83472000	-0.55223600

### **Ads**

Cu	1.69593800	2.63626500	-1.18028200
Cu	2.19835400	0.19713400	-1.19034400

Cu	1.27063700	1.29415300	0.90918300
Cu	-0.42488200	2.97451300	0.19739300
Cu	-0.13472200	0.99475600	-1.22436600
Cu	0.18762900	-1.27356400	-2.10031600
Cu	-0.90503500	-2.98541600	-0.46398500
Cu	-1.85340400	-1.65708000	1.39627000
Cu	-3.52851500	0.05996500	0.86145000
Cu	-2.46276100	1.73766400	-0.66845100
Cu	-1.13888600	0.73017400	1.19090300
Cu	0.48821000	-1.09802600	0.44076100
Cu	-1.92426500	-0.70904700	-0.88261400
O	1.47491600	-2.71988000	-1.71941500
O	1.08067300	-3.00549100	-0.30672400
C	3.20772300	-1.02849300	1.39723500
C	3.46228200	0.35273500	1.50370800
C	2.86885200	1.11246000	2.52952500
C	2.03424500	0.48080500	3.46759900
C	1.78727900	-0.88486300	3.37143100
C	2.35422900	-1.63096600	2.33207900
H	4.15204500	0.82529200	0.80683100
H	3.11925100	2.16477300	2.63780000
H	1.58154600	1.06555000	4.26213300
H	1.12720300	-1.36883500	4.08470600
H	2.14746100	-2.69514800	2.23974700
C	3.86545300	-1.83011600	0.30742500
H	3.60476400	-2.88766800	0.41604000
H	4.95588300	-1.73609200	0.39510000
O	3.50349500	-1.38833600	-1.00141400
H	2.77819600	-2.03082800	-1.35840500

## TS1

Cu	1.72794000	2.62819800	-1.17132700
Cu	2.22433500	0.19750500	-1.19121600
Cu	1.29272400	1.27565000	0.91746400
Cu	-0.38498700	2.97548200	0.21045600
Cu	-0.11112400	0.99528700	-1.22077100
Cu	0.18423900	-1.28253400	-2.09153600
Cu	-0.96734000	-2.97107600	-0.46959600
Cu	-1.87727600	-1.62797200	1.39681200
Cu	-3.52823800	0.10516200	0.84071500
Cu	-2.43417700	1.77521300	-0.67073900
Cu	-1.12623700	0.73965800	1.18805100
Cu	0.48303300	-1.11072000	0.44209900
Cu	-1.92314900	-0.67888600	-0.88836300
O	1.47031000	-2.76714700	-1.69271100
O	1.01292700	-3.05008800	-0.29410900
C	3.18377900	-1.06869300	1.38188300
C	3.45349900	0.30849800	1.51343100
C	2.87018800	1.05797900	2.55292000
C	2.02961200	0.42033500	3.48212800
C	1.76783500	-0.94016900	3.36289500
C	2.32548400	-1.67572200	2.30966700

H	4.15096500	0.78348700	0.82568400
H	3.13501300	2.10469600	2.68034100
H	1.58517400	0.99666400	4.28741400
H	1.10569400	-1.42969800	4.07064100
H	2.11004300	-2.73686900	2.20242000
C	3.81797200	-1.85309900	0.26204600
H	3.59879200	-2.91964600	0.39602900
H	4.90973500	-1.72826300	0.31516800
O	3.38251500	-1.43786400	-1.02080300
H	2.55580700	-2.13240400	-1.37596300

### Int1

Cu	1.85706500	2.53589400	-1.20503700
Cu	2.25983500	0.08968800	-1.20030400
Cu	1.37162700	1.21477100	0.90276300
Cu	-0.23096600	2.97725400	0.19477800
Cu	-0.05015700	0.99068100	-1.23267700
Cu	0.13245900	-1.28536100	-2.10269500
Cu	-1.11617500	-2.91447500	-0.47483900
Cu	-1.92372600	-1.53662800	1.40439500
Cu	-3.50889900	0.25639200	0.82539000
Cu	-2.34415500	1.88019500	-0.67678100
Cu	-1.07222300	0.78245000	1.17048300
Cu	0.46833100	-1.15075400	0.41852100
Cu	-1.93842300	-0.59498400	-0.89070000
O	1.35450300	-2.92665300	-1.73059000
O	0.86191700	-3.16268700	-0.32569800
C	3.03217800	-1.14067600	1.46562600
C	3.35512900	0.22444300	1.63982600
C	2.77581800	0.97012300	2.68483000
C	1.88848500	0.34516600	3.58086600
C	1.57549500	-0.99776200	3.42149400
C	2.12893100	-1.73154600	2.36120400
H	4.09881600	0.67877300	0.98777000
H	3.08071200	2.00093700	2.84747300
H	1.44984200	0.92023300	4.39022100
H	0.88163200	-1.47891600	4.10461300
H	1.88627800	-2.78502100	2.23178700
C	3.66803000	-1.93226900	0.34766000
H	3.37366600	-2.98759500	0.47355500
H	4.76426800	-1.89128500	0.49230400
O	3.34024700	-1.47716000	-0.93117600
H	2.23384600	-2.45855800	-1.50264700

### TS<sub>o-oc</sub>

Cu	-1.99353800	-2.40857100	-1.24353000
Cu	-2.24554100	0.07417000	-1.19486200
Cu	-1.43621300	-1.13124000	0.88379800
Cu	0.06713400	-2.97433700	0.12824500
Cu	0.00124000	-0.96662500	-1.26826900
Cu	-0.07824500	1.34870800	-2.09460500
Cu	1.32634800	2.88731800	-0.42142900

Cu	1.97348200	1.40997900	1.45250700
Cu	3.47806200	-0.43160300	0.83075300
Cu	2.24269900	-1.99211900	-0.70205800
Cu	1.01838800	-0.85674200	1.16276600
Cu	-0.40168600	1.18443400	0.41846000
Cu	1.94013700	0.49654800	-0.87187100
O	-1.25895000	2.91919800	-1.94852100
O	-0.56490200	3.13654400	-0.29276200
C	-2.91818500	1.25408400	1.53185500
C	-3.35049300	-0.08844600	1.62921700
C	-2.86010400	-0.92507900	2.65084700
C	-1.95278600	-0.41419100	3.59767600
C	-1.54362000	0.91075500	3.52066200
C	-2.01066500	1.73442600	2.48734100
H	-4.09768500	-0.45154600	0.92631400
H	-3.24287600	-1.93772300	2.75186900
H	-1.57719700	-1.06136400	4.38435400
H	-0.83518800	1.30290200	4.24452900
H	-1.68403400	2.77077900	2.41567200
C	-3.43834600	2.14285500	0.42779500
H	-2.88483400	3.09690200	0.48600500
H	-4.49368000	2.38108800	0.66622200
O	-3.36259800	1.58072600	-0.84180300
H	-2.12346300	2.56309600	-1.59991400

### Into-oc

Cu	-2.24072800	-2.31538800	-0.95744100
Cu	-2.33381400	0.14291300	-0.95986700
Cu	-1.44119600	-1.19857300	1.10651000
Cu	-0.04225500	-3.05652500	0.15429600
Cu	-0.19203200	-0.96208300	-1.18713700
Cu	-0.34662500	1.55849100	-1.79827600
Cu	1.22698900	2.86450900	-0.27205100
Cu	2.19910900	1.11491500	1.52590900
Cu	3.50770400	-0.69650600	0.58946200
Cu	1.98665100	-2.06006100	-1.00550200
Cu	1.11537900	-1.12106600	1.14579500
Cu	-0.25871300	1.00787400	0.71480300
Cu	1.80436000	0.42904100	-0.87858800
O	1.06114500	3.01238900	-2.15144800
O	0.92720800	2.50702700	1.51519500
C	-2.91447100	1.98150100	0.83771800
C	-3.89407900	0.97321700	0.74171500
C	-3.94247300	-0.07395500	1.66639200
C	-2.99710100	-0.13710200	2.70371300
C	-2.06617500	0.90064900	2.85077400
C	-2.04273800	1.97156100	1.94021500
H	-4.60822500	1.00881800	-0.08034100
H	-4.69887800	-0.84738800	1.57323000
H	-3.02859500	-0.94859100	3.42594000
H	-1.34882700	0.88036700	3.66632000
H	-1.30731600	2.76480400	2.06255800

C	-2.68374000	2.88422100	-0.35568000
H	-1.90167300	3.62175400	-0.10752000
H	-3.60013700	3.44568100	-0.60005600
O	-2.32075600	2.08667600	-1.46088200
H	1.83750300	2.70657000	-2.63158200

## TS2

O	1.91013700	-1.63238700	2.73127600
O	1.05371900	-2.12773500	-0.97698400
C	5.28622800	-0.75788700	-1.30583000
C	5.59276800	-1.27883900	-0.04392700
C	4.96268600	-0.79700600	1.09725500
C	3.99819400	0.22236200	1.02590800
C	3.73386200	0.79990700	-0.24872300
C	4.37604100	0.29972500	-1.40945600
H	5.76683500	-1.15053800	-2.19578500
H	6.31794900	-2.08294800	0.04167700
H	5.19739600	-1.22944600	2.06873800
H	3.12984600	1.71013100	-0.28212000
H	4.21027900	0.78612900	-2.36820700
C	3.18193700	0.60627400	2.19511800
H	3.77947000	0.80893900	3.10288600
H	2.62238600	-0.50930700	2.54457700
O	2.17632700	1.45689800	1.99134100
H	2.58428200	-2.32093800	2.78562600
Cu	-0.20473600	3.35109900	0.04403300
Cu	-1.48256000	1.42900100	-0.88543700
Cu	0.82001900	1.83788800	-1.61025100
Cu	0.74066100	1.02053300	0.73483000
Cu	2.37204300	-0.64830900	-0.93202300
Cu	1.11711900	-1.68565300	0.97476300
Cu	-0.81545800	-2.61797100	-0.44653400
Cu	-0.00768300	-0.46864200	-1.41905100
Cu	-2.45812800	-0.80308100	-1.41051200
Cu	-3.00219300	-2.21725700	0.54238600
Cu	-3.37419800	0.51049900	0.41909300
Cu	-1.20650900	-0.56531500	0.94063100
Cu	-1.51631400	1.81743400	1.54722700

## Int2

Cu	-2.39275000	-2.13834400	-1.05388500
Cu	-2.25612100	0.36204300	-1.04433900
Cu	-1.54986600	-0.96827600	1.02220200
Cu	-0.35145300	-2.99053600	0.14428600
Cu	-0.22709500	-0.94654300	-1.19511600
Cu	-0.04350100	1.41081500	-2.00029400
Cu	1.60032300	2.71672100	-0.57113000
Cu	2.23315500	1.16499200	1.41860700
Cu	3.38282100	-0.85952300	0.66472700
Cu	1.85818800	-2.23649200	-0.91523400
Cu	0.96031900	-1.06207500	1.13306000
Cu	-0.13861700	1.15475900	0.54820600

Cu	1.91607500	0.27244600	-0.96165800
O	-1.39870600	2.70286300	-2.96497700
O	1.03133700	2.67790000	1.22831100
C	-2.50254900	1.81691300	1.50081900
C	-3.31843300	0.64726700	1.48186400
C	-3.17599500	-0.32226500	2.48542100
C	-2.20516800	-0.14432100	3.48745400
C	-1.46949600	1.04898500	3.56144700
C	-1.61516900	2.02361000	2.58633300
H	-4.08169000	0.54403400	0.71477600
H	-3.82389500	-1.19395400	2.49645800
H	-2.06550600	-0.91642500	4.23748000
H	-0.73747800	1.18416000	4.35076000
H	-0.97238000	2.90080800	2.58065900
C	-2.44182700	2.66797800	0.33989900
H	-2.09609100	2.80432300	-2.27969400
H	-1.83741600	3.58687800	0.40874700
O	-2.99904500	2.35183500	-0.75701000
H	-1.83526700	2.28077400	-3.71270700

### Int3

Cu	3.43883200	-0.17960800	-0.21898100
Cu	1.84166800	-2.09157200	0.03355300
Cu	1.68337000	-0.12480300	1.53124800
Cu	2.13612000	1.92470100	0.18017400
Cu	1.08076100	0.01290200	-0.97948600
Cu	-0.32331900	-2.02010800	-1.31993800
Cu	-2.67305700	-1.79326100	-0.15614100
Cu	-2.55068600	0.28505500	1.15038300
Cu	-2.20667400	2.37655400	-0.10323800
Cu	0.03874100	2.25072600	-1.20996800
Cu	-0.24315200	1.26164900	1.03706400
Cu	-0.46484100	-1.30345400	1.06902000
Cu	-1.41932600	0.21723500	-1.04917000
O	-1.22683300	-2.95806200	0.12861300

### Int4

Cu	1.69386100	2.73785700	-0.39988900
Cu	2.21876400	0.24867000	-0.35413000
Cu	0.77431600	1.32945000	1.40395600
Cu	-0.69968000	3.02838700	0.32349200
Cu	-0.00756700	1.05849600	-1.00710900
Cu	0.58941400	-1.29614800	-1.64455400
Cu	-0.90301900	-3.02703300	-0.46011700
Cu	-2.25133100	-1.75250000	1.19110500
Cu	-3.79141200	-0.06198500	0.20728600
Cu	-2.42716700	1.71268800	-0.94084300
Cu	-1.58763600	0.72941100	1.17128200
Cu	0.20286700	-1.03476100	0.86983200
Cu	-1.74295000	-0.71250400	-0.97878500
O	0.84228300	-3.10973600	-1.16235700
C	3.70673100	-1.41673600	-0.56390900

C	3.72050300	-1.40173500	0.84946400
C	4.49834400	-0.44028400	1.50488900
C	5.26670400	0.47694300	0.78640100
C	5.23909900	0.47282800	-0.60595100
C	4.45024300	-0.46325100	-1.28178200
H	3.13791700	-2.18441800	-1.08972100
H	4.49985600	-0.41665100	2.59253500
H	5.86650900	1.21070300	1.31664100
H	5.81735900	1.19950000	-1.16819500
H	4.42674400	-0.47798700	-2.36749000
C	2.93408800	-2.42318800	1.62628200
H	3.44810100	-3.39491200	1.57166900
H	2.90657500	-2.13584000	2.68336200
O	1.59912900	-2.58093600	1.19680300
H	1.48605900	-2.94325700	0.22905100

### TS3

Cu	1.70634800	2.72612500	-0.39595800
Cu	2.22046500	0.23428400	-0.33434900
Cu	0.76914900	1.33266300	1.40938500
Cu	-0.69266400	3.02818400	0.31298200
Cu	0.00044400	1.05094600	-1.00556600
Cu	0.59173700	-1.30601000	-1.63089400
Cu	-0.91058200	-3.02627300	-0.44822700
Cu	-2.26496500	-1.74193800	1.18971500
Cu	-3.79406300	-0.05032400	0.19187600
Cu	-2.41896400	1.71605300	-0.95529600
Cu	-1.59256200	0.73641700	1.16484400
Cu	0.19581800	-1.03270500	0.88650200
Cu	-1.74113800	-0.71090900	-0.98014600
O	0.85285700	-3.12260800	-1.12837000
C	3.71562900	-1.41411400	-0.57945700
C	3.71636000	-1.40020600	0.83449100
C	4.48894600	-0.43765400	1.49588800
C	5.26419700	0.47882500	0.78382000
C	5.24981800	0.47382900	-0.60893700
C	4.46661700	-0.46194500	-1.29103900
H	3.15309700	-2.18336700	-1.10920700
H	4.48069200	-0.41408200	2.58357000
H	5.85946300	1.21266700	1.31916300
H	5.83378200	1.19985200	-1.16614500
H	4.45190700	-0.47614000	-2.37692200
C	2.91585600	-2.41959500	1.60219800
H	3.42987200	-3.39240700	1.54792300
H	2.89065400	-2.13433000	2.66139500
O	1.59081600	-2.56847600	1.15723800
H	1.44492100	-2.93716700	0.14637000

### Int5

Cu	0.82673100	3.30182100	-0.51414700
Cu	2.15344200	1.20794400	-0.53978900
Cu	0.49233500	1.67355100	1.32746100

Cu	-1.50651600	2.72677000	0.29057700
Cu	-0.22796600	1.08741600	-1.04754300
Cu	1.20793400	-0.95132100	-1.67803500
Cu	0.21653300	-2.96557500	-0.41029000
Cu	-1.46509600	-2.20063300	1.23081000
Cu	-3.45451300	-1.11630800	0.24347800
Cu	-2.72510700	0.93640800	-0.98834400
Cu	-1.62722000	0.34671800	1.17586100
Cu	0.59820200	-0.74720800	0.80697400
Cu	-1.29330400	-1.10598800	-1.00034400
O	1.62704200	-2.99727300	-1.73655500
C	3.85924900	0.32279100	1.14593400
C	3.61469200	-0.83728900	0.39192000
C	2.85009800	-1.86672700	0.96765000
C	2.31100700	-1.71666500	2.25766500
C	2.52765400	-0.53433200	2.97574600
C	3.31593800	0.47819700	2.42502500
H	4.48340000	1.10736800	0.71740000
H	2.69227800	-2.78114300	0.39555900
H	1.73644700	-2.52667700	2.70024500
H	2.09107000	-0.41423900	3.96247100
H	3.51255800	1.38429100	2.99166900
C	3.99209900	-0.86828200	-1.06898600
H	5.01627200	-0.48038500	-1.20129700
H	3.96633800	-1.90482000	-1.43679600
O	3.08290200	-0.06105900	-1.78124500
H	1.32947200	-3.39815000	-2.55997500

#### TS4

Cu	0.20825500	3.35591700	-0.64601600
Cu	1.86556200	1.45346300	-0.61463100
Cu	0.18885800	1.76763400	1.23817700
Cu	-2.02380200	2.50391400	0.28606100
Cu	-0.55596900	1.05968200	-1.04628900
Cu	1.07519200	-0.64203100	-1.82458500
Cu	0.84921500	-2.82448200	-0.46160400
Cu	-0.91562200	-2.42291600	1.22122600
Cu	-3.17172700	-1.74767600	0.42773500
Cu	-2.94398800	0.42124700	-0.79473500
Cu	-1.61497300	0.06759700	1.23936600
Cu	0.76765500	-0.58978500	0.72898100
Cu	-1.14454200	-1.36418000	-0.95246700
O	2.67766100	-3.14533000	-1.17039100
C	3.80521200	1.00345900	0.70635000
C	3.57778800	-0.34368600	0.34286500
C	3.12708500	-1.23229800	1.33927500
C	2.87352200	-0.77518600	2.63808700
C	3.10217300	0.55916200	2.97634400
C	3.58832600	1.44303700	2.01558300
H	4.21149300	1.68459400	-0.04316100
H	2.98813200	-2.28375500	1.09289100
H	2.49330000	-1.46903400	3.38254500

H	2.90294200	0.90507500	3.98609500
H	3.78123700	2.48071800	2.27300300
C	3.68954500	-0.73971000	-1.10077200
H	4.71224400	-0.96020700	-1.45123500
H	3.18627700	-2.05439000	-1.19230600
O	3.00262400	0.09548700	-1.92050200
H	2.76091200	-3.50602500	-2.06242500

## Int6

Cu	0.18464800	-3.35041300	-0.74030400
Cu	-1.73629500	-1.74983200	-0.39748000
Cu	0.20766900	-1.88543000	1.28688900
Cu	2.32263000	-2.18684100	-0.00740900
Cu	0.50574700	-0.94284000	-1.05467500
Cu	-1.36465000	0.52256200	-1.62112100
Cu	-1.38824100	2.60032000	-0.02018900
Cu	0.70073200	2.43078700	1.36519900
Cu	2.92739000	2.11584500	0.31116600
Cu	2.80264300	0.04369400	-1.11845400
Cu	1.76510200	0.07395000	1.13986000
Cu	-0.71557400	0.38905800	0.89025300
Cu	0.80201700	1.55983100	-0.87174400
O	-2.46250800	1.66036000	-3.01039800
C	-3.80796500	-1.15868600	0.38342200
C	-3.51710000	0.24100600	0.56674200
C	-2.77929800	0.61986500	1.74799700
C	-2.23095700	-0.36615900	2.57701300
C	-2.42881000	-1.74337200	2.31158500
C	-3.30158900	-2.12167300	1.25843300
H	-4.48710500	-1.44947400	-0.41606700
H	-2.75012900	1.66736900	2.03586300
H	-1.68671800	-0.06974500	3.46965400
H	-2.02886700	-2.49240100	2.98839900
H	-3.56688100	-3.16637700	1.12530400
C	-3.84275200	1.17568300	-0.43423700
H	-4.49606200	0.81180100	-1.24691000
O	-3.39462200	2.38806600	-0.51509800
H	-2.95165400	2.22460100	-2.37518600
H	-3.12544000	1.20684600	-3.54057900