

Electronic Supplementary Information (ESI)

DFT Studies on the Mechanism of Veratryl Alcohol Oxidation Catalyzed by Cu-phen(phen=1,10-phenanthroline) Complexes

Lisha Ma,^a Qiancheng Zhang,^a Lin Cheng,^{*a} Zhijian Wu,^{*b} Jucai Yang,^a

^aKey Laboratory of Industrial Catalysis of the Inner Mongolia Autonomous Region,
Inner Mongolia University of Technology, Huhehot 010051, China

^bState Key Laboratory of Rare Earth Resource Utilization, Changchun Institute of
Applied Chemistry, Chinese Academy of Sciences, Changchun 130022, China

Table S1 Cartesian coordinates all structures considered in this work (B3LYP level)

0				1			
Charge=0 Multiplicity = 2				Charge=0 Multiplicity = 2			
Cu	1.90853100	-0.01724400	0.02665500	Cu	0.18287100	-1.11862500	1.39846800
O	3.05843800	1.38651500	-0.25804500	O	-0.52766500	-0.62934700	3.01856400
H	3.96992700	1.08533600	-0.37870300	H	-1.01054200	-1.35648200	3.43636200
O	2.99044000	-1.47625200	0.29769400	O	-0.53903700	-2.75870100	1.00131700
H	3.91744900	-1.22242500	0.40868300	H	-1.25704300	-2.99447300	1.60572900
C	-0.91276100	-3.53255500	-0.07070200	C	2.69094500	-2.57477000	-1.84242500
C	-2.08301200	-2.80222000	-0.03574400	C	3.36712200	-1.42971000	-2.22723400
C	-2.04885400	-1.38940800	-0.01422500	C	3.11077600	-0.21165400	-1.55728800
C	-0.80500300	-0.71356200	-0.03063000	C	2.16219000	-0.25750400	-0.51316400
C	0.32590400	-2.86737300	-0.08609200	C	1.76608300	-2.51679500	-0.78048800
C	-3.27034400	-0.63710000	0.02378700	C	3.73643200	1.04823800	-1.85592700
C	-0.78578500	0.73220400	-0.00976400	C	1.82803800	0.93266800	0.21571800
C	-2.01120700	1.44006000	0.02776500	C	2.46046900	2.15701400	-0.08941600
C	-3.25228300	0.71971400	0.04443700	C	3.42944600	2.17832800	-1.15176800
C	-2.00790300	2.85335200	0.04817300	C	2.07744000	3.27315100	0.68886800
H	-2.96993800	3.38695500	0.07728000	H	2.52931300	4.24366000	0.49959600
C	-0.81871000	3.55304400	0.03162800	C	1.13221700	3.11545500	1.68794000
C	0.40182300	2.85593800	-0.00573900	C	0.55346600	1.84953500	1.90912000
H	-4.21914000	-1.19517300	0.03587800	H	4.46871900	1.08650600	-2.65804400
H	-0.93987100	-4.63182300	-0.08658000	H	2.86495700	-3.51970700	-2.34672800
H	-3.05901900	-3.31050500	-0.02344400	H	4.08903300	-1.45721600	-3.03963200
H	1.25520700	-3.45549700	-0.11370300	H	1.18920900	-3.36969400	-0.43348400
H	-4.18608000	1.30191100	0.07395200	H	3.91675100	3.11993500	-1.39053300
H	-0.81660800	4.65265400	0.04740000	H	0.82791000	3.95558800	2.30363800
H	1.34623700	3.41999700	-0.01880500	H	-0.18249800	1.64760100	2.68256200
N	0.37834100	-1.48727000	-0.06694100	N	1.52485100	-1.38641400	-0.12800500
N	0.41769100	1.47498300	-0.02584400	N	0.88736300	0.79369500	1.17738600
				C	-1.66040400	-0.61489300	-0.73856500
				H	-1.69996300	-1.69773000	-0.58802800
				O	-1.00010500	-0.00664300	0.42748800
				H	-1.63732900	-0.00923600	1.17067700
				H	-0.98617600	-0.39522200	-1.56918600
				C	-3.02559400	-0.02755700	-0.94352900
				C	-3.17285200	1.26067600	-1.47955500
				C	-4.16748300	-0.74901400	-0.57059500
				C	-4.44033800	1.81566900	-1.63905300
				H	-2.29103700	1.82473100	-1.77422100
				C	-5.43786500	-0.19443900	-0.73240700
				H	-4.06343300	-1.75297200	-0.16442500
				C	-5.57424400	1.08804100	-1.26545600

	H	-4.54720400	2.81114500	-2.06000900
	H	-6.31759200	-0.76400900	-0.44784800
	H	-6.56245500	1.51962400	-1.39525900

TS ₁₋₂				2			
Charge=0 Multiplicity = 2				Charge=0 Multiplicity = 2			
Cu	0.17658200	-1.00122200	-0.11143400	Cu	0.10881800	-0.95565600	-0.09048400
O	-0.73337100	-0.44173700	1.91487800	O	-0.48603700	-1.60003600	2.42347100
H	-0.96764000	-1.25117800	2.39396300	H	-0.38029100	-2.31730400	1.75695000
O	-0.01337200	-2.77316700	-0.56029200	O	-0.09935600	-2.80870300	-0.08189800
H	-0.92729400	-3.00819900	-0.77087100	H	-0.99218500	-3.08613600	-0.33176300
C	4.22118800	-2.51345800	0.18160400	C	4.16917200	-2.42332200	-0.55956000
C	4.96609000	-1.34768900	0.19842900	C	4.91094400	-1.25916500	-0.46915400
C	4.31154800	-0.09924400	0.09198200	C	4.25003800	-0.02458600	-0.27349300
C	2.90448200	-0.13303200	-0.01960900	C	2.84214900	-0.07148400	-0.18976400
C	2.81805900	-2.44213800	0.07097900	C	2.76405800	-2.36474700	-0.46497600
C	4.96791700	1.17924600	0.08711700	C	4.90084400	1.25104600	-0.14803700
C	2.15492400	1.08448800	-0.15049900	C	2.08843500	1.13027600	0.02818200
C	2.82374500	2.32794500	-0.15319800	C	2.75010700	2.36992700	0.16052400
C	4.25571300	2.33901700	-0.02637400	C	4.18387400	2.39525100	0.05901800
C	2.01664800	3.48067600	-0.28548500	C	1.93231200	3.49946600	0.39317600
H	2.47839600	4.46478100	-0.29159400	H	2.38697800	4.48060200	0.50424600
C	0.64661900	3.34011600	-0.40469800	C	0.56121700	3.34096800	0.48352300
C	0.07499600	2.05202700	-0.39690900	C	-0.00410700	2.05833900	0.33632200
H	6.05049100	1.20782900	0.17744700	H	5.98466200	1.28956800	-0.21628400
H	4.70197600	-3.48344400	0.25432500	H	4.65384100	-3.38361300	-0.70143500
H	6.04893300	-1.38161900	0.28866000	H	5.99532900	-1.28424900	-0.54115800
H	2.16997900	-3.31339900	0.03693600	H	2.11771100	-3.23655800	-0.51701600
H	4.76786700	3.29751200	-0.02625700	H	4.69374800	3.34987300	0.15665200
H	0.00209100	4.20730400	-0.50357100	H	-0.08789700	4.19047100	0.66823300
H	-0.99410500	1.88202300	-0.48125100	H	-1.07066200	1.86237700	0.40050100
N	2.18733800	-1.27871000	-0.01514100	N	2.12572500	-1.21426900	-0.29187600
N	0.81323600	0.95525600	-0.28195900	N	0.74552300	0.98667500	0.11115800
C	-2.84753700	-1.10564400	-0.51023800	C	-2.76702600	-1.15220800	-0.15665800
H	-2.83359500	-2.05538100	0.05741300	H	-2.88235100	-1.92081200	0.63181000
O	-1.72650400	-0.32073000	-0.17427700	O	-1.65283600	-0.33912300	0.06130300
H	-1.45149400	-0.34973400	0.97564300	H	-1.12611700	-1.01562600	1.97416100
H	-2.80901500	-1.37817600	-1.57447700	H	-2.68038300	-1.71252500	-1.11039500
C	-4.15308600	-0.38502900	-0.22219800	C	-4.05392100	-0.34341500	-0.22001500
C	-5.22966300	-0.46317300	-1.11177700	C	-4.07976800	0.89439800	-0.87539000
C	-4.30989200	0.34902400	0.96211500	C	-5.24210200	-0.82705500	0.33817400
C	-6.44172700	0.17031700	-0.82785200	C	-5.26277700	1.62618500	-0.97468000
H	-5.11761400	-1.02246400	-2.03872700	H	-3.15696100	1.27541900	-1.30314400
C	-5.51770000	0.98552700	1.24663100	C	-6.43064700	-0.09988800	0.23936900

H	-3.47725800	0.42114400	1.65734600	H	-5.23558600	-1.78128000	0.86163500
C	-6.58898700	0.89768300	0.35356000	C	-6.44501500	1.13083300	-0.41808700
H	-7.26662800	0.10094900	-1.53285700	H	-5.26516200	2.58501500	-1.48853000
H	-5.62438800	1.55173800	2.16884400	H	-7.34262700	-0.49145100	0.68377200
H	-7.52962500	1.39504900	0.57636300	H	-7.36740700	1.70139100	-0.49304100

TS _{2-3'}				¹ 3			
Charge=0 Multiplicity = 2				Charge=0 Multiplicity = 1			
Cu	-0.05535500	-0.64217500	-0.12856800	Cu	-2.32787500	-0.22905500	-0.94313900
O	-0.02193900	0.86391800	2.81563800	O	-1.05576400	-0.20452200	-2.29838100
H	-0.22139500	0.24837300	3.53620300	H	-1.09026200	0.63295600	-2.78404500
O	-1.17528500	-2.02205400	-1.00757500	C	-0.37679800	-4.03727100	-0.01718800
H	-1.37495800	-1.91671400	-1.95381300	C	-1.37709300	-4.71218300	0.65282900
C	3.48437100	-3.10356900	-0.07581300	C	-2.61887500	-4.07083100	0.86514200
C	4.47624900	-2.13717500	-0.12776400	C	-2.74810400	-2.75959000	0.35805700
C	4.11139700	-0.77499100	-0.16261300	C	-0.59299600	-2.72191000	-0.48386500
C	2.72878800	-0.47607500	-0.15313200	C	-3.73321000	-4.65900400	1.55618200
C	2.13828800	-2.70969100	-0.02899700	C	-3.97979600	-2.04408600	0.54407700
C	5.05090700	0.31234100	-0.18793800	C	-5.05827500	-2.63659500	1.23855900
C	2.28743600	0.88735400	-0.21445600	C	-4.89993800	-3.97349900	1.73906600
C	3.23148500	1.93970500	-0.19666900	C	-6.22225400	-1.84911400	1.38934500
C	4.63001600	1.61007400	-0.18471500	H	-7.08280500	-2.25699500	1.91387400
C	2.72433000	3.25622200	-0.20225200	C	-6.25143100	-0.56580100	0.87329500
H	3.40983000	4.09942400	-0.18636500	C	-5.12461900	-0.06486700	0.19253100
C	1.35367300	3.45358400	-0.21937700	H	-3.62685200	-5.67024000	1.94027400
C	0.49646200	2.34220000	-0.27118900	H	0.58821100	-4.49987700	-0.19705500
H	6.11223400	0.07865500	-0.19126900	H	-1.22353300	-5.72438500	1.01946800
H	3.73226500	-4.15962000	-0.04656800	H	0.19919900	-2.17636100	-1.00874400
H	5.52671200	-2.41570200	-0.13661300	H	-5.72996300	-4.43246800	2.26957100
H	1.33706700	-3.43863600	0.04079900	H	-7.12997300	0.06126700	0.98429800
H	5.35317200	2.42138100	-0.18244600	H	-5.06698300	0.93768200	-0.22200500
H	0.93150300	4.45307700	-0.21079300	N	-1.75560300	-2.10150400	-0.29361800
H	-0.58311700	2.45413900	-0.28996300	N	-4.02963900	-0.79621300	0.02492700
N	1.75998800	-1.43002100	-0.04345700	C	-2.17015600	2.59531700	-1.30709500
N	0.94532700	1.08984600	-0.30171800	H	-2.29245500	2.72541700	-2.40322100
C	-2.67301300	-0.81265000	0.65011500	O	-2.90816100	1.52090000	-0.81819200
H	-2.72567000	-1.53333000	1.48512100	H	-1.08758700	2.45575300	-1.13328900
O	-1.62064100	0.04531200	0.69681200	C	-2.57278300	3.90843800	-0.64859200
H	-0.70868500	0.65547400	2.14257800	C	-3.16692300	3.91934100	0.61797500
H	-2.15236600	-1.64888500	-0.36522400	C	-2.32123100	5.13452400	-1.27752100
C	-3.98710900	-0.29243100	0.23504900	C	-3.49803200	5.12359000	1.24199500
C	-4.11915500	0.95277800	-0.40943300	H	-3.36492500	2.96576300	1.09670100
C	-5.15414100	-1.06069200	0.42633000	C	-2.64711200	6.34114300	-0.65706600

C	-5.36236700	1.40746700	-0.84297200	H	-1.86843600	5.14240500	-2.26793900
H	-3.22856600	1.55844600	-0.54544000	C	-3.23912800	6.34068600	0.60834200
C	-6.39493400	-0.60609500	-0.00961500	H	-3.96025200	5.11274700	2.22716400
H	-5.07614300	-2.02456600	0.92672100	H	-2.44667900	7.28226100	-1.16463000
C	-6.50965000	0.63271800	-0.64981800	H	-3.49967000	7.27912200	1.09219200
H	-5.44000100	2.37664000	-1.33160600	H	1.84538500	2.46349900	0.95339600
H	-7.28006700	-1.21683900	0.15437300	C	2.88050600	2.21593900	1.17622600
H	-7.47900500	0.98914800	-0.98842700	C	3.69714900	2.94722500	2.06292900
				N	3.33418400	1.14099100	0.54295400
				C	5.00333400	2.54551700	2.28528200
				H	3.29214800	3.82288800	2.55964300
				C	4.60229500	0.72992500	0.76782000
				C	5.50076300	1.39702500	1.62741700
				H	5.64879100	3.10279400	2.95973900
				C	5.01262700	-0.45048100	0.06220300
				C	6.83162800	0.86921700	1.76384500
				C	6.32650400	-0.94655300	0.20557800
				N	4.07230500	-1.02949200	-0.71896700
				C	7.22728500	-0.24723400	1.08195600
				H	7.52775900	1.38104100	2.42322400
				C	6.64382700	-2.10623000	-0.53776200
				C	4.39322700	-2.11119200	-1.41821300
				H	8.23934700	-0.62669800	1.19608300
				C	5.68030900	-2.68137200	-1.34928600
				H	7.64065000	-2.53494000	-0.46967900
				H	3.58904500	-2.49982200	-2.03797700
				H	5.90343200	-3.56779000	-1.93437800
				Cu	2.26421500	-0.04564500	-0.73332400
				O	0.74254300	0.86935400	-0.26971100
				O	1.65149200	-1.21059500	-2.02683100
				H	0.06323600	0.59624100	-0.91392900
				H	0.78548900	-0.88398200	-2.34782900

³ 3				¹ TS ₃₋₄			
Charge=0	Multiplicity = 3			Charge=0	Multiplicity = 1		
Cu	-2.32787500	-0.22905500	-0.94313900	Cu	2.32941300	-0.45101200	-1.11246700
O	-1.05576400	-0.20452200	-2.29838100	O	1.18849700	0.18891600	-2.49199300
H	-1.09026200	0.63295600	-2.78404500	H	1.31790500	-0.30178800	-3.31813800
C	-0.37679800	-4.03727100	-0.01718800	C	2.27312400	3.62368400	0.39577300
C	-1.37709300	-4.71218300	0.65282900	C	3.57669900	3.77119700	0.84116000
C	-2.61887500	-4.07083100	0.86514200	C	4.45789100	2.67306100	0.75607400
C	-2.74810400	-2.75959000	0.35805700	C	3.94096900	1.47527800	0.20901300
C	-0.59299600	-2.72191000	-0.48386500	C	1.83215500	2.38240200	-0.09606700
C	-3.73321000	-4.65900400	1.55618200	C	5.82350900	2.69208700	1.20473900

C	-3.97979600	-2.04408600	0.54407700	C	4.79437600	0.33354600	0.05756000
C	-5.05827500	-2.63659500	1.23855900	C	6.12439900	0.36323100	0.54187300
C	-4.89993800	-3.97349900	1.73906600	C	6.61454000	1.58314100	1.12236200
C	-6.22225400	-1.84911400	1.38934500	C	6.88472300	-0.81571200	0.39954700
H	-7.08280500	-2.25699500	1.91387400	H	7.91182800	-0.84264100	0.75448100
C	-6.25143100	-0.56580100	0.87329500	C	6.30584800	-1.92957800	-0.19128600
C	-5.12461900	-0.06486700	0.19253100	C	4.98960400	-1.85071400	-0.67218500
H	-3.62685200	-5.67024000	1.94027400	H	6.21388900	3.61301800	1.63073200
H	0.58821100	-4.49987700	-0.19705500	H	1.57211200	4.45145600	0.43933400
H	-1.22353300	-5.72438500	1.01946800	H	3.92682800	4.71509000	1.25172600
H	0.19919900	-2.17636100	-1.00874400	H	0.80640200	2.23772100	-0.44250100
H	-5.72996300	-4.43246800	2.26957100	H	7.63945900	1.61060000	1.48348100
H	-7.12997300	0.06126700	0.98429800	H	6.86314200	-2.85370800	-0.30747300
H	-5.06698300	0.93768200	-0.22200500	H	4.49545600	-2.69490600	-1.14436600
N	-1.75560300	-2.10150400	-0.29361800	N	2.63976800	1.31861500	-0.16462200
N	-4.02963900	-0.79621300	0.02492700	N	4.25948000	-0.73959500	-0.58548400
C	-2.17015600	2.59531700	-1.30709500	C	0.69258600	-2.74305100	-0.71360100
H	-2.29245500	2.72541700	-2.40322100	H	0.37518700	-3.57527000	-1.37413100
O	-2.90816100	1.52090000	-0.81819200	O	1.92484200	-2.30081100	-0.96307500
H	-1.08758700	2.45575300	-1.13328900	H	-0.17487200	-1.88232800	-1.02802300
C	-2.57278300	3.90843800	-0.64859200	C	0.32706500	-3.01801100	0.72248300
C	-3.16692300	3.91934100	0.61797500	C	1.17292200	-2.64584600	1.77608000
C	-2.32123100	5.13452400	-1.27752100	C	-0.89154000	-3.64249700	1.03270200
C	-3.49803200	5.12359000	1.24199500	C	0.81293600	-2.89433400	3.10065700
H	-3.36492500	2.96576300	1.09670100	H	2.12330600	-2.17949500	1.53598000
C	-2.64711200	6.34114300	-0.65706600	C	-1.25275700	-3.89312400	2.35524700
H	-1.86843600	5.14240500	-2.26793900	H	-1.55874600	-3.93643300	0.22380500
C	-3.23912800	6.34068600	0.60834200	C	-0.40108900	-3.51777700	3.39837000
H	-3.96025200	5.11274700	2.22716400	H	1.48569500	-2.60569800	3.90538500
H	-2.44667900	7.28226100	-1.16463000	H	-2.19859600	-4.38363400	2.57468700
H	-3.49967000	7.27912200	1.09219200	H	-0.68030400	-3.71229300	4.43092500
H	1.84538500	2.46349900	0.95339600	H	-3.04069000	-2.14122000	-2.09219600
C	2.88050600	2.21593900	1.17622600	C	-3.87017700	-1.75926000	-1.50607200
C	3.69714900	2.94722500	2.06292900	C	-5.05244500	-2.48815900	-1.30077900
N	3.33418400	1.14099100	0.54295400	N	-3.69096600	-0.53843900	-1.00157900
C	5.00333400	2.54551700	2.28528200	C	-6.08231300	-1.93443000	-0.55280200
H	3.29214800	3.82288800	2.55964300	H	-5.15641900	-3.46998700	-1.75109500
C	4.60229500	0.72992500	0.76782000	C	-4.67195000	-0.01511600	-0.21524600
C	5.50076300	1.39702500	1.62741700	C	-5.90998600	-0.65623200	0.01723400
H	5.64879100	3.10279400	2.95973900	H	-7.01512300	-2.47242700	-0.40546800
C	5.01262700	-0.45048100	0.06220300	C	-4.40776600	1.27223000	0.34581000
C	6.83162800	0.86921700	1.76384500	C	-6.90212300	0.04238700	0.78961300
C	6.32650400	-0.94655300	0.20557800	C	-5.40863600	1.95688800	1.07147900
N	4.07230500	-1.02949200	-0.71896700	N	-3.15389100	1.76028300	0.15257100

C	7.22728500	-0.24723400	1.08195600	C	-6.67011700	1.29699700	1.27653200
H	7.52775900	1.38104100	2.42322400	H	-7.85722400	-0.44511200	0.96676000
C	6.64382700	-2.10623000	-0.53776200	C	-5.07702700	3.24056200	1.55332800
C	4.39322700	-2.11119200	-1.41821300	C	-2.87813500	2.98781800	0.58699100
H	8.23934700	-0.62669800	1.19608300	H	-7.44012200	1.81506200	1.84225100
C	5.68030900	-2.68137200	-1.34928600	C	-3.81599500	3.75947700	1.29268900
H	7.64065000	-2.53494000	-0.46967900	H	-5.80781200	3.81166200	2.12002000
H	3.58904500	-2.49982200	-2.03797700	H	-1.87785700	3.34276400	0.35930000
H	5.90343200	-3.56779000	-1.93437800	H	-3.53659000	4.74653500	1.64683000
Cu	2.26421500	-0.04564500	-0.73332400	Cu	-2.05757100	0.58521500	-1.06880000
O	0.74254300	0.86935400	-0.26971100	O	-0.95704500	-0.85541400	-1.48541400
O	1.65149200	-1.21059500	-2.02683100	O	-0.93824700	1.92479100	-1.60130000
H	0.06323600	0.59624100	-0.91392900	H	-0.16783700	-0.44671000	-1.97538400
H	0.78548900	-0.88398200	-2.34782900	H	-0.21527500	1.54109800	-2.13779300

³ TS ₃₋₄				4u			
Charge=0 Multiplicity = 3				Charge=0 Multiplicity = 1			
Cu	-2.25725300	-0.05512500	-1.23058000	Cu	-2.46844300	0.58536200	-0.58054800
O	-1.28324800	-0.93382300	-2.57578600	O	-1.20903600	0.53476300	-2.04565400
H	-1.38358100	-0.44557500	-3.40804800	H	-1.43001600	-0.13987400	-2.70358900
C	-1.78376000	-3.85183900	0.93568400	C	-2.53068000	-3.03859200	1.78775600
C	-2.98618800	-3.94224000	1.60875400	C	-3.87712400	-3.35069700	1.79432600
C	-3.92576500	-2.89376000	1.48616600	C	-4.77902600	-2.50288200	1.11715100
C	-3.56271800	-1.80933900	0.65664400	C	-4.24129200	-1.36555800	0.46689000
C	-1.50228000	-2.72400100	0.13521100	C	-2.07886500	-1.88751500	1.11836400
C	-5.19963000	-2.86182800	2.15079300	C	-6.19611400	-2.73086000	1.06857100
C	-4.46717900	-0.70363500	0.49765400	C	-5.12014300	-0.46663500	-0.23266600
C	-5.70571400	-0.68343400	1.17825000	C	-6.51735400	-0.70789100	-0.24834400
C	-6.05016200	-1.80314900	2.00934400	C	-7.03073900	-1.86990500	0.41990200
C	-6.51592200	0.45836400	0.98461600	C	-7.32704600	0.22594900	-0.92857700
H	-7.48056900	0.52337000	1.48188200	H	-8.40363600	0.07991200	-0.96506500
C	-6.06803900	1.48508700	0.17166900	C	-6.73504600	1.31831300	-1.53791000
C	-4.81864100	1.36873300	-0.46764400	C	-5.33864200	1.46097100	-1.47822200
H	-5.47294700	-3.70284200	2.78285400	H	-6.59417700	-3.60858600	1.57145900
H	-1.03891600	-4.63750700	1.01110700	H	-1.80696500	-3.66876400	2.29523400
H	-3.21722400	-4.80285800	2.23203600	H	-4.24918400	-4.23333200	2.30871200
H	-0.54708600	-2.62597700	-0.39473800	H	-1.01824600	-1.62684300	1.05818300
H	-7.00560000	-1.79266400	2.52720400	H	-8.10240400	-2.05034800	0.39832400
H	-6.66587100	2.37761400	0.01839900	H	-7.32930100	2.05712700	-2.06649000
H	-4.38967100	2.14294800	-1.09855400	H	-4.84314700	2.30288400	-1.95445500
N	-2.37400600	-1.72507300	0.00482300	N	-2.91143400	-1.05841900	0.47506700
N	-4.05699000	0.29174500	-0.32053900	N	-4.54294600	0.59514600	-0.85521600
C	-0.90146600	2.39487600	-1.79055100	C	-1.70390300	3.38938600	0.46762500

H	-0.84425300	2.84444300	-2.80050900	H	-2.12249400	4.40257100	0.32226500
O	-2.12486600	1.75456000	-1.58012100	O	-2.37350900	2.42563400	0.07754100
H	0.03115500	1.56386800	-1.72090600	H	1.54326800	1.63007200	-2.44266600
C	-0.58071300	3.43198100	-0.76313000	C	-0.40995000	3.33655300	1.13721700
C	-1.17129100	3.41251100	0.51461900	C	0.28206500	2.12574800	1.33371000
C	0.40641400	4.40931100	-1.00583300	C	0.14479700	4.54337500	1.60634400
C	-0.78949700	4.32026900	1.50363900	C	1.50517600	2.13757400	1.99895200
H	-1.94514100	2.67519600	0.70437100	H	-0.09743400	1.18164700	0.94773300
C	0.78659200	5.31920500	-0.02103800	C	1.36598600	4.54485100	2.27103900
H	0.87359100	4.45191800	-1.98845600	H	-0.39385100	5.47562500	1.44791400
C	0.19310600	5.28130700	1.24738000	C	2.04734100	3.33864300	2.46876400
H	-1.26886600	4.28479100	2.48062000	H	2.04119800	1.20359900	2.13605400
H	1.54166900	6.07062300	-0.24520900	H	1.78899100	5.47784300	2.63338000
H	0.47791200	5.99981900	2.01257100	H	3.00436200	3.33592200	2.98385000
H	1.39851200	2.05063400	0.37155500	H	3.31682400	2.64359700	-0.92475500
C	2.39496300	1.78249100	0.70438800	C	4.14567700	1.95806600	-0.76574000
C	3.16352200	2.65256400	1.50300400	C	5.45048000	2.42783700	-0.73172700
N	2.84620200	0.59343700	0.31671500	N	3.80543400	0.66806400	-0.55093600
C	4.42994000	2.27010100	1.90750900	C	6.50329200	1.53854800	-0.44866700
H	2.73724900	3.60925400	1.78420900	H	5.64127200	3.48488200	-0.88885800
C	4.09789400	0.22173400	0.69146900	C	4.84627600	-0.22230500	-0.34312000
C	4.93845800	1.01483900	1.50202800	C	6.20518900	0.18574000	-0.24330700
H	5.03726700	2.92250900	2.52996100	H	7.52967800	1.88900700	-0.38336900
C	4.54390600	-1.06090300	0.23152300	C	4.49478000	-1.57988300	-0.18300400
C	6.23226000	0.49811600	1.85731400	C	7.18459600	-0.82182200	0.07752600
C	5.81462100	-1.55428900	0.60169200	C	5.46954800	-2.55766800	0.16769900
N	3.68704200	-1.73569700	-0.57178100	N	3.17388900	-1.89832600	-0.40119000
C	6.64959300	-0.73174100	1.43343900	C	6.83413200	-2.12275400	0.29167900
H	6.87913400	1.10923700	2.48133200	H	8.22498700	-0.51587500	0.16012700
C	6.16215800	-2.83315500	0.11138700	C	5.03029500	-3.87372900	0.35175300
C	4.02573300	-2.94289200	-1.00873800	C	2.78448700	-3.15708100	-0.17174400
H	7.62954600	-1.10574900	1.71799400	H	7.59164400	-2.85953700	0.54885200
C	5.26544900	-3.52704500	-0.68463600	C	3.66999900	-4.17124800	0.19723700
H	7.12879000	-3.26228500	0.36319600	H	5.74333800	-4.65156500	0.61388100
H	3.27233900	-3.43088200	-1.62099800	H	1.72270200	-3.34076500	-0.30732600
H	5.50797300	-4.51279900	-1.06815300	H	3.30069000	-5.18256300	0.33413200
Cu	1.94952100	-0.74168600	-0.93112700	Cu	2.07750800	-0.27827900	-0.74128200
O	0.80821000	0.53290400	-1.69171600	O	1.26318800	0.72029500	-2.26895600
O	1.09770100	-2.28767200	-1.46882400	O	0.46552900	-0.82502400	0.02791400
H	0.14533100	-0.04042100	-2.15548500	H	0.20219900	0.71137900	-2.19111400
H	0.37150200	-2.04721500	-2.07731300	H	-0.23630700	-0.52118900	-0.57701900

4r				³ 4			
Charge=0 Multiplicity = 1				Charge=0 Multiplicity = 3			
Cu	-2.46824300	0.58445000	-0.58136400	Cu	2.39877300	-0.66590000	-0.65687200
O	-1.20932500	0.53027300	-2.04675100	O	1.26992800	-0.66583900	-2.23084700
H	-1.43260000	-0.14388500	-2.70440700	H	1.58566000	-0.11033700	-2.95716100
C	-2.53180900	-3.04132600	1.78375000	C	2.65221900	3.30475100	1.06354200
C	-3.87840900	-3.35282700	1.79021700	C	4.01955900	3.49223600	1.13969200
C	-4.78010800	-2.50356700	1.11460400	C	4.87648200	2.45730700	0.70960700
C	-4.24199700	-1.36561800	0.46574500	C	4.27461300	1.27188600	0.22105200
C	-2.07964800	-1.88943000	1.11603000	C	2.13698400	2.09201400	0.57406500
C	-6.19736000	-2.73061500	1.06632200	C	6.30914200	2.54640200	0.75578600
C	-5.12057500	-0.46521800	-0.23225600	C	5.10668700	0.18963600	-0.23399400
C	-6.51796500	-0.70550000	-0.24747700	C	6.51844200	0.29851300	-0.15685000
C	-7.03175200	-1.86815600	0.41935900	C	7.09687500	1.51101200	0.34871400
C	-7.32741600	0.22984400	-0.92591000	C	7.27732300	-0.80867800	-0.59107200
H	-8.40412600	0.08459400	-0.96198900	H	8.36276500	-0.76786400	-0.54863700
C	-6.73501600	1.32267900	-1.53403400	C	6.62435800	-1.93341200	-1.06385700
C	-5.33848200	1.46422300	-1.47507400	C	5.22057300	-1.93675000	-1.11791200
H	-6.59573300	-3.60884000	1.56809400	H	6.75629900	3.46224400	1.13387400
H	-1.80827600	-3.67254600	2.29018900	H	1.96154700	4.07952700	1.38131200
H	-4.25073200	-4.23603100	2.30343500	H	4.44151600	4.41812100	1.52246300
H	-1.01896900	-1.62885800	1.05639400	H	1.06312100	1.91810300	0.47683600
H	-8.10354600	-2.04786700	0.39806800	H	8.17994200	1.58843800	0.39786000
H	-7.32907600	2.06267400	-2.06117900	H	7.17793500	-2.80331400	-1.40317600
H	-4.84266000	2.30640500	-1.95049100	H	4.67896100	-2.80014000	-1.49495600
N	-2.91201700	-1.05908000	0.47407000	N	2.92302800	1.08680500	0.16703300
N	-4.54298000	0.59692800	-0.85384300	N	4.47294400	-0.90760200	-0.72635800
C	-1.70145500	3.38881200	0.46680700	C	1.42580300	-3.02382700	1.09038100
H	-2.12020800	4.40185800	0.32082700	H	1.71180400	-4.07616700	1.27123800
O	-2.37033700	2.42474000	0.07638600	O	2.11545200	-2.36342100	0.30360000
H	1.54174500	1.62781600	-2.44598500	H	-1.48366600	-1.68023000	-2.69330700
C	-0.40801800	3.33651500	1.13747800	C	0.26678200	-2.54450800	1.83102200
C	0.28419100	2.12591700	1.33470200	C	-0.23619900	-1.24481400	1.63870300
C	0.14603500	4.54361600	1.60668600	C	-0.35516300	-3.40660900	2.75435900
C	1.50691700	2.13833000	2.00067200	C	-1.34478200	-0.82061900	2.36467600
H	-0.09483800	1.18154700	0.94879400	H	0.20561600	-0.57529400	0.90635000
C	1.36680700	4.54562900	2.27214800	C	-1.45808800	-2.97307900	3.48180900
H	-0.39279500	5.47566400	1.44767400	H	0.03462400	-4.41277900	2.89521500
C	2.04841800	3.33967900	2.47052800	C	-1.95366100	-1.67852300	3.28681000
H	2.04318900	1.20458100	2.13837100	H	-1.73540900	0.17783100	2.19265900
H	1.78929900	5.47882900	2.63455400	H	-1.93677800	-3.63866700	4.19469500
H	3.00513300	3.33738000	2.98618900	H	-2.82137000	-1.34245500	3.84820400
H	3.31642000	2.64295700	-0.92791200	H	-3.10682000	-2.72258900	-1.58207000
C	4.14530200	1.95762900	-0.76819900	C	-3.96156700	-2.13789800	-1.24806100

C	5.45010200	2.42737500	-0.73486600	C	-5.20613800	-2.73034100	-1.12765000
N	3.80503200	0.66784800	-0.55181300	N	-3.71164400	-0.84155200	-0.96145000
C	6.50294500	1.53840400	-0.45082800	C	-6.30464400	-1.95692600	-0.68108300
H	5.64091700	3.48422500	-0.89328500	H	-5.32708000	-3.77891000	-1.37925200
C	4.84590100	-0.22230100	-0.34312500	C	-4.78352600	-0.08081900	-0.50641500
C	6.20481800	0.18583500	-0.24387800	C	-6.09816500	-0.61536000	-0.36035100
H	7.52933900	1.88892200	-0.38602300	H	-7.29321100	-2.39737600	-0.58390400
C	4.49443400	-1.57972200	-0.18158800	C	-4.51306100	1.25365600	-0.17806800
C	7.18424600	-0.82139100	0.07796200	C	-7.12433700	0.28189000	0.11423900
C	5.46926500	-2.55717200	0.16990500	C	-5.53580800	2.13204500	0.29434800
N	3.17352700	-1.89840300	-0.39926500	N	-3.20626200	1.67295400	-0.34061500
C	6.83383400	-2.12212800	0.29341900	C	-6.85995800	1.58386200	0.42365100
H	8.22463300	-0.51533200	0.16020400	H	-8.13319600	-0.10974800	0.22427000
C	5.03005900	-3.87311000	0.35501000	C	-5.17416200	3.44381000	0.60228700
C	2.78421000	-3.15695900	-0.16893000	C	-2.89517400	2.93589000	-0.02649900
H	7.59137700	-2.85864200	0.55127200	H	-7.65641400	2.23376500	0.77945600
C	3.66981200	-4.17084900	0.20073600	C	-3.83598500	3.85177700	0.44147400
H	5.74315600	-4.65069700	0.61774400	H	-5.92520600	4.14122300	0.96582700
H	1.72240800	-3.34076100	-0.30422900	H	-1.84880100	3.19245900	-0.16222400
H	3.30057200	-5.18209200	0.33834100	H	-3.52844800	4.86493000	0.67822400
Cu	2.07729300	-0.27837400	-0.74115300	Cu	-2.04967500	0.24137800	-1.04037000
O	1.26283200	0.71809900	-2.27022100	O	-1.16928100	-0.79353000	-2.46931900
O	0.46540800	-0.82500300	0.02831200	O	-0.46481000	1.06705700	-0.52881600
H	0.20178400	0.70710700	-2.19524100	H	-0.08490400	-0.80437300	-2.39543100
H	-0.23612700	-0.52270700	-0.57776200	H	0.24835400	0.69922400	-1.08200100

¹⁵				³⁵			
Charge=0 Multiplicity = 1				Charge=0 Multiplicity = 3			
Cu	2.03164800	-0.15951600	0.24044500	Cu	2.14547500	0.03649300	-0.08561500
O	1.03098700	-1.60836400	0.86136600	O	0.97727400	1.43217100	-0.54650900
H	0.42063500	-1.85895700	0.12800700	H	0.38859500	1.57932800	0.22544800
C	4.42413000	3.37835100	-0.69051800	C	4.77246500	-2.97223800	1.65786400
C	5.69145600	2.84242700	-0.80974000	C	6.02623600	-2.44785100	1.40235500
C	5.88198300	1.46052700	-0.58448300	C	6.13508000	-1.18862800	0.76963500
C	4.73274800	0.70596800	-0.26154500	C	4.92562100	-0.54575600	0.42874500
C	3.33684900	2.54470400	-0.35799000	C	3.62515600	-2.24825200	1.27795200
C	7.15108700	0.78950000	-0.65319400	C	7.37393000	-0.52808400	0.45968000
C	4.85315700	-0.69800500	0.00636800	C	4.94744100	0.74249500	-0.20254700
C	6.11222500	-1.33454700	-0.05230900	C	6.17531100	1.37567100	-0.49140000
C	7.26283100	-0.54742600	-0.39873900	C	7.39343100	0.69784200	-0.14254800
C	6.13574300	-2.71584400	0.24835200	C	6.09882800	2.64527000	-1.10930400
H	7.07795700	-3.25727800	0.21789700	H	7.01231400	3.18012000	-1.35681800
C	4.95944400	-3.36114400	0.58385500	C	4.85962200	3.19236900	-1.39162500
C	3.75085700	-2.63656000	0.61296500	C	3.68950900	2.47874600	-1.06130100

H	8.03108900	1.37351700	-0.90900700	H	8.30460500	-1.02608400	0.71782700
H	4.24806400	4.43750600	-0.84672000	H	4.65394600	-3.93387600	2.14563000
H	6.54166500	3.46949500	-1.06624400	H	6.92596900	-2.98901700	1.68369000
H	2.32106600	2.92178500	-0.23368800	H	2.62140000	-2.61383000	1.46668200
H	8.23175300	-1.03662000	-0.45024000	H	8.34009900	1.18144200	-0.36833700
H	4.95240600	-4.41909500	0.82478900	H	4.77472300	4.16563600	-1.86380300
H	2.78686200	-3.06751300	0.87019700	H	2.68278100	2.84431100	-1.24663300
N	3.48874600	1.23889700	-0.15928600	N	3.70013900	-1.06731800	0.67826500
N	3.70845100	-1.34152900	0.32795800	N	3.74117300	1.28621000	-0.48210200
H	-1.89653500	2.50243800	0.61955300	H	-2.42395000	-2.63540200	-1.07831400
C	-2.96443600	2.32632200	0.51100600	C	-3.45449600	-2.32568600	-0.92733000
C	-3.88537600	3.37268600	0.60871600	C	-4.50965000	-3.18123000	-1.24356100
N	-3.31981600	1.06390200	0.22805900	N	-3.62831400	-1.10384300	-0.39592700
C	-5.23925500	3.12264100	0.38816200	C	-5.82401000	-2.77855700	-0.99677100
H	-3.52980300	4.37575300	0.82199600	H	-4.29226900	-4.16456500	-1.64828200
C	-4.65752500	0.80043500	0.06309700	C	-4.92417900	-0.67605700	-0.21796500
C	-5.65336600	1.81283800	0.09905400	C	-6.05403600	-1.49817100	-0.46854000
H	-5.97037800	3.92609900	0.42824500	H	-6.66093400	-3.43917900	-1.20686800
C	-5.01295800	-0.55177400	-0.19570100	C	-5.09428800	0.64574200	0.27634200
C	-7.01188500	1.43923300	-0.18660300	C	-7.35599300	-0.97653200	-0.14935900
C	-6.35394600	-0.89207200	-0.51522100	C	-6.38470900	1.13103500	0.61499800
N	-4.00568900	-1.48481700	-0.09509100	N	-3.95721100	1.41355400	0.37032800
C	-7.34180000	0.15394300	-0.50039700	C	-7.51240100	0.26781300	0.38676400
H	-7.77567800	2.21288400	-0.16559400	H	-8.22238800	-1.60752600	-0.33246900
C	-6.63604600	-2.23538000	-0.81177600	C	-6.47551100	2.43304200	1.13225600
C	-4.31623500	-2.75593500	-0.40768400	C	-4.08357300	2.64531900	0.89492000
H	-8.37110900	-0.10707000	-0.73436300	H	-8.50402400	0.63661200	0.63735000
C	-5.59650600	-3.16785300	-0.77226800	C	-5.30714200	3.18538300	1.28601500
H	-7.64966600	-2.53667400	-1.06197700	H	-7.44428300	2.84464400	1.40277400
H	-3.50139300	-3.47077100	-0.32911200	H	-3.16272900	3.21575400	0.97560800
H	-5.77906400	-4.21623800	-0.98710600	H	-5.34445700	4.19853400	1.67429800
Cu	-2.24994500	-0.61702700	0.19890400	Cu	-2.34192500	0.36974700	-0.03708300
O	-1.05164600	-0.39413300	1.79437800	O	-1.03811500	0.12764700	-1.53131400
O	-0.96523100	-1.44682700	-0.97565900	O	-1.04136500	0.94276600	1.26179600
H	-0.25302400	-0.99911400	1.61061200	H	-0.26682900	0.75839400	-1.33532700
O	0.47490300	2.28355000	0.32907500	O	0.44788600	-2.13484800	-1.11920000
O	0.98331200	1.38570600	1.19113100	O	1.68586400	-1.66321400	-1.17833400
H	-0.58351400	0.46817500	1.74960300	H	-0.59889900	-0.75396000	-1.40860600
O	0.89450500	0.23788700	-1.51332000	O	0.79327500	-0.83009400	1.35453800
H	0.13197700	-0.44807800	-1.44815100	H	0.08757900	-0.07554700	1.38729700
H	0.47755200	1.07263500	-1.21658600	H	0.39299300	-1.47399300	0.73345200
H	-1.35579600	-1.93906800	-1.71091400	H	-1.41211200	1.18947300	2.12019800

¹TS5-6

³TS5-6

Charge=0 Multiplicity = 1				Charge=0 Multiplicity = 3			
Cu	-1.95636500	-0.62158600	-0.02375600	Cu	-2.02311800	-0.16853600	-0.17471500
O	-1.27010700	-2.15947600	-0.81197800	O	-1.00862400	-1.63098000	-0.79825800
H	-0.57901700	-2.52272400	-0.22969400	H	-0.40705600	-1.86629400	-0.05314100
C	-3.38629900	3.17575400	1.54792600	C	-4.40383600	3.35874500	0.89410000
C	-4.75531200	3.06286200	1.38207200	C	-5.68602700	2.84342200	0.90433800
C	-5.29037900	1.89596200	0.79124300	C	-5.88751200	1.48310300	0.58192700
C	-4.36273700	0.90032600	0.41488400	C	-4.73638200	0.72508000	0.26984500
C	-2.54051100	2.12560900	1.13601700	C	-3.32000600	2.52241500	0.56306400
C	-6.68704500	1.65674600	0.54692100	C	-7.17013400	0.83540000	0.54948100
C	-4.81535900	-0.30907300	-0.21269100	C	-4.86517500	-0.66450900	-0.06536200
C	-6.19119100	-0.51998900	-0.44785500	C	-6.13686200	-1.27770900	-0.10029700
C	-7.11783400	0.50223500	-0.04315900	C	-7.29063200	-0.48428100	0.22093500
C	-6.54259200	-1.73595900	-1.07754300	C	-6.16934200	-2.64526800	-0.45680600
H	-7.58756400	-1.95364300	-1.28439600	H	-7.12157700	-3.16795600	-0.49980800
C	-5.54986000	-2.63545600	-1.42576400	C	-4.98731000	-3.30101700	-0.75052500
C	-4.20205000	-2.33152200	-1.14664500	C	-3.76602800	-2.60120800	-0.68160300
H	-7.40278900	2.41986100	0.84147200	H	-8.05189000	1.42274800	0.79113500
H	-2.95085100	4.06488600	1.99223100	H	-4.21614300	4.39977000	1.13509800
H	-5.42173800	3.86272900	1.69556300	H	-6.53781100	3.47053800	1.15510800
H	-1.45633800	2.16465700	1.22810700	H	-2.29724700	2.88705700	0.53158100
H	-8.17801900	0.34130900	-0.22049300	H	-8.26917300	-0.95634000	0.19757400
H	-5.79511200	-3.57441700	-1.91155100	H	-4.98587200	-4.34915900	-1.03138900
H	-3.36590900	-2.98507500	-1.38343800	H	-2.79651900	-3.04150900	-0.90043900
N	-3.02723400	1.01552700	0.59379100	N	-3.48077400	1.23964100	0.25701000
N	-3.85322000	-1.19470200	-0.55777400	N	-3.71535200	-1.31842100	-0.34410700
H	1.43795000	2.09203400	-1.30971200	H	1.88967300	2.46094900	-0.83679100
C	2.51465100	2.07878500	-1.18361900	C	2.95666200	2.28838900	-0.71293400
C	3.34088800	3.15047000	-1.57761700	C	3.87673400	3.32705800	-0.87499200
N	3.01547800	0.98699400	-0.61806100	N	3.31058700	1.04733500	-0.34145900
C	4.70674100	3.08009300	-1.37082200	C	5.22962500	3.09647000	-0.62781700
H	2.89225400	4.02212900	-2.04282000	H	3.52039800	4.31251400	-1.15804800
C	4.34757200	0.90939400	-0.40520500	C	4.64888900	0.80011200	-0.14781700
C	5.25689400	1.92987800	-0.76309500	C	5.64284500	1.81067000	-0.24606600
H	5.35922100	3.89661700	-1.67012200	H	5.95977000	3.89687900	-0.71665600
C	4.82042000	-0.29214000	0.22157800	C	5.00777300	-0.52903300	0.20726300
C	6.65493700	1.72677900	-0.49997300	C	7.00063100	1.46269800	0.07355400
C	6.20346700	-0.47771700	0.44878300	C	6.34849100	-0.84223100	0.55621800
N	3.87672400	-1.20916600	0.54998000	N	4.00492000	-1.47077600	0.16865600
C	7.10883900	0.57420600	0.07446800	C	7.33339200	0.20324900	0.47587700
H	7.35374200	2.51200900	-0.77662400	H	7.76148100	2.23648900	0.00453600
C	6.59298100	-1.70394100	1.03085600	C	6.63363000	-2.16113200	0.94437200
C	4.27480500	-2.36303500	1.07604100	C	4.31780100	-2.71611000	0.56765800
H	8.17084000	0.43310400	0.25697600	H	8.36206100	-0.03747700	0.73323600

C	5.62800600	-2.64836400	1.33389500	C	5.59798400	-3.09854000	0.96378800
H	7.64429400	-1.89882400	1.22703100	H	7.64728500	-2.44046800	1.21891500
H	3.48315500	-3.07709700	1.28161200	H	3.50510000	-3.43711300	0.53545100
H	5.89829700	-3.60531700	1.76835100	H	5.78315000	-4.12933100	1.24964900
Cu	1.95298900	-0.65183900	-0.03380700	Cu	2.24378700	-0.63211500	-0.19572600
O	1.00692000	-0.74088900	-1.73289000	O	1.07262500	-0.57280000	-1.83045700
O	1.16605400	-2.10472600	0.91222500	O	0.97762500	-1.39175800	1.03767400
H	0.36331900	-1.48127800	-1.70220700	H	0.26623700	-1.04621700	-1.57255000
O	0.44203800	0.94306700	0.55521900	O	-0.36337900	2.14821500	-0.23181500
O	-0.49314500	0.79568800	-0.58832500	O	-0.85587800	1.24499600	-1.07112400
H	0.13034400	0.17463300	-1.24578100	H	0.24614800	0.60363400	-1.69609900
O	-0.96623500	-0.74440400	1.83116000	O	-0.96199900	0.21360900	1.66138500
H	-0.31621400	-1.46667700	1.61507200	H	-0.20775600	-0.38847100	1.56382800
H	-0.37765600	0.04660300	1.54563600	H	-0.60766500	1.07639300	1.35575000
H	1.57502900	-2.15227800	1.79110800	H	1.38812300	-1.87710500	1.76669000

¹ _g				³ _g			
Charge=0 Multiplicity = 1				Charge=0 Multiplicity = 3			
Cu	-2.01838200	-0.38950500	-0.06644900	Cu	-2.02349400	-0.16939900	-0.17314400
O	-1.14228900	-1.91529000	-0.68909900	O	-1.00929100	-1.63053500	-0.80021500
H	-0.49274000	-2.19409500	-0.01521300	H	-0.40765400	-1.86766100	-0.05572900
C	-4.01344900	3.35891600	0.94950100	C	-4.40357100	3.35572700	0.90417300
C	-5.34716200	2.99733400	0.91501100	C	-5.68583300	2.84056100	0.91339200
C	-5.69777600	1.67461600	0.56115900	C	-5.88755300	1.48102100	0.58785600
C	-4.63050600	0.79425400	0.27987500	C	-4.73657200	0.72356300	0.27385900
C	-3.01445400	2.40696000	0.65320100	C	-3.31990400	2.52001500	0.57105000
C	-7.04255800	1.17662600	0.46117100	C	-7.17027100	0.83357500	0.55408400
C	-4.90030300	-0.55691500	-0.12098100	C	-4.86560600	-0.66522700	-0.06455000
C	-6.22983900	-1.02209900	-0.22350400	C	-6.13738300	-1.27816700	-0.10073300
C	-7.29811200	-0.11234200	0.08766700	C	-7.29099800	-0.48532400	0.22249600
C	-6.39768800	-2.36264200	-0.63921300	C	-6.17010400	-2.64489100	-0.46040700
H	-7.39902100	-2.77522600	-0.73627100	H	-7.12241800	-3.16734400	-0.50449000
C	-5.28364900	-3.13326100	-0.92255300	C	-4.98820400	-3.30012200	-0.75580700
C	-3.99628200	-2.57573800	-0.78873900	C	-3.76681500	-2.60064600	-0.68543100
H	-7.86299600	1.85331800	0.68613600	H	-8.05191100	1.42048500	0.79722000
H	-3.71820800	4.37193600	1.20365300	H	-4.21570000	4.39616400	1.14755800
H	-6.12800700	3.71808700	1.14620200	H	-6.53749500	3.46721300	1.16573200
H	-1.94005300	2.62532000	0.63587400	H	-2.29709800	2.88458600	0.54027200
H	-8.32227300	-0.46877600	0.01404000	H	-8.26960800	-0.95719100	0.19817500
H	-5.38736900	-4.16354800	-1.24762700	H	-4.98695100	-4.34761100	-1.03910100
H	-3.07135700	-3.11120400	-0.98940500	H	-2.79739800	-3.04057400	-0.90542100
N	-3.32625900	1.15269300	0.33948300	N	-3.48089400	1.23797700	0.26204400
N	-3.81854500	-1.32006300	-0.39742100	N	-3.71591200	-1.31865200	-0.34497000
H	1.59653500	2.27062300	-0.64700200	H	1.88957400	2.46106700	-0.82966000

C	2.69387600	2.20178700	-0.66388300	C	2.95655600	2.28807100	-0.70635000
C	3.54166800	3.30384500	-0.91462100	C	3.87675200	3.32698400	-0.86612600
N	3.19622100	1.01216700	-0.34179500	N	3.31035800	1.04611000	-0.33780100
C	4.91234500	3.16279100	-0.82009200	C	5.22964400	3.09563500	-0.61967100
H	3.09677000	4.25815900	-1.17735900	H	3.52051500	4.31314400	-1.14684700
C	4.53745800	0.86609800	-0.22029700	C	4.64865200	0.79825100	-0.14491700
C	5.45751100	1.91114600	-0.44902700	C	5.64273600	1.80889600	-0.24096000
H	5.57603700	4.00197400	-1.01412200	H	5.95988900	3.89614600	-0.70675500
C	5.00780000	-0.42609800	0.19757800	C	5.00739900	-0.53176300	0.20703100
C	6.85938500	1.64410100	-0.28472700	C	7.00051700	1.45999300	0.07766700
C	6.39260200	-0.66291300	0.35733300	C	6.34812000	-0.84595700	0.55507500
N	4.06199800	-1.37461800	0.41918000	N	4.00440800	-1.47327400	0.16637900
C	7.30876000	0.41326000	0.10022400	C	7.33315600	0.19956900	0.47702200
H	7.56503800	2.44949000	-0.47113000	H	7.76146600	2.23383600	0.01033800
C	6.77376100	-1.96082700	0.76544600	C	6.63312700	-2.16579400	0.94013100
C	4.44865600	-2.58598700	0.80234700	C	4.31717000	-2.71957300	0.56244900
H	8.37287800	0.22905500	0.22035500	H	8.36182800	-0.04189700	0.73368200
C	5.80256200	-2.92099900	0.98630800	C	5.59735300	-3.10310000	0.95751600
H	7.82663500	-2.19495500	0.90052400	H	7.64678100	-2.44590700	1.21388600
H	3.65176200	-3.30718700	0.96015300	H	3.50436300	-3.44038600	0.52868300
H	6.06791600	-3.92586400	1.29776200	H	5.78241400	-4.13457600	1.24096100
Cu	2.18749200	-0.74080000	-0.11300000	Cu	2.24334200	-0.63352400	-0.19581600
O	1.09145000	-0.55588600	-1.57128100	O	1.07196500	-0.57025600	-1.83024400
O	1.13411700	-1.80721900	1.02570100	O	0.97724300	-1.39584800	1.03599300
H	0.35542300	-1.21320700	-1.49144600	H	0.26554600	-1.04415700	-1.57332500
O	-0.14806300	1.89454500	0.12586200	O	-0.30474000	2.20081000	-0.34066700
O	-0.79360300	1.14556000	-0.97994800	O	-0.85617900	1.24604400	-1.06643400
O	-0.86354200	-0.02862100	1.60850500	O	-0.96207000	0.20834000	1.66369100
H	-0.13874400	-0.70564100	1.53495800	H	-0.20792500	-0.39361800	1.56463500
H	-0.45756000	0.82628200	1.17068300	H	-0.60765700	1.07178000	1.36000800
H	1.59317400	-2.07190200	1.83712700	H	1.38777300	-1.88294100	1.76382600
H	-0.01414400	0.59875000	-1.32298700	H	-0.12525400	0.64288700	-1.27343800

¹ TS ₆₋₇				³ TS ₆₋₇			
Charge=0	Multiplicity = 1			Charge=0	Multiplicity = 3		
Cu	-2.03146200	-0.41845500	0.04594800	Cu	-2.03279600	-0.42315400	0.06218800
O	-1.14126500	-1.94164300	-0.55099500	O	-1.14046800	-1.94527800	-0.53402400
H	-0.46148000	-2.18956400	0.10514400	H	-0.45764000	-2.18995900	0.12023200
C	-4.06825900	3.34533900	0.95515500	C	-4.07184100	3.34279400	0.96221200
C	-5.39901700	2.98002700	0.87616600	C	-5.40238800	2.97902400	0.87338600
C	-5.73300000	1.65595500	0.51209500	C	-5.73510500	1.65600400	0.50444300
C	-4.65380400	0.77864300	0.26875000	C	-4.65510100	0.77792800	0.26738900
C	-3.05771100	2.39428700	0.69844300	C	-3.06063800	2.39110200	0.71071200
C	-7.07232200	1.15374000	0.36859700	C	-7.07392600	1.15570600	0.35000800

C	-4.90691500	-0.57097400	-0.14899700	C	-4.90682000	-0.57051800	-0.15516800
C	-6.23096400	-1.04117400	-0.29212000	C	-6.23032700	-1.03870500	-0.30939300
C	-7.31171500	-0.13611600	-0.01219300	C	-7.31205500	-0.13298200	-0.03546400
C	-6.38124800	-2.38174500	-0.71425300	C	-6.37911300	-2.37802100	-0.73603000
H	-7.37770200	-2.79840500	-0.83996800	H	-7.37513100	-2.79304600	-0.87032300
C	-5.25643600	-3.14768600	-0.96604700	C	-5.25343000	-3.14480200	-0.98128800
C	-3.97583400	-2.58502300	-0.79498400	C	-3.97344100	-2.58425100	-0.79900900
H	-7.90168900	1.82763900	0.56771000	H	-7.90391800	1.83020800	0.54441100
H	-3.78416700	4.36017800	1.21450600	H	-3.78842600	4.35691200	1.22508700
H	-6.18934900	3.69906000	1.07852400	H	-6.19335900	3.69854800	1.07143300
H	-1.98861400	2.62552500	0.71324000	H	-1.99205100	2.62259700	0.73184700
H	-8.33176800	-0.49659300	-0.11673600	H	-8.33173200	-0.49195600	-0.14848900
H	-5.34643900	-4.17817900	-1.29450000	H	-5.34226000	-4.17430700	-1.31312900
H	-3.04315100	-3.11740700	-0.96547300	H	-3.04018000	-3.11744700	-0.96371100
N	-3.35301600	1.13795700	0.37876200	N	-3.35471600	1.13553200	0.38714500
N	-3.81496800	-1.32933300	-0.39588400	N	-3.81407700	-1.32981400	-0.39540500
H	1.63846200	2.30569100	-0.63666600	H	1.64088800	2.30868000	-0.64000200
C	2.73232900	2.22285600	-0.65526500	C	2.73414000	2.22454100	-0.66110300
C	3.59093100	3.31764200	-0.90002200	C	3.59288700	3.31786000	-0.91150400
N	3.22066400	1.02394300	-0.34772700	N	3.22193600	1.02602700	-0.35141600
C	4.96048500	3.15863200	-0.81605500	C	4.96252400	3.15779500	-0.83079200
H	3.15590900	4.28003400	-1.14923300	H	3.15802600	4.27988700	-1.16236800
C	4.56115200	0.86079700	-0.23702700	C	4.56259100	0.86198300	-0.24413100
C	5.49262800	1.89643100	-0.46238200	C	5.49441600	1.89612900	-0.47489700
H	5.63301300	3.99186800	-1.00504000	H	5.63528300	3.98986100	-1.02402400
C	5.01869200	-0.44035100	0.16696200	C	5.02004100	-0.43851700	0.16198900
C	6.89234800	1.60997300	-0.31113800	C	6.89427100	1.60880600	-0.32647900
C	6.40118200	-0.69685900	0.31361100	C	6.40262900	-0.69585300	0.30596100
N	4.06235200	-1.37699700	0.39119300	N	4.06342700	-1.37374200	0.39075300
C	7.32898200	0.36984300	0.05852100	C	7.33072000	0.36933500	0.04560600
H	7.60684300	2.40812500	-0.49487900	H	7.60901100	2.40578100	-0.51431700
C	6.76771000	-2.00314000	0.70873500	C	6.76891100	-2.00139300	0.70378100
C	4.43413900	-2.59605700	0.76441400	C	4.43490800	-2.59213100	0.76643800
H	8.39159500	0.17118700	0.16867200	H	8.39343300	0.17006300	0.15365000
C	5.78508200	-2.95110300	0.93245000	C	5.78594500	-2.94784800	0.93239400
H	7.81834200	-2.25306200	0.83247000	H	7.81960500	-2.25193100	0.82573400
H	3.62678400	-3.30417500	0.92803900	H	3.62713100	-3.29889500	0.93377400
H	6.03931600	-3.96161600	1.23480300	H	6.04000600	-3.95773900	1.23696400
Cu	2.19177200	-0.72146400	-0.10230500	Cu	2.19226900	-0.71851300	-0.09881400
O	1.04583300	-0.52991100	-1.51771000	O	1.03987500	-0.52762400	-1.50891300
O	1.16417000	-1.76500700	1.07739600	O	1.16944100	-1.76152200	1.08520200
H	0.31042600	-1.18268500	-1.40443000	H	0.30498200	-1.18037800	-1.39176800
O	-0.14989400	1.94780300	0.13701200	O	-0.16144300	1.90554600	0.18636000
O	-0.80180800	1.26398700	-1.00173500	O	-0.80096000	1.27573200	-0.99793400

O	-0.84262400	0.07952700	1.54418200	O	-0.84237400	0.08466000	1.54610400
H	-0.11701900	-0.59570400	1.52554200	H	-0.11626000	-0.58952600	1.53114500
H	-0.42313000	0.97969500	1.02564700	H	-0.40712000	1.03793600	0.97812700
H	1.62850200	-1.98390500	1.89940600	H	1.63480300	-1.97471100	1.90814600
H	-0.04480800	0.67926100	-1.32251100	H	-0.04714000	0.68568600	-1.31651700

¹⁷				³⁷			
Charge=0 Multiplicity = 1				Charge=0 Multiplicity = 3			
Cu	-2.15956100	-0.56195900	0.31015200	Cu	-2.03185400	-0.41958700	0.04735500
O	-1.16091200	-1.90395600	-0.48737100	O	-1.14154400	-1.94255800	-0.54995800
H	-0.41586400	-2.11919200	0.10785800	H	-0.46156400	-2.19051800	0.10598500
C	-4.13667600	3.28597900	0.95412800	C	-4.06842200	3.34460600	0.95595400
C	-5.45811600	2.96500600	0.70798600	C	-5.39918700	2.97932800	0.87692200
C	-5.78884300	1.65031100	0.30752300	C	-5.73318500	1.65524400	0.51292100
C	-4.71669400	0.73989200	0.19066700	C	-4.65400500	0.77787800	0.26968100
C	-3.13267800	2.30450400	0.81022000	C	-3.05790400	2.39349900	0.69935800
C	-7.11879700	1.18961100	0.01349300	C	-7.07252100	1.15306800	0.36942500
C	-4.96933200	-0.61023300	-0.23002400	C	-4.90715700	-0.57175300	-0.14800300
C	-6.28138900	-1.03820100	-0.52809100	C	-6.23121900	-1.04191400	-0.29112300
C	-7.35588200	-0.09455200	-0.38755700	C	-7.31194800	-0.13680500	-0.01128000
C	-6.42640600	-2.38056900	-0.94808600	C	-6.38155500	-2.38250500	-0.71317600
H	-7.41454900	-2.76594000	-1.18727400	H	-7.37802400	-2.79913300	-0.83886900
C	-5.30775900	-3.18857800	-1.05491700	C	-5.25677100	-3.14850400	-0.96491800
C	-4.03976700	-2.66908900	-0.72690800	C	-3.97615000	-2.58588800	-0.79386500
H	-7.94302500	1.89115700	0.11327700	H	-7.90186700	1.82701100	0.56847500
H	-3.85341700	4.28910800	1.25536000	H	-3.78430500	4.35944900	1.21525800
H	-6.24314900	3.70983700	0.81420100	H	-6.18950800	3.69839600	1.07919800
H	-2.08304900	2.52230900	0.99123900	H	-1.98884700	2.62478000	0.71425500
H	-8.36829700	-0.42247300	-0.60850100	H	-8.33200900	-0.49725800	-0.11581800
H	-5.39363600	-4.21894700	-1.38467200	H	-5.34681100	-4.17901200	-1.29331500
H	-3.11281400	-3.23317200	-0.79284700	H	-3.04348700	-3.11832200	-0.96430700
N	-3.42256700	1.06266900	0.43535000	N	-3.35320300	1.13715700	0.37973100
N	-3.88839000	-1.41808100	-0.31186700	N	-3.81523600	-1.33018300	-0.39481500
H	1.94838200	2.50671800	-0.86681400	H	1.63822200	2.30486500	-0.63608300
C	3.01479700	2.31408900	-0.76242900	C	2.73209200	2.22209600	-0.65462100
C	3.98287200	3.31985200	-0.97559500	C	3.59069300	3.31695300	-0.89907100
N	3.36470600	1.07682400	-0.42277000	N	3.22041400	1.02315000	-0.34721400
C	5.32637100	3.02694700	-0.84468600	C	4.96024200	3.15796600	-0.81495600
H	3.65294900	4.31855300	-1.24155700	H	3.15568300	4.27938200	-1.14816500
C	4.68140800	0.77967100	-0.29101800	C	4.56089100	0.86003500	-0.23634400
C	5.71903800	1.71471000	-0.49347900	C	5.49237200	1.89572400	-0.46140100
H	6.08357000	3.78991900	-1.00789700	H	5.63277000	3.99125300	-1.00372100
C	5.00157600	-0.56987400	0.08456100	C	5.01840000	-0.44115500	0.16753000
C	7.08040300	1.28110400	-0.33617800	C	6.89207700	1.60926600	-0.30998400

C	6.34766500	-0.97676600	0.22489500	C	6.40086300	-0.69766800	0.31436600
N	3.95267500	-1.40621100	0.27459900	N	4.06203100	-1.37782400	0.39149200
C	7.38343700	-0.00623900	0.00438000	C	7.32868100	0.36909000	0.05956500
H	7.87546700	2.00436700	-0.49751900	H	7.60658700	2.40745700	-0.49350000
C	6.56951300	-2.32810000	0.57479500	C	6.76732100	-2.00400200	0.70938700
C	4.18484600	-2.66994200	0.61054900	C	4.43372700	-2.59692900	0.76465100
H	8.41889600	-0.31720200	0.11375600	H	8.39128300	0.17044400	0.16984800
C	5.48981200	-3.17236400	0.76533200	C	5.78465200	-2.95198600	0.93284500
H	7.58659500	-2.69426000	0.68933400	H	7.81793200	-2.25394600	0.83325600
H	3.29860400	-3.28091000	0.75597900	H	3.62629700	-3.30499700	0.92811800
H	5.63360300	-4.21420800	1.03204700	H	6.03884500	-3.96253200	1.23512800
Cu	2.15345600	-0.55783400	-0.09698300	Cu	2.19154600	-0.72241800	-0.10206100
O	0.86403900	-0.10635700	-1.31831200	O	1.04523100	-0.53085700	-1.51713900
O	1.18292700	-1.67196200	1.05870900	O	1.16440100	-1.76673000	1.07744400
H	0.11543600	-0.74462400	-1.21633400	H	0.30988800	-1.18367600	-1.40377200
O	0.16196700	2.24065100	0.73770300	O	-0.14963700	1.94631700	0.13805400
O	-0.20407500	2.20493400	-0.68394000	O	-0.80208400	1.26299000	-1.00061900
O	-1.00058600	0.07445900	1.60532900	O	-0.84266800	0.07835200	1.54501700
H	-0.23724800	-0.54407800	1.58900800	H	-0.11700700	-0.59675400	1.52574600
H	-0.28574700	1.38925500	1.08603700	H	-0.34762800	1.24695500	0.78038700
H	1.64048900	-1.81325200	1.90161900	H	1.62820400	-1.98395300	1.90021200
H	0.18560000	1.30944100	-0.96974000	H	-0.04529000	0.67819700	-1.32178000

8	Charge=0 Multiplicity = 1			9	Charge=0 Multiplicity = 1		
Cu	-1.85458500	-0.83299000	-0.13376000	Cu	0.13592700	-0.23541800	0.87590200
C	0.34358000	0.88505700	-0.08704400	C	2.54943800	0.76207700	-0.10698600
C	-1.51462000	2.23755500	-0.28884400	C	1.22804300	2.60467300	0.31924000
C	1.20920200	1.99354600	0.08480100	C	3.68268200	1.56289300	-0.39341600
C	0.86954000	-0.44731100	-0.05392700	C	2.64819600	-0.66623100	-0.16275600
C	-0.74438000	3.39345600	-0.09128000	C	2.30190000	3.47792400	0.08967200
H	-2.58670500	2.30323600	-0.45100200	H	0.24732800	2.98619100	0.58870000
C	0.62578500	3.27646900	0.08304100	C	3.53273300	2.95979300	-0.28178000
C	2.61752500	1.75241000	0.23354000	C	4.90167300	0.91572000	-0.79198200
C	2.26503800	-0.65709200	0.05989700	C	3.85061200	-1.27860900	-0.59110400
H	-1.22693600	4.36571200	-0.10105200	H	2.14969400	4.54864500	0.18252600
H	1.25102900	4.15569800	0.21458200	H	4.37624200	3.61310000	-0.48904700
C	3.12370700	0.48663700	0.20250800	C	4.97585500	-0.44118200	-0.90465300
H	3.27842900	2.60626100	0.35895500	H	5.76669600	1.53446800	-1.01661900
C	2.72858800	-1.98763700	0.03746900	C	3.87291900	-2.68520700	-0.67332900
C	0.43959900	-2.71861400	-0.14511500	C	1.60149500	-2.70829500	0.13125000
H	4.19326300	0.31951900	0.30027400	H	5.89996300	-0.91687500	-1.22273200
H	3.79239400	-2.19372300	0.11780400	H	4.77402300	-3.19598300	-1.00154100
C	1.80640400	-3.01623100	-0.08697400	C	2.73185800	-3.39449700	-0.32868600

H	-0.30096600	-3.51002600	-0.19966800	H	0.71321400	-3.24624700	0.44637000
H	2.12469200	-4.05355800	-0.11413600	H	2.70777700	-4.47818400	-0.38466700
O	-3.55107000	-0.80002400	0.68331600	O	-1.95530000	-0.63441500	0.17808300
N	-0.04473000	-1.46843700	-0.10189800	H	-1.96853600	-0.31258200	1.14839900
N	-0.99864200	1.00635500	-0.30443600	O	-1.00185100	0.26691800	2.28976000
H	-3.64989100	-1.39110900	1.44264900	N	1.54705200	-1.37307600	0.24805500
				N	1.32672900	1.27748700	0.21370200
				C	-2.65658000	0.29238100	-0.63806000
				H	-2.32642500	0.11046100	-1.66978700
				H	-2.37049000	1.32617400	-0.38973600
				C	-4.16632300	0.15000100	-0.56029500
				C	-4.99586200	1.23116000	-0.88126300
				C	-4.75427000	-1.06839800	-0.20428700
				C	-6.38448300	1.09727700	-0.85776800
				H	-4.55111300	2.18868400	-1.14709500
				C	-6.14307200	-1.20379200	-0.17405900
				H	-4.10931300	-1.90091900	0.05871600
				C	-6.96331500	-0.12305500	-0.50327300
				H	-7.01424300	1.94800200	-1.10642200
				H	-6.58593700	-2.15575200	0.10887700
				H	-8.04491900	-0.22832100	-0.47794000
				H	-0.94610400	-0.29243200	3.07699100

TS ₉₋₁₀				10			
Charge=0	Multiplicity = 1			Charge=0	Multiplicity = 1		
Cu	0.09342700	-0.23210000	0.84188300	Cu	-0.03182300	-0.21187600	0.83508800
C	2.52414400	0.75978000	-0.08528000	C	-2.59326000	-0.60178100	-0.11762400
C	1.20460800	2.58669800	0.41527000	C	-1.66340900	-2.66850100	0.34276300
C	3.63545700	1.57518200	-0.41179500	C	-3.78523700	-1.18342300	-0.61339100
C	2.63067400	-0.66688200	-0.17085100	C	-2.45036500	0.82381100	-0.08265400
C	2.25593300	3.47246300	0.13694900	C	-2.82061500	-3.32725700	-0.09204200
H	0.23465200	2.95803600	0.73261300	H	-0.80729600	-3.22929700	0.70411700
C	3.47591900	2.97006200	-0.28665400	C	-3.88419200	-2.58902200	-0.58814300
C	4.84699600	0.94500800	-0.85734400	C	-4.81505700	-0.31915100	-1.12075700
C	3.82844000	-1.26174800	-0.63590000	C	-3.47071900	1.65169100	-0.61269600
H	2.09573800	4.54071100	0.24308300	H	-2.86048600	-4.41120500	-0.05351800
H	4.30340700	3.63333600	-0.52418500	H	-4.78290300	-3.07653000	-0.95602500
C	4.93496900	-0.41046200	-0.97584100	C	-4.65843700	1.03520300	-1.13494800
H	5.69567100	1.57568600	-1.10922500	H	-5.72418200	-0.77183200	-1.50799100
C	3.86353900	-2.66749500	-0.73223900	C	-3.25710900	3.04446700	-0.58283300
C	1.60658000	-2.71995700	0.10824000	C	-1.14009100	2.63586400	0.48861500
H	5.85423200	-0.87358000	-1.32493800	H	-5.44025000	1.67539200	-1.53541200
H	4.76217100	-3.16491500	-1.08681100	H	-4.01217600	3.71680800	-0.98145200
C	2.73904300	-3.39244700	-0.36958700	C	-2.07931200	3.53334600	-0.04006500

H	0.72406500	-3.27016400	0.41955100	H	-0.21871200	2.99671500	0.93666500
H	2.72556700	-4.47583700	-0.43426300	H	-1.88067200	4.59966100	0.00037300
O	-1.90789600	-0.54735300	0.29840100	O	1.80334100	0.11664700	0.45894900
H	-1.83475400	-0.31536000	1.41393900	H	1.73415800	-0.44069700	2.03545500
O	-1.06222200	0.02216000	2.40884800	O	1.01735100	-0.70702900	2.69407400
N	1.53727000	-1.38763500	0.23097200	N	-1.30862200	1.31046700	0.48880700
N	1.31339400	1.25934700	0.30447200	N	-1.52201000	-1.33575600	0.31970400
C	-2.60010100	0.46200500	-0.40112900	C	2.48584800	-0.59426000	-0.52211400
H	-2.19651800	0.51293700	-1.42450100	H	2.06040800	-0.39712200	-1.52650500
H	-2.42089100	1.45337400	0.05134100	H	2.40523200	-1.69316400	-0.38544600
C	-4.10029300	0.22526800	-0.48204100	C	3.97067000	-0.25113300	-0.58457600
C	-4.95508000	1.25267300	-0.90171000	C	4.84342100	-1.00551300	-1.38002900
C	-4.65087300	-1.01996100	-0.16720500	C	4.48778300	0.82870200	0.13530800
C	-6.32902000	1.04028500	-1.01040900	C	6.19874300	-0.68728900	-1.45823000
H	-4.54080400	2.23084400	-1.14220700	H	4.45573200	-1.85418200	-1.94254700
C	-6.02696900	-1.23544000	-0.27089300	C	5.84538700	1.15074200	0.06233700
H	-3.98466200	-1.80977100	0.16395600	H	3.80424200	1.40407900	0.75090100
C	-6.87114200	-0.20805800	-0.69397700	C	6.70653800	0.39560700	-0.73467100
H	-6.97801800	1.85014000	-1.33521300	H	6.86104700	-1.28585400	-2.07973400
H	-6.44054600	-2.20937800	-0.01929900	H	6.23199200	1.99428800	0.63046600
H	-7.94240200	-0.37522600	-0.77321200	H	7.76348400	0.64445400	-0.79122800
H	-1.03695200	-0.67222700	3.08304000	H	1.05861900	-0.05966100	3.41505100

¹ 11				³ 11			
Charge=0 Multiplicity = 1				Charge=0 Multiplicity = 1			
Cu	0.17967500	-0.99280100	-0.52993900	Cu	0.01917800	-1.00810600	0.20638800
C	-2.32832600	0.13811300	0.29862200	C	2.55404600	0.22019200	-0.21677200
C	-2.31442700	-2.10468700	0.84774300	C	2.73618300	-2.05394400	-0.58080800
C	-3.62976400	0.33461600	0.81166800	C	3.91513400	0.45214700	-0.52147400
C	-1.61549600	1.23772800	-0.28958600	C	1.70071600	1.31687200	0.14550400
C	-3.61509000	-2.01118900	1.38005700	C	4.09890100	-1.92436600	-0.90642200
H	-1.76329200	-3.03974900	0.84259400	H	2.22498700	-3.00935600	-0.60623200
C	-4.27213200	-0.79537100	1.36589100	C	4.68943500	-0.67480100	-0.87527300
C	-4.20870100	1.64799300	0.73893200	C	4.42094800	1.79493000	-0.45620400
C	-2.20467400	2.51936100	-0.34878900	C	2.22425300	2.62805700	0.20325000
H	-4.08360600	-2.89673400	1.79621700	H	4.66828200	-2.80642000	-1.17943800
H	-5.27503100	-0.69933500	1.77389700	H	5.74069200	-0.54939100	-1.12151700
C	-3.52720900	2.69333200	0.18485200	C	3.61078900	2.83692900	-0.10666200
H	-5.20921300	1.79516300	1.13646600	H	5.46788900	1.96706500	-0.69025900
C	-1.43147200	3.54424900	-0.94131100	C	1.32478100	3.65607800	0.56913100
C	0.33041300	1.93945900	-1.31843600	C	-0.41557900	1.99908400	0.76270800
H	-3.98048200	3.67985400	0.13860400	H	4.00676100	3.84768200	-0.05715300
H	-1.83608100	4.55065600	-1.01261000	H	1.67664200	4.68291200	0.62875000
C	-0.16880900	3.25322100	-1.42369000	C	0.00897300	3.34061300	0.84810700

H	1.30952600	1.63836600	-1.67877700	H	-1.43605400	1.69569400	0.97548100
H	0.44420300	4.02134900	-1.88341900	H	-0.70403800	4.10767500	1.13158100
O	1.75944100	-0.70148600	-1.50775000	O	-1.58745600	-0.85929800	1.14015200
H	0.68081300	-2.00314800	-2.53369300	H	-0.70318600	-2.08496600	2.15803400
O	-0.21054300	-2.37212800	-2.35002000	O	0.08158500	-2.64963300	2.37421800
N	-0.37775000	0.96570000	-0.76204200	N	0.40552100	1.01929300	0.41314500
N	-1.68832700	-1.05732200	0.32280000	N	1.98779100	-1.01107300	-0.24106100
C	3.02084300	-1.03368900	-0.98809800	C	-2.84188900	-1.34074900	0.72865100
H	3.76331200	-0.98040600	-1.80279400	H	-3.40511800	-1.66003700	1.62188200
H	3.04522900	-2.06664300	-0.60303100	H	-2.74666300	-2.23125400	0.08385800
C	3.45246000	-0.08885300	0.12335200	C	-3.64089100	-0.27546000	-0.00167300
C	4.16998100	1.08011400	-0.16132600	C	-4.15846100	0.81835900	0.71160700
C	3.08979800	-0.34181500	1.45458600	C	-3.84805400	-0.32055600	-1.38399900
C	4.51675400	1.97672600	0.85161500	C	-4.85894200	1.83449100	0.06367700
H	4.46736500	1.28207900	-1.18901100	H	-4.01038400	0.86135900	1.78899500
C	3.43251900	0.55213300	2.47107700	C	-4.54796000	0.69650100	-2.04186000
H	2.54596700	-1.25473300	1.68857300	H	-3.45644600	-1.16359700	-1.94959000
C	4.14668100	1.71517400	2.17250100	C	-5.05590600	1.77625100	-1.32042100
H	5.08249300	2.87444200	0.61236600	H	-5.26408100	2.66642900	0.63564900
H	3.15104700	0.33588200	3.49912300	H	-4.70035500	0.64038300	-3.11716200
H	4.42028600	2.40813800	2.96442700	H	-5.60966400	2.56218800	-1.82794800
H	-0.03110800	-3.12304800	-1.73499000	H	-0.10766700	-3.47598800	1.89932600
O	0.40486100	-3.70791200	-0.02602700	O	-0.86712100	-3.59652700	-0.34892900
O	0.72879900	-2.54713000	0.51517500	O	-0.18323400	-2.58911800	-0.82675300

¹ TS ₁₁₋₁₂				³ TS ₁₁₋₁₂			
Charge=0 Multiplicity = 1				Charge=0 Multiplicity = 3			
Cu	-0.03598500	-0.40706600	0.48918600	Cu	-0.09251700	-0.61095500	0.68685500
C	2.69186900	-0.29158000	-0.33177000	C	2.51076800	-0.19354900	-0.43510400
C	1.93761700	-2.46975200	-0.54878300	C	1.89980200	-2.38511100	-0.83479300
C	3.99208100	-0.61040500	-0.77883800	C	3.76719200	-0.34734800	-1.06189600
C	2.36762500	1.05785200	0.04004000	C	2.13938100	1.07828400	0.12234500
C	3.20692900	-2.88438900	-1.00203000	C	3.12894900	-2.63864200	-1.47498400
H	1.09333400	-3.14682000	-0.41736200	H	1.13827300	-3.15078700	-0.71525900
C	4.22980300	-1.96197100	-1.11989900	C	4.06130800	-1.62475000	-1.59016900
C	4.96878500	0.44089000	-0.85830800	C	4.64964900	0.78543400	-1.12609900
C	3.34201700	2.07574700	-0.05622100	C	3.01797600	2.18056400	0.03550300
H	3.36459100	-3.92796700	-1.25336800	H	3.32740200	-3.62932400	-1.87017300
H	5.21386800	-2.26349500	-1.46986800	H	5.01511000	-1.79817100	-2.08183900
C	4.65795800	1.72587600	-0.51597400	C	4.29129300	1.99510600	-0.60406800
H	5.96939400	0.19345500	-1.20248300	H	5.61616600	0.66134700	-1.60699300
C	2.93623900	3.37851900	0.31242200	C	2.56300600	3.39802000	0.59155000
C	0.73839000	2.51318700	0.79922300	C	0.50469500	2.30213100	1.20946000
H	5.40804600	2.50888900	-0.58615400	H	4.96966500	2.84167700	-0.66640300

H	3.64698000	4.19917800	0.25831300	H	3.20018400	4.27788700	0.55386500
C	1.63646100	3.59605400	0.73272500	C	1.30861600	3.45828700	1.17193900
H	-0.29554300	2.62684000	1.11097200	H	-0.49522900	2.28327200	1.63425600
H	1.29827000	4.58766500	1.01447900	H	0.93440500	4.38285900	1.59886700
O	-1.64178800	0.58296300	0.59582700	O	-1.65452700	0.22502200	1.25762300
H	-0.53388400	-1.53731400	2.93976500	H	-0.19862600	-1.95087100	3.02670500
O	0.11398800	-1.71286400	2.24100300	O	0.41982200	-2.10730800	2.29609000
N	1.10107500	1.27976600	0.46853700	N	0.91970500	1.14735800	0.70378200
N	1.69411200	-1.20128300	-0.23482600	N	1.59887800	-1.19173000	-0.33355900
C	-2.70781700	-0.24765300	0.65162900	C	-2.76717400	-0.52881600	0.90044900
H	-2.86387900	-0.77979800	1.61069900	H	-3.29338700	-0.95847900	1.77472100
H	-2.16525300	-1.34831700	0.00419000	H	-2.28783600	-1.47853300	0.32129900
C	-3.96087800	0.18166000	0.01175800	C	-3.74243600	0.15928100	-0.00915100
C	-3.97493400	1.23043400	-0.92721700	C	-3.36098000	1.27299500	-0.77112200
C	-5.17120100	-0.48342800	0.29031200	C	-5.05047400	-0.33024200	-0.15774500
C	-5.15902400	1.60264700	-1.55791900	C	-4.25678100	1.87868500	-1.65246000
H	-3.04247600	1.74399100	-1.13823900	H	-2.35453800	1.65969400	-0.64529400
C	-6.35226500	-0.11314700	-0.34532900	C	-5.94664300	0.27050400	-1.03950400
H	-5.17471900	-1.29691700	1.01332400	H	-5.36500700	-1.19145700	0.42936900
C	-6.35367400	0.93370700	-1.27345300	C	-5.55386900	1.38064600	-1.79311500
H	-5.15378000	2.41888900	-2.27687800	H	-3.94322100	2.74518500	-2.23114700
H	-7.27676400	-0.63743800	-0.11551900	H	-6.95592000	-0.12323200	-1.13634900
H	-7.27649800	1.22460700	-1.76867000	H	-6.25291700	1.85299100	-2.47884700
H	-0.32064600	-2.45386700	1.62661700	H	-0.03645700	-2.79345400	1.71279000
O	-0.93061100	-3.08442800	0.43402300	O	-0.93222800	-3.30995800	0.42052300
O	-1.11279700	-1.89836400	-0.30915300	O	-1.20191900	-2.09165800	-0.10125500

12r	Charge=0 Multiplicity = 1			12u	Charge=0 Multiplicity = 1		
Cu	-0.11102900	-0.68075500	-0.28134500	Cu	-0.80481400	-1.07258500	-0.05814100
C	-2.87275500	-0.07930300	-0.23199800	C	-3.36333900	0.03070200	-0.08072700
C	-2.58893900	-2.33029800	-0.73121100	C	-3.62741600	-2.26325500	-0.09338500
C	-4.28645600	-0.18267500	-0.25688300	C	-4.75213200	0.25476600	-0.25121500
C	-2.23683200	1.15908800	0.04045700	C	-2.46040100	1.13781000	-0.00264900
C	-3.97693000	-2.52412500	-0.77562800	C	-5.00779100	-2.14088700	-0.30524600
H	-1.87374700	-3.12779400	-0.90655300	H	-3.15626200	-3.23812500	-0.01005800
C	-4.82980300	-1.44852900	-0.53739700	C	-5.58047100	-0.87842400	-0.36869400
C	-5.05135800	1.00574200	0.00664200	C	-5.23164100	1.60902100	-0.27365300
C	-3.00684700	2.32203300	0.29248500	C	-2.96147600	2.46244800	0.01238500
H	-4.37038100	-3.51131700	-0.99289900	H	-5.61676700	-3.03583400	-0.38682400
H	-5.90857000	-1.57897500	-0.56600200	H	-6.65207400	-0.75507800	-0.50201700
C	-4.44108900	2.19838900	0.26867600	C	-4.37844800	2.66244200	-0.12490900
H	-6.13607600	0.93745400	-0.00673800	H	-6.29855500	1.77845700	-0.39536600
C	-2.30847800	3.51542200	0.54386000	C	-2.03016700	3.51018900	0.14751200

C	-0.23273900	2.30819600	0.27935400	C	-0.26890000	1.86272400	0.17190000
H	-5.03736800	3.08576600	0.46468900	H	-4.75756800	3.68125200	-0.12353600
H	-2.85523600	4.43228400	0.74657200	H	-2.37157200	4.54163300	0.16898000
C	-0.91144300	3.50367700	0.52725200	C	-0.68173700	3.19767900	0.25096300
H	0.85082700	2.25551200	0.26098500	H	0.78456300	1.60330200	0.21149700
H	-0.34366700	4.40992300	0.70945100	H	0.06573600	3.97691100	0.36289900
O	1.67011000	0.06633000	-0.39227900	O	2.72419300	0.23140200	0.96032100
H	1.21066900	-2.51964000	-1.11319800	H	0.32677900	-2.24781900	-1.89567900
O	0.37026300	-2.46683400	-0.63386300	O	-0.10336300	-2.50942600	-1.06971800
N	-0.86634600	1.15308700	0.03981500	N	-1.12135200	0.83673800	0.01507900
N	-2.04775000	-1.14076200	-0.47062800	N	-2.81179700	-1.21297300	0.03848000
C	2.72564300	-0.54469700	0.01038200	C	3.63109400	-0.49609400	0.55966400
H	2.61428000	-1.51573700	0.50860100	H	3.47292700	-1.58775000	0.53028300
C	4.04599500	-0.01788100	-0.14557000	C	4.93970500	0.00049600	0.10565400
C	4.28838700	1.21456500	-0.80608200	C	5.23339300	1.37403400	0.11446000
C	5.15547300	-0.73393300	0.37163100	C	5.90182400	-0.91820000	-0.33854600
C	5.58131900	1.70106400	-0.93310600	C	6.47709100	1.81895200	-0.31822100
H	3.44451900	1.76080000	-1.21531200	H	4.47466500	2.06688000	0.46496400
C	6.44412000	-0.23721900	0.23942400	C	7.14800800	-0.47013600	-0.77263100
H	4.98410400	-1.68144300	0.87809300	H	5.66654400	-1.98005000	-0.34085300
C	6.66795200	0.98380100	-0.41232700	C	7.43364700	0.89711000	-0.76190600
H	5.75339100	2.64562800	-1.44353800	H	6.70880800	2.88033300	-0.31231500
H	7.28292100	-0.79860000	0.64295500	H	7.89366400	-1.18078100	-1.11711700
H	7.67795500	1.37042200	-0.51569500	H	8.40510900	1.24823400	-1.09964000
H	0.69659400	-2.84432700	0.87914000	H	0.90773100	-2.77839400	0.02651400
O	0.86760000	-2.80558400	1.88370000	O	1.40375100	-2.69533400	0.94117200
O	0.28838500	-1.48540000	2.12674000	O	0.62421800	-1.56316900	1.45364500
H	1.06611400	-1.01233200	2.47001300	H	1.30248500	-0.85058800	1.42155500

³12

Charge=0 Multiplicity = 3

Cu	-0.11102900	-0.68075500	-0.28134500
C	-2.87275500	-0.07930300	-0.23199800
C	-2.58893900	-2.33029800	-0.73121100
C	-4.28645600	-0.18267500	-0.25688300
C	-2.23683200	1.15908800	0.04045700
C	-3.97693000	-2.52412500	-0.77562800
H	-1.87374700	-3.12779400	-0.90655300
C	-4.82980300	-1.44852900	-0.53739700
C	-5.05135800	1.00574200	0.00664200
C	-3.00684700	2.32203300	0.29248500
H	-4.37038100	-3.51131700	-0.99289900
H	-5.90857000	-1.57897500	-0.56600200
C	-4.44108900	2.19838900	0.26867600

H	-6.13607600	0.93745400	-0.00673800
C	-2.30847800	3.51542200	0.54386000
C	-0.23273900	2.30819600	0.27935400
H	-5.03736800	3.08576600	0.46468900
H	-2.85523600	4.43228400	0.74657200
C	-0.91144300	3.50367700	0.52725200
H	0.85082700	2.25551200	0.26098500
H	-0.34366700	4.40992300	0.70945100
O	1.67011000	0.06633000	-0.39227900
H	1.21066900	-2.51964000	-1.11319800
O	0.37026300	-2.46683400	-0.63386300
N	-0.86634600	1.15308700	0.03981500
N	-2.04775000	-1.14076200	-0.47062800
C	2.72564300	-0.54469700	0.01038200
H	2.61428000	-1.51573700	0.50860100
C	4.04599500	-0.01788100	-0.14557000
C	4.28838700	1.21456500	-0.80608200
C	5.15547300	-0.73393300	0.37163100
C	5.58131900	1.70106400	-0.93310600
H	3.44451900	1.76080000	-1.21531200
C	6.44412000	-0.23721900	0.23942400
H	4.98410400	-1.68144300	0.87809300
C	6.66795200	0.98380100	-0.41232700
H	5.75339100	2.64562800	-1.44353800
H	7.28292100	-0.79860000	0.64295500
H	7.67795500	1.37042200	-0.51569500
H	0.69659400	-2.84432700	0.87914000
O	0.86760000	-2.80558400	1.88370000
O	0.28838500	-1.48540000	2.12674000
H	1.06611400	-1.01233200	2.47001300