

Supporting information

Mechanistic insight into the alcohol oxidation mediated by an efficient green
Cu^{II}-bipy catalyst with and without TEMPO by density functional methods

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

0				1			
Charge=1 Multiplicity = 2				Charge=1 Multiplicity = 2			
C	-2.63128500	0.31814400	0.00207400	C	-0.86066200	2.27081800	-0.43436600
C	-3.48637900	-0.78034400	-0.01010500	C	-0.36649100	3.56627600	-0.31742800
C	-2.92849300	-2.05751300	-0.01132100	C	0.97994000	3.73586200	0.00037400
C	-1.54027100	-2.20154100	-0.00294900	C	1.78490900	2.61240500	0.18426100
C	-0.74123800	-1.06034800	0.00759000	C	1.22450100	1.34233700	0.04907400
N	-1.29658300	0.17869300	0.01217100	N	-0.09032000	1.18728000	-0.25503100
H	-3.56472000	-2.93692700	-0.02043300	H	1.40324500	4.73033000	0.10081500
H	-3.00830400	1.33559600	0.00135400	H	-1.89966800	2.08232000	-0.68265100
H	-4.56003400	-0.62969000	-0.01907600	H	-1.02405200	4.41411900	-0.47386000
H	-1.09573600	-3.18979200	-0.00664700	H	2.83503600	2.73039100	0.42403400
H	3.56414300	-2.93760400	-0.01638500	H	4.94839400	-1.37743600	0.95426600
C	2.92806200	-2.05806700	-0.00912900	C	3.90373300	-1.28512400	0.67408500
C	3.48617300	-0.78099200	-0.01040100	C	3.13313800	-2.42110400	0.43089900
C	1.53981500	-2.20184900	-0.00061600	C	3.32302700	-0.02117200	0.55988800
C	2.63126900	0.31766900	-0.00032600	C	1.79705800	-2.25400400	0.07552300
H	4.55985800	-0.63056200	-0.01954700	H	3.55172700	-3.41792400	0.51428300
C	0.74098200	-1.06048900	0.00761500	C	1.97905400	0.07404700	0.20032800
H	1.09511600	-3.19003300	-0.00207500	H	3.91281900	0.86714800	0.75341000
N	1.29654900	0.17843600	0.00988100	N	1.24517000	-1.03843000	-0.03495400
H	3.00846800	1.33504800	-0.00313200	H	1.13211300	-3.08759300	-0.12413100
Cu	0.00013000	1.61981700	0.02352500	Cu	-0.63332900	-0.69794600	-0.49054100
O	0.00046300	3.35075000	-0.14928200	O	-1.16892500	-2.25981400	-1.22036500
H	0.00214600	3.95534800	0.60902000	H	-0.61478500	-2.63920000	-1.91686300
O	0.00046300	3.35075000	-0.14928200	C	-3.69911100	0.07365900	0.53823600
H	0.00214600	3.95534800	0.60902000	H	-4.13644000	0.47289700	-0.38606000
				O	-2.54053600	-0.73108800	0.20848500
				H	-2.79663600	-1.54831800	-0.26808200
				C	-4.71620100	-0.73056700	1.32933500
				H	-5.57097500	-0.09719600	1.58989000
				H	-5.09518400	-1.57506300	0.74237300
				H	-4.27487200	-1.11623400	2.25315700
				H	-3.30982800	0.90687100	1.12878800

TS₁₋₂

Charge=1 Multiplicity = 2

C	-0.71557900	2.36343300	-0.13889100
C	-0.12261000	3.62193100	-0.09478100
C	1.26529000	3.69892200	0.00054700
C	2.01374100	2.52292100	0.04939100

2

Charge=1 Multiplicity = 2

C	0.85100300	2.31531800	0.42121900
C	0.31217200	3.59691800	0.34649500
C	-1.04754800	3.73130200	0.07312800
C	-1.82467600	2.58775400	-0.11079000

C	1.35581600	1.29490100	-0.00082100	C	-1.22197100	1.33362600	-0.01710400
N	0.00250300	1.23157800	-0.09922400	N	0.10401200	1.21568000	0.24731800
H	1.76411700	4.66223300	0.03901100	H	-1.50290000	4.71420100	0.00368800
H	-1.79061900	2.24429500	-0.20628400	H	1.90335500	2.15053000	0.62414900
H	-0.73962600	4.51274100	-0.13175200	H	0.94896100	4.46147400	0.49739200
H	3.09345000	2.56905500	0.12805600	H	-2.88344000	2.67961000	-0.32231100
H	4.98377700	-1.67511500	0.29815200	H	-4.90736300	-1.46613600	-0.81136200
C	3.91396800	-1.51142200	0.21393200	C	-3.85153700	-1.35370000	-0.58578700
C	3.03425500	-2.59136100	0.16547100	C	-3.03995300	-2.47417700	-0.41542900
C	3.41154800	-0.21026800	0.15647200	C	-3.29694600	-0.07977700	-0.46284500
C	1.66990200	-2.33388400	0.05387900	C	-1.69199300	-2.27983500	-0.12807500
H	3.39034500	-3.61447300	0.21197200	H	-3.43621500	-3.47976300	-0.50200500
C	2.03456700	-0.02301400	0.04945200	C	-1.93792400	0.04380700	-0.17493300
H	4.08784500	0.63546400	0.19649600	H	-3.91966500	0.79761500	-0.59119100
N	1.19268700	-1.08255100	-0.00094300	N	-1.15764000	-1.05420700	-0.01723200
H	0.92404900	-3.12080700	0.01143300	H	-1.00967600	-3.10998400	0.02175800
Cu	-0.70239600	-0.61010100	-0.14162800	Cu	0.73535100	-0.65226500	0.28443500
O	-1.42697100	-2.37669100	-0.48118700	O	1.17643700	-2.34765200	1.41622600
H	-1.57499400	-2.63300700	-1.40639000	H	1.10499700	-2.36708000	2.38475200
C	-3.70180500	0.14772700	-0.05728100	C	3.39765000	0.13429600	-0.63583800
H	-3.75139000	0.17468300	-1.15751100	H	3.83599800	0.82996500	0.10164400
O	-2.54316500	-0.56807000	0.37494300	O	2.50601500	-0.75120100	-0.00063500
H	-2.35569500	-1.71734900	-0.06995900	H	2.13277800	-2.26175600	1.20070600
C	-4.96043600	-0.49045400	0.51480400	C	4.52319600	-0.65091800	-1.30618200
H	-5.84621400	0.07813400	0.21052400	H	5.23268700	0.03118200	-1.78800200
H	-5.07643800	-1.51908000	0.15624900	H	5.06578200	-1.24773600	-0.56593200
H	-4.91659900	-0.50907800	1.60788900	H	4.11865400	-1.32715800	-2.06629200
H	-3.61972100	1.18356200	0.29741000	H	2.87779800	0.74353400	-1.39408700

3				3			
Charge=1 Multiplicity = 3				Charge=1 Multiplicity = 1			
C	-3.39455400	1.59596100	0.70556600	C	-3.39455400	1.59596100	0.70556600
C	-4.65209700	1.46950100	1.29290800	C	-4.65209700	1.46950100	1.29290800
C	-5.19672100	0.19461200	1.43166900	C	-5.19672100	0.19461200	1.43166900
C	-4.48084300	-0.90928500	0.96812800	C	-4.48084300	-0.90928500	0.96812800
C	-3.22786600	-0.70636300	0.38834000	C	-3.22786600	-0.70636300	0.38834000
N	-2.70059100	0.53336500	0.28177800	N	-2.70059100	0.53336500	0.28177800
H	-6.17265000	0.05645900	1.88671300	H	-6.17265000	0.05645900	1.88671300
H	-2.91494100	2.55389500	0.54261500	H	-2.91494100	2.55389500	0.54261500
H	-5.18571700	2.35231300	1.62757100	H	-5.18571700	2.35231300	1.62757100
H	-4.90151900	-1.90428100	1.05460100	H	-4.90151900	-1.90428100	1.05460100
H	-2.14658700	-5.10017600	-0.84983700	H	-2.14658700	-5.10017600	-0.84983700
C	-1.88416900	-4.04712300	-0.82211500	C	-1.88416900	-4.04712300	-0.82211500
C	-0.70013700	-3.59367700	-1.40161100	C	-0.70013700	-3.59367700	-1.40161100

C	-2.73554900	-3.13078200	-0.20879100	C	-2.73554900	-3.13078200	-0.20879100
C	-0.40676100	-2.23470500	-1.33229700	C	-0.40676100	-2.23470500	-1.33229700
H	-0.01525300	-4.27322500	-1.89685100	H	-0.01525300	-4.27322500	-1.89685100
C	-2.38233200	-1.77965200	-0.18839400	C	-2.38233200	-1.77965200	-0.18839400
H	-3.66195200	-3.46686900	0.24159700	H	-3.66195200	-3.46686900	0.24159700
N	-1.22300300	-1.35123100	-0.74227700	N	-1.22300300	-1.35123100	-0.74227700
H	0.50281200	-1.82849500	-1.75944400	H	0.50281200	-1.82849500	-1.75944400
Cu	-0.85067600	0.61593100	-0.52893200	Cu	-0.85067600	0.61593100	-0.52893200
H	4.30514100	-2.31120700	1.96143300	H	4.30514100	-2.31120700	1.96143300
C	3.93592500	-1.73741600	1.10434600	C	3.93592500	-1.73741600	1.10434600
C	5.08472300	-0.93101100	0.46195900	C	5.08472300	-0.93101100	0.46195900
C	2.73057600	-0.90160300	1.58255300	C	2.73057600	-0.90160300	1.58255300
H	3.55815200	-2.47713200	0.38797300	H	3.55815200	-2.47713200	0.38797300
H	5.53649300	-1.53658800	-0.33067800	H	5.53649300	-1.53658800	-0.33067800
C	4.62790100	0.42827200	-0.09843200	C	4.62790100	0.42827200	-0.09843200
H	5.88052800	-0.75231500	1.19231700	H	5.88052800	-0.75231500	1.19231700
N	2.26051600	-0.07048000	0.41988300	N	2.26051600	-0.07048000	0.41988300
C	3.18306900	0.47605000	-0.63832400	C	3.18306900	0.47605000	-0.63832400
H	5.29096900	0.74239600	-0.91190800	H	5.29096900	0.74239600	-0.91190800
H	4.72253200	1.19942100	0.67315500	H	4.72253200	1.19942100	0.67315500
O	1.00392100	0.22659400	0.38921900	O	1.00392100	0.22659400	0.38921900
C	2.81233200	1.93772600	-0.92902400	C	2.81233200	1.93772600	-0.92902400
H	1.78388200	2.03501100	-1.27613100	H	1.78388200	2.03501100	-1.27613100
H	2.93833500	2.55792400	-0.03625700	H	2.93833500	2.55792400	-0.03625700
H	3.47941600	2.32321400	-1.70677900	H	3.47941600	2.32321400	-1.70677900
C	3.02255700	-0.36910700	-1.91919100	C	3.02255700	-0.36910700	-1.91919100
H	3.72611900	-0.01484700	-2.67993200	H	3.72611900	-0.01484700	-2.67993200
H	3.22900300	-1.42930400	-1.74049100	H	3.22900300	-1.42930400	-1.74049100
H	2.01368800	-0.25810400	-2.32842600	H	2.01368800	-0.25810400	-2.32842600
C	3.07285800	0.02599400	2.76859800	C	3.07285800	0.02599400	2.76859800
H	2.21169500	0.65567000	3.01328500	H	2.21169500	0.65567000	3.01328500
H	3.31240200	-0.58142800	3.64797900	H	3.31240200	-0.58142800	3.64797900
H	3.92825000	0.67520600	2.56873900	H	3.92825000	0.67520600	2.56873900
C	1.59697200	-1.84963000	2.00315500	C	1.59697200	-1.84963000	2.00315500
H	0.73499700	-1.30149400	2.38792100	H	0.73499700	-1.30149400	2.38792100
H	1.26906800	-2.47325500	1.16548700	H	1.26906800	-2.47325500	1.16548700
H	1.96761500	-2.50949200	2.79386300	H	1.96761500	-2.50949200	2.79386300
H	-1.10522100	5.10183500	-0.37469900	H	-1.10522100	5.10183500	-0.37469900
C	-0.13574800	4.71113500	-0.04667800	C	-0.13574800	4.71113500	-0.04667800
C	-0.26911000	3.26476700	0.42420000	C	-0.26911000	3.26476700	0.42420000
H	0.23969000	5.34996100	0.76122700	H	0.23969000	5.34996100	0.76122700
H	0.55898300	4.77799500	-0.89131300	H	0.55898300	4.77799500	-0.89131300
O	-0.77705800	2.46107700	-0.61718200	O	-0.77705800	2.46107700	-0.61718200
H	-0.94068800	3.23391100	1.30278800	H	-0.94068800	3.23391100	1.30278800

O	-0.32875400	1.02019100	-2.66483200	O	-0.32875400	1.02019100	-2.66483200
H	-0.97436400	0.96771800	-3.38748100	H	-0.97436400	0.96771800	-3.38748100
H	-0.35927000	1.94874100	-2.32435600	H	-0.35927000	1.94874100	-2.32435600
H	0.70851000	2.89808000	0.77164900	H	0.70851000	2.89808000	0.77164900

3r							
Charge=1 Multiplicity = 1							
C	-3.47124300	1.58122100	0.60328400				
C	-4.81948000	1.45096700	0.93443200				
C	-5.39268200	0.18088100	0.91271400				
C	-4.61080500	-0.91697900	0.55209200				
C	-3.26956200	-0.70777900	0.22903400				
N	-2.72247500	0.52459300	0.27199000				
H	-6.43814400	0.04155900	1.17009100				
H	-2.94678800	2.53087200	0.57874200				
H	-5.39921300	2.32794800	1.20107400				
H	-5.04343100	-1.91051000	0.52891700				
H	-2.00492500	-5.01567800	-1.11281500				
C	-1.72946400	-3.98830800	-0.89578900				
C	-0.41537500	-3.55398800	-1.05268100				
C	-2.69303600	-3.08210300	-0.45826600				
C	-0.11752600	-2.22653000	-0.75908400				
H	0.36737600	-4.22243800	-1.39400800				
C	-2.32431600	-1.76218000	-0.19475200				
H	-3.72265800	-3.39728700	-0.33746900				
N	-1.03804000	-1.35135200	-0.34388700				
H	0.89236600	-1.84058300	-0.83443100				
Cu	-0.72965100	0.58840300	-0.12863500				
H	3.91481100	-2.06708200	2.31691600				
C	3.63778700	-1.64008600	1.34691800				
C	4.87486100	-1.03278300	0.65402800				
C	2.48601400	-0.64820100	1.57955000				
H	3.24774200	-2.47622800	0.75354300				
H	5.37189200	-1.81730700	0.07374100				
C	4.52657500	0.16567600	-0.25019700				
H	5.60480200	-0.70473000	1.40126700				
N	2.09055600	-0.07927100	0.23353500				
C	3.11451500	0.12763600	-0.88184100				
H	5.24645000	0.23782800	-1.07299300				
H	4.62079700	1.10213400	0.30841600				
O	1.11416200	0.78664600	0.28560400				
C	2.84272100	1.46061600	-1.59066600				
H	1.87400900	1.46632500	-2.09422200				
H	2.88361200	2.30064900	-0.89238500				

H	3.62235900	1.60867600	-2.34527200
C	3.01604200	-1.01456100	-1.91424200
H	3.79227100	-0.87906000	-2.67472900
H	3.16411800	-2.00241100	-1.46678500
H	2.05059800	-0.99246700	-2.42932900
C	2.88147200	0.50279100	2.53309000
H	2.04626700	1.19755500	2.65689000
H	3.12852700	0.08729900	3.51555800
H	3.74680700	1.06817200	2.18286700
C	1.28873000	-1.38734100	2.19879900
H	0.41862000	-0.73104600	2.28609000
H	1.01107200	-2.27261400	1.62056900
H	1.55764200	-1.71986400	3.20586300
H	-0.46686300	5.04693700	-0.80502100
C	0.42461400	4.48281000	-0.51052300
C	0.04444100	3.31808200	0.40617900
H	1.10930500	5.16842100	0.00204100
H	0.91756200	4.12025000	-1.41963800
O	-0.85117100	2.44479300	-0.21310300
H	-0.38736800	3.70226900	1.34655500
O	-0.54839700	1.19282800	-2.53401800
H	-1.12113700	1.28381800	-3.31109400
H	-0.65771800	2.01676200	-2.00497400
H	0.96638300	2.76714300	0.68465200

TS₃₋₄ Charge=1 Multiplicity =3		TS₃₋₄ Charge=1 Multiplicity = 1	
C	-3.50139400	-1.73452200	-0.41228700
C	-4.87441900	-1.69241200	-0.64293200
C	-5.50984200	-0.45237300	-0.65478400
C	-4.76007900	0.70355200	-0.43839200
C	-3.38744000	0.58827200	-0.21786700
N	-2.78226500	-0.62158800	-0.21519800
H	-6.57919700	-0.38092100	-0.82762500
H	-2.94238600	-2.66292600	-0.37496400
H	-5.42527900	-2.61250000	-0.80383600
H	-5.24415600	1.67304200	-0.43754900
H	-2.19516400	5.10620400	0.19396500
C	-1.90633500	4.05981900	0.20885100
C	-0.58186700	3.69084300	0.43266500
C	-2.86250000	3.06872300	-0.00887500
C	-0.25838700	2.33581400	0.44261300
C	3.43949100	-1.69832900	0.61877400
C	4.80176300	-1.63405500	0.90540800
C	5.43675600	-0.39582700	0.83696200
C	4.69661900	0.73359300	0.48853000
C	3.33500200	0.59146500	0.21626000
N	2.73058700	-0.61407600	0.28907200
H	6.49704900	-0.30498600	1.05180100
H	2.87650200	-2.62613500	0.64648400
H	5.34430100	-2.53429900	1.17264900
H	5.17974200	1.70196000	0.43257200
H	2.22136600	5.04549900	-0.73897100
C	1.91093800	4.01140100	-0.62543700
C	0.57909300	3.64386200	-0.80361700
C	2.84599400	3.03441600	-0.28968000
C	0.23423900	2.30393100	-0.64934000

H	0.19266600	4.43275100	0.59310400	H	-0.18171300	4.37467800	-1.05521300
C	-2.47204400	1.72970300	0.01728900	C	2.43149100	1.70844700	-0.15266700
H	-3.89346300	3.34077900	-0.20166500	H	3.88358700	3.30688300	-0.13780200
N	-1.18239000	1.38277100	0.25223200	N	1.13426600	1.35943200	-0.34128900
H	0.75973900	1.98166000	0.57264000	H	-0.78987500	1.95711400	-0.74125600
Cu	-0.85228100	-0.57946900	0.28678000	Cu	0.78390500	-0.60026500	-0.25991800
H	4.77961600	1.37504000	-1.95708000	H	-4.19999000	1.50236000	2.44834600
C	3.92547700	1.60718300	-1.31049500	C	-3.42764300	1.66847800	1.68864500
C	4.41281100	1.80435800	0.13515700	C	-4.09039700	2.07635400	0.36129700
C	2.87094500	0.46562700	-1.48549000	C	-2.55738600	0.37324900	1.60199600
H	3.50798900	2.54937600	-1.68281800	H	-2.81211000	2.49754400	2.05497400
H	3.73606200	2.47913100	0.67417900	H	-3.40146100	2.69027000	-0.23249600
C	4.48863200	0.46550900	0.86522400	C	-4.49966600	0.84361300	-0.44323500
H	5.39341500	2.29278800	0.13231200	H	-4.96377800	2.70607000	0.56249100
N	2.24170000	0.23467800	-0.14321800	N	-2.19888700	0.17604400	0.15798600
C	3.09198000	-0.18863500	1.02580200	C	-3.27274600	0.00469400	-0.88531900
H	4.92577700	0.58621300	1.86301900	H	-5.05872300	1.12817800	-1.34168000
H	5.15876200	-0.20962300	0.31948700	H	-5.18010100	0.22706400	0.15649500
O	1.09669000	-0.56433600	-0.26428100	O	-1.16937500	-0.73123200	-0.01445700
C	3.24423700	-1.71462800	1.17737900	C	-3.68776300	-1.46283000	-1.10478200
H	2.29384900	-2.19311500	1.43053500	H	-2.87544600	-2.05125900	-1.53986800
H	3.64181100	-2.18804200	0.27620200	H	-4.01595900	-1.94857800	-0.18240300
H	3.94527400	-1.92009100	1.99387400	H	-4.52673000	-1.49154100	-1.80836300
C	2.41141500	0.36105100	2.29503400	C	-2.71189200	0.55637900	-2.20982300
H	2.95000600	0.02669000	3.18848500	H	-3.41581800	0.36052600	-3.02545800
H	2.39953900	1.45612000	2.30117300	H	-2.55232600	1.63868800	-2.16112000
H	1.37985900	0.00239500	2.37012600	H	-1.76183800	0.07489900	-2.46308900
C	3.51985900	-0.80063700	-2.09098400	C	-3.30147500	-0.83682200	2.21222800
H	2.81089000	-1.63500100	-2.13096600	H	-2.74304600	-1.76817700	2.06716100
H	3.83426500	-0.59214000	-3.11960200	H	-3.40843300	-0.68721600	3.29212200
H	4.40649900	-1.12555600	-1.54090900	H	-4.30549500	-0.96645000	1.80146100
C	1.77495000	0.95028800	-2.45049600	C	-1.26034100	0.58918500	2.39981600
H	1.05426900	0.16248600	-2.68448800	H	-0.66072000	-0.32299900	2.47139300
H	1.23410400	1.80427000	-2.02984500	H	-0.64898300	1.37864400	1.95253700
H	2.24021100	1.27422800	-3.38727200	H	-1.51737700	0.89802400	3.41806200
H	0.07178700	-5.01450400	-0.55452200	H	-0.45554700	-5.03565200	-0.51740700
C	0.85374300	-4.25006000	-0.43675600	C	-1.07466700	-4.12755400	-0.54281300
C	0.28214100	-2.87030800	-0.62866600	C	-0.46865900	-3.06792500	0.35311300
H	1.63549400	-4.45594500	-1.17559100	H	-2.08298100	-4.40109100	-0.21668300
H	1.27769100	-4.36547500	0.56643600	H	-1.12287700	-3.78916800	-1.58425600
O	-0.60437300	-2.45682200	0.30426300	O	0.67661800	-2.52120200	-0.01721600
H	-0.00282500	-2.63847800	-1.67160900	H	-0.57208500	-3.25256200	1.43643500
H	1.16249500	-1.75198100	-0.50490200	H	-1.28085500	-1.90453400	0.25144200
O	-1.09346200	-1.08895000	2.51372300	O	1.25219000	-1.40473700	-2.38031500

H	-0.66826100	-0.83649900	3.34786400	H	0.81983600	-1.39871300	-3.24844200
H	-0.82664200	-2.00894700	2.32691300	H	1.08888700	-2.28414600	-1.98667700

4				4			
Charge=1 Multiplicity = 3				Charge=1 Multiplicity = 1			
C	-3.52982500	-1.63920500	-0.39432400	C	-2.42465500	1.81802200	1.86337300
C	-4.89287800	-1.56112600	-0.67201300	C	-3.64806400	2.08578200	2.46628500
C	-5.49090700	-0.30374300	-0.72324000	C	-4.78175900	1.42114300	1.99803000
C	-4.71583400	0.83348600	-0.49558300	C	-4.64274200	0.51697600	0.94890400
C	-3.35549900	0.68156700	-0.22636700	C	-3.38018000	0.29715200	0.39148700
N	-2.78627200	-0.54462200	-0.18980900	N	-2.27538900	0.94589200	0.84840600
H	-6.55107500	-0.20412900	-0.93451200	H	-5.75689800	1.60565600	2.43770500
H	-2.99863400	-2.58158900	-0.32133100	H	-1.51626200	2.30218100	2.20752700
H	-5.46495800	-2.46726400	-0.83813100	H	-3.70520900	2.79483500	3.28535500
H	-5.17171500	1.81614000	-0.52463400	H	-5.51319100	0.00622600	0.55303000
H	-2.06273000	5.16687000	0.23458600	H	-4.41431600	-3.25338500	-2.48225400
C	-1.79917500	4.11383400	0.25002200	C	-3.72816300	-2.46796200	-2.18100700
C	-0.48988600	3.71213800	0.50497500	C	-2.52069300	-2.27677000	-2.85314800
C	-2.77287600	3.14718300	0.00299200	C	-4.03802800	-1.63759500	-1.10774700
C	-0.19943700	2.34980800	0.51450800	C	-1.67235700	-1.26474600	-2.41698500
H	0.29776900	4.43427700	0.68975100	H	-2.23926800	-2.89517100	-3.69893400
C	-2.41601900	1.79881400	0.03134300	C	-3.13767300	-0.63599000	-0.73245400
H	-3.79234700	3.44482600	-0.21162200	H	-4.95944000	-1.78361100	-0.55556700
N	-1.14063700	1.41974900	0.29481600	N	-1.95943800	-0.45465700	-1.38335200
H	0.80827700	1.97292300	0.66430400	H	-0.72251700	-1.08297000	-2.90966700
Cu	-0.85894200	-0.54654200	0.34479300	Cu	-0.73375900	0.75524100	-0.34669600
H	4.86556700	1.21151400	-2.01174200	H	3.85202900	-1.58343700	2.44307500
C	4.05661000	1.50391400	-1.33270700	C	2.77610600	-1.76861600	2.55981600
C	4.60280300	1.61340900	0.10094100	C	2.43235600	-3.13970400	1.97917300
C	2.89565600	0.46928400	-1.50518400	C	1.96361700	-0.63851900	1.87799600
H	3.71786700	2.49047500	-1.66719800	H	2.57413400	-1.73267600	3.63661100
H	3.99888700	2.32040100	0.68274300	H	1.35659100	-3.32298500	2.07959800
C	4.59387500	0.24686100	0.78281000	C	2.84362100	-3.21747800	0.49957300
H	5.61905600	2.02159200	0.07924200	H	2.93872900	-3.93018000	2.54409400
N	2.30136000	0.25791700	-0.14242000	N	1.63763000	-1.08842000	0.48416600
C	3.15411200	-0.29769500	0.97328300	C	2.61602300	-1.89231900	-0.30336600
H	5.07268000	0.29370900	1.76744500	H	2.29385600	-4.03194000	0.01625900
H	5.18643400	-0.45934700	0.18849200	H	3.90636600	-3.47723000	0.42761200
O	1.10026300	-0.52911100	-0.27404400	O	1.17882500	0.04333300	-0.29323000
C	3.18675000	-1.83769600	1.05474900	C	3.96475600	-1.18517500	-0.58255300
H	2.21443100	-2.25665100	1.33290000	H	3.82113400	-0.21211400	-1.06871600
H	3.51212300	-2.30293000	0.12037900	H	4.55680300	-1.03707900	0.32451600
H	3.90197300	-2.13317400	1.82973500	H	4.56341400	-1.79744700	-1.26590900
C	2.56780800	0.25202100	2.28774600	C	1.96183400	-2.23844100	-1.65260000

H	3.11148600	-0.15697900	3.14640200	H	2.57085200	-2.98643000	-2.17149200
H	2.64247000	1.34367500	2.32985800	H	0.96325100	-2.65597500	-1.49126000
H	1.51410600	-0.02620300	2.39348400	H	1.87482000	-1.36353300	-2.30391800
C	3.40021500	-0.82403400	-2.18560500	C	2.74340400	0.69165400	1.96920300
H	2.62067000	-1.59403100	-2.23095400	H	2.14826300	1.54433100	1.62448600
H	3.68672600	-0.60094200	-3.21893000	H	2.99682300	0.88087000	3.01783000
H	4.27768900	-1.24934500	-1.69233300	H	3.68160700	0.66779800	1.40741700
C	1.81092300	1.09176300	-2.40264700	C	0.60135700	-0.46128400	2.57290700
H	1.01080200	0.38346400	-2.63436600	H	-0.04937300	0.14398000	1.93608300
H	1.37015700	1.97370300	-1.92668400	H	0.10917300	-1.42711100	2.72375900
H	2.26440400	1.40922100	-3.34739200	H	0.71274700	0.03088900	3.54552800
H	-0.71391500	-5.08763200	-0.48335500	H	4.47985400	4.92731600	-1.06051300
C	0.21723400	-4.49566100	-0.48487800	C	3.90444200	4.36502000	-1.80792300
C	-0.04906700	-3.02903100	-0.63629900	C	3.77340600	2.94588600	-1.36494600
H	0.83975800	-4.86360000	-1.30748000	H	4.49005100	4.40283100	-2.73628800
H	0.73116300	-4.70793100	0.46049000	H	2.92972900	4.83319100	-1.96016100
O	-0.68341100	-2.41523500	0.38570000	O	2.71118200	2.35922400	-1.20174200
H	-0.29517600	-2.66757100	-1.64562900	H	4.71601400	2.40024700	-1.17845800
O	-0.98822200	-1.02161600	2.56493000	O	-0.03614600	2.59231700	-1.03868300
H	-0.51734800	-0.79389200	3.38123800	H	-0.51939900	3.07070600	-1.72839200
H	-0.77867100	-1.95395800	2.36028500	H	0.92002200	2.72309700	-1.21408200
H	1.29369500	-1.48488000	-0.48197400	H	1.92847100	0.65623300	-0.45010800

TS₅₋₆				
Charge=1 Multiplicity = 3				
C	3.36580100	-1.88951500	-0.58130900	
C	4.70489900	-1.84176300	-0.96167000	
C	5.34094600	-0.60328300	-0.99949200	
C	4.62241100	0.54169700	-0.65867600	
C	3.28241600	0.41926300	-0.28801700	
N	2.67108400	-0.78873700	-0.25818300	
H	6.38385500	-0.52448300	-1.29031600	
H	2.82065800	-2.82574700	-0.53034100	
H	5.22749700	-2.75643000	-1.21906200	
H	5.10605700	1.51091900	-0.68409800	
H	2.27245200	4.92678800	0.53706900	
C	1.94854700	3.89143300	0.49543200	
C	0.63270400	3.54554900	0.79574800	
C	2.85056700	2.89273200	0.13091800	
C	0.26657700	2.20351400	0.72578800	
H	-0.10045200	4.29467800	1.07399700	
C	2.41795400	1.56611500	0.08767400	
H	3.87392500	3.15067300	-0.11392400	
N	1.13712600	1.24262900	0.38937600	

H	-0.75054200	1.86806900	0.90602800
Cu	0.75778200	-0.70944100	0.38303800
H	-5.25022200	0.52694900	1.27159300
C	-4.46703900	0.67913400	0.52079400
C	-5.01617400	0.38752400	-0.89157300
C	-3.25540800	-0.18487000	0.91511400
H	-4.17631900	1.73270400	0.60375400
H	-5.48037600	1.29868000	-1.28384800
C	-3.92722300	-0.11851800	-1.86002000
H	-5.81663200	-0.35807200	-0.83964300
N	-2.15740300	0.08256800	-0.07725400
C	-2.50434100	0.38606000	-1.52575200
H	-4.16498600	0.18279600	-2.88682900
H	-3.90702700	-1.21386200	-1.86911000
O	-1.14003500	-0.83281100	0.08683500
C	-1.50180600	-0.28168400	-2.47767000
H	-0.47837000	0.05936800	-2.29415100
H	-1.52193400	-1.37299900	-2.40895300
H	-1.76310700	-0.00906400	-3.50519600
C	-2.41317100	1.91414200	-1.73349700
H	-2.67688800	2.16850200	-2.76615000
H	-3.08526000	2.46707900	-1.07284700
H	-1.39299400	2.26734900	-1.55142600
C	-3.64386100	-1.67937800	0.99158100
H	-2.80335100	-2.28911100	1.33358900
H	-4.45678700	-1.80380600	1.71465100
H	-3.99053800	-2.08036400	0.03607900
C	-2.74889600	0.25383100	2.30135100
H	-1.83702300	-0.28756700	2.57231200
H	-2.54099500	1.32945500	2.32252100
H	-3.50541400	0.04516700	3.06532200
O	-0.53761000	-3.10540800	-0.29071500
O	0.58638800	-2.69997100	0.29553400
H	-1.10675600	-2.18307200	-0.27111400
H	0.92510300	-0.74525500	3.42637400
O	1.10054400	-1.22467600	2.60141500
H	0.86138100	-2.14975100	2.77314200

6				6			
Charge=1 Multiplicity = 3				Charge=1 Multiplicity = 1			
C	-2.87996600	-2.44510600	0.46348100	C	-2.88423500	-2.44133300	0.47574800
C	-3.81546000	-2.88832000	1.39596700	C	-3.81900100	-2.87843300	1.41184500
C	-4.59840300	-1.94274800	2.05569100	C	-4.59903200	-1.92831800	2.06848500
C	-4.43027500	-0.58778800	1.76683800	C	-4.42888000	-0.57503600	1.77300500

C	-3.47703200	-0.21302200	0.82061600	C	-3.47656900	-0.20648400	0.82340800
N	-2.71938800	-1.14292100	0.19354700	N	-2.72168700	-1.14072900	0.19947700
H	-5.33685300	-2.25238900	2.78877500	H	-5.33678700	-2.23314900	2.80428000
H	-2.23733600	-3.11520100	-0.09908400	H	-2.24373500	-3.11525000	-0.08468100
H	-3.92264800	-3.94914300	1.59344300	H	-3.92785500	-3.93812000	1.61444200
H	-5.03659200	0.15565700	2.27093500	H	-5.03291600	0.17189300	2.27467900
H	-3.97985000	4.45513600	0.83484500	H	-3.97200500	4.46248200	0.81531200
C	-3.48357200	3.57065300	0.44768800	C	-3.47762000	3.57532100	0.43187500
C	-2.49206900	3.68240800	-0.52516100	C	-2.48729100	3.68072000	-0.54287800
C	-3.83728200	2.30835300	0.92378500	C	-3.83262300	2.31594700	0.91471400
C	-1.88398800	2.51929500	-0.99005900	C	-1.88162300	2.51437800	-1.00281200
H	-2.19088600	4.64660500	-0.91933200	H	-2.18519000	4.64248500	-0.94225300
C	-3.18986300	1.18423100	0.41183800	C	-3.18765500	1.18829800	0.40744900
H	-4.60599500	2.20889100	1.68116000	H	-4.60047000	2.22144300	1.67359900
N	-2.22779400	1.30572900	-0.53574600	N	-2.22669300	1.30361800	-0.54203100
H	-1.10192300	2.53642700	-1.74166500	H	-1.10050200	2.52657600	-1.75549700
Cu	-1.45247300	-0.41473400	-1.13905000	Cu	-1.45490600	-0.42104300	-1.13777400
H	6.01960000	0.36898000	-0.96033700	H	6.01868200	0.36470400	-0.96569100
C	5.29406600	0.46946300	-0.14560200	C	5.29413700	0.46900500	-0.15055900
C	5.67183500	-0.46748200	1.02054600	C	5.67428500	-0.46121100	1.02017800
C	3.88827800	0.24705200	-0.74146300	C	3.88781200	0.24215900	-0.74343600
H	5.35379900	1.51376600	0.18137300	H	5.35345800	1.51512700	0.17060600
H	6.36849000	0.06296300	1.67800200	H	6.37161400	0.07332700	1.67359400
C	4.45072900	-0.96319100	1.82242700	C	4.45471200	-0.95320300	1.82665500
H	6.21905700	-1.33887600	0.64610200	H	6.22148400	-1.33432800	0.64973500
N	2.89200400	0.28133000	0.38111900	N	2.89281500	0.28091800	0.38004300
C	3.23488600	-0.01651500	1.81110600	C	3.23798300	-0.00766600	1.81139500
H	4.72966600	-1.13823400	2.86730700	H	4.73522900	-1.12189400	2.87215800
H	4.11839300	-1.93288700	1.43365000	H	4.12261200	-1.92540200	1.44397300
O	1.67829600	0.64989600	0.13779400	O	1.67711300	0.64171500	0.13508400
C	2.03347900	-0.72265700	2.46018400	C	2.03832600	-0.71091200	2.46677200
H	1.16252100	-0.06600400	2.50451600	H	1.16678100	-0.05488700	2.50855700
H	1.76199300	-1.62585900	1.90372400	H	1.76675300	-1.61777500	1.91637800
H	2.30149000	-1.01573100	3.48036500	H	2.30843600	-0.99737100	3.48827600
C	3.50927300	1.31276600	2.54560600	C	3.51220700	1.32635700	2.53732900
H	3.65881000	1.11972500	3.61333600	H	3.66363100	1.13997600	3.60597800
H	4.39932800	1.82349200	2.16849900	H	4.40111200	1.83574500	2.15574700
H	2.65296400	1.98507600	2.43386500	H	2.65501400	1.99710900	2.42292400
C	3.77655100	-1.11074200	-1.46746400	C	3.77650900	-1.11935900	-1.46248400
H	2.74735400	-1.29996400	-1.78985100	H	2.74706900	-1.31104600	-1.78262700
H	4.41619200	-1.10589700	-2.35658000	H	4.41505600	-1.11845300	-2.35239300
H	4.08788800	-1.94532800	-0.83350300	H	4.08934700	-1.95041900	-0.82462300
C	3.57961900	1.39491000	-1.71816700	C	3.57677100	1.38488200	-1.72544300
H	2.63989800	1.24779500	-2.25466600	H	2.63654300	1.23418300	-2.26004100

H	3.53016500	2.35438800	-1.19435700	H	3.52701900	2.34686800	-1.20625600
H	4.38177400	1.45010400	-2.46088400	H	4.37793600	1.43730500	-2.46943200
O	0.03001500	-2.15327100	-2.69379000	O	0.02324800	-2.16910600	-2.68579200
O	-1.20025400	-2.06889700	-1.91002600	O	-1.20639700	-2.07899900	-1.90172500
H	-0.32550700	-2.41933800	-3.56060900	H	-0.33334600	-2.43751000	-3.55145200
O	0.15514500	0.34386000	-1.97601900	O	0.15414900	0.33074900	-1.97855700
H	0.85512400	0.48921300	-1.26694800	H	0.85427800	0.47759700	-1.27003400
H	0.43059200	-0.45710200	-2.49288400	H	0.42781000	-0.47316300	-2.49179900

7				7			
Charge=1 Multiplicity = 3				Charge=1 Multiplicity = 1			
C	1.93622400	-1.82947200	-2.02475900	C	2.16730400	-1.67879600	-2.06672000
C	2.87112600	-2.84483900	-2.21609700	C	3.20714500	-2.57874600	-2.29188700
C	3.81976600	-3.07472100	-1.22166600	C	4.16271400	-2.75594000	-1.29290400
C	3.80157400	-2.29505800	-0.06548200	C	4.04801100	-2.04128700	-0.10053200
C	2.83284900	-1.29903900	0.06338500	C	2.97626500	-1.16178100	0.05846600
N	1.92530000	-1.07822000	-0.91622000	N	2.06138700	-0.99234400	-0.92282600
H	4.56721300	-3.85321000	-1.33966400	H	4.98989200	-3.44453200	-1.43525600
H	1.15865100	-1.60030700	-2.74548100	H	1.38298800	-1.49344100	-2.79186400
H	2.85105100	-3.43568600	-3.12529800	H	3.26224800	-3.12183700	-3.22900100
H	4.53422300	-2.46255800	0.71537900	H	4.78376200	-2.17105300	0.68463800
H	3.78750500	0.30032100	4.37359400	H	3.76353400	0.41237300	4.41271000
C	3.20631600	0.36872200	3.45918500	C	3.16000700	0.42298800	3.51032600
C	2.20924400	1.33351600	3.32261300	C	2.02880000	1.23311000	3.42290300
C	3.45007100	-0.51669300	2.41031600	C	3.51176100	-0.38093100	2.42705000
C	1.48983800	1.37968300	2.13118200	C	1.28680500	1.21045500	2.24470600
H	1.98755400	2.03502100	4.11932300	H	1.72271400	1.86865900	4.24656200
C	2.69036700	-0.41147400	1.24381900	C	2.72237600	-0.35164000	1.27600400
H	4.21430100	-1.27884200	2.50813500	H	4.38515600	-1.01993600	2.48507800
N	1.73212700	0.53564100	1.12025000	N	1.63003100	0.44378900	1.20244100
H	0.69792200	2.10136000	1.96250700	H	0.39060900	1.80727700	2.11402600
Cu	0.70503000	0.47909600	-0.59312500	Cu	0.62617500	0.37191400	-0.52305800
H	-4.06802300	-2.95331700	1.46902200	H	-4.05847400	-2.96799900	1.46232400
C	-3.89651900	-1.88219400	1.31441200	C	-3.90235000	-1.89831800	1.28390300
C	-5.05122100	-1.27119500	0.49355300	C	-5.05349300	-1.32722500	0.42971200
C	-2.49621400	-1.71494000	0.68915200	C	-2.49451600	-1.72663900	0.67467900
H	-3.86986300	-1.43423700	2.31445500	H	-3.89781300	-1.42575600	2.27281200
H	-5.84248500	-0.96258300	1.18477300	H	-5.85986700	-1.01303800	1.10060800
C	-4.61072600	-0.07948200	-0.38209100	C	-4.61772200	-0.15211700	-0.47041100
H	-5.50015900	-2.03142800	-0.15421100	H	-5.48049700	-2.11124200	-0.20427200
N	-2.28400100	-0.25317200	0.40704700	N	-2.30374300	-0.26424100	0.36648200
C	-3.40449800	0.71382900	0.15625200	C	-3.43775900	0.67698700	0.07004600
H	-5.44142200	0.62348800	-0.50785000	H	-5.45780300	0.53235300	-0.63031200
H	-4.35694100	-0.42680400	-1.38985200	H	-4.33824600	-0.52099000	-1.46345800

O	-1.09673000	0.23398100	0.55049300	O	-1.14047600	0.25837800	0.55839100
C	-2.94643300	1.73075700	-0.90145400	C	-2.97685500	1.67819200	-1.00092500
H	-2.16206000	2.38201300	-0.50910600	H	-2.19667100	2.33843200	-0.61551500
H	-2.57093600	1.22259400	-1.79379000	H	-2.59415400	1.15536500	-1.88087800
H	-3.80017400	2.35652800	-1.18192400	H	-3.83254900	2.29476300	-1.29525300
C	-3.72860500	1.44772700	1.47495600	C	-3.79872600	1.43329400	1.36644800
H	-4.46193100	2.23786900	1.28151800	H	-4.54943600	2.19796400	1.14093000
H	-4.14429900	0.78108400	2.23554000	H	-4.20865100	0.77574900	2.13790700
H	-2.82303600	1.91175200	1.87733700	H	-2.91236700	1.93247900	1.76907600
C	-2.35483400	-2.51184000	-0.62517700	C	-2.32601400	-2.55605700	-0.61534100
H	-1.39138400	-2.30893300	-1.10038400	H	-1.35517800	-2.36661600	-1.07953100
H	-2.41954000	-3.58347000	-0.40593800	H	-2.39552900	-3.62037100	-0.36468200
H	-3.13850100	-2.26615200	-1.34559100	H	-3.09573500	-2.33141100	-1.35669600
C	-1.43298600	-2.18386700	1.69382200	C	-1.43865600	-2.15479900	1.70484100
H	-0.42876200	-2.15056000	1.26575400	H	-0.42806100	-2.11714700	1.29157300
H	-1.44348400	-1.56845400	2.59843000	H	-1.47167700	-1.52076500	2.59586900
H	-1.65037800	-3.21851600	1.97790100	H	-1.64437800	-3.18624600	2.00805900
O	-0.76571500	-0.33690300	-2.79209600	O	-0.86494800	-0.46649400	-2.69951300
O	0.11551400	0.73598900	-2.33838500	O	0.03815900	0.59877800	-2.26536800
H	-0.67694500	-0.22790400	-3.75561700	H	-0.78553700	-0.36682500	-3.66455400
H	0.02955200	2.51330300	-1.54230100	H	0.06295700	2.43886500	-1.58213700
O	0.57053600	2.60779200	-0.72825200	O	0.57282000	2.56893400	-0.75523700
C	1.69004700	3.48558500	-1.00646300	C	1.63678800	3.51738100	-0.99172300
H	2.26422500	3.08687300	-1.85198200	H	2.29084700	3.14723000	-1.79207900
C	1.22406100	4.90673300	-1.27510900	C	1.09185500	4.89774100	-1.32278300
H	2.31966400	3.43937100	-0.11376100	H	2.21556800	3.53717500	-0.06392800
H	2.08745900	5.56053100	-1.44085900	H	1.91526100	5.60774400	-1.45856800
H	0.59329100	4.95404000	-2.17017300	H	0.51006500	4.88052500	-2.25180600
H	0.65233400	5.29599400	-0.42697200	H	0.44731400	5.26430100	-0.51772800

TS₇₋₈				TS₇₋₈			
Charge=1 Multiplicity = 3				Charge=1 Multiplicity = 1			
C	-0.00709500	-0.19410200	0.18316300	C	1.65226300	-2.03610800	-1.87336700
C	0.08503600	-0.04256500	1.56470500	C	2.41092600	-3.19908000	-1.98267900
C	1.34237200	0.16780400	2.12808200	C	3.34174400	-3.48203600	-0.98447500
C	2.46326800	0.22337700	1.30037100	C	3.48449100	-2.60267500	0.08841500
C	2.29714600	0.06804900	-0.07631900	C	2.68724000	-1.45856600	0.13702800
N	1.07060500	-0.14035100	-0.61052800	N	1.79038600	-1.19311800	-0.84171500
H	1.45411600	0.28462000	3.20156800	H	3.95498400	-4.37618100	-1.03866500
H	-0.95319300	-0.36738100	-0.31847700	H	0.91610900	-1.75151300	-2.61758800
H	-0.80845400	-0.09262300	2.17716700	H	2.27335900	-3.85923100	-2.83191500
H	3.44722800	0.37821800	1.72738000	H	4.21051300	-2.80780900	0.86643400
H	6.71212700	0.64567200	-1.56837300	H	4.05650500	0.39933900	4.22661600
C	5.67350700	0.41979900	-1.78915600	C	3.45635800	0.46634800	3.32450100

C	5.26784700	0.15584400	-3.09621400	C	2.61883300	1.55950200	3.10988900
C	4.73144100	0.39793200	-0.76109800	C	3.51539300	-0.54978400	2.37117700
C	3.92457800	-0.12839400	-3.32918400	C	1.86897500	1.60059200	1.93715500
H	5.97132400	0.16974500	-3.92129900	H	2.54282200	2.36502700	3.83183800
C	3.40138700	0.10639800	-1.06663400	C	2.73519000	-0.44437800	1.21898100
H	5.03249000	0.61443900	0.25716700	H	4.15318800	-1.41088700	2.53253600
N	3.02510100	-0.16155700	-2.33866400	N	1.93789600	0.63054800	1.01735200
H	3.54076300	-0.34050000	-4.32138800	H	1.19646400	2.42066500	1.70864500
Cu	1.07554300	-0.42079300	-2.59238100	Cu	0.81602200	0.53768800	-0.61554200
H	-1.10932800	5.54995900	-3.21971500	H	-4.25354000	-2.92086000	1.21119300
C	-0.64756600	4.78332900	-3.85199100	C	-3.91930000	-1.87891500	1.27037200
C	-1.38363100	4.69248200	-5.20612100	C	-5.07743700	-0.92524100	0.90811800
C	-0.60420800	3.46805500	-3.04421400	C	-2.65740900	-1.73791400	0.39239500
H	0.38787700	5.10644500	-4.01127700	H	-3.61566100	-1.71860100	2.31148600
H	-0.91261000	5.39107500	-5.90549300	H	-5.63123300	-0.68821100	1.82253300
C	-1.39239100	3.26840400	-5.79682600	C	-4.60261000	0.37005500	0.21841300
H	-2.41971500	5.03049200	-5.09915200	H	-5.79194400	-1.42810100	0.24798700
N	-0.02695900	2.39801600	-3.93120500	N	-2.23175900	-0.29509900	0.41816800
C	-0.17785200	2.39640000	-5.42678800	C	-3.19137000	0.84530900	0.61206100
H	-1.44405000	3.31390300	-6.89009900	H	-5.29764800	1.18871000	0.43445300
H	-2.29624900	2.73701500	-5.47923500	H	-4.62294000	0.24370500	-0.86979700
O	0.81175500	1.56110600	-3.41887200	O	-0.97084400	-0.02761200	0.47971300
C	-0.42938200	0.95504800	-5.89735700	C	-2.77258500	2.00212200	-0.30917800
H	0.41851400	0.29971900	-5.69079000	H	-1.79323700	2.40479600	-0.04574700
H	-1.31287500	0.53532500	-5.40636400	H	-2.73620500	1.67233500	-1.35211100
H	-0.60715000	0.96336200	-6.97801500	H	-3.51248800	2.80539300	-0.22663000
C	1.13003600	2.93127600	-6.04618400	C	-3.12005200	1.29397800	2.08656800
H	1.07580000	2.85516900	-7.13715000	H	-3.73915900	2.18612400	2.22737400
H	1.31404200	3.97845800	-5.78891100	H	-3.47757400	0.52242300	2.77470900
H	1.97985100	2.33559700	-5.70079300	H	-2.08902500	1.54423300	2.35264400
C	-2.00681000	3.02927000	-2.57040600	C	-2.91487300	-2.16239200	-1.06949800
H	-1.96319000	2.03773400	-2.11027300	H	-2.04000700	-1.94820000	-1.69034100
H	-2.37981700	3.74449200	-1.82893500	H	-3.11551800	-3.23893900	-1.10473300
H	-2.72964700	2.98814500	-3.38843500	H	-3.77211700	-1.64729000	-1.50889300
C	0.31185300	3.65412000	-1.82643000	C	-1.53315200	-2.60005400	0.98444100
H	0.31493900	2.77207300	-1.18243900	H	-0.64318200	-2.59507000	0.35171800
H	1.34147100	3.86257000	-2.13147900	H	-1.25008200	-2.25327000	1.98258400
H	-0.05340200	4.50409200	-1.24097400	H	-1.89003400	-3.63181100	1.06606600
O	-1.86459100	-0.53254000	-2.95695400	O	-1.01169100	0.23124800	-2.92486000
O	-0.70906800	-1.37234400	-2.67553400	O	0.29902800	0.75088000	-2.56185200
H	-2.58073000	-1.18393300	-2.83991800	H	-0.98189500	0.35521500	-3.89156100
H	-0.17385600	-1.63495200	-3.64413600	H	0.19069400	1.78649500	-2.09190500
O	1.04520800	-1.54684200	-4.17643700	O	0.52091900	2.42356700	-0.97795300
C	1.72408400	-2.80273800	-4.18503700	C	1.62475200	3.30810700	-1.17503400

H	1.42314500	-3.41364400	-3.31807000	H	2.30550500	2.91423000	-1.94749200
C	1.42828800	-3.55381500	-5.47702900	C	1.12712400	4.69038600	-1.57768300
H	2.80617900	-2.63098600	-4.09400900	H	2.20457200	3.37712100	-0.24367300
H	1.96407900	-4.50978400	-5.49807700	H	1.96915200	5.37976000	-1.70857400
H	0.35657600	-3.75987600	-5.57060100	H	0.57254600	4.64445200	-2.52110700
H	1.73838500	-2.96162200	-6.34411700	H	0.46049300	5.09647400	-0.80998900

8 Charge=1 Multiplicity = 3				8 Charge=1 Multiplicity = 1			
C	1.45132300	-2.16281500	-1.76565700	C	1.30207400	-2.24200000	-1.65635400
C	2.14187400	-3.36909700	-1.85424200	C	1.95224500	-3.47078200	-1.74403500
C	3.12350200	-3.64432600	-0.90392700	C	2.99138300	-3.73887400	-0.85483200
C	3.38092500	-2.71370700	0.10163100	C	3.34525800	-2.77921800	0.09257900
C	2.64765800	-1.52663800	0.13182100	C	2.64756200	-1.57102500	0.12647700
N	1.70073600	-1.26721500	-0.80074900	N	1.64456600	-1.31945500	-0.74723700
H	3.68627200	-4.57183000	-0.94287200	H	3.52476200	-4.68347900	-0.89654600
H	0.67752100	-1.89037900	-2.47583500	H	0.48846400	-1.97169800	-2.32166000
H	1.91260200	-4.06894400	-2.65025800	H	1.64870900	-4.19334000	-2.49355800
H	4.14587200	-2.91266200	0.84300400	H	4.15507800	-2.97277800	0.78615200
H	4.37126300	0.45927100	4.02252700	H	4.69204100	0.51491100	3.80392400
C	3.71879100	0.51313800	3.15655600	C	3.97883500	0.55215600	2.98634200
C	2.92293400	1.63614100	2.93734500	C	3.19003900	1.68342100	2.78440900
C	3.66675900	-0.55065800	2.25621400	C	3.84050300	-0.54144000	2.13195500
C	2.10350500	1.65913800	1.81150300	C	2.29153200	1.68447900	1.72042500
H	2.93122600	2.47827000	3.62043600	H	3.26353200	2.54864500	3.43391400
C	2.82054100	-0.46121300	1.15006500	C	2.91725200	-0.47331300	1.08776300
H	4.26964900	-1.43526700	2.42443300	H	4.43774800	-1.43211400	2.28788200
N	2.06816900	0.64332300	0.94041800	N	2.17329400	0.63978100	0.89143200
H	1.45625800	2.49791700	1.57858700	H	1.64431200	2.52775200	1.50468500
Cu	0.83975200	0.53747600	-0.61430300	Cu	0.85125200	0.51075400	-0.58218600
H	-4.37911400	-2.68304400	1.54742900	H	-4.49072200	-2.52335800	1.69172000
C	-3.97419300	-1.66568400	1.50473900	C	-4.02615200	-1.53403600	1.61301600
C	-5.09411700	-0.65673000	1.17309600	C	-5.09937100	-0.45803300	1.34548500
C	-2.78706300	-1.66924600	0.51858600	C	-2.90985600	-1.61864900	0.55112500
H	-3.57046300	-1.45880700	2.50281800	H	-3.54559900	-1.34851800	2.58090000
H	-5.54201100	-0.31259600	2.11116600	H	-5.46212300	-0.08054700	2.30723900
C	-4.60010800	0.54595700	0.34359800	C	-4.58720600	0.70525900	0.47315500
H	-5.90064000	-1.15048100	0.62094000	H	-5.96969700	-0.90355900	0.85224500
N	-2.26536300	-0.26206300	0.41610800	N	-2.30907000	-0.24808700	0.39961100
C	-3.13285500	0.95386100	0.57883900	C	-3.08435400	1.02243300	0.60456100
H	-5.22135300	1.42461300	0.54867100	H	-5.13708900	1.62288100	0.70868000
H	-4.72399000	0.33933000	-0.72502200	H	-4.79366900	0.49923000	-0.58282100
O	-0.98735900	-0.09178900	0.37776100	O	-1.03516700	-0.17349500	0.22021000
C	-2.72437100	1.99748600	-0.47334200	C	-2.68996000	2.03069400	-0.48682400

H	-1.71103000	2.37063000	-0.31373100	H	-1.65427000	2.36188600	-0.39146800
H	-2.78543900	1.57276000	-1.48111400	H	-2.83023300	1.59583600	-1.48233500
H	-3.41666500	2.84449000	-0.41832400	H	-3.34028900	2.90829500	-0.40495600
C	-2.91085900	1.52130600	1.99595800	C	-2.73124000	1.58623200	1.99621000
H	-3.46801100	2.45750100	2.10618300	H	-3.22530200	2.55346400	2.13627800
H	-3.24781000	0.83263300	2.77652300	H	-3.04954300	0.92243200	2.80561200
H	-1.84940600	1.73228800	2.15447000	H	-1.65108600	1.73924000	2.07763700
C	-3.19290300	-2.15890600	-0.88877700	C	-3.43544700	-2.09056200	-0.82205100
H	-2.36171300	-2.03160900	-1.58939600	H	-2.64152500	-2.02626600	-1.57272500
H	-3.45095400	-3.22277100	-0.84421700	H	-3.76211300	-3.13379300	-0.74944800
H	-4.05701700	-1.62284300	-1.28800400	H	-4.28390100	-1.49861000	-1.17306200
C	-1.67679800	-2.57477900	1.07031100	C	-1.82365800	-2.58759900	1.03992400
H	-0.84309100	-2.66567400	0.37093300	H	-1.04456800	-2.73477100	0.28934400
H	-1.29005100	-2.19580000	2.02082800	H	-1.35376200	-2.22537600	1.95917200
H	-2.09339700	-3.57280500	1.24055700	H	-2.28811700	-3.55668100	1.24909800
O	-1.00613000	0.03791900	-3.05826700	O	-1.03673800	-0.03664200	-3.04119300
O	0.23820500	0.65833300	-2.63613100	O	0.20328400	0.60394100	-2.63967700
H	-0.91137100	0.10011600	-4.02784000	H	-0.95013500	0.01161900	-4.01222400
H	0.00938600	1.59857300	-2.32014000	H	-0.04635300	1.52865300	-2.31938200
O	0.55997500	2.36785600	-0.94299700	O	0.56611200	2.32847200	-0.92804700
C	1.66216000	3.20457700	-1.25757300	C	1.65072600	3.14973000	-1.33100900
H	2.22884100	2.81256100	-2.12055400	H	2.15968300	2.73374900	-2.21836800
C	1.17193600	4.61430000	-1.57309800	C	1.14804400	4.55477100	-1.64914700
H	2.37082300	3.24778600	-0.41416200	H	2.41322900	3.21058200	-0.53684600
H	2.01428900	5.27420400	-1.81081300	H	1.97698100	5.20405900	-1.95367600
H	0.49044200	4.60375300	-2.43073200	H	0.41481000	4.52843600	-2.46262100
H	0.63210400	5.03248900	-0.71694100	H	0.66372100	4.99562700	-0.77140500

9				10			
Charge=0 Multiplicity =2				Charge=0 Multiplicity =2			
C	-2.61285900	0.12284800	0.11204000	C	-0.69786400	-2.61784600	-0.23796900
C	-3.47727600	-0.97009500	0.08013400	C	-1.74482200	-3.42091600	0.21237200
C	-2.93225100	-2.25248000	0.01239600	C	-2.90588400	-2.80547300	0.67848900
C	-1.54751300	-2.40692200	-0.02628100	C	-2.99059200	-1.41378500	0.68265600
C	-0.74331600	-1.26533100	0.01741100	C	-1.90056600	-0.67393200	0.21904600
N	-1.28385900	-0.03153600	0.09591100	N	-0.78415700	-1.28348100	-0.22810300
H	-3.57709800	-3.12612900	-0.01886900	H	-3.74129900	-3.40054600	1.03620400
H	-2.93638300	1.16017300	0.13102800	H	0.24351900	-2.99509500	-0.62903000
H	-4.55087800	-0.81487300	0.10176000	H	-1.64721400	-4.50128400	0.19545800
H	-1.10716700	-3.39534000	-0.09973800	H	-3.88808400	-0.92056800	1.03912000
H	3.56907000	-3.13438200	0.01827900	H	-3.40182500	3.72589300	0.89673400
C	2.92626200	-2.25922500	-0.01264700	C	-2.63466900	3.04168000	0.54574600
C	3.47424300	-0.97808300	-0.07994500	C	-1.44083100	3.52580300	0.01365300
C	1.54117900	-2.41036900	0.02605900	C	-2.83591900	1.66492100	0.63288400

C	2.61246900	0.11690300	-0.11138800	C	-0.48445600	2.61049300	-0.42321900
H	4.54820000	-0.82532900	-0.10161400	H	-1.24650600	4.59055800	-0.06003600
C	0.73961900	-1.26693300	-0.01724800	C	-1.83313600	0.80790100	0.17534300
H	1.09841700	-3.39772500	0.09924200	H	-3.75305600	1.27108600	1.05657000
N	1.28295700	-0.03425700	-0.09531400	N	-0.68679100	1.28999200	-0.35013000
H	2.93848400	1.15347100	-0.12990500	H	0.48289700	2.88994400	-0.83126400
Cu	0.00251700	1.53886800	-0.00031900	Cu	0.70597000	-0.07968600	-0.89478000
O	1.40715000	2.65372000	0.39716300	O	1.98796300	1.28530000	-1.04906600
H	1.12094700	3.57337600	0.48881000	H	2.76841500	1.00605800	-1.54927800
O	-1.39970100	2.65655700	-0.39686600	C	3.23778300	-0.53246700	1.45649400
H	-1.11320700	3.57603400	-0.48947500	H	2.98490800	-1.20306800	0.62006200
				O	2.31559100	0.54576500	1.52573100
				H	2.31545100	0.97442600	0.62814300
				C	4.68431800	-0.05275100	1.33056400
				H	5.38631000	-0.89692600	1.32522200
				H	4.82451900	0.51002000	0.39887500
				H	4.94185100	0.61058200	2.16376100
				H	3.11883300	-1.10827400	2.38305300
				H	2.50644300	-1.34463100	-1.81054900
				O	1.59746500	-1.54914100	-1.54955800

11				TS₁₁₋₁₂			
Charge=0 Multiplicity =2				Charge=0 Multiplicity =2			
C	-0.01952500	0.29408200	0.04150500	C	-0.48208800	2.46496300	0.28801200
C	-0.00835700	0.31827600	1.43501900	C	0.22721800	3.64338600	0.11428900
C	1.21653100	0.22410800	2.09499300	C	1.61082600	3.57235300	-0.10496100
C	2.38887700	0.11553900	1.34871100	C	2.21996100	2.32561700	-0.15496600
C	2.29948900	0.09327600	-0.04515500	C	1.44424600	1.17471900	0.03903000
N	1.10627400	0.17253200	-0.67110700	N	0.10453000	1.25178600	0.28361400
H	1.26324000	0.24136400	3.18014300	H	2.19499700	4.47527000	-0.25639200
H	-0.91402100	0.39105100	-0.56794200	H	-1.55760800	2.45140000	0.43366100
H	-0.93918900	0.41288000	1.98435400	H	-0.28852600	4.59755500	0.15170700
H	3.35112600	0.05724400	1.84544000	H	3.27916900	2.23879900	-0.37479000
H	6.80693500	-0.43342600	-1.26752400	H	4.71165800	-2.17536900	0.20422200
C	5.76833500	-0.29255700	-1.55301600	C	3.67383900	-1.88506500	0.07077900
C	5.40633700	-0.21118000	-2.89743400	C	2.68229300	-2.85140800	-0.15696900
C	4.78242400	-0.20095900	-0.57171000	C	3.30211500	-0.54954700	0.14153200
C	4.06145400	-0.03292500	-3.21808800	C	1.36911100	-2.43723900	-0.30838200
H	6.14728400	-0.28837000	-3.68624100	H	2.92770400	-3.90655200	-0.22154600
C	3.45550600	-0.01759300	-0.96819500	C	1.95707900	-0.19624100	-0.02810600
H	5.04439900	-0.27976400	0.47769700	H	4.04035900	0.21665200	0.35516600
N	3.12125200	0.07325700	-2.27197600	N	0.99606300	-1.13967700	-0.27034900
H	3.67094000	0.01265200	-4.23142500	H	0.56466100	-3.14473100	-0.48104300

Cu	1.13649800	0.22500100	-2.71039800	Cu	-0.81548100	-0.47716700	0.00754400
O	1.50226600	-0.25514600	-4.44255900	O	-1.81014400	-1.96075400	0.85429200
H	0.75282600	-0.09999700	-5.03259100	H	-1.88119400	-1.97762600	1.82441100
H	-1.14672200	-1.21590300	-4.35305200	H	-4.61652800	0.42042900	1.00584400
C	-1.97295200	-0.52811900	-4.13738800	C	-4.79691000	-0.08681500	0.04998300
C	-1.42134400	0.86766800	-3.81809800	C	-3.50457500	-0.65805600	-0.50657000
H	-2.64987600	-0.51221000	-5.00258100	H	-5.54295600	-0.87515100	0.20989100
H	-2.52435900	-0.92306500	-3.27533000	H	-5.23374700	0.65425700	-0.63649600
H	-0.90983200	1.26084700	-4.71969100	H	-2.89295600	-1.53865900	0.36336100
O	-0.59239700	0.88014400	-2.69997300	O	-2.48049900	0.19211000	-0.62682300
H	-2.27198900	1.55182000	-3.64186400	H	-3.65378600	-1.33403600	-1.37141000

12				13			
Charge=0 Multiplicity =2				Charge=0 Multiplicity =2			
C	-0.00565200	0.01571900	0.00021600	C	-0.10444300	0.05730300	-0.17024800
C	-0.00470100	0.00192800	1.38280800	C	-0.15665600	0.56550300	1.11397800
C	1.23661300	-0.01137500	2.05266600	C	1.05182800	0.84670500	1.77992000
C	2.40175400	0.00135600	1.30854700	C	2.24858500	0.59225500	1.13127800
C	2.33570200	0.00097700	-0.09909800	C	2.23779400	0.08243500	-0.17800400
N	1.11951300	-0.01842900	-0.74236700	N	1.05426300	-0.16012700	-0.83358800
H	1.27897300	-0.00600900	3.13806200	H	1.04777100	1.23504500	2.79400100
H	-0.92928100	0.05457600	-0.56974100	H	-1.00544100	-0.18993700	-0.72291800
H	-0.94207200	0.00193700	1.92932000	H	-1.11634600	0.74266800	1.58825200
H	3.36604000	0.04656100	1.80453500	H	3.19309400	0.75277100	1.64118900
H	6.85321200	-0.43047500	-1.20613100	H	6.78503200	0.19804500	-1.27014300
C	5.83545100	-0.19653900	-1.50427000	C	5.78013900	-0.15714500	-1.47817000
C	5.53684700	0.14322400	-2.84232400	C	5.52568800	-0.98164400	-2.59272400
C	4.80651800	-0.24758700	-0.58345800	C	4.72372200	0.20971100	-0.66216700
C	4.22586400	0.42222900	-3.17364700	C	4.23003500	-1.40319300	-2.82336200
H	6.31229800	0.19549000	-3.59941800	H	6.32460500	-1.29397200	-3.25731400
C	3.48713100	0.04808100	-0.97892400	C	3.42717800	-0.25444400	-0.94524300
H	5.00470000	-0.54659400	0.44085100	H	4.88614000	0.87620900	0.17884300
N	3.20838400	0.41166400	-2.28221500	N	3.19176400	-1.08230500	-2.01743500
H	3.94875800	0.69157500	-4.18876300	H	3.97819600	-2.03709100	-3.66823500
Cu	1.30239500	0.46147500	-2.64383400	Cu	1.29152700	-1.32075200	-2.38933000
O	1.17823800	-0.45316500	-4.51919600	O	1.22774700	-1.44812300	-4.39699400
H	1.01199000	-1.40930900	-4.57295600	H	1.01058400	-0.60674800	-4.85261100
H	-2.57020900	0.30394900	-3.82499000	H	1.20923500	3.71148200	-5.69681500
C	-2.27951400	1.24539400	-4.30810800	C	1.95383300	3.33200800	-4.99402100
C	-0.81576500	1.53112700	-4.10336500	C	1.79265700	1.85290600	-4.79762600
H	-2.53280600	1.18873000	-5.37359600	H	2.96570200	3.54750700	-5.36150000
H	-2.90864900	2.03605200	-3.86269500	H	1.85541400	3.84267400	-4.02708800
H	0.34847000	0.00062000	-4.82869900	O	0.93751600	1.18400900	-5.35004500
O	-0.29725100	1.42308600	-2.91369500	H	2.50974900	1.37414100	-4.10066400

H	-0.32972400	2.21010900	-4.82363400	H	0.38923000	-2.01648400	-4.37794000
				O	-0.74734800	-2.79198400	-3.46444300
				O	-0.26384900	-2.42609300	-2.28193000

TS₁₃₋₁₄				14			
Charge=0 Multiplicity =2				Charge=0 Multiplicity =2			
C	-0.01857600	-0.55817900	0.37438000	C	-0.68980300	2.63636800	-0.25790600
C	-0.13193300	-1.11771400	1.63653600	C	-1.66779000	3.53121400	0.17207400
C	1.03902400	-1.45078800	2.33490800	C	-2.87229300	3.02182900	0.65729000
C	2.26874100	-1.22582500	1.73165000	C	-3.06420500	1.64181000	0.70446200
C	2.31668900	-0.65633900	0.45233900	C	-2.03900800	0.80405900	0.25989100
N	1.17191700	-0.30464900	-0.20865800	N	-0.87906500	1.31174200	-0.21202800
H	0.98663300	-1.89277800	3.32533700	H	-3.65782100	3.69047300	0.99738500
H	-0.88865300	-0.28945100	-0.21548900	H	0.28195900	2.93283200	-0.64529100
H	-1.11324000	-1.28577800	2.06776600	H	-1.48513700	4.59943700	0.12388900
H	3.18641600	-1.51304600	2.23428200	H	-3.99337400	1.23071700	1.08340500
H	6.92474100	-0.06585800	-0.14899800	H	-3.98449700	-3.44353000	0.77925900
C	5.92131700	-0.09376600	-0.56325700	C	-3.13236000	-2.83066900	0.49992200
C	5.70268500	0.16512500	-1.92609000	C	-1.95666200	-3.42009500	0.03504100
C	4.83392800	-0.36611800	0.25416700	C	-3.21212100	-1.44188200	0.59677300
C	4.40447600	0.13394200	-2.40824100	C	-0.88945300	-2.59481100	-0.31407000
H	6.52635000	0.38597000	-2.59697900	H	-1.86485800	-4.49685800	-0.06001800
C	3.54558200	-0.39592500	-0.29913200	C	-2.10132000	-0.67816400	0.23244800
H	4.97440800	-0.53035900	1.31739900	H	-4.12440900	-0.96836600	0.94254900
N	3.34542500	-0.16383500	-1.63016800	N	-0.96479000	-1.26363000	-0.20355100
H	4.16551600	0.34500200	-3.44566000	H	0.05838500	-2.95185600	-0.70800600
Cu	1.45754000	0.08294100	-2.10181000	Cu	0.54428900	-0.02848500	-0.70267700
O	1.52024000	1.28910600	-3.62706000	O	1.64394300	-1.36675800	-1.40577200
H	1.38885500	2.23328300	-3.42169700	H	2.20579800	-1.65559300	-0.66140500
H	1.47541600	6.10980400	-5.62025500	H	4.12224600	-0.21293500	3.22630900
C	1.69086600	5.16098000	-6.11653900	C	4.29768600	0.34231500	2.30127000
C	1.61783000	4.01985900	-5.13999100	C	3.68314700	-0.36358300	1.12093700
H	0.97542000	4.99277000	-6.93235500	H	3.87070700	1.35088700	2.37615500
H	2.68773700	5.19301300	-6.57567700	H	5.37578500	0.47127300	2.13737900
O	1.34402400	4.15044300	-3.96125300	O	3.06925400	-1.41602100	1.22139700
H	1.82892000	3.01074400	-5.54504800	H	3.80754100	0.12601900	0.13870000
H	0.43155500	0.80116500	-3.99840900	H	2.68879400	0.00662400	-1.81296100
O	-0.52967300	0.10145700	-3.93598800	O	2.94109100	0.95408900	-1.62529100
O	-0.15265500	-0.60820500	-2.83496400	O	1.80653400	1.31866400	-0.77526500

15				TS₁₅₋₁₆			
Charge=0 Multiplicity =2				Charge=0 Multiplicity =2			
C	0.08557900	-0.33142500	0.07369200	C	-0.00745900	-0.07995200	0.01893000
C	0.06795900	-0.22150300	1.46363100	C	0.00351900	-0.02474600	1.41231800

C	1.27801300	-0.05748500	2.13570600	C	1.23393500	0.04536400	2.06314500
C	2.46631100	-0.01013300	1.40723100	C	2.40574500	0.05601600	1.30844400
C	2.40821700	-0.13187300	0.01758400	C	2.31035800	-0.01033700	-0.08425200
N	1.22932200	-0.29343100	-0.61920300	N	1.11552600	-0.08205000	-0.70401400
H	1.30117300	0.03606200	3.21762600	H	1.28463500	0.09967900	3.14673300
H	-0.80238500	-0.45664400	-0.54128700	H	-0.92956700	-0.11706900	-0.55453000
H	-0.87465800	-0.25996300	1.99920100	H	-0.92959400	-0.02951300	1.96580100
H	3.41476600	0.12222100	1.91592400	H	3.36952800	0.13141800	1.79977400
H	6.94899200	0.24854600	-1.13528700	H	6.85868000	-0.23555000	-1.23577400
C	5.91386400	0.11780700	-1.43731100	C	5.82088100	-0.14422900	-1.54292900
C	5.57849500	-0.00863500	-2.78484900	C	5.48594900	-0.05280200	-2.89366100
C	4.90690500	0.07875000	-0.47367100	C	4.80945900	-0.13324200	-0.58479300
C	4.23670100	-0.17473200	-3.12356600	C	4.14110700	0.05613200	-3.23785900
H	6.33658500	0.02259300	-3.56035100	H	6.24616300	-0.07087200	-3.66731700
C	3.58376000	-0.08757900	-0.88904300	C	3.48032600	-0.01221800	-1.00050300
H	5.15189800	0.18011100	0.57774400	H	5.05270600	-0.23137000	0.46709500
N	3.27453000	-0.21716500	-2.19623500	N	3.17494200	0.09003000	-2.31225600
H	3.87166600	-0.27857000	-4.14237200	H	3.78779000	0.09457200	-4.26378800
Cu	1.29737500	-0.41513700	-2.63302700	Cu	1.25688100	0.31467300	-2.79359800
O	1.58337000	-0.60748800	-4.51787400	O	1.37574100	-0.56089600	-4.46481700
H	1.67054900	-1.53117500	-4.79777000	H	1.35791600	-1.52693400	-4.38531100
O	-1.03884400	-0.28974500	-3.91851400	O	-1.05792800	0.43247600	-4.43087000
O	-0.50423500	-0.90883600	-2.69726500	O	-0.74698500	0.53103400	-3.00853900
H	-0.29552200	-0.52448100	-4.53014100	H	-0.22637200	-0.05563400	-4.71845900
H	-0.14323000	1.33877800	-3.63638200	H	-0.34468500	1.57675600	-2.85434800
O	0.73321700	1.78146100	-3.53719600	O	0.74249800	2.28213800	-2.49927500
H	1.21240600	1.41114300	-4.30149700	H	0.98570900	2.85379300	-3.24337900

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Charge=0 Multiplicity =2

C	-0.00475900	-0.14559600	0.04668000
C	0.01866500	-0.07367600	1.43981400
C	1.25436000	0.03494000	2.07442100
C	2.41439800	0.06648400	1.30274200
C	2.30085500	-0.02006500	-0.08862900
N	1.10435700	-0.12821200	-0.69515100
H	1.31747500	0.10664800	3.15642600
H	-0.93862200	-0.21059900	-0.50541100
H	-0.90758700	-0.09440000	2.00472600
H	3.38266300	0.18197900	1.77766100
H	6.83437200	-0.42326000	-1.22749700
C	5.81007200	-0.23212100	-1.53420700
C	5.50208900	0.00560700	-2.87326500
C	4.78534000	-0.24487600	-0.59119000

C	4.17176800	0.23215800	-3.21537100
H	6.27000400	0.00733900	-3.63954600
C	3.47234600	0.00386100	-1.00558800
H	5.00080500	-0.46908200	0.44743800
N	3.19345400	0.24969900	-2.30254400
H	3.85123600	0.38258000	-4.24114100
Cu	1.27910000	0.59068400	-2.82791000
O	1.30507600	-0.52985600	-4.33666500
H	1.16684000	-1.47523400	-4.17857300
O	-0.95735000	0.72248500	-4.62044300
O	-0.81803800	0.85711900	-3.17428600
H	-0.14816200	0.12780200	-4.76595200
O	0.95939900	2.38526100	-2.30768700
H	1.49872400	3.01274900	-2.81140700
H	-0.51951200	1.80684800	-3.03903800