

Supporting information

**Mechanistic Insight into the Aerobic Oxidation of
Benzylic Alcohol Catalyzed by the Cu^{II}-TEMPO
Catalyst in Alkaline Water Solution**

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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			
Cu	1.24806700	0.66643300	0.05856700	Cu	-0.69336700	0.34941900	0.03333700
C	2.51561600	-3.23360300	-0.18526600	O	3.44571600	1.34015000	0.08007100
N	2.37759000	-0.96045000	0.04449900	C	-1.83317000	4.26766300	0.31402000
C	3.81264600	-2.71332400	-0.08697100	N	-0.66112200	2.31632200	0.08868000
H	2.22661300	-4.27134900	-0.30040600	C	-0.46673100	4.56618700	0.26706000
C	3.67252300	-1.31022300	0.04880400	H	-2.65839300	4.96212700	0.41437300
H	4.74442500	-3.26448200	-0.11105500	C	0.21559200	3.33075500	0.13190300
H	4.44670200	-0.55854100	0.14192500	H	-0.00685200	5.54448600	0.32491900
C	0.23646200	-1.99551000	-0.13933600	H	1.28217300	3.14580200	0.07341300
H	-0.37033800	-2.89452600	-0.27797300	C	-3.01004500	1.95531900	0.19251700
N	-0.31136100	-0.80780300	-0.03571200	H	-4.02718500	2.33901400	0.30036600
C	-1.70799100	-0.64139500	-0.00905500	N	-2.77570900	0.66502000	0.08267100
C	-2.23157200	0.62047500	-0.35679800	C	-3.82593900	-0.26798500	-0.00031400
C	-2.60512800	-1.65864600	0.37860200	C	-3.56457300	-1.60279000	0.36843200
C	-3.60860300	0.84145400	-0.36754600	C	-5.11649100	0.06098800	-0.46459600
C	-3.98508100	-1.44342900	0.36769800	C	-4.57247800	-2.56544700	0.32295900
C	-4.46102600	-0.19722500	-0.01563900	C	-6.13077900	-0.89804000	-0.50933300
H	-4.01531400	1.81119500	-0.63514600	C	-5.84053600	-2.19361500	-0.10495200
H	-4.68018500	-2.22060200	0.66915400	H	-4.37467200	-3.59386600	0.60652300
C	1.64525100	-2.12208500	-0.09856100	H	-7.12428800	-0.65200400	-0.87022700
H	-1.54146900	1.42610500	-0.59002800	C	-1.92674900	2.86021000	0.19982800
H	-2.23152500	-2.61920600	0.71819500	H	-2.55716800	-1.87743500	0.66407100
F	-5.81575600	0.01726600	-0.02407000	H	-5.33150400	1.06263600	-0.82220100
O	1.54382000	4.26192100	0.04175600	F	6.83309000	-3.13733700	-0.15164000
C	1.45769500	3.03457000	0.05392300	O	1.65124800	-2.40380700	0.01683000
O	2.47897200	2.18910600	0.14953300	C	0.85105700	-1.46938800	0.01677300
O	0.30978200	2.34908000	-0.02843200	O	1.19146900	-0.17714400	-0.06124600
				O	-0.47078200	-1.57673500	0.08777300
				H	2.66161800	0.74370600	0.12687700
				C	4.30552500	0.85098400	-0.93780900
				H	4.84269400	1.71323000	-1.35425900
				H	3.71182700	0.40549100	-1.74967300
				C	5.31789200	-0.16864100	-0.44087200
				C	4.89496300	-1.43537300	-0.00294800
				C	6.68472000	0.13603400	-0.40799100
				C	5.82930800	-2.36758700	0.45390400
				H	3.83669000	-1.69551100	-0.01812000
				C	7.62190900	-0.79833100	0.04770300
				H	7.01925100	1.11745600	-0.73938000
				C	7.19417700	-2.05565800	0.48090200

	H	5.48646700	-3.34371000	0.78756300			
	H	8.67901800	-0.54276900	0.06675200			
	H	7.91648600	-2.78658500	0.83699000			
TS1-2	2						
Charge=-1 Multiplicity = 2	Charge=-1 Multiplicity = 2						
Cu	0.79356400	-1.08811100	0.27489600	Cu	0.00690000	0.02652400	-0.48451000
O	-1.11999400	-0.80360500	-0.46768000	O	-1.75718600	-0.69950400	-0.15747100
C	4.32299900	-2.02644000	-1.62775100	C	0.02772800	4.13063100	-0.72848900
N	2.31381800	-2.13895000	-0.52959300	N	-0.53163800	1.91935400	-0.60556600
C	3.98109300	-3.37153100	-1.45446200	C	-1.35264500	4.00391200	-0.94704000
H	5.20706900	-1.62541400	-2.10818300	H	0.61460300	5.04099100	-0.71897200
C	2.73785200	-3.38594700	-0.77133600	C	-1.64752700	2.62501900	-0.86518900
H	4.54697700	-4.23889600	-1.77036600	H	-2.06202000	4.79822800	-1.14162500
H	2.15717800	-4.24219400	-0.45042100	H	-2.60236600	2.12840300	-0.98250600
C	3.03424700	0.10067500	-0.88403500	C	1.79815900	2.28990500	-0.26760400
H	3.77552400	0.82538400	-1.22903200	H	2.64926000	2.97237500	-0.18705700
N	1.93875100	0.49790600	-0.27653400	N	1.95736100	0.99572300	-0.15431900
C	1.64688800	1.85886700	-0.07987100	C	3.21656700	0.47132500	0.20837200
C	0.95162400	2.22927500	1.08770600	C	3.60995000	-0.78339000	-0.29597100
C	2.00239300	2.85637500	-1.00755200	C	4.08393400	1.15217000	1.08646700
C	0.65158900	3.56784100	1.33763900	C	4.85707500	-1.31679400	0.02893800
C	1.70677800	4.19926400	-0.76086800	C	5.33537800	0.62384800	1.41323100
C	1.04071800	4.52824100	0.41160300	C	5.70055300	-0.59879900	0.86751100
H	0.12071000	3.86436400	2.23620700	H	5.16435400	-2.28371600	-0.35548800
H	1.96844600	4.97585200	-1.47225700	H	6.00664600	1.13772400	2.09381800
C	3.26863200	-1.28193300	-1.04652800	C	0.50876300	2.82046800	-0.52005000
H	0.66001600	1.45377300	1.79093300	H	2.90957000	-1.33716400	-0.91343600
H	2.48532700	2.58188900	-1.94020900	H	3.77017000	2.08503500	1.54456900
F	0.74587500	5.84401100	0.65409000	F	6.92639700	-1.12183300	1.18861200
O	-1.03550100	-2.27071900	3.37959900	O	1.10070500	-3.81932200	-1.32798300
C	-0.41840700	-1.78981600	2.44110800	C	0.38593900	-2.87911800	-0.98828100
O	-0.47510900	-2.47529300	1.16323100	O	-0.89831500	-3.09597000	-0.62520200
O	0.31887800	-0.75193600	2.35531500	O	0.80926800	-1.63340400	-0.95324000
H	-1.09778100	-1.90689100	0.53273300	H	-1.33077100	-2.21330000	-0.40604000
C	-1.90173300	0.34630300	-0.30550700	C	-2.43110800	-0.34823000	1.01292200
H	-1.54509100	1.15654400	-0.96616600	H	-2.12731400	-0.99035000	1.86339900
H	-1.84661600	0.73505700	0.72845800	H	-2.19566200	0.68786100	1.31548400
C	-3.36135100	0.06803700	-0.63263400	C	-3.94706500	-0.45258700	0.87495300
C	-4.18475700	-0.58744700	0.29612200	C	-4.54123100	-0.81446200	-0.33886200
C	-3.91068500	0.42462300	-1.87121400	C	-4.77569500	-0.18140500	1.97477700
C	-5.51745500	-0.87692300	-0.00444600	C	-5.93352200	-0.89954300	-0.45249000
H	-3.77185200	-0.87570100	1.26002800	H	-3.89241700	-1.02932200	-1.18143000
C	-5.24545700	0.14026300	-2.17880200	C	-6.16501200	-0.26299700	1.86487700
H	-3.28129100	0.92728700	-2.60232300	H	-4.32574700	0.09713400	2.92656500

C	-6.05441700	-0.51251800	-1.24461500	C	-6.75184600	-0.62366500	0.64584700
H	-6.13809800	-1.38569600	0.72916400	H	-6.37856600	-1.18556900	-1.40260600
H	-5.65191200	0.42625900	-3.14630400	H	-6.79032100	-0.04799500	2.72838100
H	-7.09231000	-0.73602200	-1.47923100	H	-7.83329600	-0.69071500	0.55708200
3				TS3-4			
Charge=-1 Multiplicity = 2				Charge=-1 Multiplicity = 2			
Cu	1.03380600	0.19976600	-0.00055700	Cu	1.06113800	0.46524500	0.35012600
O	5.16973600	2.43899800	0.33110700	O	0.43487800	1.49164900	2.00868700
C	1.40078200	-3.87701400	-0.16564700	C	2.40665800	-3.34530400	-0.46278900
N	1.77776000	-1.62658100	0.00229000	N	2.28364900	-1.10568200	0.01400500
C	2.78168500	-3.65762900	-0.08909100	C	3.70525100	-2.84462200	-0.32225600
H	0.88618100	-4.82635700	-0.25089200	H	2.11089300	-4.36264800	-0.68844500
C	2.96222700	-2.25614800	0.00968400	C	3.57372800	-1.46218900	-0.03238900
H	3.56643600	-4.40325300	-0.10327100	H	4.63434000	-3.39242300	-0.41831200
H	3.88672500	-1.69642800	0.07923900	H	4.35752000	-0.73289700	0.13269900
C	-0.54057500	-2.15424800	-0.12906600	C	0.13821800	-2.09762900	-0.27424300
H	-1.34189600	-2.88970600	-0.23492100	H	-0.49725000	-2.95187700	-0.52150700
N	-0.79976900	-0.86871700	-0.04827400	N	-0.38150800	-0.91465500	-0.04222000
C	-2.12263700	-0.38931300	-0.00064100	C	-1.76477800	-0.67931700	-0.05659200
C	-2.36670000	0.93879000	-0.40294100	C	-2.21656800	0.57799300	-0.50503900
C	-3.20786700	-1.16343400	0.46009000	C	-2.70899700	-1.62876000	0.37711000
C	-3.66084500	1.45881900	-0.39479800	C	-3.58038300	0.86493700	-0.54866800
C	-4.50614400	-0.64898500	0.46805500	C	-4.07686500	-1.34730100	0.33292800
C	-4.70886900	0.65242300	0.02996800	C	-4.48494500	-0.10569800	-0.13405800
H	-3.85259000	2.48095500	-0.70420000	H	-3.93990900	1.82623500	-0.90088500
H	-5.34450600	-1.23807700	0.82582400	H	-4.81389100	-2.06771800	0.67284400
C	0.80120400	-2.59753400	-0.10404000	C	1.54295800	-2.24488700	-0.24708800
H	-1.52648700	1.56136700	-0.69357600	H	-1.48085600	1.31099300	-0.82792100
H	-3.04270800	-2.16518500	0.84307100	H	-2.37455200	-2.57977200	0.77978100
F	-5.98144700	1.16087100	0.03986800	F	-5.82616300	0.17494400	-0.17422200
O	2.13852300	3.64080700	-0.06079700	O	2.11857500	3.88512600	-0.91628000
C	1.76166800	2.46939200	-0.03745700	C	1.65877900	2.80387200	-0.57185900
O	2.57140900	1.41419600	0.07607800	O	2.24357300	2.15208200	0.57462900
O	0.49799100	2.05848600	-0.11830700	O	0.71683100	2.09536000	-1.06543400
H	4.88315200	3.35976100	0.26730100	H	1.49934100	2.16133800	1.36905600
H	4.30755500	1.97233600	0.26130400	H	-0.41736000	1.92423700	1.87140100
4				5			
Charge=-1 Multiplicity = 2				Charge=-1 Multiplicity = 2			
Cu	1.08081200	-0.35415600	-0.00309900	Cu	-0.58089500	0.35642100	-0.51599100
O	0.27216400	-2.06635400	-0.01990400	O	0.86518300	0.09990200	-1.79308800
C	1.42429500	3.75523600	-0.14887200	C	-1.01883200	4.29438500	0.55550800
N	1.74925200	1.49553300	-0.04145100	N	-0.28491000	2.27942800	-0.22891000
C	2.80019600	3.49831700	-0.11266400	C	0.31266000	4.43319700	0.13641200
H	0.93214000	4.71907100	-0.19915100	H	-1.66087200	5.05683600	0.97929200

C	2.94969100	2.08954100	-0.04939300	C	0.72244300	3.16562500	-0.33443400
H	3.60293300	4.22466900	-0.13093000	H	0.92075500	5.32813300	0.16936400
H	3.84956700	1.48884500	-0.01364000	H	1.68949200	2.86392400	-0.71700900
C	-0.55325300	2.07017300	-0.11366400	C	-2.53293200	2.18417400	0.54635800
H	-1.34916000	2.81774900	-0.18630000	H	-3.41121400	2.66863000	0.98162500
N	-0.83203200	0.78674700	-0.07435200	N	-2.54174500	0.90636800	0.25645800
C	-2.16530100	0.35096100	-0.02747400	C	-3.73615100	0.16357100	0.37933600
C	-3.17604900	1.05578700	0.65931000	C	-3.66676200	-1.19537800	0.74091800
C	-2.50805500	-0.85642800	-0.67018200	C	-4.99913400	0.73403600	0.12257700
C	-4.49553900	0.59619600	0.67018300	C	-4.83120200	-1.94866400	0.88895800
C	-3.82256600	-1.32243600	-0.66127800	C	-6.16916600	-0.01440600	0.27283900
C	-4.79440000	-0.58280200	0.00214100	C	-6.06028400	-1.34171600	0.66346900
H	-5.27590900	1.13102200	1.20214000	H	-4.78295600	-2.99709600	1.16356800
H	-4.09282500	-2.24878100	-1.15783700	H	-7.14531500	0.41449600	0.07057700
C	0.79344500	2.48902000	-0.10067800	C	-1.36195900	2.94619100	0.31765400
H	-2.92528100	1.95500400	1.21332800	H	-2.69034800	-1.65113300	0.86821700
H	-1.71717200	-1.42530100	-1.14795300	H	-5.07096400	1.75896500	-0.22791800
F	-6.08691100	-1.04016500	0.01362400	F	-7.20560000	-2.07991200	0.80793700
O	4.65037700	-2.40281700	0.19027500	O	-0.78951800	-3.72115900	-0.38475700
C	3.43855000	-2.19591000	0.13048000	C	-0.44189200	-2.60385500	-0.75661100
O	2.57671200	-3.24190700	0.13986100	O	0.36116500	-2.46951100	-1.84054600
O	2.91947400	-0.99159600	0.05476700	O	-0.81409900	-1.49616800	-0.15400900
H	1.63442500	-2.89188700	0.08955600	H	0.58837400	-1.50409400	-1.96388000
H	-0.33648700	-2.17889200	0.72122400	O	3.41421700	0.39307800	-0.96116300
				H	0.75116600	0.71733800	-2.52718500
				C	3.72986000	-0.73858800	-0.18100400
				H	3.07559400	-0.80360600	0.70493900
				H	3.57224200	-1.66856300	-0.75127700
				C	5.16979300	-0.69050100	0.28717300
				C	5.68167300	-1.73204400	1.07682400
				C	6.01360900	0.37455000	-0.04843300
				C	7.00429800	-1.71074400	1.52200600
				H	5.03589900	-2.56654300	1.34341100
				C	7.34020400	0.39818700	0.39680800
				H	5.61318200	1.17602000	-0.65921000
				C	7.84220300	-0.64173100	1.18297800
				H	7.38186200	-2.52727700	2.13263500
				H	7.98242500	1.23354600	0.12762500
				H	8.87273400	-0.62233800	1.52846500
				H	2.47472800	0.29831900	-1.27127300
TS5-6				6			
Charge=-1 Multiplicity = 2				Charge=-1 Multiplicity = 2			
Cu	-0.10049500	0.34632500	0.45963400	Cu	-0.27630400	0.34082800	0.48026900
O	-0.49335900	0.00666600	2.75881600	O	-0.98440800	0.25472800	3.51077000

C	0.13868300	4.37220700	-0.29968200	C	-0.10898000	4.34288400	-0.47189700
N	-0.50217500	2.26202300	0.29528300	N	-0.68644900	2.25786500	0.25726000
C	-1.18201500	4.41879400	0.17100700	C	-1.40858500	4.39476500	0.05598000
H	0.74216100	5.19681400	-0.65875400	H	0.46378900	5.15689200	-0.89916800
C	-1.53174700	3.09514200	0.52352100	C	-1.72099400	3.08578000	0.48732100
H	-1.81949400	5.29022900	0.25097200	H	-2.05541600	5.26051900	0.12153200
H	-2.46459700	2.71819100	0.92209000	H	-2.63113400	2.71120300	0.93791500
C	1.73221800	2.33104900	-0.51267500	C	1.50389000	2.31407600	-0.66211800
H	2.58256800	2.88237700	-0.92336000	H	2.31828800	2.85642900	-1.14988300
N	1.80020200	1.03786500	-0.31968600	N	1.60502300	1.03465400	-0.40252500
C	3.01525200	0.35365500	-0.53552200	C	2.81800400	0.35879600	-0.65938800
C	2.98699400	-0.95395600	-1.05328400	C	2.78125600	-0.99498700	-1.03864400
C	4.26024300	0.93486000	-0.22427900	C	4.07072300	0.99025600	-0.52494500
C	4.17274900	-1.64797600	-1.29123200	C	3.95807900	-1.68625400	-1.32292800
C	5.45218900	0.24916800	-0.46791200	C	5.25342600	0.30698200	-0.81440700
C	5.38252800	-1.02869600	-1.00563600	C	5.17069900	-1.01846300	-1.21876400
H	4.15416800	-2.66336800	-1.67158500	H	3.93395100	-2.73578200	-1.59441000
H	6.41589900	0.68417300	-0.22359500	H	6.22290800	0.78218900	-0.70510100
C	0.53393900	3.02023600	-0.20715300	C	0.31207800	3.00334400	-0.32966100
H	2.02912000	-1.42867000	-1.23184800	H	1.82717500	-1.50775500	-1.06346100
H	4.29856100	1.91502300	0.24085700	H	4.12792800	2.01110800	-0.16050700
F	6.55011800	-1.70655300	-1.23902900	F	6.33008100	-1.69291600	-1.49763000
O	1.19574300	-3.49757200	0.50648500	O	1.61622300	-3.15429200	1.31815600
C	0.77818700	-2.43236400	0.95733000	C	0.98262400	-2.12974100	1.55315400
O	0.86099000	-2.18714400	2.28461100	O	0.99091900	-1.63763400	2.82877000
O	0.24166400	-1.49960700	0.20062800	O	0.29163800	-1.47337300	0.65865200
H	0.39960100	-1.33345700	2.53464400	H	0.32646500	-0.92638900	2.96985100
O	-2.15353200	0.00879300	1.06081300	O	-2.08022500	0.02914100	1.15546800
H	-0.37197600	0.74909800	3.36002000	H	-0.76071100	1.18680000	3.62005100
C	-2.82446700	-1.21332900	0.84189000	C	-2.72579500	-1.19668200	0.95402400
H	-2.12515200	-1.97263000	0.46169600	H	-2.00190800	-2.02053800	0.85604400
H	-3.22099400	-1.59401700	1.79784300	H	-3.34373100	-1.42993000	1.84162300
C	-3.97604900	-1.07434000	-0.13767600	C	-3.64305100	-1.22157100	-0.26383600
C	-4.78938500	-2.18451200	-0.41587500	C	-4.30226400	-2.40918600	-0.61989000
C	-4.24964000	0.13431400	-0.78794000	C	-3.85849800	-0.08030600	-1.04473100
C	-5.85114400	-2.08978300	-1.31683500	C	-5.15718700	-2.45568000	-1.72235300
H	-4.58312100	-3.13332700	0.07606400	H	-4.13600100	-3.30808100	-0.02852900
C	-5.31192000	0.23216400	-1.69374000	C	-4.71218700	-0.12302200	-2.15305400
H	-3.61746500	0.98951800	-0.57711000	H	-3.34445100	0.83498400	-0.77191900
C	-6.11864800	-0.87631500	-1.96173600	C	-5.36733200	-1.30813800	-2.49674700
H	-6.46826000	-2.96214400	-1.51853400	H	-5.65452800	-3.38728000	-1.98262500
H	-5.50626200	1.17893800	-2.19213900	H	-4.86257800	0.77365200	-2.74993200
H	-6.94356200	-0.79962500	-2.66562200	H	-6.02879800	-1.34179000	-3.35894400
H	-1.54395700	0.00821200	2.02481400	H	-1.53779500	0.20268500	2.66795800

7				7			
Charge=0 Multiplicity = 1				Charge=0 Multiplicity = 3			
Cu	-0.09472000	-1.15599800	-1.39613200	Cu	0.09387200	-1.16200700	1.39768000
H	-2.60398500	5.02945500	-0.31332400	H	2.62392700	5.01951200	0.31144300
C	-2.08768400	4.41389900	0.43175700	C	2.10361900	4.40570500	-0.43229900
C	-1.20656600	5.30051500	1.33578400	C	1.22444800	5.29549600	-1.33514100
C	-1.34099700	3.29285600	-0.31803800	C	1.35380700	3.28826600	0.31968700
H	-2.87623500	3.94409600	1.02977800	H	2.88912200	3.93239300	-1.03154500
H	-1.82180400	5.67605500	2.16067600	H	1.83961300	5.66765000	-2.16163000
C	0.03412900	4.56353700	1.88443500	C	-0.02063300	4.56366500	-1.88062500
H	-0.87007800	6.18640400	0.78631700	H	0.89309300	6.18332100	-0.78567600
N	-0.55259700	2.49444900	0.67755700	N	0.55917700	2.49295900	-0.67335900
C	-0.11468800	3.03306600	2.00763600	C	0.12131800	3.03245900	-2.00316900
H	0.30402300	4.95809700	2.87048500	H	-0.29098100	4.95886800	-2.86629900
H	0.89536600	4.75746000	1.23513000	H	-0.87960800	4.76157500	-1.22952700
O	-0.21322600	1.29343900	0.36290000	O	0.20892100	1.29644900	-0.35354600
C	1.25060800	2.42227000	2.36085800	C	-1.24714200	2.42738000	-2.35384400
H	1.18380100	1.34102200	2.48856700	H	-1.18518200	1.34582300	-2.48132900
H	1.98773400	2.62629000	1.57898500	H	-1.98218200	2.63466700	-1.57089800
H	1.60840600	2.86364700	3.29667000	H	-1.60447200	2.87000600	-3.28924600
C	-1.14646300	2.63056100	3.08455900	C	1.14948100	2.62491500	-3.08166300
H	-0.78758700	2.93348600	4.07432000	H	0.79056200	2.92972000	-4.07084300
H	-2.12173200	3.09626400	2.92276700	H	2.12731200	3.08573600	-2.92140800
H	-1.28149400	1.54508600	3.08574500	H	1.27913000	1.53877500	-3.08324100
C	-0.37640300	3.85188100	-1.38657900	C	0.39460900	3.85200200	1.39061200
H	0.18495900	3.03304900	-1.84507000	H	-0.16959200	3.03591300	1.85048400
H	-0.94634000	4.35968200	-2.17201300	H	0.96900200	4.35697800	2.17460900
H	0.33727200	4.56713300	-0.96848800	H	-0.31656300	4.57075900	0.97424400
C	-2.36623500	2.36456100	-0.98832900	C	2.37654800	2.35536100	0.98749200
H	-1.87995600	1.57169900	-1.55722500	H	1.88797500	1.56364300	1.55602200
H	-3.01693200	1.89979800	-0.24141200	H	3.02432500	1.88900200	0.23901000
H	-2.98880400	2.95082600	-1.67201100	H	3.00246300	2.93831900	1.67094600
C	2.53569000	0.05950700	-1.17980100	C	-2.53222900	0.06400400	1.19562100
O	1.68854600	-1.03813800	-1.36819100	O	-1.68909500	-1.03813200	1.37600700
H	2.56468000	0.64750600	-2.11547800	H	-2.55966800	0.64461400	2.13593000
H	2.14461900	0.73532200	-0.40408700	H	-2.13816500	0.74439300	0.42544900
C	-3.61981400	-1.27441600	-3.39925300	C	3.62599200	-1.29507600	3.38751500
N	-1.43343400	-0.97805200	-2.80101500	N	1.43798600	-0.99203700	2.79852800
C	-2.92685200	-0.72879600	-4.48668800	C	2.93824100	-0.75196500	4.47946700
H	-4.66827100	-1.53898200	-3.35248300	H	4.67372200	-1.56160500	3.33585100
C	-1.58661000	-0.56439700	-4.07209200	C	1.59676800	-0.58332000	4.07046400
H	-3.32653200	-0.48084000	-5.46080600	H	3.34205300	-0.50837200	5.45298000
H	-0.75178300	-0.17404300	-4.64055700	H	0.76488500	-0.19322200	4.64340100
C	-2.72510000	-1.91218200	-1.04177700	C	2.72116500	-1.92242900	1.03112500

H	-3.66418000	-2.27504400	-0.62146000	H	3.65792600	-2.28563200	0.60598900
N	-1.62398200	-1.89822600	-0.32286900	N	1.61732100	-1.90367000	0.31642400
C	-1.56978600	-2.43367300	0.98080000	C	1.55681100	-2.43441400	-0.98887000
C	-0.71576100	-1.82775700	1.91874900	C	0.69866300	-1.82478700	-1.92063400
C	-2.31103200	-3.56659500	1.36273300	C	2.29572400	-3.56630200	-1.37841600
C	-0.62194800	-2.32347800	3.21806300	C	0.59864400	-2.31568500	-3.22132900
C	-2.22704100	-4.06581900	2.66351800	C	2.20550900	-4.06069900	-2.68060700
C	-1.38524500	-3.43146300	3.56803300	C	1.35987000	-3.42263800	-3.57892700
H	0.03052100	-1.86367800	3.95251000	H	-0.05713100	-1.85297900	-3.95099100
H	-2.78654700	-4.94346800	2.96895600	H	2.76317400	-4.93748500	-2.99183200
C	-2.67121600	-1.42185700	-2.36492400	C	2.67323400	-1.43677200	2.35617000
H	-0.14779100	-0.95191000	1.62093200	H	0.13211600	-0.95000000	-1.61700700
H	-2.93180600	-4.08128500	0.63623800	H	2.91956500	-4.08401700	-0.65672600
F	-1.29437100	-3.92010500	4.83542900	F	1.26293400	-3.90657400	-4.84767400
C	3.95940800	-0.34889700	-0.83175200	C	-3.95712900	-0.33661100	0.84348600
C	4.89655200	0.63504200	-0.48387100	C	-4.89136400	0.65371600	0.50601400
C	4.36502800	-1.68698700	-0.86136400	C	-4.36657600	-1.67378100	0.85843100
C	6.21363800	0.29055200	-0.17467600	C	-6.20925600	0.31634000	0.19250700
H	4.59376100	1.68043700	-0.45497900	H	-4.58560900	1.69850600	0.48865200
C	5.68399500	-2.03488200	-0.55054100	C	-5.68637800	-2.01453500	0.54324700
H	3.63702300	-2.44548600	-1.12784500	H	-3.64085900	-2.43718000	1.11705700
C	6.61292000	-1.05002400	-0.20672600	C	-6.61234800	-1.02338000	0.20974100
H	6.92700300	1.06565100	0.09263900	H	-6.92031700	1.09633500	-0.06658300
H	5.98468300	-3.07898700	-0.57637000	H	-5.99003000	-3.05800400	0.55765300
H	7.63657400	-1.32159800	0.03538900	H	-7.63665400	-1.28940500	-0.03575100
7				TS7-14			
Charge=-1 Multiplicity = 1				Charge=0 Multiplicity = 3			
Cu	-0.62744800	1.35264100	0.51399000	Cu	-1.45111900	1.45952200	-0.36291400
O	1.07168700	0.35464800	0.08393300	H	1.97223000	-1.74132400	4.53687100
C	-1.60455400	4.60075100	-1.82012300	C	2.05103900	-1.97155900	3.46803000
N	-0.55924300	3.00784400	-0.55210900	C	3.39795500	-2.66160000	3.17207400
C	-0.26631400	4.98156500	-1.64182100	C	1.80052400	-0.66644000	2.67701700
H	-2.37486900	5.12776800	-2.37036400	H	1.22639100	-2.65647600	3.24483000
C	0.33148000	3.97286700	-0.85560800	H	3.28222200	-3.73824900	3.33971900
H	0.22130300	5.87192300	-2.01876200	C	3.90875700	-2.39380500	1.73978900
H	1.35263500	3.92054000	-0.49907400	H	4.15998300	-2.32837800	3.88535100
C	-2.88984900	2.53261800	-0.97019700	N	2.05327700	-0.90566400	1.22058700
H	-3.84023000	2.85196000	-1.41485200	C	2.80362000	-2.08120800	0.71148400
N	-2.79738200	1.43190900	-0.27823800	H	4.48393500	-3.25173600	1.37426500
C	-3.88477700	0.55683100	-0.14564900	H	4.59951300	-1.54304200	1.74576400
C	-3.97971400	-0.20315300	1.03879900	O	1.09345900	-0.45250600	0.36807300
C	-4.85609400	0.36790800	-1.15083100	C	3.46106600	-1.69169400	-0.62574900
C	-5.03719400	-1.09173900	1.23012300	H	2.70878100	-1.46259400	-1.38369200
C	-5.91717800	-0.52257000	-0.96495400	H	4.10023000	-0.81244400	-0.50578800

C	-5.99010700	-1.22929100	0.22736300	H	4.07481000	-2.52199600	-0.99108400
H	-5.11838200	-1.67525000	2.14147900	C	1.88065700	-3.30065800	0.46922000
H	-6.66521000	-0.68054200	-1.73560700	H	2.45150700	-4.11476800	0.00892300
C	-1.75692200	3.37455000	-1.13757800	H	1.43293400	-3.68231600	1.38978600
H	-3.20285200	-0.08442100	1.78980800	H	1.07306000	-3.02295700	-0.21297000
H	-4.76878600	0.89639500	-2.09532000	C	2.74460300	0.45889800	3.16181700
F	-7.02910700	-2.10755900	0.41002700	H	2.57672100	1.37045800	2.57981000
O	-0.77238300	-0.91970700	3.95209400	H	2.55736200	0.68863000	4.21726200
C	-0.35847100	-0.42564700	2.90514500	H	3.79632300	0.18059400	3.05328000
O	0.92837800	-0.70327300	2.51139800	C	0.34433800	-0.23141900	2.91036800
O	-1.04415400	0.34122200	2.11278000	H	0.12376300	0.72845300	2.43885200
H	1.08425300	-0.29859900	1.61715500	H	-0.35961100	-0.97061400	2.51931000
C	2.06770100	0.83211600	-0.71208800	H	0.17650500	-0.12652700	3.98744200
H	2.55082600	-0.07433900	-1.22119500	C	1.35612000	1.85135400	-0.73240400
H	1.67762500	1.40763500	-1.57192200	O	0.08947800	1.85847100	-1.22859100
H	-0.85158300	-4.05757400	-0.77595800	H	1.48945300	2.44918000	0.18183900
C	-0.18623800	-3.25687100	-0.42902200	H	1.40231900	0.55131700	-0.11684400
C	0.58213400	-3.70883100	0.83003100	C	-4.39831200	2.76508900	2.09633000
C	0.70091600	-2.84264100	-1.63902500	N	-2.51818200	2.60424500	0.80590400
C	1.94665200	-4.30684200	0.48565300	C	-3.68033400	3.96140500	2.19787600
H	-0.01768000	-4.43994300	1.38370200	H	-5.33410800	2.51621300	2.57966000
C	2.87197700	-3.28156700	-0.20535300	C	-2.53116100	3.81598400	1.38813500
H	1.82688800	-5.19347200	-0.15057500	H	-3.94203900	4.83550800	2.77871100
H	0.72118000	-2.85727400	1.50142400	H	-1.73807800	4.53225000	1.21396800
H	-0.82787600	-2.41285100	-0.16130100	C	-3.84040700	0.63545100	0.71247400
H	2.45375800	-4.64864000	1.39548000	H	-4.71306800	0.04427900	0.99196100
C	0.06459400	-1.65190400	-2.36767400	N	-2.92139700	0.14254900	-0.09363800
H	0.60911600	-1.39905300	-3.28052200	C	-3.06451000	-1.10982100	-0.72764500
H	-0.96334800	-1.92084500	-2.63301400	C	-1.90795600	-1.86367200	-0.99462600
H	0.04096900	-0.78027800	-1.71100100	C	-4.31648300	-1.61127200	-1.12949300
C	0.86228000	-4.00769500	-2.65381400	C	-2.00060700	-3.10574300	-1.62076000
H	-0.11065200	-4.21898000	-3.11106100	C	-4.41712800	-2.85609600	-1.75165600
H	1.56148000	-3.72071500	-3.44568200	C	-3.25528100	-3.58212400	-1.98226400
H	1.21651200	-4.92933700	-2.18563800	H	-1.11730400	-3.70040500	-1.82681900
C	3.51687000	-2.34096500	0.83160700	H	-5.37495800	-3.25151900	-2.07218800
H	4.23255100	-2.91179600	1.43370700	C	-3.65875100	1.93650600	1.22418500
H	4.05607100	-1.53367400	0.33063100	H	-0.93876300	-1.47602800	-0.69250500
H	2.77338600	-1.90577300	1.50088300	H	-5.21321600	-1.01747100	-0.98442500
C	3.98732300	-3.99927500	-0.99813200	F	-3.34839300	-4.79267800	-2.59613500
H	4.64872700	-3.26975800	-1.47169800	C	2.46203600	1.95139600	-1.69456300
H	4.57618000	-4.61599200	-0.31027600	C	3.76213200	2.26983000	-1.24789100
H	3.57383800	-4.65069700	-1.77388200	C	2.26997900	1.68932900	-3.06638900
N	2.06680900	-2.44487100	-1.16209500	C	4.83119600	2.32336800	-2.13982500
O	2.73783800	-1.63304600	-1.89083600	H	3.92614600	2.48456700	-0.19412400

C	3.18025400	1.62441000	-0.04650100	C	3.34253800	1.74577500	-3.95540500
C	3.20207800	1.87245400	1.33192900	H	1.27023700	1.45651200	-3.41773600
C	4.22798800	2.12856900	-0.83587400	C	4.62862300	2.05956900	-3.50021600
C	4.24432000	2.60853300	1.90565300	H	5.82337600	2.57877700	-1.77739900
H	2.40044600	1.48946300	1.95387800	H	3.17547100	1.54873000	-5.01111100
C	5.26913600	2.86203700	-0.26615200	H	5.46096100	2.10465000	-4.19650200
H	4.22073500	1.94346100	-1.90851200				
C	5.28157400	3.10574300	1.11269100				
H	4.24052000	2.79390600	2.97678000				
H	6.06939500	3.24514700	-0.89494400				
H	6.08961500	3.67836000	1.56083400				
8				9			
Charge=0 Multiplicity =2				Charge=0 Multiplicity =2			
Cu	1.18968600	0.58568100	0.02028600	Cu	0.00756700	0.46143300	0.31681600
C	2.66049400	-3.15860700	-0.17211300	C	0.59880400	4.41962900	-0.30696700
N	2.40236800	-0.89693500	0.00180700	N	-0.27325700	2.37009000	0.19479800
C	3.92477400	-2.56989500	-0.04537600	C	-0.72697800	4.58698600	0.11513900
H	2.43294000	-4.21170000	-0.27186500	H	1.29428200	5.19072400	-0.61143300
C	3.71888700	-1.17872200	0.05717300	C	-1.22318800	3.30144800	0.41277600
H	4.88241500	-3.07199400	-0.03240600	H	-1.27444300	5.51569300	0.20174300
H	4.45965800	-0.39612700	0.15974900	H	-2.20589700	3.02834000	0.77557200
C	0.32285800	-2.01871400	-0.20270400	C	1.99181700	2.23221700	-0.49659700
H	-0.28494900	-2.91824100	-0.30343900	H	2.92445900	2.68200900	-0.83982700
N	-0.24592400	-0.83193800	-0.15887800	N	1.89988900	0.93245100	-0.32592300
C	-1.64700600	-0.67327900	-0.08108300	C	3.03025800	0.09466700	-0.45298500
C	-2.25471200	0.40440000	-0.74725900	C	2.88303000	-1.17849900	-1.02858900
C	-2.44591300	-1.56003200	0.66435300	C	4.29959200	0.49845900	-0.00054600
C	-3.63691700	0.57215600	-0.70483800	C	3.98409700	-2.01850800	-1.18416200
C	-3.83114200	-1.40302400	0.70559200	C	5.40875000	-0.33266300	-0.15865200
C	-4.40047800	-0.34046600	0.01427300	C	5.22910900	-1.57541500	-0.75330800
H	-4.11970200	1.39853800	-1.21463700	H	3.88239100	-3.00487600	-1.62298800
H	-4.46016700	-2.07659900	1.27733200	H	6.39218200	-0.03595500	0.18960200
C	1.72951100	-2.10080900	-0.13794500	C	0.85771400	3.03581300	-0.24407900
H	-1.63758100	1.11555500	-1.28294500	H	1.89919000	-1.51087000	-1.33859700
H	-1.98390200	-2.35996000	1.23415900	H	4.41721600	1.45309700	0.50222400
F	-5.74855900	-0.17920400	0.05802600	F	6.30600400	-2.39188400	-0.90240400
O	1.04613300	4.32281100	0.17145800	O	0.92385700	-3.12811600	1.83902200
C	1.08491700	3.11685500	0.13041500	C	0.76069000	-1.94346600	1.60237200
O	2.33269000	2.42299800	0.22662800	O	1.23571900	-0.97015100	2.46232200
O	0.17412100	2.21332800	0.00549900	O	0.14372200	-1.42399200	0.58117300
H	3.07712000	3.03846000	0.31141300	H	1.68120000	-1.43624600	3.18624400
				C	-2.91001900	0.12625900	-0.86211500
				H	-2.40819200	-0.25151400	-1.76005600
				O	-2.04765700	-0.07569400	0.29370300

	H	-1.90338600	-1.02947000	0.43633200			
	H	-3.00526100	1.21018800	-0.94798300			
	C	-4.24695300	-0.54311200	-0.67530300			
	C	-4.55775800	-1.71654700	-1.37498900			
	C	-5.19077500	-0.01125900	0.21705600			
	C	-5.79026600	-2.34946400	-1.18932900			
	H	-3.83437200	-2.13625100	-2.06994400			
	C	-6.41997400	-0.64249800	0.40609100			
	H	-4.95713000	0.89692300	0.76644800			
	C	-6.72194600	-1.81360600	-0.29792000			
	H	-6.01977800	-3.25766800	-1.73862200			
	H	-7.14348300	-0.22175500	1.09817900			
	H	-7.68005000	-2.30378000	-0.15217900			
TS9-10	10						
Charge=0 Multiplicity =2	Charge=0 Multiplicity =2						
Cu	-0.07982200	0.12229400	-0.17433700	Cu	-0.14883300	-0.36133900	-0.45295900
C	-0.71402200	4.06676300	0.46837900	C	0.47450200	-4.04594200	-1.97359900
N	-0.96879600	1.82676100	0.11462500	N	-0.43839000	-2.06519200	-1.29161100
C	-2.07876700	3.76031300	0.47943500	C	-0.89737200	-4.06648200	-2.24306200
H	-0.25590900	5.03672600	0.61107100	H	1.19622400	-4.82630100	-2.17599300
C	-2.19083700	2.36925900	0.25779500	C	-1.41912800	-2.82872600	-1.80494600
H	-2.90275000	4.44533900	0.62567900	H	-1.46424800	-4.86869500	-2.69525300
H	-3.08565400	1.76396200	0.19739300	H	-2.44383100	-2.48156800	-1.83930200
C	1.31088500	2.46513000	0.14048000	C	1.89392200	-2.15011300	-0.89637800
H	2.11018500	3.20191700	0.22075700	H	2.86702600	-2.63981700	-0.93599100
N	1.59704000	1.19529700	-0.08139000	N	1.76873500	-0.94621600	-0.36992100
C	2.94175200	0.75310700	-0.12221800	C	2.88056700	-0.17357700	0.02335800
C	3.33722300	-0.15739300	-1.11415100	C	2.74452300	0.70926800	1.10820400
C	3.88875400	1.20194400	0.81410200	C	4.11406300	-0.23746600	-0.65143300
C	4.65846300	-0.59134700	-1.19293800	C	3.81892300	1.48541900	1.53719100
C	5.21567900	0.77579200	0.74257300	C	5.19814700	0.52956200	-0.22489000
C	5.57452300	-0.11171600	-0.26385900	C	5.03108400	1.37463400	0.86533700
H	4.97869100	-1.29220400	-1.95598300	H	3.72585100	2.16645100	2.37597300
H	5.95680800	1.10913400	1.46086900	H	6.15245200	0.49269500	-0.73896200
C	-0.03956100	2.84699800	0.24370800	C	0.74012500	-2.79118800	-1.38332600
H	2.60330100	-0.52578300	-1.82228700	H	1.78902500	0.77939900	1.61680500
H	3.58266200	1.86604600	1.61638400	H	4.22201100	-0.86593800	-1.52937400
F	6.86460800	-0.53575300	-0.33482900	F	6.08245800	2.12893400	1.27838000
O	0.44361000	-3.89386800	1.00360300	O	-3.53640600	2.89659900	-0.93763700
C	1.08252000	-2.93621900	0.61628400	C	-2.71170200	3.27324500	-1.75725000
O	2.35145000	-2.67197300	1.01162300	O	-3.01370600	4.11007800	-2.77580700
O	0.66705400	-2.01784200	-0.24756600	O	-1.43384200	2.95436900	-1.80012000
H	2.59926100	-3.38367400	1.62195800	H	-3.95720100	4.31296700	-2.68809500
C	-2.55792600	-1.15113800	-1.33709500	C	-1.39260500	1.53570400	1.33617100

H	-2.58908700	-2.12709500	-1.84571300	O	-0.84034200	1.23575100	0.05042900
O	-1.45918700	-1.16698900	-0.44254700	H	-1.21361200	2.30522100	-1.05401200
H	-0.44500900	-1.98052200	-0.41921400	H	-2.04561600	2.40734600	1.21569000
H	-2.41901500	-0.39152200	-2.11954600	C	-2.17357100	0.37702300	1.91272400
C	-3.88260700	-0.91133200	-0.63575100	C	-3.47730900	0.12183100	1.45675700
C	-4.93690800	-0.29136200	-1.31982500	C	-1.61039100	-0.47277900	2.87449900
C	-4.08820100	-1.33981200	0.68204600	C	-4.19562900	-0.96840400	1.95058100
C	-6.17856400	-0.10937700	-0.70416900	H	-3.91684000	0.78649300	0.71733000
H	-4.78665300	0.05536800	-2.34024100	C	-2.32903900	-1.56584800	3.36934600
C	-5.32700900	-1.15411000	1.30099800	H	-0.60792600	-0.27354700	3.24775300
H	-3.26971600	-1.81018000	1.21744700	C	-3.62274700	-1.81567200	2.90605300
C	-6.37671500	-0.54051500	0.61037700	H	-5.20564800	-1.15453000	1.59605200
H	-6.98538000	0.37474400	-1.24740300	H	-1.88184300	-2.21523500	4.11662900
H	-5.47263400	-1.48948700	2.32413400	H	-4.18476300	-2.66186200	3.29090400
H	-7.33895300	-0.39647000	1.09335900	H	-0.57324200	1.81790400	2.01400600
11				12			
Charge=0 Multiplicity =2				Charge=0 Multiplicity =2			
Cu	-1.21130400	1.29698300	-0.11029300	Cu	-0.09390100	-0.36077600	0.27230100
C	-3.29831100	-2.14204100	0.20573500	C	-1.12709000	-4.22745600	-0.41810700
N	-2.66504500	0.04095800	-0.03626200	N	-0.00995700	-2.28218100	0.02393500
C	-4.44726500	-1.35081600	0.09426700	C	0.22800700	-4.52200900	-0.22622500
H	-3.24898500	-3.21598300	0.32879400	H	-1.92662000	-4.92217000	-0.64028100
C	-4.01025300	-0.01647000	-0.04983800	C	0.87462300	-3.29618700	0.04301100
H	-5.47610600	-1.68332000	0.11486900	H	0.69968100	-5.49436100	-0.27075600
H	-4.61088600	0.87808000	-0.15584000	H	1.92231500	-3.12129800	0.25180100
C	-0.80234600	-1.41507400	0.16616200	C	-2.33344800	-1.92839200	-0.30158400
H	-0.35986800	-2.40113600	0.30819900	H	-3.34177600	-2.28362400	-0.52125600
N	-0.04715400	-0.34154300	0.05946800	N	-2.10298000	-0.64905800	-0.10015500
C	1.36227900	-0.38365900	0.03006100	C	-3.15674900	0.28827400	-0.05742100
C	2.07542500	0.75237300	0.45252300	C	-2.96959800	1.55686300	-0.63450900
C	2.07687900	-1.50770800	-0.42579000	C	-4.38503300	-0.00383900	0.56402300
C	3.46919800	0.75478900	0.45903000	C	-3.99479100	2.50196600	-0.62099100
C	3.47164800	-1.51403500	-0.41785400	C	-5.41799300	0.93471500	0.57817300
C	4.14271600	-0.38313800	0.03105900	C	-5.20331900	2.17014800	-0.01923500
H	4.02905800	1.62347900	0.78807700	H	-3.86543500	3.48109600	-1.06945400
H	4.03354000	-2.37214800	-0.77053700	H	-6.36753600	0.72301900	1.05789700
C	-2.20267300	-1.25749800	0.12037200	C	-1.25028500	-2.83143100	-0.25408600
H	1.52540900	1.63519000	0.76451000	H	-2.01411100	1.79100800	-1.09078100
H	1.54974500	-2.37377100	-0.81216700	H	-4.52585800	-0.95859400	1.06081600
F	5.50250600	-0.38472100	0.03303200	F	-6.20488900	3.09100200	-0.00237000
O	-0.46892600	2.92193300	-0.10977100	O	0.02823100	1.46468400	0.59610800
H	-0.12362000	3.26789900	-0.94335700	H	-0.71861600	1.88670700	1.03542000
				O	2.03013500	-0.01338900	0.45777500
				C	2.89482100	0.05078400	-0.70233900

				H	3.03757600	-0.98735100	-1.01179000
				H	2.38519700	0.58837300	-1.51075800
				H	1.76279700	0.89714100	0.72446400
				C	4.21240400	0.71040200	-0.37692800
				C	4.45230900	2.04093100	-0.74474000
				C	5.20703700	0.00885200	0.32077600
				C	5.66229900	2.66193900	-0.42174700
				H	3.68859100	2.59355500	-1.28672800
				C	6.41539800	0.62604300	0.64579600
				H	5.02933800	-1.02303400	0.61265300
				C	6.64541400	1.95522500	0.27450500
				H	5.83566700	3.69348000	-0.71423500
				H	7.17847100	0.07180200	1.18468400
				H	7.58704100	2.43507300	0.52515000
TS12-13				13			
Charge=0 Multiplicity =2				Charge=0 Multiplicity =2			
Cu	-0.07556500	0.24689400	-0.01879300	Cu	0.01129600	-0.26374000	-0.32440800
C	-0.90455600	4.21545200	0.13025600	C	-0.36073900	3.77702100	-0.03627300
N	0.12433300	2.17853100	0.00874800	N	-0.76181600	1.53350900	-0.22385800
C	0.47733800	4.41493000	0.03555200	C	-1.74089000	3.57304500	-0.12335100
H	-1.67559900	4.97169500	0.19920600	H	0.16173400	4.71941500	0.06499800
C	1.06917800	3.13489200	-0.03739100	C	-1.94144900	2.17824100	-0.23640400
H	1.00343300	5.35973500	0.01850300	H	-2.51791200	4.32519300	-0.10483100
H	2.11884100	2.88564800	-0.12466200	H	-2.87732400	1.64059200	-0.31152000
C	-2.23528400	1.98283300	0.14327500	C	1.55289600	2.02368300	-0.03375100
H	-3.23611800	2.40918200	0.22327200	H	2.38501800	2.72146500	0.06966800
N	-2.06488200	0.67708900	0.09836600	N	1.77532600	0.72597300	-0.12058300
C	-3.17117200	-0.20015100	0.03626600	C	3.08527800	0.21652000	0.03441300
C	-3.12767400	-1.41414800	0.74397100	C	3.52968200	-0.82005900	-0.80431000
C	-4.31049300	0.10051800	-0.73299700	C	3.95670700	0.71140600	1.02229400
C	-4.20877800	-2.29415300	0.71137400	C	4.82003700	-1.33342300	-0.68068000
C	-5.39868000	-0.77284100	-0.76789300	C	5.25218700	0.20696100	1.15152300
C	-5.32773900	-1.95369900	-0.04011800	C	5.66009900	-0.80579000	0.29347200
H	-4.19077200	-3.22962000	1.26012500	H	5.17584700	-2.12714500	-1.32866400
H	-6.28003200	-0.55429700	-1.36115500	H	5.93036500	0.57882100	1.91205500
C	-1.10052800	2.81804700	0.10799000	C	0.22867300	2.49473500	-0.09646600
H	-2.23951200	-1.66184000	1.31376200	H	2.85733700	-1.21985700	-1.55444100
H	-4.33789800	1.00767500	-1.32843500	H	3.61274200	1.47769100	1.70999400
F	-6.38253100	-2.81189100	-0.07593300	F	6.91911500	-1.30658900	0.41807700
O	-0.05836500	-1.74920200	0.02621100	O	0.84585900	-2.25422000	-0.11269600
H	-0.45022800	-2.23192700	-0.71334100	H	1.13260700	-2.58047500	0.75031400
O	1.79710600	-0.41672000	-0.22462000	O	-1.40374300	-1.44343000	-0.66865500
C	2.81040600	-0.25150300	0.75472600	C	-2.62562400	-1.18633500	-1.29707800
H	2.90150900	0.81881800	0.99036100	H	-2.56984900	-0.28307600	-1.92704200

H	2.53712100	-0.76095200	1.69206100	H	-2.84041000	-2.01935400	-1.98932500
H	1.06530100	-1.41199000	-0.13964200	H	-0.07956300	-2.55568700	-0.28211800
C	4.15650600	-0.77304800	0.28035800	C	-3.81100000	-1.04352800	-0.34890800
C	5.14384100	-1.10519900	1.21842700	C	-5.05400400	-0.62581400	-0.84894700
C	4.44890800	-0.89586700	-1.08305100	C	-3.70131000	-1.34058000	1.01321400
C	6.40373400	-1.54240100	0.80359300	C	-6.16220000	-0.50980500	-0.00780500
H	4.92530100	-1.02601800	2.28147100	H	-5.15503000	-0.38822000	-1.90665500
C	5.70814300	-1.33775600	-1.50006000	C	-4.80906500	-1.22396500	1.85990200
H	3.68055700	-0.64978400	-1.80841100	H	-2.73929300	-1.65916000	1.40051500
C	6.69020600	-1.66036900	-0.55994200	C	-6.04289100	-0.80899400	1.35392800
H	7.15726200	-1.79818100	1.54339400	H	-7.11652600	-0.18348700	-0.41240900
H	5.92117100	-1.43089100	-2.56156100	H	-4.70637000	-1.45683300	2.91653700
H	7.66757600	-2.00534200	-0.88509200	H	-6.90282300	-0.71720700	2.01130600
14				14			
Charge=0 Multiplicity =1				Charge=0 Multiplicity =3			
Cu	0.56438600	0.55891400	-1.89407700	Cu	0.33205700	-1.47684400	0.26178000
H	0.98707600	-5.36565300	0.75865900	H	0.46283400	4.06694500	3.41119500
C	0.79339400	-4.47371700	1.36635600	C	0.25987900	3.95577800	2.33948400
C	-0.54910500	-4.62428300	2.11175500	C	-0.51383400	5.18427600	1.81976100
C	0.87553300	-3.23512600	0.44290800	C	-0.45951500	2.60159400	2.12767100
H	1.61767800	-4.41960800	2.08423100	H	1.24069400	3.90076300	1.85608900
H	-0.37083100	-5.13677500	3.06379600	H	0.20714300	5.95912900	1.53531900
C	-1.23796000	-3.26643800	2.36019800	C	-1.43306900	4.84440500	0.62780600
H	-1.22952700	-5.27114400	1.54609200	H	-1.12007800	5.61918000	2.62225100
N	0.42430800	-1.95719600	1.13932700	N	-1.00066800	2.46007500	0.72020700
C	-0.26240000	-2.07872600	2.46441100	C	-0.96912400	3.63000800	-0.20044900
H	-1.83635000	-3.30305600	3.27773100	H	-1.52350700	5.70576300	-0.04342200
H	-1.94164000	-3.04991400	1.54659200	H	-2.44535700	4.62670400	0.98732300
O	1.53012000	-1.04963800	1.33166800	O	-0.43788100	1.32370100	0.03007200
C	-1.06734200	-0.78250100	2.67694100	C	-2.00760100	3.36343700	-1.30809400
H	-0.40622700	0.08787300	2.68273600	H	-1.71668100	2.50354500	-1.91818500
H	-1.80620500	-0.64807200	1.88011000	H	-2.98974100	3.16026000	-0.87081300
H	-1.59909000	-0.81298400	3.63460200	H	-2.09096600	4.23306000	-1.96949700
C	0.69387900	-2.24221400	3.67141600	C	0.39857000	3.89011800	-0.87684100
H	0.10609100	-2.28885500	4.59509000	H	0.31112800	4.73573300	-1.56825100
H	1.30272500	-3.14606100	3.61970600	H	1.19455200	4.12252000	-0.16701200
H	1.36784100	-1.38600800	3.73672000	H	0.70239200	3.01474200	-1.45580400
C	-0.06076500	-3.42214600	-0.77265100	C	-1.67609200	2.49063700	3.07457400
H	0.01286700	-2.55600700	-1.43865700	H	-2.18640200	1.53531300	2.91842800
H	0.22116800	-4.31482700	-1.34356400	H	-1.35933400	2.54972600	4.12300700
H	-1.10684400	-3.53417400	-0.47151400	H	-2.40385000	3.28604300	2.89203800
C	2.31669300	-3.11247000	-0.07666400	C	0.53200100	1.48150400	2.47944800
H	2.42966400	-2.28672700	-0.78258300	H	0.06215500	0.49543300	2.44671200
H	3.02769100	-2.96192000	0.73805300	H	1.39505900	1.47531000	1.80930900

H	2.57553000	-4.04058400	-0.59842600	H	0.89191500	1.64332100	3.50126500
C	-2.19717300	-0.09166200	-1.23705600	C	-2.42201900	-2.09875600	-0.21812500
O	-1.34072600	0.54604200	-1.87158000	O	-1.40605800	-1.22472200	-0.21103600
H	-1.88014200	-0.90725200	-0.57032800	H	-2.35829700	-2.94129500	0.47093400
H	1.38135800	-0.34714500	0.67857200	H	-1.18326900	0.70177300	-0.05591000
C	4.59117900	0.49482000	-2.38550700	C	2.19994100	-3.54111500	3.19536700
N	2.33282800	0.14255200	-2.55551100	N	0.63407000	-2.58951400	1.83343200
C	4.35501500	-0.35074400	-3.47435800	C	0.92757800	-3.85859000	3.68138800
H	5.54633700	0.85759800	-2.02742200	H	3.15482700	-3.83927000	3.60792700
C	2.95603200	-0.53410200	-3.53906400	C	-0.00635600	-3.24961100	2.81311400
H	5.08823200	-0.78133100	-4.14337500	H	0.68839100	-4.44858900	4.55558800
H	2.39347300	-1.11676000	-4.25827500	H	-1.08716700	-3.26024200	2.87429000
C	2.95057500	1.59455800	-0.73033400	C	2.84417400	-2.12868200	1.10647700
H	3.73330300	2.14432000	-0.20010600	H	3.92760200	-2.21123400	1.18974800
N	1.68714200	1.70746600	-0.38273700	N	2.29513000	-1.42398300	0.13500800
C	1.30477000	2.51675700	0.70454000	C	3.04894600	-0.85381300	-0.91431800
C	0.05129100	3.15366300	0.64756800	C	2.59381200	0.34626700	-1.48812400
C	2.09186300	2.68948000	1.86054700	C	4.21189100	-1.46152100	-1.42141400
C	-0.39329200	3.96834000	1.68829300	C	3.29969200	0.94434800	-2.53076100
C	1.65635000	3.50112800	2.90921400	C	4.92796100	-0.86368700	-2.45825400
C	0.42285400	4.13050300	2.80117900	C	4.45860500	0.33088900	-2.99188300
H	-1.35311100	4.47199900	1.64368100	H	2.96377800	1.87283700	-2.97932000
H	2.25307200	3.63235900	3.80573800	H	5.82314000	-1.32224100	-2.86411900
C	3.32502200	0.78483500	-1.82888600	C	1.99574000	-2.75160000	2.04253300
H	-0.56378000	3.01200200	-0.23561800	H	1.69286900	0.81455200	-1.10034700
H	3.03553200	2.16260300	1.95775300	H	4.54422800	-2.41690000	-1.02832900
F	-0.00772800	4.92045500	3.82599400	F	5.14999900	0.90981800	-4.00815200
C	-3.62659000	0.18606400	-1.33166600	C	-3.54940600	-1.94536900	-1.05813700
C	-4.52125700	-0.59682000	-0.57965100	C	-4.61802100	-2.88860300	-0.99283900
C	-4.12030900	1.21253400	-2.16071100	C	-3.67101500	-0.87204800	-1.98885500
C	-5.89261700	-0.35777400	-0.65270700	C	-5.73477800	-2.76016800	-1.80492700
H	-4.13623200	-1.38704400	0.05950900	H	-4.54849700	-3.71760400	-0.29228800
C	-5.48911900	1.44694600	-2.22970600	C	-4.79688700	-0.75828800	-2.79516600
H	-3.41934800	1.80654400	-2.73799400	H	-2.86889200	-0.14541600	-2.06272700
C	-6.37559200	0.66349000	-1.47672600	C	-5.83930600	-1.69425600	-2.71533200
H	-6.58209300	-0.96178200	-0.07123700	H	-6.53529000	-3.49199800	-1.73475700
H	-5.87277700	2.23718400	-2.86771600	H	-4.86832100	0.06848700	-3.49735300
H	-7.44376600	0.85123700	-1.53436200	H	-6.71550500	-1.59703500	-3.34898600
15				15			
Charge=0 Multiplicity =1				Charge=0 Multiplicity =3			
Cu	1.54742400	1.00502300	0.00818300	Cu	1.53080600	0.95857400	0.20435100
O	-0.29700400	1.10169600	0.10067100	O	-0.30024600	0.95043000	0.51573900
C	4.54873100	3.71343200	-0.13806200	C	4.33991800	3.81720800	-0.34089100
N	2.49357100	2.72265200	0.01338200	N	2.36715000	2.73594800	0.07491800

C	3.57998100	4.70915900	0.00476200	C	3.34089300	4.77144200	-0.13532800
H	5.61900000	3.84510400	-0.22995200	H	5.38545900	3.99510700	-0.55703500
C	2.32948900	4.05225100	0.09144200	C	2.14398700	4.05858900	0.11384200
H	3.73828300	5.77851100	0.03714600	H	3.44596800	5.84756400	-0.16197100
H	1.34594300	4.49187600	0.19949400	H	1.15504800	4.45402000	0.31087900
C	4.25740600	1.13573300	-0.21170100	C	4.18774300	1.23107800	-0.29722900
H	5.31277100	0.88335400	-0.31708200	H	5.23962300	1.04513000	-0.51654700
N	3.33876800	0.18429700	-0.18161300	N	3.34648100	0.22231300	-0.14034900
C	3.67348600	-1.18551600	-0.15353900	C	3.78196300	-1.11925700	-0.13571300
C	2.79365100	-2.10422800	-0.75218000	C	2.89384800	-2.11464400	-0.57921400
C	4.83359100	-1.67050000	0.47860000	C	5.05438500	-1.50647200	0.32505500
C	3.07037100	-3.47004400	-0.74808400	C	3.26686400	-3.45748900	-0.59380700
C	5.12371700	-3.03487700	0.48226500	C	5.44018600	-2.84710900	0.31037900
C	4.23731500	-3.90997000	-0.13408100	C	4.53984400	-3.79878800	-0.15246900
H	2.40046900	-4.18474500	-1.21330300	H	2.58922600	-4.22929600	-0.94204100
H	6.01102500	-3.42128700	0.97195700	H	6.41545800	-3.15657400	0.67038900
C	3.85361800	2.48139500	-0.12722900	C	3.71497700	2.55503900	-0.20420600
H	1.89426900	-1.73804100	-1.23939100	H	1.90766800	-1.82563300	-0.93210200
H	5.49790900	-0.98663700	0.99658400	H	5.73794000	-0.76554500	0.72641600
F	4.51391000	-5.23988500	-0.12416000	F	4.91083600	-5.10640900	-0.16031000
H	-2.74418800	1.15408600	1.15406000	H	-2.97437400	1.32984600	1.01199500
H	-5.30106100	-3.01815000	0.01188300	H	-5.21453200	-3.11023400	0.31357200
C	-4.45369800	-2.36864600	-0.24024900	C	-4.37697000	-2.45574800	0.04255800
C	-4.65801900	-1.78574400	-1.64857600	C	-4.46611000	-2.10529900	-1.45237200
C	-4.31965600	-1.28968800	0.88491100	C	-4.40621100	-1.21332200	0.99320500
C	-5.56105000	-0.55480700	-1.58369300	C	-5.42529800	-0.93450200	-1.66398500
H	-5.09307000	-2.54782000	-2.30638600	H	-4.79931500	-2.98240900	-2.02003300
C	-4.90722500	0.59912100	-0.78017100	C	-4.90757100	0.36432100	-0.99244100
H	-6.51722200	-0.83523200	-1.12328200	H	-6.40956200	-1.19882900	-1.25609300
H	-3.69098400	-1.50904700	-2.08406000	H	-3.47392700	-1.84089200	-1.83571900
H	-3.56439000	-3.00889100	-0.24058100	H	-3.46329300	-3.03267100	0.22410200
H	-5.80073200	-0.18612600	-2.58800900	H	-5.57869000	-0.73601800	-2.73116100
C	-3.13898900	-1.67355400	1.79742200	C	-3.30914000	-1.38343700	2.06176200
H	-3.06051900	-1.00260700	2.65637000	H	-3.35145400	-0.58786000	2.80977500
H	-3.28065100	-2.69420100	2.16973400	H	-3.44214800	-2.34295700	2.57348500
H	-2.19870000	-1.63779000	1.23709500	H	-2.31833400	-1.37541300	1.59523700
C	-5.59786800	-1.22793500	1.75621200	C	-5.76727600	-1.09704700	1.72132700
H	-5.69101800	-2.14978400	2.34210000	H	-5.87635600	-1.92262500	2.43421500
H	-5.54361800	-0.38541100	2.45154600	H	-5.82332700	-0.15682400	2.27753200
H	-6.50646300	-1.13055200	1.15619700	H	-6.61465300	-1.14894700	1.03292500
C	-4.03208100	1.45713300	-1.71713900	C	-3.98377400	1.12231200	-1.96885200
H	-4.65308800	1.97143000	-2.45952300	H	-4.55145000	1.48282200	-2.83422000
H	-3.48967400	2.21451400	-1.14375900	H	-3.53353100	1.98866100	-1.47504000
H	-3.29839600	0.83777500	-2.24248100	H	-3.17673600	0.47504800	-2.32660000

C	-6.00283400	1.50246500	-0.17310200	C	-6.09672000	1.28208400	-0.63550400
H	-5.56474300	2.36375200	0.33528500	H	-5.75047800	2.22946400	-0.21746200
H	-6.65036500	1.86715500	-0.97913000	H	-6.66927200	1.49349100	-1.54612400
H	-6.62958500	0.96784400	0.54365800	H	-6.77432500	0.81978100	0.08509300
N	-3.96939800	-0.00052700	0.22293800	N	-4.04545600	-0.02277000	0.17126000
O	-3.70265700	0.98858500	1.22899500	O	-3.92424000	1.12384400	1.03255200
O	-0.85807400	1.59449300	1.15460500	O	-1.04326400	1.90680700	0.89741100
16				16			
Charge=0	Multiplicity =1			Charge=0	Multiplicity =3		
Cu	0.36137100	0.86941300	-0.56413400	Cu	1.61849500	1.30269600	-0.24970600
O	-1.27950900	0.00740800	-1.05840600	O	-0.15161700	1.06213100	-0.54436500
C	1.97037200	4.49784900	0.52365900	C	5.38242300	2.54699000	0.55384200
N	0.48869600	2.86035800	-0.11134600	N	3.14276700	2.44777900	0.09657000
C	0.71818300	5.08589900	0.33028000	C	4.88674900	3.85255100	0.45949600
H	2.88907200	4.98557500	0.82511600	H	6.40046700	2.24304900	0.76030800
C	-0.15258000	4.03948800	-0.06157500	C	3.50859400	3.74119100	0.17419800
H	0.45585000	6.12930400	0.44802800	H	5.44052300	4.77423200	0.57694200
H	-1.20497800	4.11453200	-0.31134300	H	2.79061800	4.53741700	0.02206300
C	2.72438000	2.04798100	0.25684000	C	4.13569600	0.28831800	0.27770100
H	3.76418900	2.25335200	0.52237300	H	5.00254800	-0.35790800	0.42550300
N	2.34008300	0.83241000	-0.07523100	N	2.94929300	-0.21820400	0.01981900
C	3.22638700	-0.25814800	-0.01222400	C	2.70644500	-1.60596100	-0.00449400
C	3.00245100	-1.34686100	-0.87612600	C	1.69961600	-2.09127600	-0.85841200
C	4.30343600	-0.33452600	0.89369500	C	3.41031500	-2.51714100	0.80504100
C	3.84164300	-2.45990800	-0.86861700	C	1.42456300	-3.45583600	-0.93151500
C	5.14986700	-1.44460800	0.91013100	C	3.14224700	-3.88510300	0.73642900
C	4.90663700	-2.48582900	0.02402500	C	2.15638900	-4.32924700	-0.13551500
H	3.67806000	-3.29579800	-1.54048500	H	0.65717600	-3.84128300	-1.59415500
H	5.97655200	-1.51255400	1.60953000	H	3.67406200	-4.59634000	1.35934300
C	1.80306000	3.11937900	0.24430400	C	4.28271300	1.69223900	0.32702600
H	2.16231400	-1.30164400	-1.56306900	H	1.13717200	-1.39081900	-1.46820400
H	4.46906000	0.46249700	1.61116500	H	4.15126100	-2.15927800	1.51254700
F	5.72817100	-3.57471200	0.04237100	F	1.88820100	-5.66287800	-0.20021000
H	-1.65579300	-0.62461900	-2.80463600	H	-1.41461500	0.39209700	-1.76922800
H	-4.10613500	1.40423800	1.45408400	H	-5.44136900	2.10072900	1.49484300
C	-3.28092500	0.94611800	0.89667100	C	-4.39529800	1.84408900	1.28896100
C	-2.26767500	0.31897700	1.87630900	C	-3.95587100	0.74971500	2.26925400
C	-3.92075000	-0.03175800	-0.12341300	C	-4.27784700	1.45549900	-0.22060700
C	-2.54837000	-1.16001100	2.14581900	C	-4.51829600	-0.60115600	1.82878800
H	-2.27947100	0.87530200	2.81914400	H	-4.30397300	1.00256800	3.27697800
C	-2.45446100	-2.03044900	0.87521100	C	-3.87225100	-1.07828600	0.51105500
H	-3.53334500	-1.27766900	2.61293700	H	-5.60678200	-0.51903400	1.70895900
H	-1.25633800	0.42735000	1.47234100	H	-2.86182600	0.70084400	2.32016400
H	-2.78527500	1.75165700	0.34937100	H	-3.81252500	2.75285800	1.47003500

H	-1.82374800	-1.55658500	2.86549900	H	-4.34849800	-1.37229200	2.58813600
C	-4.15839700	0.65360000	-1.47307100	C	-3.42214500	2.49463000	-0.96146900
H	-4.65454900	-0.01250400	-2.18237600	H	-3.37749000	2.28984900	-2.03232300
H	-4.80682800	1.51845400	-1.30186100	H	-3.87167600	3.48168300	-0.81297100
H	-3.21755800	1.00835600	-1.89436900	H	-2.40168300	2.51320900	-0.56872600
C	-5.27998700	-0.58194700	0.38027200	C	-5.67159100	1.37416800	-0.88460600
H	-5.99392300	0.24720400	0.39429000	H	-6.13835500	2.36495200	-0.87524500
H	-5.66280600	-1.35012900	-0.29779200	H	-5.57901800	1.04340000	-1.92317500
H	-5.23191100	-0.98888100	1.39109000	H	-6.33702000	0.68705100	-0.35369600
C	-1.00701300	-2.44370400	0.57305900	C	-2.50920300	-1.74332900	0.78387400
H	-0.70745400	-3.19702100	1.30796100	H	-2.65901300	-2.64407800	1.38734200
H	-0.93022100	-2.87669000	-0.42566500	H	-2.03041400	-2.02717800	-0.15485900
H	-0.31936900	-1.60061400	0.63589500	H	-1.83280500	-1.07163600	1.31918500
C	-3.31522400	-3.30502000	1.00626400	C	-4.78894000	-2.06914900	-0.23147500
H	-3.20975100	-3.93391600	0.11965700	H	-4.32369900	-2.39356000	-1.16521100
H	-2.96230800	-3.86620200	1.87691900	H	-4.96094000	-2.94760500	0.39946200
H	-4.37341300	-3.08073600	1.15602200	H	-5.75969900	-1.62127700	-0.46267700
N	-3.00541400	-1.24138800	-0.33198600	N	-3.61227000	0.11268500	-0.37019500
O	-3.11516800	-1.87721500	-1.38544600	O	-3.05235600	-0.14439800	-1.50271700
O	-0.98569600	-0.86289300	-2.13995100	O	-0.47439800	0.69137200	-1.87126400

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Charge=0 Multiplicity =2

Cu	0.70895200	0.71832700	0.88751000
O	2.00057400	0.12856200	2.11440400
C	1.19136000	3.88729100	-1.62633400
N	1.49370800	2.22995100	-0.07916400
C	2.49900400	3.95956000	-1.13927100
H	0.72623500	4.52721400	-2.36516300
C	2.63620900	2.92340300	-0.18381800
H	3.26462100	4.67034800	-1.42011100
H	3.48991800	2.67589900	0.43276000
C	-0.71456500	2.25824700	-0.95257100
H	-1.49099800	2.68778700	-1.58779800
N	-0.98901800	1.25056700	-0.14455600
C	-2.27229200	0.66333100	-0.14257000
C	-2.83307800	0.25339500	1.08035200
C	-3.00602900	0.45484300	-1.32611000
C	-4.10056500	-0.32511800	1.12860100
C	-4.27792800	-0.12027000	-1.28838500
C	-4.80254500	-0.49750000	-0.05914500
H	-4.54444000	-0.63474600	2.06867900
H	-4.84909100	-0.28821600	-2.19518300
C	0.58244400	2.80341600	-0.95141500
H	-2.26823400	0.39893800	1.99459100

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Charge=0 Multiplicity =2

Cu	-0.66001300	0.66534700	-0.82962100
O	-2.25485000	0.08791400	-2.00017000
C	-0.87312600	4.19079600	1.14915600
N	-1.31859200	2.30762300	-0.06315800
C	-2.21496500	4.21497400	0.75527500
H	-0.34563100	4.93254800	1.73470100
C	-2.44406500	3.03669500	0.00730600
H	-2.94634800	4.98214900	0.97053100
H	-3.35550400	2.70007300	-0.46964100
C	0.93630700	2.38603600	0.65693800
H	1.77162900	2.87033400	1.16470700
N	1.10788900	1.23718700	0.02951100
C	2.34301900	0.55667200	0.07170100
C	2.78179100	-0.12931200	-1.07481800
C	3.14305400	0.52743900	1.22958200
C	4.00296800	-0.80167700	-1.07892700
C	4.36947900	-0.13936600	1.23300900
C	4.77812900	-0.78887200	0.07524400
H	4.35467700	-1.32700600	-1.96034700
H	4.99278700	-0.17108600	2.12020200
C	-0.33390000	2.99235600	0.62980800
H	2.15338300	-0.13313700	-1.95870000

H	-2.57336400	0.72296800	-2.28501500	H	2.79803800	1.00850800	2.13948000
F	-6.03913100	-1.06485800	-0.01719900	F	5.96969200	-1.44532700	0.07562700
H	3.85678700	0.43836800	2.13210800	H	-3.25666500	-1.00943000	-0.76340300
O	3.11029400	0.98960100	2.41713900	O	-3.48483000	-0.22665000	-1.30102300
C	-0.25678800	-2.33715500	0.58912800	C	-0.06829900	-2.29143500	-0.91770000
H	-1.08764500	-1.99247700	-0.02891500	H	0.92621300	-2.22747800	-0.46087100
H	-0.60444000	-3.18124000	1.19460700	H	-0.05610700	-3.12763200	-1.62933200
O	0.01914100	-1.22739000	1.48539600	O	-0.30662900	-1.09183300	-1.65564200
H	0.79542000	-1.42639700	2.04317900	H	-1.49343500	-0.79754500	-1.99306500
C	0.93467900	-2.73016800	-0.24789800	C	-1.11654600	-2.53611400	0.15007600
C	1.29161100	-1.97695900	-1.37674300	C	-0.95634800	-2.01772200	1.44436800
C	1.71765900	-3.83799200	0.10336800	C	-2.29556000	-3.23779600	-0.15158000
C	2.41360600	-2.31907600	-2.13249100	C	-1.95173900	-2.18581300	2.41069900
H	0.68819000	-1.11949900	-1.66418900	H	-0.04321100	-1.48395700	1.69673700
C	2.83969900	-4.18588600	-0.65372000	C	-3.29396400	-3.40841300	0.81357800
H	1.44548600	-4.43569400	0.97042000	H	-2.42630600	-3.66272500	-1.14447900
C	3.18997200	-3.42514000	-1.77176600	C	-3.12421400	-2.87901400	2.09658700
H	2.67973300	-1.72688900	-3.00304400	H	-1.81161400	-1.77797500	3.40755800
H	3.43597700	-5.04894200	-0.37230500	H	-4.19759500	-3.95782400	0.56559800
H	4.06081800	-3.69430400	-2.36236900	H	-3.89789400	-3.01066100	2.84709700

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Charge=0 Multiplicity =2

Cu	-0.78546800	-0.60713700	0.64303500
O	-2.52695200	-0.16155100	2.00612500
C	-1.15914300	-3.90710500	-1.67098300
N	-1.52265100	-2.13397500	-0.27563100
C	-2.51328300	-3.88162800	-1.31977500
H	-0.66014700	-4.61666500	-2.31803800
C	-2.68947500	-2.77636100	-0.45777100
H	-3.28481800	-4.57048900	-1.63598700
H	-3.59620300	-2.43856300	0.02717000
C	0.74640500	-2.29586800	-0.94198900
H	1.56505800	-2.79040200	-1.46679800
N	0.97398300	-1.22949400	-0.20208000
C	2.25656900	-0.64739200	-0.12340600
C	2.69403900	-0.12549100	1.10652500
C	3.10626500	-0.56343600	-1.24201700
C	3.96470700	0.43422300	1.22852400
C	4.38151100	-0.00779900	-1.12779300
C	4.78831500	0.47606300	0.10906800
H	4.31641900	0.83422700	2.17338100
H	5.04483100	0.06551200	-1.98287400
C	-0.56370600	-2.80969400	-1.01209500
H	2.02385200	-0.15480400	1.95884400

H	2.76342400	-0.91318300	-2.21076000
F	6.02849100	1.02296800	0.22440100
H	-3.46362400	-0.94135400	3.44837500
O	-2.52532300	-0.98941800	3.20366000
C	0.03271500	2.17156200	0.93391400
H	1.02411900	2.02656000	0.47959300
H	0.14667600	2.93709900	1.71566000
O	-0.39270000	0.97710800	1.56631300
C	-0.93944000	2.66189400	-0.12240600
C	-0.75365200	2.33700900	-1.47378700
C	-2.06863400	3.41300000	0.23680000
C	-1.67610500	2.74284600	-2.44282200
H	0.12511600	1.76830500	-1.76954600
C	-2.99264300	3.82245600	-0.72683000
H	-2.22045200	3.68103800	1.27998300
C	-2.79911900	3.48607700	-2.07066000
H	-1.51546400	2.48382400	-3.48568600
H	-3.85960600	4.40736700	-0.43209800
H	-3.51558800	3.80601500	-2.82183400
H	-1.86290500	0.56880800	2.21321800

Table S2 Cartesian coordinates all structures considered in this work (H₂O level)

0				TS1-2			
Charge=-1 Multiplicity = 2				Charge=-1 Multiplicity = 2			
Cu	1.03380600	0.19976600	-0.00055700	Cu	0.83643000	-1.02058900	-0.12298800
O	5.16973600	2.43899800	0.33110700	O	-1.07096700	-0.67765500	-0.78314800
C	1.40078200	-3.87701400	-0.16564700	C	4.54660000	-1.63521100	-1.76538700
N	1.77776000	-1.62658100	0.00229000	N	2.46494200	-1.91715600	-0.85236700
C	2.78168500	-3.65762900	-0.08909100	C	4.25882100	-3.00329900	-1.71675400
H	0.88618100	-4.82635700	-0.25089200	H	5.44610400	-1.16200100	-2.13935500
C	2.96222700	-2.25614800	0.00968400	C	2.96776900	-3.12422500	-1.14343000
H	3.56643600	-4.40325300	-0.10327100	H	4.89128100	-3.81904200	-2.04304300
H	3.88672500	-1.69642800	0.07923900	H	2.40639800	-4.02564700	-0.93084100
C	-0.54057500	-2.15424800	-0.12906600	C	3.09630600	0.37050800	-0.97529200
H	-1.34189600	-2.88970600	-0.23492100	H	3.82455700	1.15582600	-1.19077000
N	-0.79976900	-0.86871700	-0.04827400	N	1.93348600	0.66306200	-0.43726100
C	-2.12263700	-0.38931300	-0.00064100	C	1.56326100	1.98606700	-0.13810000
C	-2.36670000	0.93879000	-0.40294100	C	0.81078500	2.21976000	1.02837600
C	-3.20786700	-1.16343400	0.46009000	C	1.89986500	3.07479000	-0.96350600
C	-3.66084500	1.45881900	-0.39479800	C	0.43079600	3.51443600	1.37922800
C	-4.50614400	-0.64898500	0.46805500	C	1.52395900	4.37488300	-0.61701500
C	-4.70886900	0.65242300	0.02996800	C	0.79970200	4.56823900	0.55142800
H	-3.85259000	2.48095500	-0.70420000	H	-0.14304600	3.70568500	2.27981500
H	-5.34450600	-1.23807700	0.82582400	H	1.77012600	5.22232600	-1.24847600
C	0.80120400	-2.59753400	-0.10404000	C	3.41419600	-0.98211600	-1.22450300

H	-1.52648700	1.56136700	-0.69357600	H	0.54003300	1.37388200	1.65370900
H	-3.04270800	-2.16518500	0.84307100	H	2.43288300	2.90372000	-1.89374000
F	-5.98144700	1.16087100	0.03986800	F	0.42695800	5.84061900	0.89063400
O	2.13852300	3.64080700	-0.06079700	O	-0.96436700	-2.81681300	2.72791500
C	1.76166800	2.46939200	-0.03745700	C	-0.38580800	-2.13649400	1.88194900
O	2.57140900	1.41419600	0.07607800	O	-0.42559500	-2.56065000	0.52491600
O	0.49799100	2.05848600	-0.11830700	O	0.29077000	-1.05756800	2.02114200
H	4.88315200	3.35976100	0.26730100	H	-1.03204600	-1.84202000	-0.03409600
H	4.30755500	1.97233600	0.26130400	C	-1.92278700	0.37226500	-0.38815300
				H	-1.60101600	1.31274200	-0.86324100
				H	-1.88529600	0.53055800	0.70272900
				C	-3.35870400	0.08195700	-0.79024100
				C	-4.21424900	-0.61998500	0.07118100
				C	-3.84822400	0.47344200	-2.04419100
				C	-5.52430600	-0.92323700	-0.30934100
				H	-3.84629300	-0.93537700	1.04468300
				C	-5.15780400	0.17532800	-2.43040800
				H	-3.19106700	1.01262000	-2.72259400
				C	-6.00119600	-0.52541800	-1.56227200
				H	-6.17148100	-1.46961700	0.37207300
				H	-5.52007800	0.48847600	-3.40678000
				H	-7.02048800	-0.75908000	-1.85953800
				O	-0.17564800	-1.00796300	4.90411700
				H	0.21871800	-0.69164300	4.07228700
				H	-0.63482500	-1.79619600	4.56458000
TS3-4				TS5-6			
Charge=-1 Multiplicity = 2				Charge=-1 Multiplicity = 2			
Cu	0.98496200	0.00114900	0.63940700	Cu	-0.19498400	0.59049000	0.47304600
O	0.27390800	0.88697900	2.31102900	O	-0.58694100	0.58502600	2.81808600
C	2.02352700	-3.61680000	-0.99470600	C	-0.06049800	4.50492200	-0.73223800
N	2.06071200	-1.54452300	-0.01892800	N	-0.66509300	2.45139200	0.06224200
C	3.35118100	-3.27600800	-0.71411400	C	-1.39227900	4.56555000	-0.29407100
H	1.65797300	-4.52580900	-1.45626600	H	0.53077600	5.30391500	-1.16225000
C	3.32026100	-1.99028400	-0.11799800	C	-1.71887000	3.27727400	0.18578100
H	4.23655900	-3.86586400	-0.91444000	H	-2.05152400	5.42399000	-0.31688400
H	4.15147400	-1.38661600	0.22487000	H	-2.65047900	2.92135700	0.60585600
C	-0.14279300	-2.24412800	-0.57765600	C	1.58243400	2.48906900	-0.70172500
H	-0.84023000	-2.95072100	-1.03407200	H	2.43402300	3.00679600	-1.15065400
N	-0.56398200	-1.10106100	-0.08805100	N	1.66624800	1.22474700	-0.37334800
C	-1.91649500	-0.72599400	-0.09019600	C	2.89439900	0.53905100	-0.50846100
C	-2.22493100	0.63292100	-0.29579000	C	2.89452700	-0.78718300	-0.97141200
C	-2.96458600	-1.63898900	0.12666800	C	4.12083700	1.14682200	-0.18007900
C	-3.55046800	1.06472300	-0.31074100	C	4.09014500	-1.48316700	-1.14210100
C	-4.29518100	-1.21325300	0.11035900	C	5.32480000	0.45998900	-0.35239400

C	-4.56087700	0.13104900	-0.11111500	C	5.28314200	-0.84048800	-0.83826700
H	-3.79964000	2.10715000	-0.47913300	H	4.07724100	-2.51065800	-1.48912900
H	-5.11267600	-1.90506900	0.28546200	H	6.27669600	0.91291700	-0.09481900
C	1.24134900	-2.52485300	-0.55148000	C	0.36401600	3.18067900	-0.49450200
H	-1.40960200	1.33271300	-0.46088800	H	1.95563700	-1.28371000	-1.17906600
H	-2.73984100	-2.67957200	0.33937900	H	4.13320000	2.14825800	0.23948500
F	-5.86398000	0.55116700	-0.12148300	F	6.46460000	-1.51282000	-1.00283300
O	2.69001400	3.37496600	0.05090400	O	1.23742700	-3.14769700	1.18950400
C	2.01484900	2.35311100	0.18825600	C	0.78720400	-2.01834500	1.43639300
O	2.32083900	1.48212900	1.26461400	O	0.86835200	-1.54740500	2.68993900
O	1.03875400	1.91904800	-0.51992700	O	0.22568000	-1.27041100	0.52196200
H	1.42852300	1.45994400	1.94856100	H	0.36059500	-0.68163200	2.80189100
H	-0.48683400	1.45609900	2.13830000	O	-2.22013000	0.26914300	1.11984200
O	1.19521400	4.22279000	-2.30750300	H	-0.48394400	1.41655000	3.29261300
H	1.88515200	4.32562200	-1.62689000	C	-2.85523400	-0.99204200	1.09011900
H	0.83909100	3.36114400	-2.02733600	H	-2.12012300	-1.79000400	0.91215400
				H	-3.31512200	-1.19213400	2.07201600
				C	-3.93364600	-1.07150700	0.02501900
				C	-4.64219200	-2.27031900	-0.15401000
				C	-4.24800200	0.02029200	-0.79180900
				C	-5.64405600	-2.37480500	-1.12004800
				H	-4.40066500	-3.13098800	0.46697900
				C	-5.24974800	-0.08238600	-1.76379600
				H	-3.69474500	0.94321500	-0.65984100
				C	-5.95380300	-1.27698200	-1.93157500
				H	-6.17948500	-3.31297500	-1.24396300
				H	-5.47645500	0.77510400	-2.39276300
				H	-6.73061100	-1.35625600	-2.68781000
				H	-1.63530100	0.43635900	2.07360600
				O	1.42835300	-3.88337100	-1.44840600
				H	0.58765900	-3.57783500	-1.80895700
				H	1.36670300	-3.65489600	-0.48589500
8				TS9-10			
Charge=0 Multiplicity = 2				Charge=0 Multiplicity = 2			
Cu	-1.23260600	0.53081700	-0.06940800	Cu	-0.22538400	-0.33088200	0.20237300
C	-3.22641300	-2.93988700	0.34925500	C	-1.17670800	-4.09203900	-0.94851400
N	-2.64265100	-0.75350900	0.05255800	N	-1.24940500	-1.89810200	-0.32354000
C	-4.39130800	-2.18279700	0.17260800	C	-2.50884400	-3.66494900	-0.95439500
H	-3.15455300	-4.00736600	0.51033500	H	-0.79903600	-5.07448900	-1.19998700
C	-3.98581000	-0.84429600	-0.00658500	C	-2.50826600	-2.30760300	-0.56286800
H	-5.41173200	-2.54056300	0.17979700	H	-3.38330000	-4.24993100	-1.20493700
H	-4.60402800	0.03072300	-0.16048100	H	-3.35005700	-1.63792600	-0.44745400
C	-0.74715400	-2.14957600	0.32434300	C	0.96608300	-2.73473200	-0.37069100
H	-0.26841600	-3.11948900	0.46163800	H	1.69903400	-3.52735500	-0.52183900

N	-0.01587600	-1.05955600	0.22139500	N	1.35499700	-1.53430400	0.01666200
C	1.38841600	-1.10403000	0.08399300	C	2.73130700	-1.22779100	0.14986300
C	2.17430800	-0.14555600	0.74399700	C	3.16664500	-0.48250500	1.25629000
C	2.01153300	-2.06991100	-0.72858400	C	3.67111700	-1.64942300	-0.80598500
C	3.56066300	-0.15757100	0.61684500	C	4.51729900	-0.18799200	1.42658900
C	3.40024900	-2.10137800	-0.84649900	C	5.02708700	-1.36280800	-0.64344600
C	4.14717300	-1.14313100	-0.16909300	C	5.42346300	-0.63931400	0.47399700
H	4.16687100	0.59719300	1.10408400	H	4.86797000	0.38594300	2.27718600
H	3.89948700	-2.83633200	-1.46848400	H	5.76370400	-1.67673500	-1.37497400
C	-2.15163100	-2.03206800	0.26755900	C	-0.40826100	-2.97485900	-0.55656300
H	1.70315000	0.61737600	1.35147600	H	2.44050400	-0.13104900	1.98079100
H	1.40927800	-2.78001100	-1.28674100	H	3.33935400	-2.18091900	-1.69238600
F	5.49853100	-1.16411000	-0.29827100	F	6.74269100	-0.35212400	0.63458900
O	-0.60424700	4.22530700	-0.49104800	O	0.71511900	3.76135700	-0.30452100
C	-0.82407900	3.03995700	-0.39213100	C	1.25587800	2.67610000	-0.11269900
O	-2.13293500	2.51989700	-0.52468900	O	2.47309000	2.34932700	-0.55206500
O	-0.03642000	2.04043200	-0.15938300	O	0.70062800	1.68536300	0.57407000
H	-2.77708900	3.23282900	-0.65750900	H	2.84264100	3.13291200	-1.03065300
O	2.47557200	3.05595500	1.01432000	C	-2.60841000	1.00329800	1.48977700
H	1.68613000	2.80875900	0.50266900	H	-2.58828700	1.93032100	2.08367700
H	2.46793100	4.02037500	1.03496000	O	-1.50212300	1.03513200	0.60631500
				H	-0.41156900	1.74450600	0.71720400
				H	-2.52359800	0.17054800	2.20291300
				C	-3.93937400	0.90651800	0.76563400
				C	-5.04568300	0.33441200	1.40839600
				C	-4.09708000	1.41727700	-0.52898100
				C	-6.29003600	0.27939600	0.77485200
				H	-4.93359300	-0.07598900	2.40990800
				C	-5.33923700	1.35808500	-1.16657200
				H	-3.23826900	1.84999600	-1.03176800
				C	-6.44002900	0.79113700	-0.51728000
				H	-7.13734800	-0.16936300	1.28580500
				H	-5.44721600	1.75511300	-2.17221100
				H	-7.40460800	0.74520600	-1.01466200
				O	2.88295500	4.81500400	-1.61740800
				H	2.87008500	5.10088800	-2.53852200
				H	1.96730900	4.87714700	-1.27562600
11				TS12-13			
Charge=0 Multiplicity = 2				Charge=0 Multiplicity = 2			
Cu	1.21147000	1.04172500	0.10335900	Cu	0.02957800	0.42794700	0.04177200
C	2.88550300	-2.63740700	-0.23177900	C	0.88124700	4.36916800	-0.38558200
N	2.50127000	-0.39586800	-0.00400300	N	-0.16627700	2.35243100	-0.15691800
C	4.11600400	-1.98054100	-0.11391400	C	-0.50178200	4.58234100	-0.34749900
H	2.71513000	-3.69967000	-0.34903800	H	1.65964100	5.11454400	-0.48366200

C	3.83032900	-0.60465600	0.02428700	C	-1.10560800	3.31454300	-0.20419400
H	5.10068000	-2.42793300	-0.12287700	H	-1.02094900	5.52876600	-0.41416700
H	4.52386600	0.21754100	0.14663300	H	-2.15924400	3.07809800	-0.13240900
C	0.48759000	-1.63288400	-0.19884200	C	2.19289700	2.13113100	-0.20084100
H	-0.06444800	-2.56585300	-0.32388600	H	3.20253200	2.53892900	-0.26482800
N	-0.14998600	-0.48501600	-0.10911900	N	2.00680800	0.83280600	-0.07989400
C	-1.55904800	-0.42623600	-0.06373100	C	3.10985900	-0.04007100	0.09304500
C	-2.22336300	0.61067300	-0.74254500	C	3.18585500	-1.22265300	-0.66109600
C	-2.31794400	-1.36607700	0.65784600	C	4.12510700	0.25159800	1.02135600
C	-3.61529800	0.69086600	-0.72876900	C	4.26678400	-2.08980200	-0.50455900
C	-3.71180700	-1.29570300	0.67302700	C	5.21309100	-0.60897300	1.17984100
C	-4.33423500	-0.26873100	-0.02505300	C	5.26155000	-1.76453600	0.41054900
H	-4.14021500	1.48092400	-1.25489400	H	4.33916300	-3.00156900	-1.08724600
H	-4.30788500	-2.01117400	1.22921000	H	6.00192500	-0.39916700	1.89414500
C	1.89743300	-1.63275000	-0.15772400	C	1.06597500	2.97622300	-0.26194000
H	-1.63637800	1.34944000	-1.27702900	H	2.41172900	-1.46391500	-1.38064400
H	-1.81742700	-2.14021100	1.23084800	H	4.05201700	1.14283500	1.63722800
F	-5.69236400	-0.19182700	-0.00773600	F	6.31535400	-2.61076400	0.56603400
O	0.15525600	2.56542700	0.24194900	O	0.00804700	-1.63710600	0.25102400
H	-0.67472100	2.49667600	0.72691200	H	0.37607000	-2.01349900	1.06206400
O	2.63830600	2.69099700	0.20735800	O	-1.80719200	-0.20653700	0.32614700
H	1.81013800	3.21958900	0.32676800	C	-2.84807500	-0.11068200	-0.63158800
H	3.05143500	2.97255300	-0.61985000	H	-2.98384800	0.94654800	-0.90344900
				H	-2.58521700	-0.64324600	-1.55923800
				H	-1.05796000	-1.26960400	0.36588000
				C	-4.16139200	-0.65968600	-0.10032600
				C	-5.13857900	-1.11921700	-0.99401700
				C	-4.43555000	-0.68174200	1.27266400
				C	-6.37151900	-1.58149700	-0.52758600
				H	-4.93370600	-1.11847000	-2.06265700
				C	-5.66692500	-1.14856600	1.74159700
				H	-3.67489900	-0.33661600	1.96522100
				C	-6.63968800	-1.59789600	0.84439300
				H	-7.11772500	-1.93547900	-1.23354900
				H	-5.86611500	-1.16179100	2.80976400
				H	-7.59559300	-1.96184200	1.21009900
				O	0.70535900	-2.90489000	-2.17390800
				H	0.16449900	-3.65247900	-2.45272000
				H	0.35884300	-2.61213700	-1.30925300

Table S3 Cartesian coordinates all structures considered in this work (2H₂O level)

0				TS1-2			
	Charge=-1 Multiplicity = 2				Charge=-1 Multiplicity = 2		
Cu	1.05039800	-0.13407300	0.02776100	Cu	1.09852600	-0.78378300	-0.37293800
O	5.05072400	2.78781600	-0.01274900	O	-0.86935600	-0.97297400	-0.84985700

C	1.37370300	-4.20968900	-0.11854800	C	4.67393900	-0.21445000	-2.27726200
N	1.77840800	-1.96326400	0.03014500	N	2.83936200	-1.13013200	-1.26044500
C	2.75733300	-4.00680100	-0.04155000	C	4.78381100	-1.60916400	-2.32232500
H	0.84787200	-5.15331100	-0.19632400	H	5.37163400	0.51598700	-2.66757800
C	2.95529500	-2.60776400	0.04487200	C	3.63221400	-2.12653900	-1.68011000
H	3.53251700	-4.76227400	-0.04740800	H	5.58909400	-2.19014400	-2.75324100
H	3.88690300	-2.05990100	0.11201200	H	3.36473300	-3.16126000	-1.50543000
C	-0.54412100	-2.45815900	-0.11364900	C	2.79323900	1.24457700	-1.23104300
H	-1.36176800	-3.17585100	-0.21390400	H	3.25007900	2.21833200	-1.42111400
N	-0.77747000	-1.16636000	-0.05985500	N	1.64530900	1.15707100	-0.59888200
C	-2.09146900	-0.66082200	-0.03347700	C	0.95068700	2.30089800	-0.15822900
C	-2.32613000	0.62758700	-0.55054600	C	0.32826800	2.26298800	1.10278400
C	-3.17494600	-1.37638800	0.51404900	C	0.85165300	3.46763300	-0.93723100
C	-3.61165900	1.16737200	-0.56464700	C	-0.35041000	3.37792500	1.59228300
C	-4.46578900	-0.84398000	0.50038300	C	0.17235800	4.58873000	-0.45420200
C	-4.66012400	0.41656400	-0.04767700	C	-0.41103500	4.52106800	0.80423500
H	-3.79702400	2.16043700	-0.96013900	H	-0.81757400	3.35701900	2.57094800
H	-5.30464600	-1.38543200	0.92550000	H	0.08028700	5.49330200	-1.04636300
C	0.78989100	-2.92333400	-0.07012500	C	3.45524900	0.05682400	-1.61454300
H	-1.48467900	1.20498000	-0.91751000	H	0.39238600	1.36022500	1.70062900
H	-3.01045700	-2.34178000	0.98181600	H	1.28250100	3.49000400	-1.93355000
F	-5.92375600	0.94136900	-0.05845700	F	-1.07739300	5.61869000	1.27638300
O	2.20320500	3.29107100	0.01433400	O	0.20505100	-3.24771300	2.43128000
C	1.81706000	2.10955900	0.02483500	C	0.44858000	-2.36156700	1.60329900
O	2.61443400	1.05586100	0.03921100	O	0.36845200	-2.68757600	0.23532300
O	0.54026900	1.74033900	0.02317100	O	0.78862600	-1.14590800	1.79456000
H	4.20372400	3.27445200	-0.00408400	H	-0.45326900	-2.10155300	-0.21203300
H	4.71430700	1.87868200	0.00117100	C	-1.94240000	-0.22834400	-0.34535700
O	-0.31933900	4.63625100	0.25169500	H	-1.76645900	0.84771200	-0.50926300
H	0.63698800	4.46025700	0.14150400	H	-2.04667700	-0.35717100	0.74612800
H	-0.64664900	3.72732200	0.31757000	C	-3.27158300	-0.58302700	-1.00031600
				C	-4.46073500	-0.00585800	-0.52836700
				C	-3.33885500	-1.46673600	-2.08284500
				C	-5.68763200	-0.30044600	-1.12546800
				H	-4.42350300	0.67800400	0.31782100
				C	-4.56717500	-1.76550700	-2.68296900
				H	-2.41623800	-1.91230900	-2.43968500
				C	-5.74619700	-1.18427400	-2.20957600
				H	-6.59814300	0.15549600	-0.74387900
				H	-4.60165600	-2.45644100	-3.52208800
				H	-6.70038200	-1.41816000	-2.67497900
				O	0.21891400	0.08675100	4.32317900
				H	0.48597600	-0.29027800	3.46127100
				H	0.03063800	-0.71368500	4.84437300

	O	-0.24764800	-2.71997400	5.08199700			
	H	0.00395700	-2.92033000	4.14463400			
	H	-1.17695700	-2.97104500	5.13804700			
TS3-4	TS5-6						
Charge=-1 Multiplicity = 2	Charge=-1 Multiplicity = 2						
Cu	-0.68031600	0.27473600	0.52643300	Cu	-0.11738600	0.74197200	-0.06796600
O	-0.27976800	-0.94910000	2.04688700	O	-0.75363900	-0.02000100	2.11862800
C	-0.77447100	4.09952000	-0.91189300	C	0.19993000	4.81615800	-0.22732900
N	-1.32756100	2.03595700	-0.09010600	N	-0.52775100	2.65422500	-0.13624500
C	-2.16091700	4.04306000	-0.73343200	C	-1.20288900	4.81270000	-0.20926300
H	-0.19009700	4.93090300	-1.28594800	H	0.85774600	5.67538400	-0.26889800
C	-2.45249600	2.75137200	-0.22992000	C	-1.60388200	3.45881600	-0.15331900
H	-2.88176900	4.82291800	-0.94219800	H	-1.86057200	5.67207200	-0.23628700
H	-3.41702200	2.32702200	0.01927400	H	-2.60205700	3.04247700	-0.12880400
C	1.00734200	2.25884500	-0.46954700	C	1.83933100	2.79570300	-0.17958300
H	1.87593900	2.81360600	-0.83189500	H	2.76853100	3.37058600	-0.20268700
N	1.12874300	1.02360300	-0.03951100	N	1.86681100	1.48593300	-0.17279100
C	2.36350700	0.35705300	0.00817000	C	3.10290800	0.80844400	-0.06993600
C	2.39415700	-1.01016600	-0.32676800	C	3.35092200	-0.31734600	-0.87393500
C	3.55713000	0.99214800	0.39558500	C	4.09318100	1.23460100	0.83454800
C	3.59333700	-1.72081000	-0.29996200	C	4.57459800	-0.98202100	-0.80206200
C	4.76279600	0.28713100	0.42251500	C	5.32245300	0.57637100	0.91036300
C	4.75634600	-1.05587800	0.07145800	C	5.53890900	-0.51757800	0.08331700
H	3.63038200	-2.77143000	-0.56791900	H	4.76766000	-1.85356500	-1.41777100
H	5.68928300	0.76238900	0.72769500	H	6.09081800	0.88900500	1.60980800
C	-0.27882800	2.84002300	-0.50349300	C	0.59027900	3.46127000	-0.18067300
H	1.46952100	-1.49496300	-0.62817100	H	2.58623300	-0.67777300	-1.55139000
H	3.53893100	2.03246500	0.70543600	H	3.88881100	2.06604100	1.50226600
F	5.93507800	-1.74942200	0.10245700	F	6.74132700	-1.16484000	0.15655100
O	-3.28307600	-2.38051100	-0.47741600	O	1.07150400	-3.15228900	-0.45537600
C	-2.32408800	-1.65140800	-0.18437800	C	0.62577800	-2.12770000	0.10167900
O	-2.40621200	-0.88949800	1.00043000	O	0.46533200	-2.14099000	1.43071700
O	-1.23372700	-1.46547900	-0.82107000	O	0.31041000	-1.05882500	-0.56659700
H	-1.51434900	-1.16276100	1.65421700	H	0.02030100	-1.28992700	1.78450200
H	0.30637500	-1.67878000	1.80922900	O	-2.16726300	0.31545400	0.24381100
O	-1.78443100	-3.37480000	-2.89800800	H	-0.75267100	0.45935400	2.95311900
H	-2.60485300	-3.45085700	-2.38554400	C	-2.77357300	-0.85337500	-0.27481700
H	-1.33707400	-2.67760100	-2.38075400	H	-2.49823700	-0.95730700	-1.33257600
O	-5.27799700	-1.90862000	1.49188800	H	-2.38717500	-1.74777400	0.23452400
H	-4.67275200	-1.28640400	1.91732600	C	-4.28982500	-0.83347900	-0.15851100
H	-4.72851700	-2.20727400	0.73618400	C	-5.03090900	-1.93176300	-0.62250300
H	-2.54483857	-5.95972918	-0.87365161	C	-4.97588800	0.25056800	0.39891000
C	-2.90151141	-6.46412737	-0.00000010	C	-6.42367400	-1.94448500	-0.53518700
H	-2.54485699	-7.47293737	-0.00000010	H	-4.50983200	-2.78453100	-1.05337900

H	-2.54483857	-5.95972918	0.87365140	C	-6.37235500	0.24037400	0.48924100
H	-3.97151141	-6.46411418	-0.00000010	H	-4.40126900	1.09688200	0.75958700
H	13.14373350	-6.46411418	-0.00000010	C	-7.10265600	-0.85491100	0.02272300
C	14.21373350	-6.46412737	-0.00000010	H	-6.97952000	-2.80488300	-0.89939100
H	14.57038792	-7.47293737	-0.00000010	H	-6.88890100	1.09139200	0.92658000
H	14.57040634	-5.95972918	0.87365140	H	-8.18724000	-0.86298500	0.09321300
H	14.57040634	-5.95972918	-0.87365161	H	-1.73139800	0.14971200	1.25985200
				O	1.48770900	-2.48644700	-3.13973800
				H	0.86043900	-1.75261400	-3.13068800
				H	1.38860100	-2.84966800	-2.22958400
				O	1.31281900	-5.13476100	1.58503200
				H	1.03807700	-4.47623700	2.23657700
				H	1.29969600	-4.60157300	0.76294400

8

Charge=0 Multiplicity = 2

Cu	-1.07083000	-0.08413300	-0.00287800
C	-1.82989000	-4.02792300	0.31108200
N	-1.99013800	-1.76216400	0.09289700
C	-3.18270300	-3.67988100	0.20687300
H	-1.41337800	-5.02025100	0.42300400
C	-3.23511900	-2.27698300	0.07495800
H	-4.03358200	-4.34686900	0.22980800
H	-4.10627000	-1.64161000	-0.01989100
C	0.26164100	-2.47874100	0.25620000
H	1.03212500	-3.24532000	0.34256600
N	0.59684900	-1.20757800	0.18411100
C	1.93980900	-0.79342300	0.03621500
C	2.38727300	0.34705700	0.72181000
C	2.82761700	-1.48440500	-0.80906500
C	3.70247300	0.78457900	0.58694700
C	4.15133600	-1.06453300	-0.93611800
C	4.56210000	0.06275500	-0.23295300
H	4.04207300	1.67918000	1.09584900
H	4.84990000	-1.58261500	-1.58413600
C	-1.10690600	-2.82057800	0.23536700
H	1.70646600	0.90047900	1.35688500
H	2.47698800	-2.33454800	-1.38598100
F	5.84747700	0.48068000	-0.37013200
O	-1.74034500	3.58819700	-0.27482800
C	-1.52786400	2.38556200	-0.21822000
O	-2.55659800	1.45061900	-0.31707100
O	-0.41646900	1.74845600	-0.06122300
H	-3.44450200	1.89857500	-0.40910200
O	1.65155200	3.48073900	1.10434200

TS9-10

Charge=0 Multiplicity = 2

Cu	-0.34602000	-0.56970500	0.23500000
C	-1.43593800	-4.13328600	-1.34486300
N	-1.42347800	-2.02220800	-0.47755500
C	-2.74666400	-3.64407900	-1.32925700
H	-1.09751400	-5.09848300	-1.69837400
C	-2.69327200	-2.34062600	-0.78720300
H	-3.64021500	-4.15419300	-1.66245400
H	-3.50558700	-1.64670500	-0.61553900
C	0.75179000	-2.95391400	-0.57438100
H	1.45172100	-3.75939500	-0.79747300
N	1.18442500	-1.82388900	-0.04814800
C	2.56809300	-1.60207700	0.15373700
C	3.00210000	-1.01235900	1.35078700
C	3.51673200	-1.95171700	-0.82192000
C	4.35856300	-0.80185200	1.58754300
C	4.87832300	-1.74714400	-0.59443100
C	5.27205100	-1.17804700	0.60964800
H	4.70835300	-0.35078900	2.50964500
H	5.62174000	-2.00557400	-1.34064000
C	-0.62740300	-3.10560900	-0.81364200
H	2.27041900	-0.71666700	2.09442800
H	3.18862200	-2.35904700	-1.77308100
F	6.59764300	-0.96967000	0.83452700
O	0.77222500	3.44407200	0.11508000
C	1.25032500	2.31305000	0.18153300
O	2.40270200	1.92649600	-0.33790100
O	0.63995900	1.31605100	0.82166300
H	2.87212600	2.68256700	-0.80391700
C	-2.71825400	0.68781800	1.62143500

H	0.96982500	3.00409800	0.59924200	H	-2.65396500	1.49416300	2.36882500
H	1.31602000	4.38074700	1.19212000	O	-1.58935300	0.78926000	0.77389300
O	-4.46795600	3.24994900	-0.46412600	H	-0.46602200	1.43077300	0.97507100
H	-4.99994500	3.51864900	-1.22307700	H	-2.71003500	-0.25950500	2.17981400
H	-3.67597600	3.82679200	-0.43704100	C	-4.03250400	0.81125400	0.87035900
				C	-5.19587500	0.23120500	1.39456900
				C	-4.11600300	1.53286900	-0.32702500
				C	-6.42301000	0.37645100	0.74199000
				H	-5.14245400	-0.34234100	2.31779900
				C	-5.34128600	1.67491200	-0.98411400
				H	-3.21362700	1.97117100	-0.74077400
				C	-6.49901000	1.09989100	-0.45168700
				H	-7.31515500	-0.08124300	1.16038000
				H	-5.39140300	2.23525700	-1.91372000
				H	-7.45047500	1.21039400	-0.96397900
				O	3.67673800	3.86854300	-1.60747800
				H	4.57162400	4.08497100	-1.31937600
				H	3.12795000	4.68660300	-1.50955000
				O	1.83818200	5.71389000	-0.99632000
				H	1.23333900	6.14902900	-1.60847000
				H	1.33354400	4.99322100	-0.55439500
11				TS12-13			
Charge=0 Multiplicity = 2				Charge=0 Multiplicity = 2			
Cu	1.20308700	0.65927700	0.02651300	Cu	-0.01908100	0.79036000	-0.30493600
C	3.41659300	-2.70921100	-0.08673800	C	-1.82272900	4.36209600	0.46591700
N	2.69818200	-0.54444100	0.05227400	N	-0.32826100	2.71075900	-0.05229300
C	4.53253400	-1.87127300	0.01967800	C	-0.56505500	4.93963800	0.26884800
H	3.40998400	-3.78827800	-0.16689800	H	-2.74675500	4.86564700	0.71899400
C	4.04395800	-0.54961400	0.09992000	C	0.32214500	3.88388000	-0.04872100
H	5.57309300	-2.16522500	0.03670400	H	-0.30707400	5.98796900	0.33646900
H	4.60834600	0.37037500	0.18485500	H	1.37927900	3.94055900	-0.27451700
C	0.89503100	-2.07406000	-0.12634500	C	-2.51749200	1.86365100	0.29323600
H	0.49146300	-3.08099200	-0.22999600	H	-3.57601600	1.99543200	0.52324600
N	0.10057300	-1.02448100	-0.07811700	N	-2.02725200	0.66151300	0.06330000
C	-1.30715800	-1.11413400	-0.05357900	C	-2.87862500	-0.46246300	-0.01350000
C	-2.05630300	0.00047800	-0.46987600	C	-2.44632100	-1.69359100	0.51047300
C	-1.98743200	-2.26265700	0.39476300	C	-4.14681900	-0.39212500	-0.62066700
C	-3.44931100	-0.04048700	-0.47957200	C	-3.26764200	-2.81917700	0.45939100
C	-3.38082500	-2.31352200	0.38196100	C	-4.97773500	-1.51254500	-0.67329200
C	-4.08716600	-1.20204900	-0.06191500	C	-4.52246800	-2.70590800	-0.12781200
H	-4.03525900	0.81463900	-0.79819000	H	-2.94439800	-3.76963500	0.87002000
H	-3.91562000	-3.19132400	0.72820200	H	-5.95441100	-1.46989600	-1.14336100
C	2.28735900	-1.86415200	-0.06258100	C	-1.65168800	2.97409200	0.25931900
H	-1.53552600	0.90406300	-0.77123100	H	-1.46573000	-1.76462000	0.96535100

H	-1.43656600	-3.11438400	0.77928800	H	-4.47583700	0.53506500	-1.07913200
F	-5.44578700	-1.24785300	-0.06778800	F	-5.32628600	-3.80289400	-0.18243600
O	0.46454000	2.28570200	-0.07769300	O	0.46638600	-1.18971500	-0.96945100
H	0.08527800	2.69899000	0.72270500	H	0.01646000	-1.51706500	-1.75940000
O	0.12902200	4.78622600	-1.11766700	O	1.75685700	0.73683000	-1.16698300
H	0.32981700	3.82696700	-1.01178000	C	2.98280900	1.07968600	-0.52754900
H	-0.41652900	4.87431700	-1.90770200	H	3.50834000	1.79818700	-1.17420300
O	-0.73633000	4.33593400	1.48356700	H	2.78706300	1.57561100	0.43118300
H	-0.38115200	4.89799500	2.18171700	H	1.31889200	-0.47995800	-1.21850900
H	-0.54759300	4.78814600	0.63447500	C	3.86817300	-0.12922100	-0.29199000
				C	4.16189700	-0.57076100	1.00529400
				C	4.40273100	-0.83718800	-1.38014900
				C	4.96971400	-1.69488400	1.21373800
				H	3.75143700	-0.03171600	1.85506800
				C	5.20312000	-1.96301100	-1.17756500
				H	4.18756700	-0.50004200	-2.39115200
				C	5.48913200	-2.39613600	0.12201800
				H	5.19769000	-2.01707200	2.22647100
				H	5.61067400	-2.49832600	-2.03069200
				H	6.11780100	-3.26765800	0.28113900
				O	1.13869700	-2.46640700	1.34287500
				H	2.07115900	-2.72003900	1.36154500
				H	0.94077700	-2.22857600	0.40776600
				O	0.75089200	0.18197900	1.86878900
				H	0.14314400	0.40190000	2.58524900
				H	0.89690200	-0.79375000	1.89271600

Table S4 Cartesian coordinates all structures considered in this work (3H₂O level)

0				TS1-2			
	Charge=-1 Multiplicity = 2				Charge=-1 Multiplicity = 2		
Cu	0.30938300	1.17336600	-0.11368400	Cu	-1.09481400	-0.31480600	-0.64079200
C	-2.50315700	4.11044800	0.30804000	O	0.43341700	0.91468400	-1.05915600
N	-0.57398600	2.92698600	-0.01139600	C	-3.43904600	-3.23053600	-2.26580400
C	-1.43921400	5.01276200	0.17200200	N	-2.59712400	-1.24019000	-1.51655800
H	-3.54870100	4.34220600	0.46950000	C	-4.33006200	-2.20686400	-2.60895300
C	-0.27281300	4.23530600	-0.01966000	H	-3.53867700	-4.28888600	-2.47168500
H	-1.48794300	6.09362000	0.20602600	C	-3.76964200	-1.00121100	-2.12247900
H	0.74881200	4.56688500	-0.15680800	H	-5.27039200	-2.30510100	-3.13569900
C	-2.46631800	1.51121800	0.23992800	H	-4.17148800	0.00250700	-2.18166000
H	-3.53665000	1.36381300	0.40226300	C	-1.18830700	-3.07172200	-0.97129200
N	-1.65541200	0.48672700	0.11201900	H	-0.97170200	-4.14133700	-0.92693100
C	-2.14741500	-0.83379100	0.06424000	N	-0.38228300	-2.20352000	-0.40403100
C	-1.33267900	-1.87236300	0.54717700	C	0.78428700	-2.60758300	0.27559900
C	-3.40261600	-1.15817500	-0.48649800	C	1.08502900	-2.00546000	1.51082800
C	-1.75892900	-3.19870900	0.50842800	C	1.65592100	-3.58028400	-0.24476100

C	-3.84620800	-2.48205500	-0.51661100	C	2.21732100	-2.38859700	2.22821900
C	-3.01558000	-3.47570500	-0.01397000	C	2.79305800	-3.96893600	0.46772100
H	-1.10693400	-3.99293500	0.85495000	C	3.04748200	-3.36628500	1.69264000
H	-4.80739400	-2.74577700	-0.94591500	H	2.44533300	-1.93863200	3.18841600
C	-1.93638700	2.82209100	0.18890400	H	3.47972700	-4.71232400	0.07639700
H	-0.35184400	-1.63659800	0.93970900	C	-2.36856400	-2.60298900	-1.59003100
H	-4.02331900	-0.38300800	-0.92498200	H	0.41888300	-1.24848000	1.91128700
F	-3.44920800	-4.77318000	-0.05987300	H	1.45836500	-4.01474700	-1.22003300
O	3.67041500	-0.13575100	-0.41393300	F	4.16132800	-3.74508100	2.38945300
C	2.51222900	0.32367300	-0.31993600	O	-2.33348100	2.62446700	1.53805200
O	2.21424500	1.59793900	-0.34559400	C	-1.82787600	1.66509600	0.92033300
O	1.42857000	-0.43127500	-0.18354900	O	-1.69452400	1.76864600	-0.46014200
O	1.72573300	-3.26449500	0.43355500	O	-1.41610900	0.55904300	1.39555700
H	1.58513800	-2.33598200	0.16408200	H	-0.60773300	1.66326100	-0.72562800
H	2.69528400	-3.34212100	0.42745500	C	1.65170900	1.05274000	-0.37586800
O	4.55192400	-2.63303200	-0.11240500	H	2.15003900	0.07368800	-0.30193000
H	4.13807700	-1.73461000	-0.24783900	H	1.49208800	1.39719300	0.65984100
H	4.74117500	-2.95802000	-1.00078700	C	2.60833100	2.01642800	-1.06523100
O	6.46615900	-0.27517100	0.41006300	C	3.84555200	2.31132000	-0.47191800
H	6.18944500	-1.20365100	0.45815300	C	2.29051200	2.61472300	-2.28899000
H	5.63956700	0.16728300	0.14815000	C	4.74614700	3.18202200	-1.08749300
				H	4.10252700	1.85686100	0.48327700
				C	3.19031000	3.48989700	-2.90754000
				H	1.33220600	2.38518400	-2.74243700
				C	4.42096200	3.77689300	-2.31221800
				H	5.69897600	3.39996200	-0.61121000
				H	2.92553700	3.95026500	-3.85633100
				H	5.11825700	4.45860600	-2.79239300
				O	-0.66575800	0.33601600	4.15327100
				H	-0.95010000	0.33919800	3.21783000
				H	-1.09947200	1.13488400	4.50039700
				O	-2.16445100	2.88237400	4.27045700
				H	-2.28544900	2.73164700	3.30030000
				H	-1.62225700	3.67840000	4.32228600
				O	-3.66638400	5.03077400	0.96734300
				H	-4.24544100	4.90683000	1.72870700
				H	-3.12613800	4.21212600	0.95960100
TS5-6				8			
Charge=-1 Multiplicity = 2				Charge=0 Multiplicity = 2			
Cu	-0.19942300	-0.93617600	0.06106900	Cu	0.71887600	0.48476400	0.05359500
O	-0.73250900	0.06296200	-2.08441900	C	0.42542600	4.49757600	0.31340200
C	-0.10509500	-5.02033000	-0.05065600	N	1.17103700	2.34858700	0.13504100
N	-0.71542900	-2.82105400	-0.00533100	C	1.82530900	4.50943200	0.25937000
C	-1.50513500	-4.93973300	-0.08606900	H	-0.23611400	5.34970200	0.39737500

H	0.50534800	-5.91468400	-0.05912600	C	2.24159700	3.16649000	0.15119500
C	-1.83296700	-3.56566500	-0.05613800	H	2.47430800	5.37354100	0.29944500
H	-2.20789200	-5.76205900	-0.12569800	H	3.24952600	2.77545500	0.09666700
H	-2.80765200	-3.09652300	-0.06640800	C	-1.19306700	2.45965300	0.22602600
C	1.63910200	-3.09177900	0.05676400	H	-2.13734800	3.00219000	0.27959700
H	2.53746500	-3.71380900	0.04872100	N	-1.18569700	1.14446300	0.16904400
N	1.73385000	-1.78745200	0.14115700	C	-2.37440000	0.39684600	0.00514000
C	3.00434300	-1.16941800	0.09260800	C	-2.52441700	-0.81638200	0.69510800
C	3.30716600	-0.12297500	0.98045200	C	-3.39580600	0.82931000	-0.86046300
C	3.97498200	-1.57721200	-0.84093800	C	-3.67882100	-1.58075300	0.54387400
C	4.56414600	0.48035400	0.95992900	C	-4.56327800	0.07990400	-1.00443700
C	5.23728900	-0.98076500	-0.86561600	C	-4.68099700	-1.11132300	-0.29697400
C	5.50695900	0.03435000	0.04233100	H	-3.78391000	-2.52959900	1.05703800
H	4.80095900	1.29168900	1.63934900	H	-5.36012700	0.39584200	-1.66898600
H	5.99104700	-1.27851500	-1.58698900	C	0.04099300	3.14409400	0.23309600
C	0.35750300	-3.68862100	-0.00114200	H	-1.73533700	-1.17002200	1.34711100
H	2.55878800	0.22307700	1.68309600	H	-3.26740600	1.73731400	-1.44142800
H	3.72950800	-2.34274500	-1.57066400	F	-5.81190200	-1.84927800	-0.45097300
F	6.74118800	0.62093900	0.02007500	O	2.34422100	-2.86348800	-0.15464900
O	-2.19561200	-0.36734300	-0.27091700	C	1.81785600	-1.75830000	-0.10960300
H	-0.76444000	-0.25780500	-2.99122800	O	2.52533300	-0.57701100	-0.22802800
C	-2.76197600	0.78029000	0.33587900	O	0.57054200	-1.46501200	0.05442200
H	-2.46111600	0.81182500	1.39117800	H	3.52895300	-0.65150000	-0.40152300
H	-2.36465500	1.69460400	-0.12796600	O	-1.01599400	-3.66447200	1.15706700
C	-4.28023700	0.80119000	0.25263900	H	-0.45288200	-3.02641300	0.68397100
C	-4.98586200	1.87810900	0.81168700	H	-0.45859300	-4.43909200	1.29589000
C	-5.00192800	-0.22433000	-0.36680700	O	5.05576500	-0.77618600	-0.65893600
C	-6.37943900	1.92689900	0.75656700	H	5.38446700	-0.51714200	-1.52853400
H	-4.43674400	2.68551200	1.29226100	H	5.27442000	-1.73654300	-0.53085800
C	-6.39932100	-0.17788500	-0.42469200	O	5.02990600	-3.37599700	-0.13674200
H	-4.45433100	-1.05374700	-0.80107700	H	5.31649800	-4.18135700	-0.58185600
C	-7.09438200	0.89567100	0.13636600	H	4.04532500	-3.37033900	-0.12747800
H	-6.90789200	2.77003500	1.19434200				
H	-6.94412200	-0.98338100	-0.91103800				
H	-8.17965600	0.93206900	0.09075400				
H	-1.73607800	-0.13353100	-1.26200200				
O	1.19767800	2.84870200	0.76386400				
C	0.69522800	1.90408900	0.11155200				
O	0.53597700	2.04254900	-1.20570300				
O	0.32348300	0.80469200	0.68786900				
H	0.05097200	1.23498900	-1.64083400				
O	1.44759000	1.95967800	3.41490900				
H	0.80862500	1.24219600	3.32064700				
H	1.41585900	2.38050500	2.52633800				

O	0.84613400	4.67300200	-2.73087300				
H	0.68461100	3.77261200	-2.40577900				
H	1.25639200	5.10227900	-1.95691800				
O	1.86615100	5.35560700	-0.10702800				
H	1.67824900	4.42611500	0.17590400				
H	1.27697700	5.89725800	0.43078000				
TS9-10				11			
Charge=0 Multiplicity = 2				Charge=0 Multiplicity = 2			
Cu	-0.27378100	-1.18932900	0.57819100	Cu	1.10177100	0.61846600	0.02511600
C	-0.98352100	-4.43916100	-1.72856200	C	4.03991500	-2.14428500	-0.06444300
N	-1.20180500	-2.59348400	-0.40139200	N	2.83690000	-0.20590400	0.06620300
C	-2.34440600	-4.19779200	-1.51281000	C	4.92961800	-1.06947400	0.04362000
H	-0.54050500	-5.23144400	-2.31769900	H	4.28503000	-3.19534700	-0.14237500
C	-2.43235400	-3.05336700	-0.68960000	C	4.14631600	0.10256500	0.11836600
H	-3.17981800	-4.76793500	-1.89584400	H	6.00994800	-1.11310900	0.06521300
H	-3.31971200	-2.55923300	-0.31710600	H	4.47996100	1.12909800	0.20217100
C	1.06860900	-3.09383700	-0.86923700	C	1.43967200	-2.11240500	-0.11770700
H	1.85122600	-3.69815700	-1.32814100	H	1.28205200	-3.18570700	-0.22075700
N	1.38001500	-2.04650900	-0.13065900	N	0.42301300	-1.27543100	-0.07671300
C	2.71846300	-1.61066500	0.00405300	C	-0.92548800	-1.68928900	-0.06179500
C	3.16038000	-1.13474600	1.24860800	C	-1.91087600	-0.77173000	-0.46696200
C	3.61358300	-1.62769200	-1.07940000	C	-1.32444900	-2.97017100	0.36622500
C	4.47656200	-0.71337200	1.42182700	C	-3.25683800	-1.13273600	-0.48622900
C	4.93552200	-1.21290300	-0.91536300	C	-2.66850400	-3.34075400	0.34437700
C	5.34207700	-0.76637100	0.33542600	C	-3.61105100	-2.41590700	-0.08857900
H	4.83101500	-0.34550600	2.37835400	H	-4.02334600	-0.43117400	-0.79667800
H	5.63585900	-1.21489900	-1.74351900	H	-2.98710200	-4.32333200	0.67525500
C	-0.29011000	-3.42661100	-1.03137200	C	2.74470000	-1.58503000	-0.04674400
H	2.46609000	-1.09348100	2.08073700	H	-1.61281100	0.23256500	-0.75168300
H	3.27052700	-1.93837000	-2.06115800	H	-0.59371100	-3.67826800	0.74216200
F	6.62776600	-0.35521500	0.49913400	F	-4.92269600	-2.77352200	-0.10383900
O	-0.20422700	2.88439900	0.60867700	O	0.05091600	2.06173400	-0.08572700
C	0.59568300	1.94816100	0.53701300	H	-0.38726100	2.39917500	0.72927400
O	1.70452600	1.93819700	-0.17778600	O	-1.96995200	5.35803700	0.21927300
O	0.42188400	0.81417100	1.20336300	H	-1.51833400	5.01470900	-0.58978100
H	1.85019500	2.79735100	-0.67868400	H	-2.87627700	5.56981800	-0.03160100
C	-2.85126500	-0.30002300	2.07829900	O	-1.34150700	3.33978700	1.95435000
H	-2.99206000	0.34437400	2.95941300	H	-0.90440100	3.69850100	2.73553700
O	-1.46629500	-0.31239700	1.79311200	H	-1.64481200	4.11677300	1.42625200
H	-0.62726300	0.62460000	1.64447000	O	-0.54830600	4.09670900	-1.73486500
H	-3.16170700	-1.31123400	2.37201500	H	-0.28076400	3.28600500	-1.22437600
C	-3.73987200	0.19250900	0.94928100	H	-0.84195600	3.80099200	-2.60386500
C	-4.97522300	-0.42669200	0.71514400	H	-10.95421660	1.51295823	0.00000008
C	-3.37406400	1.29138400	0.15847200	C	-11.31087103	2.52176823	0.00000008

C	-5.83230100	0.03873100	-0.28675100	H	-10.95419819	3.02616642	0.87365158
H	-5.27165000	-1.27992100	1.32219000	H	-10.95419819	3.02616642	-0.87365143
C	-4.22594000	1.75320400	-0.84785400	H	-12.38087103	2.52178142	0.00000008
H	-2.42583000	1.79333700	0.32855300				
C	-5.45727700	1.12998000	-1.07403400				
H	-6.78551200	-0.45472900	-0.45531800				
H	-3.92700900	2.60459100	-1.45294900				
H	-6.11740400	1.49150100	-1.85725800				
O	2.35209800	4.03581900	-1.61097300				
H	2.39474400	3.87900000	-2.56156300				
H	1.98731400	4.95053200	-1.48791300				
O	1.24150600	6.45657400	-1.25338300				
H	0.39252100	6.23703800	-0.79633900				
H	1.70212500	7.10129900	-0.70380800				
O	-0.95270000	5.42085400	-0.08948800				
H	-1.52148500	5.72554200	0.62645500				
H	-0.67096700	4.50781700	0.14272100				
TS12-13							
Charge=0 Multiplicity = 2							
Cu	-0.02709600	0.89942600	-0.26901700				
C	-1.83655300	4.44778600	0.59176200				
N	-0.33102000	2.80806300	0.07112700				
C	-0.56871200	5.02432300	0.46768000				
H	-2.76720100	4.94684100	0.82889200				
C	0.32465400	3.97607800	0.14443200				
H	-0.30787700	6.06723700	0.58799600				
H	1.39001300	4.03595900	-0.03766600				
C	-2.53387700	1.96076500	0.29377900				
H	-3.60534300	2.08627400	0.45951400				
N	-2.03424700	0.76459300	0.05832400				
C	-2.89269200	-0.34219600	-0.14072100				
C	-2.62866000	-1.55695300	0.51453900				
C	-3.99942200	-0.25584400	-1.00463500				
C	-3.46503600	-2.65687000	0.32529900				
C	-4.84309300	-1.35207800	-1.19716500				
C	-4.55716800	-2.53354600	-0.52606300				
H	-3.27982400	-3.59570200	0.83605500				
H	-5.69744500	-1.29928400	-1.86345900				
C	-1.66395300	3.06812600	0.34040000				
H	-1.79051700	-1.63572300	1.19804100				
H	-4.18693200	0.66667300	-1.54565400				
F	-5.37107600	-3.60941000	-0.71319700				
O	0.45059900	-1.05654800	-1.08065800				
H	-0.04979600	-1.33906100	-1.85731100				

O	1.70301200	0.89965400	-1.23972200
C	2.97160100	1.23663100	-0.69178600
H	3.45181000	1.95566700	-1.37258100
H	2.84738700	1.73374700	0.27870500
H	1.27487200	-0.30173900	-1.33575600
C	3.87114800	0.02674800	-0.52050600
C	4.30497800	-0.38041100	0.74790400
C	4.27518400	-0.71855000	-1.64038000
C	5.11890800	-1.50957200	0.89933500
H	3.99796900	0.18629100	1.62322800
C	5.08109700	-1.84888600	-1.49457100
H	3.95093800	-0.40820700	-2.63053200
C	5.50501200	-2.24975200	-0.22169700
H	5.45180100	-1.80688300	1.89012300
H	5.38556600	-2.41363400	-2.37137600
H	6.13809300	-3.12512400	-0.10760500
O	1.52615400	-2.54184300	0.89557800
H	2.45990600	-2.71213400	0.71370600
H	1.12671800	-2.18798900	0.06183600
O	0.85545900	0.11681900	1.76720100
H	0.20211400	-0.11686100	2.44478400
H	1.29223100	-0.73764300	1.58441800
O	-0.32689100	-2.30014700	2.96912600
H	0.35629800	-2.67664800	2.38162500
H	-0.40560000	-2.88759500	3.72931300

Table S5 Cartesian coordinates all structures considered in this work (4H₂O level)

0				TS5-6			
Charge=-1 Multiplicity = 2				Charge=-1 Multiplicity = 2			
Cu	0.66810900	0.59541500	0.03352100	Cu	0.46540000	1.10040300	0.02266400
C	0.36223300	4.65152800	0.32712100	O	0.81711900	-0.19472800	-2.05009300
N	1.10759600	2.50350300	0.10527400	C	0.96346300	5.12111500	-0.49453500
C	1.76247300	4.66367500	0.27506800	N	1.24731800	2.87066800	-0.24125400
H	-0.30158700	5.50117600	0.42807000	C	2.33406500	4.82901600	-0.55916900
C	2.17582600	3.31716700	0.14162700	H	0.49044200	6.09151700	-0.57845200
H	2.41274300	5.52725400	0.32784400	C	2.45886200	3.43101200	-0.39786300
H	3.18094500	2.91830000	0.07681600	H	3.14704900	5.52925400	-0.70151100
C	-1.26119800	2.62129700	0.21469600	H	3.35296900	2.82230300	-0.38611200
H	-2.18991600	3.18860400	0.30499000	C	-1.03701600	3.49340100	-0.14283600
N	-1.27828600	1.31036000	0.12172800	H	-1.83533000	4.23816500	-0.18320700
C	-2.49161600	0.59855600	0.01147600	N	-1.31556300	2.23083100	0.07234000
C	-2.55292500	-0.71200700	0.51528000	C	-2.66383500	1.80888300	0.13622500
C	-3.62886400	1.13458500	-0.62348300	C	-3.06819400	0.91335500	1.14067100
C	-3.71909700	-1.46835800	0.41266800	C	-3.61381400	2.26692900	-0.79500200
C	-4.80794400	0.39247700	-0.71565600	C	-4.40015500	0.51258600	1.23693400

C	-4.82985900	-0.89394000	-0.19120900	C	-4.95021300	1.87262200	-0.70418000
H	-3.73962500	-2.49192800	0.77000700	C	-5.31684800	1.00668000	0.31738800
H	-5.68815000	0.79053900	-1.21002200	H	-4.71599800	-0.18038300	2.00893000
C	-0.01871800	3.29558700	0.21894200	H	-5.69078200	2.21009600	-1.42161400
H	-1.67295800	-1.14664800	0.97234200	C	0.31364700	3.88496900	-0.29707800
H	-3.58731600	2.11864000	-1.07970200	H	-2.34114100	0.52505700	1.84327000
F	-5.98293500	-1.62188200	-0.29966300	H	-3.29944200	2.91057600	-1.61093600
O	2.46581100	-2.55698300	-0.03858100	F	-6.62367100	0.62070600	0.41028300
C	1.84411500	-1.47950900	-0.03569500	O	2.34052200	0.22137700	-0.28084100
O	2.41974000	-0.29020700	-0.10961100	H	0.89333600	-0.02228700	-2.99386100
O	0.53130800	-1.36163500	0.04419600	C	2.76502000	-0.92102700	0.44194500
O	-1.17615600	-3.75781000	0.31215300	H	2.47851000	-0.80468600	1.49499400
H	-0.66627100	-2.94804100	0.12751800	H	2.24669900	-1.81894300	0.07540200
H	-0.47311500	-4.42472700	0.41706800	C	4.26650100	-1.14562800	0.35749500
O	1.40577600	-5.05233000	0.42985800	C	4.84546400	-2.20196700	1.07791600
H	1.79075400	-4.14940600	0.31079200	C	5.09452000	-0.33362100	-0.42433600
H	1.73015500	-5.55789400	-0.32427800	C	6.21947200	-2.43926600	1.02082900
O	5.40983600	-2.57123800	-0.27156900	H	4.21278600	-2.84403800	1.68773700
H	4.44417300	-2.66586000	-0.16798100	C	6.47252800	-0.56964300	-0.48451300
H	5.53819300	-1.60758900	-0.27585200	H	4.64616600	0.48201700	-0.98124800
O	5.03092700	0.37635000	-0.59972100	C	7.04141200	-1.62141900	0.23687900
H	5.09099900	0.43697500	-1.56065300	H	6.64905800	-3.26262100	1.58582500
H	4.09255600	0.12793900	-0.41994400	H	7.10104700	0.07112100	-1.09803000
				H	8.11160700	-1.80464000	0.18986600
				H	1.84365100	-0.05001800	-1.24049300
				O	-1.43161800	-2.38251700	1.05580000
				C	-0.81214400	-1.57849800	0.31601200
				O	-0.68156700	-1.86514200	-0.97864500
				O	-0.29610000	-0.49113100	0.78830800
				H	-0.08880200	-1.17064300	-1.49698500
				O	-1.59369900	-1.32778800	3.64517200
				H	-0.82766200	-0.74231800	3.60698100
				H	-1.58291200	-1.75859600	2.76023800
				O	-1.06829600	-4.59393100	-2.11170900
				H	-0.91289300	-3.65292200	-1.91763400
				H	-1.30907500	-4.95060600	-1.23775100
				O	-2.38779700	-4.81127800	0.42930100
				H	-2.07797000	-3.88787100	0.63622300
				H	-2.29395800	-5.30871700	1.24946100
				O	-3.96959900	-5.26207900	-2.08849000
				H	-3.79692200	-5.13022600	-1.14207000
				H	-3.11440000	-5.01841000	-2.48351200
8				TS9-10			
Charge=0 Multiplicity = 2				Charge=0 Multiplicity = 2			

Cu	-0.42909700	0.81985700	0.36484400	Cu	0.39829300	-1.26676700	0.13650400
C	0.51970600	4.57900600	-0.75074600	C	1.38749300	-4.70997100	-1.74562700
N	-0.55886900	2.69146700	-0.05585000	N	0.26313900	-2.98876700	-0.75523400
C	-0.81965100	4.89555700	-0.49017100	C	0.01345500	-4.96631200	-1.82218500
H	1.29858900	5.24747700	-1.09336900	H	2.19342700	-5.32499800	-2.12394000
C	-1.44593500	3.70507000	-0.06583400	C	-0.64037400	-3.88085900	-1.20036100
H	-1.29638400	5.86053500	-0.59533100	H	-0.46869300	-5.82630500	-2.26655800
H	-2.47945600	3.55204900	0.21741300	H	-1.70282600	-3.72424900	-1.06593000
C	1.72759900	2.28381100	-0.52064900	C	2.60814100	-2.65631300	-0.71333000
H	2.72673200	2.59571300	-0.82693800	H	3.63343800	-2.96064000	-0.92431500
N	1.49259800	1.02673200	-0.20916900	N	2.36656100	-1.52278900	-0.08494500
C	2.53577400	0.07445400	-0.12918600	C	3.41967700	-0.63393000	0.24157200
C	2.36204000	-1.18835600	-0.71780900	C	3.43433000	-0.01909800	1.50284000
C	3.73501300	0.36618700	0.54386100	C	4.44494800	-0.34632800	-0.67470700
C	3.37805900	-2.14004700	-0.65664700	C	4.46774200	0.84439700	1.85909700
C	4.76056400	-0.57823100	0.60267700	C	5.48635600	0.51490800	-0.32724600
C	4.56004200	-1.81379800	-0.00114400	C	5.47775400	1.09149900	0.93630600
H	3.25238100	-3.11877800	-1.10596200	H	4.49462600	1.32363300	2.83153700
H	5.69135200	-0.37257500	1.12005100	H	6.28101700	0.75247600	-1.02601300
C	0.65914600	3.20434600	-0.47191100	C	1.51944400	-3.47217100	-1.08196500
H	1.43788100	-1.42864300	-1.23156900	H	2.63097600	-0.21991200	2.20306600
H	3.85631400	1.32362700	1.04125900	H	4.41428900	-0.77332900	-1.67214400
F	5.55392000	-2.73918600	0.06231200	F	6.48594500	1.93714100	1.27811100
O	-2.55964300	-2.01793400	1.44021800	O	-0.74699000	2.72988100	0.34500500
C	-1.83148900	-1.07208600	1.15534200	C	0.24197700	1.99260000	0.33757400
O	-2.33593300	0.20928000	1.01108600	O	1.40683100	2.27646300	-0.19541300
O	-0.56296100	-1.05164200	0.92887600	O	0.22824800	0.78401300	0.90849600
H	-3.33347800	0.21942700	0.76561800	H	1.39638400	3.16721800	-0.68918900
O	-0.23746700	-3.21290900	-1.11457200	C	-2.33823600	-1.55300800	1.37651700
H	-0.21746500	-2.68708600	-0.29825100	H	-2.17436100	-1.40028900	2.45388200
H	-1.12747400	-3.59734700	-1.13641400	O	-1.40465900	-0.80789700	0.61618200
O	-4.77410600	0.17602700	0.25034300	H	-0.77122900	0.30872100	0.97624700
H	-5.44055200	0.07050700	0.94113600	H	-2.18496100	-2.62490200	1.18180500
H	-4.88279900	-0.59684900	-0.36663600	C	-3.76808500	-1.17930500	1.02684000
O	-4.97415900	-1.96543600	-1.36658800	C	-4.76716800	-1.19965600	2.00765600
H	-4.92795400	-1.86270400	-2.32453600	C	-4.11860100	-0.84181000	-0.28907000
H	-4.36463800	-2.70142400	-1.12397500	C	-6.09348100	-0.89887400	1.68341500
O	-3.15357400	-3.82615900	-0.45433200	H	-4.50736000	-1.44521900	3.03491900
H	-2.91521400	-3.32699200	0.36344500	C	-5.44362300	-0.53575600	-0.61475700
H	-3.41786500	-4.71282300	-0.17904600	H	-3.34535800	-0.81350600	-1.05077800
				C	-6.43594500	-0.56456800	0.37110400
				H	-6.85483300	-0.91413300	2.45805600
				H	-5.70084000	-0.27688700	-1.63828300
				H	-7.46425200	-0.32340000	0.11854300

	O	1.40344800	4.47365800	-1.56545000			
	H	2.07947200	5.14162300	-1.40035500			
	H	0.51247600	4.91855100	-1.46223700			
	O	-0.97696000	5.33432400	-0.87295000			
	H	-1.80941300	5.25125800	-1.38827800			
	H	-1.01000000	4.58612000	-0.25006300			
	O	-3.55136700	2.62950200	-0.06921300			
	H	-3.93767000	1.74477800	-0.12982600			
	H	-2.61603100	2.50566300	0.18315800			
	O	-3.47816000	4.66951800	-1.92621100			
	H	-4.20815200	5.28039100	-1.77068900			
	H	-3.62994800	3.90183000	-1.32858900			
11	TS12-13						
Charge=0 Multiplicity = 2	Charge=0 Multiplicity = 2						
Cu	0.54344700	-0.81565700	-0.09123700	Cu	0.07425400	1.03892300	-0.12262400
C	-1.13824900	-4.47599200	0.13044300	C	-1.57311000	4.49275700	1.28209300
N	0.31901000	-2.71726200	0.05660900	N	-0.13391300	2.85697700	0.58984200
C	0.16900100	-4.97357300	0.16458200	C	-0.26135700	4.94660700	1.45145200
H	-2.05878100	-5.04431900	0.15313000	H	-2.48869400	5.02284000	1.51056000
C	1.03204300	-3.85716900	0.11436100	C	0.58915400	3.90527500	1.01055300
H	0.47437400	-6.00963900	0.21728400	H	0.05597200	5.90553200	1.83884100
H	2.11459000	-3.84447700	0.11429900	H	1.67112600	3.88990300	0.98268000
C	-1.94110600	-2.00508800	0.00590400	C	-2.40215800	2.21321500	0.34536700
H	-3.01361700	-2.19794700	-0.00778900	H	-3.47404300	2.41135800	0.40209200
N	-1.47081100	-0.77565200	-0.05606300	N	-1.96438200	1.04868900	-0.08795900
C	-2.29183300	0.37055900	-0.04807400	C	-2.86503400	0.10505800	-0.63450000
C	-1.78643100	1.56027400	-0.60174700	C	-2.77249600	-1.24588200	-0.25810000
C	-3.58379000	0.37601100	0.51191200	C	-3.84226100	0.49104800	-1.57011100
C	-2.56377800	2.71664800	-0.63586600	C	-3.65255300	-2.18746500	-0.79131700
C	-4.36937000	1.52781100	0.47717700	C	-4.72891700	-0.44594500	-2.10567200
C	-3.84641400	2.67709200	-0.10274500	C	-4.61510200	-1.76993100	-1.70345600
H	-2.18480400	3.63785900	-1.06498000	H	-3.59933500	-3.23096200	-0.49974800
H	-5.36439400	1.54424900	0.90857400	H	-5.48356700	-0.16162600	-2.83119700
C	-1.02200300	-3.07117500	0.06512000	C	-1.46847400	3.19004200	0.74460100
H	-0.77356700	1.57097200	-0.99226900	H	-2.03745800	-1.55717600	0.47634700
H	-3.97530900	-0.51003100	1.00023000	H	-3.89259700	1.52476500	-1.89844000
F	-4.60805400	3.80334800	-0.13170600	F	-5.47202400	-2.69199300	-2.22585600
O	1.52286600	0.66617100	-0.33470600	O	0.51020300	-0.73910000	-1.30654500
H	1.74305600	1.18605700	0.47372300	H	0.10721700	-0.79047800	-2.18296800
O	5.62782100	1.61964100	-0.81470900	O	1.91489600	1.06884300	-0.86434000
H	4.81939100	1.47800500	-1.37131300	C	3.10395800	1.12859800	-0.08748800
H	6.26200300	2.10353700	-1.35542400	H	3.57070000	2.11079600	-0.25804900
O	4.99612700	2.30620500	1.72645600	H	2.87590700	1.05666100	0.98436700
H	5.51511100	1.73482400	2.30476900	H	1.41155300	-0.03696600	-1.27897400

H	5.27140900	2.08690700	0.80112400	C	4.08336800	0.03260300	-0.46436500
O	3.33271900	1.22132300	-2.20055600	C	4.57411600	-0.86029700	0.49741400
H	2.62111100	1.00216900	-1.53471100	C	4.51636400	-0.10576300	-1.79276700
H	2.97528100	1.92687900	-2.75212400	C	5.47926700	-1.86842800	0.14533100
O	2.29406300	2.06548300	1.92558700	H	4.24835300	-0.76403900	1.53056400
H	1.93458200	2.93604400	2.13192400	C	5.41520500	-1.11228400	-2.14925800
H	3.27748900	2.17027100	1.89797200	H	4.14064900	0.58106300	-2.54645700
				C	5.90026800	-1.99832600	-1.18021200
				H	5.85478300	-2.54784700	0.90588000
				H	5.74274800	-1.20400500	-3.18124200
				H	6.60317600	-2.77907100	-1.45674200
				O	1.28756400	-2.69793800	0.38314200
				H	2.15307700	-3.05199500	0.14487900
				H	0.98042500	-2.14866200	-0.37984200
				O	0.66611500	-0.24327900	1.73902200
				H	-0.07799900	-0.69881300	2.17548300
				H	1.18560500	-1.00038100	1.40975900
				O	-0.88018600	-2.55495700	2.24118000
				H	-0.16951300	-2.97935900	1.72947900
				H	-1.10902400	-3.14660800	2.97960200
				O	-1.66094800	-4.18664500	4.46597400
				H	-2.58447400	-4.46874200	4.47328500
				H	-1.48425700	-3.81735100	5.34059200

Table S6 relative corrections to Gibbs free energies for each reported structures

complexes	sp(scrf)	thermal	D3-gep
	Total free energy in solution: - with all non electrostatic terms (a.u.)	Thermal correction to Gibbs Free Energy	The sum of the geometrical counterpoise correction and the dispersion correction
Catalyst Activation			
path A			
0_-12	-2538.116566	0.135386	-0.004842236
1_-12	-2885.006889	0.255229	0.004232776
1-2_-12	-2884.962112	0.253738	-0.000972771
2_-12	-2884.995787	0.256486	0.000994824
path B			
0_-12	-2538.116566	0.135386	-0.004842236
3_-12	-2614.594409	0.154079	0.00504409

3-4_-12	-2614.550474	0.154679	0.002885161
4_-12	-2614.583537	0.158161	0.004607887
5_-12	-2961.475652	0.278978	0.013785248
5-6_-12	-2961.454455	0.276466	0.010328994
6_-12	-2961.469003	0.277853	0.008527404
path C			
8_02	-2538.563345	0.146084	-0.001800681
9_02	-2885.461699	0.267813	0.002682467
9-10_02	-2885.432869	0.264261	0.003721628
10_02	-2885.447364	0.264892	0.003971529
path D			
11_02	-2349.906803	0.136586	-0.004878498
12_02	-2696.79806	0.257763	0.000509539
12-13_02	-2696.787632	0.254664	0.001526502
13_02	-2696.793086	0.255778	-0.001618948
substrate oxidation			
7_03	-3104.176095	0.47314	0.009540499
7_01	-3104.176069	0.473789	0.009533239
7-14_03	-3104.130013	0.473019	0.010309462
14_03	-3104.154281	0.477972	0.01092878
14r_01	-3104.193117	0.475203	0.008502831
catalyst regeneration			
15_03	-2908.903492	0.376783	0.022646636
16_03	-2908.924627	0.380748	0.022147464
15_01	-2908.90005	0.378931	0.022605956
16_01u	-2908.924598	0.381752	0.022147464
16_01r	-2908.88812	0.384316	0.017039715
17_02	-2771.951481	0.259336	-0.00146235
17-18_02	-2771.938717	0.257397	-0.00152605
18_02	-2771.942324	0.256282	-0.000563843
Water involvement			
<u>1H2O</u>			
path A			
0_-12	-2614.594409	0.154079	0.00504409

1-2_-12	-2961.441563	0.272369	0.009078427
path B			
0_-12	-2614.594409	0.154079	0.00504409
3-4_-12	-2691.029813	0.173852	0.013116635
5-6_-12	-3037.933672	0.295817	0.020003673
path C			
8_02	-2615.039909	0.165148	0.007508517
9-10_02	-2961.909861	0.284829	0.015321688
path D			
11_02	-2426.381925	0.158663	0.002823606
12-13_02	-2773.264825	0.273293	0.010430454
<u>2H2O</u>			
path A			
0_-12	-2691.07082	0.175003	0.01539013
1-2_-12	-3037.923381	0.29373	0.020353624
path B			
0_-12	-2691.07082	0.175003	0.01539013
3-4_-12	-2767.508193	0.192786	0.023353798
5-6_-12	-3114.412138	0.316201	0.031131355
path C			
8_02	-2691.518007	0.187725	0.019314805
9-10_02	-3038.391266	0.307446	0.026737189
path D			
11_02	-2502.858827	0.177265	0.016099058
12-13_02	-2849.73675	0.299942	0.017086163
<u>3H2O</u>			
path A			
0_-12	-2767.551365	0.198129	0.027269662
1-2_-12	-3114.402102	0.310542	0.030240604
path B			
0_-12	-2767.551365	0.198129	0.027269662
5-6_-12	-3190.891959	0.33681	0.042280462
path C			
8_02	-2767.99975	0.208825	0.030727036

9-10_02	-3114.868203	0.327223	0.036325078
path D			
11_02	-2579.340463	0.198383	0.026942963
12-13_02	-2926.209768	0.322368	0.027764395
<u>4H2O</u>			
path A			
0_-12	-2844.032572	0.21888	0.036763446
path B			
0_-12	-2844.032572	0.21888	0.036763446
5-6_-12	-3267.367672	0.356629	0.053954963
path C			
8_02	-2844.478758	0.233279	0.042611388
9-10_02	-3191.348066	0.352677	0.049499795
path D			
11_02	-2655.819389	0.21889	0.037416913
12-13_02	-3002.685239	0.335963	0.039059873