

Supporting Information

Mechanistic Insight into the 2° Alcohol Oxidation Mediated by an Efficient Cu^I/L-Proline-TEMPO catalyst, A density functional theory study

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Table S1A. Comparison of the energy barriers for processes ${}^1\mathbf{7} \rightarrow {}^1\mathbf{TS}_{7-8}$ and ${}^2\mathbf{13} \rightarrow {}^2\mathbf{TS}_{13-14}$ between the optimized structures in the gas phase and the solvent.

process	M06//B3LYP_gas ^[a]	M06//B3LYP_sol ^[b]
${}^1\mathbf{7} \rightarrow {}^1\mathbf{TS}_{7-8}$	21.8	21.7
${}^2\mathbf{13} \rightarrow {}^2\mathbf{TS}_{13-14}$	22.8	23.4
[a] M06/6-311+G(d,p)/SMD(DMF)//B3LYP/6-31+G(d) with geometrical counterpoise correction and the dispersion correction. [b] M06/6-311+G(d,p)/SMD(DMF)//B3LYP/6-31+G(d)/SMD(DMF) with geometrical counterpoise correction and the dispersion correction.		

Table S1B. Comparison of energetic spans (δE) for path A and path B at different levels of theories.

routes	M06 ^[a]	TPssh ^[b]	Wb97xd ^[c]
Path A	23.6	25.5	25.8
Path B	22.8	23.7	25.0
[a] M06/6-311+G(d,p)/SMD(DMF)//B3LYP/6-31+G(d). [b] TPssh/6-311+G(d,p)/SMD(DMF)//B3LYP/6-31+G(d). [c] Wb97xd/6-311+G(d,p)/SMD(DMF)//B3LYP/6-31+G(d).			

Table S2. Cartesian coordinates of all structures considered in this work (B3LYP level).

0				1			
Charge=-2 Multiplicity =1				Charge=-2 Multiplicity =1			
C	2.42823500	-1.86138900	0.24715300	C	-2.00794500	2.72721100	-0.72480100
C	3.73857200	-1.39693500	-0.46508600	C	-3.41117500	3.34421600	-1.03073400
C	3.65812800	0.15128800	-0.35582400	C	-4.35932100	2.53424500	-0.10233600
C	2.30715800	0.40476300	0.39048800	C	-3.40074600	1.54695900	0.63757800
H	2.02353300	-2.79771800	-0.16339700	H	-1.33910400	2.73332800	-1.59712300
H	2.69971700	-2.07673900	1.32525000	H	-1.52112000	3.38460900	0.05479400
H	3.73469200	-1.72156600	-1.51514100	H	-3.66921900	3.19456700	-2.08816000
H	4.64353400	-1.81385800	0.00933700	H	-3.44205900	4.42839100	-0.83167600
H	4.50868000	0.58626800	0.18375100	H	-4.91450300	3.16839200	0.59985900
H	3.62377100	0.62702300	-1.34190600	H	-5.09689900	1.96361300	-0.67697600
H	2.56545000	0.45069500	1.48542700	H	-3.09506400	2.06514500	1.58739500
N	1.51614300	-0.77104100	0.10185600	N	-2.27549100	1.40308900	-0.25838700
C	1.66276300	1.79332700	0.08412400	C	-4.07423600	0.22397500	1.10811900
O	2.47486100	2.76810900	0.04608200	O	-5.21305200	0.34445700	1.64473800
Cu	-0.35389900	-0.81298600	0.11964900	Cu	-1.27534900	-0.17097100	-0.31389700
O	0.40838200	1.84281200	-0.05520600	O	-3.41603200	-0.84848700	0.95151400
O	-2.22576800	-1.04061800	0.09915300	C	2.48506500	0.25810800	-0.34894300
C	-4.54378400	-0.52513400	-0.06135800	H	1.77939400	0.64011500	0.41014200
H	-4.66092800	-1.25863200	-0.86990000	O	2.36888500	-1.13511000	-0.45964000
H	-4.72930700	-1.04084400	0.88990900	O	-0.11699000	-1.67911900	-0.53168900
H	-5.30052100	0.26543200	-0.18846400	H	1.35816000	-1.38313400	-0.48402800
C	-2.84001200	0.75117700	-1.42422000	C	0.54297300	-3.98519900	-0.59061100

H	-1.82198800	1.15530300	-1.43174900	H	0.69493700	-3.92722500	-1.67572200
H	-2.93716500	0.02861800	-2.24560900	H	1.49810500	-3.75418200	-0.10459300
H	-3.55014000	1.57747300	-1.59588900	H	0.25813600	-5.01530700	-0.33137900
C	-2.94030500	1.06821100	1.07143900	C	-1.87374500	-3.31323200	-0.86394100
H	-1.92480800	1.47870500	1.05356000	H	-2.65127000	-2.61039900	-0.54644400
H	-3.66078700	1.89844500	0.97989900	H	-1.74319400	-3.23415000	-1.95098400
H	-3.10076600	0.56911100	2.03647100	H	-2.20458500	-4.33574900	-0.62370400
C	-3.09120400	0.02864900	-0.07248000	C	-0.74799400	-3.04848800	1.37296900
				H	-1.53029500	-2.34189700	1.66896200
				H	-1.04689600	-4.05901000	1.69317000
				H	0.18675400	-2.78348600	1.88336100
				C	-0.54314100	-2.97074800	-0.15818400
				C	3.89403800	0.62649200	0.10053400
				C	4.20741900	1.93825900	0.49452300
				C	4.91648000	-0.33292000	0.12480200
				C	5.50177800	2.28544100	0.88918600
				H	3.42340800	2.69227300	0.49998700
				C	6.21506400	0.01093900	0.51564000
				H	4.65845800	-1.34804800	-0.15763300
				C	6.51744400	1.32163400	0.89862100
				H	5.71686700	3.30710500	1.19620000
				H	6.99300500	-0.75051900	0.52794700
				H	7.52594800	1.58816400	1.20814500
				C	2.13359700	0.95285100	-1.68263600

	H	2.80509500	0.59679800	-2.47389900					
	H	1.10093800	0.69980000	-1.94327700					
	H	2.21276100	2.04495900	-1.61072700					
TS₁₋₂	2								
Charge=-2 Multiplicity =1	Charge=-2 Multiplicity =1								
C	2.48327300	-2.83218100	-0.73605600	C	-3.29644000	-2.54847400	0.69023900		
C	3.82787400	-2.44721900	-1.43595100	C	-4.74410300	-2.07045400	1.04156900		
C	4.51583000	-1.53997900	-0.37891500	C	-4.98333400	-0.90866400	0.03606000		
C	3.45267500	-1.44901100	0.78229900	C	-3.65966800	-0.86108400	-0.79501800		
H	1.66894400	-3.01832100	-1.44863600	H	-2.74348600	-2.91694600	1.56597100		
H	2.66639400	-3.80548800	-0.19567100	H	-3.40074700	-3.42692100	-0.01351800		
H	3.62228000	-1.88950000	-2.35897100	H	-4.78473800	-1.71096200	2.07893200		
H	4.43621800	-3.32848600	-1.70284400	H	-5.48618300	-2.88008200	0.94117900		
H	5.47066200	-1.94910100	-0.02181200	H	-5.86213500	-1.06745400	-0.60128800		
H	4.71523800	-0.53991300	-0.78150600	H	-5.12338800	0.04702700	0.55339800		
H	3.73784200	-2.22660100	1.52982400	H	-3.82915600	-1.52474300	-1.68544500		
N	2.18114000	-1.76263500	0.16694900	N	-2.66420100	-1.41840900	0.08850500		
C	3.52935100	-0.08785000	1.52992800	C	-3.32463100	0.53673500	-1.39044000		
O	4.52404400	0.08090200	2.28548000	O	-4.26120000	1.10871800	-2.01803500		
Cu	1.03311400	-0.24233900	-0.06001200	Cu	-0.90397300	-0.79558100	0.07704900		
O	2.60445000	0.75997100	1.30130900	O	-2.14422400	0.96961500	-1.22176000		
C	-2.16064500	-0.84879700	-0.48187500	C	1.84070200	-1.25135300	0.74566700		
H	-1.75936900	-1.85095500	-0.20497300	H	1.45908800	-2.28650500	0.63327700		
O	-1.40202100	0.15517900	0.05661600	O	0.95060700	-0.33129200	0.22166600		
O	0.17590100	1.66695100	-1.12265700	O	1.56724900	2.22479500	0.86969000		

H	-0.63175700	1.16025400	-0.71414100	H	1.23831000	1.31292100	0.61778100
C	-0.61848000	3.93874800	-1.25015800	C	1.25895600	4.55188500	1.02396400
H	-0.45524000	3.92750400	-2.33483700	H	1.48152100	4.50621000	2.09729500
H	-1.65418200	3.63322100	-1.05820500	H	2.20242200	4.71457800	0.48808800
H	-0.48755200	4.96803700	-0.88575900	H	0.59685000	5.40710700	0.83758700
C	1.81540500	3.36088900	-0.85480100	C	-0.70254400	2.98860500	1.33152600
H	2.48627500	2.65268200	-0.35855300	H	-1.17743900	2.06495300	0.98641100
H	1.99993800	3.33268600	-1.93633200	H	-0.49513300	2.91111300	2.40641900
H	2.02912300	4.37460600	-0.48789600	H	-1.41757000	3.80546400	1.16624500
C	0.12041300	2.94784200	0.96125100	C	0.32801400	3.27900300	-0.95137000
H	0.84811000	2.28779700	1.44373100	H	-0.20475300	2.37890900	-1.27456000
H	0.22774900	3.96003900	1.37777900	H	-0.30862300	4.13657600	-1.20773800
H	-0.88751400	2.57913900	1.18201300	H	1.27543500	3.36978100	-1.49882400
C	0.36151300	2.96375300	-0.56001300	C	0.60822500	3.23670600	0.56264700
C	-3.61241000	-0.83795000	0.04416800	C	3.19442600	-1.23686200	0.01262200
C	-4.52256500	-1.87116400	-0.23664500	C	4.16371900	-2.22749000	0.24412700
C	-4.05161400	0.22225300	0.84867900	C	3.48325200	-0.24031700	-0.92947500
C	-5.83254900	-1.83947000	0.25095000	C	5.38824700	-2.22020400	-0.43046600
H	-4.19675600	-2.71686500	-0.84014800	H	3.95150600	-3.02272500	0.95726000
C	-5.36097800	0.26253200	1.33954800	C	4.70813500	-0.22475600	-1.60469800
H	-3.31829100	0.99013800	1.07789500	H	2.72116600	0.50838800	-1.11601100
C	-6.26207600	-0.76613100	1.04218700	C	5.66918600	-1.21179700	-1.36062000
H	-6.51804500	-2.65388600	0.01982800	H	6.12025200	-3.00289400	-0.23580300
H	-5.67847200	1.09579900	1.96490400	H	4.91060200	0.56117500	-2.33003000

H	-7.27989800	-0.73892700	1.42732500	H	6.61955700	-1.20167300	-1.89123900
C	-2.18050000	-0.81127400	-2.03688000	C	2.05773200	-1.02269900	2.26534400
H	-2.62098300	0.13296000	-2.38172500	H	2.45276000	-0.01490500	2.43486700
H	-1.14739100	-0.85924100	-2.39606200	H	1.08467600	-1.09806800	2.76277600
H	-2.74770200	-1.64526900	-2.47580200	H	2.74514400	-1.75698200	2.71044000
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C	1.27186100	2.16089600	-0.93001300	C	1.25083100	2.13941100	-0.95269900
C	1.64244500	2.82886600	0.42825600	C	1.60347600	2.82113300	0.40312000
C	3.03089600	2.22056400	0.76045700	C	2.99574800	2.23109700	0.75139900
C	3.24701300	1.13497200	-0.36524700	C	3.23601000	1.14291200	-0.36579500
H	0.19211500	2.02844800	-1.05551500	H	0.17411900	1.99107900	-1.08381800
H	1.63171100	2.82864900	-1.75486800	H	1.60819100	2.80344000	-1.78031900
H	0.90131000	2.53988200	1.18186600	H	0.85961600	2.52939000	1.15282400
H	1.66238700	3.92982500	0.37485400	H	1.61134700	3.92164500	0.34114200
H	3.83564400	2.96819700	0.75048100	H	3.79192300	2.98774800	0.74604900
H	3.03672800	1.75108800	1.75095000	H	2.99682200	1.76600700	1.74389700
H	3.95872500	1.56491500	-1.10339300	H	3.94546100	1.57780200	-1.10222800
N	1.94586900	0.88940500	-0.95037000	N	1.94269900	0.87589500	-0.96208200
C	3.88420900	-0.15317900	0.19385800	C	3.88522700	-0.13288300	0.20674300
O	5.11046200	-0.16264800	0.45013600	O	5.11073100	-0.12595300	0.46725900
Cu	1.14802200	-0.74491200	-0.23061000	Cu	1.15304700	-0.75281200	-0.23425100
O	3.07231000	-1.13130200	0.38776700	O	3.08185500	-1.11590900	0.40644800
C	-1.76433900	-0.86611600	0.31142500	C	-1.75246400	-0.86708900	0.31138800
O	-0.67892000	-0.04934900	0.10839600	O	-0.66441600	-0.04900500	0.12147600

C	-3.08477900	-0.09958500	0.12078100	C	-3.07043200	-0.09677700	0.12359300
C	-4.32503400	-0.75633200	0.04370200	C	-4.30977000	-0.75269900	0.02659500
C	-3.07620600	1.29904300	0.01480000	C	-3.06213700	1.30346500	0.04087400
C	-5.51754100	-0.04454400	-0.11994200	C	-5.50141500	-0.03891600	-0.13411800
H	-4.35213400	-1.84322600	0.10297300	H	-4.33629400	-1.84041000	0.06747400
C	-4.26520700	2.01855100	-0.14499200	C	-4.25036400	2.02492800	-0.11583300
H	-2.10414700	1.78206500	0.04891700	H	-2.09111000	1.78715000	0.08998400
C	-5.49516400	1.35328200	-0.21233600	C	-5.47934600	1.36025100	-0.20335100
H	-6.46474600	-0.57930600	-0.18293700	H	-6.44770900	-0.57312800	-0.21320500
H	-4.23241700	3.10435500	-0.22593200	H	-4.21760700	3.11193300	-0.17870300
H	-6.42052200	1.91179700	-0.34403300	H	-6.40402600	1.92036800	-0.33295800
O	0.73461300	-2.70373400	-0.16426400	O	0.74498700	-2.71478400	-0.17809700
O	-0.03014000	-3.13991100	-1.15990000	O	-0.06807600	-3.14943300	-1.14256000
C	-1.75325000	-1.50347800	1.73189600	C	-1.74637800	-1.52037200	1.72414200
H	-0.84221600	-2.10113600	1.82769500	H	-0.83812900	-2.12339000	1.81342500
H	-1.73941400	-0.70817900	2.48891700	H	-1.73080500	-0.73407600	2.49054700
H	-2.62281000	-2.15320700	1.91534600	H	-2.61890700	-2.16862400	1.89793900
H	-1.78995000	-1.70964400	-0.40797700	H	-1.77472500	-1.70274500	-0.41675100
TS₃₋₄				TS₃₋₄			
Charge=-2 Multiplicity =3				Charge=-2 Multiplicity =1			
C	1.52890900	2.28240200	-0.06928400	C	1.46400700	2.27259700	0.06771900
C	2.36125700	2.45162000	1.23557900	C	2.34846600	2.36653600	1.34812300
C	3.66466700	1.66487600	0.93589400	C	3.62767200	1.57774800	0.96347200
C	3.36711700	0.95045200	-0.44059400	C	3.28590100	0.97048900	-0.45282400
H	0.44966600	2.29705900	0.11081300	H	0.39295000	2.26702600	0.29730100

H	1.77700400	3.13494300	-0.75102300	H	1.67261200	3.17113100	-0.56613100
H	1.81480600	1.99613400	2.06966900	H	1.82675900	1.88120600	2.18141400
H	2.55030900	3.50655300	1.49232600	H	2.56323900	3.40586600	1.64553300
H	4.54412000	2.31823700	0.85932600	H	4.52091000	2.21528100	0.91706200
H	3.87927800	0.92565100	1.71641300	H	3.83793600	0.77736000	1.68235200
H	3.92104400	1.50718400	-1.22637200	H	3.81883500	1.58352000	-1.21097800
N	1.93418700	1.02223100	-0.63938900	N	1.84771600	1.05731800	-0.60343300
C	3.87859800	-0.50294700	-0.45710300	C	3.78801400	-0.47895900	-0.58761200
O	5.10524000	-0.71633500	-0.58567300	O	5.00333100	-0.68876200	-0.80419400
Cu	1.06629700	-0.66401600	-0.23582300	Cu	0.99499400	-0.66016900	-0.21037600
O	2.97589200	-1.40668600	-0.30050500	O	2.88984200	-1.38513600	-0.42478900
C	-1.78381500	-0.54981900	0.69693200	C	-1.74238600	-0.55612700	0.82935600
O	-0.68306900	0.18948300	0.46153200	O	-0.60777600	0.13736100	0.61620400
H	-1.61291300	-1.57814100	-0.11929300	H	-1.60368700	-1.63834000	0.15359900
O	-0.98712000	-2.46323600	-0.75994400	O	-1.07451700	-2.62279700	-0.48197100
O	0.27877800	-2.44537200	-0.18983300	O	0.29714700	-2.45955600	-0.33436500
C	-3.06920100	0.04748600	0.23470100	C	-2.96957200	0.05937100	0.22992200
C	-3.03857500	1.15934100	-0.64372300	C	-2.83053700	1.03175500	-0.78783700
C	-4.34737200	-0.46562500	0.56819200	C	-4.28701700	-0.30816300	0.58866800
C	-4.20911100	1.71465100	-1.15760300	C	-3.94214900	1.59645600	-1.41080800
H	-2.06103000	1.55772400	-0.89506100	H	-1.82106400	1.32268700	-1.05948400
C	-5.51809700	0.09385400	0.05454400	C	-5.40088400	0.26098500	-0.03434500
H	-4.42295000	-1.32190100	1.23268100	H	-4.44365100	-1.05397000	1.36281200
C	-5.46639600	1.19207000	-0.81754700	C	-5.24285600	1.21994300	-1.04300800

H	-4.14392100	2.56942300	-1.83050800	H	-3.79534900	2.34151400	-2.19188200
H	-6.48183000	-0.33055200	0.33621200	H	-6.40073700	-0.04764700	0.27048200
H	-6.37963800	1.62710900	-1.21936900	H	-6.11005500	1.66266400	-1.52959300
C	-1.78739900	-1.23270000	2.07294500	C	-1.87430100	-1.07486800	2.27205500
H	-2.64507000	-1.89917200	2.22979900	H	-2.70344900	-1.78199100	2.40296300
H	-0.87373000	-1.83052300	2.15241500	H	-0.94664100	-1.59696900	2.52428500
H	-1.77831300	-0.47568500	2.87434800	H	-2.00779600	-0.24113400	2.98083600
4 Charge=-2 Multiplicity =3				4 Charge=-2 Multiplicity =1			
C	-1.13597800	-1.90963500	-1.34026000	C	2.32648700	0.42437500	-2.11946800
C	-1.17309200	-2.83198800	-0.08380100	C	1.52571300	1.60709600	-2.73979400
C	-2.51003400	-2.45521800	0.60848900	C	1.24778200	2.51734300	-1.51518400
C	-3.08795100	-1.29273700	-0.28107600	C	1.91132100	1.76084900	-0.31299400
H	-0.12092600	-1.59656900	-1.60536900	H	2.15246700	-0.53032600	-2.63933300
H	-1.54749900	-2.48365600	-2.20549000	H	3.41842800	0.65596500	-2.24701000
H	-0.31849400	-2.60758900	0.56455000	H	0.58871000	1.24514000	-3.18250900
H	-1.11774300	-3.90022800	-0.34413500	H	2.09186700	2.12002400	-3.53328200
H	-3.21181700	-3.29672000	0.67132300	H	1.66356900	3.52692300	-1.63008300
H	-2.34047800	-2.09825100	1.63072900	H	0.17198400	2.61337100	-1.33252200
H	-3.86147400	-1.73251900	-0.94437600	H	2.94856200	2.14900700	-0.21867800
N	-1.96757400	-0.76857800	-1.03881600	N	1.90407500	0.36445700	-0.73878900
C	-3.76778000	-0.20764900	0.57753600	C	1.19466400	2.14616000	1.02091100
O	-4.90377700	-0.42991100	1.05026800	O	1.73640800	3.07767800	1.67680300
Cu	-1.34949500	0.90479600	-0.34297300	Cu	2.40002300	-1.08363400	0.33120200

O	-3.07009200	0.85643600	0.77484600	O	0.10179000	1.56239600	1.30432700
C	1.64285700	0.47192500	0.49602700	C	-3.79634000	0.60186100	1.12839900
O	0.81980800	0.49898800	-0.50602300	O	-5.00926600	0.83467900	1.17068700
H	0.63293700	2.37047800	-1.08445700	H	1.31023400	-2.58075600	2.39608900
O	0.01098300	3.11694100	-1.18225400	O	1.74077700	-3.28599100	1.89141400
O	-0.98485500	2.76793500	-0.13718700	O	2.93518100	-2.53853400	1.35574400
C	2.98907100	0.01855900	0.31899000	C	-3.21893200	-0.21180300	0.00870300
C	3.44636100	-0.38501100	-0.98596600	C	-4.10176600	-0.91427400	-0.83600900
C	3.95825500	-0.07868100	1.37710100	C	-1.83279100	-0.28836500	-0.21614900
C	4.74017100	-0.82753000	-1.20076800	C	-3.60694600	-1.69361000	-1.87817000
H	2.73348900	-0.33122300	-1.80228100	H	-5.16907300	-0.83424500	-0.65059700
C	5.25194000	-0.52461300	1.14476500	C	-1.34236600	-1.06758400	-1.27225700
H	3.67633000	0.19586900	2.38925100	H	-1.10506600	0.27551000	0.37815900
C	5.67890500	-0.90808400	-0.14549100	C	-2.22144700	-1.77249600	-2.09505400
H	5.03853000	-1.12235000	-2.20727100	H	-4.29319700	-2.24211100	-2.52139100
H	5.94903300	-0.58088500	1.98149800	H	-0.26494700	-1.08784000	-1.41738000
H	6.69319300	-1.25977100	-0.31992000	H	-1.83376600	-2.38393300	-2.90771100
C	1.11242100	0.92657700	1.84150600	C	-2.87577100	1.08893500	2.21988700
H	1.89835700	1.22529400	2.54334100	H	-1.96882400	1.58904900	1.84846300
H	0.43577900	1.77289500	1.67535900	H	-3.43824000	1.74084000	2.89265700
H	0.52176500	0.12758100	2.31565800	H	-2.49867800	0.22481900	2.78307200
5				TS₅₋₆			
Charge=-2 Multiplicity =1				Charge=-2 Multiplicity =1			
C	3.46430100	-2.40410500	0.24840200	C	2.61335300	-2.58658400	-0.12276200
C	4.86454900	-2.13002900	-0.39725800	C	4.02308000	-2.30864500	-0.74294200

C	5.17529300	-0.67535800	0.05217300	C	4.48526100	-1.03194000	0.01300700
C	3.92870700	-0.28225800	0.92543700	C	3.27432800	-0.71042300	0.96670600
H	2.84000100	-3.07651600	-0.35372900	H	1.92337300	-3.07000800	-0.82607800
H	3.65398600	-2.92892700	1.22630500	H	2.76953700	-3.30944200	0.72624200
H	4.79899300	-2.20076300	-1.49103400	H	3.93014600	-2.11700400	-1.81981600
H	5.62929500	-2.85033000	-0.06110000	H	4.71757000	-3.15560900	-0.61078600
H	6.11314800	-0.58919500	0.61655800	H	5.41743100	-1.17847300	0.57465100
H	5.24199000	-0.00257900	-0.81081600	H	4.64225700	-0.19631100	-0.67877200
H	4.18793100	-0.54939600	1.97631100	H	3.50130800	-1.21158000	1.93661000
N	2.85192800	-1.12182400	0.43841000	N	2.11838200	-1.32164400	0.34026200
C	3.68745200	1.25614500	0.93157200	C	3.18042900	0.80595000	1.29372000
O	4.52188300	1.93614100	1.58661900	O	4.08074600	1.27250300	2.03622600
Cu	1.51387100	-0.27752400	-0.56394400	Cu	0.99592800	-0.10011500	-0.59077000
O	2.70020400	1.71046400	0.26811200	O	2.21176100	1.46415200	0.78267400
C	-2.69165700	0.44388400	-0.02434900	C	-2.11744900	0.82519000	0.16710500
O	-2.34689600	0.28785300	-1.37215700	O	-1.38070700	0.47494500	-0.93805800
H	-2.00988100	-0.14630500	0.61514100	H	-1.56757500	0.62648100	1.11454200
H	-1.31782600	0.44738600	-1.45836200	H	-0.39139900	1.37260200	-1.49375400
O	0.15670400	0.63266500	-1.53098200	O	0.54570100	1.67190600	-1.87872200
O	0.34801600	2.09462100	-1.28617700	O	0.89545800	2.86281800	-1.09615800
H	1.17935800	2.09856000	-0.76169700	H	1.47153100	2.46122400	-0.39249600
C	-4.10412700	-0.07914500	0.21190900	C	-3.41972200	0.00859100	0.27113400
C	-4.61545200	-0.22840500	1.51187300	C	-4.25204900	0.06127200	1.40169200
C	-4.93618700	-0.41214200	-0.86674600	C	-3.80069900	-0.82721900	-0.78764000

C	-5.91833600	-0.68356600	1.73023300	C	-5.43518800	-0.68081400	1.46856800
H	-3.98035400	0.00964700	2.36245600	H	-3.96313800	0.68611200	2.24531600
C	-6.24231900	-0.86596700	-0.65357700	C	-4.98323900	-1.57207000	-0.72870600
H	-4.52262200	-0.31357900	-1.86485300	H	-3.12163500	-0.87100900	-1.63456200
C	-6.74337000	-1.00305200	0.64505800	C	-5.81091400	-1.50233200	0.39795900
H	-6.28858500	-0.79492900	2.74768300	H	-6.06131700	-0.62524600	2.35819500
H	-6.87014800	-1.11973000	-1.50606400	H	-5.25717000	-2.21896400	-1.56122100
H	-7.75770400	-1.36019000	0.81143000	H	-6.72813300	-2.08669000	0.44806500
C	-2.56878300	1.92059200	0.41583300	C	-2.45969700	2.34180600	0.17408300
H	-2.75967400	2.04405200	1.49053100	H	-3.01257700	2.64775700	1.07477800
H	-1.55634700	2.26599400	0.18284300	H	-1.52474200	2.90832700	0.11973100
H	-3.28700900	2.53424100	-0.14278600	H	-3.06468400	2.58537900	-0.70940200
6				7_gas			
Charge=-2 Multiplicity =1				Charge=-2 Multiplicity =1			
C	1.96059500	-2.75187300	0.53054000	H	-1.32745900	-2.11374500	-0.16423100
C	2.96406200	-3.05995700	-0.62949000	O	-0.37017200	-2.04593700	-0.37257400
C	3.87393100	-1.79986600	-0.64469600	O	-0.15279300	-0.57148200	-0.29456900
C	3.28723600	-0.90603600	0.50841200	H	5.89736200	-1.06444700	-1.10264700
H	0.96902600	-3.19258900	0.36657600	C	4.89545200	-0.69976400	-1.37321700
H	2.37826400	-3.23380100	1.45966700	C	4.96054600	0.81912700	-1.59591300
H	2.42255900	-3.16644400	-1.57865700	C	3.88427200	-1.13176100	-0.25672000
H	3.53071500	-3.99119900	-0.46076200	H	4.63038200	-1.19321300	-2.31613200
H	4.93434700	-2.03312900	-0.48050700	H	4.10407700	1.14543600	-2.19626500
H	3.79369300	-1.26598700	-1.59864900	C	4.94087200	1.53650400	-0.24627500
H	3.86700400	-1.16100800	1.42692400	H	5.86850500	1.07723100	-2.16116700

N	1.90798900	-1.32403200	0.63764800	N	3.00253700	0.02501600	0.03928500
C	3.53310800	0.60668800	0.26026400	C	3.59921300	1.30882000	0.49846800
O	4.71311600	1.01660500	0.41150800	H	5.10156500	2.61679900	-0.36555900
Cu	0.52450100	-0.14175600	0.18737100	H	5.77781900	1.16449000	0.36344900
O	2.52284600	1.29511200	-0.09664300	O	1.99816800	-0.35794200	0.97016700
C	-2.06197300	1.10556700	0.58530500	C	3.82599000	1.40641400	2.02700000
O	-0.93288700	1.02803700	-0.20140900	H	2.88187600	1.25501900	2.55397000
H	-1.83451600	0.94997400	1.66241000	H	4.54045300	0.65889200	2.38390100
H	-0.17866600	2.46191700	-0.81993500	H	4.22245100	2.40072000	2.27625100
O	0.24759000	3.25021800	-1.26047500	C	2.58500800	2.40124100	0.09406200
O	1.26383600	3.65147100	-0.28715400	H	2.89744800	3.38542200	0.47059900
H	1.86057900	2.84872100	-0.25996900	H	2.48764000	2.45301300	-0.99541600
C	-3.11933400	0.04410800	0.22580700	H	1.59994500	2.15957500	0.50098400
C	-4.23553700	-0.19567200	1.04269700	C	4.63412400	-1.69359000	0.98163300
C	-2.98589600	-0.70789900	-0.94908800	H	3.92060500	-1.83807200	1.79824900
C	-5.20097400	-1.14562900	0.69401500	H	5.09043600	-2.66360800	0.74050300
H	-4.34413700	0.36385700	1.97094400	H	5.43617000	-1.02913100	1.32289400
C	-3.94839500	-1.65838800	-1.30534400	C	2.97879700	-2.24850100	-0.81119700
H	-2.09896800	-0.53025700	-1.54980300	H	2.28631800	-2.61816100	-0.05324200
C	-5.06287700	-1.88200500	-0.48897600	H	2.36770200	-1.86573000	-1.63350700
H	-6.05598400	-1.31714600	1.34661200	H	3.60023300	-3.07887200	-1.17526500
H	-3.82129300	-2.23760500	-2.21829900	H	1.09247200	-0.45036300	0.42578200
H	-5.80727100	-2.62764200	-0.76258900	C	-4.05878600	2.25840600	0.05865700
C	-2.69882400	2.51528300	0.46817600	C	-5.06026200	1.98371800	-1.11193200

H	-3.59011300	2.62253900	1.10266500	C	-5.47281400	0.50442500	-0.87431600
H	-1.95628700	3.26508700	0.75753300	C	-4.65189800	0.08891500	0.40206700
H	-2.98215000	2.70637500	-0.57381100	H	-3.27910700	2.98370900	-0.20726700
				H	-4.65535300	2.71816300	0.89627000
				H	-4.55232500	2.10118900	-2.07821800
				H	-5.92183700	2.67261000	-1.10034600
				H	-6.55278900	0.37801300	-0.72192300
				H	-5.18098000	-0.12836700	-1.72057700
				H	-5.31756400	0.27944500	1.27609500
				N	-3.51302500	0.98520100	0.42467700
				C	-4.35620600	-1.43998200	0.42624500
				O	-5.34907600	-2.18327300	0.65077700
				Cu	-1.84018400	0.23488600	0.04191500
				O	-3.16402100	-1.82299800	0.19722100
7_sol				TS7-8_gas			
Charge=-2 Multiplicity =1				Charge=-2 Multiplicity =1			
H	-1.57791500	-2.15165200	-0.45933000	H	-0.12039400	-3.49786000	-0.26415300
O	-0.66151800	-2.13556200	-0.81471200	O	0.44253600	-4.28607800	-0.13208000
O	-0.30250500	-0.69512900	-0.63596300	O	-0.56525300	-1.41605700	0.28270800
H	6.13677500	-0.83801800	-0.89198800	H	5.21341300	-0.08714800	-1.58304800
C	5.13863500	-0.50733900	-1.20806000	C	4.12941300	0.10358300	-1.61950100
C	5.12181400	1.02619400	-1.32938400	C	3.88851000	1.61641700	-1.50184000
C	4.09585800	-1.08266300	-0.19345700	C	3.43368500	-0.74597200	-0.49990900
H	4.96718000	-0.94783100	-2.19833800	H	3.78742100	-0.24322500	-2.60307900
H	4.36259400	1.33994200	-2.05695200	H	2.89132100	1.86867100	-1.88223100

C	4.82545200	1.66321300	0.02682900	C	3.99771800	2.03642000	-0.03680500
H	6.08758000	1.37872300	-1.71510200	H	4.61727200	2.16454300	-2.12017400
N	3.02916700	-0.05199400	-0.01511900	N	2.43439700	0.12425800	0.18490100
C	3.41267700	1.28820200	0.54675600	C	2.87569000	1.39687000	0.82186200
H	4.89591300	2.75724500	-0.02876800	H	3.94767800	3.12998500	0.07238500
H	5.58828000	1.34022700	0.74813100	H	4.98485300	1.73095300	0.34403200
O	1.97736400	-0.59566100	0.80270000	O	1.74426900	-0.62917000	1.17698100
C	3.39462600	1.37284400	2.08806700	C	3.36586400	1.25561500	2.28447700
H	2.38453500	1.23659400	2.48487000	H	2.57131300	0.84552000	2.91242000
H	4.04756800	0.62930800	2.55348900	H	4.23601500	0.59599400	2.36443200
H	3.75011300	2.36572900	2.39460800	H	3.65368900	2.24576400	2.66988500
C	2.38036300	2.29387400	-0.00117000	C	1.63399600	2.31537300	0.81981400
H	2.55232900	3.29359200	0.41879500	H	1.83428100	3.24811100	1.36885200
H	2.44036500	2.36712400	-1.09405700	H	1.33912100	2.56872600	-0.20509300
H	1.36243700	1.98636200	0.26314200	H	0.78768800	1.80258700	1.28516800
C	4.78839700	-1.52826800	1.11732200	C	4.48641000	-1.36292400	0.45720100
H	4.04512500	-1.81275500	1.87013400	H	3.97476800	-1.83052000	1.30405800
H	5.42189900	-2.40347700	0.92076800	H	5.06284600	-2.13780800	-0.06817700
H	5.43210900	-0.75056300	1.53902000	H	5.19982000	-0.61764700	0.83303300
C	3.44452300	-2.32712900	-0.82359100	C	2.65672300	-1.89826100	-1.16552400
H	2.78130500	-2.83858500	-0.11933700	H	2.17209800	-2.58549700	-0.46214700
H	2.86143300	-2.05509900	-1.71197700	H	1.86563400	-1.49232500	-1.80622000
H	4.22639400	-3.03266000	-1.13215500	H	3.34812400	-2.48258500	-1.79187000
H	1.17190300	-0.65390900	0.20701600	H	0.83445500	-0.90086600	0.77163200

C	-3.95497100	2.28046600	0.03792300	C	-1.77404500	1.08816800	-1.58551600
C	-4.90095100	1.95016100	-1.15147900	C	-2.74783500	0.30728200	-2.50253600
C	-5.38652900	0.51184700	-0.82876000	C	-4.12193600	0.48134300	-1.80080700
C	-4.62688000	0.14761100	0.49827000	C	-3.76272500	1.13418100	-0.41394400
H	-3.14593900	2.96834200	-0.23691500	H	-0.74602100	0.72129900	-1.62044800
H	-4.56015300	2.79243900	0.82102700	H	-1.77028900	2.15748800	-1.89604600
H	-4.34393000	1.97307700	-2.09665300	H	-2.45172700	-0.74755700	-2.52307400
H	-5.73018400	2.66564500	-1.23977800	H	-2.75015600	0.67898000	-3.53836700
H	-6.47503300	0.45095600	-0.70240600	H	-4.80503000	1.12722400	-2.36834900
H	-5.10813300	-0.18787900	-1.62728500	H	-4.62706200	-0.48158400	-1.66149900
H	-5.30666800	0.41508600	1.33353900	H	-4.03259400	2.20563400	-0.45363900
N	-3.44314500	1.00494400	0.52152500	N	-2.31472400	1.00359400	-0.23527800
C	-4.39732600	-1.37929400	0.61059500	C	-4.52014800	0.48796800	0.75711300
O	-5.36036100	-2.05620700	1.06308500	O	-5.68220100	0.83381700	1.02544900
Cu	-1.87276100	0.19143000	-0.10825200	Cu	-2.06223000	-0.67891500	0.66859500
O	-3.28724000	-1.86349200	0.21136500	O	-3.85178700	-0.43872200	1.37201500
TS7-8_sol				8			
Charge=-2 Multiplicity =1				Charge=-2 Multiplicity =1			
H	0.99950400	3.13247700	-1.84531200	H	-7.76438000	0.39790500	0.01198600
O	0.47109300	3.72583500	-1.28924400	O	-6.86646500	0.42153200	-0.36167300
O	0.52451400	1.49153900	-0.79113800	O	1.02326100	-1.59078100	0.34546700
H	-4.71271700	-2.04923000	-1.11636000	H	-5.04875200	0.94463600	0.67702800
C	-3.67154500	-1.83410400	-0.84145300	C	-4.02686600	1.31307900	0.87459700
C	-3.41262200	-2.30877400	0.59884100	C	-3.54432000	2.02388200	-0.39039800
C	-3.41492000	-0.30748200	-1.06785900	C	-3.07150100	0.15547600	1.27357900

H	-3.04480800	-2.41585400	-1.52916800	H	-4.09051900	2.01493600	1.72159100
H	-2.34978100	-2.54698400	0.73292700	H	-2.51491900	2.39370600	-0.27093200
C	-3.82281800	-1.22693000	1.59628100	C	-3.63804100	1.04367900	-1.57006100
H	-3.96772100	-3.23684800	0.78993200	H	-4.18629000	2.89277700	-0.59486000
N	-2.49795600	0.15727100	0.01580300	N	-2.34723200	-0.30968100	0.05071000
C	-2.96693700	0.05787800	1.43922200	C	-3.09182700	-0.38961400	-1.24213000
H	-3.72446000	-1.58697400	2.62870000	H	-3.09725900	1.45380400	-2.43674000
H	-4.88571300	-0.99036100	1.45126800	H	-4.69667000	0.95464900	-1.84077800
O	-2.10978400	1.51618500	-0.23758200	O	-1.74764200	-1.58636900	0.33405800
C	-3.77185700	1.27583600	1.94298000	C	-4.25185400	-1.41634000	-1.25779700
H	-3.15945200	2.18208200	1.95278700	H	-3.91842000	-2.36780900	-0.82479700
H	-4.65921300	1.47058100	1.33428600	H	-5.14829900	-1.04210500	-0.74563800
H	-4.10902500	1.08091700	2.97001700	H	-4.55124600	-1.60492200	-2.30023100
C	-1.69620200	-0.06580600	2.30388100	C	-2.05756100	-0.78888100	-2.31436400
H	-1.95382400	-0.06966600	3.37122600	H	-2.51753300	-0.71502500	-3.30990600
H	-1.15362000	-0.99180500	2.07909000	H	-1.18740800	-0.12145900	-2.27777500
H	-1.02005800	0.77600700	2.11931100	H	-1.70548600	-1.81431600	-2.16511300
C	-4.75109600	0.46965500	-1.16256000	C	-3.87491600	-0.94336700	2.00678200
H	-4.56844800	1.54939800	-1.19554600	H	-4.31567200	-0.51301800	2.91791200
H	-5.27795700	0.18881000	-2.08440300	H	-4.69894700	-1.31310100	1.39263300
H	-5.42420800	0.25425700	-0.32735200	H	-3.22584800	-1.77886500	2.28913600
C	-2.68214500	-0.13520000	-2.41046500	C	-1.97115300	0.67678800	2.22517900
H	-2.55562600	0.91998600	-2.67085200	H	-1.22573400	-0.10188700	2.42094200
H	-1.69115800	-0.60265900	-2.37628400	H	-1.45403900	1.53537400	1.77895300

H	-3.25943200	-0.62009200	-3.20820500	H	-2.41038100	0.99332200	3.18268000
H	-1.12113800	1.48681700	-0.43930500	H	-0.76663100	-1.43255000	0.29365100
C	1.80007500	-2.04733700	-0.49643800	C	2.09698600	1.64516300	0.09246800
C	2.82687200	-2.08256400	-1.65214600	C	3.06704300	2.87035400	0.06278700
C	4.15047000	-1.65187700	-0.96876600	C	4.46934900	2.26388700	-0.27457200
C	3.70704300	-1.18528000	0.46703300	C	4.14222300	0.78035000	-0.52463700
H	0.77129000	-1.87300800	-0.82694000	H	1.31911400	1.71223200	0.85773500
H	1.81534200	-3.02888300	0.01958000	H	1.59581900	1.53996700	-0.88664100
H	2.53917900	-1.36229000	-2.42785200	H	3.08376200	3.36785400	1.03921200
H	2.89687900	-3.07047600	-2.12454500	H	2.74521600	3.61149800	-0.67962700
H	4.87220500	-2.47379000	-0.90312600	H	4.94066100	2.73371100	-1.14536800
H	4.63485800	-0.83523000	-1.51708200	H	5.16178000	2.35376400	0.56872600
H	3.97385900	-1.98113400	1.18364900	H	3.84143300	0.67550900	-1.59211800
N	2.24920200	-1.01119300	0.43283300	N	3.01357400	0.55490500	0.37742600
C	4.41245200	0.10468700	0.89337200	C	5.16942300	-0.33291000	-0.27954700
O	5.55909200	0.07193300	1.37644900	O	6.38598000	-0.15857300	-0.41082600
Cu	1.93612600	0.83841700	-0.03127400	Cu	2.67625700	-1.27212400	0.25587000
O	3.74111400	1.19214500	0.67582700	O	4.58722600	-1.46141100	0.01920200
9				TS9-10			
Charge=-1 Multiplicity =1				Charge=-1 Multiplicity =1			
O	0.30550800	-0.31299000	0.16903100	O	0.18031300	-1.34800800	-0.20425600
H	-5.85882600	0.43380400	-0.85782000	H	-5.35829300	0.82587400	-0.76345600
C	-5.06460100	-0.16651400	-1.32502000	C	-4.82457500	-0.08638400	-1.06946000
C	-5.01366100	-1.53686400	-0.64896200	C	-5.03413600	-1.16445900	-0.00628600
C	-3.70579200	0.57451300	-1.21880100	C	-3.31962100	0.22141900	-1.27653500

H	-5.33268900	-0.25900400	-2.38648700	H	-5.25774400	-0.38894800	-2.03277300
H	-4.20783900	-2.13255700	-1.09375900	H	-4.46683500	-2.06236100	-0.27900200
C	-4.77068800	-1.37654600	0.86210800	C	-4.56884600	-0.64717700	1.36376600
H	-5.94917000	-2.08803500	-0.82179000	H	-6.09240100	-1.45859100	0.04535500
N	-3.00263600	0.10361400	0.00941800	N	-2.59453100	-0.03699900	-0.00105600
C	-3.79092900	-0.21252800	1.22725600	C	-3.25036200	0.19461300	1.31010300
H	-4.38094100	-2.31994600	1.26410500	H	-4.43276400	-1.49806700	2.04319200
H	-5.72889300	-1.19487600	1.37010600	H	-5.36242800	-0.02504800	1.80245000
O	-1.97645100	1.04458700	0.33001400	O	-1.32282800	0.52622700	-0.03706300
C	-4.55908600	0.99277600	1.83096600	C	-3.53871000	1.69236300	1.59266100
H	-3.88252600	1.84622900	1.94580800	H	-2.63304300	2.28251300	1.41734900
H	-5.41197000	1.29960100	1.21576400	H	-4.34291100	2.08628300	0.96107400
H	-4.95049500	0.72860100	2.82323000	H	-3.84557300	1.82921000	2.63913100
C	-2.79974600	-0.71845000	2.29338000	C	-2.28724600	-0.31952700	2.39757300
H	-3.35556100	-1.14540500	3.13948500	H	-2.79575100	-0.31165300	3.37147900
H	-2.14603600	-1.48805700	1.87000300	H	-1.96802300	-1.34154000	2.16773100
H	-2.16593700	0.09192000	2.66276200	H	-1.39133900	0.30280200	2.46041000
C	-3.93735800	2.10193800	-1.28574800	C	-3.14474100	1.66320200	-1.80651400
H	-2.98426800	2.63656600	-1.26872500	H	-2.08811800	1.87484500	-1.98950000
H	-4.46344200	2.34859400	-2.21864900	H	-3.69802500	1.77861800	-2.74901600
H	-4.54517100	2.46473600	-0.45161700	H	-3.52407900	2.40747400	-1.09890100
C	-2.79763400	0.17251600	-2.40070700	C	-2.72514400	-0.75408300	-2.31548800
H	-1.79285800	0.58108000	-2.25733000	H	-1.63732400	-0.64790300	-2.35224600
H	-2.70443000	-0.91716700	-2.46784100	H	-2.94307400	-1.79324100	-2.04469500

H	-3.20228200	0.55138300	-3.34972500	H	-3.13977400	-0.55478500	-3.31378200
H	-1.12015800	0.51817600	0.25652300	H	-0.62192900	-0.38357400	-0.12964600
C	3.40914800	2.04397000	0.39305800	C	2.19156400	1.89200800	-0.07965900
C	4.92966100	2.38744100	0.49175800	C	3.44954400	2.78963300	0.14531400
C	5.66030600	1.09075700	0.02419400	C	4.66257400	1.81395200	0.01959700
C	4.50522000	0.19134300	-0.45378400	C	3.99912900	0.48596900	-0.39159000
H	2.81377100	2.44077500	1.22250600	H	1.33823700	2.15119100	0.55410400
H	2.98898200	2.45546900	-0.54411900	H	1.85788100	1.96628400	-1.13147100
H	5.20027400	2.64051100	1.52303900	H	3.41827400	3.24765600	1.14023200
H	5.18032500	3.25359300	-0.13244700	H	3.49179100	3.60394400	-0.58815800
H	6.39357400	1.27356800	-0.76762600	H	5.40488400	2.14578900	-0.71349800
H	6.18538200	0.60318700	0.85161800	H	5.17930400	1.68690200	0.97608400
H	4.29290000	0.43072500	-1.51837200	H	3.90668000	0.47246500	-1.49945100
N	3.38644100	0.59467500	0.38905500	N	2.68144700	0.56195400	0.22866500
C	4.63118800	-1.34431300	-0.40735000	C	4.63471100	-0.86866400	-0.02751100
O	5.72569100	-1.89883100	-0.54694300	O	5.85734300	-0.99954900	0.07925200
Cu	1.99978200	-0.70345100	0.11790000	Cu	1.90541200	-1.18271800	0.03437600
O	3.47922900	-1.92547200	-0.26599400	O	3.74419400	-1.80981900	0.08469300
10				11			
Charge=-1 Multiplicity =1				Charge=-1 Multiplicity =2			
O	2.48498000	3.29092200	-0.50180300	O	2.98446900	0.13157300	-0.29990400
H	-3.55664100	-2.19274600	1.40436200	H	3.45053500	0.23883800	0.54359400
C	-2.69863700	-1.81667100	0.82458200	C	-0.10227100	2.06048600	0.56395000
C	-1.96390400	-0.75880000	1.64880300	C	-0.95332700	2.18634200	-0.71977800
C	-3.21627200	-1.30134900	-0.53596300	C	-2.01479500	1.07646500	-0.53905600

H	-2.03232800	-2.66546600	0.63217800	C	-1.39720200	0.12518400	0.55675100
H	-1.03677100	-0.46070100	1.14948400	H	0.91236100	2.46188600	0.45628100
C	-2.88602000	0.43692500	1.88877500	H	-0.59626300	2.62967000	1.38188000
H	-1.66381800	-1.19418300	2.61128300	H	-0.32126700	1.97901700	-1.59272400
N	-3.87378900	0.04358700	-0.36179500	H	-1.39634500	3.18387200	-0.85478900
C	-3.38155900	1.10195700	0.58788900	H	-2.96923100	1.48874400	-0.18802600
H	-2.37994600	1.20609700	2.48755600	H	-2.22168600	0.54000400	-1.47167900
H	-3.76275500	0.10802000	2.46885300	H	-2.05406400	0.14166000	1.44315600
O	-4.59697600	0.45639300	-1.34558800	N	-0.06884500	0.64524700	0.89731800
C	-4.57258700	2.02236100	0.90629500	C	-1.32190600	-1.33465900	0.07025000
H	-4.90562600	2.56383200	0.01756400	O	-2.34219700	-2.03317200	0.03704900
H	-5.41993600	1.44426700	1.29371700	Cu	1.25543100	-0.44330500	-0.03224000
H	-4.26873200	2.74801400	1.67079300	O	-0.14135000	-1.72433500	-0.31922800
C	-2.26199800	1.92662100	-0.08494400				
H	-2.02803000	2.80049600	0.53563300				
H	-1.33801400	1.35790900	-0.21377400				
H	-2.60054600	2.28068700	-1.06459900				
C	-4.29095700	-2.26502900	-1.06945400				
H	-4.62845100	-1.97064600	-2.06636800				
H	-3.86750500	-3.27532700	-1.12130400				
H	-5.16239500	-2.28803400	-0.40394100				
C	-2.07266500	-1.19041000	-1.56807700				
H	-2.43816600	-0.68930100	-2.47133200				
H	-1.20371600	-0.65605800	-1.17834500				

H	-1.73128900	-2.19694200	-1.83657900	
H	2.38806600	3.53018000	-1.43641200	
C	5.07675800	-0.04331200	-0.08237400	
C	5.37790600	-1.47469300	0.47117400	
C	4.00281400	-2.21012100	0.40839300	
C	3.09161600	-1.16476700	-0.26842800	
H	5.65072400	0.74237000	0.42438400	
H	5.34968200	-0.01032100	-1.16182100	
H	5.74145900	-1.41487800	1.50381200	
H	6.15125000	-1.98245200	-0.12067800	
H	4.04596300	-3.15047800	-0.15292900	
H	3.62296300	-2.43982900	1.40926000	
H	3.17977600	-1.31217900	-1.37344900	
N	3.65815100	0.10839100	0.14318100	
C	1.58399700	-1.16349100	0.00573500	
O	0.95711500	-2.20690300	0.23139800	
Cu	2.39569700	1.48060600	-0.22957400	
O	1.05464100	0.02470300	-0.08573600	
12				TS₁₂₋₁₃
Charge=-1 Multiplicity =2				Charge=-1 Multiplicity =2
O	0.19522700	0.89783800	-1.38789100	O -0.29249900 -2.27788800 0.34583700
H	0.13691400	0.83490700	-2.35324500	H -0.41907700 -2.96035800 -0.33081400
C	-2.01623500	-2.03073200	-0.82655600	C -3.67731900 -1.64549300 -0.05970900
C	-2.24944700	-2.44225400	0.64029500	C -4.29944000 -0.89218300 1.13395500
C	-3.67182700	-1.91080300	0.89931200	C -4.59862500 0.49340900 0.52790600

C	-3.80319100	-0.69430900	-0.08157000	C	-3.57756900	0.61979900	-0.66216500
H	-0.95922400	-1.99092400	-1.11555800	H	-3.06844800	-2.50673700	0.23984200
H	-2.50581200	-2.77203400	-1.49297900	H	-4.49452800	-2.02997500	-0.70845600
H	-1.52062700	-1.93320500	1.28457400	H	-3.55605800	-0.81309000	1.93807100
H	-2.15585100	-3.52336400	0.81277400	H	-5.19348800	-1.38182200	1.54657500
H	-4.41545900	-2.67798000	0.64645500	H	-5.62707400	0.53294500	0.14573600
H	-3.84928200	-1.61789900	1.93897200	H	-4.49146300	1.31309700	1.24607500
H	-4.73914400	-0.79201000	-0.65472900	H	-4.14114100	0.84013000	-1.58448500
N	-2.64999700	-0.72706800	-0.99805200	N	-2.87547900	-0.66730000	-0.78044300
C	-3.89916100	0.65147900	0.67329300	C	-2.60031700	1.79996400	-0.45874100
O	-4.89840500	0.90173100	1.35339000	O	-3.02163500	2.96124200	-0.51814800
Cu	-1.50877500	0.81789000	-0.62175000	Cu	-1.04110700	-0.43814500	-0.30309200
O	-2.87290300	1.44464700	0.54473300	O	-1.36441700	1.47269100	-0.21104900
O	2.52239100	2.21036700	-0.92069700	O	1.06589100	-0.50087700	-0.36749400
C	3.09841700	1.76862300	0.29487200	C	1.83257000	0.35477300	0.44999200
H	3.93427900	2.45676500	0.48548400	H	1.51471200	1.38534200	0.23221500
H	1.63868000	1.76457900	-1.06434300	H	0.67588600	-1.52869100	0.05894500
C	3.68544800	0.35918400	0.20486900	C	3.32377800	0.24939200	0.12522500
C	2.93993200	-0.70131100	-0.33613400	C	3.83464100	-0.82060900	-0.61967100
C	4.97448100	0.09444100	0.68589700	C	4.22011800	1.22977000	0.58007600
C	3.47627400	-1.99031000	-0.38407200	C	5.20409900	-0.91886600	-0.88835100
H	1.94175300	-0.50422400	-0.72444600	H	3.13939900	-1.56272900	-0.99924700
C	5.51327100	-1.19639700	0.64122100	C	5.58809200	1.13836000	0.31284300
H	5.56798800	0.91024200	1.09748800	H	3.83999400	2.08104900	1.14292100

C	4.76308600	-2.24582400	0.10469700	C	6.08862700	0.05777000	-0.42210000
H	2.88535500	-2.80107200	-0.80576100	H	5.57974300	-1.75851400	-1.47049100
H	6.51817200	-1.37856300	1.01805100	H	6.26258400	1.91360600	0.67181400
H	5.17652000	-3.25163000	0.06423600	H	7.15315900	-0.01584300	-0.63519200
C	2.10739000	1.88288600	1.46675500	C	1.57998600	0.09210700	1.94830700
H	1.73620500	2.91184200	1.53730800	H	0.51756500	0.23570700	2.17392000
H	1.24865700	1.22008700	1.31191600	H	1.85645100	-0.93628300	2.21114300
H	2.58422700	1.61045000	2.41737100	H	2.16169100	0.77896400	2.57562100
13_gas				13_sol			
Charge=-1 Multiplicity =2				Charge=-1 Multiplicity =2			
O	1.36759100	-3.41129400	-0.19167200	O	1.10800500	-3.74863500	-1.00821600
H	0.98098300	-3.53063200	-1.07135300	H	1.34532500	-3.54580200	-1.92694700
C	-3.54690200	-1.58849600	-0.00046700	C	-3.64996300	-1.26967200	0.00853100
C	-4.64302700	-0.73818700	0.66803700	C	-4.50188500	-0.28632800	0.82618400
C	-4.83429800	0.39015000	-0.35801000	C	-4.53770100	0.93954900	-0.09815400
C	-3.40023700	0.61497400	-0.89050800	C	-3.12980100	0.93244400	-0.74628100
H	-2.96991400	-2.19806900	0.70879700	H	-3.16229200	-2.04407600	0.61564900
H	-4.00998300	-2.29911900	-0.71331900	H	-4.28998200	-1.79992200	-0.72078700
H	-4.27454600	-0.32819400	1.61768600	H	-3.99559300	-0.04170200	1.76975400
H	-5.56180500	-1.30243000	0.87517400	H	-5.49786400	-0.67691400	1.06536300
H	-5.49251800	0.04901500	-1.16967300	H	-5.30457800	0.80224300	-0.87114300
H	-5.25351900	1.31067800	0.05774900	H	-4.74681500	1.88062300	0.41866500
H	-3.42267900	0.90692300	-1.95197000	H	-3.18667200	1.28858400	-1.78643900
N	-2.67493900	-0.65963100	-0.72529800	N	-2.64778000	-0.46295000	-0.70483400
C	-2.65951900	1.77474200	-0.15056300	C	-2.13134700	1.88610000	-0.03619600

O	-3.21720500	2.87090400	-0.03396900	O	-2.41858100	3.08771400	0.09329000
Cu	-0.91976900	-0.37529400	-0.16658300	Cu	-0.86555500	-0.59018400	-0.15066600
O	-1.46742100	1.49197200	0.27591500	O	-1.01674700	1.35814800	0.35938600
O	0.88786200	-0.75548100	0.13811200	O	0.84998300	-1.32070700	0.14853400
C	1.68250100	0.12505600	0.89104300	C	1.75121100	-0.74230300	1.05849500
H	1.19540200	1.11183700	0.95402400	H	1.21184000	-0.10504500	1.78064400
H	1.21225600	-2.44523300	0.00861400	H	1.06451300	-2.85979500	-0.55152600
C	3.05309900	0.34527300	0.24599700	C	2.78967800	0.15354600	0.37364600
C	3.74130100	-0.70304100	-0.38465100	C	3.12091800	-0.01394700	-0.97802500
C	3.66647900	1.60508300	0.29910000	C	3.45687500	1.15081700	1.10416700
C	5.00983900	-0.49532600	-0.93328300	C	4.09841700	0.78527600	-1.58321800
H	3.27281400	-1.68073200	-0.45168400	H	2.59622500	-0.76866100	-1.55688300
C	4.93568900	1.81798300	-0.24933000	C	4.43353000	1.95279800	0.50533600
H	3.13610100	2.43350900	0.76657500	H	3.20480600	1.30544600	2.15244200
C	5.61541500	0.76483600	-0.86805200	C	4.76064400	1.77132600	-0.84408000
H	5.52669500	-1.32152700	-1.41869800	H	4.33925600	0.64021800	-2.63442900
H	5.38720900	2.80752800	-0.20250700	H	4.93398500	2.72254800	1.08910500
H	6.60108800	0.92516400	-1.30100800	H	5.51735600	2.39553900	-1.31385400
C	1.85306100	-0.39769200	2.33427700	C	2.46031000	-1.84116200	1.87487300
H	0.86617700	-0.49464600	2.80271100	H	1.71499500	-2.45957200	2.39076900
H	2.33074900	-1.38543600	2.32554800	H	3.05318800	-2.49031600	1.21817100
H	2.46632700	0.28137100	2.94269700	H	3.13126500	-1.41024300	2.62897700
TS13-14_gas				TS13-14_sol			
Charge=-1 Multiplicity =2				Charge=-1 Multiplicity =2			
O	-1.75842200	4.06164500	0.01714300	O	-2.43185400	3.60622000	-0.29345900

H	-0.93759000	4.53343000	0.22038100	H	-3.23105400	3.21787500	-0.68449500
C	0.88102900	-2.01882900	-0.87430800	C	0.95891600	-1.89257200	-1.03998300
C	2.17355400	-2.83977000	-0.68095100	C	2.27664800	-2.68242300	-0.94956900
C	2.67064300	-2.37442200	0.69701500	C	2.75743400	-2.35863500	0.47238600
C	2.28151400	-0.88628900	0.69328100	C	2.33732500	-0.88561800	0.63575600
H	0.67178900	-1.79432100	-1.92881200	H	0.70312700	-1.59579700	-2.06522300
H	0.00712600	-2.56951700	-0.48894900	H	0.12339800	-2.50459100	-0.66345400
H	2.91120400	-2.57192100	-1.44816400	H	2.99683700	-2.30546200	-1.68803600
H	2.00152700	-3.92183600	-0.74364600	H	2.13904700	-3.75448600	-1.13090800
H	2.12923200	-2.90309300	1.49480400	H	2.22103100	-2.97960500	1.20196800
H	3.74444300	-2.51022500	0.84731300	H	3.83053200	-2.50270700	0.62014200
H	2.09656700	-0.50556600	1.70942000	H	2.11615700	-0.63859900	1.68531100
N	1.05055100	-0.77106200	-0.10667500	N	1.12338000	-0.69991800	-0.18278100
C	3.42010800	0.05107200	0.11087800	C	3.45918200	0.13647600	0.21884800
O	4.59680100	-0.27858700	0.29926900	O	4.64107300	-0.14462200	0.48088400
Cu	1.12606700	1.37243600	-0.54590000	Cu	1.15595000	1.46763500	-0.45913400
O	3.02944300	1.13066500	-0.48543300	O	3.08309000	1.24625300	-0.32811400
O	-0.70827800	1.50840600	-0.10159800	O	-0.70524500	1.52277100	-0.04048100
C	-1.10212000	0.50076200	0.74185500	C	-1.04742500	0.46588100	0.77193600
H	-0.10590700	-0.37752700	0.51459700	H	-0.04534300	-0.36937200	0.47220100
H	-1.46980200	3.11432300	-0.03922400	H	-1.80247900	2.83956500	-0.19731200
C	-2.34647400	-0.21079900	0.31545100	C	-2.29775500	-0.24785500	0.36302400
C	-2.85028900	-0.02653800	-0.98985200	C	-2.78080700	-0.13117400	-0.95956300
C	-3.02816400	-1.12476700	1.14930700	C	-3.00869700	-1.09910100	1.23961300

C	-3.97394100	-0.72157400	-1.43800000	C	-3.91392500	-0.82856200	-1.38473800
H	-2.34287600	0.68529800	-1.63259000	H	-2.25275100	0.52087600	-1.64867800
C	-4.15225100	-1.81996200	0.69979300	C	-4.14248600	-1.79610300	0.81325700
H	-2.67518500	-1.29939900	2.16223200	H	-2.67740900	-1.22139900	2.26687800
C	-4.63549400	-1.62670200	-0.59957900	C	-4.60462600	-1.66885600	-0.50241300
H	-4.34067000	-0.55117100	-2.44910000	H	-4.26074300	-0.71486700	-2.41015800
H	-4.65516900	-2.51573300	1.36983200	H	-4.66911900	-2.44009300	1.51490000
H	-5.51241300	-2.16768100	-0.94932200	H	-5.48737000	-2.21159000	-0.83226200
C	-0.99425100	0.87091500	2.22512900	C	-0.87863000	0.75797700	2.26464200
H	-0.00669800	1.30594000	2.41518600	H	0.08440800	1.25505000	2.42792400
H	-1.75068600	1.62314900	2.49848100	H	-1.66893300	1.43083900	2.63584400
H	-1.11423800	0.00701700	2.89022000	H	-0.89298400	-0.14923000	2.87991900
14a				14a			
Charge=-1 Multiplicity =3				Charge=-1 Multiplicity =1			
H	-2.05697500	-0.45087100	-0.75170800	H	3.96638000	-2.39580900	-1.52470700
C	-3.10103400	-0.76831300	-0.83970400	C	3.35225500	-1.76170900	-0.86915200
C	-3.96650200	0.45321500	-1.21886700	C	3.55138100	-2.18539300	0.59908600
C	-3.49618800	-1.46281000	0.47939400	C	1.87338000	-1.84552500	-1.35913500
H	-3.14495000	-1.52525700	-1.63367900	H	3.71906800	-0.73607000	-0.99694900
H	-4.02768900	0.51049000	-2.31273400	H	3.39921100	-1.32078200	1.25689500
C	-5.38346100	0.40894200	-0.61274900	C	2.57007200	-3.29222800	0.98691500
H	-3.46383000	1.36486300	-0.88146400	H	4.58719900	-2.51779600	0.75713200
N	-4.96239600	-1.79033000	0.43088600	N	0.98474300	-1.75513100	-0.15998600
C	-5.94877100	-1.00492500	-0.37463200	C	1.09673800	-2.81500700	0.90304100
H	-6.09103100	0.95098100	-1.25306700	H	2.76508500	-3.64599000	2.00877100

H	-5.38616200	0.93440200	0.34883800	H	2.72408000	-4.15851200	0.32951300
O	-5.39819800	-2.81283900	1.08088500	O	-0.32234800	-1.58242100	-0.52036000
C	-7.25958900	-0.90839500	0.42470400	C	0.15394200	-4.01493400	0.66036600
H	-7.68490600	-1.89798700	0.60253000	H	-0.88500400	-3.68013900	0.60836200
H	-7.08615600	-0.43255200	1.39504000	H	0.38718800	-4.53845900	-0.27101300
H	-7.98064600	-0.30212500	-0.13515800	H	0.25901500	-4.73240700	1.48607800
C	-6.21439000	-1.75116200	-1.70142500	C	0.69287500	-2.15913100	2.23979600
H	-7.00751200	-1.24498300	-2.26472400	H	0.67062800	-2.91151200	3.03891200
H	-5.32169900	-1.78966100	-2.33120400	H	1.39530900	-1.37013800	2.52909700
H	-6.53563600	-2.77633400	-1.49221000	H	-0.30547300	-1.71834100	2.16226200
C	-3.20934700	-0.57299600	1.70836200	C	1.62890500	-3.12664700	-2.20124000
H	-3.56275400	-1.07110200	2.61754000	H	0.55795600	-3.23946100	-2.39884600
H	-2.13224400	-0.39848700	1.78670700	H	2.15115300	-3.03964300	-3.16391900
H	-3.68332600	0.40753400	1.63134900	H	1.99520600	-4.03530900	-1.71344400
C	-2.71359400	-2.77846000	0.61458900	C	1.57772300	-0.64306400	-2.27246800
H	-2.94755100	-3.28401400	1.55349700	H	0.59791800	-0.74108700	-2.74681300
H	-2.95041300	-3.46175300	-0.20739500	H	1.58654700	0.29331800	-1.71129600
H	-1.64286000	-2.55417200	0.58493200	H	2.34560800	-0.59418600	-3.05656800
C	3.92796800	-0.64884400	0.73759800	C	0.91239900	1.29299500	0.83859700
O	3.05378000	-0.13680200	-0.21543800	O	-0.18697800	1.28887300	-0.01053800
C	2.66661800	3.67833600	0.06120900	C	-2.76831600	2.44381100	0.57819100
C	1.94380500	4.26814100	-1.16695100	C	-3.92152800	2.85437200	-0.39008900
C	0.51012100	4.47280800	-0.63783000	C	-4.48065900	1.51030300	-0.89203800
C	0.38675800	3.43588700	0.53875300	C	-4.12193900	0.55587400	0.27470400

H	3.58341600	3.13257200	-0.18670400	H	-1.77475900	2.72556000	0.21034900
H	2.95784200	4.50646100	0.74051300	H	-2.89093600	2.94486300	1.55603000
H	1.95563700	3.53454200	-1.98251700	H	-3.57007900	3.49578500	-1.20843900
H	2.39840300	5.19510100	-1.54018300	H	-4.69981500	3.41306400	0.14828500
H	0.38154700	5.49134000	-0.25324700	H	-5.55439000	1.52935200	-1.11039500
H	-0.25870300	4.31807200	-1.40067100	H	-3.95451800	1.18379600	-1.79871700
H	0.08417500	3.97265700	1.45225800	H	-4.88482200	0.67185400	1.06621300
N	1.70305200	2.80840700	0.72587100	N	-2.81570500	0.99314900	0.77051000
C	-0.70891700	2.38877200	0.26851900	C	-4.06290000	-0.90477200	-0.15712800
O	-1.90126800	2.72002000	0.29040500	O	-5.07784700	-1.59293700	-0.29091300
Cu	1.61892900	0.97220500	0.11123600	Cu	-1.42925500	-0.11162500	-0.01544400
O	-0.28642100	1.18496500	0.00229400	O	-2.84996400	-1.31977000	-0.40555900
C	4.80087300	-1.75626200	0.13499400	C	1.97705400	2.27293400	0.33017400
C	5.55901500	-2.60731700	0.95384000	C	3.27135100	2.27041200	0.87538400
C	4.86450300	-1.93743700	-1.25210700	C	1.68484700	3.20472800	-0.67446200
C	6.37035100	-3.60350500	0.40465400	C	4.24285400	3.17427100	0.43840000
H	5.50852400	-2.49387800	2.03533400	H	3.52405000	1.54631900	1.64854600
C	5.67693000	-2.93140200	-1.80733600	C	2.65319100	4.11334200	-1.11490700
H	4.25297600	-1.29043400	-1.87210400	H	0.69070500	3.19061100	-1.10958400
C	6.43532500	-3.76846100	-0.98343900	C	3.93652800	4.10506000	-0.56087400
H	6.94645300	-4.25442700	1.05855000	H	5.24051200	3.14868000	0.87339600
H	5.71183400	-3.05789600	-2.88722100	H	2.40470300	4.82724100	-1.89840500
H	7.06268900	-4.54470300	-1.41482100	H	4.69098600	4.80938600	-0.90577000
C	4.81973400	0.46458400	1.33470400	C	0.51567300	1.66093600	2.28971300

H	5.41230800	0.92809500	0.53758100	H	0.08351500	2.66848500	2.31733100
H	4.18512200	1.23332500	1.78766200	H	-0.24026900	0.95826100	2.65572600
H	5.50561000	0.07645200	2.09829500	H	1.37894100	1.63412600	2.96894600
H	3.38059700	-1.11185800	1.58419600	H	1.38636500	0.29221900	0.84893300
TS14a-15a_N				TS14a-15a_N			
Charge=-1 Multiplicity =3				Charge=-1 Multiplicity =1			
H	4.14172800	0.09383900	-2.18839000	H	4.55837800	-1.10138600	-1.30043000
C	3.50018300	0.27530900	-1.31515800	C	3.77193900	-0.71269600	-0.63926700
C	4.30437900	0.03060000	-0.02241800	C	3.97558100	-1.25514400	0.79057500
C	2.23981900	-0.62257200	-1.46580600	C	2.40376300	-1.08731300	-1.27266500
H	3.20333400	1.32878300	-1.36250100	H	3.88151200	0.37751300	-0.63075600
H	3.91867200	0.66944100	0.78199600	H	3.61040800	-0.52072000	1.51844600
C	4.22038900	-1.43321000	0.41609000	C	3.23604200	-2.57902800	1.00262500
H	5.35223200	0.32423200	-0.17090300	H	5.04701800	-1.38193500	0.99431000
N	1.75991000	-1.01785100	-0.05749700	N	1.38495700	-1.26190600	-0.13256400
C	2.77043400	-1.85522600	0.76568300	C	1.70005500	-2.42332900	0.85259800
H	4.84884000	-1.60692700	1.30027200	H	3.43961600	-2.97312800	2.00724900
H	4.62551500	-2.07457600	-0.37660900	H	3.61678200	-3.33026900	0.29957700
O	0.57108300	-1.67580300	-0.11103900	O	0.13139700	-1.41401000	-0.64666100
C	2.56279300	-3.36344000	0.53240800	C	1.04606500	-3.73407600	0.38110900
H	1.56820400	-3.66767200	0.86375500	H	-0.04016500	-3.63216200	0.34658600
H	2.67667000	-3.65923800	-0.51079200	H	1.38435500	-4.05734400	-0.60354900
H	3.31753000	-3.90229600	1.12121400	H	1.30902600	-4.51888500	1.10276500
C	2.49229700	-1.58098300	2.25162300	C	1.08469400	-2.06746200	2.21496900
H	2.98469400	-2.35082100	2.85858800	H	1.06848100	-2.96774100	2.84112900

H	2.88350000	-0.61080400	2.56436300	H	1.66659600	-1.30800900	2.73912900
H	1.41780800	-1.61019100	2.45185700	H	0.05653400	-1.71045700	2.10662500
C	2.52234400	-1.86941500	-2.33151500	C	2.49701000	-2.35709600	-2.14436200
H	1.67064900	-2.55351400	-2.28631900	H	1.49583700	-2.67915500	-2.44361700
H	2.64220000	-1.54274900	-3.37169200	H	3.06149300	-2.10594400	-3.05076300
H	3.43489500	-2.40337300	-2.05467100	H	3.01617900	-3.18875100	-1.66311700
C	1.11362600	0.14446100	-2.17224800	C	1.91439700	0.03436200	-2.19873300
H	0.23616400	-0.48705300	-2.33204500	H	0.98143700	-0.25053300	-2.69032900
H	0.80771400	1.02829800	-1.61444500	H	1.75574800	0.97079800	-1.66761500
H	1.48977500	0.48277100	-3.14669400	H	2.68271100	0.20778200	-2.96317100
C	0.71137900	1.14529500	1.36442200	C	0.78269300	1.15914000	1.15654600
O	-0.39128400	0.42916100	1.55779800	O	-0.53888900	0.96299500	1.04981400
C	-3.59068700	-0.23122700	2.00913400	C	-3.31247000	1.09473600	1.65940300
C	-4.36644000	0.89794600	1.28091600	C	-4.52235500	1.80151300	0.97890300
C	-4.74954400	0.26392700	-0.08225800	C	-4.67390100	1.04824200	-0.35280400
C	-4.00207800	-1.11797100	-0.09573200	C	-4.18048700	-0.36835800	0.03085500
H	-2.81398900	0.14208100	2.68485700	H	-2.39166900	1.70498000	1.62296600
H	-4.30591800	-0.82433400	2.61865100	H	-3.50705500	0.92417700	2.73468600
H	-3.70954800	1.76450900	1.13778000	H	-4.36143200	2.88008400	0.84977100
H	-5.24152000	1.24211300	1.85026200	H	-5.43197800	1.67700000	1.58425700
H	-5.83121200	0.12377000	-0.19196900	H	-5.69447300	1.04921100	-0.75214500
H	-4.42253000	0.88796500	-0.92167400	H	-4.00821300	1.47146900	-1.11750700
H	-4.74348400	-1.91430200	0.09748400	H	-5.01541700	-0.89648300	0.52936500
N	-3.01716500	-1.07828000	0.98040200	N	-3.07731900	-0.16766200	0.97288600

C	-3.34929800	-1.40472900	-1.46379700	C	-3.74997000	-1.20187900	-1.18434000
O	-4.06535700	-1.72397700	-2.42471200	O	-4.60086300	-1.70879200	-1.92843100
Cu	-1.24568800	-0.85412000	0.27074300	Cu	-1.39480900	-0.42539500	0.04777400
O	-2.06425900	-1.24473200	-1.50492300	O	-2.46575400	-1.28183700	-1.35337800
C	0.60381300	2.34291200	0.44730300	C	1.32073000	2.28463200	0.33985600
C	1.68904600	3.21453900	0.22173400	C	2.63193900	2.78793800	0.51162000
C	-0.61355500	2.64077000	-0.19337800	C	0.51458200	2.91697300	-0.63433000
C	1.56803500	4.32271700	-0.61892200	C	3.11422900	3.84798700	-0.25801300
H	2.64486700	3.02299100	0.70370800	H	3.28439300	2.34480500	1.26024000
C	-0.73735800	3.74928300	-1.03248900	C	0.99703500	3.97710100	-1.40074900
H	-1.46000500	1.98306600	-0.02523700	H	-0.49934700	2.55474400	-0.76943700
C	0.35228100	4.59767200	-1.25583500	C	2.30299100	4.45297300	-1.22581700
H	2.42592000	4.97440200	-0.77683900	H	4.12966200	4.20786500	-0.09711800
H	-1.69126900	3.94859300	-1.51666700	H	0.34593000	4.44030700	-2.14050700
H	0.25692400	5.45878700	-1.91376100	H	2.67795900	5.28008000	-1.82477700
C	1.41996700	1.50889400	2.68705800	C	1.24417800	1.19988300	2.62687800
H	0.91553300	2.37482700	3.14151400	H	1.07760300	2.20715400	3.04365900
H	1.34211500	0.67384500	3.38567000	H	0.64524300	0.50245500	3.21598700
H	2.47793700	1.77289700	2.56461600	H	2.30577100	0.96181600	2.77716400
H	1.48936000	0.14252700	0.62485900	H	1.34752600	-0.17734100	0.49332500
TS14a-15a_O				TS14a-15a_O			
Charge=-1 Multiplicity =3				Charge=-1 Multiplicity =1			
H	3.06434400	-3.55367200	-2.03441600	H	3.93732000	-2.19829800	-2.30849800
C	3.22701700	-2.69847700	-1.36580000	C	3.80008200	-1.50510800	-1.46885600
C	3.78089000	-3.20581500	-0.02489800	C	4.41044100	-2.10724600	-0.18857900

C	1.87927000	-1.91114500	-1.24658400	C	2.27325500	-1.18227000	-1.35803000
H	3.97995900	-2.06551200	-1.85006000	H	4.34670600	-0.59025900	-1.72717600
H	4.31257200	-2.39773700	0.49131500	H	4.75849200	-1.30162700	0.46833700
C	2.63958000	-3.71159000	0.85648500	C	3.38306100	-2.95624800	0.56117400
H	4.51490300	-4.00291100	-0.20272200	H	5.29379800	-2.70891800	-0.43969600
N	1.68842300	-1.52937000	0.18621900	N	1.99098000	-0.98878400	0.09380600
C	1.68142400	-2.56560600	1.26531800	C	2.18385900	-2.10700800	1.06135600
H	3.02227000	-4.18795700	1.76806100	H	3.83997300	-3.44779000	1.42940600
H	2.08336100	-4.48687600	0.31330400	H	3.02453200	-3.75980000	-0.09301700
O	0.64794700	-0.65386600	0.35410700	O	0.81673600	-0.27277800	0.34736700
C	0.27391700	-3.12595200	1.56033700	C	0.94543700	-3.00676000	1.25358400
H	-0.40095100	-2.33059000	1.88317200	H	0.13235400	-2.46467100	1.74270800
H	-0.16632600	-3.60073200	0.68080400	H	0.55829600	-3.38743600	0.30765100
H	0.33992600	-3.87713100	2.35769400	H	1.21437700	-3.85744800	1.89288800
C	2.21241700	-1.86965500	2.53619100	C	2.54089500	-1.46460300	2.41862700
H	2.17433300	-2.55398600	3.39240800	H	2.65029800	-2.23863000	3.18768900
H	3.24667700	-1.53603500	2.39937200	H	3.47574300	-0.89750400	2.35597100
H	1.59866400	-0.99500200	2.76651300	H	1.74936000	-0.78082800	2.73377200
C	0.69688900	-2.73410800	-1.81264700	C	1.42588000	-2.28253100	-2.04419400
H	-0.25753100	-2.23213600	-1.62831800	H	0.35867400	-2.14419100	-1.85393800
H	0.81599300	-2.85145800	-2.89712400	H	1.59740300	-2.24388100	-3.12775000
H	0.65326000	-3.73938400	-1.38197100	H	1.70274300	-3.28758500	-1.71243000
C	1.99338900	-0.60660500	-2.05546000	C	1.99973300	0.15012500	-2.07595700
H	1.05070100	-0.05651100	-2.06048400	H	0.93104700	0.36539800	-2.12956000

H	2.76862900	0.04213400	-1.63540100	H	2.49315400	0.98118000	-1.56289300
H	2.26180200	-0.84683500	-3.09094800	H	2.39083500	0.09004700	-3.09827700
C	0.65783600	1.84005000	0.68876100	C	0.19418400	1.93189300	1.27841900
O	-0.42661500	1.92827600	-0.11288500	O	-1.03223000	1.42356400	1.10427900
C	-3.86131500	1.78093200	1.08630000	C	-3.83329700	0.68040500	1.11430400
C	-4.92665900	1.86724300	-0.02380900	C	-4.84469100	0.81434000	-0.06922600
C	-5.44159800	0.41743600	-0.08538200	C	-4.42429500	-0.29951100	-1.04773500
C	-4.21207300	-0.43719600	0.37987700	C	-3.74016200	-1.32357600	-0.10369300
H	-3.12867600	2.59507500	1.06446200	H	-3.15297500	1.54258000	1.19841500
H	-4.36562400	1.82612200	2.07399500	H	-4.37435900	0.63078400	2.07747300
H	-4.44755200	2.14982200	-0.96954500	H	-4.81942500	1.80957100	-0.52895000
H	-5.72019700	2.59662300	0.18514100	H	-5.87216500	0.64477900	0.27936200
H	-6.27697600	0.28255000	0.61286600	H	-5.25873900	-0.73193800	-1.60972500
H	-5.79497100	0.11596600	-1.07561800	H	-3.68730300	0.07373700	-1.77008100
H	-4.53878900	-1.14593300	1.15703000	H	-4.52818800	-1.94562600	0.35938400
N	-3.20382000	0.48646900	0.92915300	N	-3.05244200	-0.53100400	0.91257800
C	-3.64200100	-1.30101600	-0.76940000	C	-2.77296700	-2.26159700	-0.83825500
O	-4.31161100	-2.23418300	-1.22332400	O	-3.19068600	-3.22860900	-1.48305800
Cu	-1.64190700	0.47470400	-0.23858100	Cu	-1.20106200	-0.37680300	0.37426100
O	-2.46091000	-0.95955900	-1.20084300	O	-1.51503700	-1.92445100	-0.74219700
C	1.85365200	2.60545900	0.20317600	C	0.59944800	3.02233000	0.34567200
C	3.05252200	2.68157200	0.94174800	C	1.75878900	3.80436000	0.54933300
C	1.81358800	3.24982000	-1.04903100	C	-0.16797700	3.29210000	-0.80879200
C	4.16032000	3.37517900	0.45189400	C	2.13225300	4.79835900	-0.35663600

H	3.12385600	2.18545900	1.90513400	H	2.37867700	3.63196500	1.42383700
C	2.92028200	3.94579300	-1.53709500	C	0.20786400	4.28456900	-1.71266400
H	0.89083100	3.19080500	-1.61571700	H	-1.06866700	2.70977400	-0.96921200
C	4.10303600	4.01427500	-0.79212400	C	1.36246100	5.04768500	-1.49830000
H	5.07270400	3.41554100	1.04281700	H	3.03110900	5.38209400	-0.16900000
H	2.85982800	4.43966600	-2.50458300	H	-0.40706700	4.46739100	-2.59133900
H	4.96562600	4.55496200	-1.17349000	H	1.65457800	5.82082800	-2.20425400
C	0.34126700	1.95960100	2.18627400	C	0.60997500	2.05900300	2.74727700
H	0.03152500	2.98786300	2.42270100	H	0.12075300	2.92574100	3.21903500
H	-0.48682200	1.28881800	2.43170000	H	0.28408600	1.16232700	3.28175400
H	1.19460000	1.70461400	2.82331300	H	1.69147900	2.16526000	2.88565600
H	0.96875900	0.55179400	0.55861300	H	0.91847700	0.83470000	0.79010000
15a				15a			
Charge=-1 Multiplicity =3				Charge=-1 Multiplicity =1			
H	5.00827700	-1.66384600	2.14843500	H	4.53375000	-1.78635100	2.31816600
C	5.16122400	-2.28324000	1.25470600	C	4.42847100	-2.54755900	1.53358500
C	6.59562200	-2.09980200	0.75893800	C	5.78265500	-2.75573300	0.85522100
C	4.12260600	-1.90334000	0.16611200	C	3.33441800	-2.11344100	0.52023300
H	4.97875500	-3.32017300	1.56407000	H	4.09407300	-3.46367900	2.03782400
H	6.74480100	-2.69458300	-0.14928900	H	5.67822300	-3.50244900	0.05975700
C	6.87480000	-0.61574200	0.46256700	C	6.29768200	-1.43152200	0.26190100
H	7.31168700	-2.47282300	1.50343500	H	6.51484600	-3.15505200	1.57066400
N	4.74544500	-0.87657600	-0.71710900	N	4.01024200	-1.40439300	-0.60150700
C	5.65452700	0.15116500	-0.15176400	C	5.16967100	-0.51802900	-0.32820000
H	7.73140600	-0.54150000	-0.21808200	H	7.03262100	-1.65444500	-0.52145400

H	7.16929200	-0.10612600	1.38927400	H	6.83219300	-0.86521100	1.03640500
O	3.78840300	-0.32794600	-1.61502700	O	3.06152300	-0.82117800	-1.48522100
C	5.02041500	1.09825400	0.90325200	C	4.88815400	0.68293300	0.61390900
H	4.10404300	1.55994400	0.52548000	H	4.02091700	1.25653800	0.27452700
H	4.78761800	0.57729800	1.83701000	H	4.71056200	0.36208000	1.64494700
H	5.72921500	1.90030200	1.14714200	H	5.76051700	1.35032400	0.62788700
C	6.15609500	1.01728300	-1.32419000	C	5.64856600	0.04510000	-1.68033900
H	6.97385600	1.66097000	-0.97719900	H	6.61804200	0.54078500	-1.54345200
H	6.52684300	0.37833300	-2.13205200	H	5.76298500	-0.76631100	-2.40646000
H	5.36070000	1.64794800	-1.72651200	H	4.93793600	0.76826300	-2.08515500
C	2.79545400	-1.48348200	0.83761600	C	2.23652300	-1.31023300	1.25347400
H	2.01319700	-1.27347500	0.10445700	H	1.42912500	-1.00850200	0.58183900
H	2.44567300	-2.30188000	1.47969500	H	1.80858500	-1.93528900	2.04889000
H	2.91424000	-0.59541000	1.46287200	H	2.63276700	-0.40434300	1.71846600
C	3.84301300	-3.12276800	-0.73900000	C	2.68210200	-3.36409300	-0.11009500
H	3.21873000	-2.81900900	-1.58285100	H	2.01063600	-3.05721800	-0.91574300
H	4.77703500	-3.53385800	-1.13687700	H	3.44410300	-4.02721800	-0.53449000
H	3.32111900	-3.90856700	-0.17906500	H	2.10625200	-3.92118000	0.63981600
C	-4.10857100	-0.95003700	0.15835400	C	-3.52813800	-0.88905500	-0.22803800
H	3.15521600	0.26090400	-1.13283500	H	2.63127000	-0.01204100	-1.07746900
O	-3.60162800	0.13935700	-0.38917700	O	-3.51954100	0.34770500	-0.01791000
C	-2.16516300	3.23384000	0.66978800	C	-1.41530500	4.62511300	0.24780400
C	-1.24104000	3.12553600	1.89893300	C	-0.15557400	5.02242400	1.07728800
C	0.16348800	3.25545800	1.27523900	C	0.91854700	3.98771600	0.64022100

C	-0.03625400	2.78357900	-0.20915000	C	0.18579900	3.11712900	-0.42592900
H	-3.16145500	2.80440400	0.81584800	H	-2.35368400	4.77840500	0.79380100
H	-2.30548700	4.30089900	0.40683700	H	-1.45898300	5.27659600	-0.65627900
H	-1.36938700	2.14118800	2.36526200	H	-0.36423900	4.93813000	2.15028500
H	-1.44168800	3.88653300	2.66278100	H	0.15352800	6.05829100	0.88346500
H	0.50100500	4.29777700	1.29251600	H	1.82192000	4.45205100	0.23236200
H	0.92234400	2.66321900	1.79429200	H	1.22680800	3.35869100	1.48150600
H	0.32217300	3.57040100	-0.89054100	H	0.40073900	3.56965600	-1.42004100
N	-1.47367600	2.56339500	-0.42579600	N	-1.22126300	3.24067600	-0.10164400
C	0.77609000	1.52026000	-0.53952900	C	0.69377100	1.66296900	-0.52696500
O	2.01620000	1.59770200	-0.60565100	O	1.93824800	1.51901400	-0.70458100
Cu	-1.79434800	0.62870000	-0.56731000	Cu	-2.24914500	1.72569600	-0.08303100
O	0.10447100	0.42883400	-0.70609800	O	-0.15682100	0.72712300	-0.44630600
C	-5.51444500	-1.17536300	0.07100200	C	-4.81052100	-1.60796200	-0.07581800
C	-6.18190700	-2.31754000	0.62152200	C	-4.91726600	-2.99757500	-0.29242800
C	-6.34568800	-0.21942500	-0.60295500	C	-5.97169800	-0.89512300	0.29474200
C	-7.55645300	-2.47972700	0.50801600	C	-6.14138100	-3.64975500	-0.14308900
H	-5.61181900	-3.08174700	1.14026500	H	-4.04149300	-3.57034200	-0.57794200
C	-7.71665500	-0.39773000	-0.70740000	C	-7.19034000	-1.54984700	0.44285100
H	-5.86544700	0.65256900	-1.03243000	H	-5.88789600	0.17353500	0.45991400
C	-8.35048800	-1.52710300	-0.15549700	C	-7.28379600	-2.93155200	0.22489500
H	-8.02206500	-3.36327700	0.94098100	H	-6.20344500	-4.72117900	-0.31417400
H	-8.31060500	0.35177500	-1.22763600	H	-8.07369000	-0.98485800	0.72879200
H	-9.42527000	-1.66127100	-0.24094600	H	-8.23644600	-3.44112500	0.34092500

C	-3.14825700	-1.89030000	0.83982900	C	-2.27589200	-1.62132600	-0.62683300
H	-2.58091900	-1.35587400	1.61605300	H	-2.05531900	-2.42571700	0.08637700
H	-3.63112400	-2.74959700	1.31020800	H	-2.40315800	-2.09173600	-1.61082300
H	-2.40832200	-2.27371300	0.12100600	H	-1.42767600	-0.93302900	-0.66139900
15				16			
Charge=-1 Multiplicity =2				Charge=-1 Multiplicity =1			
C	2.18098500	2.47662900	-0.35622900	C	-1.35622600	2.36169600	1.97874900
C	2.56980900	2.36131500	1.12688500	C	-1.84712400	3.81135700	1.78136000
C	3.65655300	1.25099900	1.15273200	C	-2.29729100	3.84886200	0.31256700
C	3.63757200	0.61689800	-0.27185400	C	-1.26565100	2.94140900	-0.37353500
H	1.14330900	2.79484100	-0.50699300	H	-0.49068600	2.31437000	2.64749100
H	2.84424800	3.20030900	-0.87072700	H	-2.14290300	1.71845800	2.38748000
H	1.69507600	2.05200800	1.70841800	H	-1.02242500	4.51923800	1.93434100
H	2.92523500	3.31492600	1.53483600	H	-2.64596000	4.07218300	2.48622500
H	4.65269500	1.64630400	1.37584600	H	-3.29985700	3.41400000	0.21147200
H	3.42747100	0.49782200	1.91338200	H	-2.29185600	4.85187400	-0.12081900
H	4.50752900	0.97957300	-0.84220800	H	-1.67590200	2.48588200	-1.28258200
N	2.37037100	1.10552400	-0.83408300	N	-1.00747000	1.84038800	0.60996200
C	3.74546800	-0.92967800	-0.22362900	C	0.03177500	3.69989300	-0.81666900
O	4.88838800	-1.41003900	-0.21789700	O	-0.12393200	4.79960500	-1.37506200
Cu	0.91230900	-0.84166700	-0.16646000	Cu	0.85832500	1.23846000	0.36278800
O	2.64786900	-1.60192400	-0.15100300	O	1.14598400	3.09543200	-0.61144400
H	2.34109200	1.02964600	-1.84860000	H	-1.67701300	1.06024500	0.41482300
C	-1.97495700	-0.92075500	0.11829300	C	3.31199300	-0.00933400	-0.47538400
O	-0.86435700	-0.27803600	-0.15011200	O	2.41931800	0.12785700	0.40236700

C	-3.22290900	-0.23472500	0.04348800	C	4.46847200	-0.86324000	-0.16879300
C	-4.47681500	-0.87070700	0.32434600	C	5.48421800	-1.14127300	-1.11205900
C	-3.27935700	1.15046600	-0.32462600	C	4.56991100	-1.45445600	1.11412400
C	-5.67708900	-0.17517100	0.24156900	C	6.55673800	-1.96847700	-0.78350300
H	-4.49500200	-1.91965000	0.60884800	H	5.43360400	-0.71510400	-2.10877100
C	-4.48568900	1.82887300	-0.40268500	C	5.64475500	-2.27464000	1.43735900
H	-2.34356300	1.65524400	-0.54275500	H	3.78723100	-1.25155600	1.83758000
C	-5.70804700	1.18377400	-0.12228400	C	6.64774200	-2.53871900	0.49246500
H	-6.60853500	-0.69600200	0.46325800	H	7.32601800	-2.16936500	-1.52583900
H	-4.48667600	2.88137400	-0.68647600	H	5.70444500	-2.71625500	2.42968300
H	-6.65087100	1.72255800	-0.18548700	H	7.48660200	-3.18197500	0.74716700
C	-1.91507300	-2.38228200	0.50613200	C	3.15087000	0.67060500	-1.81100700
H	-2.48367100	-3.02294300	-0.18691400	H	2.59700300	0.01237400	-2.49844800
H	-0.87201400	-2.71512600	0.49767600	H	2.56431800	1.58740100	-1.68002500
H	-2.32377800	-2.56504500	1.51308700	H	4.10686600	0.91766100	-2.28157400
				H	-2.58798900	-4.42002100	0.92242000
				C	-3.38665500	-3.66860900	0.83625200
				C	-4.09416500	-3.83950900	-0.51769700
				C	-2.76120700	-2.24903700	1.05062000
				H	-4.09859600	-3.88419800	1.64430000
				H	-5.10450600	-3.41468200	-0.46994200
				C	-3.29598500	-3.13271600	-1.61224900
				H	-4.20836000	-4.90929900	-0.74786300
				N	-3.35398800	-1.30521500	0.07007500

	C	-3.25742300	-1.60069900	-1.38578600			
	H	-3.72040500	-3.33464000	-2.60625600			
	H	-2.27356000	-3.53821100	-1.62634600			
	O	-3.07704600	0.01549600	0.34871200			
	C	-1.99751900	-1.00868000	-2.06136800			
	H	-1.99527700	0.08050500	-1.97571700			
	H	-1.07696100	-1.38757100	-1.60720000			
	H	-1.98654600	-1.27653800	-3.12763100			
	C	-4.49927500	-0.94552300	-2.03204200			
	H	-4.44952300	-1.00393300	-3.12854500			
	H	-5.42013000	-1.43885400	-1.69706600			
	H	-4.54615500	0.10442400	-1.72912400			
	C	-1.20936800	-2.31923600	0.99216200			
	H	-0.78683000	-1.30898800	0.99580600			
	H	-0.81528000	-2.85973700	1.86516700			
	H	-0.85264800	-2.84150100	0.09747100			
	C	-3.15529100	-1.74791700	2.45405000			
	H	-2.67226000	-0.79493400	2.68036900			
	H	-4.24026500	-1.59932400	2.50849000			
	H	-2.85978400	-2.49111900	3.20806000			
17	18						
Charge=-1 Multiplicity =1				Charge=-2 Multiplicity =3			
C	2.16962000	2.31279100	-1.93534500	C	-2.72794000	1.07998900	0.86761200
C	1.80685400	3.81654900	-1.93429200	C	-3.60996400	0.74087500	-0.37850700
C	1.83779700	4.18848400	-0.42890200	C	-3.25121300	-0.73719800	-0.69017400

C	1.97359500	2.81091800	0.31512900	C	-2.21655700	-1.11149900	0.43163100
H	1.76710200	1.76996200	-2.79954200	H	-2.35983200	2.11132800	0.85863400
H	3.27674300	2.21708900	-1.97869300	H	-3.36150600	0.95255800	1.78179000
H	0.79847400	3.95352700	-2.34633000	H	-3.33813300	1.39701100	-1.21367400
H	2.49798200	4.42165100	-2.53884900	H	-4.68545800	0.87974300	-0.18118100
H	2.67574200	4.84957700	-0.17829500	H	-4.12181900	-1.40676700	-0.68018600
H	0.92047700	4.70578300	-0.12466000	H	-2.77689200	-0.82893500	-1.67440800
H	3.01992600	2.70985300	0.65493800	H	-2.78864200	-1.59575900	1.25366000
N	1.65545700	1.77702200	-0.68136700	N	-1.63407300	0.14118300	0.86554000
C	1.08439800	2.76829300	1.58391900	C	-1.16745000	-2.12954200	-0.05800100
O	1.45479200	3.41813500	2.57662200	O	-1.50712000	-3.33225000	-0.17416100
Cu	-0.12901500	1.18027300	-0.38121300	Cu	0.11344500	0.46930500	0.11202800
O	-0.00878400	2.08349700	1.49977800	O	-0.01493800	-1.64243000	-0.33767200
H	2.49071600	0.33107400	-0.39212800	O	-0.14432000	2.34935500	-0.75920000
H	0.96359400	-4.33829900	-1.49632900	O	-0.71796000	3.35582800	-0.13309300
C	1.43035000	-3.84400900	-0.63293800	O	2.02233500	0.77312600	0.11408600
C	0.40280800	-3.56473800	0.46404200	C	4.38772500	0.59757800	0.18703800
C	2.11655100	-2.53949600	-1.11832200	H	4.46975400	1.36417700	-0.59358000
H	2.18413500	-4.54579800	-0.24748100	H	4.40542500	1.10604500	1.15944000
H	-0.14446600	-4.48260300	0.72340000	H	5.25962900	-0.07370900	0.12117100
C	1.09859100	-2.99702500	1.71340900	C	3.03369900	-0.87081600	-1.35673400
H	-0.33864800	-2.84644400	0.09495300	H	2.09110600	-1.41280000	-1.47740800
N	2.10064700	-1.54659000	-0.00212300	H	3.10972900	-0.11488400	-2.14938300
C	2.28576800	-2.02910600	1.39439100	H	3.87116000	-1.58046900	-1.46556400

H	1.48259600	-3.82528300	2.32664600	C	2.93883200	-1.23516200	1.14138000
H	0.35788900	-2.47185300	2.32830000	H	1.99759700	-1.78196300	1.03104300
O	3.05319500	-0.52371500	-0.29269000	H	3.77470100	-1.95385700	1.10648400
C	2.18982200	-0.81028200	2.32967200	H	2.94508700	-0.73982500	2.12144600
H	3.05917300	-0.15600000	2.22404700	C	3.03832100	-0.15906700	0.02482600
H	1.29342000	-0.21949400	2.11803600				
H	2.14060000	-1.15413200	3.37171200				
C	3.65119800	-2.71718700	1.65783300				
H	3.79118800	-2.86405400	2.73762400				
H	3.72903700	-3.70122000	1.18279100				
H	4.46529000	-2.08309200	1.29102900				
C	1.28573200	-1.91406100	-2.25880000				
H	1.70062600	-0.94032700	-2.53576100				
H	1.29436600	-2.56290300	-3.14604300				
H	0.24758400	-1.75641700	-1.94711100				
C	3.52231900	-2.86391100	-1.67637400				
H	3.99884000	-1.96052300	-2.06545800				
H	4.18092200	-3.29448900	-0.91687700				
H	3.42831700	-3.59304300	-2.49363400				
C	-2.95434300	0.87766600	-0.16032700				
O	-1.85612200	0.41072700	-0.55438300				
C	-4.11603000	-0.03020100	-0.08872800				
C	-5.40841700	0.39891400	0.28151600				
C	-3.93766200	-1.39348500	-0.41863300				

C	-6.47644600	-0.49812100	0.32057400				
H	-5.58623000	1.43641500	0.54335800				
C	-5.00433000	-2.28483900	-0.37557200				
H	-2.94551800	-1.72774800	-0.70291200				
C	-6.28294100	-1.84399100	-0.00633600				
H	-7.46321000	-0.14396700	0.61051400				
H	-4.84161300	-3.33004600	-0.62875200				
H	-7.11604500	-2.54209700	0.02776800				
C	-3.01714600	2.33419400	0.21181300				
H	-2.25387300	2.52462500	0.97949600				
H	-2.72687200	2.93373700	-0.66339400				
H	-3.99272700	2.67229700	0.56624700				
18				20			
Charge=-2 Multiplicity =1				Charge=-1 Multiplicity =3			
C	-2.72205400	1.06411700	0.89037400	C	-4.24848200	-0.28126000	-1.01751200
C	-3.59420900	0.73272100	-0.36203300	C	-4.81102800	0.34818900	0.28168100
C	-3.25914000	-0.75395000	-0.65932800	C	-3.94222100	1.61741600	0.46808100
C	-2.20286800	-1.12568000	0.44539200	C	-2.75628700	1.42946000	-0.55436500
H	-2.35598700	2.09596800	0.89159700	H	-4.40012800	-1.36566400	-1.07526400
H	-3.35719500	0.92473900	1.80133100	H	-4.77719000	0.16343500	-1.88743500
H	-3.29296800	1.37639500	-1.19632500	H	-4.66381800	-0.34561200	1.11810100
H	-4.66951100	0.89544200	-0.18315600	H	-5.88431100	0.57321800	0.22180100
H	-4.13711100	-1.41249500	-0.61594000	H	-4.49833500	2.53450500	0.24549300
H	-2.81303500	-0.86739700	-1.65430000	H	-3.57045100	1.70938000	1.49360800
H	-2.75563500	-1.62453900	1.27113800	H	-2.88986800	2.15853600	-1.37202700

N	-1.62472400	0.12822500	0.88295700	N	-2.83799500	0.05995100	-1.05800400
C	-1.14647500	-2.12206100	-0.07008200	C	-1.39647000	1.73566500	0.09421600
O	-1.46267600	-3.32956100	-0.19092900	O	-1.04969400	2.89700500	0.31297600
Cu	0.10357400	0.47386100	0.08952100	Cu	-1.50016700	-0.98215600	-0.21440800
O	-0.00693500	-1.61068500	-0.36680200	O	-0.68240900	0.68147200	0.41813100
O	-0.19897400	2.32585900	-0.79799800	C	2.35125500	-0.32716500	1.44379900
O	-0.72099300	3.34334200	-0.12737900	H	1.65737600	-1.12335100	1.13467700
O	2.01422500	0.77772000	0.10089300	O	1.62865300	0.78453900	1.93320700
C	4.37902300	0.61459500	0.20989000	H	0.81023800	0.89507200	1.39214500
H	4.46852400	1.37288600	-0.57790200	O	-0.41144800	-2.60861900	0.18346200
H	4.38049700	1.13371400	1.17673800	O	-1.60932000	-3.02223900	-0.22100000
H	5.25485100	-0.05327200	0.16372200	C	3.22543800	0.02015600	0.23691500
C	3.05520400	-0.87661300	-1.33730600	C	3.71204700	-0.99351300	-0.60195700
H	2.11803800	-1.42588300	-1.46617900	C	3.57751100	1.34658700	-0.04094200
H	3.13709400	-0.12821300	-2.13641800	C	4.54315800	-0.69348000	-1.68400900
H	3.89893500	-1.58148800	-1.42697100	H	3.42313200	-2.02599900	-0.41529900
C	2.92576400	-1.21471100	1.16342600	C	4.40843600	1.65105700	-1.12350900
H	1.98783700	-1.76582200	1.04722900	H	3.17006500	2.13075400	0.58886200
H	3.76414000	-1.93102900	1.14660000	C	4.89865800	0.63365200	-1.94740400
H	2.91786000	-0.70914400	2.13819900	H	4.90197400	-1.49258700	-2.32846000
C	3.03574300	-0.15054800	0.03659500	H	4.66318500	2.68777200	-1.33049400
				H	5.53807700	0.87196800	-2.79382800
				C	3.20941000	-0.85732100	2.60176800
				H	2.56094300	-1.14896700	3.43413500

	H	3.80622300	-1.72256900	2.29358400					
	H	3.88888100	-0.07095200	2.94949400					
20	21								
Charge=-1 Multiplicity =1	Charge=-3 Multiplicity =3								
C	O	-2.32583800	-1.80878300	-1.31510800	O	-0.01148600	-0.47615300	0.60627200	
C	O	-2.10214300	-2.52013900	0.03601300	O	0.14896700	-1.47813300	1.66576700	
C	C	-3.38636400	-2.17529700	0.82597300	C	2.37971500	-1.85447200	-2.45513500	
C	C	-3.98371200	-0.92968500	0.06983700	C	3.90744000	-1.62158200	-2.22377700	
H	C	-1.40352300	-1.60013800	-1.86523000	C	4.34704500	-2.88224000	-1.42899800	
H	C	-2.95628700	-2.44928900	-1.96354900	C	3.00463300	-3.68220000	-1.22434700	
H	H	-1.21715100	-2.09812500	0.52605100	H	1.80208400	-0.92371400	-2.48668400	
H	H	-1.94297400	-3.60102900	-0.06531900	H	2.25964000	-2.34488900	-3.45629300	
H	H	-4.10265000	-3.00408600	0.80769900	H	4.06095300	-0.71076200	-1.63159500	
H	H	-3.18311800	-1.95086500	1.87752600	H	4.46424200	-1.50143200	-3.16891500	
H	H	-4.96494100	-1.20382100	-0.34741000	H	5.09875500	-3.48437000	-1.96079600	
N	H	-3.05742900	-0.58047700	-1.01729000	H	4.77533700	-2.60991100	-0.45609800	
C	H	-4.19781300	0.27034300	1.00085300	H	2.97592500	-4.47355800	-2.00898300	
O	N	-5.12591200	0.31199600	1.80494700	N	1.94132600	-2.71984500	-1.39296600	
Cu	C	-2.04223600	0.89732300	-0.45931800	C	2.94877800	-4.39324000	0.14420400	
O	O	-3.29066000	1.21622000	0.88311800	O	3.64163300	-5.42413500	0.32055000	
O	Cu	-0.70027300	2.18404400	-0.57716700	Cu	1.16838200	-2.21108900	0.28321500	
O	O	-0.52061900	1.08664600	-1.45044800	O	2.19562900	-3.84207700	1.02834200	
C	C	2.66539900	0.75890900	-0.14428200	C	-4.31218900	-0.61858200	-1.82828600	
O	C	1.77823100	-0.22083700	-0.65516900	C	-5.16239500	0.65972800	-1.57202100	
H	C	0.92895000	0.21992300	-0.90018500	C	-4.29132700	1.79800900	-2.16467600	

H	2.75794100	1.58851800	-0.86542500	C	-2.94082800	1.07778000	-2.54713000
C	2.14248500	1.33908700	1.18274400	H	-4.46695700	-1.38042200	-1.05777500
H	2.81380100	2.11535600	1.56938200	H	-4.61208900	-1.05353200	-2.81732400
H	1.15301400	1.77796500	1.01905400	H	-5.28155000	0.78387300	-0.49015300
H	2.06373600	0.54294600	1.93142700	H	-6.16627700	0.60834900	-2.02977100
C	4.04348400	0.13645100	0.02113700	H	-4.74918100	2.27319700	-3.04498300
C	5.16996900	0.95247500	0.20678500	H	-4.10875400	2.59012100	-1.42801100
C	4.22010000	-1.25334700	0.01576100	H	-2.94812600	0.93088500	-3.65012800
C	6.43831000	0.39838600	0.39373800	N	-2.93718100	-0.19160400	-1.85004000
H	5.05346500	2.03427400	0.20026100	C	-1.71181800	1.94154100	-2.20464500
C	5.48865200	-1.81163600	0.20376100	O	-1.47269300	2.95764500	-2.90047100
H	3.35261900	-1.88271100	-0.14853700	Cu	-1.82281000	-0.15554000	-0.24263900
C	6.60333200	-0.99076400	0.39545600	O	-1.03713400	1.55838400	-1.18305000
H	7.29752800	1.05014800	0.53279500	O	-3.27546400	-0.64290300	1.00283800
H	5.60595400	-2.89273400	0.19580100	C	-3.31255600	-1.07045100	2.31963500
H	7.58918100	-1.42588600	0.53865900	C	-2.42776800	-0.19622500	3.24476100
				C	-2.86681200	-2.55102100	2.44114100
				C	-4.78936800	-0.95663900	2.80393400
				H	-1.37992600	-0.28938900	2.94410500
				H	-2.73505000	0.85579000	3.15511000
				H	-2.51512000	-0.49534500	4.30424900
				H	-3.49929500	-3.17497300	1.79291400
				H	-1.82561900	-2.63585000	2.11294800
				H	-2.94548200	-2.92907900	3.47593600

	H	-5.43723600	-1.56078000	2.15355600			
	H	-4.91646700	-1.29954800	3.84569500			
	H	-5.12221200	0.08851500	2.73526300			
	O	1.56401700	1.54649500	1.50949000			
	H	0.99724400	0.77235600	1.20943500			
	C	1.08300500	2.70908100	0.86418900			
	H	0.71540500	2.46374900	-0.14201200			
	C	-0.11042900	3.30679600	1.64148900			
	H	-0.50775400	4.20211300	1.14464500			
	H	-0.90838000	2.56022700	1.68600400			
	H	0.19574900	3.56677300	2.66487300			
	C	2.20418900	3.72918600	0.75049500			
	C	2.05442800	4.86353800	-0.06665500			
	C	3.40231200	3.58111500	1.46539500			
	C	3.06027800	5.83000300	-0.15018800			
	H	1.14612200	4.97093900	-0.65647700			
	C	4.41067700	4.54837500	1.38595800			
	H	3.52543700	2.68411300	2.06446700			
	C	4.24558300	5.68165800	0.58198100			
	H	2.92492300	6.69433600	-0.80009000			
H	5.33551000	4.40971700	1.94625400				
H	5.03425100	6.43093400	0.51311900				
21	22						
Charge=-3 Multiplicity =1				Charge=-3 Multiplicity =3			
O	0.21817800	-0.70748000	0.12931300	O	-0.43594600	-0.25373900	-0.53171000

O	0.85914300	-1.63149000	1.00526300	O	-1.15447700	-0.73839100	-1.71511000
C	3.74097900	0.07219400	-2.27765400	C	-3.39845700	0.11510200	2.35477300
C	4.78294400	1.01536800	-1.59429900	C	-4.29041400	1.39562700	2.24381300
C	5.65716600	0.03672300	-0.76249000	C	-5.38794800	0.98498900	1.22333200
C	4.99884800	-1.36907500	-1.02748500	C	-5.00364400	-0.49235400	0.83933500
H	2.76618000	0.54880300	-2.43241600	H	-2.34005100	0.34046900	2.52700800
H	4.14008800	-0.18962500	-3.29393600	H	-3.75430400	-0.46673400	3.24492800
H	4.26869900	1.73414300	-0.94437500	H	-3.69688200	2.23772800	1.86601200
H	5.37290700	1.59186500	-2.32743700	H	-4.71163600	1.69876400	3.21771200
H	6.71713500	0.04984200	-1.05664300	H	-6.40571000	1.04631100	1.63654600
H	5.60909400	0.27537600	0.30729900	H	-5.35764200	1.62262900	0.33066000
H	5.58433300	-1.85259400	-1.84333900	H	-5.62471400	-1.16417000	1.47748900
N	3.64063300	-1.09568300	-1.44273500	N	-3.59711200	-0.62032100	1.13533600
C	5.08414900	-2.29204400	0.20869000	C	-5.33459000	-0.82607000	-0.63050600
O	6.18523200	-2.83856700	0.47060400	O	-6.53483200	-0.98983300	-0.95823200
Cu	2.38737900	-1.39756600	-0.03319100	Cu	-2.52184500	-0.63199400	-0.44792200
O	4.01090900	-2.40504700	0.90095700	O	-4.32914900	-0.88801300	-1.42830000
C	-3.93176900	-2.65150600	-1.35309300	C	2.40061000	-3.75629200	1.57951100
C	-5.15819000	-1.74563500	-1.05415800	C	3.89224900	-3.31256900	1.60796300
C	-4.91649300	-0.51696500	-1.96644400	C	3.87498800	-2.05906000	2.52165700
C	-3.44602900	-0.72846100	-2.50205200	C	2.33964800	-1.81173100	2.78929200
H	-3.67123600	-3.29808000	-0.50727800	H	2.13035200	-4.24463500	0.63819900
H	-4.18546000	-3.31966500	-2.21996600	H	2.23461900	-4.49064600	2.41111300
H	-5.12170400	-1.45632300	0.00150700	H	4.19591400	-3.04835200	0.58885300

H	-6.12351600	-2.24472300	-1.25098500	H	4.56935900	-4.10233900	1.97950400
H	-5.63229000	-0.46059700	-2.79972800	H	4.42271000	-2.20810000	3.46412500
H	-4.99498800	0.42357200	-1.40829500	H	4.32149600	-1.19124700	2.02077700
H	-3.52892400	-1.05809800	-3.56221900	H	2.11975800	-2.19041600	3.81234700
N	-2.84940000	-1.76352100	-1.68180800	N	1.61913200	-2.56473200	1.78380800
C	-2.63964800	0.58826500	-2.49366200	C	1.98577800	-0.31354600	2.76132600
O	-2.93634800	1.47160000	-3.33433400	O	2.33971900	0.41233100	3.72155600
Cu	-1.62175200	-1.04182700	-0.33342900	Cu	1.01748700	-1.41565600	0.31005700
O	-1.74229700	0.68768600	-1.58476200	O	1.37314100	0.08694300	1.70778600
O	-2.62974400	-1.38257000	1.31973500	O	1.94431700	-2.37832800	-1.14220200
C	-2.30976600	-2.12472300	2.44899500	C	1.54022700	-2.94740500	-2.33772300
C	-1.36996900	-1.34101700	3.40158900	C	1.35397200	-1.87608400	-3.44505400
C	-1.64870800	-3.47861700	2.08261900	C	0.21832600	-3.74141600	-2.17978300
C	-3.64226600	-2.41387400	3.20107200	C	2.65885300	-3.93273000	-2.79266200
H	-0.41845600	-1.14065800	2.90025700	H	0.56040900	-1.18464700	-3.14353400
H	-1.83639000	-0.38230400	3.66725900	H	2.29236600	-1.31658500	-3.57000600
H	-1.16649700	-1.90008100	4.33180300	H	1.08231200	-2.32456800	-4.41758900
H	-2.31971600	-4.05187200	1.42754300	H	0.33583200	-4.49981700	-1.39296100
H	-0.70801000	-3.29405400	1.55364800	H	-0.58214000	-3.05074100	-1.89409800
H	-1.43321400	-4.08677200	2.97782600	H	-0.07495900	-4.25036800	-3.11466800
H	-4.32242200	-2.97833900	2.54889900	H	2.79992900	-4.71110100	-2.03014600
H	-3.47928900	-2.99084600	4.12788500	H	2.42342400	-4.41973000	-3.75516800
H	-4.13175600	-1.46485300	3.45972800	H	3.60717400	-3.38716000	-2.89803600
O	0.48385500	1.80929200	1.28059200	H	2.12150900	5.04411900	1.47908000

H	0.41924100	0.88354100	0.91562600	C	2.08093900	3.98165700	1.18644400
C	-0.58754200	2.56547200	0.74095600	C	3.33779600	3.62145100	0.37586700
H	-0.79775400	2.24355800	-0.28864500	C	0.74433700	3.72866400	0.41194300
C	-1.87608300	2.35036100	1.56336000	H	2.07790800	3.38853200	2.10710700
H	-2.71459400	2.92469400	1.14580900	H	3.51592100	2.54373900	0.45378500
H	-2.14577400	1.28916100	1.54755000	C	3.15518200	4.01007800	-1.09285000
H	-1.71376200	2.66235000	2.60507200	H	4.21887500	4.12636400	0.80344400
C	-0.20293800	4.03634100	0.72598300	N	1.05581600	2.79593400	-0.69540900
C	-0.97474600	4.96578200	0.00728100	C	2.01375800	3.19162800	-1.75429700
C	0.91123300	4.50924500	1.43552000	H	4.08035000	3.84897700	-1.66665400
C	-0.65574800	6.32620300	0.01181900	H	2.93520700	5.08834200	-1.15561500
H	-1.82030200	4.60812200	-0.57692000	O	-0.13809100	2.31712700	-1.30840800
C	1.23217800	5.87133100	1.44475100	C	1.39229800	3.99584000	-2.92629400
H	1.52475900	3.78243000	1.95865500	H	0.58475900	3.41956200	-3.38660400
C	0.44946500	6.79008800	0.73703300	H	0.98523800	4.95868500	-2.59880600
H	-1.26287900	7.02441400	-0.56405400	H	2.16388300	4.19494600	-3.68620900
H	2.10630900	6.21451700	1.99817800	C	2.58257200	1.87655700	-2.32861800
H	0.70456400	7.84978900	0.73655100	H	3.28089300	2.08326400	-3.15466200
				H	3.10428900	1.30569300	-1.55419700
				H	1.77315500	1.24434100	-2.70204900
				C	0.09311600	5.06770700	-0.04050700
				H	-0.75607800	4.86083000	-0.70197200
				H	-0.28089100	5.61580900	0.83728600
				H	0.79736200	5.72670000	-0.56411000

	C	-0.23979600	3.01824900	1.35948000			
	H	-1.22502200	2.90601100	0.89763000			
	H	0.14546800	2.02811000	1.62481800			
	H	-0.34842900	3.61457800	2.27769000			
	H	-0.21674200	1.35799200	-0.99876100			
22	24						
Charge=-3 Multiplicity =1	Charge=-2 Multiplicity =4						
O	0.43837700	-0.35277700	0.43939100	C	-2.93644600	-2.70168600	-1.05080500
O	1.10604500	-0.87863100	1.63435500	C	-3.33527600	-3.45258100	0.26015100
C	3.46609200	-0.05890900	-2.37892700	C	-4.31863300	-2.47814400	0.96157700
C	4.43022700	1.16439200	-2.23039000	C	-4.41843100	-1.26946000	-0.03508200
C	5.48325400	0.67207900	-1.19921900	H	-1.88748900	-2.86284000	-1.31787100
C	5.00714900	-0.78727100	-0.85121800	H	-3.57046600	-3.09408500	-1.88337500
H	2.42597200	0.23259400	-2.56330000	H	-2.44320600	-3.62267800	0.87397400
H	3.80157700	-0.64443500	-3.27488900	H	-3.79050900	-4.43464600	0.05678800
H	3.88126000	2.03410400	-1.84767200	H	-5.30292200	-2.92204100	1.15958700
H	4.88568500	1.45798700	-3.19174200	H	-3.91612700	-2.13373900	1.92141100
H	6.51040100	0.68235000	-1.59308200	H	-5.31360900	-1.44089800	-0.67081100
H	5.47228400	1.29355600	-0.29485900	N	-3.20303000	-1.30098000	-0.82472700
H	5.59866000	-1.48183400	-1.49331600	C	-4.62181100	0.07086800	0.69431300
N	3.60072500	-0.82662600	-1.17109900	O	-5.74626300	0.33340400	1.17803800
C	5.29386100	-1.16885900	0.61623900	Cu	-1.92342300	0.03145500	-0.28695300
O	6.47709100	-1.40706200	0.95923700	O	-3.57878300	0.81857800	0.76902000
Cu	2.50170200	-0.81316000	0.39708400	O	-0.11919400	-1.00044400	-0.10058400
O	4.27300400	-1.19038700	1.39658900	O	0.13976800	-2.21683300	-0.55309300

C	-2.77862100	-3.56990800	-1.53228500	O	-0.79767800	1.60960300	-0.47352300
C	-4.22610000	-2.99782800	-1.52318600	C	-0.08388400	3.82523800	-0.98638200
C	-4.12542700	-1.75806300	-2.45012500	H	0.81395500	3.69652900	-0.36951900
C	-2.58230100	-1.64807900	-2.76236600	H	0.16496800	3.52285600	-2.01128800
H	-2.52559200	-4.07542400	-0.59506800	H	-0.35508000	4.89255900	-0.98945000
H	-2.70154900	-4.32210500	-2.36114800	C	-1.55754600	3.37295200	1.01011100
H	-4.47550900	-2.69959300	-0.49881100	H	-2.36361100	2.74763800	1.40400100
H	-4.97997700	-3.72827800	-1.86728400	H	-0.66709300	3.23737100	1.63841300
H	-4.71039100	-1.86638500	-3.37562800	H	-1.86418200	4.43047200	1.06336300
H	-4.48012100	-0.85059200	-1.94618300	C	-2.48321700	3.14807500	-1.32952200
H	-2.42552200	-2.05256400	-3.78722900	H	-3.31126500	2.54393400	-0.94768300
N	-1.90218900	-2.45293100	-1.76887000	H	-2.79707700	4.20416600	-1.35069300
C	-2.09909200	-0.18590000	-2.76033200	H	-2.26023100	2.82937500	-2.35610000
O	-2.41109600	0.55764600	-3.72154500	C	-1.23011500	2.92948600	-0.44113500
Cu	-1.17166800	-1.34382800	-0.32175000	H	2.42345400	1.95040800	1.09682900
O	-1.42994900	0.17110700	-1.72554800	C	3.16044900	1.38955200	0.51086100
O	-2.15003600	-2.17433700	1.17178700	C	2.53207700	0.97436200	-0.84147300
C	-1.75723500	-2.81920700	2.33274900	C	3.67500300	0.22762300	1.39023100
C	-1.42585700	-1.80478500	3.45997200	H	4.01039900	2.06733500	0.34455700
C	-0.52462700	-3.72959100	2.10012800	H	2.81467500	1.72317100	-1.59353100
C	-2.94739700	-3.70678200	2.80675900	C	2.96225700	-0.43037600	-1.29720200
H	-0.58230100	-1.18250200	3.14370600	H	1.43818400	1.00246100	-0.77114600
H	-2.30042300	-1.16276500	3.63944000	N	4.59189700	-0.62244200	0.55723500
H	-1.16044800	-2.30665300	4.40779600	C	4.39859400	-0.82790600	-0.91318800

H	-0.74364400	-4.45056900	1.30009700	H	2.87525800	-0.51121900	-2.38857500
H	0.32671200	-3.10918500	1.80017900	H	2.26591500	-1.17189200	-0.89518800
H	-0.24663100	-4.29093200	3.00928100	O	5.62348900	-1.16617300	1.10838800
H	-3.19172300	-4.44547100	2.03113500	C	4.62400700	-2.31789100	-1.22658500
H	-2.72341400	-4.24199000	3.74609900	H	5.63181200	-2.63187700	-0.94219700
H	-3.83415800	-3.07688200	2.96488600	H	3.89659300	-2.93393800	-0.68991800
H	-1.73591900	5.22952600	-1.38843200	H	4.48275800	-2.48434900	-2.30056300
C	-1.79353200	4.16186000	-1.11900900	C	5.45487600	0.02275600	-1.65439300
C	-3.04873000	3.91251900	-0.26479800	H	5.40104600	-0.17296500	-2.73221000
C	-0.45984700	3.75653000	-0.40708600	H	5.28800400	1.09237800	-1.49534300
H	-1.88682500	3.59498000	-2.05157800	H	6.45914800	-0.23164500	-1.29908300
H	-3.34607200	2.86301400	-0.36316200	C	2.51964000	-0.63287200	1.94658100
C	-2.76696700	4.23322400	1.20449300	H	2.92593000	-1.51882100	2.44786600
H	-3.88674900	4.52151800	-0.64044900	H	1.95930300	-0.04505500	2.68307600
N	-0.81682500	2.82565100	0.68817700	H	1.80246200	-0.93946300	1.18170100
C	-1.69304900	3.28071900	1.79445500	C	4.49336700	0.79929300	2.55998700
H	-3.68032700	4.15172000	1.81294300	H	4.83331000	0.00756800	3.23148200
H	-2.43108400	5.27960000	1.28710500	H	5.37465800	1.34135300	2.20054500
O	0.35186000	2.22950500	1.24427000	H	3.85803900	1.49352800	3.12079700
C	-0.95174200	3.97947800	2.96409500				
H	-0.19255900	3.31007900	3.37798900				
H	-0.45903600	4.90562500	2.64818600				
H	-1.67248700	4.23256400	3.75716200				
C	-2.37135300	2.01084400	2.35065800				

H	-3.01254000	2.25782300	3.21128700				
H	-2.97840900	1.52294800	1.58172900				
H	-1.61794700	1.28666400	2.67013100				
C	0.33592800	5.01225900	0.05268400				
H	1.18469300	4.70461800	0.67408000				
H	0.72879300	5.54701200	-0.82511400				
H	-0.28045000	5.72054000	0.62087100				
C	0.41202900	2.98173600	-1.41247200				
H	1.40013800	2.76504000	-0.99640800				
H	-0.07550300	2.03870000	-1.68203300				
H	0.53952000	3.58922200	-2.32098700				
H	0.33628700	1.27310100	0.91893500				
25				TS25-26			
Charge=-2 Multiplicity =4				Charge=-2 Multiplicity =4			
C	-0.09084200	-2.97868200	-2.75313900	C	-2.12189000	-1.34094800	2.91317400
C	-1.13270400	-3.99252700	-3.32434000	C	-2.59534400	-2.72019100	3.48377000
C	-2.33649300	-3.87899200	-2.34310100	C	-2.90897500	-3.57243000	2.21872500
C	-1.89764900	-2.75064500	-1.37814100	C	-2.35687700	-2.69774100	1.07593900
H	0.94575500	-3.32254100	-2.87190100	H	-2.54099800	-0.49087500	3.46875100
H	-0.18450800	-2.01201000	-3.29522600	H	-1.01920800	-1.24959000	2.96392000
H	-0.71994300	-5.00972600	-3.32445500	H	-3.48681900	-2.60336500	4.11382700
H	-1.40909700	-3.75184400	-4.36063100	H	-1.81710300	-3.18045200	4.10734700
H	-3.28106400	-3.64593700	-2.84658200	H	-2.44994700	-4.56699200	2.24371000
H	-2.48692800	-4.80603100	-1.77975100	H	-3.98686100	-3.71046900	2.08170100
H	-2.21016000	-1.78301700	-1.83960500	H	-1.26382500	-2.90767600	0.99671000

N	-0.44742700	-2.83422100	-1.36106000	N	-2.57134900	-1.33508900	1.53701200
C	-2.51326000	-2.71976200	0.03822900	C	-2.89480400	-2.88554200	-0.35661500
O	-3.71015300	-3.07595700	0.17432500	O	-3.32713700	-4.00208900	-0.71634600
Cu	0.33485400	-1.76060400	-0.03244100	Cu	-2.22988100	-0.10666900	0.14951800
O	-1.74739500	-2.24858200	0.94509000	O	-2.78962500	-1.83194400	-1.08348100
C	3.80361400	0.24394600	-0.41571100	C	-0.48305900	3.13476300	0.70005300
H	2.80418600	0.69835900	-0.48948100	H	-0.20631200	1.70236000	0.53830300
O	3.93803200	-0.43119400	0.81371200	O	-1.19690200	3.47564100	-0.43184200
O	1.63653900	-1.50425900	1.40385000	O	-2.71257000	1.49105600	-0.88309700
H	3.04164500	-0.85539900	1.05460600	H	-1.86031500	2.70714600	-0.64664400
C	2.75230800	-1.83807500	3.50730200	C	-3.90779000	2.96193700	-2.35613600
H	3.56259700	-2.39672300	3.02391100	H	-4.37477200	3.46857500	-1.50289400
H	3.04950000	-0.78386300	3.54119600	H	-2.98970800	3.50553200	-2.60666000
H	2.64009300	-2.20490000	4.53771800	H	-4.59235000	3.01929400	-3.21432900
C	1.05365000	-3.49638400	2.66450300	C	-4.89862400	0.76125700	-1.63434500
H	0.11576500	-3.62328200	2.11473600	H	-4.68413100	-0.28149800	-1.38208900
H	1.84076300	-4.06376900	2.15226500	H	-5.36922300	1.24400800	-0.76862600
H	0.92424900	-3.91182100	3.67548800	H	-5.60950700	0.77990900	-2.47391600
C	0.31359900	-1.20308500	3.40897400	C	-2.91667500	0.79548200	-3.19499500
H	-0.62122800	-1.32342900	2.85386300	H	-2.69620200	-0.24457300	-2.93753700
H	0.15565200	-1.54575200	4.44322300	H	-3.56421700	0.80982900	-4.08489200
H	0.57891200	-0.13888400	3.43125500	H	-1.97761700	1.30676600	-3.43962800
C	1.43833300	-1.99907600	2.70698700	C	-3.58657000	1.49406300	-1.98945100
C	4.84031100	1.35577800	-0.51010300	C	0.86008200	3.71059100	0.75318000

C	4.76439300	2.32025600	-1.52894400	C	1.65327800	3.68299400	1.92872600
C	5.90043600	1.44008300	0.40363400	C	1.44144900	4.29125200	-0.40389700
C	5.72264900	3.33067300	-1.64017100	C	2.94581200	4.20378900	1.94262300
H	3.93576700	2.28371200	-2.23251200	H	1.25657600	3.22603200	2.82879400
C	6.86434900	2.44831400	0.29374600	C	2.73267400	4.81298800	-0.38092900
H	5.93704600	0.70763000	1.20301700	H	0.84432300	4.31844000	-1.30861300
C	6.78354100	3.39848000	-0.72914500	C	3.50277400	4.77720100	0.79082700
H	5.63670500	4.07118100	-2.43287100	H	3.52912600	4.15457600	2.86039200
H	7.67823500	2.49601500	1.01508000	H	3.14703300	5.25234600	-1.28729300
H	7.52959900	4.18619000	-0.81120700	H	4.51316000	5.17974800	0.80469000
C	3.95101500	-0.73786000	-1.59904800	C	-1.29922300	3.06472900	1.98341900
H	4.93603900	-1.21987700	-1.56428000	H	-1.46061300	4.06889300	2.41267000
H	3.17670000	-1.50609800	-1.52123300	H	-2.27454400	2.62489700	1.75975400
H	3.83429000	-0.23271300	-2.56554900	H	-0.81699300	2.43414200	2.73785000
O	0.53790400	0.14281500	-0.76036500	O	-0.21512700	0.56849000	0.45566500
O	-0.10294700	0.47797700	-1.86180800	O	0.53417400	0.05961400	1.52051700
H	-1.18669400	3.98494200	1.14901200	H	3.60673500	0.73697500	-1.79861000
C	-2.08690300	3.35704000	1.17261900	C	3.50929400	-0.35325700	-1.72996400
C	-1.70134100	1.86218500	1.22984500	C	2.01730300	-0.75516300	-1.73900600
C	-2.97272100	3.75377900	-0.02824800	C	4.30585400	-0.81986900	-0.49162100
H	-2.63326000	3.64056000	2.08257300	H	4.01526600	-0.76467400	-2.61479700
H	-1.63786100	1.55583700	2.28028400	H	1.71212600	-0.94270500	-2.77593300
C	-2.68298500	0.95207800	0.46867200	C	1.71109700	-1.97834500	-0.85395100
H	-0.70565500	1.69686900	0.80892200	H	1.39363400	0.06522800	-1.37518900

N	-4.17545400	2.86006900	-0.04165400	N	4.11699500	-2.30194800	-0.35002100
C	-4.14132600	1.43877200	0.44890500	C	2.85253800	-3.00504300	-0.74435400
H	-2.65207300	-0.05811400	0.88821200	H	0.82171600	-2.49546500	-1.23033900
H	-2.34239100	0.84059700	-0.56502300	H	1.44431400	-1.62532500	0.14745600
O	-5.29214200	3.33958600	-0.47233800	O	5.09526100	-3.01805300	0.08915000
C	-4.95700100	0.56361300	-0.51692400	C	2.51108900	-4.03565100	0.34544400
H	-6.00874900	0.86235500	-0.52527500	H	3.30307600	-4.78279100	0.44199800
H	-4.56485900	0.65282900	-1.53496100	H	2.37709600	-3.53952300	1.31105200
H	-4.87117300	-0.48435100	-0.21168200	H	1.57065700	-4.53337300	0.08758800
C	-4.78408000	1.39175900	1.85229500	C	3.10677100	-3.73404800	-2.08305500
H	-4.83678300	0.35130700	2.18934200	H	2.22762000	-4.33045500	-2.35135800
H	-4.20043100	1.95825300	2.58519600	H	3.29675300	-3.02660200	-2.89633400
H	-5.79700500	1.80762700	1.81621000	H	3.97190400	-4.39933600	-1.99069400
C	-2.21208800	3.63434900	-1.36921700	C	3.84911000	-0.10221400	0.79749300
H	-2.90202400	3.80937700	-2.20210800	H	4.36905000	-0.53551800	1.65992200
H	-1.42250800	4.39515300	-1.41002300	H	4.11597100	0.95957900	0.73433700
H	-1.73574100	2.66070300	-1.50358200	H	2.76837500	-0.15208500	0.97174000
C	-3.45325400	5.20399600	0.15110100	C	5.80210500	-0.55077400	-0.72297800
H	-4.05295200	5.53158700	-0.70085200	H	6.39488600	-0.84339000	0.14624400
H	-4.06518000	5.30545400	1.05341800	H	6.17553300	-1.10648000	-1.58995000
H	-2.57784900	5.85694700	0.24586000	H	5.94037100	0.52087400	-0.90437000
26				27			
Charge=-2 Multiplicity =4				Charge=-2 Multiplicity =3			
C	0.52201700	-2.48526000	2.61636200	C	2.54886800	-2.74828600	-0.94935900
C	1.16752900	-3.77477700	3.23533600	C	3.90410800	-3.48882700	-1.20431100

C	1.34913100	-4.74034300	2.02894900	C	4.91352800	-2.74644800	-0.27544800
C	1.18576500	-3.79157900	0.83029100	C	4.01271400	-1.71113700	0.44616100
H	-0.35893400	-2.14701700	3.17667400	H	1.91496400	-2.69232400	-1.84441600
H	1.23073600	-1.63585400	2.60987400	H	1.97134500	-3.31493700	-0.18003900
H	0.52664000	-4.21486100	4.01002700	H	4.20010000	-3.39474500	-2.25847600
H	2.13005700	-3.54169500	3.70912800	H	3.83562100	-4.56484000	-0.97721300
H	2.31315000	-5.26111600	2.03110500	H	5.42333500	-3.41928500	0.42746200
H	0.55979300	-5.49942500	1.99922600	H	5.68720800	-2.22552800	-0.85142000
H	2.16126500	-3.26667200	0.69070800	H	3.62282000	-2.21537200	1.37191300
N	0.15276800	-2.86249400	1.26573100	N	2.95191300	-1.44514500	-0.49639100
C	0.83660500	-4.34400200	-0.56439800	C	4.64103500	-0.39926100	0.94394000
O	1.16340600	-5.50000300	-0.89236400	O	5.81688300	-0.38515400	1.37061100
Cu	-0.27630600	-1.77092700	-0.24103800	Cu	2.00458900	0.16308200	-0.08872000
O	0.24091100	-3.47699200	-1.31514300	O	3.83555300	0.60465000	0.91592300
C	-2.97249000	1.68313100	0.86701400	O	1.22792400	1.90818000	-0.24796300
H	-0.64995700	0.67316000	0.09052000	C	0.81995500	4.23231200	-0.49647700
O	-2.30433600	1.26241000	-0.16589700	H	0.59116900	4.09402100	-1.56178700
O	-1.97104100	-1.04740200	-1.43924400	H	-0.11852000	4.13050200	0.06399800
H	-2.24318300	-0.19922800	-0.98829800	H	1.21166900	5.25263500	-0.34875300
C	-4.21272900	-0.96365000	-2.35441100	C	3.13486300	3.29959200	-0.84923000
H	-4.52741500	-0.18373400	-1.65377700	H	3.85754400	2.54216800	-0.52935200
H	-3.83009900	-0.47656200	-3.25812500	H	2.91909500	3.15139200	-1.91685100
H	-5.09345600	-1.55902500	-2.62660100	H	3.58750400	4.29781200	-0.72094500
C	-3.63626600	-2.51686300	-0.44349500	C	2.13584700	3.36159900	1.47127500

H	-2.84307000	-3.11690100	0.01341300	H	2.84337000	2.59843000	1.81007500
H	-3.94661600	-1.75088300	0.27582800	H	2.56567000	4.35903500	1.66695100
H	-4.49709800	-3.16678400	-0.64759900	H	1.20753900	3.26324900	2.05125100
C	-2.65818500	-2.91816800	-2.74297800	C	1.82436800	3.14256100	-0.03343000
H	-1.80775200	-3.47962100	-2.34450500	O	0.05868500	-0.53690800	-0.38033200
H	-3.47720800	-3.61048000	-2.97658300	O	-0.34540200	-1.56705600	0.35210300
H	-2.33646800	-2.43363500	-3.67212600	H	-6.43841300	-0.10570600	1.86613100
C	-3.12777200	-1.86114700	-1.73840900	C	-5.55963500	0.19236700	1.27646200
C	-4.20369600	2.39389500	0.71155700	C	-5.98461100	1.08522700	0.08887800
C	-5.02027400	2.81410400	1.81714200	C	-4.78567900	-1.07642400	0.86678900
C	-4.69316700	2.73198500	-0.59753800	H	-4.90912800	0.76338100	1.95047200
C	-6.21028600	3.50238000	1.62262000	H	-5.96934400	2.13485000	0.41174300
H	-4.70682900	2.58191100	2.83074900	C	-5.07583100	0.89673800	-1.14431300
C	-5.88118400	3.42175900	-0.77401400	H	-7.02507200	0.87139100	-0.19605600
H	-4.08864500	2.43955400	-1.45001700	N	-3.55108000	-0.63859600	0.18358700
C	-6.67022400	3.82240400	0.32801700	C	-3.61558800	0.50067500	-0.81052800
H	-6.79899600	3.79736500	2.49128000	H	-5.05505400	1.82281300	-1.73622800
H	-6.21086600	3.66114000	-1.78499900	H	-5.49910100	0.12829500	-1.80337200
H	-7.60361900	4.36094100	0.18287100	O	-2.90713800	-1.79946300	-0.34509700
C	-2.40107800	1.40099200	2.24489600	C	-2.90273000	0.13697400	-2.12414100
H	-2.48931600	2.26696300	2.91498700	H	-1.84751500	-0.08573100	-1.94676200
H	-2.92442400	0.56381200	2.73523300	H	-3.36833600	-0.72729800	-2.60984200
H	-1.34167300	1.13323100	2.16101200	H	-2.96402200	0.99995500	-2.80232600
O	0.18851700	0.14541500	0.05273300	C	-2.86461900	1.69251000	-0.17442900

O	0.92418500	0.56637600	1.26628100	H	-2.87577300	2.56168400	-0.84827400
H	2.25711000	3.58621200	-1.99312200	H	-3.32006800	1.99213700	0.77739100
C	3.11294200	2.95627100	-1.72020100	H	-1.82060100	1.42239500	0.01313700
C	2.72486300	1.46370600	-1.80818900	C	-5.67980100	-2.04198300	0.03897200
C	3.61956500	3.42203400	-0.33671300	H	-5.07059200	-2.87673000	-0.31980000
H	3.90591200	3.18208000	-2.44717900	H	-6.48871600	-2.44092900	0.66833300
H	2.94710400	1.10761200	-2.82284700	H	-6.14017400	-1.56016100	-0.82878700
C	3.42592500	0.59081800	-0.74829800	C	-4.35054000	-1.82273400	2.14621000
H	1.64963000	1.33644500	-1.65802000	H	-3.77478300	-2.71555300	1.88552200
N	4.75473600	2.52547300	0.06131700	H	-3.71118500	-1.17760300	2.75840700
C	4.82135300	1.07691400	-0.31855000	H	-5.22754400	-2.12540700	2.73744500
H	3.53151400	-0.43465700	-1.12236100	H	-1.94346600	-1.71390400	-0.04109500
H	2.76923800	0.52406200	0.13062400				
O	5.75245600	3.02560700	0.70699700				
C	5.28015100	0.27665100	0.91308200				
H	6.26469000	0.60886100	1.25273400				
H	4.56308500	0.39461300	1.73026500				
H	5.32531300	-0.78675300	0.65439300				
C	5.86587600	0.93212900	-1.44933300				
H	6.01126600	-0.12848700	-1.68495900				
H	5.54149100	1.44051200	-2.36311300				
H	6.82414300	1.35887200	-1.13429900				
C	2.51159800	3.38043200	0.73799200				
H	2.93671000	3.66266800	1.70844800				

H	1.73587900	4.11338700	0.48173400	
H	2.01968200	2.40205700	0.84097700	
C	4.16459800	4.85505100	-0.45956700	
H	4.51590500	5.22805500	0.50462600	
H	5.00004400	4.90451300	-1.16666800	
H	3.35944000	5.50491200	-0.82037300	
27				29
Charge=-2 Multiplicity =1				Charge=-1 Multiplicity =2
C	2.45004200	-2.66784500	-1.19420400	C -3.03307500 -1.78202000 -0.79357100
C	3.75254200	-3.52433600	-1.32623200	C -3.73180200 -1.72932200 0.59416900
C	4.69254200	-2.94487500	-0.22449100	C -3.99351500 -0.21535100 0.80833500
C	3.80486100	-1.86729900	0.44783600	C -3.22204000 0.48039400 -0.37752100
H	1.95237900	-2.49540000	-2.15857800	H -2.35207700 -2.63537200 -0.89984500
H	1.72309900	-3.21058100	-0.54697100	H -3.81746600 -1.89636700 -1.57572500
H	4.19525000	-3.39773500	-2.32407100	H -3.05259300 -2.11707900 1.36316200
H	3.55430200	-4.59917300	-1.18908600	H -4.65257900 -2.32856600 0.63358000
H	5.03654200	-3.70635800	0.48829200	H -5.06066900 0.03296400 0.77869900
H	5.58316000	-2.47441700	-0.65703500	H -3.61182700 0.12659200 1.77658400
H	3.24412000	-2.37925000	1.27413900	H -3.97408100 0.81584200 -1.11610000
N	2.90733900	-1.43830500	-0.60203400	N -2.33289400 -0.52512500 -0.94718100
C	4.47615400	-0.65603700	1.11681500	C -2.46006100 1.73580300 0.09199100
O	5.59403000	-0.77716400	1.66499100	O -3.07373200 2.78877100 0.31276300
Cu	2.02568400	0.19176700	-0.14380200	Cu -0.56111200 -0.19826300 -0.29903900
O	3.75937700	0.41239000	1.08641600	O -1.17700300 1.57743100 0.26061400
O	1.42033700	1.99936800	-0.34212700	H 3.07726600 1.00025600 2.57304300

C	1.25115700	4.35226100	-0.60209400	C	3.05472500	0.73219500	1.50935600
H	1.12047700	4.23950000	-1.68689000	C	2.64305800	1.92907100	0.65092700
H	0.25511100	4.33373400	-0.14069200	C	2.08062500	-0.45986200	1.32292700
H	1.71564600	5.33244100	-0.40225400	H	4.07830000	0.43146200	1.24624800
C	3.49680300	3.21200400	-0.72857700	H	3.26438900	2.80316100	0.88512000
H	4.11264000	2.39336100	-0.34210400	C	2.77799100	1.57920700	-0.84069800
H	3.38115600	3.08143600	-1.81378900	H	1.60632200	2.20510900	0.87105200
H	4.02101400	4.16568900	-0.54589400	N	1.48215200	-0.39145300	-0.06839900
C	2.27509100	3.35443400	1.47756800	C	2.35704800	0.11473700	-1.18510100
H	2.86919100	2.52517400	1.87450800	H	3.81908400	1.72010200	-1.16259600
H	2.77493800	4.30511600	1.73138700	H	2.17042500	2.27799600	-1.42576000
H	1.28750700	3.34064200	1.95930100	O	0.82482700	-1.59740600	-0.40389900
C	2.09996900	3.17315300	-0.05399800	C	1.52743900	0.12497600	-2.48129500
O	0.02206300	-0.37306400	-0.38149000	H	1.24201600	-0.88741800	-2.77347600
O	-0.37661100	-1.50059200	0.20315500	H	0.61500700	0.71928000	-2.36398700
H	-6.43471000	-0.25447500	1.93190700	H	2.12468600	0.57932700	-3.28135300
C	-5.57349500	0.10750500	1.35220900	C	3.58558700	-0.79357600	-1.43210400
C	-6.03867400	1.08714700	0.25195400	H	4.06708300	-0.51151400	-2.37638000
C	-4.78773000	-1.10792000	0.82105200	H	4.33949100	-0.70867800	-0.64511700
H	-4.91886200	0.63236000	2.05895900	H	3.26364500	-1.83683700	-1.50566800
H	-6.05099400	2.10457700	0.66554900	C	0.91397300	-0.32467700	2.32236000
C	-5.13930400	1.03406900	-1.00178900	H	0.19189600	-1.13310800	2.17495500
H	-7.07561000	0.86701400	-0.04055800	H	1.29543800	-0.38998100	3.34866000
N	-3.57215900	-0.59296200	0.15756400	H	0.39049700	0.62796100	2.19915800

C	-3.66896000	0.63627900	-0.71848400	C	2.78840600	-1.80334200	1.59216500
H	-5.14285900	2.01141900	-1.50517800	H	2.09819100	-2.62834500	1.40273400
H	-5.55378700	0.32133300	-1.72568200	H	3.67221800	-1.94437600	0.96626300
O	-2.92847700	-1.68886000	-0.49421500	H	3.10987700	-1.83649700	2.64048300
C	-2.95824800	0.41798100	-2.06483200				
H	-1.89821800	0.19713300	-1.91485500				
H	-3.41263700	-0.40210900	-2.63074400				
H	-3.03872000	1.34286100	-2.65345500				
C	-2.93403800	1.77433600	0.02694500				
H	-2.95766000	2.70267400	-0.56247600				
H	-3.38933400	1.97782100	1.00393600				
H	-1.88756000	1.49631900	0.18596100				
C	-5.68391100	-2.00993100	-0.07319400				
H	-5.07413900	-2.80954900	-0.50358600				
H	-6.48448700	-2.46265200	0.53008900				
H	-6.15507500	-1.46265300	-0.89533700				
C	-4.31831100	-1.95677600	2.02177800				
H	-3.73222300	-2.81230700	1.67353900				
H	-3.67841000	-1.35753100	2.67837700				
H	-5.17924400	-2.32679100	2.59825200				
H	-1.95780400	-1.62351100	-0.19680600				
30				TS₃₀₋₃₁			
Charge=-1 Multiplicity =2				Charge=-1 Multiplicity =2			
C	1.27375000	3.31080700	0.13007900	C	2.23964200	-2.69789900	0.40136600

C	2.22036200	3.64120200	1.31347800	C	1.84561400	-3.79656700	1.40552900
C	3.62685600	3.33505400	0.73925900	C	1.08284000	-4.78007400	0.50308300
C	3.33632100	2.57708600	-0.61297800	C	0.40254700	-3.85104900	-0.54844700
H	0.26462700	3.02597000	0.45087600	H	2.48346700	-1.73894200	0.87140100
H	1.16440500	4.22120900	-0.49930500	H	3.14752800	-3.02561800	-0.14638800
H	1.99577500	2.97780500	2.15753400	H	1.17939200	-3.37929100	2.17157300
H	2.12158700	4.67604000	1.66920100	H	2.70468700	-4.25281600	1.91436700
H	4.20576000	4.24678400	0.55432800	H	1.79313600	-5.45277400	0.00500000
H	4.21737900	2.71420900	1.42135600	H	0.35028600	-5.40060700	1.02641700
H	3.58814800	3.25958000	-1.44443900	H	0.47489400	-4.31485900	-1.54552500
N	1.91285400	2.24672600	-0.61785600	N	1.11283100	-2.55767200	-0.52386300
C	4.22560000	1.32879200	-0.76942600	C	-1.11609400	-3.69015200	-0.28248000
O	5.41742200	1.44657400	-1.07714400	O	-1.84727700	-4.68550600	-0.28121300
Cu	1.72166500	0.39608800	-0.19239800	Cu	-0.12995500	-1.13643100	-0.21099100
O	3.63567000	0.19073800	-0.51984600	O	-1.53056700	-2.47098900	-0.08006200
H	2.62840300	-3.80417400	1.73972000	C	5.64790700	2.89362600	0.77990700
C	1.94568700	-3.52262800	0.92880500	C	4.39985900	2.93855000	1.40783200
C	2.70796100	-3.32694700	-0.38293800	C	3.31422100	2.23524900	0.87624000
C	1.19690800	-2.23128600	1.35065900	C	3.45433000	1.48079200	-0.29493800
H	1.23640900	-4.35436800	0.82225100	C	4.71379800	1.43409900	-0.91225500
H	3.32096700	-4.20967600	-0.60484400	C	5.80174300	2.13336500	-0.38442900
C	1.72657900	-3.07200700	-1.54084300	H	6.49294600	3.43631800	1.19613800
H	3.39196700	-2.47660500	-0.29298400	H	4.27145100	3.51773400	2.31928400
N	0.85519700	-1.44644300	0.09994600	H	2.34707700	2.24401900	1.36759500

C	0.47975600	-2.21943300	-1.13954400	H	4.84549700	0.83523600	-1.81147300
H	1.36592300	-4.02777000	-1.94418800	H	6.77017200	2.07885200	-0.87616500
H	2.26307800	-2.56913000	-2.35246400	C	2.26729900	0.73607100	-0.90475300
O	-0.03260400	-0.37589600	0.38962700	H	2.62757500	-0.25357400	-1.22710000
C	0.17487300	-1.21837100	-2.26800100	C	1.74714300	1.47118300	-2.15497600
H	-0.73131300	-0.64586500	-2.06122400	H	2.54263100	1.58837700	-2.89940900
H	1.00074300	-0.51492800	-2.41828000	H	0.92663700	0.90402400	-2.60474300
H	0.03556100	-1.77557200	-3.20180200	H	1.37440000	2.46650200	-1.88806800
C	-0.77702000	-3.10486300	-0.96047600	O	1.24644400	0.54100600	0.05107200
H	-1.07707200	-3.49720500	-1.93970400	H	0.20536700	0.97120900	-0.17123800
H	-0.59913300	-3.96559400	-0.31138600	H	-4.85407200	2.89119400	-1.29021400
H	-1.61291300	-2.52409100	-0.56096100	C	-4.35296100	2.32911800	-0.49133200
C	2.13722800	-1.35162400	2.19928100	C	-4.05003000	3.23303400	0.70389800
H	1.64432900	-0.41101300	2.46171500	C	-3.06157400	1.69337500	-1.07132000
H	2.38875700	-1.87391400	3.13000100	H	-5.05408100	1.54328000	-0.18356800
H	3.06322000	-1.12137900	1.66429600	H	-4.96283000	3.74016100	1.04457000
C	-0.04318500	-2.56408800	2.20441700	C	-3.43598100	2.41918700	1.85922200
H	-0.55387100	-1.64895300	2.51145400	H	-3.35130800	4.01820700	0.39267100
H	-0.76196700	-3.19484000	1.67879000	N	-2.06024000	1.56459200	0.02940000
H	0.28071800	-3.10138200	3.10421100	C	-2.54672300	1.21784800	1.39437700
C	-7.45654500	0.56098500	-0.50208700	H	-4.23462700	2.02056600	2.49852900
C	-6.81735700	-0.43604900	0.23992300	H	-2.83930600	3.09091500	2.48816000
C	-5.43698000	-0.38191300	0.45888200	O	-1.00860400	0.71892900	-0.42543800
C	-4.67317300	0.67265700	-0.05764700	C	-1.32231800	1.14446900	2.32522200

C	-5.32288200	1.66595800	-0.80610200	H	-0.71829700	0.25377900	2.13791800
C	-6.70093700	1.61446400	-1.02750700	H	-0.68658300	2.02540400	2.18966500
H	-8.52871000	0.51566700	-0.67535500	H	-1.66076700	1.11143600	3.36792800
H	-7.39378100	-1.26376500	0.64632300	C	-3.32222200	-0.11934600	1.51865700
H	-4.93025800	-1.15943700	1.01972500	H	-3.47475400	-0.35388400	2.58048400
H	-4.74216800	2.48454700	-1.22619500	H	-4.31307400	-0.06768400	1.05832000
H	-7.18319500	2.39196000	-1.61489100	H	-2.77710700	-0.95052700	1.06503300
C	-3.17633500	0.76392200	0.20018500	C	-2.43470000	2.65818300	-2.10147300
O	-2.70094000	-0.49286000	0.64413100	H	-1.46189700	2.27539300	-2.41949100
H	-1.70689500	-0.49019800	0.58315400	H	-3.07986500	2.75584500	-2.98387600
H	-2.68774600	1.03298700	-0.75096100	H	-2.28345300	3.65138800	-1.66443700
C	-2.85201000	1.86595900	1.22670600	C	-3.40504300	0.37052600	-1.79127000
H	-1.77010200	1.91345900	1.38311900	H	-2.52600100	-0.03854600	-2.29259100
H	-3.19630700	2.84869700	0.88429200	H	-3.77510100	-0.39315300	-1.10546300
H	-3.33610600	1.63789100	2.18266000	H	-4.17922500	0.56144500	-2.54616700
31				32			
Charge=-1 Multiplicity =2				Charge=-2 Multiplicity =2			
C	3.45403900	1.05463800	1.12379400	C	4.00694100	0.94047900	-0.49186400
C	3.84849900	0.06626800	2.23678100	C	4.44775600	0.62222600	0.97173800
C	4.98312800	-0.72810300	1.56604500	C	4.02625200	-0.86016300	1.16468900
C	4.60722100	-0.69905700	0.04742300	C	3.28384700	-1.21545600	-0.18170400
H	2.45463400	1.48642000	1.24364900	H	3.69737300	1.98232800	-0.62645600
H	4.16961500	1.90180600	1.12176300	H	4.88580200	0.75366900	-1.16272100
H	2.99883200	-0.58941300	2.46454100	H	3.90406300	1.27656600	1.66300100
H	4.15747900	0.55715900	3.16833900	H	5.52656000	0.77916100	1.13712700

H	5.94246600	-0.21962200	1.72390900	H	4.88130000	-1.52810700	1.33886800
H	5.09089700	-1.75068500	1.93824400	H	3.34514700	-0.97459200	2.01634200
H	5.49741900	-0.43594800	-0.54466100	H	4.00215200	-1.78896000	-0.80887500
N	3.56193500	0.32535600	-0.13927500	N	2.92027200	0.04403900	-0.79073000
C	4.15925400	-2.09002400	-0.46491100	C	2.05302900	-2.11220400	0.04795000
O	4.97283100	-3.01737300	-0.49376600	O	2.21362800	-3.33951300	0.24210300
Cu	1.92076600	-0.57730300	-0.73593200	Cu	1.05881400	0.51070200	-0.38574300
O	2.91187400	-2.18843500	-0.83021800	O	0.92135200	-1.49942300	0.04765600
C	-1.16512000	4.81426900	1.34819700	H	-3.93195600	-0.37779300	2.60082300
C	-1.49966400	3.46437700	1.48767400	C	-3.75565300	-0.37858400	1.51554700
C	-0.94812000	2.50317100	0.63383500	C	-3.57189000	-1.79887200	0.98268800
C	-0.05428000	2.87507600	-0.37810300	C	-2.51786100	0.50607700	1.20778000
C	0.28017600	4.23266400	-0.50584200	H	-4.65474300	0.06047400	1.05614300
C	-0.26808700	5.19589100	0.34446600	H	-4.40032000	-2.44830700	1.30628700
H	-1.59074500	5.55914700	2.01616200	C	-3.49884600	-1.76608000	-0.55145200
H	-2.19072600	3.15487600	2.26851200	H	-2.64645700	-2.22412800	1.38484500
H	-1.20065500	1.45362300	0.74229700	N	-1.84026200	-0.02511100	-0.00009400
H	0.98883400	4.53726100	-1.27398400	C	-2.64883300	-0.57403400	-1.10983700
H	0.01109500	6.24093800	0.23048100	H	-4.51841900	-1.69889800	-0.96225800
C	0.54916300	1.83579200	-1.32921300	H	-3.07739200	-2.71259600	-0.91057400
H	1.61962900	2.08931400	-1.42651700	O	-0.89380200	0.89932800	-0.48343800
C	-0.07853000	1.95706100	-2.73503600	C	-1.65987500	-1.12685900	-2.15634800
H	0.03522000	2.96788900	-3.14555000	H	-1.13393200	-0.31351600	-2.66136500
H	0.40784300	1.24558700	-3.41081300	H	-0.91238100	-1.75344600	-1.66055100

H	-1.14645400	1.71707300	-2.69427700	H	-2.20952500	-1.71886000	-2.90327200
O	0.41089700	0.52978900	-0.83731800	C	-3.55676900	0.47139700	-1.82209100
H	-0.99486400	-0.40650700	-1.00354900	H	-3.95566900	0.05930200	-2.76105700
H	-5.92453800	-0.54764300	0.32994100	H	-4.41168000	0.77156800	-1.20504100
C	-5.02355900	-1.15566000	0.48042700	H	-2.95908700	1.35838300	-2.05557400
C	-4.45688800	-0.96198900	1.88606000	C	-1.49106000	0.37821200	2.35631200
C	-3.98826600	-0.78246000	-0.61311800	H	-0.58436100	0.93101500	2.09907400
H	-5.33472400	-2.20191000	0.36094200	H	-1.90208800	0.78322100	3.29285500
H	-5.23338500	-1.13639300	2.64254000	H	-1.20983500	-0.66898800	2.50512700
C	-3.27203400	-1.91602700	2.11947600	C	-2.95476500	1.99243800	1.12668900
H	-4.12899200	0.07687300	2.00569300	H	-2.08742700	2.64213700	0.99014700
N	-2.61198800	-0.99545400	-0.06309400	H	-3.65269500	2.16928500	0.30264800
C	-2.38063200	-2.14860600	0.85526300	H	-3.45797300	2.27628600	2.06324900
H	-3.64735700	-2.89118200	2.45717300	O	0.18736700	3.28898700	-0.36719800
H	-2.65171100	-1.52465400	2.93393100	H	-0.49292400	2.57819000	-0.41440000
O	-1.71190200	-1.07967800	-1.17507500	O	1.41109900	2.44715800	-0.34695600
C	-0.90231800	-2.10976400	1.28415500				
H	-0.23603600	-2.37788200	0.46122500				
H	-0.63153900	-1.10905800	1.63394000				
H	-0.73904100	-2.82267600	2.10101800				
C	-2.64989200	-3.53813100	0.22424400				
H	-2.26541800	-4.32546900	0.88396200				
H	-3.71545400	-3.73269800	0.07107500				
H	-2.13297700	-3.61676500	-0.73623800				

C	-4.09032300	0.72343900	-0.93058500				
H	-3.29735700	1.01420000	-1.62432800				
H	-5.05813400	0.95760400	-1.39154900				
H	-3.97820300	1.32530800	-0.02378600				
C	-4.29553400	-1.56763400	-1.90932700				
H	-3.60469000	-1.28338200	-2.70528200				
H	-4.22274500	-2.64809600	-1.76701200				
H	-5.31905600	-1.33817400	-2.23239000				
33				TS33-34			
Charge=-2 Multiplicity =2				Charge=-2 Multiplicity =2			
C	-1.18387600	3.09138400	0.28211200	C	2.02914300	2.41464600	-0.92118200
C	-0.61956900	3.86562500	1.51150300	C	1.38845900	3.46369600	-1.85954500
C	0.77688700	4.34162300	1.02982100	C	0.57706200	4.35802700	-0.89182000
C	0.94109700	3.65626400	-0.38208500	C	0.48351900	3.50604000	0.43510500
H	-1.86289700	2.28141000	0.56412200	H	2.29198100	1.46708500	-1.40208400
H	-1.76815500	3.81072500	-0.34198800	H	2.96599400	2.84413800	-0.50062900
H	-0.52596200	3.17849100	2.36108400	H	0.72398900	2.95556700	-2.56860400
H	-1.26671700	4.69976100	1.82608400	H	2.12830400	4.03008900	-2.44414500
H	0.84825600	5.43463500	0.95118800	H	1.08374500	5.31175700	-0.69660100
H	1.57133300	4.01384500	1.71051200	H	-0.41796500	4.59870700	-1.28200400
H	0.74920800	4.43536700	-1.15006700	H	1.06068100	4.03068200	1.21819400
N	-0.03916800	2.59147200	-0.44108100	N	1.06139800	2.19628900	0.14411800
C	2.36735900	3.12754500	-0.60505900	C	-0.96939100	3.39385000	0.92634600
O	3.28477700	3.92206800	-0.90188700	O	-1.51046400	4.36208100	1.49208400
Cu	0.78152700	0.86664700	-0.07490700	Cu	-0.27344800	0.87656800	-0.04856000

O	2.51274600	1.85679000	-0.43100000	O	-1.55249300	2.26722400	0.66683200
H	5.27817600	-2.23339400	2.11869900	H	-5.20727000	0.70329900	0.04826200
C	4.79758000	-2.28785100	1.13165800	C	-4.98172100	-0.36740600	0.11332700
C	5.57203200	-1.48277500	0.08903400	C	-4.91329500	-0.77055100	1.59754900
C	3.33320000	-1.78712800	1.25935400	C	-3.66684300	-0.66316800	-0.68368800
H	4.80705800	-3.34934100	0.84070300	H	-5.81210900	-0.89733400	-0.37654900
H	6.63666100	-1.76256700	0.09113600	H	-5.92877400	-0.91258500	1.99699900
C	4.96734200	-1.72709300	-1.30169300	C	-4.08470800	-2.04508100	1.76618200
H	5.51360600	-0.41662500	0.33146800	H	-4.45211200	0.03886400	2.17341800
N	2.92910300	-1.17657900	-0.03023500	N	-2.57355500	-0.74587200	0.31569900
C	3.40101000	-1.76856900	-1.30194400	C	-2.60838300	-1.81996400	1.34222100
H	5.34758000	-2.67968600	-1.70163200	H	-4.53146600	-2.84894400	1.16412400
H	5.30968600	-0.94055000	-1.98437300	H	-4.10288700	-2.39389800	2.80806000
O	1.53712600	-0.96265500	-0.06619300	O	-1.29091100	-0.69722700	-0.27742500
C	2.89006300	-0.86276500	-2.44037600	C	-1.80453400	-1.28472600	2.54939300
H	1.80909800	-0.96026300	-2.56293900	H	-0.77903500	-1.06458200	2.24330500
H	3.11152800	0.18247500	-2.20546900	H	-2.24590800	-0.35809500	2.92949900
H	3.38271700	-1.14618100	-3.38173800	H	-1.77575400	-2.02986600	3.35634100
C	2.88221600	-3.21011200	-1.57201800	C	-1.96962100	-3.15832900	0.90081200
H	3.09119500	-3.50527300	-2.61051700	H	-1.98340400	-3.86870000	1.73962400
H	3.35366500	-3.95231400	-0.91787100	H	-2.50440100	-3.61498500	0.06379900
H	1.79919700	-3.23577800	-1.41525100	H	-0.93471100	-2.99799000	0.59290900
C	3.26414300	-0.65333000	2.30745900	C	-3.37335000	0.53764200	-1.60348300
H	2.25215300	-0.24269700	2.33837300	H	-2.53645800	0.32422500	-2.27245900

H	3.52240500	-1.03235800	3.30673300	H	-4.26301400	0.74880000	-2.21325500
H	3.94373400	0.16132200	2.04001200	H	-3.12802200	1.41807000	-1.00273500
C	2.43709700	-2.94976500	1.76112600	C	-3.84605600	-1.91467600	-1.59100200
H	1.42329500	-2.60022900	1.96781900	H	-2.90374800	-2.17803000	-2.07997300
H	2.37953300	-3.76646500	1.03615000	H	-4.21461100	-2.78468000	-1.03722600
H	2.85627500	-3.35492300	2.69397700	H	-4.58258000	-1.69406800	-2.37701300
O	-0.76417100	-1.38230700	1.01450100	O	-0.44206100	-2.25580700	-2.40792500
H	0.14925500	-1.53389300	0.65878600	H	-0.77571300	-1.70539900	-1.65377800
O	-0.94069400	0.02462600	0.58542300	O	0.46421900	-1.31697900	-3.07820600
C	-3.89132200	-1.18174700	0.11695100	C	2.97922300	-1.82322800	-0.92637300
O	-3.17155100	-0.25579400	-0.64583400	O	2.11857100	-0.81040500	-1.24224500
H	-2.23940000	-0.12203300	-0.21708800	H	1.18387300	-1.14185000	-2.32996700
H	-3.63264000	-1.07621400	1.18497900	H	3.48816700	-2.24148000	-1.83373100
C	-5.38945800	-0.91803400	-0.02125000	C	4.12227100	-1.37221400	0.00294600
C	-6.32997000	-1.62930500	0.74262300	C	5.33116700	-2.08145900	0.08729900
C	-5.86408600	0.04474200	-0.92339700	C	3.96572900	-0.23415800	0.80878300
C	-7.70096400	-1.39555800	0.60586600	C	6.35375000	-1.68005900	0.95361400
H	-5.98293700	-2.37103800	1.45903700	H	5.47322100	-2.95911500	-0.54303100
C	-7.23569500	0.27943100	-1.06700000	C	4.98227200	0.16954900	1.68032300
H	-5.12710900	0.60324700	-1.49065200	H	3.04023800	0.32801000	0.72065700
C	-8.16321800	-0.43881500	-0.30566900	C	6.18207400	-0.54838600	1.75999800
H	-8.40878900	-1.95631600	1.21370600	H	7.28480500	-2.24460900	0.99598900
H	-7.58078900	1.03322400	-1.77209800	H	4.83800400	1.05603900	2.29518000
H	-9.22973300	-0.25239100	-0.41388100	H	6.97473700	-0.22692000	2.43365600

C	-3.54103900	-2.62837200	-0.29859100	C	2.25285600	-3.03205300	-0.26268600
H	-2.46581700	-2.76105100	-0.15135800	H	1.44800600	-3.35934100	-0.92835100
H	-4.08152600	-3.37494600	0.29989500	H	2.93312300	-3.87507300	-0.06287800
H	-3.78781700	-2.77916800	-1.35664200	H	1.80353700	-2.71022300	0.68489000
34				35			
Charge=-2 Multiplicity =2				Charge=-2 Multiplicity =1			
C	-2.06334200	2.25301000	1.36223800	H	-0.03240000	-0.02997300	0.06857200
C	-1.06609600	3.14414700	2.15195900	O	-0.13897400	0.27426000	0.99798500
C	-0.36651700	3.96455800	1.03916500	O	-0.01255900	-0.85286600	-1.72207000
C	-0.80069700	3.24065700	-0.29823700	C	1.21307600	0.25416100	-5.04134900
H	-2.30958600	1.31526600	1.87118900	C	1.47891500	0.18166000	-6.58165700
H	-3.01724300	2.82511800	1.24709800	C	0.34211700	-0.74164200	-7.12822000
H	-0.34365300	2.50630100	2.67513200	C	-0.50406800	-1.01313000	-5.86682000
H	-1.55687300	3.78016000	2.90529400	H	2.12784400	0.29666900	-4.44031200
H	-0.68937300	5.01403800	1.03403700	H	0.62306200	1.16905200	-4.81796300
H	0.72343400	3.96536500	1.15484100	H	2.46564800	-0.25549600	-6.77894900
H	-1.49383200	3.92095100	-0.83353900	H	1.46294000	1.18033200	-7.04124500
N	-1.44485700	1.99505800	0.07969100	H	-0.24294500	-0.27102900	-7.92837700
C	0.39960600	2.98638600	-1.22483400	H	0.73935700	-1.68508700	-7.51766800
O	0.85108700	3.91278800	-1.92908000	H	-1.24940600	-0.18346200	-5.78185100
Cu	-0.18724900	0.48788300	-0.07998400	N	0.47895200	-0.96632200	-4.79569000
O	0.88745300	1.79217100	-1.16834000	C	-1.31908500	-2.30547600	-5.72006800
H	4.47169800	1.45230700	1.10355200	O	-1.80421400	-2.89240000	-6.70111400
C	4.60842500	0.41222300	0.78344000	Cu	-0.42765800	-1.52705000	-3.22996500
C	4.97720500	0.39568500	-0.71030000	O	-1.46801900	-2.64787300	-4.47749300

C	3.31434100	-0.40649000	1.11753600	H	6.19005300	0.53141300	2.76948500
H	5.44323000	0.00684600	1.37517800	C	5.48628400	0.64637600	1.93108700
H	6.03968400	0.65343200	-0.83896900	C	6.15253300	1.42296400	0.77229900
C	4.67778700	-0.97969900	-1.30888000	C	4.18399200	1.28548800	2.45019000
H	4.39138000	1.15423100	-1.23938400	H	5.23274300	-0.36627000	1.59155700
N	2.55386800	-0.53639800	-0.14708500	H	6.62467800	0.70603500	0.08632700
C	3.15438800	-1.28424100	-1.27652700	C	5.14973800	2.30800200	0.00297500
H	5.23116200	-1.74653300	-0.74690800	H	6.96750400	2.05643700	1.15356400
H	5.02866800	-1.04492300	-2.34810900	N	3.21774000	1.36374300	1.33471300
O	1.20927300	-0.93485400	0.04750100	C	3.69900300	1.76202300	-0.03362600
C	2.49803400	-0.73497000	-2.56309200	H	5.50027600	2.45243100	-1.03093900
H	1.42150800	-0.91503300	-2.53659300	H	5.12104100	3.30751400	0.45513600
H	2.63506800	0.34677300	-2.63701400	O	2.02802200	1.93674400	1.72246100
H	2.91997800	-1.23081700	-3.44947300	C	2.79673600	2.85974700	-0.62342300
C	2.92423900	-2.81710100	-1.23863200	H	1.77299200	2.50189300	-0.74654500
H	3.33953800	-3.27814900	-2.14655400	H	2.76450800	3.73429900	0.03492100
H	3.39895900	-3.28700500	-0.37284600	H	3.19055700	3.15840700	-1.60678700
H	1.85423900	-3.03378000	-1.19581700	C	3.61777100	0.51792200	-0.95152900
C	2.45661000	0.41216600	2.10103200	H	3.91740500	0.76974500	-1.98126600
H	1.59722600	-0.16305000	2.45270400	H	4.27212000	-0.28613800	-0.59224400
H	3.07003700	0.69516700	2.96798300	H	2.59481300	0.12820000	-0.97761300
H	2.09721500	1.32291000	1.61245900	C	4.44390300	2.65986100	3.13588700
C	3.68743300	-1.74003800	1.83276300	H	3.47210300	3.15436400	3.24952000
H	2.79842900	-2.35910900	1.98332600	H	4.90079900	2.52869200	4.12884000

H	4.43297500	-2.31456000	1.27255700	H	5.10268000	3.31099600	2.55023000
H	4.12103400	-1.51990500	2.81940100	C	3.56003500	0.34850000	3.50716100
O	0.49443000	-3.00429400	1.56356100	H	2.62427600	0.77956100	3.87315700
H	0.82752100	-2.25033100	0.98183800	H	3.32352200	-0.62088000	3.05383800
O	-0.36659200	-2.27345800	2.50216100	H	4.25292200	0.19591000	4.34936500
C	-2.23923800	-1.74637900	-0.14488100	H	0.65301300	0.83465500	1.21176500
O	-1.51486400	-0.86614500	0.65395600				
H	-0.88622000	-1.68945400	1.84760300				
H	-2.21796300	-2.75763700	0.30963100				
C	-3.71969800	-1.35569500	-0.25800500				
C	-4.73388800	-2.31960200	-0.16730200				
C	-4.08685100	-0.01759800	-0.48393400				
C	-6.08365200	-1.97211200	-0.30618300				
H	-4.46089900	-3.35639900	0.02570900				
C	-5.43223200	0.33131200	-0.62565900				
H	-3.30113800	0.73917800	-0.52577800				
C	-6.43925000	-0.64037800	-0.53970900				
H	-6.85394100	-2.73788400	-0.22312300				
H	-5.69799700	1.37264800	-0.79846600				
H	-7.48635900	-0.36043700	-0.64344400				
C	-1.64455800	-1.89540900	-1.56505600				
H	-0.59634400	-2.19513700	-1.47996700				
H	-2.19203800	-2.64496600	-2.15469000				
H	-1.69096300	-0.93704600	-2.09705500				
36				37			

Charge=-1 Multiplicity =1				Charge=-1 Multiplicity =1			
O	0.02088200	0.00295600	0.04749600	O	0.45962300	1.18609700	-0.03850800
C	-0.00482700	0.00386200	3.51966700	C	-0.20052100	0.24598500	3.73833700
C	1.48995100	-0.00195400	3.91406000	C	0.70166200	-0.43452300	4.78457400
C	1.79594700	1.49611600	4.17487400	C	1.34807700	0.77539900	5.48016300
C	0.55325900	2.25391400	3.57726600	C	1.49187600	1.79568600	4.32730500
H	-0.30437400	-0.84243000	2.89641800	H	-0.45060600	-0.37890500	2.87424300
H	-0.62005400	-0.01825600	4.44409900	H	-1.15963800	0.54358800	4.20412300
H	2.08309600	-0.37754700	3.07161400	H	1.46549400	-1.04163500	4.28169000
H	1.70191100	-0.63771600	4.78507200	H	0.14711800	-1.08790300	5.46956000
H	1.90073400	1.71569900	5.24408300	H	0.67506900	1.16732700	6.25538000
H	2.72558400	1.81260100	3.68916100	H	2.31522300	0.56386600	5.94494800
H	-0.04734500	2.65779000	4.40982500	H	1.32393700	2.82605000	4.67671900
N	-0.24538400	1.26974000	2.83869900	N	0.49004800	1.46429800	3.30967100
C	0.95438200	3.42625800	2.66789000	C	2.91714400	1.80965400	3.68700600
O	1.32725500	4.50092600	3.14728600	O	3.90375800	1.90200600	4.41971900
Cu	0.25922100	1.39615600	1.00103600	Cu	1.23256000	1.47988800	1.50447300
O	0.89545700	3.15512200	1.39314300	O	2.93359800	1.74720600	2.39537000
				C	-1.13815900	1.52591600	-2.86627300
				O	-0.95055400	0.34868900	-2.11583900
				H	-0.41434000	0.59205100	-1.29645300
				H	-1.61073300	2.30166500	-2.23699900
				C	0.21047700	2.08784800	-3.36166300
				H	0.07904000	3.02474200	-3.91984600
				H	0.85319500	2.27685200	-2.49533000

	H	0.70218200	1.35658700	-4.01499700
	C	-2.07772000	1.23949900	-4.02950700
	C	-2.64953300	2.29262100	-4.76043100
	C	-2.38006200	-0.07497400	-4.40961600
	C	-3.49051400	2.04411400	-5.84800600
	H	-2.43747600	3.32078900	-4.47078400
	C	-3.22106500	-0.32845100	-5.49854900
	H	-1.95327600	-0.88667300	-3.82977100
	C	-3.77927500	0.72769200	-6.22468300
	H	-3.92469400	2.87712600	-6.39795500
	H	-3.44461200	-1.35670600	-5.77755600
	H	-4.43564600	0.52965100	-7.06977000
38	39			
Charge=-1 Multiplicity =1	Charge=-1 Multiplicity =1			
O	O	-1.19411300	2.71100800	0.02743400
C	C	-0.70015100	-0.65051300	-1.10776800
C	C	-0.73531400	-2.14438100	-0.72446100
C	C	-2.20562400	-2.55495600	-0.94155600
C	C	-2.97955600	-1.22890300	-0.78751600
H	H	-0.01330600	-0.02141700	-0.42173500
H	H	-0.25063000	-0.44227900	-2.09840600
H	H	-0.45255700	-2.25428100	0.33022100
H	H	-0.03332000	-2.74816100	-1.31101600
H	H	-2.34654800	-2.95028400	-1.95609500
H	H	-2.56697800	-3.30704000	-0.23417500
	O	-1.23316000	-0.42513700	1.20862000
	C	2.19184000	-0.85232000	4.36057200
	C	3.37806100	-0.19724000	3.60911200
	C	3.02208400	1.31109900	3.58347000
	C	1.55661100	1.36549500	4.14592800
	H	1.97287500	-1.87187200	4.03159000
	H	2.40861200	-0.88621400	5.44676100
	H	3.43088500	-0.60060400	2.59079500
	H	4.34427600	-0.39525600	4.09278000
	H	3.69590500	1.91400400	4.20316700
	H	3.06828000	1.71997500	2.56792200

H	-3.80242400	-1.15956700	-1.51731100	H	1.58827500	1.75347100	5.17729900
N	-2.03570200	-0.14735500	-1.07195600	N	1.02985900	-0.00114900	4.15960900
C	-3.68062000	-1.00746400	0.58789300	C	0.64670100	2.26335700	3.31547900
O	-4.31678600	-1.92064800	1.10805100	O	0.65850400	3.48978400	3.39603100
Cu	-2.30921100	1.32801100	0.19841000	Cu	-0.00644700	-0.27216600	2.57890100
O	-3.57140000	0.20182600	1.05897500	O	-0.11458200	1.59510500	2.47743900
C	2.12752900	1.15195400	-0.43698300	C	-0.39010800	-2.99855500	1.86549800
O	1.01956500	1.03541600	0.36622600	O	0.36006400	-2.08851300	2.61416000
H	-0.29915500	2.32483900	0.21280600	H	-1.47071600	0.49592100	1.00784000
H	1.87791800	0.91912400	-1.50190700	H	-0.98593500	-2.46854200	1.10735800
C	2.65929900	2.61053000	-0.43496300	C	0.58945200	-3.94279100	1.13158000
H	3.52998500	2.73565500	-1.09440700	H	0.05918200	-4.69194800	0.52866800
H	1.86148500	3.28388600	-0.76785100	H	1.23158100	-3.34967000	0.47041700
H	2.94902900	2.89417400	0.58443500	H	1.22525700	-4.46732200	1.85626100
C	3.26140700	0.18484200	-0.04890000	C	-1.36343000	-3.79914400	2.73855700
C	4.32288300	-0.09426700	-0.92356600	C	-2.32915200	-4.63506100	2.15469500
C	3.25683500	-0.43483300	1.20730200	C	-1.31426400	-3.72169600	4.13631300
C	5.35763700	-0.95850000	-0.55383700	C	-3.20948300	-5.38337900	2.94019400
H	4.33565500	0.36673100	-1.91110300	H	-2.40151600	-4.68998800	1.06932900
C	4.29019500	-1.29857400	1.58516500	C	-2.19316800	-4.46843100	4.92824000
H	2.41640700	-0.22945300	1.86444300	H	-0.58783000	-3.05103700	4.58477000
C	5.34692400	-1.56437300	0.70791500	C	-3.14283200	-5.30629900	4.33613100
H	6.16880100	-1.16430900	-1.25067400	H	-3.95373600	-6.01964400	2.46381400
H	4.26750200	-1.77181500	2.56562500	H	-2.14072600	-4.38818500	6.01279300

H	6.14838700	-2.24080700	0.99911700	H	-3.82977300	-5.88376300	4.95201600
TS₃₉₋₄₀				TS₃₉₋₄₁			
Charge=-1 Multiplicity =1				Charge=-1 Multiplicity =1			
O	-0.44466500	-1.14567000	-0.60933500	O	-0.15441000	0.21598500	-0.27219700
C	1.83592600	1.81047200	-0.92760200	C	-0.09101400	-0.09113600	4.37449100
C	2.84338400	2.67182000	-0.12155000	C	1.08916800	0.08215000	5.36009400
C	3.71868700	1.62306500	0.58161400	C	1.41981800	1.58232500	5.26954900
C	3.74634100	0.47602500	-0.45787600	C	1.09667900	1.89281800	3.80279000
H	0.86621600	1.74760000	-0.41372100	H	-0.02381600	-1.02760600	3.80675400
H	1.62766700	2.25120900	-1.91717800	H	-1.05935900	-0.10358400	4.89368800
H	2.34419200	3.35728300	0.57394000	H	1.95181300	-0.50486600	5.02320600
H	3.45899100	3.27815000	-0.80110200	H	0.83696100	-0.24660100	6.37548200
H	4.72151300	1.97961600	0.84059400	H	0.76628800	2.16465200	5.93427900
H	3.23438000	1.27192600	1.50287400	H	2.46161900	1.81440400	5.50704600
H	4.52128500	0.70292000	-1.21105500	H	0.86774200	2.95379900	3.63316400
N	2.42284400	0.46964500	-1.09651300	N	-0.06760000	1.07105100	3.44809300
C	4.09195100	-0.88443300	0.17681700	C	2.26766200	1.52394200	2.81863800
O	5.25940800	-1.14418500	0.48164600	O	3.42286800	1.82896900	3.13196900
Cu	1.42960200	-1.05269300	-0.35001400	Cu	-0.08837800	0.73308800	1.49801000
O	3.07304700	-1.67083600	0.38682000	O	1.89061100	0.93792000	1.73431000
C	-2.06064800	0.45084400	0.90609500	C	-2.43283500	1.82160800	2.68194100
O	-1.63518200	1.69979900	0.83093100	O	-2.05144200	1.16208000	1.57592200
H	-0.68141000	-0.93345900	-1.52636800	H	-1.08674300	0.32479900	-0.52241400
H	-1.30277500	-0.18814400	0.17619700	H	-1.39564000	1.68154100	3.40614300
C	-1.80892400	-0.23866500	2.27132300	C	-2.56655800	3.34274800	2.48132600

H	-1.98923600	-1.31807000	2.22985300	H	-2.69754700	3.89318600	3.42115600
H	-0.76850000	-0.07063500	2.56634600	H	-1.66283800	3.71587200	1.98749600
H	-2.46598900	0.19661300	3.03709100	H	-3.42265400	3.56626100	1.82806100
C	-3.44657500	0.18294800	0.32112600	C	-3.54528900	1.16323900	3.46743400
C	-3.92959400	-1.12444000	0.13880500	C	-4.13403200	1.76247500	4.59890600
C	-4.26579600	1.25366300	-0.06939300	C	-4.00355400	-0.11315800	3.09040100
C	-5.19780700	-1.35323700	-0.40132100	C	-5.13919900	1.11484700	5.32099100
H	-3.29747500	-1.96884800	0.40159700	H	-3.80065800	2.74447700	4.92530100
C	-5.53602800	1.02803400	-0.60708500	C	-5.00731100	-0.76217400	3.81227400
H	-3.88237000	2.26235400	0.05455200	H	-3.55607100	-0.57144200	2.21395300
C	-6.01095000	-0.27708200	-0.77406600	C	-5.58372200	-0.15413900	4.93313900
H	-5.54896600	-2.37435400	-0.53880900	H	-5.57590300	1.60274500	6.19090200
H	-6.15737100	1.87389300	-0.89688800	H	-5.34505400	-1.74758300	3.49547100
H	-6.99918600	-0.45443600	-1.19374600	H	-6.36704400	-0.65889100	5.49492400
40				41			
Charge=-1 Multiplicity =1				Charge=-1 Multiplicity =1			
O	-0.16773400	2.42318800	-1.31177200	O	-3.48842100	-2.66186200	-1.12314200
C	-1.53844200	-2.32411800	-0.43317700	C	-4.54212400	1.47693700	-0.50369300
C	-1.45612700	-2.48349400	1.11697000	C	-4.62921100	1.25417900	1.01803700
C	-2.36848000	-1.34472300	1.64816000	C	-3.17244200	1.46160200	1.52282700
C	-2.91215900	-0.65628200	0.35031900	C	-2.31461900	1.63616000	0.23410900
H	-0.59700100	-2.58156900	-0.93578200	H	-5.25842800	0.86925700	-1.06847900
H	-2.30860600	-3.03515000	-0.81449500	H	-4.72831300	2.54466300	-0.74352300
H	-0.42135700	-2.34941800	1.45739100	H	-4.95712200	0.22938500	1.21849100
H	-1.78639200	-3.47918500	1.44948500	H	-5.34323800	1.93844700	1.49205800

H	-3.18544400	-1.70709600	2.28385700	H	-3.06890200	2.33741300	2.17158700
H	-1.79047800	-0.62159400	2.23635500	H	-2.83348300	0.58811900	2.08906200
H	-3.87977600	-1.13566200	0.10261600	H	-2.12205500	2.71067600	0.07154400
N	-1.93122000	-0.95981600	-0.69436000	N	-3.17472500	1.06128800	-0.79958000
C	-3.21867300	0.85016600	0.58987400	C	-0.93399600	0.94997400	0.34836400
O	-4.26147500	1.12593700	1.21232900	O	0.00641800	1.64534900	0.78255900
Cu	-0.88532200	0.54835700	-1.00455100	Cu	-2.23308200	-1.45010500	-0.57056900
O	-2.34659500	1.69596800	0.15849900	O	-0.84255600	-0.28874300	0.02533600
C	2.83721000	1.51953300	0.67117300	C	3.37940200	-1.50616500	0.88530900
O	2.25684200	2.45692800	0.10037900	O	4.10509200	-2.49687800	0.94967500
H	-0.89842200	2.75166300	-0.74159800	H	-3.11364200	-3.55582100	-1.08815700
H	0.66515300	2.53130100	-0.79943600	H	-2.87177500	1.28176400	-1.74500600
C	3.63465000	1.82193000	1.93077700	C	2.00751600	-1.50093800	1.51830600
H	4.64800900	1.40535900	1.88875200	H	1.94243600	-0.71766400	2.28467700
H	3.68869800	2.90564100	2.05622000	H	1.21020100	-1.27298800	0.79826800
H	3.13728400	1.39313700	2.81128800	H	1.82608100	-2.47670400	1.97510900
C	2.75306200	0.13527000	0.17788000	C	3.85972200	-0.26495000	0.18435100
C	3.25233500	-0.95511400	0.92670000	C	3.04216800	0.86726300	0.03207300
C	2.12189800	-0.12955000	-1.06097100	C	5.17015100	-0.24632600	-0.32640200
C	3.14893300	-2.25565100	0.44773700	C	3.53965500	1.99945700	-0.62264700
H	3.71358800	-0.78452500	1.89520400	H	2.01723000	0.89243600	0.40107500
C	2.03868700	-1.43820100	-1.54510500	C	5.66076300	0.88454900	-0.97502600
H	1.77237700	0.69587800	-1.66850900	H	5.78484900	-1.13305200	-0.20188600
C	2.54728000	-2.50063200	-0.79932500	C	4.84304300	2.01336700	-1.12424500

H	3.52804200	-3.08362300	1.04213900	H	2.89409200	2.86662400	-0.73664500
H	1.55192600	-1.62159600	-2.49880900	H	6.67633200	0.89032700	-1.36596400
H	2.46589800	-3.51816800	-1.17374600	H	5.22376300	2.89754100	-1.63224000
42				43			
Charge=-1 Multiplicity =1				Charge=-1 Multiplicity =2			
O	2.87518200	1.19025000	-0.11094800	O	-0.16583800	2.15393000	-1.50089300
C	-1.42341000	1.99515000	0.74229900	C	2.12361700	-1.65346000	-1.29893100
C	-1.84073700	1.89789800	-0.74054100	C	2.95763300	-2.78277400	-0.66075700
C	-1.96463300	0.37012400	-1.01037100	C	3.63323400	-2.07925300	0.53955200
C	-1.56336100	-0.31201300	0.32722800	C	2.76705700	-0.79840100	0.79387000
H	-0.74361200	2.83182600	0.94332000	H	2.75468100	-1.03145000	-1.95006700
H	-2.32370300	2.12229000	1.38027400	H	1.27552400	-2.00601400	-1.89538200
H	-1.06246300	2.33529500	-1.37427700	H	3.68232200	-3.22950600	-1.35543500
H	-2.77525700	2.43905300	-0.93399600	H	2.28714100	-3.58382900	-0.31898900
H	-2.97345800	0.06879000	-1.31068400	H	3.67013000	-2.72532100	1.42422000
H	-1.27519500	0.06481300	-1.80427400	H	4.66367700	-1.78660500	0.31809300
H	-2.47761000	-0.53784500	0.90451000	H	2.34541000	-0.80664100	1.80619400
N	-0.74800900	0.72166400	0.96492700	N	1.65571400	-0.83113900	-0.17704900
C	-0.83086700	-1.66122500	0.10713500	C	3.62855400	0.50317900	0.72324700
O	-1.54520500	-2.67840000	0.06252600	O	4.71552900	0.47654300	1.32611700
Cu	1.62913700	-0.15471800	-0.06351700	Cu	1.45875700	1.71378000	-0.72460700
O	0.44378200	-1.63558000	-0.04812200	O	3.15716100	1.51705100	0.09160000
H	3.71424400	0.83275200	-0.44177100	H	-0.11528500	3.06457300	-1.82981800
H	-0.54387200	0.52843600	1.94225700	H	0.82688600	-1.25742400	0.23846300
				H	-4.57373800	-0.13875600	-1.74650600

	C	-4.09983500	-0.08021100	-0.75775000
	C	-3.82974600	1.39065000	-0.38170500
	C	-2.85217300	-0.98595200	-0.78173800
	H	-4.81886100	-0.51800700	-0.05263100
	H	-4.74601900	1.80747400	0.05914600
	C	-2.62444900	1.56142500	0.56936000
	H	-3.62863000	1.97624300	-1.28646800
	N	-2.14926400	-0.86322200	0.53657600
	C	-2.29520100	0.32901600	1.43655200
	H	-2.79723000	2.40826900	1.24758900
	H	-1.73423700	1.81173100	-0.02365400
	O	-1.34998100	-1.81071400	0.88502800
	C	-0.96213800	0.57152900	2.16097100
	H	-0.69545000	-0.27458000	2.79988700
	H	-0.15376500	0.74483400	1.44444200
	H	-1.05829700	1.46813400	2.78507000
	C	-3.39083200	0.02602900	2.48610500
	H	-3.44212300	0.84727900	3.21250300
	H	-4.38273300	-0.08757100	2.03652400
	H	-3.14938600	-0.89641600	3.02711700
	C	-1.88107800	-0.60405900	-1.91831500
	H	-1.03638800	-1.30090500	-1.92761800
	H	-2.40136600	-0.68904900	-2.88271600
	H	-1.47015500	0.40805300	-1.82458600

	C	-3.30068500	-2.44891400	-0.94939900
	H	-2.44035400	-3.12180000	-0.96535200
	H	-3.96131600	-2.75756900	-0.12980200
	H	-3.84827000	-2.55155700	-1.89451200
TS43-44	44			
Charge=-1 Multiplicity =2	Charge=-1 Multiplicity =2			
O	O	-0.51995100	-0.46755900	-0.15221700
C	C	-0.10847400	-0.00482800	3.90108700
C	C	0.63619900	0.13238700	5.23711400
C	C	1.70493400	-0.97613900	5.14315700
C	C	1.91236000	-1.18230800	3.61446600
H	H	-0.81406700	-0.85029800	3.94969500
H	H	-0.67274900	0.88758700	3.61486600
H	H	-0.02453900	0.01846600	6.10652300
H	H	1.10695700	1.12109000	5.28640400
H	H	2.63759400	-0.69692600	5.64365200
H	H	1.36125600	-1.91091700	5.59890400
H	H	2.92722100	-0.89121900	3.32001000
N	N	0.95894100	-0.27312400	2.90951800
C	C	1.73542000	-2.65349700	3.17003300
O	O	2.26943900	-3.55911600	3.81489300
Cu	Cu	0.29791700	-1.25719500	1.28913800
O	O	1.03098000	-2.82886700	2.08840300
H	H	-1.48651600	-0.44203900	-0.08229600
H	H	1.57536100	0.81612300	2.68263000
	O	-0.14810700	0.30240700	-0.50068000
	C	-0.02923900	0.40970100	3.51848800
	C	0.61574700	0.48679600	4.91251000
	C	1.71597000	-0.59097300	4.82716800
	C	2.03840400	-0.67977000	3.30724400
	H	-0.72391400	-0.45307300	3.49507500
	H	-0.60988800	1.30037700	3.25293100
	H	-0.09889400	0.30719900	5.72555100
	H	1.05568700	1.48067600	5.05491500
	H	2.60019300	-0.33507800	5.41863300
	H	1.35867500	-1.56142400	5.18650600
	H	3.07088300	-0.35476300	3.11498700
	N	1.11355600	0.24595100	2.60662000
	C	1.95268000	-2.11925600	2.74675300
	O	2.45292100	-3.06812800	3.35474500
	Cu	0.61902100	-0.60122100	0.90586600
	O	1.35415700	-2.21780000	1.58910500
	H	-1.11274200	0.27008800	-0.50796300
	H	2.00221000	1.87164900	2.32563000

H	0.74443700	4.99074100	-0.14234900	H	0.81206800	5.59240100	-0.48006100
C	1.56791400	4.28203100	0.02076700	C	1.67465100	4.93240800	-0.32358800
C	1.74440300	3.37172700	-1.21344700	C	1.81685900	3.94465200	-1.50095100
C	1.29813000	3.51508400	1.33245200	C	1.51610800	4.24905800	1.04975100
H	2.46954200	4.89012900	0.16775500	H	2.55370600	5.58588600	-0.27216100
H	2.39565200	3.88007800	-1.93818400	H	2.39192100	4.42942800	-2.30070700
C	2.31903300	1.98713300	-0.84355500	C	2.48158300	2.61633600	-1.07697600
H	0.78077500	3.22834400	-1.71889300	H	0.83178600	3.72010000	-1.92607500
N	2.45058700	2.62095200	1.58760900	N	2.74834200	3.45153600	1.29669300
C	3.18144400	1.99053800	0.44168700	C	3.42451800	2.75578800	0.14213200
H	2.92400000	1.59763200	-1.67515700	H	3.05471200	2.19985200	-1.91602600
H	1.50079000	1.27316500	-0.70318500	H	1.70842400	1.87791400	-0.84499400
O	2.30006900	1.84248200	2.74333400	O	2.60950800	2.65750000	2.47350200
C	3.58179500	0.54179500	0.75603000	C	3.92147500	1.35775100	0.54105100
H	4.18339600	0.48519200	1.66672400	H	4.58542600	1.40392700	1.40760600
H	2.70748600	-0.10156100	0.88165800	H	3.09724100	0.68223200	0.77824900
H	4.17065600	0.14438100	-0.08074800	H	4.47400200	0.92762300	-0.30206200
C	4.49652700	2.78553700	0.21606400	C	4.67317300	3.59674600	-0.22820500
H	5.09564200	2.33464200	-0.58903400	H	5.23058000	3.12261500	-1.04714500
H	4.30661500	3.83039000	-0.04802900	H	4.41054100	4.61090300	-0.54069500
H	5.08890800	2.77913300	1.13819600	H	5.33087300	3.67890800	0.64313400
C	-0.07281900	2.79688500	1.25853400	C	0.19371900	3.44532100	1.10109500
H	-0.32709100	2.38112900	2.23649800	H	0.01593700	3.07674900	2.11425300
H	-0.85795500	3.51883000	0.99065900	H	-0.64254100	4.10723700	0.84044200

H	-0.09687800	1.97650600	0.53647600	H	0.17228400	2.58548800	0.42709900
C	1.24551200	4.53040200	2.49438400	C	1.46512000	5.33418300	2.14531700
H	1.15127800	3.99957400	3.44601400	H	1.45482700	4.86538600	3.13291600
H	2.16745600	5.12384700	2.52654500	H	2.34745600	5.98031400	2.08372000
H	0.39027800	5.21157900	2.37918600	H	0.56423900	5.95251400	2.03906300

Table S3. Relative corrections to Gibbs free energies for each reported structures.

complexes	sp(scrf) (M06)	Thermal (B3LYP)	D3-gep (M06)
	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
Path A			
0_-21	-2273.485878	0.192891	0.067396786
1_-21	-2659.42764	0.337532	0.112356044
TS₁₋₂_-21	-2659.402241	0.340241	0.112408152
2_-21	-2659.426585	0.338603	0.111884935
3_-21	-2576.138848	0.218211	0.077595835
TS₃₋₄_-21	-2576.120466	0.215467	0.080396848
4_-21	-2576.179261	0.214133	0.075793961
3_-23	-2576.141684	0.2169	0.077509011
TS₃₋₄_-23	-2576.1102	0.214175	0.080745813
4_-23	-2576.150106	0.216284	0.078738538
5_-21	-2577.392028	0.23801	0.090337242
TS₅₋₆_-21	-2577.368227	0.238029	0.090461608
6_-21	-2577.39754	0.239232	0.089760873
Path B			

7_-21	-2675.578289	0.345535	0.127366808
TS7-8_-21	-2675.539046	0.346597	0.121771655
8_-21	-2675.540846	0.342940	0.121251815
9_-11	-2599.650663	0.338802	0.115647962
TS9-10_-11	-2599.644396	0.333342	0.116564397
10_-11	-2599.706763	0.336352	0.11283197
11_-12	-2116.206173	0.094312	0.038643684
12_-12	-2502.142825	0.240038	0.082887295
TS12-13_-12	-2502.133498	0.237868	0.084669715
13_-12	-2502.144683	0.238284	0.08251689
TS13-14_-12	-2502.105359	0.234450	0.083347363
14_-12	-2502.168565	0.236253	0.081604761
15_-12	-2425.730372	0.215859	0.070248228
16_-11	-2909.237891	0.464319	0.145918361
17_-11	-2909.249887	0.465152	0.14664364
Path B'			
32_-22	-2674.958012	0.338554	0.121060002
33_-22	-3060.895468	0.484444	0.168021333
TS33-34_-22	-3060.877869	0.487124	0.166196281
34_-22	-3060.897421	0.488832	0.168708322
14a_-13	-2909.205564	0.455641	0.143896512
TS14a-15a_O_-13	-2909.172525	0.458065	0.146574041
15a_O_-13	-2909.202567	0.460744	0.148819587
14a_-11r	-2909.203627	0.4721	0.146903031
14a_-11u	-2909.205584	0.460521	0.143805507

TS _{14a-15a_O_-11u}	-2909.180823	0.464756	0.148267002
TS _{14a-15a_O_-11r}	-2909.178678	0.464614	0.148655682
15a_O_-11	-2909.23938	0.46209	0.150554484
TS _{14a-15a_N_-11r}	-2909.18095	0.471101	0.1498902
TS _{14a-15a_N_-13}	-2909.176975	0.467131	0.149250547
7' → 44			
7'_-21	-2675.571712	0.350776	0.127544068
TS _{7'-35_-21}	-2675.525685	0.344914	0.124336425
35_-21	-2675.549598	0.343815	0.120501113
36_-11	-2115.519208	0.085907	0.035107965
37_-11	-2501.469138	0.227536	0.079216546
38_-11	-2501.463904	0.229175	0.07991362
39_-11	-2501.505756	0.234639	0.079462836
TS _{39-40_-11}	-2501.462645	0.222488	0.078102973
40_-11	-2501.552603	0.230572	0.078955854
TS _{39-41_-11}	-2501.489947	0.228858	0.078770019
41_-11	-2501.576477	0.226665	0.076816242
42_-12	-2116.848289	0.104997	0.042438755
43_-12	-2600.358084	0.351235	0.117561203
TS _{43-44_-12}	-2600.31549	0.347964	0.120969798
44_-12	-2600.326769	0.351550	0.120185128
Path C			
18_-23	-2423.799686	0.194438	0.074422362
18_-21	-2423.794176	0.196148	0.074491611
20_-11	-2576.63828	0.234207	0.083471188

20_-13	-2576.638301	0.226887	0.081886961
21_-33	-4850.13295	0.448208	0.15309869
21_-31	-4850.108083	0.449043	0.153302311
22_-31	-4948.323558	0.559728	0.189318347
22_-33	-4948.322768	0.557925	0.189239083
Path D			
24_-24	-2907.296872	0.43922	0.150389985
25_-24	-3293.244642	0.582486	0.19326486
TS₂₅₋₂₆_-24	-3293.194767	0.591151	0.196426882
26_-24	-3293.222761	0.582937	0.196675578
Path F			
29_-12	-2523.907748	0.328929	0.106662064
30_-12	-2909.843988	0.476076	0.151056569
TS₃₀₋₃₁_-12	-2909.819218	0.474541	0.153259849
31_-12	-2909.836208	0.474998	0.150214939

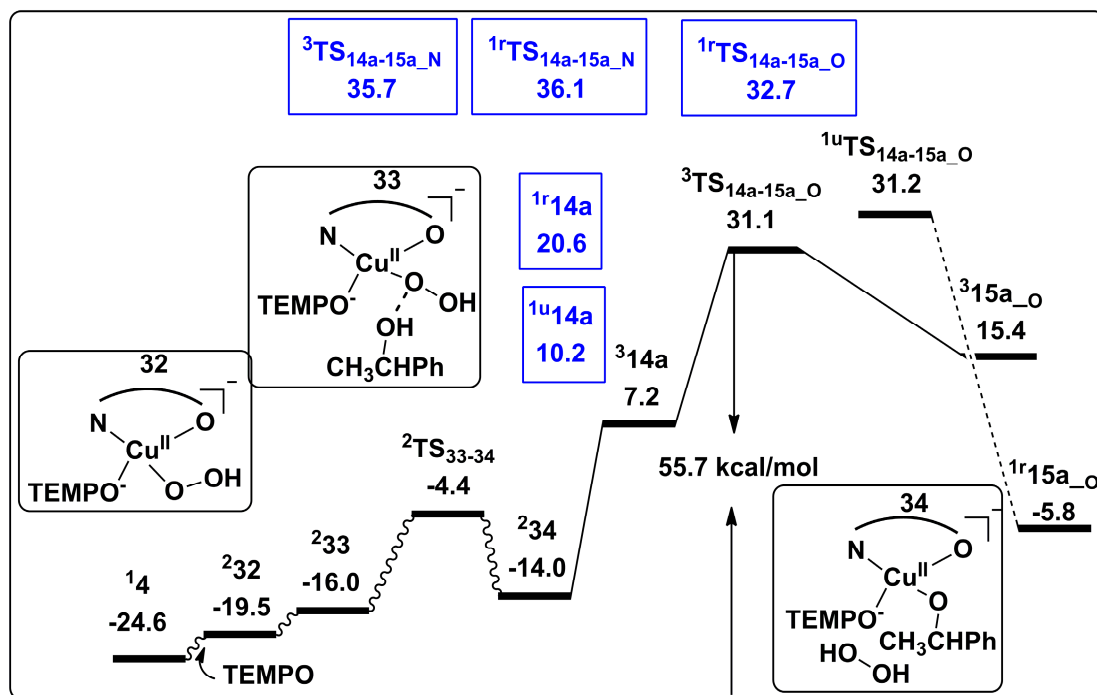


Figure S1. The calculated Gibbs free energy profiles for path B'. The energy values are in kcal/mol.

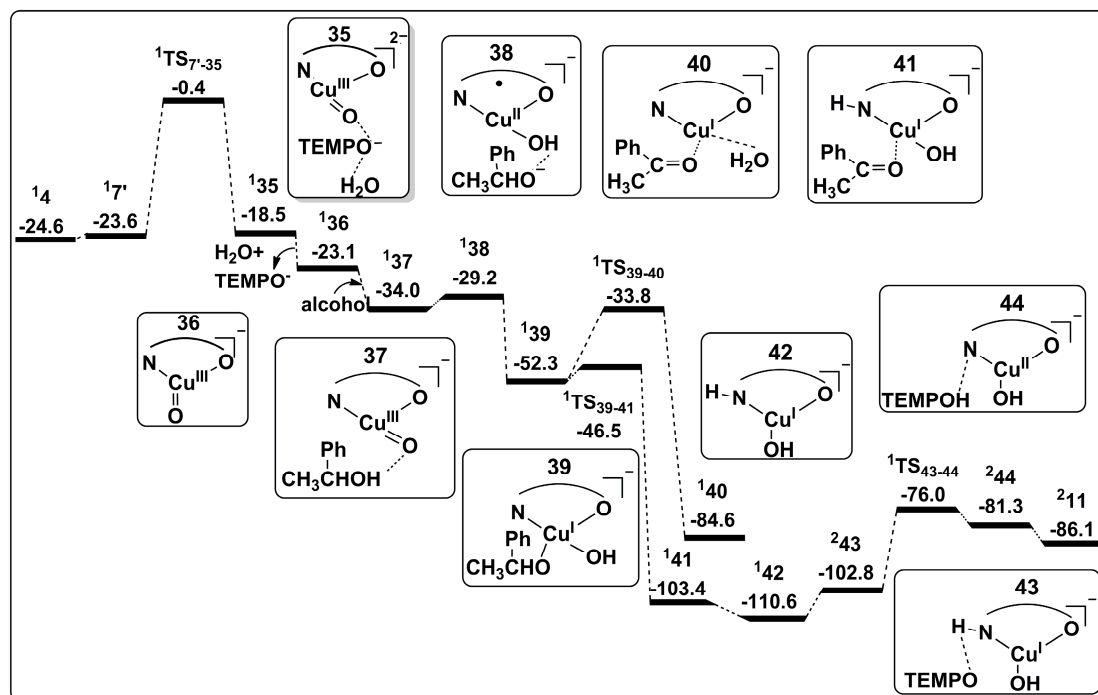


Figure S2. The calculated Gibbs free energy profiles for the process of **7***→**44**. The energy values are in kcal/mol.

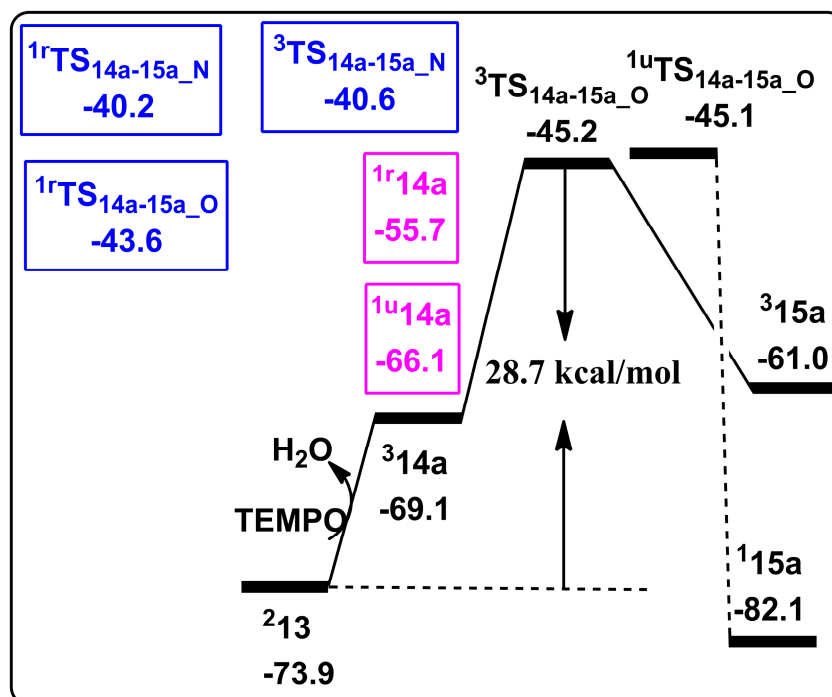


Figure S3. The calculated Gibbs free energy profiles for the process of $^2\mathbf{13} \rightarrow ^1\mathbf{15a}$. The energy values are in kcal/mol.

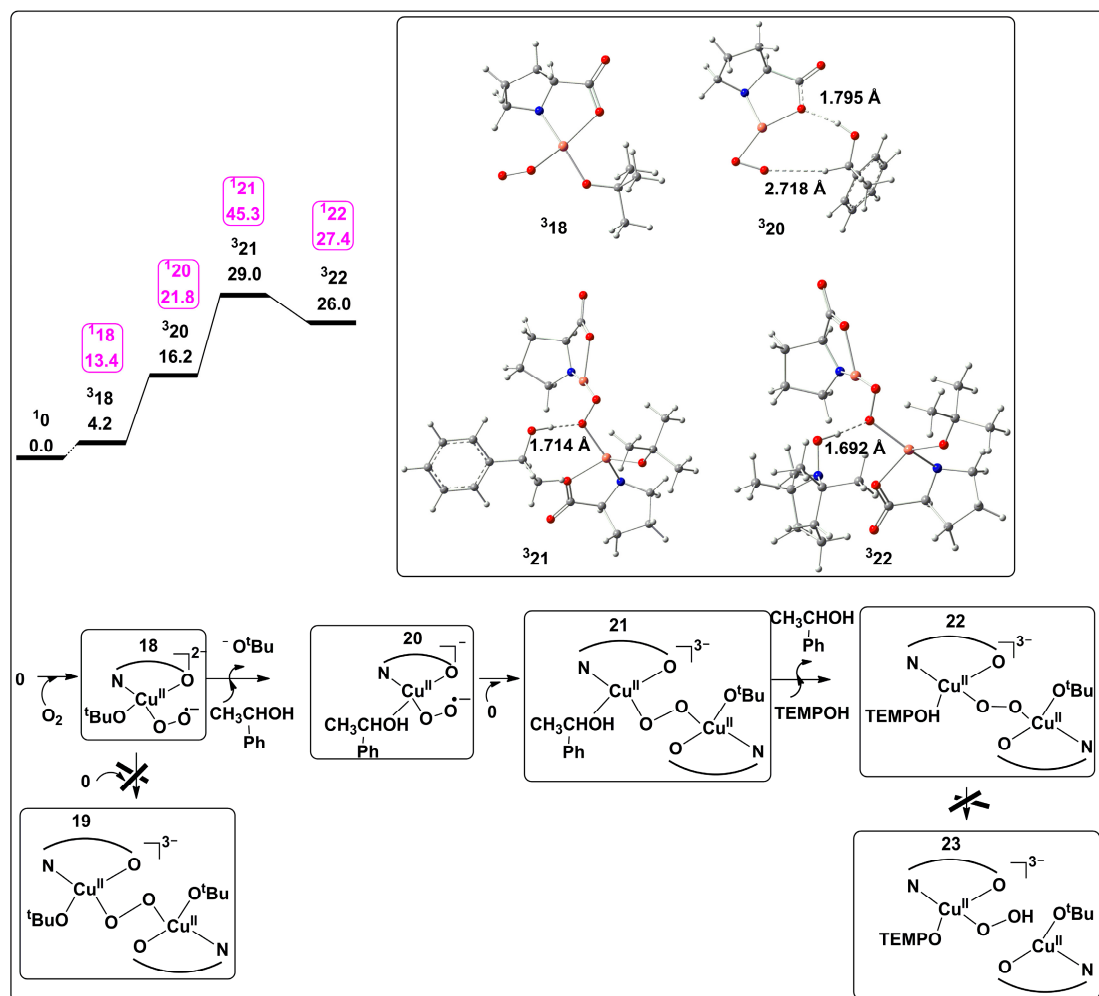


Figure S4. The calculated Gibbs free energy profiles for Path C. The energy values are in kcal/mol.

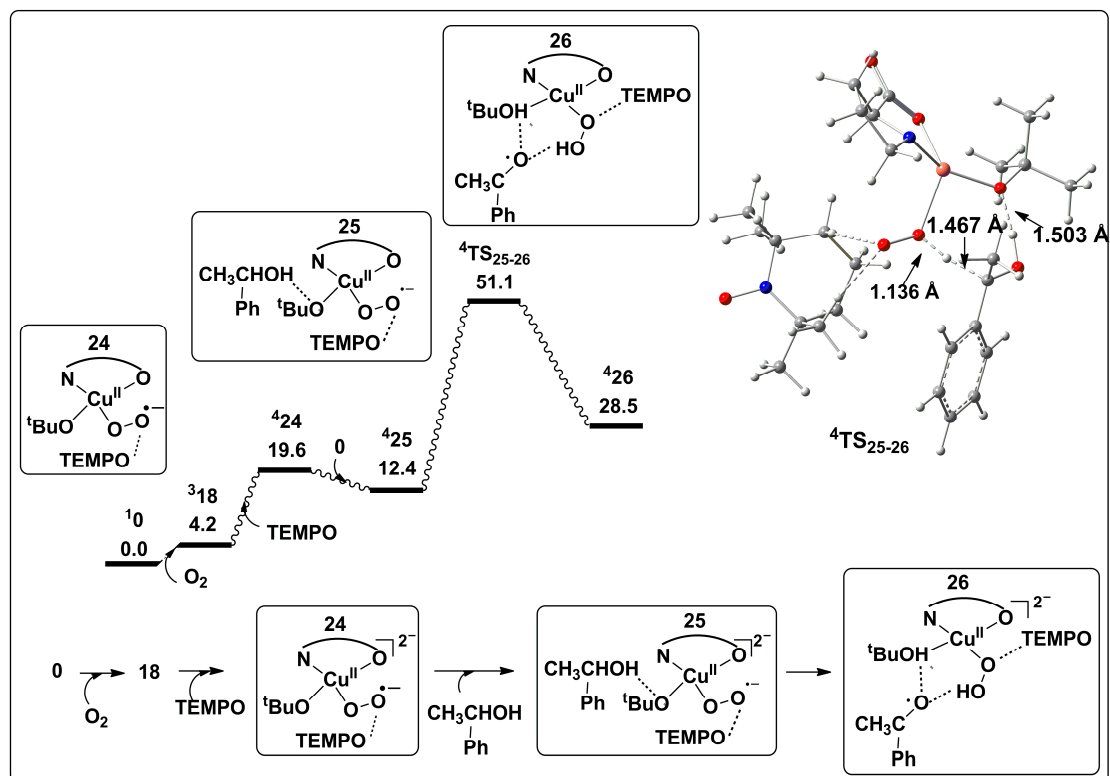


Figure S5. The calculated Gibbs free energy profiles for Path D. The energy values are in kcal/mol.