Supplementary Data

Mechanistic Unveiling of NH_3BH_3 Hydrolysis Catalyzed by a Cu–CAAC Complex

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To investigate the potential transition state for the direct reaction of **INT3** with $[NH_3BH_2(H_2O)]^+$ to form H_2, a potential energy surface scan was performed by varying the distance between the two relevant H atoms, as shown in Figure S2. When the interatomic distance between the two H atoms reached 1.00 Å, a L502 error occurred in Gaussian. Notably, the system was still far from the expected convergence region of the transition state at this point.

Subsequently, attempts were made to optimize the transition state by adjusting the structure parameters. these efforts not only failed to yield the desired transition state structure but also did not result in product formation. Instead, the optimization process directly reverted to the initial reactants (**INT3** and $[NH_3BH_2(H_2O)]^+$), as illustrated in Figure S3. Based on these observations, we conclude that a direct reaction between **INT3** and $[NH_3BH_2(H_2O)]^+$ to generate H_2 is unlikely.

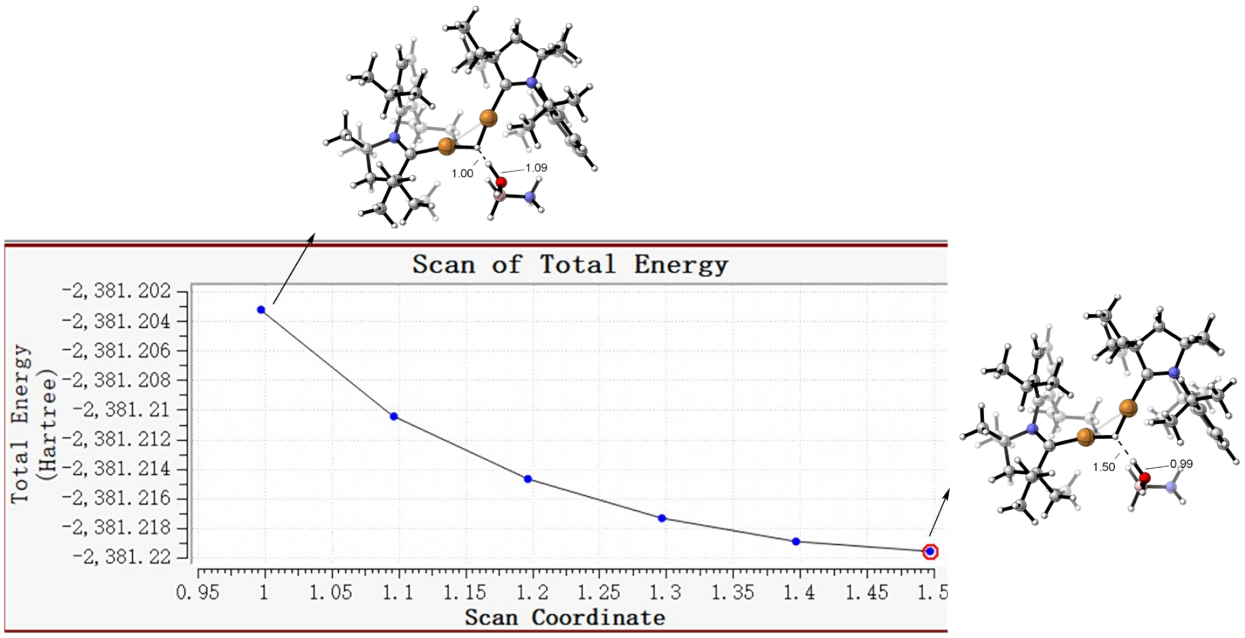

Figure S1. Potential energy surface scan of the H…H distance between **INT3** and $[NH_3BH_2(H_2O)]^+$.

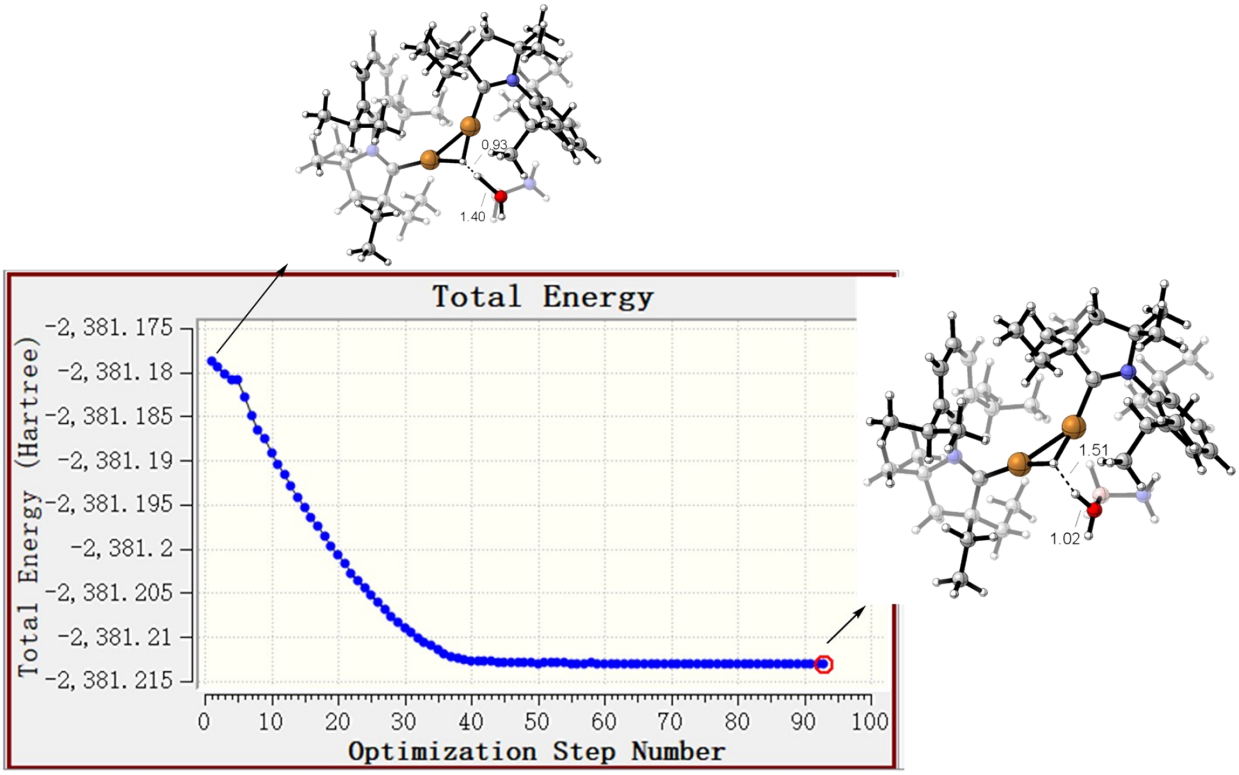

Figure S2. The attempt at transition state optimization.

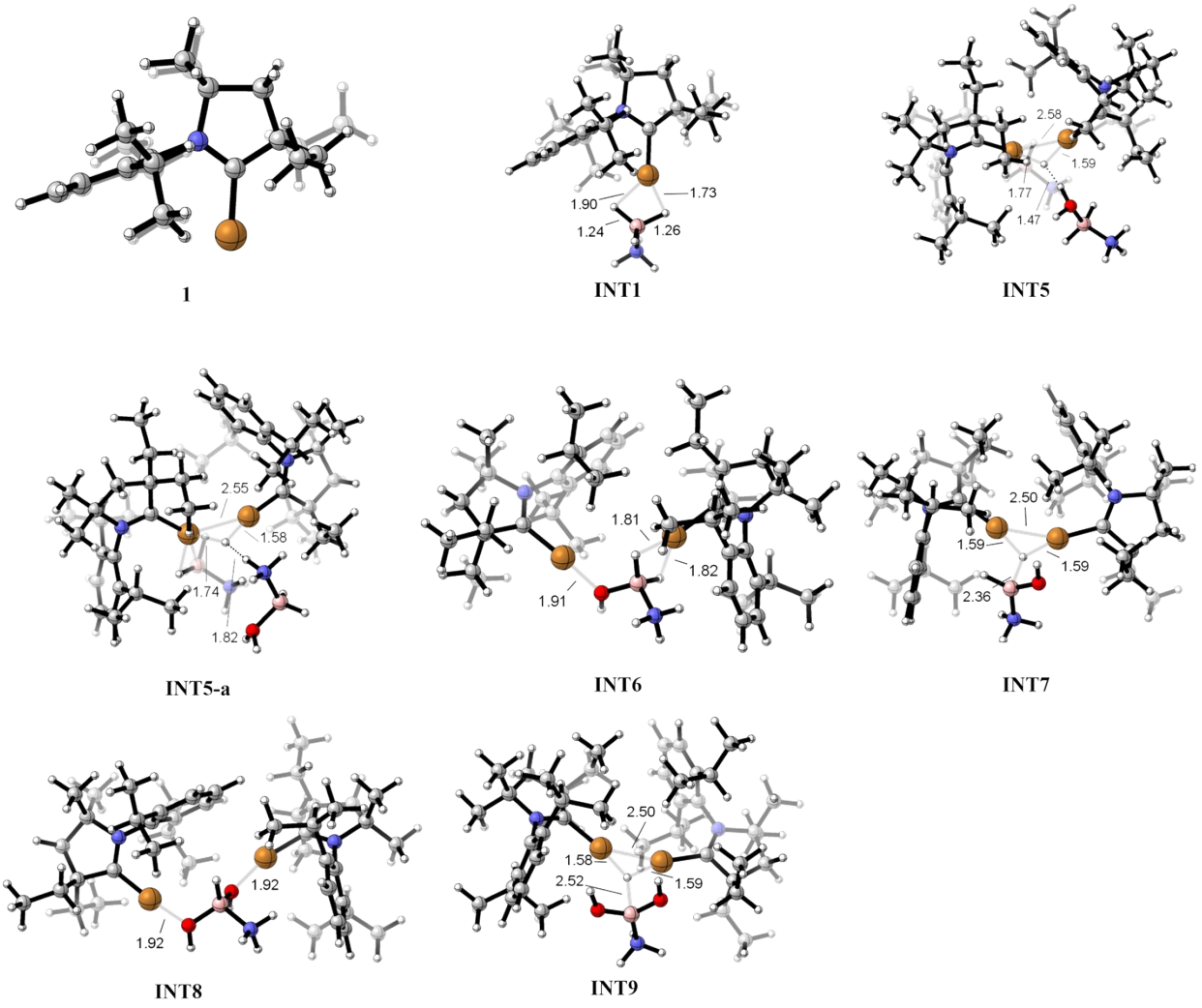

Figure S3. Optimized 3D structures of **1**, **INT1**, **INT5**, **INT5-a**, **INT6**, **INT7, INT8, INT9**

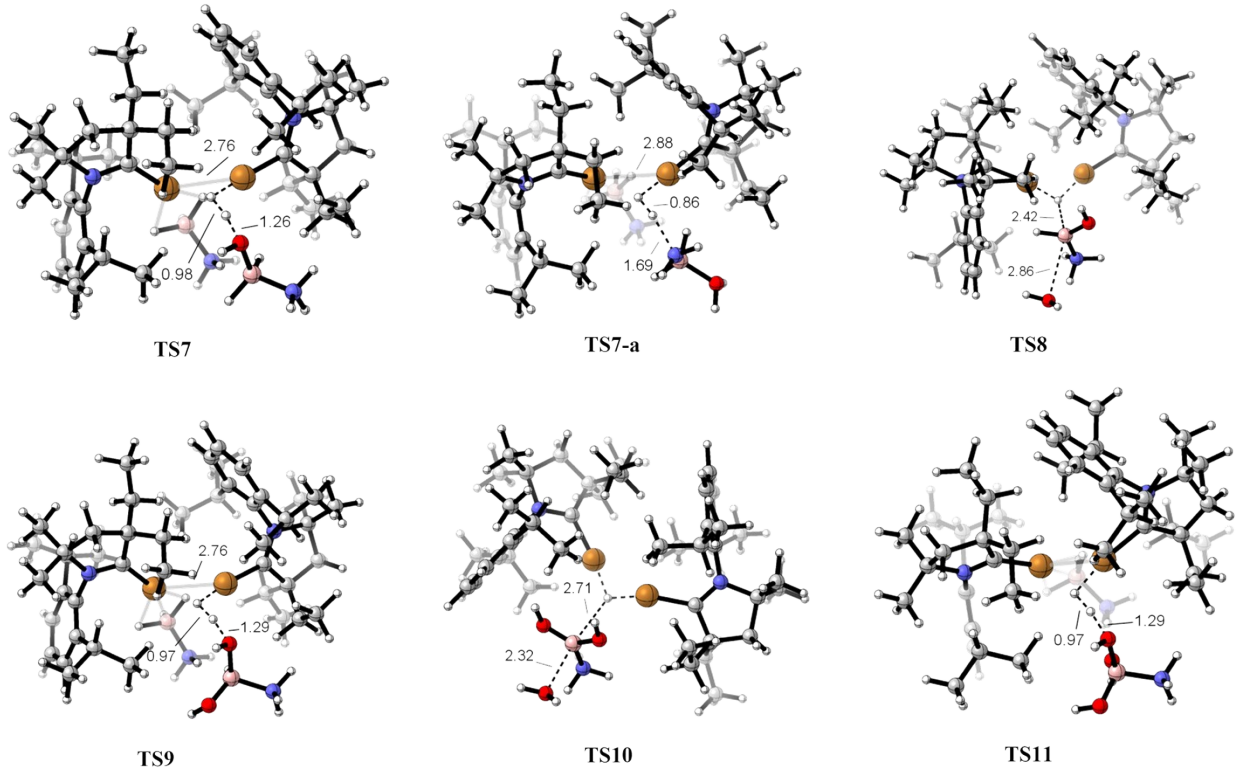

Figure S4. Optimized 3D structures of **TS7**, **TS7-a**, **TS8**, **TS9**, **TS10**, **TS11**

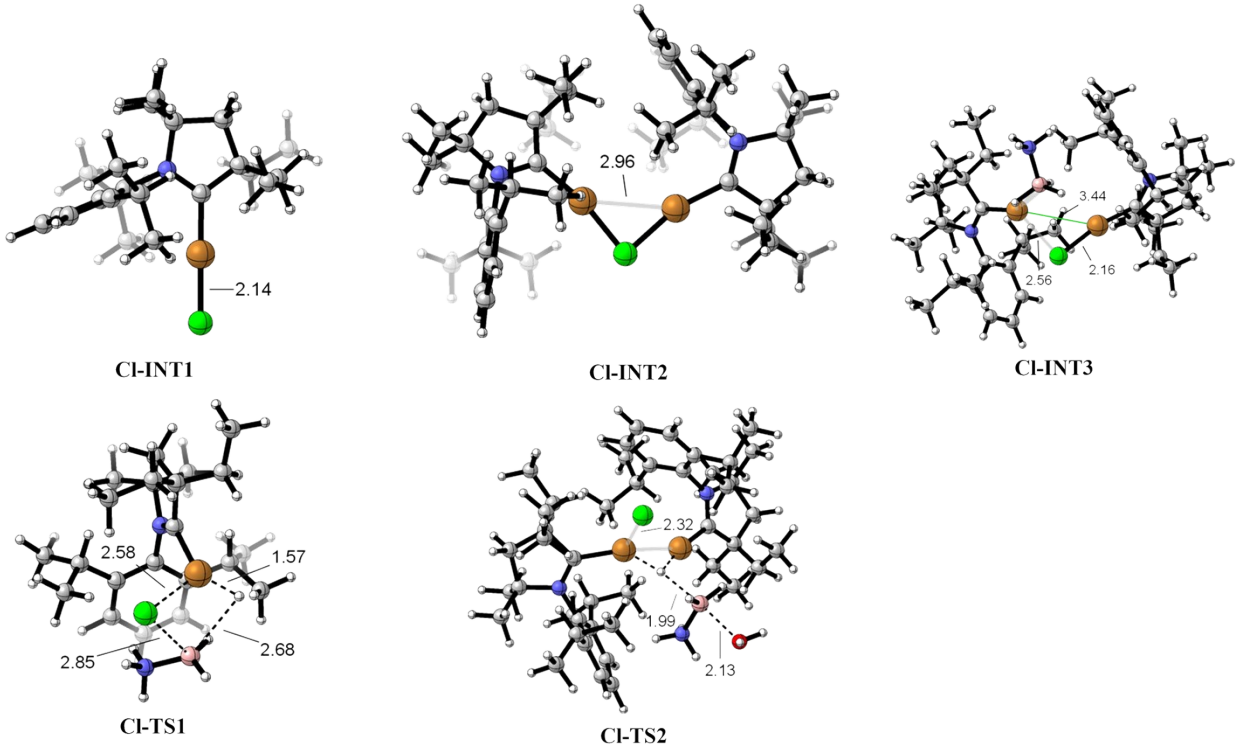

Figure S5. Optimized 3D structures of **Cl-INT1**, **Cl-INT2**, **Cl-INT3, Cl-TS1, Cl-TS2**

Coordinates for all structures.

NH_3BH_3

E_{solv} = -83.196393 a.u.

Zero-point energy correction = 0.04633 a.u.

N	-0.71892000	0.00002300	-0.00002200
H	-1.10078900	0.14888700	-0.93195500
H	-1.10053100	0.73255900	0.59513600
H	-1.10061700	-0.88158800	0.33685400
B	0.91485100	0.00000800	0.00005600
H	1.25488700	1.09059800	-0.41773000
H	1.25510900	-0.90683300	-0.73571600
H	1.25508900	-0.18357100	1.15330800

H_2O

E_{solv} = --76.431298 a.u.

Zero-point energy correction = 0.004028 a.u.

O	0.00000000	0.00000000	0.11738100
H	0.00000000	0.75468100	-0.47931400
H	0.00000000	-0.75468100	-0.47931400

H_2

E_{solv} = -1.167911 a.u.

Zero-point energy correction = -0.001365 a.u.

H	0.88295500	0.20691800	-0.30336900
H	0.14049500	0.20691800	-0.30336900

$[NH_3BH_2(H_2O)]^+$

E_{solv} = -158.901811 a.u.

Zero-point energy correction = 0.061332 a.u.

N	1.25999500	-0.25012300	-0.00054100
H	1.31624900	-0.85231800	0.82183400
H	2.10757500	0.31911100	-0.00149300
H	1.31474100	-0.85281000	-0.82265800
B	-0.01649300	0.69824000	0.00029400
H	-0.05302500	1.31502700	1.02303600
H	-0.05414100	1.31528000	-1.02225400
O	-1.22464500	-0.30079000	0.00077100
H	-1.78819600	-0.28543400	-0.78850900
H	-1.78687700	-0.28624300	0.79099800

$NH_3BH_2(OH)$

E_{solv} = -158.467008 a.u.

Zero-point energy correction = 0.050257 a.u.

N	-0.64773300	0.04331000	-0.04404300
H	-0.92420200	0.24652100	-1.00320900
H	-1.04687400	0.77584200	0.54051000
H	-1.09283400	-0.83392800	0.21929500
B	1.02162900	-0.00957200	0.13947900
H	1.36046200	-0.89507600	-0.63543600
H	1.15784200	-0.32117100	1.31330400
O	1.53030300	1.30188500	-0.12548000
H	1.69475500	1.41432000	-1.06401000

$[NH_3BH(OH)(H_2O)]^+$

E_{solv} = -234.182694 a.u.

Zero-point energy correction = 0.067221 a.u.

N	1.27637200	-0.25380900	0.00693200
H	1.33221600	-0.76389300	0.89088000
H	2.15632300	0.25272000	-0.09587200
H	1.23553900	-0.94158800	-0.74525100
B	0.05464200	0.76945000	-0.00258600
H	-0.00995700	1.35166200	-1.04741500
O	-1.19598600	-0.28448100	-0.03167100
H	-1.82901600	-0.14454600	-0.75311600
H	-1.68476500	-0.26937900	0.80868200
O	0.04275300	1.42321600	1.21672700
H	-0.36381800	2.29234900	1.17569100

$NH_3BH(OH)_2$

E_{solv} = -233.747267 a.u.

Zero-point energy correction = 0.05327 a.u.

N	-0.70703200	0.06722200	-0.08511600
H	-0.93134800	0.30745400	-1.04862600
H	-1.08707100	0.80307700	0.50841700
H	-1.20601200	-0.79161500	0.13802300
B	1.00597500	-0.04040800	0.21117000
H	1.33518300	-0.94338700	-0.55456700
O	1.50290200	1.26047700	-0.08286000
H	1.70159200	1.34306800	-1.01685100
O	1.11219700	-0.31245300	1.60450500
H	1.05682000	-1.25502200	1.76936000

$[NH_3B(OH)_2(H_2O)]^+$

E_{solv} = -309.465657 a.u.

Zero-point energy correction = 0.068703 a.u.

N	1.31031600	-0.29210100	0.03074000
H	1.23363600	-0.89017500	0.85402500
H	2.23293800	0.14369700	0.05709800
H	1.28351300	-0.89397600	-0.79295400
B	0.17917500	0.82668500	-0.00849800
O	-1.17526700	-0.24003900	-0.02807500
H	-1.70869800	-0.13000600	-0.83019900
H	-1.75373800	-0.10491000	0.73833800
O	0.13356100	1.45807500	1.21702800
H	-0.27852000	2.32598600	1.20856600
O	0.19234300	1.42728300	-1.25033500
H	-0.22268300	2.29312800	-1.28313500

$NH_3B(OH)_3$

E_{solv} = -309.031998 a.u.

Zero-point energy correction = 0.057366 a.u.

N	-0.82203000	0.14575500	0.03397900
H	-1.14629100	0.42309300	-0.89019900
H	-1.08241900	0.88170900	0.68611100
H	-1.33608500	-0.69356700	0.29381800
B	0.88530300	-0.09367100	0.08078200
O	1.46010000	1.16265100	-0.27334300
H	1.45503900	1.25020100	-1.22923000
O	1.19492600	-0.39601200	1.44007900
H	1.01533200	-1.32518000	1.60093500
O	1.00186500	-1.16351900	-0.87447200
H	1.92840000	-1.40438000	-0.95748400

1^-

E_{solv} = - -1110.987245 a.u.

Zero-point energy correction = 0.466617 a.u.

Cu	0.57876200	-0.01674300	-2.22880500
N	0.12130800	-0.02310000	0.54455700
C	-1.81284800	1.42400200	0.08142700
C	-1.29280300	0.13065500	0.26962800
C	2.39971900	-0.17610800	0.17677300
C	-0.94276600	2.66034600	-0.02110300
C	-2.08786700	-1.02307700	0.15506000
C	2.16013500	-0.37273100	1.68897300
C	3.06866100	1.18322500	-0.13781900
C	1.01435800	-0.09765800	-0.39855500
C	0.68332500	-0.05362100	1.96733300
C	-1.51638700	-2.42599200	0.12840800
C	-4.00698900	0.42251400	-0.17500700
C	-3.45594600	-0.84531500	-0.05634700
C	3.18507900	-1.32952100	-0.46511700
C	-3.18762100	1.54145600	-0.12968300
C	-1.44274900	3.81934100	0.83598300
C	0.48628100	1.29866600	2.63683300
C	-1.55857000	-2.97106900	-1.30019500
C	2.47498600	-2.67471800	-0.44766200
C	-0.00264800	-1.12368300	2.79755800
C	-2.22617000	-3.37906900	1.08555700
C	-0.82033400	3.08767100	-1.48433500
C	4.52755800	1.27615700	0.28001200
H	0.06649300	2.40788900	0.32124100
H	2.49343300	1.98102700	0.35657700
H	4.14722900	-1.41394300	0.05785600
H	-1.79865500	3.35208800	-1.90468200
H	-4.09701900	-1.71999800	-0.14708500
H	2.98407000	1.37400300	-1.21870900
H	2.81262400	0.26996100	2.29072100

H	-1.57083700	3.52655400	1.88444100
H	0.44424900	-1.11919400	3.79759900
H	0.87309300	1.23469400	3.65950500
H	2.37827100	-1.40606200	1.98260700
H	2.22866100	-3.00210200	0.57050500
H	4.66753500	1.02886000	1.33939000
H	-0.46024800	-2.38055900	0.42173300
H	-0.40188100	2.27993800	-2.10491400
H	0.13496900	-2.12620200	2.37924100
H	1.53940900	-2.65017600	-1.02297700
H	5.16241000	0.60460800	-0.30743500
H	-2.40459300	4.20417200	0.47601200
H	3.42176700	-1.04979900	-1.50352700
H	-3.61973500	2.52924500	-0.27686100
H	-3.26670200	-3.55076300	0.78448100
H	-0.15992900	3.95753900	-1.57814000
H	1.02871400	2.10300400	2.12883300
H	-1.09247300	-3.96252900	-1.34700900
H	-2.59179700	-3.06344300	-1.65745300
H	-2.23389500	-2.99730500	2.11266500
H	-0.57557000	1.56393200	2.69909800
H	-1.02540500	-2.31149700	-1.99962200
H	-5.07632700	0.53788200	-0.33342300
H	-0.72662600	4.64802700	0.79947400
H	4.89802200	2.29468300	0.12928200
H	-1.72271700	-4.35255100	1.08730300
H	3.10621900	-3.45111000	-0.89035100
H	-1.07443200	-0.92245200	2.91072100

INT1

E_{solv}= -1194.222687 a.u.

Zero-point energy correction = 0.539578 a.u.

Cu	-0.09444700	1.52054900	-1.11424700
N	0.46612600	-0.74933900	0.42752800
C	-1.59939800	-0.15101000	1.61524000
C	-0.97466900	-0.83608900	0.55752900
C	2.50676100	0.14754800	-0.14474400
C	-0.84868900	0.74562300	2.57980600
C	-1.70844800	-1.50093500	-0.44024100
C	2.77658300	-1.22132900	0.52005400
C	2.93381600	1.32780400	0.75927800
C	1.01055300	0.23453700	-0.23538300
C	1.43225000	-1.75221100	1.04654500
C	-1.08225900	-2.06005100	-1.70187600
C	-3.73423500	-0.92572700	0.76362900
C	-3.09722600	-1.54258200	-0.30338700
C	3.13673000	0.27814100	-1.53888700
C	-2.99051500	-0.22253900	1.70111800
C	-1.22753500	0.49809500	4.03683700
C	1.34075200	-1.72882400	2.56591900
C	-1.44240800	-1.18229000	-2.90200600
C	2.55910600	-0.66274100	-2.58521500
C	1.12461100	-3.15808500	0.55722800
C	-1.47295700	-3.51239700	-1.96022500
C	-1.05164800	2.21522000	2.20723700
C	4.43736600	1.49109800	0.91346400
H	0.22201500	0.54382000	2.47974700
H	2.47362600	1.19298100	1.75092600
H	4.21749700	0.10576200	-1.44250000
H	-2.11604700	2.48390500	2.20052600
H	-3.69076200	-2.05063600	-1.06112900
H	2.50238700	2.25372600	0.34824400
H	3.50253700	-1.13825200	1.33722500
H	-1.12837300	-0.55942800	4.30841200
H	1.83736900	-3.85008600	1.01868800
H	2.00777500	-2.50113600	2.96395000
H	3.19982700	-1.92790900	-0.20367700
H	2.63937800	-1.71589600	-2.28490700
H	4.91672200	0.56664700	1.25843400
H	0.00815000	-2.02068200	-1.59794100
H	-0.64275600	2.42734300	1.20781900
H	1.23070200	-3.25146500	-0.52879100
H	1.49769400	-0.45180400	-2.77609700
H	4.91298300	1.78193300	-0.02932300
H	-2.26049100	0.80222400	4.24573000
H	3.01625100	1.31972500	-1.87509100
H	-3.50085100	0.30010400	2.50776900
H	-2.54469900	-3.61000700	-2.17223700
H	-0.53688400	2.86718900	2.92292000
H	1.65826100	-0.77127100	2.99179700
H	-0.97446600	-1.57100400	-3.81460500
H	-2.52751500	-1.14965300	-3.06238800
H	-1.24178300	-4.15451400	-1.10252200
H	0.32519100	-1.95764500	2.91068700
H	-1.09793300	-0.14611100	-2.76260200
H	-4.81702200	-0.97099400	0.85092800
H	-0.57712600	1.08203700	4.69791200
H	4.66092600	2.27043700	1.64859200
H	-0.93114100	-3.89883800	-2.83111000
H	3.08735100	-0.55872900	-3.53799200
H	0.11569400	-3.47413300	0.84904700
B	-1.63075600	2.74154700	-2.00182200
H	-0.41411500	2.72061300	-2.32125100
H	-1.95035800	1.92160300	-1.13161900
H	-2.27466000	2.56450200	-2.99947200
N	-1.91186300	4.20237100	-1.41138100
H	-2.89670200	4.31909800	-1.17432200
H	-1.38036200	4.41094000	-0.56616300
H	-1.68665100	4.93319400	-2.08589100

TS1

E_{solv} = -1270.604187 a.u.

Zero-point energy correction = 0.55373 a.u.

Cu	0.35862700	-1.09318700	-1.49672200
N	-1.02064700	0.38728300	0.49977800
C	1.07496800	0.20773400	1.77379200
C	0.28056100	0.91343100	0.85123700
C	-2.58739400	-0.91514500	-0.56154800
C	0.67104600	-1.12783100	2.36492800
C	0.74923400	2.06450800	0.19167100
C	-3.34951100	0.06849000	0.35278900
C	-2.62853200	-2.36551100	-0.02454800
C	-1.14797200	-0.49172700	-0.46051100
C	-2.30414200	0.78564700	1.22065900
C	0.01251400	2.71937700	-0.95965000
C	2.79110200	1.90456000	1.49458600
C	2.01016500	2.55054700	0.54554700
C	-3.05645400	-0.86852000	-2.02299800
C	2.33419400	0.73123800	2.08294100
C	0.82807200	-1.17242400	3.88210800
C	-2.29299000	0.28901700	2.66002200
C	0.73121200	2.41882500	-2.27623100
C	-2.76738900	0.44069400	-2.74217600
C	-2.47835500	2.29522700	1.22634000
C	-0.16246000	4.22347200	-0.77163900
C	1.45324100	-2.26277200	1.70397600
C	-3.98688600	-3.04040300	-0.12880900
H	-0.38453400	-1.30023700	2.13525300
H	-2.30040800	-2.36106800	1.02662200
H	-4.13619200	-1.07169400	-2.04301900
H	2.53493100	-2.14495600	1.85681400
H	2.39500500	3.44011700	0.05080600
H	-1.87919900	-2.95806500	-0.57197900
H	-4.08757200	-0.44303800	0.98149900
H	0.30758800	-0.34115100	4.37186600
H	-3.41866800	2.53360900	1.73533000
H	-3.21112500	0.62995700	3.15060500
H	-3.90205300	0.80230100	-0.24622500
H	-3.22090100	1.30323000	-2.23635800
H	-4.77623000	-2.45056700	0.35327400
H	-0.98466300	2.27039300	-1.03659800

H	1.26544000	-2.29972100	0.62019700
H	-2.53656600	2.71131800	0.21521200
H	-1.68707100	0.62846900	-2.81634000
H	-4.28102900	-3.20273500	-1.17128400
H	1.88222500	-1.12999300	4.18244300
H	-2.57372500	-1.69663800	-2.56502600
H	2.96780900	0.20609600	2.79524600
H	0.80063400	4.74810100	-0.79003400
H	1.15686200	-3.22873800	2.12966900
H	-2.27099600	-0.80386700	2.72818600
H	0.18122100	2.85068500	-3.12093600
H	1.74424400	2.84252300	-2.28336200
H	-0.65439700	4.46075100	0.17839400
H	-1.44545900	0.70116300	3.22051200
H	0.80945500	1.33351800	-2.44905300
H	3.76950200	2.29974800	1.75629300
H	0.41595000	-2.10956600	4.27308900
H	-3.96283400	-4.01847600	0.36183400
H	-0.77294200	4.63441500	-1.58381200
H	-3.16496700	0.42098600	-3.76174100
H	-1.66861700	2.79269400	1.77406700
B	3.49902400	-1.75813200	-1.63026900
H	1.60197900	-1.49952700	-2.32136400
H	3.74399100	-1.92537100	-2.77608700
H	3.10112600	-2.57146900	-0.86985300
N	3.53868700	-0.26367700	-1.14095100
H	3.00044300	0.33540600	-1.76743600
H	3.16501700	-0.12920600	-0.19483000
H	4.49895000	0.08413700	-1.13355300
O	5.43632300	-2.12111600	-1.08979700
H	5.73792900	-2.10911800	-0.17383500
H	6.18234500	-1.84826800	-1.63654600

TS2

E_{solv} = -1270.615174 a.u.

Zero-point energy correction = 0.55335 a.u.

Cu	-0.95195300	1.53229100	-0.23300300
N	0.14929200	-1.05856200	0.17810300
C	1.99079600	-0.35757200	-1.29055300
C	1.46100600	-0.47034300	0.00902100
C	-2.14938700	-1.20999600	0.20140200
C	1.21681500	-0.72798500	-2.54055500
C	2.12807300	0.04721400	1.13412000
C	-1.59416200	-2.58639900	0.62833300
C	-2.78324400	-1.24671600	-1.20957600
C	-0.93327400	-0.33570000	0.07490000
C	-0.06815400	-2.54435900	0.44345300
C	1.49524400	0.14367700	2.50774700
C	3.96626100	0.66949600	-0.32313800
C	3.39549100	0.60108500	0.93970000
C	-3.13397400	-0.60929800	1.21631700
C	3.25773000	0.21457500	-1.42732700
C	2.01742700	-1.61526500	-3.48973000
C	0.40679800	-3.37869600	-0.73768300
C	1.16629900	1.60297700	2.82844300
C	-2.52544900	-0.26295300	2.56668000
C	0.68445900	-2.98330600	1.68836700
C	2.36679000	-0.46205900	3.60436900
C	0.73129200	0.53074700	-3.26131800
C	-4.09317400	-2.01361100	-1.29389800
H	0.32253700	-1.28404300	-2.24200900
H	-2.05509900	-1.68367200	-1.91073400
H	-3.95890200	-1.32155400	1.35472900
H	1.57302100	1.16876000	-3.56153700
H	3.93329900	1.00789400	1.79383500
H	-2.94139400	-0.21002200	-1.54571200
H	-2.02959900	-3.40107600	0.03820100
H	2.41253000	-2.50396400	-2.98420300
H	0.49219600	-4.04920700	1.85198000
H	0.26845200	-4.43689100	-0.49067000
H	-1.83712400	-2.79462100	1.67708600
H	-2.05966800	-1.13307500	3.04754300
H	-3.99676400	-3.03523700	-0.90625300
H	0.54272000	-0.39957900	2.49313900
H	0.06583100	1.12792700	-2.62137100
H	0.35346600	-2.44656900	2.58377900
H	-1.75768000	0.51783800	2.47553500
H	-4.89164200	-1.51704400	-0.73231300
H	2.86530200	-1.07619600	-3.92981500
H	-3.57619400	0.29656200	0.77104900
H	3.68951100	0.31681000	-2.42099300
H	3.29666100	0.10433400	3.73747800
H	0.17200000	0.26029700	-4.16466500
H	-0.16196200	-3.17821000	-1.65169400
H	0.66672800	1.67661300	3.80191800
H	2.07532900	2.21692800	2.86667600
H	2.63707700	-1.50127700	3.38593700
H	1.47369000	-3.22141200	-0.93612000
H	0.49965800	2.03956200	2.07163400
H	4.95337600	1.10614000	-0.45206700
H	1.38013800	-1.94923800	-4.31644300
H	-4.42176900	-2.08801600	-2.33519800
H	1.83333000	-0.44294500	4.56165000
H	-3.29049700	0.11267000	3.25323300
H	1.76720800	-2.85451400	1.57056900
B	-1.10124700	3.59519600	-0.50331600
H	-1.03088600	3.14932900	0.63732100
H	-1.27247800	2.85031400	-1.46389500
H	-0.89277300	4.74534100	-0.69214000
N	1.17960900	3.22306400	-0.71497500
H	1.68725400	2.34038500	-0.77611900
H	1.38794800	3.72812500	-1.57275600
H	1.60664400	3.74592600	0.04577300
O	-3.13975100	3.74085100	-0.28468800
H	-3.52701300	4.15761700	-1.06515000
H	-3.34786700	4.33516800	0.44761500

TS3

E_{solv} = -1270.614578 a.u.

Zero-point energy correction = 0.558674 a.u.

Cu	2.14419100	-0.83173700	-1.25269600
N	-0.76959600	0.45783200	0.57836300
C	-2.72421500	-0.30617700	-0.69792400
C	-1.64939400	-0.61412900	0.15843800
C	0.90231800	2.02382500	0.50522700
C	-2.92874200	1.06053800	-1.32302800
C	-1.39516500	-1.93162600	0.57829700
C	-0.03675100	2.41737700	1.67096000
C	0.82937800	3.04718500	-0.65401400
C	0.31412100	0.76485100	-0.08429800
C	-1.06727400	1.28916000	1.82836300
C	-0.13768400	-2.34172300	1.31568000
C	-3.39878000	-2.63437700	-0.59535800
C	-2.29843700	-2.92596000	0.19645500
C	2.36616300	1.82319600	0.92181300
C	-3.59240200	-1.33927100	-1.05404600
C	-4.34671000	1.59433300	-1.13395100
C	-2.49445400	1.80903200	1.84949400
C	0.75432900	-3.17054300	0.38924400
C	2.61223800	0.84481100	2.05832800
C	-0.84621900	0.43433800	3.06776800
C	-0.41835700	-3.11385500	2.60180900
C	-2.57802000	1.01980700	-2.81109600
C	1.33091500	4.44281400	-0.31757100
H	-2.23628800	1.76668700	-0.84873200
H	-0.21840400	3.10712500	-0.99164200
H	2.78140900	2.80002600	1.20434600
H	-3.26529800	0.36121300	-3.35741900
H	-2.12224700	-3.95224000	0.51379800
H	1.39818800	2.64382700	-1.50631100
H	-0.55773000	3.35516900	1.44011700
H	-4.64959000	1.59975800	-0.08102100

H	-1.01608600	1.05112300	3.95740500
H	-2.63860400	2.37830500	2.77469400
H	0.50556400	2.58575000	2.60843700
H	2.18515500	1.20063600	3.00329800
H	0.84180300	4.84999900	0.57595300
H	0.41861000	-1.43513600	1.58203400
H	-1.56174400	0.64571500	-2.97837200
H	0.17110400	0.03394400	3.12609700
H	2.19122700	-0.14876200	1.85347200
H	2.41198300	4.45975900	-0.14228100
H	-5.07777800	0.99297900	-1.68807400
H	2.92548600	1.50534700	0.02523500
H	-4.42997700	-1.12416400	-1.71511400
H	-0.91053700	-4.07225100	2.39541100
H	-2.65283000	2.02244100	-3.24868300
H	-2.70341300	2.48402200	1.01370100
H	1.72715800	-3.36632600	0.85676200
H	0.29101800	-4.13627800	0.15039500
H	-1.06115800	-2.55003300	3.28697400
H	-3.22543100	0.99171300	1.84598900
H	0.92746300	-2.65682900	-0.57114500
H	-4.09192000	-3.42291900	-0.87823400
H	-4.41575100	2.62028400	-1.51417200
H	1.12503400	5.12975600	-1.14464900
H	0.52125100	-3.33361300	3.12202300
H	3.68707800	0.70964600	2.22410600
H	-1.55817800	-0.39899500	3.10130400
B	4.03324900	-1.63595100	-0.66945400
H	3.19886400	-1.08933300	0.09454100
H	3.65476300	-1.81136900	-1.83379800
H	4.33315000	-2.68508000	-0.16784700
N	5.30345600	-0.65958300	-0.71867200
H	6.07516800	-1.08682800	-1.23029600
H	5.11168800	0.23221000	-1.17497800
H	5.65735700	-0.44466000	0.21329700
O	0.70305600	-0.44177500	-2.60414300
H	1.00871800	0.10859600	-3.33765800
H	0.35331100	0.16373000	-1.89174500

TS4

E_{solv} = -1194.134085 a.u.

Zero-point energy correction = 0.528421 a.u.

Cu	-0.18785300	-0.77539700	1.85752200
N	-0.09294700	-0.00758800	-0.77974400
C	2.03182000	1.21944100	-0.41912000
C	1.32017800	0.00668700	-0.43981700
C	-2.38790700	-0.13595700	-0.50907000
C	1.40171500	2.57973300	-0.63645400
C	1.93234500	-1.21735600	-0.08935900
C	-2.04478500	-0.58348700	-1.94514500
C	-3.06821200	1.25854400	-0.48547900
C	-1.02517100	-0.02520500	0.14122100
C	-0.59727300	-0.16551300	-2.21624500
C	1.17627900	-2.52712300	0.04316200
C	4.02333000	-0.02769500	0.20003200
C	3.29091000	-1.20570000	0.22513200
C	-3.29089100	-1.14815300	0.21907800
C	3.39246700	1.16723000	-0.10655200
C	2.03550800	3.32710300	-1.80970400
C	-0.48715400	1.14110100	-2.98683700
C	1.04747500	-2.95099000	1.51264900
C	-2.64823600	-2.47422800	0.59200500
C	0.19270800	-1.23716600	-2.94587300
C	1.82386300	-3.66930600	-0.73876400
C	1.50852900	3.43233600	0.63042900
C	-4.43753200	1.30493900	-1.14476000
H	0.33391000	2.43755500	-0.84720200
H	-2.40496300	1.99304600	-0.96369100
H	-4.15355600	-1.33867700	-0.43358100
H	2.55394000	3.67976900	0.85268900
H	3.78258300	-2.13689500	0.49851000
H	-3.16192600	1.57701100	0.55906300
H	-2.72447700	-0.15613800	-2.68970300
H	2.05861400	2.73058600	-2.72818900
H	-0.21568200	-1.33356300	-3.95768300
H	-0.92484300	0.99038400	-3.97962100
H	-2.13138500	-1.67488400	-2.02748800
H	-2.14417000	-2.95735200	-0.25560000
H	-4.41325000	0.97921000	-2.19120500
H	0.16497000	-2.39746500	-0.35904900
H	1.08582900	2.91945800	1.50102400
H	0.10438400	-2.21568700	-2.46312200
H	-1.90788100	-2.35511100	1.39918100
H	-5.16834900	0.68323400	-0.61658000
H	3.06980700	3.61164700	-1.57980300
H	-3.69153700	-0.67337800	1.12619000
H	3.96421700	2.09282600	-0.08901000
H	2.80913900	-3.92842700	-0.33485600
H	0.96641700	4.37565800	0.49363800
H	-1.02269900	1.96707600	-2.50852300
H	0.32557400	-3.76506500	1.63252900
H	2.01553000	-3.28656700	1.90585700
H	1.95326300	-3.40608700	-1.79382600
H	0.55847300	1.43005500	-3.13007200
H	0.79033900	-2.16651000	2.28063600
H	5.08336100	-0.03979800	0.43959500
H	1.47947100	4.24897200	-2.01526200
H	-4.81640400	2.33179600	-1.13454500
H	1.19767700	-4.56654800	-0.68282000
H	-3.39823500	-3.17768700	0.96586800
H	1.25295700	-0.97330100	-3.03733000
B	-1.01046300	1.10831000	1.98519100
H	-0.92413200	2.04791200	1.25346300
H	-2.05952400	0.73633600	2.43017100
H	0.05522300	0.80568500	2.57540000
N	-1.02150300	2.86068300	3.82885000
H	-0.22940100	3.49598800	3.79837100
H	-1.84553700	3.42098400	3.63278300
H	-1.10631700	2.55185300	4.79277300

TS5

E_{solv} = -1194.141054 a.u.

Zero-point energy correction = 0.53753 a.u.

Cu	-0.75533800	0.64022000	-2.06198900
N	-0.02248900	-0.13332900	0.59478700
C	2.26045100	-0.95601700	-0.01267300
C	1.37234400	0.11198400	0.21687200
C	-2.35116400	-0.08611700	0.42105100
C	1.93602700	-2.41553300	0.21852900
C	1.78836600	1.45521600	0.06196100
C	-1.97371500	0.12955900	1.89946700
C	-3.11178600	-1.41619200	0.20149800
C	-0.99953800	-0.11824700	-0.28106200
C	-0.50423000	-0.26235400	2.05501800
C	0.95845300	2.67967000	0.40230400
C	3.96436700	0.64726200	-0.65724200
C	3.08925200	1.68610600	-0.38874200
C	-3.23141000	1.05748900	-0.13281400
C	3.55087700	-0.65808200	-0.45476300
C	2.73166700	-2.96233400	1.40677600
C	-0.35559300	-1.69775100	2.54584800
C	0.75055500	3.60248300	-0.79790800
C	-2.65803900	2.46485000	-0.12431300
C	0.26416500	0.65209200	2.98546500
C	1.61022200	3.47883800	1.53577200
C	2.21607300	-3.27798900	-1.01542000
C	-4.50536500	-1.47899200	0.81135300
H	0.87024100	-2.49276800	0.47917200
H	-2.52016500	-2.23882500	0.63007700
H	-4.15026400	1.05374100	0.46746400
H	3.29250000	-3.36867000	-1.19527700
H	3.42236200	2.71290000	-0.52274300

H	-3.20986300	-1.58380900	-0.88187200
H	-2.60320500	-0.45700700	2.57701700
H	2.64835700	-2.32135300	2.29185700
H	-0.09572600	0.47962000	4.00526900
H	-0.80935500	-1.75492000	3.54107600
H	-2.10691700	1.18146000	2.17757700
H	-2.33839500	2.78762800	0.87450600
H	-4.50555500	-1.19888300	1.87088300
H	-0.03198200	2.35232500	0.74179300
H	1.78258600	-2.85972100	-1.93258900
H	0.10303900	1.70793300	2.75546200
H	-1.80430500	2.57110800	-0.80537500
H	-5.21342400	-0.82953600	0.28855600
H	3.79691800	-3.02755500	1.15535700
H	-3.53532600	0.79214200	-1.15783800
H	4.24569400	-1.47333400	-0.64318000
H	2.52733000	3.96934100	1.18805000
H	1.83668700	-4.29688200	-0.86796800
H	-0.86986300	-2.42988700	1.91506000
H	0.09716400	4.43689500	-0.51421800
H	1.70180500	4.03021000	-1.13763100
H	1.87793400	2.85544500	2.39498600
H	0.69122200	-1.99145600	2.65148200
H	0.29480900	3.07840100	-1.64615000
H	4.97123600	0.85495900	-1.00961700
H	2.38690500	-3.96856100	1.67132800
H	-4.88852500	-2.50135200	0.74315600
H	0.92752400	4.26488100	1.87964000
H	-3.42175900	3.17404600	-0.45857900
H	1.33934400	0.43538700	2.97138400
B	-0.78669500	-1.43886900	-2.29353100
H	0.32739400	-1.22813500	-2.68450800
H	-1.75851500	-1.15132800	-2.93343000
H	-0.67182200	1.71569000	-3.15990500
N	-0.93135800	-2.84279400	-1.63526800
H	-1.80743900	-2.99065400	-1.12952300
H	-0.93567200	-3.52619900	-2.40052600
H	-0.15964200	-3.11808900	-1.02338100

INT2

E_{solv} = -2305.25595 a.u.

Zero-point energy correction = 1.029203 a.u.

Cu	-1.48484700	-0.77068100	-0.21805300
N	-3.85884800	0.65766500	-0.11054200
C	-4.72831700	-1.55537700	-0.74088700
C	-4.39230400	-0.63662400	0.27035100
C	-2.25697600	2.18379400	-0.75523600
C	-4.53517500	-1.27632500	-2.21816900
C	-4.41459400	-0.98140000	1.63395300
C	-3.58217100	2.95821700	-0.56607900
C	-1.82842800	2.10411200	-2.23740800
C	-2.58290700	0.78256400	-0.34387500
C	-4.68981500	1.92291800	-0.29663300
C	-3.86804600	-0.09015900	2.73144200
C	-5.25667300	-3.16531800	0.99530800
C	-4.86934800	-2.25738900	1.97067800
C	-1.11006300	2.71653700	0.11489900
C	-5.16955000	-2.81965000	-0.34610500
C	-5.78372900	-1.58074300	-3.04135900
C	-5.64083600	1.76304400	-1.47423900
C	-2.56697400	-0.66911900	3.29121400
C	-1.33995500	2.59690900	1.61251800
C	-5.49794000	2.22628900	0.95337400
C	-4.87741200	0.14252100	3.85247100
C	-3.33220800	-2.04964900	-2.76012500
C	-1.30262000	3.40955800	-2.81121900
H	-4.30709500	-0.21396300	-2.34555100
H	-2.68770000	1.75731100	-2.83243600
H	-0.94008700	3.76957400	-0.15006700
H	-3.45760500	-3.13146100	-2.62001900
H	-4.89858800	-2.55044900	3.01835900
H	-1.05853600	1.32173900	-2.33416800
H	-3.82644200	3.55701100	-1.45122500
H	-6.66474500	-1.06091700	-2.64787500
H	-6.08735100	3.13172700	0.77350100
H	-6.24657500	2.67210100	-1.55381900
H	-3.50990500	3.65759700	0.27483700
H	-2.26606600	3.09012800	1.93522300
H	-2.01392300	4.23327100	-2.67374300
H	-3.61808100	0.88496300	2.29825000
H	-2.40073500	-1.73832200	-2.25793800
H	-4.86354000	2.41453000	1.82562400
H	-1.39005000	1.54659100	1.93192000
H	-0.35617300	3.70698700	-2.34256800
H	-6.00780300	-2.65430600	-3.05591000
H	-0.18591300	2.17885800	-0.15951500
H	-5.43594300	-3.55096000	-1.10666200
H	-5.09853100	-0.78550100	4.39366200
H	-3.20038600	-1.85864100	-3.83136000
H	-5.11221800	1.63724800	-2.42518400
H	-2.15224200	-0.00307200	4.05809200
H	-2.73074300	-1.65294000	3.74863100
H	-5.82451500	0.54080800	3.47120000
H	-6.32574400	0.91949600	-1.32681700
H	-1.80567700	-0.79089500	2.50632200
H	-5.60700200	-4.15413700	1.28056400
H	-5.63601300	-1.26328100	-4.07971100
H	-1.11914100	3.30623600	-3.88560100
H	-4.47463600	0.85750800	4.57901000
H	-0.51775800	3.06400900	2.16488800
H	-6.19764900	1.41413600	1.18525400
B	-0.23700400	-2.54960200	-0.05631600
H	0.03038400	-1.64999400	-0.90479700
H	-1.27706400	-2.32804600	0.57763900
H	0.62847100	-2.67747200	0.81398800
N	-0.40218000	-3.89596800	-0.86023400
H	-0.60842200	-4.68127200	-0.24037900
H	-1.16266100	-3.85873200	-1.54177800
H	0.44184300	-4.14822600	-1.37863700
Cu	1.66968200	-1.50915000	-0.06518500
N	3.99890500	0.20067300	0.12446400
C	2.93152600	2.16762800	-0.88447800
C	3.21277700	1.40669700	0.26491300
C	4.59138500	-1.99104300	-0.27326800
C	3.13422200	1.62523900	-2.28432100
C	2.78654000	1.79790200	1.54543600
C	5.88265000	-1.23369700	0.09693400
C	4.53585800	-2.34824700	-1.77850900
C	3.49342300	-0.98298300	-0.06624100
C	5.52677300	0.25775100	0.19556400
C	2.82438100	0.86613200	2.73880900
C	2.00439400	3.87426700	0.56657700
C	2.19773700	3.05735000	1.67176100
C	4.35334300	-3.24257600	0.58491800
C	2.33255400	3.41488900	-0.70217100
C	3.70500700	2.64581400	-3.26223300
C	6.09493500	1.07934800	-0.95160100
C	1.42106400	0.29864500	2.97279300
C	4.10485900	-2.97017300	2.06082200
C	5.96274000	0.87198100	1.51536400
C	3.35439700	1.51998700	4.01039300
C	1.80815900	1.06873300	-2.80707100
C	5.50498200	-3.43948400	-2.20391500
H	3.83412400	0.78410500	-2.23448400
H	4.73008400	-1.43552400	-2.36254800
H	5.22619500	-3.90034300	0.47555100
H	1.06884800	1.87346100	-2.91988300
H	1.87717900	3.39804900	2.65474600
H	3.50665600	-2.65248800	-2.02769800
H	6.67342300	-1.39262300	-0.64521000
H	4.63164900	3.09676500	-2.88895700

H	7.05700900	0.85013000	1.56098800
H	7.18306100	1.12445500	-0.83444300
H	6.27763900	-1.58724700	1.05657200
H	4.93462500	-2.42333800	2.52674200
H	6.53625900	-3.20763300	-1.91116000
H	3.48050500	0.01920200	2.50104400
H	1.38616000	0.31929700	-2.12041000
H	5.58335300	0.30904900	2.37540800
H	3.19028900	-2.38137900	2.22130300
H	5.24368900	-4.40924800	-1.76746200
H	2.99293200	3.45571100	-3.46386700
H	3.49827500	-3.79569000	0.16180700
H	2.11304300	4.03369300	-1.57047100
H	2.68489000	2.31119600	4.36898100
H	1.94595000	0.59525500	-3.78640100
H	5.88753500	0.63490200	-1.93079700
H	1.43240600	-0.45923900	3.76565000
H	0.72056800	1.09162000	3.26754800
H	4.34562100	1.96166700	3.85743400
H	5.71711300	2.10838400	-0.93571900
H	1.01546100	-0.16871000	2.06027900
H	1.55350800	4.85658300	0.68937200
H	3.92345200	2.16245900	-4.22100100
H	5.49065800	-3.55383200	-3.29212600
H	3.43266700	0.77474500	4.80993800
H	3.98645400	-3.90709700	2.61371800
H	5.64497800	1.91773300	1.60193800

TS6

E_{solv}(B3LYP-D3BJ/Def2TZVP) = -2381.669121 a.u.

Zero-point energy correction = 1.048957 a.u.

Cu	0.98991200	-0.12349200	0.24806500
N	3.57712100	0.89999100	0.15455900
C	4.02759800	-0.90616200	1.75680300
C	3.95517500	-0.47314700	0.41893600
C	2.18911000	2.71812100	-0.12508700
C	3.60238200	-0.04564500	2.93013000
C	4.15533900	-1.34842300	-0.66416600
C	3.64308700	3.24552400	-0.13658400
C	1.39023900	3.19302400	1.11032500
C	2.32207800	1.23597600	0.04232800
C	4.58555500	2.03807600	0.02559400
C	3.87461400	-0.96289100	-2.10223400
C	4.69604900	-3.09160000	0.93936100
C	4.53671500	-2.66225000	-0.37339400
C	1.40085800	3.02208800	-1.40650300
C	4.41840400	-2.22677900	1.99006400
C	4.63838700	-0.01572400	4.04998600
C	5.45298000	2.13633800	1.27055200
C	2.55752400	-1.58604700	-2.57099100
C	1.98835200	2.46435400	-2.69114400
C	5.48165700	1.81373200	-1.18256000
C	5.01124700	-1.33198800	-3.05049900
C	2.24677300	-0.51115300	3.46586900
C	1.18126400	4.69444600	1.20887400
H	3.46441900	0.98138100	2.57465400
H	1.89895900	2.83292100	2.02091100
H	1.29291900	4.11232000	-1.49587700
H	2.30680500	-1.53137400	3.86734500
H	4.70837900	-3.36011900	-1.19087000
H	0.40997400	2.69026200	1.08681600
H	3.80628100	3.95431900	0.68352000
H	5.62776900	0.28077500	3.68400600
H	6.19774600	2.64055300	-1.24056900
H	6.17292800	2.94868000	1.12409300
H	3.86675500	3.78486500	-1.06409900
H	2.99609700	2.84853800	-2.89390200
H	2.12864800	5.24631500	1.21760500
H	3.74440900	0.12334200	-2.14786300
H	1.47566500	-0.50496500	2.68051600
H	4.92094200	1.79623300	-2.12299500
H	2.04313000	1.36658100	-2.67241000
H	0.57792000	5.07812200	0.37842200
H	4.73873100	-0.99503200	4.53334200
H	0.38531100	2.62232800	-1.26896200
H	4.49248800	-2.58704200	3.01410400
H	5.12333500	-2.41871900	-3.14636300
H	1.90669600	0.15112300	4.27127900
H	4.87066800	2.37235900	2.16725700
H	2.33015800	-1.27335600	-3.59768000
H	2.60614000	-2.68340500	-2.55604700
H	5.97092900	-0.92366100	-2.71387600
H	6.02312200	1.21503000	1.44016800
H	1.71267600	-1.27462100	-1.93622900
H	5.00583700	-4.11371300	1.14263400
H	4.33252500	0.69850300	4.82273600
H	0.65176400	4.93699300	2.13686100
H	4.80485100	-0.93623100	-4.05118900
H	1.36323400	2.74197900	-3.54772500
H	6.05632300	0.88428500	-1.08876600
B	0.01210400	-3.30598000	0.13819800
H	0.30015800	-1.54451400	0.61174800
H	-0.05394300	-3.09305800	-1.02930200
H	-0.91125100	-3.40467700	0.88726900
N	1.39560700	-3.69712400	0.72172400
H	1.46654600	-4.71506900	0.60669100
H	2.20621600	-3.28339300	0.24609500
H	1.48786700	-3.49489000	1.71857100
Cu	-1.24857200	-1.24049700	0.31822400
N	-3.69627000	0.15255300	-0.25986900
C	-2.78613100	2.22052000	0.71964100
C	-2.99014300	1.40603300	-0.40723900
C	-4.15717200	-2.06796500	0.14776100
C	-2.98758100	1.72837100	2.13904800
C	-2.56314500	1.78381900	-1.69421000
C	-5.45994400	-1.41391400	-0.35611300
C	-4.22648900	-2.43046200	1.64969400
C	-3.12216900	-0.97928700	0.03052900
C	-5.21760600	0.09980600	-0.40876200
C	-2.49760900	0.79963000	-2.84473900
C	-1.96445200	3.94518300	-0.77529000
C	-2.07011900	3.07800000	-1.85595400
C	-3.74937100	-3.29351100	-0.68594000
C	-2.27569400	3.50340700	0.50234500
C	-3.75471700	2.70973500	3.01943200
C	-5.87525200	0.84463600	0.74382300
C	-1.07665600	0.23524500	-2.93856200
C	-3.33936800	-2.98599800	-2.11838300
C	-5.66329900	0.71626900	-1.72348200
C	-2.92670900	1.38837600	-4.18372200
C	-1.62950200	1.39930000	2.76518800
C	-5.14033600	-3.60172600	1.97311300
H	-3.55725700	0.79205800	2.10596400
H	-4.55488200	-1.54224000	2.21079000
H	-4.59344100	-3.99656700	-0.68728800
H	-1.00889200	2.30140600	2.86149900
H	-1.73715800	3.40516300	-2.83967300
H	-3.20797800	-2.65208300	2.00490600
H	-6.31209900	-1.64684100	0.29273500
H	-4.71772600	2.99000500	2.57758100
H	-6.75251900	0.62151600	-1.79318500
H	-6.96172200	0.79321600	0.61522600
H	-5.71522100	-1.78429200	-1.35619400
H	-4.14243200	-2.49865900	-2.68645700
H	-6.15359200	-3.45056400	1.58131500
H	-3.16251000	-0.04460100	-2.62310900
H	-1.07138700	0.67292100	2.15298400
H	-5.23156200	0.20147400	-2.58863700
H	-2.45998500	-2.32788000	-2.15769000
H	-4.75897900	-4.54138200	1.55935800
H	-3.18373400	3.63022300	3.19159800

H	-2.92318100	-3.80887800	-0.17296200
H	-2.11866400	4.16479700	1.35278700
H	-2.22021600	2.14922100	-4.53769600
H	-1.75899900	0.96953100	3.76566600
H	-5.63460900	0.40426300	1.71772800
H	-1.01250100	-0.53830300	-3.71433700
H	-0.35559900	1.02653500	-3.18518600
H	-3.91884100	1.85080800	-4.12639300
H	-5.59131000	1.90351300	0.74949900
H	-0.75700800	-0.21410500	-1.98316900
H	-1.59210600	4.95650300	-0.92620800
H	-3.94871400	2.26034400	3.99985700
H	-5.22303700	-3.72884700	3.05687400
H	-2.96014400	0.60058600	-4.94451900
H	-3.07827200	-3.90575500	-2.65192200
H	-5.41734300	1.78308200	-1.77962900
O	-0.24763200	-5.53749500	-0.32227700
H	-0.45433600	-5.65963600	-1.25661300
H	-0.98052300	-5.94216900	0.15706100

INT3

E_{solv} = -2222.771288 a.u.

Zero-point energy correction = 0.966997 a.u.

Cu	-1.04333200	-0.57782400	0.08698400
N	-3.64118100	0.40583400	-0.05925300
C	-3.98726600	-1.67286400	-1.32046400
C	-3.97253400	-1.00540000	-0.08126700
C	-2.29812900	2.27507500	-0.09686500
C	-3.58634800	-1.01072800	-2.62419000
C	-4.15177800	-1.68474300	1.13690900
C	-3.76540000	2.76389200	-0.13241500
C	-1.55003400	2.54078200	-1.42266600
C	-2.39334700	0.78207000	0.00159300
C	-4.67457900	1.52074000	-0.13823600
C	-3.91707000	-1.04077400	2.48832200
C	-4.53141900	-3.71662700	-0.13296800
C	-4.44603500	-3.04839900	1.08021400
C	-1.48667800	2.82324200	1.08506500
C	-4.28437300	-3.03641600	-1.31757100
C	-4.60458100	-1.23230900	-3.73875000
C	-5.50209600	1.40374300	-1.40931000
C	-2.60564400	-1.55005000	3.09109800
C	-2.00846800	2.44625200	2.46141300
C	-5.60666800	1.46356100	1.06182500
C	-5.07421900	-1.25640000	3.45915500
C	-2.19849600	-1.48571800	-3.05848100
C	-1.36725400	4.00476600	-1.78353300
H	-3.50973700	0.06861000	-2.45520500
H	-2.08164100	2.02531800	-2.24043500
H	-1.43774100	3.91801000	0.99530500
H	-2.19118600	-2.56500100	-3.25741600
H	-4.59029100	-3.59952400	2.00759200
H	-0.56236200	2.05902900	-1.34896400
H	-3.95700800	3.37122600	-1.02459600
H	-5.61122100	-0.91840400	-3.43946300
H	-6.33969700	2.27272200	0.97202400
H	-6.25650300	2.19791100	-1.40503600
H	-3.99383500	3.39936200	0.73108900
H	-3.03995100	2.78421700	2.62565800
H	-2.32188300	4.54029800	-1.84862400
H	-3.80196900	0.03907000	2.34357000
H	-1.44250500	-1.28547300	-2.28381100
H	-5.07510600	1.60192500	2.00938600
H	-1.98174500	1.35907800	2.62200700
H	-0.73816500	4.52693200	-1.05381100
H	-4.65673100	-2.28720300	-4.03472500
H	-0.45384600	2.45819400	0.97535400
H	-4.30390000	-3.57824100	-2.26126000
H	-5.18691300	-2.31466500	3.72482000
H	-1.88723700	-0.96730400	-3.97400300
H	-4.89836400	1.52939400	-2.31410800
H	-2.39664600	-1.04042100	4.04008700
H	-2.65236000	-2.62881000	3.28696400
H	-6.02729900	-0.91328000	3.04040500
H	-6.02998300	0.44365200	-1.45828400
H	-1.75416800	-1.37272600	2.41628100
H	-4.76423700	-4.77846500	-0.15389200
H	-4.31903000	-0.65831500	-4.62783000
H	-0.87598500	4.09045900	-2.75944600
H	-4.89257400	-0.70414200	4.38838300
H	-1.39402600	2.90458200	3.24458300
H	-6.15846600	0.51629700	1.09469200
H	-0.22723900	-1.95077500	0.14844400
Cu	1.26536000	-1.40981600	0.05248300
N	3.72633500	0.06020900	0.04409700
C	2.65262300	1.88668400	-1.20341300
C	2.99081400	1.30552100	0.03221500
C	4.19771400	-2.19035600	-0.04776600
C	2.77365300	1.14238900	-2.51832100
C	2.64429900	1.90047100	1.25866000
C	5.52999800	-1.45430600	0.20317900
C	4.11007600	-2.76583200	-1.48155200
C	3.15239100	-1.11018700	0.01855400
C	5.25339700	0.04852100	0.05154300
C	2.74035200	1.16534500	2.58000300
C	1.83426300	3.81733100	0.01516200
C	2.07822500	3.17551500	1.22173600
C	3.90600300	-3.28464300	0.98995400
C	2.08243500	3.16124800	-1.18257700
C	3.36668800	1.98442800	-3.64298600
C	5.79577500	0.62209800	-1.24966700
C	1.34769200	0.67398100	2.98507900
C	3.66120200	-2.77482800	2.40236800
C	5.79229800	0.86140200	1.21655400
C	3.35934400	1.99965900	3.69649300
C	1.40522600	0.59125800	-2.92760000
C	5.01664000	-3.95901600	-1.73862100
H	3.43076300	0.27867500	-2.36801900
H	4.34827100	-1.96393900	-2.19728600
H	4.75124700	-3.98657700	0.99205600
H	0.69794200	1.40595700	-3.13896300
H	1.80081300	3.66391500	2.15473900
H	3.06446200	-3.04816300	-1.68048100
H	6.31308400	-1.77517500	-0.49360800
H	4.33174500	2.42202000	-3.36257100
H	6.88561500	0.79091100	1.20978900
H	6.89006200	0.61917300	-1.19999500
H	5.90262900	-1.66381600	1.21313800
H	4.50523800	-2.18509500	2.78322900
H	6.06246000	-3.73973800	-1.49062900
H	3.36639400	0.27532100	2.43938400
H	0.96739300	-0.03296500	-2.13178500
H	5.44138600	0.48104200	2.18215100
H	2.76356000	-2.14260400	2.45437600
H	4.71179100	-4.83472500	-1.15583600
H	2.69717600	2.80409100	-3.93134900
H	3.02860100	-3.85759400	0.65061000
H	1.81948400	3.64298600	-2.12283300
H	2.72170300	2.84998100	3.96741900
H	1.49154000	-0.02432900	-3.83121400
H	5.50277000	0.03005900	-2.12345600
H	1.39753100	0.08144200	3.90688300
H	0.66922900	1.52009600	3.16003200
H	4.34243100	2.39343800	3.41393800
H	5.47288000	1.65982400	-1.39483800
H	0.89647300	0.04559300	2.19991100
H	1.40709700	4.81824200	0.00970900
H	3.52041900	1.36407400	-4.53319400
H	4.98212000	-4.23963000	-2.79590500
H	3.48292600	1.38753200	4.59708900
H	3.51148500	-3.60806200	3.09599000

H	5.52578200	1.92150700	1.13006500

INT4

E_{solv} = -2305.98365 a.u.

Zero-point energy correction = 1.035723 a.u.

Cu	1.47777100	0.86880300	0.17583200
N	4.09261800	-0.30827600	-0.21214800
C	4.58348000	1.39938900	-1.91335300
C	4.57629600	1.00873900	-0.56256800
C	2.64504300	-2.01636800	0.28459200
C	4.01344800	0.54509800	-3.02793500
C	4.96035100	1.88471000	0.46825800
C	4.07782300	-2.53733500	0.50918200
C	1.97964700	-2.57022100	-1.00028700
C	2.82253800	-0.53652300	0.02644500
C	5.02201600	-1.51443000	-0.12309600
C	4.80338400	1.55940600	1.94133400
C	5.49455300	3.53920600	-1.22411200
C	5.42882800	3.14901800	0.10619000
C	1.72600100	-2.26860600	1.48873700
C	5.06061200	2.67504400	-2.21943300
C	4.97227400	0.39463400	-4.20601200
C	5.50694700	-1.94243400	-1.50262500
C	3.65795000	2.36848900	2.55346600
C	2.15677200	-1.59553400	2.78277300
C	6.23205600	-1.21748700	0.74577800
C	6.09189500	1.78322200	2.72947100
C	2.66904400	1.09878200	-3.49969800
C	1.98819300	-4.08352000	-1.13870600
H	3.81686100	-0.45440800	-2.62837000
H	2.45075000	-2.12514300	-1.89182200
H	1.64036800	-3.35479100	1.64514000
H	2.77850200	2.11235500	-3.90769900
H	5.73333800	3.84605700	0.88498900
H	0.94123200	-2.20896700	-1.00645500
H	4.24111700	-3.53795100	0.09582600
H	5.95941000	0.03567900	-3.89148500
H	6.84833800	-2.12175800	0.80218900
H	6.17951800	-2.79867000	-1.38002900
H	4.28640100	-2.60560500	1.58349300
H	3.13441300	-1.94357900	3.13746600
H	2.99627000	-4.47999400	-1.30657700
H	4.52837500	0.50135800	2.03727300
H	1.94560100	1.14544400	-2.67508400
H	5.94898600	-0.94645100	1.76803800
H	2.21176300	-0.50487400	2.66127600
H	1.57503600	-4.57776200	-0.25102500
H	5.11723200	1.34670300	-4.73171600
H	0.71490500	-1.92002600	1.21908300
H	5.07467800	3.00160900	-3.25778400
H	6.35712800	2.84683500	2.77207100
H	2.25246200	0.45910500	-4.28818300
H	4.68984100	-2.25751700	-2.16063600
H	3.55472600	2.13367300	3.62017000
H	3.83808600	3.44757000	2.45874900
H	6.93961900	1.24565000	2.28934900
H	6.07483000	-1.14406000	-1.99391800
H	2.70065800	2.14247700	2.06317300
H	5.86626500	4.52756400	-1.48421900
H	4.56650300	-0.31936700	-4.93228100
H	1.37741500	-4.38567500	-1.99702700
H	5.96722200	1.43725000	3.76227200
H	1.43509800	-1.79747300	3.58233400
H	6.85071400	-0.41819400	0.31981800
H	0.47107200	1.16469500	1.53294100
Cu	-0.93749700	0.78696800	0.92292200
N	-3.36719200	-0.57436700	0.13204600
C	-2.11736800	-2.12748700	-1.30398300
C	-2.63497100	-1.81034400	-0.03479800
C	-3.79661600	1.65966900	0.45531000
C	-2.09589500	-1.14043600	-2.45385000
C	-2.44118600	-2.64267200	1.08111700
C	-5.15977800	0.94859700	0.33295100
C	-3.46858600	2.49689300	-0.80443600
C	-2.78394900	0.54508200	0.46314300
C	-4.87621600	-0.50094700	-0.08849600
C	-2.79742600	-2.22567700	2.49370400
C	-1.36552500	-4.24390800	-0.38840900
C	-1.80231000	-3.86687400	0.87334800
C	-3.67842100	2.51291800	1.72604700
C	-1.50007300	-3.36924400	-1.45826900
C	-2.58752900	-1.73185900	-3.77097500
C	-5.22865100	-0.77365900	-1.54351500
C	-1.52543600	-1.86584200	3.26258500
C	-3.66372600	1.71907100	3.02390600
C	-5.59283300	-1.51347500	0.78937400
C	-3.59778400	-3.28503800	3.24553400
C	-0.68815700	-0.56536000	-2.61840900
C	-4.26600600	3.78431300	-0.93339000
H	-2.74978300	-0.29958000	-2.19996600
H	-3.63681800	1.87036200	-1.69376600
H	-4.51365800	3.22675500	1.73804100
H	0.01752600	-1.33405700	-2.96327900
H	-1.63711800	-4.53168400	1.71931400
H	-2.39083000	2.72469500	-0.80359700
H	-5.81539400	1.44358200	-0.39322800
H	-3.58845100	-2.16866100	-3.67738400
H	-6.67154100	-1.40919600	0.62883200
H	-6.31869200	-0.73982300	-1.64661100
H	-5.68914100	0.95998800	1.29338700
H	-4.55350000	1.08530400	3.13317600
H	-5.34618500	3.60268100	-0.87089600
H	-3.40719900	-1.31511500	2.44548800
H	-0.30376500	-0.16312100	-1.66817400
H	-5.39887100	-1.34630700	1.85426200
H	-2.78083500	1.06698300	3.08655800
H	-4.00294800	4.50563000	-0.15212600
H	-1.91316200	-2.51508200	-4.13845000
H	-2.75952900	3.11602000	1.65829500
H	-1.09898800	-3.64570700	-2.43225600
H	-3.00232500	-4.18862200	3.42479200
H	-0.68762600	0.24940500	-3.35391300
H	-4.80959300	-0.02702100	-2.22635300
H	-1.77228800	-1.51386300	4.27187700
H	-0.86382600	-2.73758600	3.35785700
H	-4.49923400	-3.58158400	2.69712600
H	-4.89707000	-1.77109600	-1.85519300
H	-0.95965800	-1.07078100	2.75212800
H	-0.88783000	-5.21029600	-0.53325700
H	-2.62804600	-0.95172100	-4.53988300
H	-4.06754700	4.25837900	-1.89962100
H	-3.90551100	-2.89896100	4.22418300
H	-3.63606800	2.38829900	3.88956400
H	-5.31435200	-2.54216700	0.53074400
B	1.13600200	2.99955900	-0.77290800
H	0.39002500	2.05882500	-1.06980600
H	1.37368500	3.67144500	-1.74864400
H	2.18530800	2.62947600	-0.24690400
N	0.37406700	3.90923600	0.31857700
H	0.98014900	4.64147000	0.68615100
H	-0.45524200	4.37249400	-0.05093600
H	0.08070200	3.33301200	1.11373800

INT5

E_{solv} = -2464.908956 a.u.

Zero-point energy correction = 1.124383 a.u.

Cu	1.54690200	0.92398400	0.11000900
N	4.12512100	-0.29476100	-0.25394900
C	4.58522400	1.41666300	-1.95999800
C	4.60604900	1.02233700	-0.61050500
C	2.67332900	-1.99446400	0.26509300
C	3.99990000	0.56212000	-3.06633200

C	5.00983900	1.89568000	0.41525300
C	4.10641500	-2.51999800	0.47659000
C	1.98972200	-2.54813600	-1.01030600
C	2.85850600	-0.51715600	0.00114400
C	5.04712000	-1.50819700	-0.17910800
C	4.88746600	1.56611700	1.89069100
C	5.50217000	3.55775000	-1.28189600
C	5.46672200	3.16257700	0.04807400
C	1.76219900	-2.22987500	1.47779900
C	5.05121000	2.69527100	-2.27097200
C	4.93958900	0.42035800	-4.26079200
C	5.50035500	-1.94300900	-1.56723200
C	3.76513800	2.38196000	2.53523900
C	2.24278900	-1.59495500	2.77332800
C	6.27597500	-1.21714300	0.66433400
C	6.19638300	1.77948600	2.64738900
C	2.64394400	1.10827800	-3.51273200
C	2.00092500	-4.06118200	-1.15067900
H	3.81705500	-0.43983700	-2.66661700
H	2.44453700	-2.10022900	-1.90863300
H	1.63089000	-3.31255400	1.62244100
H	2.73709000	2.12631200	-3.91321000
H	5.78648300	3.85752300	0.82254000
H	0.95039200	-2.18989700	-0.99906700
H	4.25997500	-3.52625600	0.07372400
H	5.93413300	0.06780700	-3.96285600
H	6.88634600	-2.12582300	0.71141700
H	6.16811800	-2.80441900	-1.45580100
H	4.32979700	-2.57485200	1.54850400
H	3.15702100	-2.05844600	3.16070100
H	3.00662500	-4.45396500	-1.33946200
H	4.60741300	0.50954600	1.99166600
H	1.93289400	1.14103300	-2.67641200
H	6.01557000	-0.94130900	1.69129700
H	2.45157300	-0.52421200	2.63440400
H	1.60739400	-4.55830500	-0.25571700
H	5.06913400	1.37410600	-4.78735800
H	0.76333800	-1.83474800	1.22624200
H	5.04361100	3.02514900	-3.30825500
H	6.46933200	2.84119500	2.68502200
H	2.21980500	0.47101800	-4.29896800
H	4.66828100	-2.25268900	-2.20870200
H	3.68724300	2.13791600	3.60288200
H	3.95099800	3.46057700	2.44945800
H	7.02878300	1.23766000	2.18449400
H	6.06533400	-1.15047000	-2.07118100
H	2.79598600	2.17549600	2.05784700
H	5.86482100	4.54823100	-1.54628400
H	4.52651200	-0.29551700	-4.98092800
H	1.37413900	-4.36371900	-1.99710900
H	6.09556000	1.43152600	3.68206300
H	1.48118300	-1.68539100	3.55674800
H	6.89195500	-0.42431900	0.22286400
H	0.57255700	0.97345200	1.59244200
Cu	-0.87398300	0.72864600	0.98765100
N	-3.32564600	-0.56169200	0.20008000
C	-2.10410500	-2.12856600	-1.24039600
C	-2.60791100	-1.80713100	0.03357900
C	-3.71225800	1.68586200	0.49312600
C	-2.09730000	-1.14539100	-2.39408700
C	-2.40992700	-2.63893600	1.14909900
C	-5.08972700	1.00812300	0.33510500
C	-3.33756600	2.51338400	-0.75964900
C	-2.72537600	0.55030500	0.52188900
C	-4.83586900	-0.46753600	-0.01147600
C	-2.75207700	-2.22006100	2.56468700
C	-1.35150700	-4.24561800	-0.32737500
C	-1.77756900	-3.86588000	0.93718000
C	-3.60723200	2.53626900	1.76594100
C	-1.49242700	-3.37249600	-1.39782700
C	-2.60437900	-1.74289000	-3.70255500
C	-5.21373700	-0.81240500	-1.44399900
C	-1.46988600	-1.88821100	3.32942500
C	-3.66519500	1.74308300	3.06227500
C	-5.55688400	-1.41689200	0.93160900
C	-3.56924700	-3.26588100	3.31718100
C	-0.69438100	-0.56546700	-2.57986800
C	-4.09352000	3.82392100	-0.90066800
H	-2.74997900	-0.30510000	-2.13559700
H	-3.50792300	1.89031600	-1.65105500
H	-4.41940900	3.27569900	1.74959600
H	0.00841300	-1.32976600	-2.93970300
H	-1.60940000	-4.53098400	1.78226900
H	-2.25416300	2.70856900	-0.74068700
H	-5.68884800	1.49076100	-0.44604200
H	-3.60290900	-2.18141000	-3.59393100
H	-6.63548200	-1.30987200	0.77284800
H	-6.30466300	-0.76767100	-1.53118000
H	-5.66938300	1.07988600	1.26295300
H	-4.56283400	1.11411900	3.12425600
H	-5.17925800	3.67550900	-0.84821800
H	-3.34361600	-1.29758900	2.52206600
H	-0.29492100	-0.16651600	-1.63454100
H	-5.35297100	-1.18750300	1.98335500
H	-2.79187000	1.08371600	3.17553600
H	-3.81571300	4.53891700	-0.11849700
H	-1.93287900	-2.52582900	-4.07560500
H	-2.66742200	3.11052000	1.73149500
H	-1.10230000	-3.65258300	-2.37517900
H	-2.99287800	-4.18416500	3.48320600
H	-0.70916600	0.25283300	-3.31129300
H	-4.79717600	-0.10825100	-2.17169300
H	-1.70413400	-1.49935400	4.32841300
H	-0.83915300	-2.77941900	3.44899600
H	-4.48271000	-3.53769400	2.77616800
H	-4.90165600	-1.82975800	-1.70777500
H	-0.87528000	-1.13023800	2.79663200
H	-0.87866700	-5.21396000	-0.47465500
H	-2.65650600	-0.96563000	-4.47363000
H	-3.87068100	4.28837900	-1.86610800
H	-3.85843400	-2.88007000	4.30155900
H	-3.69116200	2.41475800	3.92677500
H	-5.29236200	-2.46235300	0.73273300
B	1.15069500	3.00277500	-0.71624300
H	0.40129100	2.02627600	-0.91620400
H	1.35451600	3.56388100	-1.76298600
H	2.21401700	2.70218300	-0.17301100
N	0.39478200	4.01489200	0.28040000
H	0.98904500	4.81350200	0.50136200
H	-0.46214400	4.39595300	-0.12066300
H	0.14319100	3.58356000	1.17398200
B	0.04162300	3.09965700	3.92035200
H	1.05280400	3.74061600	3.84029200
H	-0.74820700	3.23018600	3.01773500
N	-0.69585400	3.41070200	5.28886200
H	-1.05147800	4.36762000	5.28123100
H	-1.49780300	2.79944800	5.44933700
H	-0.09108600	3.33519400	6.10812500
O	0.34955800	1.58099100	3.97182100
H	0.37873600	1.21463600	3.03186500
H	1.16226600	1.32330700	4.43545700

INT5-a

E_{solv} = -1270.62894 a.u.

Zero-point energy correction = 0.558058 a.u.

Cu	1.55071300	0.91788300	0.10655600
N	4.14558800	-0.30605400	-0.20546900
C	4.66891500	1.37492000	-1.92380100
C	4.64300300	1.00272400	-0.56814300
C	2.67098600	-1.98655300	0.30723100
C	4.11982900	0.50256100	-3.03473600

C	5.01462400	1.89191000	0.45604700
C	4.09452900	-2.51768200	0.56378000
C	2.01518600	-2.55948200	-0.97477900
C	2.87088500	-0.51493400	0.02309000
C	5.05828100	-1.52257800	-0.08366600
C	4.84475400	1.58360500	1.93100600
C	5.56860200	3.52486700	-1.25023700
C	5.48760000	3.15155400	0.08410800
C	1.72999200	-2.19800500	1.50144000
C	5.14854400	2.64725400	-2.23976500
C	5.09883500	0.34011000	-4.19443000
C	5.54782400	-1.98783700	-1.44934700
C	3.71558800	2.41956300	2.53583600
C	2.16572900	-1.52487700	2.79379700
C	6.26513500	-1.22303400	0.78832400
C	6.13401300	1.79118000	2.72263500
C	2.77973000	1.04100200	-3.53484300
C	2.02196900	-4.07491600	-1.08742600
H	3.92217900	-0.49209900	-2.62445000
H	2.49399000	-2.12961800	-1.86959400
H	1.60567600	-3.27847100	1.66931000
H	2.88779300	2.05061600	-3.95276300
H	5.78424200	3.85793400	0.85756600
H	0.97745700	-2.19640400	-0.99615400
H	4.25173400	-3.53122800	0.18098900
H	6.08265000	-0.00771400	-3.85757300
H	6.86726800	-2.13470800	0.87119500
H	6.20598700	-2.85125600	-1.30177200
H	4.28966500	-2.55748100	1.64198900
H	3.09576100	-1.94157500	3.19748400
H	3.03010100	-4.47589600	-1.24328100
H	4.54762200	0.53230900	2.03595600
H	2.04315500	1.09105100	-2.72215200
H	5.97774400	-0.92421800	1.80157300
H	2.32310500	-0.44678300	2.64420400
H	1.60331500	-4.55357900	-0.19368000
H	5.24700900	1.28477400	-4.73244300
H	0.73497300	-1.81889200	1.21297900
H	5.17671300	2.96006200	-3.28200100
H	6.41950300	2.84992100	2.75213000
H	2.37997600	0.38858500	-4.32154200
H	4.73164300	-2.30526500	-2.10714000
H	3.59703500	2.17734300	3.59994600
H	3.92749200	3.49427000	2.45549500
H	6.97280700	1.23229900	2.29273600
H	6.13230700	-1.20961400	-1.95329400
H	2.75695400	2.22934700	2.02975900
H	5.94299700	4.50995900	-1.51852700
H	4.70946000	-0.38761300	-4.91593700
H	1.41510000	-4.39023900	-1.94355400
H	5.99869300	1.46039800	3.75909200
H	1.39967100	-1.64283000	3.56950600
H	6.89931800	-0.44351600	0.34880500
H	0.55500900	1.16395400	1.50850300
Cu	-0.85954500	0.75938200	0.92101100
N	-3.30745100	-0.58925300	0.12356000
C	-2.07683400	-2.12489300	-1.34773800
C	-2.59323100	-1.83232500	-0.07194500
C	-3.70140400	1.65042700	0.45870800
C	-2.04660100	-1.11598300	-2.47835000
C	-2.41555000	-2.69614700	1.02226600
C	-5.07650500	0.96414000	0.33583400
C	-3.36487900	2.47352100	-0.80913800
C	-2.70794100	0.51801100	0.46383400
C	-4.81744700	-0.48884900	-0.09143600
C	-2.77146100	-2.31065500	2.44340100
C	-1.35075600	-4.27156000	-0.48206300
C	-1.78990700	-3.92199800	0.78668000
C	-3.56138500	2.50245500	1.72722300
C	-1.47206400	-3.36921700	-1.53006700
C	-2.56277600	-1.67371200	-3.80101300
C	-5.17810200	-0.75533100	-1.54533300
C	-1.49487200	-1.99351300	3.22207900
C	-3.59929600	1.71249500	3.02637200
C	-5.54794600	-1.48967600	0.78822900
C	-3.59223600	-3.37380500	3.16677700
C	-0.62932300	-0.56658300	-2.64753300
C	-4.09679700	3.80099600	-0.91457400
H	-2.68127300	-0.26703300	-2.20244900
H	-3.59271900	1.85768800	-1.69211400
H	-4.36137200	3.25518400	1.73022500
H	0.05707000	-1.34175800	-3.01584800
H	-1.63745300	-4.61027700	1.61599600
H	-2.27709200	2.64184700	-0.84587100
H	-5.72223100	1.47404000	-0.38896500
H	-3.57155300	-2.09134800	-3.70562300
H	-6.62476900	-1.37215700	0.62438700
H	-6.26741400	-0.70075400	-1.64583800
H	-5.60678200	0.98065600	1.29536300
H	-4.54577800	1.17353600	3.15932700
H	-5.18168300	3.67615400	-0.80879900
H	-3.36375000	-1.38796200	2.41647500
H	-0.22630500	-0.19209100	-1.69408300
H	-5.35524700	-1.32020100	1.85306600
H	-2.79223000	0.96586200	3.06600600
H	-3.76517700	4.50998300	-0.14791200
H	-1.90813800	-2.46416600	-4.18791700
H	-2.61387800	3.06292900	1.67128400
H	-1.07113900	-3.62645000	-2.50937000
H	-3.01435900	-4.29307800	3.32157600
H	-0.62026300	0.26320300	-3.36609100
H	-4.74649800	-0.01817200	-2.23033600
H	-1.73661900	-1.64365600	4.23387900
H	-0.85591900	-2.88194200	3.31405200
H	-4.49876500	-3.63816100	2.61065600
H	-4.86648800	-1.75934700	-1.85640800
H	-0.90637400	-1.21408000	2.71260700
H	-0.88295500	-5.23908500	-0.64919800
H	-2.59386600	-0.87946500	-4.55576000
H	-3.91130900	4.25989300	-1.89055400
H	-3.89335700	-3.00821700	4.15528700
H	-3.48059700	2.37518600	3.89029500
H	-5.28235500	-2.52269000	0.53345800
B	1.18527200	2.97839500	-0.85898500
H	0.48587400	1.98376800	-1.11135200
H	1.43206500	3.57273800	-1.87917200
H	2.22348100	2.69917200	-0.25886000
N	0.33305100	3.93647700	0.11650800
H	0.88364600	4.73435700	0.43149200
H	-0.50344000	4.31664000	-0.32592800
H	0.03322300	3.42589100	0.95164300
B	-0.19932500	3.11975000	4.27326500
H	-0.75980700	3.39932700	5.29122700
H	-0.75948300	3.39597200	3.24567400
N	0.18139800	1.58008100	4.26341800
H	-0.63656600	1.02658200	4.52213300
H	0.46747500	1.26634900	3.32285900
H	0.91677400	1.32820500	4.92621800
O	1.18781400	3.85577700	4.25179200
H	1.30648600	4.52424300	3.55976500
H	1.48018000	4.23194600	5.09712800

TS7

E_{solv} = -2464.904311 a.u.

Zero-point energy correction = 1.116938 a.u.

Cu	-1.25046300	0.47440300	0.53291200
N	-3.58601400	-0.70780400	-0.47206200
C	-4.49149300	-0.21656000	1.76400500
C	-4.25468400	0.19574200	0.44091800
C	-1.88633800	-1.83305400	-1.53408700
C	-3.98048500	-1.52611900	2.32963400

C	-4.57438000	1.48947100	-0.00799200
C	-3.20237900	-2.15986900	-2.26766200
C	-1.36363400	-2.98898000	-0.64063100
C	-2.28132900	-0.74482400	-0.56394400
C	-4.34326900	-1.68647500	-1.36408300
C	-4.16243800	2.02735400	-1.36445900
C	-5.51344200	1.94328100	2.18197700
C	-5.21709200	2.34590800	0.88726200
C	-0.76052500	-1.37523300	-2.47152400
C	-5.13732100	0.68035000	2.61660300
C	-5.05221200	-2.30457100	3.08702100
C	-4.95389300	-2.81515300	-0.54331700
C	-3.00041000	3.01096700	-1.21429300
C	-1.10726800	-0.21181600	-3.38692100
C	-5.45040400	-0.98327400	-2.12982000
C	-5.32087300	2.67721000	-2.11618600
C	-2.76229700	-1.27961500	3.21992300
C	-1.24599100	-4.33868300	-1.32950000
H	-3.64072000	-2.15312500	1.49959000
H	-1.99726400	-3.09714700	0.25397400
H	-0.42747200	-2.23155800	-3.07558000
H	-3.00996200	-0.62121000	4.06284900
H	-5.47543100	3.35353600	0.56721000
H	-0.37685600	-2.68264900	-0.26434000
H	-3.30406400	-3.22085200	-2.51663400
H	-5.95470900	-2.45313100	2.48252600
H	-5.94314900	-1.71710500	-2.77697700
H	-5.49716700	-3.47852700	-1.22518400
H	-3.24720200	-1.60894600	-3.21410800
H	-1.80777700	-0.49432800	-4.17992200
H	-2.22480300	-4.77144700	-1.56565200
H	-3.79443200	1.19389900	-1.97611500
H	-1.94521600	-0.80590600	2.65627700
H	-5.06620900	-0.18380500	-2.77151500
H	-1.56318700	0.62063100	-2.83091600
H	-0.67193600	-4.27679900	-2.26203400
H	-5.34959800	-1.79091600	4.00953600
H	0.10329700	-1.10537500	-1.83975200
H	-5.33295200	0.38711600	3.64620700
H	-5.66319800	3.59239600	-1.61823700
H	-2.38644300	-2.22783300	3.62392800
H	-4.20190700	-3.42034800	-0.02620000
H	-2.72241800	3.42881300	-2.19042500
H	-3.26063100	3.84708100	-0.55154000
H	-6.17927200	2.00107400	-2.20061900
H	-5.67388800	-2.43402100	0.18996400
H	-2.11170100	2.51758800	-0.79104400
H	-6.01935300	2.62472700	2.86155300
H	-4.66770600	-3.29022900	3.37301600
H	-0.73091300	-5.04888200	-0.67327700
H	-5.00399400	2.95546500	-3.12779900
H	-0.20736100	0.17367700	-3.88041600
H	-6.21007100	-0.57025300	-1.45536600
H	0.03774200	1.24165400	-1.16113600
Cu	1.34118000	0.94486600	-0.27817800
N	3.72114900	-0.47441600	0.44889200
C	2.50899700	-2.59732800	0.65842700
C	3.17333300	-1.66700300	-0.16324200
C	3.81817700	1.63785600	1.35498600
C	2.18224200	-2.32700100	2.11376400
C	3.29032800	-1.84493700	-1.55297700
C	5.22650000	1.02249200	1.49301200
C	3.08724100	1.69821900	2.71935500
C	3.04109600	0.63464600	0.54483900
C	5.13676800	-0.43840300	1.02643200
C	3.83871400	-0.78516700	-2.48775800
C	2.21119300	-4.00281000	-1.29526500
C	2.79772100	-3.03388000	-2.09592600
C	3.83946900	3.01462600	0.67909500
C	2.05136700	-3.77391800	0.06485100
C	2.55654500	-3.47912400	3.04103100
C	5.30621000	-1.43410600	2.16343300
C	2.70821200	-0.18445700	-3.32388700
C	4.25183400	2.98903700	-0.78480400
C	6.14541000	-0.76212600	-0.06372200
C	4.94748500	-1.31347500	-3.39416100
C	0.70125000	-1.98181900	2.26947700
C	3.60526300	2.76678000	3.66787500
H	2.74217600	-1.44249800	2.43409700
H	3.16384600	0.70981000	3.19849200
H	4.52660700	3.65875800	1.24413100
H	0.06191100	-2.85185500	2.06483100
H	2.87259000	-3.19845500	-3.16925900
H	2.01148500	1.85098700	2.53920300
H	5.59000900	1.07715000	2.52574200
H	3.60956600	-3.76450900	2.93874300
H	7.15154300	-0.69313800	0.36381700
H	6.34815400	-1.39384600	2.49882100
H	5.95164600	1.56792600	0.87758800
H	5.21101900	2.47817800	-0.93944400
H	4.68892800	2.68913900	3.81886100
H	4.25624400	0.03018800	-1.88407600
H	0.40196300	-1.18114500	1.57594400
H	6.09118900	-0.05576400	-0.89911100
H	3.50495600	2.47426500	-1.40837400
H	3.39034700	3.77607400	3.29956900
H	1.94739900	-4.36933900	2.84246100
H	2.84264000	3.47410500	0.76853500
H	1.54137000	-4.51489200	0.67872000
H	4.56676000	-2.06390700	-4.09766200
H	0.49113900	-1.63903200	3.29123200
H	4.67526600	-1.20315600	3.02780400
H	3.08670100	0.62717900	-3.95742700
H	2.25005300	-0.94049100	-3.97546300
H	5.76035000	-1.77404200	-2.82163200
H	5.10560300	-2.45969100	1.83270600
H	1.91405500	0.22639900	-2.68346300
H	1.85130000	-4.92926900	-1.73684900
H	2.38197800	-3.19183900	4.08428200
H	3.12835400	2.66548800	4.64751300
H	5.37029700	-0.49437900	-3.98732400
H	4.37896800	4.00631200	-1.17170900
H	6.01383000	-1.78187900	-0.44490000
B	-0.96118100	1.92006900	2.18189000
H	-0.09030600	1.17536500	1.64824700
H	-0.93673700	1.68867500	3.36207400
H	-2.08881200	1.78588200	1.71770400
N	-0.50463800	3.42922400	1.90320000
H	-1.22758100	4.08238800	2.20542900
H	0.33870200	3.68125500	2.41952800
H	-0.31114100	3.63751000	0.91814000
B	0.52140200	4.20193700	-1.51568300
H	-0.51152200	4.81630400	-1.39365900
H	0.98699600	3.78728100	-0.46762500
N	1.62975200	5.18633900	-2.13623700
H	1.86677000	5.93335100	-1.48349800
H	2.49429300	4.68762200	-2.35066400
H	1.32311500	5.63515200	-2.99956400
O	0.42109400	3.03652900	-2.43581200
H	0.29040400	2.00133700	-1.72140100
H	-0.28805000	3.10639500	-3.08784700

TS7-a

E_{solv} = -2464.878561 a.u.

Zero-point energy correction = 1.117697 a.u.

Cu	-1.30180400	0.47784000	0.52039200
N	-3.63715100	-0.70643400	-0.44031600
C	-4.52395400	-0.05906500	1.76464200
C	-4.28172500	0.26573000	0.41860400
C	-1.96024300	-1.91698700	-1.44463400
C	-4.04659900	-1.34597600	2.40676200

C	-4.56661800	1.53787400	-0.10893400
C	-3.28670000	-2.27411800	-2.14510900
C	-1.44327900	-3.01935900	-0.48320900
C	-2.33466600	-0.76846400	-0.53864400
C	-4.41579600	-1.72126400	-1.27215700
C	-4.13918000	1.97680700	-1.49534400
C	-5.48124600	2.15132900	2.05180200
C	-5.17979200	2.46597800	0.73382600
C	-0.84460700	-1.53392600	-2.42691600
C	-5.14009800	0.90689300	2.56222200
C	-5.13545400	-2.04505600	3.21535100
C	-5.04815000	-2.78492300	-0.38395100
C	-2.93758800	2.91765900	-1.40104200
C	-1.17521100	-0.39219500	-3.37696500
C	-5.50929700	-1.04122400	-2.07752500
C	-5.27098200	2.62775800	-2.28505100
C	-2.81512400	-1.08248900	3.27376500
C	-1.32314500	-4.40722300	-1.09045000
H	-3.73117400	-2.03218400	1.61483700
H	-2.08426900	-3.07404700	0.41116400
H	-0.56760500	-2.42349600	-3.01070800
H	-3.03267700	-0.35848600	4.06994300
H	-5.41113900	3.45903700	0.35336500
H	-0.45852400	-2.69200800	-0.11882500
H	-3.40478000	-3.34892000	-2.31506700
H	-6.04442400	-2.20615100	2.62393000
H	-6.01941400	-1.80211100	-2.67822100
H	-5.60777300	-3.47542100	-1.02423700
H	-3.32850200	-1.79453800	-3.12964500
H	-1.90863100	-0.67959500	-4.13793500
H	-2.30101100	-4.84699200	-1.31705200
H	-3.80609500	1.09527900	-2.05726300
H	-1.98397300	-0.67932000	2.67654700
H	-5.11055500	-0.29027700	-2.76714600
H	-1.58177400	0.48203900	-2.84763300
H	-0.73272500	-4.40347300	-2.01448300
H	-5.41440800	-1.46635100	4.10438500
H	0.05153500	-1.28179600	-1.83376100
H	-5.33867700	0.68392800	3.60873300
H	-5.57782200	3.58199000	-1.84006900
H	-2.46965600	-2.01349800	3.73987100
H	-4.30722400	-3.37492000	0.16593200
H	-2.62056000	3.24117600	-2.40034500
H	-3.17362400	3.81397200	-0.81134200
H	-6.15487500	1.98156600	-2.33385100
H	-5.75747400	-2.34546700	0.32673700
H	-2.07697500	2.42240300	-0.92294300
H	-5.96371200	2.88755600	2.68997100
H	-4.77678500	-3.02105000	3.56152700
H	-0.82429700	-5.08064400	-0.38482600
H	-4.94286300	2.83631800	-3.30967900
H	-0.27655300	-0.05978600	-3.91007500
H	-6.25806700	-0.57235900	-1.42788700
H	0.08967300	0.96396200	-1.36932800
Cu	1.39611900	0.95036300	-0.36717100
N	3.72961400	-0.48439700	0.45125800
C	2.45778900	-2.55632100	0.78947200
C	3.14461200	-1.69507500	-0.08745400
C	3.90882000	1.67532700	1.22653300
C	2.13629700	-2.18926500	2.22469200
C	3.25953400	-1.96441800	-1.46303600
C	5.29299400	1.01658900	1.39814600
C	3.17530400	1.83781800	2.58091500
C	3.09414200	0.65510700	0.47324300
C	5.14633000	-0.46604200	1.02909000
C	3.83978900	-0.98393700	-2.46299200
C	2.12939800	-4.07574600	-1.07192900
C	2.73932800	-3.17338700	-1.93054700
C	3.99194100	3.01520700	0.48427600
C	1.97331900	-3.75722900	0.27033500
C	2.47588800	-3.29181700	3.22300800
C	5.27944500	-1.39009700	2.22946700
C	2.73382900	-0.42372600	-3.35826300
C	4.35275900	2.89532500	-0.98754800
C	6.14057400	-0.89815900	-0.03617500
C	4.94800100	-1.59697800	-3.31554300
C	0.66450400	-1.79763600	2.35364600
C	3.73342300	2.93355400	3.47371300
H	2.71795100	-1.30137500	2.49248100
H	3.20435000	0.87493200	3.11430600
H	4.73498300	3.63966900	0.99902200
H	0.00306500	-2.66071200	2.19472000
H	2.81211300	-3.40800300	-2.99087100
H	2.10926200	2.02989000	2.38149300
H	5.66840400	1.12666400	2.42227500
H	3.51943800	-3.61565800	3.14144000
H	7.14922500	-0.83474200	0.38620000
H	6.32279500	-1.36588000	2.56212400
H	6.03002800	1.49336600	0.74098100
H	5.31065000	2.38054600	-1.13973200
H	4.80978400	2.81168000	3.64608300
H	4.26609300	-0.13579200	-1.91255600
H	0.39217700	-1.03061200	1.61252100
H	6.10825000	-0.24806300	-0.91717800
H	3.58652500	2.33387000	-1.54179800
H	3.57402100	3.92801700	3.04277700
H	1.83965100	-4.17358700	3.07964900
H	3.02983600	3.53917500	0.58284400
H	1.44621600	-4.44620400	0.92869900
H	4.55937700	-2.38793900	-3.96847600
H	0.45956400	-1.39116600	3.35264700
H	4.65947800	-1.07872300	3.07625300
H	3.13698900	0.34052500	-4.03422200
H	2.27857800	-1.21285200	-3.97132100
H	5.74493700	-2.03186800	-2.70251000
H	5.04095800	-2.42742500	1.96807000
H	1.93254800	0.03651500	-2.76304600
H	1.75002900	-5.02044100	-1.45461600
H	2.30971700	-2.93428800	4.24569200
H	3.23941200	2.91373200	4.44993100
H	5.39371100	-0.83054000	-3.96006200
H	4.43409800	3.88213900	-1.45402800
H	5.97324700	-1.93627000	-0.34704000
B	-0.83546700	2.00117300	2.04042600
H	-0.01484600	1.30640600	1.36693500
H	-0.59129200	1.78546800	3.19784900
H	-2.01367400	1.77813700	1.77331300
N	-0.53455700	3.52534300	1.67302900
H	-1.23064200	4.13981400	2.09541500
H	0.37161600	3.83521700	2.02667800
H	-0.53248700	3.72201500	0.66587700
B	0.68343800	3.90624200	-1.51354600
H	1.25506900	3.37843200	-0.56791800
H	-0.41004500	4.34960100	-1.22751200
N	0.66718500	3.03805500	-2.71817700
H	1.56608900	2.82719200	-3.14201200
H	0.36889100	1.63403700	-1.82427900
H	-0.00095300	3.25561800	-3.44819900
O	1.66427900	5.19507900	-1.78012700
H	1.31273800	5.82470300	-2.42893500
H	1.86319000	5.69377400	-0.97249900

INT6

E_{solv} = -2380.524526 a.u.

Zero-point energy correction = 1.036285 a.u.

Cu	1.51450000	-0.24550000	-0.52224900
N	4.08091600	0.49332300	0.29332400
C	4.07401800	-1.74504100	1.33102300
C	4.35798500	-0.92784300	0.21924200
C	2.85991700	2.44446800	0.19095000
C	3.46440800	-1.24125900	2.62451100

C	4.81248400	-1.46227400	-1.00300500
C	4.33623300	2.83303000	0.41031100
C	1.98760100	2.67989300	1.44478600
C	2.89303800	0.95538200	0.00445400
C	5.10400000	1.54170000	0.72773600
C	4.98835200	-0.64662200	-2.26867700
C	4.80421400	-3.66123800	0.02632600
C	5.03819500	-2.83891800	-1.06779200
C	2.22743100	3.11297400	-1.03875300
C	4.31359700	-3.11651700	1.20562000
C	4.33445800	-1.57694000	3.83488800
C	5.41807800	1.39552000	2.20965400
C	3.95430600	-1.05096000	-3.32003000
C	2.84623800	2.72299000	-2.37263400
C	6.39467600	1.41131200	-0.06044800
C	6.39888600	-0.76999200	-2.84185600
C	2.05488600	-1.79866300	2.82281200
C	1.76701700	4.13716400	1.81375500
H	3.37005100	-0.15150200	2.56486800
H	2.43535500	2.14929900	2.29960800
H	2.28630600	4.20258000	-0.90804900
H	2.05736700	-2.89529900	2.86400200
H	5.39003400	-3.27550500	-2.00025600
H	1.01507200	2.19773100	1.26569400
H	4.45435000	3.56141900	1.22051100
H	5.36960400	-1.24110700	3.70829700
H	7.08992100	2.18282300	0.28769300
H	6.15077100	2.16248900	2.48284300
H	4.74917600	3.29737500	-0.49307700
H	3.91515300	2.96559400	-2.42639300
H	2.71148800	4.67174700	1.96957600
H	4.80614900	0.40903700	-2.03311100
H	1.38105000	-1.49249700	2.01301900
H	6.24534300	1.56351300	-1.13391300
H	2.73905000	1.64713800	-2.57037600
H	1.20492500	4.67700600	1.04265200
H	4.35765000	-2.65795200	4.01954500
H	1.15638200	2.85694800	-1.04760800
H	4.10248200	-3.77007400	2.04967900
H	6.59532600	-1.78800100	-3.19983200
H	1.63219900	-1.42817000	3.76429400
H	4.53818400	1.53925000	2.84562300
H	4.07359600	-0.43960400	-4.22245900
H	4.06698600	-2.10356900	-3.60905400
H	7.16785700	-0.52320000	-2.10169900
H	5.86532400	0.41951500	2.42876300
H	2.92920400	-0.91206400	-2.95336300
H	4.98643600	-4.73041900	-0.04562100
H	3.92853600	-1.09877800	4.73356200
H	1.19647400	4.20692100	2.74682000
H	6.51739800	-0.09360700	-3.69606600
H	2.35525400	3.25316700	-3.19459500
H	6.87041000	0.43706500	0.10496000
B	0.47606000	-2.04375900	-1.10461800
H	0.42141200	-1.56787700	0.04472600
H	1.01827400	-1.28347700	-1.92858400
N	1.38869600	-3.35447000	-1.00236800
H	1.56472600	-3.78383800	-1.91305000
H	2.30957300	-3.18659100	-0.58019700
H	0.93239400	-4.06564800	-0.42728300
Cu	-2.39331600	-1.61152100	-0.67326700
N	-4.17476900	0.39539600	0.22957700
C	-2.35083200	1.84321900	1.00713000
C	-3.18165300	1.41203200	-0.04433600
C	-5.14692300	-1.67407200	0.52114000
C	-2.26381500	1.10965200	2.33064300
C	-3.07980700	1.93980400	-1.34322200
C	-6.24941100	-0.61831700	0.74283800
C	-4.70079600	-2.33732800	1.84740100
C	-3.95684700	-0.87905000	0.06033100
C	-5.57588800	0.76281500	0.72103800
C	-3.79230600	1.34599400	-2.54086800
C	-1.44911500	3.52086300	-0.49643400
C	-2.19710200	3.00391400	-1.54312800
C	-5.53013700	-2.74061100	-0.51459900
C	-1.50896300	2.92718800	0.75803900
C	-2.09578800	2.03149600	3.53318100
C	-5.52961300	1.42049800	2.09253300
C	-2.78315800	0.58762000	-3.40630400
C	-5.70148900	-2.21990200	-1.93367400
C	-6.23655600	1.71564800	-0.26148800
C	-4.53432700	2.38502100	-3.37661200
C	-1.12841800	0.08475100	2.28505300
C	-5.72868200	-3.27499400	2.46010500
H	-3.18888200	0.54223300	2.47409800
H	-4.44941300	-1.54400000	2.56854400
H	-6.46282900	-3.21677600	-0.18265400
H	-0.15420600	0.57675600	2.14545900
H	-2.10184700	3.43719800	-2.53666400
H	-3.76451900	-2.88739800	1.66576400
H	-6.77688900	-0.77472900	1.69072700
H	-2.85837900	2.81852900	3.55681400
H	-7.25423600	1.92051800	0.08821700
H	-6.54949700	1.71375800	2.36409100
H	-7.00492100	-0.67664000	-0.04937300
H	-6.46253000	-1.43160200	-1.99794700
H	-6.69908800	-2.78400100	2.60213100
H	-4.52883000	0.61451400	-2.18441200
H	-1.26486300	-0.63070400	1.46010500
H	-6.31172200	1.28532200	-1.26605500
H	-4.76354900	-1.80794000	-2.33241700
H	-5.89063000	-4.16261100	1.83941700
H	-1.11008000	2.51584000	3.53946300
H	-4.76047700	-3.52825200	-0.50194500
H	-0.88756500	3.31644400	1.56168300
H	-3.84149000	3.08875900	-3.85354400
H	-1.08676100	-0.48516500	3.22140200
H	-5.16539600	0.74490700	2.87345100
H	-3.29010700	0.07570100	-4.23301800
H	-2.03918000	1.27170100	-3.83421500
H	-5.24009100	2.96726300	-2.77391900
H	-4.91575000	2.32885500	2.08495300
H	-2.23771400	-0.16614000	-2.81931900
H	-0.79781000	4.37668300	-0.66361500
H	-2.17354600	1.45225400	4.45977600
H	-5.38826100	-3.61809000	3.44196900
H	-5.09675900	1.88988900	-4.17636400
H	-6.01394200	-3.02392500	-2.60716000
H	-5.70382700	2.67231300	-0.31842600
O	-0.86952900	-2.41915300	-1.50346400
H	-0.97431000	-2.56389000	-2.45196600

INT7

E_{solv} = -2380.523607 a.u.

Zero-point energy correction = 1.035521 a.u.

Cu	-1.04792200	-0.34697100	-0.40357600
N	-3.64566800	0.74013300	-0.07713800
C	-4.34066600	-1.41128900	-1.05334200
C	-4.08901800	-0.62959100	0.08948400
C	-2.19688400	2.48971800	-0.45753500
C	-4.10840400	-0.92199300	-2.46947000
C	-4.16648700	-1.16011100	1.38995400
C	-3.59213000	3.10133000	-0.20163400
C	-1.74130000	2.66444000	-1.92370100
C	-2.38457200	1.01602100	-0.25800600
C	-4.59417200	1.93717900	-0.10664600
C	-3.68766100	-0.41208900	2.61822500
C	-4.90887100	-3.25539100	0.41913800
C	-4.60099100	-2.47939100	1.52797400
C	-1.11647300	2.99487800	0.50795600
C	-4.75646600	-2.73012600	-0.85638900

C	-5.32810100	-1.12343900	-3.36514900
C	-5.50929500	1.85045700	-1.31935900
C	-2.34521900	-0.97703700	3.08640900
C	-1.36702600	2.67119800	1.97158700
C	-5.44480900	1.99188200	1.15089600
C	-4.70307700	-0.42440600	3.75650300
C	-2.87916600	-1.59424600	-3.08196400
C	-1.31987900	4.07835200	-2.28902700
H	-3.89434100	0.15109000	-2.43652000
H	-2.55884900	2.33800100	-2.58518700
H	-1.02064700	4.08273200	0.38318400
H	-3.00910800	-2.68373400	-3.13636200
H	-4.67259700	-2.91377800	2.52331800
H	-0.90484300	1.97299400	-2.11245600
H	-3.88157500	3.79018800	-1.00393600
H	-6.22980200	-0.67506300	-2.93259000
H	-6.11950300	2.85126800	1.07335600
H	-6.19314100	2.70579700	-1.29840300
H	-3.60251200	3.68172200	0.72818800
H	-2.31997400	3.07851200	2.33325800
H	-2.09466500	4.81435200	-2.04047500
H	-3.50688000	0.63272200	2.34244800
H	-1.97023700	-1.37494300	-2.49951100
H	-4.84322400	2.12741100	2.05567000
H	-1.37701100	1.58705000	2.15111000
H	-0.40062400	4.37378400	-1.76835300
H	-5.53276400	-2.18757000	-3.53469600
H	-0.14925600	2.56440400	0.19689500
H	-4.95868100	-3.35773200	-1.72243800
H	-4.84680600	-1.43414400	4.15979700
H	-2.70940900	-1.22930300	-4.10167700
H	-4.95745700	1.89401600	-2.26444400
H	-1.97671700	-0.41840800	3.95572800
H	-2.43834600	-2.03227200	3.37608300
H	-5.68105900	-0.05050600	3.43275600
H	-6.11756400	0.93831800	-1.29851400
H	-1.58403700	-0.90543700	2.29366300
H	-5.24433800	-4.28134400	0.54868900
H	-5.15542400	-0.66316500	-4.34463400
H	-1.12631000	4.15140300	-3.36414200
H	-4.35147200	0.20824500	4.57947300
H	-0.57635100	3.09587800	2.59980800
H	-6.06313200	1.09258200	1.25960800
B	-0.95271800	-3.44455300	0.55173000
H	-0.15242600	-1.62432100	-0.71832300
H	-1.94394800	-2.84676400	0.79656200
N	-0.90066100	-4.20776200	-0.79277200
H	-1.46495600	-5.06302500	-0.74407900
H	-1.28051700	-3.65887900	-1.56868300
H	0.05120000	-4.49243600	-1.04123900
Cu	1.33076500	-1.10191800	-0.47259600
N	3.84573200	0.17333800	0.11559500
C	2.97431100	2.35591300	-0.60796000
C	3.16985900	1.41585000	0.41945900
C	4.20999300	-1.99528300	-0.56852700
C	3.19902100	2.02506900	-2.06925600
C	2.73449700	1.64332400	1.73672300
C	5.56276000	-1.44236000	-0.07269300
C	4.17903800	-2.17477400	-2.10460400
C	3.22082100	-0.90182800	-0.27123500
C	5.36582800	0.05203400	0.22569800
C	2.68994500	0.54788000	2.78242300
C	2.10445200	3.88535100	1.06079500
C	2.21967400	2.90532400	2.03724200
C	3.79203800	-3.29385500	0.13721100
C	2.44473400	3.59843400	-0.25427500
C	3.92094700	3.12578800	-2.83917200
C	6.05010300	0.95123500	-0.79334200
C	1.25948600	0.01349400	2.89157100
C	3.53123400	-3.15042800	1.62872200
C	5.83213500	0.43596200	1.62021700
C	3.20088200	0.98847900	4.14991000
C	1.85823500	1.70081200	-2.73007200
C	5.04432200	-3.31123900	-2.62527700
H	3.81084100	1.11853300	-2.13130200
H	4.49157500	-1.22848000	-2.57314300
H	4.57775400	-4.04336900	-0.02890700
H	1.19232600	2.57457100	-2.70585200
H	1.89175900	3.11769200	3.05327700
H	3.13463200	-2.33528300	-2.41561300
H	6.35521000	-1.58357400	-0.81658000
H	4.86454300	3.41005300	-2.35926800
H	6.91988200	0.31446000	1.66533700
H	7.13364600	0.85700300	-0.66292200
H	5.88806000	-1.96497900	0.83449900
H	4.41884900	-2.80252900	2.17258300
H	6.08270900	-3.22607000	-2.28220900
H	3.31775500	-0.28539700	2.44435100
H	1.34519100	0.87235800	-2.21577800
H	5.39587600	-0.20565400	2.39335400
H	2.71878500	-2.43821000	1.83153800
H	4.66656800	-4.28868900	-2.30654000
H	3.30435100	4.02856200	-2.92915900
H	2.88693300	-3.67941300	-0.35912900
H	2.28684100	4.35004000	-1.02577900
H	2.54283600	1.73756400	4.60683900
H	2.00198400	1.41184200	-3.77802200
H	5.81684500	0.66906600	-1.82565500
H	1.20866700	-0.82461200	3.59913800
H	0.57449200	0.79726000	3.24213700
H	4.20758500	1.41753000	4.08945100
H	5.78832700	2.00475400	-0.63982200
H	0.88428900	-0.34090300	1.91553400
H	1.70487300	4.86393800	1.31801500
H	4.14563900	2.78497400	-3.85609500
H	5.05902500	-3.30532800	-3.71954100
H	3.23588100	0.13018500	4.83035100
H	3.23881900	-4.10977900	2.06682700
H	5.60355400	1.48317700	1.85113100
O	0.08671300	-3.69151700	1.33799700
H	0.05473700	-3.27656800	2.20914100

TS8

E_{solv} = -2456.964011 a.u.

Zero-point energy correction = 1.055095 a.u.

Cu	0.98984900	0.16096100	-0.55301700
N	3.52662200	-1.07053600	-0.02486600
C	4.54482900	0.96016300	-0.97563700
C	4.10740000	0.24415000	0.15262900
C	1.95776100	-2.70527000	-0.44423700
C	4.27794000	0.51447500	-2.39920600
C	4.18243200	0.77808400	1.45269900
C	3.28550400	-3.42391900	-0.11925500
C	1.54131000	-2.88837800	-1.92098300
C	2.25814200	-1.24461200	-0.27065300
C	4.37261400	-2.34428400	0.01451300
C	3.51846500	0.12887000	2.65000900
C	5.34119400	2.69499100	0.52457700
C	4.81497400	2.01114600	1.61355200
C	0.80754800	-3.09837600	0.49421700
C	5.17513500	2.18859800	-0.75816500
C	5.51894700	0.56800400	-3.28563000
C	5.35190700	-2.35481900	-1.15001300
C	2.21971100	0.86444100	2.98713000
C	1.03298900	-2.75480300	1.95706400
C	5.14844700	-2.44601400	1.31657800
C	4.42506900	0.05522400	3.87443000
C	3.15091200	1.35374900	-3.00370600
C	1.02745600	-4.27730400	-2.26376500
H	3.92530800	-0.52246700	-2.37996900
H	2.40445500	-2.64355700	-2.55949300

H	0.63654400	-4.17942200	0.39368300
H	3.40673900	2.42199900	-3.00078000
H	4.89615900	2.44339100	2.60867000
H	0.76536100	-2.14407400	-2.16116800
H	3.55475500	-4.14023800	-0.90430800
H	6.35886100	0.01712200	-2.84740700
H	5.73836400	-3.36862600	1.29360600
H	5.95117500	-3.26953500	-1.08853200
H	3.20687300	-3.99591700	0.81242100
H	1.94141200	-3.21933700	2.36154900
H	1.73673400	-5.06166400	-1.97136900
H	3.23675400	-0.89490300	2.38078200
H	2.21322500	1.22546800	-2.43996200
H	4.49093400	-2.49840500	2.19057500
H	1.11401800	-1.66971600	2.11030200
H	0.07282500	-4.48966800	-1.76687300
H	5.84859300	1.59941800	-3.45963600
H	-0.11525600	-2.60867100	0.13857800
H	5.54226900	2.75681600	-1.61077000
H	4.64116900	1.05054900	4.28104600
H	2.95752600	1.05158900	-4.03944800
H	4.84494500	-2.35718600	-2.12106500
H	1.72364700	0.39623300	3.84594200
H	2.42145300	1.91411100	3.24356400
H	5.38089600	-0.42803100	3.64301500
H	6.04121700	-1.50330100	-1.10464300
H	1.52000200	0.83325100	2.13646000
H	5.87475100	3.63198700	0.67716600
H	5.29758700	0.12830000	-4.26455700
H	0.86262400	-4.36525900	-3.34245700
H	3.93485400	-0.52032500	4.66759600
H	0.19325600	-3.10552100	2.56673500
H	5.84646500	-1.60915000	1.43902100
B	1.12031500	3.14932400	0.26510500
H	0.10227400	1.38759200	-1.03690300
H	2.07669600	2.44517700	0.25134100
N	0.84133400	4.00356700	-0.97672500
H	1.61673100	4.69987200	-0.96797200
H	0.89104700	3.48579500	-1.85549300
H	-0.05583100	4.49182500	-0.94098500
Cu	-1.36716400	1.02239200	-0.56589100
N	-3.95465900	-0.04321800	0.12146200
C	-3.21362600	-2.27323300	-0.61639600
C	-3.37001400	-1.33304200	0.41703000
C	-4.16019400	2.15597200	-0.53082800
C	-3.39717800	-1.92352300	-2.07904200
C	-2.97649900	-1.60028200	1.74021100
C	-5.53784400	1.70424900	-0.00319900
C	-4.15528000	2.35291100	-2.06498600
C	-3.25394900	0.98462700	-0.26449700
C	-5.46225200	0.18689200	0.22094400
C	-2.88804200	-0.51590700	2.79434800
C	-2.46119700	-3.86669400	1.05073500
C	-2.54143500	-2.89241400	2.03684300
C	-3.62325700	3.41023500	0.17580600
C	-2.76147400	-3.54745900	-0.26627700
C	-4.20579500	-2.95917600	-2.85348500
C	-6.18362500	-0.60606800	-0.85973900
C	-1.43172500	-0.06447600	2.92641500
C	-3.30665500	3.22657800	1.65219800
C	-5.99274700	-0.23256500	1.58122700
C	-3.44662700	-0.93273300	4.15018800
C	-2.02822400	-1.71700000	-2.72935800
C	-4.93110300	3.56795900	-2.54793400
H	-3.92899300	-0.96783900	-2.14550800
H	-4.56226000	1.44511200	-2.53646300
H	-4.36071500	4.21510500	0.05256900
H	-1.43587500	-2.64190000	-2.69404400
H	-2.24727100	-3.13426400	3.05666100
H	-3.10956100	2.42569100	-2.40375700
H	-6.34510500	1.95095600	-0.70244700
H	-5.17509900	-3.15798100	-2.38189200
H	-7.06848600	-0.02722700	1.60754900
H	-7.26057500	-0.43710400	-0.75302700
H	-5.77470200	2.20864900	0.94121500
H	-4.18636100	2.91748500	2.23133000
H	-5.96261200	3.56994100	-2.17493700
H	-3.46127000	0.35336300	2.45006800
H	-1.45331200	-0.93052800	-2.21436500
H	-5.53012500	0.32932100	2.39947500
H	-2.52361700	2.47126100	1.80594400
H	-4.45968100	4.50427200	-2.23064200
H	-3.67038300	-3.91307700	-2.93481300
H	-2.71535200	3.74084300	-0.35460600
H	-2.63280100	-4.29941800	-1.04305200
H	-2.84492500	-1.72559200	4.61088800
H	-2.13755800	-1.42316900	-3.78003500
H	-5.89796600	-0.29352600	-1.87000200
H	-1.34624000	0.79005900	3.61032900
H	-0.80397900	-0.87698600	3.31589400
H	-4.47767500	-1.29606600	4.07085300
H	-6.00412100	-1.68240400	-0.75336300
H	-1.01533500	0.23465800	1.94970800
H	-2.12214700	-4.86893600	1.30353400
H	-4.39048900	-2.60334900	-3.87335500
H	-4.97766400	3.57740100	-3.64127000
H	-3.43743500	-0.07886000	4.83708600
H	-2.94394900	4.16182900	2.09004600
H	-5.85403600	-1.30556200	1.75878900
O	3.13590900	5.14456200	-0.10298500
H	3.19241400	5.70737500	0.67656000
H	3.84320800	4.49294400	-0.00900300
O	0.30558400	3.39172700	1.28785200
H	0.50853800	2.90534600	2.09649200

TS9

E_{solv} = -2540.184903 a.u.

Zero-point energy correction = 1.123077 a.u.

Cu	-1.25614600	0.30550400	0.64970800
N	-3.56222900	-0.76887400	-0.52989100
C	-4.51406900	-0.52942000	1.72960300
C	-4.25601600	0.02320400	0.46363400
C	-1.83392700	-1.72497100	-1.70392300
C	-4.00895400	-1.89220300	2.15781200
C	-4.57693100	1.35530300	0.14655500
C	-3.13664000	-1.96946300	-2.49093600
C	-1.30575500	-2.97977200	-0.95920300
C	-2.25622900	-0.77363200	-0.60953500
C	-4.29190100	-1.64809900	-1.54150800
C	-4.13864100	2.03168700	-1.13752000
C	-5.55607500	1.57018900	2.35466700
C	-5.24130800	2.10927400	1.11476700
C	-0.70495300	-1.13601900	-2.56070800
C	-5.17977000	0.26998700	2.66067000
C	-5.09276700	-2.74796000	2.80689100
C	-4.86694800	-2.89001500	-0.87163700
C	-2.97120600	2.97927300	-0.86029700
C	-1.05285400	0.13390100	-3.32138400
C	-5.42154700	-0.89002600	-2.21619800
C	-5.27615100	2.77148600	-1.83546500
C	-2.80595700	-1.74556800	3.08985500
C	-1.18971600	-4.23580000	-1.80702200
H	-3.65480800	-2.42498300	1.26995400
H	-1.93615800	-3.19599800	-0.08210000
H	-0.35646900	-1.90390100	-3.26668200
H	-3.06744700	-1.18200800	3.99513700
H	-5.50206700	3.14349200	0.89829600
H	-0.31782600	-2.72072200	-0.55161200
H	-3.21583100	-2.98572300	-2.88922800
H	-5.98395300	-2.82983900	2.17346600
H	-5.89169600	-1.55332200	-2.95039900

H	-5.38015900	-3.48342700	-1.63634400
H	-3.18500000	-1.29037100	-3.34981000
H	-1.75698000	-0.04555900	-4.14064700
H	-2.16919800	-4.64492300	-2.07945800
H	-3.76528900	1.26549500	-1.82892300
H	-1.97915100	-1.21521800	2.59503300
H	-5.06521000	-0.00509800	-2.75263000
H	-1.50127700	0.89334400	-2.66411900
H	-0.63020400	-4.05712700	-2.73334500
H	-5.40814400	-2.33645800	3.77353700
H	0.14979700	-0.94242000	-1.88877400
H	-5.39179900	-0.13105700	3.64994500
H	-5.61691300	3.63394200	-1.24988600
H	-2.43648400	-2.73257900	3.39453800
H	-4.09783700	-3.52734200	-0.42295500
H	-2.64665000	3.48359100	-1.77898700
H	-3.25072500	3.74790500	-0.12601800
H	-6.14068000	2.11941900	-2.00489100
H	-5.60635500	-2.62817800	-0.10618300
H	-2.10485200	2.43402600	-0.45511600
H	-6.07778800	2.17371100	3.09341500
H	-4.71203600	-3.75885100	2.99197800
H	-0.66068100	-5.01578000	-1.24842500
H	-4.93742500	3.15071600	-2.80629800
H	-0.15326000	0.57314100	-3.76836000
H	-6.19287800	-0.58861700	-1.49740000
H	0.01761500	1.40952000	-0.92126900
Cu	1.32061300	0.89617900	-0.14074000
N	3.70789600	-0.61530500	0.44246300
C	2.51621900	-2.76259100	0.42452300
C	3.17719800	-1.74598500	-0.28968700
C	3.79584600	1.42157100	1.50856700
C	2.17250600	-2.64720700	1.89634700
C	3.31100500	-1.77682200	-1.68914700
C	5.20520500	0.80138900	1.60731100
C	3.06802000	1.38922400	2.87405600
C	3.02239800	0.47779200	0.62773600
C	5.11975600	-0.62153600	1.03289600
C	3.86164900	-0.61976300	-2.49892500
C	2.25326100	-3.95965800	-1.66850200
C	2.83649900	-2.90689500	-2.35848000
C	3.80644700	2.83920400	0.91967100
C	2.07879700	-3.87608900	-0.29356700
C	2.55053500	-3.88519000	2.70374100
C	5.27569800	-1.69654900	2.09726000
C	2.73213300	0.08100300	-3.25415900
C	4.26528700	2.91241300	-0.53002400
C	6.14176900	-0.86894600	-0.06470300
C	4.96599200	-1.04357200	-3.46325500
C	0.68625500	-2.33569000	2.07235200
C	3.57550000	2.40293100	3.88620200
H	2.71867200	-1.79429800	2.31181800
H	3.15740200	0.37387800	3.28980700
H	4.46207600	3.46098100	1.54364900
H	0.05812000	-3.18359300	1.76603600
H	2.92321700	-2.95829800	-3.44223800
H	1.99080300	1.53730100	2.70296100
H	5.56144900	0.77859900	2.64368800
H	3.60602100	-4.15229300	2.57986200
H	7.14148500	-0.83595700	0.38168100
H	6.31202000	-1.67659200	2.45133200
H	5.93465200	1.39131900	1.04029400
H	5.21544200	2.38816800	-0.69327300
H	4.65983000	2.32580400	4.03274800
H	4.28548700	0.11904700	-1.80827200
H	0.38615200	-1.46564300	1.46871500
H	6.10402800	-0.10411800	-0.84765900
H	3.52825600	2.47271400	-1.21882900
H	3.35322100	3.43096100	3.57856200
H	1.94896600	-4.75430800	2.41111900
H	2.79387800	3.26853300	1.01142200
H	1.57238900	-4.68326900	0.23374100
H	4.58121700	-1.70421200	-4.24960400
H	0.46288900	-2.11064400	3.12350100
H	4.62964100	-1.53142200	2.96551500
H	3.11235600	0.96122700	-3.78737500
H	2.26815800	-0.58969900	-3.98959700
H	5.77733800	-1.57180800	-2.95000700
H	5.08564100	-2.69596300	1.68948300
H	1.94218400	0.41647700	-2.56570900
H	1.90757600	-4.83854900	-2.20781300
H	2.36749200	-3.70723500	3.76964800
H	3.09919500	2.23866200	4.85754600
H	5.39167500	-0.16226100	-3.95676000
H	4.44829000	3.94976000	-0.83434500
H	6.01248500	-1.85766100	-0.52085000
B	-0.95307600	1.51788500	2.47212400
H	-0.08541200	0.86354500	1.82683500
H	-0.90947300	1.12122400	3.60676500
H	-2.08715500	1.44139200	2.00834300
N	-0.50995800	3.05456500	2.40755100
H	-1.22597500	3.64784700	2.82684200
H	0.34788000	3.23587700	2.92970700
H	-0.35112000	3.41077400	1.45911300
B	0.47397400	4.43429500	-1.16522100
H	0.57194900	4.05217900	-0.00646900
N	1.80767900	5.32919600	-1.45578000
H	1.88030900	6.11075500	-0.80548500
H	2.66778300	4.78497700	-1.38182900
H	1.77814900	5.72552300	-2.39627100
O	0.64697400	3.24568400	-2.05558300
H	0.37576400	2.16955700	-1.39828900
H	0.07124000	3.32012900	-2.83059500
O	-0.64165500	5.21045600	-1.52973200
H	-1.26606500	5.33355500	-0.81334500

INT8

E_{solv} = -2455.813249 a.u.

Zero-point energy correction = 1.04309 a.u.

Cu	1.52549800	0.03913400	-0.60193700
N	4.23616500	0.46173300	-0.23561400
C	3.98520100	-1.19882300	1.57038200
C	4.26384400	-0.91182400	0.22187700
C	3.41026800	2.45898800	-1.03876000
C	3.53290900	-0.16064100	2.57694300
C	4.51344000	-1.92716300	-0.72205600
C	4.95069500	2.52286100	-1.10117700
C	2.82948000	3.39900200	0.04169200
C	3.12443600	1.04396500	-0.60392100
C	5.48371300	1.33948300	-0.28652400
C	4.60942200	-1.67184500	-2.21282800
C	4.36077600	-3.54856600	1.07711900
C	4.56959600	-3.24380100	-0.26198000
C	2.74399300	2.74750700	-2.39478100
C	4.04712100	-2.53643200	1.97474900
C	4.38547100	-0.16158400	3.84341900
C	5.89790900	1.72318200	1.12800900
C	3.33887900	-2.16560600	-2.90602800
C	2.96560200	1.69218300	-3.46741600
C	6.64678600	0.63528100	-0.96142100
C	5.84399000	-2.30678400	-2.84679200
C	2.05911300	-0.37313400	2.92489700
C	2.97540600	4.88163500	-0.26166600
H	3.61272100	0.83186400	2.11784900
H	3.29994200	3.17268800	1.01017600
H	3.11505600	3.71844100	-2.75023600
H	1.88652800	-1.36507100	3.36384000
H	4.76354600	-4.04679900	-0.97010200
H	1.76378500	3.16364600	0.16129100
H	5.34338900	3.47003500	-0.71482000

H	5.45277700	-0.05005300	3.62140300
H	7.50145600	1.32047200	-0.96859400
H	6.78251000	2.36632500	1.06968900
H	5.29348800	2.43796900	-2.13999700
H	4.03092600	1.50172200	-3.65322200
H	4.01766500	5.16483300	-0.45051200
H	4.66221800	-0.58921800	-2.38063400
H	1.41498000	-0.28529100	2.03733900
H	6.42990400	0.37133400	-2.00096200
H	2.49826100	0.73543000	-3.19577000
H	2.38397000	5.17708100	-1.13481900
H	4.25918700	-1.09101200	4.41193200
H	1.66208100	2.87536100	-2.22991700
H	3.83911000	-2.78664400	3.01325300
H	5.79340100	-3.40194200	-2.81850200
H	1.72966100	0.37842800	3.65315900
H	5.11902700	2.27712700	1.66243400
H	3.36348700	-1.92012400	-3.97445300
H	3.23201500	-3.25371300	-2.80945600
H	6.76713700	-2.00194100	-2.34142500
H	6.17068700	0.83765000	1.71377900
H	2.44295600	-1.70090600	-2.47023200
H	4.41331100	-4.58008700	1.41622700
H	4.08588600	0.66524600	4.49710500
H	2.62391800	5.47443000	0.58835700
H	5.91731500	-2.01175200	-3.89967400
H	2.52524400	2.00951200	-4.41774700
H	6.94994000	-0.26552600	-0.41465200
B	-0.17696000	-2.31690400	0.22653900
H	-0.25582400	-1.79595600	1.30966000
N	0.99830400	-3.42966300	0.30373300
H	1.22676900	-3.87503300	-0.58824600
H	1.87254900	-3.02894000	0.66107400
H	0.74322600	-4.17607900	0.95269800
Cu	-2.94675300	-1.85647200	-0.13285300
N	-4.16835300	0.59825500	0.36776900
C	-2.38663900	0.79974800	2.05631500
C	-2.84725800	1.05378500	0.75019500
C	-5.82593000	-0.85505100	-0.30786900
C	-3.15875700	-0.00461900	3.08310700
C	-2.03733800	1.66606000	-0.22265300
C	-6.45831200	0.54852400	-0.18941300
C	-6.31269800	-1.81466000	0.80362000
C	-4.36481400	-0.62567900	-0.04348500
C	-5.42177600	1.46180500	0.48213100
C	-2.43451900	1.79847200	-1.67924400
C	-0.30854900	1.90237600	1.46594400
C	-0.76718300	2.09348700	0.16917600
C	-6.02257900	-1.49042600	-1.69276400
C	-1.10913000	1.24891200	2.39102800
C	-3.31189100	0.73635200	4.40943900
C	-5.73701100	1.73413900	1.94644200
C	-1.65979400	0.79986700	-2.53921700
C	-5.32282500	-0.76652000	-2.83324400
C	-5.24854400	2.78904500	-0.23546500
C	-2.25652900	3.21714200	-2.21319600
C	-2.49573200	-1.36420300	3.30706400
C	-7.76095200	-2.25632600	0.66587500
H	-4.16262600	-0.20042900	2.69128600
H	-6.16947200	-1.32505100	1.77919700
H	-7.10144300	-1.53944300	-1.89380900
H	-1.46610800	-1.25168100	3.67306200
H	-0.13005400	2.58790300	-0.56370200
H	-5.65723800	-2.69914600	0.81012000
H	-7.38840700	0.53051600	0.38997500
H	-3.74531300	1.73403300	4.27605800
H	-6.16728700	3.37170300	-0.10796200
H	-6.62966800	2.36678100	1.99601000
H	-6.71268600	0.94176000	-1.18084300
H	-5.64044600	0.28070500	-2.91914900
H	-8.44507900	-1.40229600	0.59047300
H	-3.49340500	1.53260000	-1.77587900
H	-2.45288400	-1.95140000	2.37860400
H	-5.08520000	2.66507600	-1.31070700
H	-4.23132900	-0.77359600	-2.70848300
H	-7.91240200	-2.88487000	-0.21809100
H	-2.34630700	0.85761700	4.91548200
H	-5.66748200	-2.53167600	-1.64607200
H	-0.72947600	1.06683100	3.39457600
H	-1.19766500	3.50226300	-2.25890000
H	-3.05916600	-1.94405400	4.04756300
H	-5.94953600	0.81905000	2.50919700
H	-1.97668600	0.87225800	-3.58644500
H	-0.57684300	0.99167700	-2.49909400
H	-2.77496100	3.95602400	-1.59185600
H	-4.91931700	2.27544500	2.43648700
H	-1.83536900	-0.22950800	-2.19744800
H	0.68328500	2.24737400	1.75667600
H	-3.96471000	0.16914900	5.08263300
H	-8.06223000	-2.84119700	1.54040100
H	-2.65538500	3.28701100	-3.23153600
H	-5.54291900	-1.24789200	-3.79109900
H	-4.42383300	3.37302300	0.19080200
O	-1.42202000	-3.01804400	-0.10643400
H	-1.38586100	-3.63511200	-0.84890000
O	0.17819300	-1.31779400	-0.78375600
H	0.02783700	-1.59361000	-1.69679100

INT9

E_{solv} = -2455.816647 a.u.

Zero-point energy correction = 1.039098 a.u.

Cu	-1.10141300	-0.33004900	-0.48433400
N	-3.68956200	0.77573900	-0.06699700
C	-4.55862000	-1.31247100	-1.03651000
C	-4.16880200	-0.58044500	0.10009400
C	-2.22649300	2.50325500	-0.48726200
C	-4.32717900	-0.82347100	-2.45185600
C	-4.16593600	-1.14584300	1.38750300
C	-3.59862100	3.13802800	-0.16921200
C	-1.83221000	2.68170300	-1.97092500
C	-2.43177800	1.03006600	-0.29610200
C	-4.61339600	1.99066000	-0.01844800
C	-3.55693900	-0.45762000	2.59176300
C	-5.13918300	-3.15461500	0.43114100
C	-4.66404600	-2.44514800	1.52768700
C	-1.09884600	2.98687800	0.43479000
C	-5.06460400	-2.59808200	-0.83792900
C	-5.54964300	-0.98047000	-3.35072700
C	-5.61565600	1.94116300	-1.16201800
C	-2.21229000	-1.10087000	2.93467600
C	-1.29433900	2.66118800	1.90612300
C	-5.36613900	2.03817800	1.30068500
C	-4.47851600	-0.45682600	3.80760600
C	-3.11833300	-1.54279300	-3.05509100
C	-1.40284700	4.09098600	-2.34448100
H	-4.07504600	0.24165200	-2.41589000
H	-2.68460900	2.37374800	-2.59660600
H	-0.99473500	4.07407900	0.31091300
H	-3.29374100	-2.62443400	-3.12339500
H	-4.68329900	-2.90455500	2.51447900
H	-1.01708800	1.97780000	-2.20177300
H	-3.91457500	3.82497800	-0.96313900
H	-6.43730400	-0.50226500	-2.92103300
H	-6.01844200	2.91808400	1.29579600
H	-6.27586100	2.81128600	-1.08008200
H	-3.55663100	3.72624900	0.75472900
H	-2.23063800	3.07236700	2.30483800
H	-2.15391000	4.83804600	-2.05868400
H	-3.34992000	0.58575400	2.32803500
H	-2.21381500	-1.39093500	-2.44557600
H	-4.69334900	2.13139600	2.15982200

H	-1.30028900	1.57692200	2.08550300
H	-0.45787200	4.36733400	-1.86078100
H	-5.79016800	-2.03583900	-3.52776800
H	-0.14988800	2.54667600	0.08312600
H	-5.37878000	-3.18441700	-1.69893200
H	-4.63678800	-1.46984500	4.19686800
H	-2.91319100	-1.16491900	-4.06378800
H	-5.13180900	1.98646300	-2.14364100
H	-1.74936500	-0.59272100	3.78958800
H	-2.33595100	-2.15949400	3.20095900
H	-5.46033200	-0.03034800	3.57292900
H	-6.24254100	1.04302100	-1.10942600
H	-1.51056600	-1.04040500	2.08694500
H	-5.53680100	-4.15771600	0.56370000
H	-5.35641000	-0.52318800	-4.32771400
H	-1.25293100	4.16844700	-3.42616300
H	-4.03292800	0.13640800	4.61411200
H	-0.47769200	3.08276600	2.50241000
H	-6.00098500	1.15399800	1.43521600
B	-0.68829700	-3.92584500	-0.06227800
H	-0.15555100	-1.56647000	-0.76928600
N	-0.10263200	-4.29240800	-1.45175100
H	-0.75262400	-4.85952500	-2.00151900
H	0.07436600	-3.44074700	-1.99582200
H	0.78428700	-4.79600400	-1.38341000
Cu	1.29010000	-1.04590100	-0.36869500
N	3.82512100	0.21322900	0.19604900
C	2.94856000	2.34888600	-0.66104600
C	3.17370200	1.48475000	0.42470600
C	4.13594600	-2.01071600	-0.31813900
C	3.12564800	1.91977200	-2.10315900
C	2.78465300	1.81157100	1.73577800
C	5.50636500	-1.44653900	0.11291700
C	4.07948400	-2.33592700	-1.82910200
C	3.17410200	-0.87348400	-0.10627200
C	5.34500800	0.07258600	0.27460400
C	2.77895000	0.79471300	2.85859700
C	2.13094900	3.99870600	0.91819300
C	2.27924900	3.09291900	1.96004300
C	3.70030400	-3.23104500	0.50786600
C	2.43167100	3.61584700	-0.38164500
C	3.88436300	2.93690300	-2.94949200
C	6.00183300	0.85697400	-0.85186700
C	1.35418400	0.27495800	3.06193300
C	3.43920100	-2.95350900	1.97992400
C	5.87152600	0.58122200	1.60593400
C	3.34782600	1.32846700	4.16851500
C	1.75666100	1.62574800	-2.71901700
C	4.90794100	-3.53989800	-2.24775000
H	3.69109600	0.98121400	-2.12095500
H	4.40716500	-1.44860600	-2.39274500
H	4.47546300	-4.00319900	0.40951900
H	1.13577000	2.53227700	-2.74296700
H	1.98493700	3.38042600	2.96795900
H	3.02607100	-2.49980300	-2.10979200
H	6.28887700	-1.67317400	-0.62057500
H	4.85418700	3.19427500	-2.50839800
H	6.95831000	0.44436200	1.62049400
H	7.08812800	0.75005800	-0.76055600
H	5.82779000	-1.89147300	1.06222800
H	4.32010600	-2.54181600	2.48949600
H	5.95057600	-3.45373900	-1.91807600
H	3.38922500	-0.06405400	2.55494100
H	1.21203400	0.86175200	-2.14095800
H	5.45773900	0.02747200	2.45536700
H	2.61221000	-2.24350000	2.11877700
H	4.50458900	-4.47256900	-1.83879100
H	3.31472800	3.86614000	-3.07260400
H	2.78645800	-3.64643200	0.05512000
H	2.25095300	4.31004200	-1.20074200
H	2.71500800	2.11677400	4.59401100
H	1.86387500	1.26068400	-3.74737500
H	5.71493700	0.48723200	-1.84224900
H	1.33624500	-0.53080000	3.80681900
H	0.69067600	1.07649900	3.41241600
H	4.35519000	1.73987200	4.03695000
H	5.76674400	1.92579300	-0.78563800
H	0.93023200	-0.11667500	2.12235100
H	1.73934300	4.99425300	1.11510700
H	4.06362200	2.53120200	-3.95162000
H	4.91513600	-3.63478500	-3.33797300
H	3.40245400	0.52219600	4.90881900
H	3.16561800	-3.87511500	2.50354800
H	5.66820300	1.65023000	1.74097200
O	0.22651500	-3.94588000	0.91263500
H	-0.07296800	-3.72964500	1.80305700
O	-1.99965400	-3.69070200	-0.11198300
H	-2.46567400	-3.40686700	0.68686800

TS10

E_{solv} = -2532.253882 a.u.

Zero-point energy correction = 1.062268 a.u.

Cu	1.02001200	0.04621200	-0.62771000
N	3.54869600	-1.14592300	0.01438300
C	4.60374700	0.81081000	-1.03920300
C	4.11739100	0.18085900	0.12022100
C	1.99820000	-2.80796900	-0.35688200
C	4.38513700	0.25850100	-2.43325300
C	4.12240400	0.82002600	1.37376200
C	3.32895900	-3.50451600	0.00634700
C	1.59277400	-3.06036800	-1.82604100
C	2.28729000	-1.33854700	-0.25348200
C	4.39469900	-2.40758500	0.17779300
C	3.41168200	0.26055000	2.58894700
C	5.29441700	2.68051900	0.34424600
C	4.72694700	2.07757600	1.46062600
C	0.84462600	-3.16638700	0.59114000
C	5.21044600	2.06027800	-0.89323200
C	5.64714400	0.27487600	-3.29047900
C	5.47156400	-2.46686100	-0.89483100
C	2.11211700	1.03142700	2.83079500
C	1.06301700	-2.76240400	2.03932100
C	5.05501700	-2.43638000	1.54642100
C	4.27542500	0.26384100	3.84621000
C	3.25560800	1.02762100	-3.12283600
C	1.11196900	-4.47317500	-2.11433300
H	4.05347700	-0.78219100	-2.34885100
H	2.45408100	-2.82149800	-2.46982200
H	0.67878400	-4.25147800	0.53497900
H	3.49772800	2.09510400	-3.20909800
H	4.75340000	2.59049400	2.42037500
H	0.80266100	-2.34267800	-2.09793200
H	3.63304700	-4.20841500	-0.77740200
H	6.48428000	-0.23125000	-2.79622800
H	5.65538200	-3.34951400	1.62125800
H	6.06833900	-3.37122500	-0.73438200
H	3.23419800	-4.08787500	0.92941100
H	1.97903800	-3.19686400	2.46030200
H	1.83869100	-5.22844500	-1.78984400
H	3.12993800	-0.77677600	2.37851200
H	2.31072200	0.94622800	-2.56349900
H	4.32333700	-2.45539700	2.36131000
H	1.12619900	-1.67095900	2.14906700
H	0.16170700	-4.68800000	-1.61022700
H	5.96479700	1.29797800	-3.52551000
H	-0.07864500	-2.69565100	0.21236400
H	5.60082500	2.56708200	-1.77320800
H	4.49804200	1.28351100	4.18318800
H	3.08511400	0.63185000	-4.13109400
H	5.05099700	-2.52474400	-1.90447100

H	1.55663800	0.60032400	3.67271100
H	2.31937300	2.08270800	3.07606400
H	5.22869500	-0.25191100	3.68539200
H	6.14943600	-1.60711200	-0.83410500
H	1.45491000	0.99474100	1.94638000
H	5.77184200	3.65283200	0.43553300
H	5.45753700	-0.23250300	-4.24308900
H	0.95122300	-4.60823900	-3.18879900
H	3.74823700	-0.24164500	4.66317100
H	0.22912200	-3.10202100	2.66298200
H	5.72954500	-1.58328700	1.68759200
B	0.86727900	3.62878300	-0.11602900
H	0.11872100	1.24169600	-1.14664700
N	0.30963000	4.10092200	-1.48862300
H	0.65243900	5.05188400	-1.65680000
H	0.62723400	3.50237400	-2.25388600
H	-0.71033900	4.13354700	-1.51226100
Cu	-1.33374400	0.89640000	-0.59790200
N	-3.91697700	-0.16623100	0.13048600
C	-3.15822200	-2.41985100	-0.51601700
C	-3.32265900	-1.43898700	0.47747600
C	-4.13873400	2.01331100	-0.57959500
C	-3.33898500	-2.13364200	-1.99279300
C	-2.93120700	-1.65079400	1.81170400
C	-5.53305300	1.54396700	-0.11105300
C	-4.07800100	2.21755600	-2.11071600
C	-3.22151400	0.85758000	-0.27766300
C	-5.42813700	0.04577100	0.21109900
C	-2.85383900	-0.52514400	2.82271800
C	-2.40463000	-3.94136800	1.21654800
C	-2.49201500	-2.92786400	2.16177600
C	-3.65801300	3.27365700	0.15647000
C	-2.70145900	-3.67688500	-0.11306500
C	-4.16981600	-3.18837100	-2.71660400
C	-6.13412100	-0.82364300	-0.81902000
C	-1.40884300	-0.02895500	2.91442700
C	-3.42840900	3.09713500	1.64875100
C	-5.95442500	-0.29524100	1.59525500
C	-3.37883500	-0.90336000	4.20311800
C	-1.96851000	-1.98426200	-2.65511600
C	-4.85292200	3.42230700	-2.61999400
H	-3.85068500	-1.17063100	-2.10119300
H	-4.45394200	1.30432300	-2.59780500
H	-4.39590500	4.06938700	-0.01364400
H	-1.39846000	-2.92148800	-2.58982200
H	-2.20062700	-3.12694200	3.19148100
H	-3.02169300	2.30522300	-2.41176900
H	-6.29587100	1.71703600	-0.87904600
H	-5.14447400	-3.34097800	-2.23897400
H	-7.03657700	-0.12536200	1.60303800
H	-7.21330300	-0.65843800	-0.73015500
H	-5.85428400	2.09797600	0.77884000
H	-4.33222300	2.75788000	2.17137300
H	-5.89557300	3.41239100	-2.27923800
H	-3.45540300	0.31521300	2.45749500
H	-1.37363900	-1.19395900	-2.17057200
H	-5.51595300	0.33849300	2.37348600
H	-2.63139400	2.36908600	1.84968100
H	-4.40301700	4.36456800	-2.28900100
H	-3.65582900	-4.15687400	-2.74672500
H	-2.72052700	3.61433400	-0.31001600
H	-2.56541700	-4.45847400	-0.85877500
H	-2.74092400	-1.65094600	4.69019700
H	-2.07631600	-1.72640800	-3.71538400
H	-5.84427900	-0.57241800	-1.84523300
H	-1.33629600	0.84137800	3.57996100
H	-0.75110000	-0.81543700	3.30827800
H	-4.39603800	-1.30884900	4.15525600
H	-5.94519500	-1.88916000	-0.64303200
H	-1.01953600	0.26450000	1.92495400
H	-2.06226500	-4.93103900	1.51104800
H	-4.34417300	-2.88115100	-3.75402100
H	-4.86519900	3.43065600	-3.71427800
H	-3.39384300	-0.01989400	4.85142000
H	-3.12543100	4.04332700	2.10806400
H	-5.78036200	-1.34768000	1.84870900
O	1.33183400	5.87793100	0.22149700
H	0.82573800	6.26282900	0.94591000
H	2.25690800	5.98051400	0.47231200
O	-0.08514500	3.47469400	0.82532100
H	0.20252200	3.12957300	1.67714500
O	2.14423900	3.22265400	-0.20856800
H	2.58533100	2.85609300	0.56956200

TS11

E_{solv} = -2615.470962 a.u.

Zero-point energy correction = 1.128644 a.u.

Cu	-1.26739800	0.17872300	0.69169400
N	-3.57436100	-0.86296600	-0.52592300
C	-4.52826400	-0.64566300	1.73643100
C	-4.27186300	-0.08306500	0.47497800
C	-1.83343200	-1.76856600	-1.72090800
C	-4.04212300	-2.02152200	2.14396400
C	-4.58988200	1.25302700	0.16972200
C	-3.13306400	-2.01691100	-2.51221200
C	-1.27568800	-3.03282600	-1.01627200
C	-2.26792900	-0.85604000	-0.60071100
C	-4.29245800	-1.73027000	-1.55629000
C	-4.16287400	1.93230600	-1.11630700
C	-5.54743100	1.45762500	2.38771600
C	-5.24126900	2.00405000	1.14857900
C	-0.72147900	-1.12733700	-2.56302100
C	-5.18021100	0.15149700	2.67937000
C	-5.14089800	-2.86972700	2.77790400
C	-4.84639200	-2.99534400	-0.91219400
C	-3.00273600	2.89008500	-0.84647800
C	-1.08572200	0.18080700	-3.24748900
C	-5.43487500	-0.97754600	-2.21495900
C	-5.30939000	2.65932900	-1.81255700
C	-2.83635600	-1.91179000	3.07700900
C	-1.13832900	-4.26100300	-1.90058300
H	-3.69710300	-2.54480600	1.24732800
H	-1.89645800	-3.28683600	-0.14226400
H	-0.38173600	-1.85551700	-3.31423100
H	-3.08744100	-1.36133000	3.99320300
H	-5.49855400	3.04103000	0.94112900
H	-0.29157500	-2.76384600	-0.60618600
H	-3.19766600	-3.02720600	-2.92799300
H	-6.03212800	-2.92634200	2.14161200
H	-5.90027200	-1.63668900	-2.95590000
H	-5.34540600	-3.58373200	-1.69007300
H	-3.19175900	-1.32489100	-3.36002000
H	-1.84930400	0.05492200	-4.02271400
H	-2.11055600	-4.68464900	-2.17681700
H	-3.78398200	1.16808000	-1.80636300
H	-2.00210600	-1.38574700	2.59030000
H	-5.09309700	-0.08090200	-2.74111100
H	-1.46270500	0.92465300	-2.53049400
H	-0.59100900	-4.04259800	-2.82574300
H	-5.45150900	-2.46827000	3.75035800
H	0.14303600	-0.96321200	-1.89540200
H	-5.38922000	-0.25685600	3.66634200
H	-5.66660200	3.50997600	-1.21949700
H	-2.48336000	-2.91045600	3.36268000
H	-4.06574000	-3.62579300	-0.47355800
H	-2.63634700	3.31093600	-1.79335600
H	-3.30798700	3.71857100	-0.19326500
H	-6.16252100	1.99521300	-1.99230900
H	-5.59326700	-2.76319700	-0.14444100
H	-2.15825600	2.38301900	-0.35951700
H	-6.05743100	2.05918300	3.13620800

H	-4.77747500	-3.88970000	2.94746300
H	-0.58642000	-5.04411200	-1.36903800
H	-4.97321200	3.05370200	-2.77845600
H	-0.20655600	0.61356700	-3.73900800
H	-6.20636600	-0.69604200	-1.48820200
H	-0.02005000	1.43526900	-0.70491000
Cu	1.30037700	0.81574700	-0.03143500
N	3.73024200	-0.70005300	0.39647200
C	2.56930700	-2.86421000	0.31056700
C	3.20082100	-1.80742000	-0.37097700
C	3.81784600	1.29433100	1.54039300
C	2.24623700	-2.81883700	1.79106900
C	3.30836600	-1.77581300	-1.77284600
C	5.23831000	0.69363200	1.57608800
C	3.13260700	1.20184500	2.92481300
C	3.03226400	0.37111200	0.64801100
C	5.15665100	-0.70763100	0.95014100
C	3.81715300	-0.57145300	-2.54008400
C	2.29195300	-3.97725600	-1.82686800
C	2.84307700	-2.88523300	-2.48169800
C	3.79173100	2.73067900	0.99743600
C	2.13901200	-3.95417600	-0.44724900
C	2.68079100	-4.07396100	2.54201900
C	5.34872500	-1.81997000	1.96883000
C	2.65307100	0.14536800	-3.22425300
C	4.20015300	2.85590600	-0.46392300
C	6.15607600	-0.89984600	-0.17894100
C	4.89785400	-0.92661000	-3.55711900
C	0.75167500	-2.57191100	2.00047800
C	3.63538300	2.20480200	3.94979600
H	2.76772000	-1.96285100	2.23259800
H	3.26802300	0.17975200	3.30965000
H	4.45627800	3.34289600	1.62158900
H	0.15339100	-3.43520600	1.67774500
H	2.91049400	-2.88914800	-3.56804200
H	2.04517200	1.31198900	2.78996200
H	5.62435700	0.63732700	2.60058300
H	3.74395700	-4.29589600	2.39760300
H	7.16495100	-0.87819800	0.24714300
H	6.38962200	-1.79509900	2.30880700
H	5.94202400	1.31587000	1.01126500
H	5.16488700	2.37321400	-0.66520100
H	4.72553600	2.15871000	4.06226300
H	4.24960200	0.14023100	-1.82672700
H	0.40584200	-1.69739800	1.42971000
H	6.09645000	-0.10228900	-0.92713700
H	3.45468100	2.40759100	-1.13541200
H	3.37297200	3.23360000	3.67779800
H	2.10924000	-4.95213700	2.21789600
H	2.77613000	3.14037900	1.13497500
H	1.65526300	-4.79160700	0.05363100
H	4.50103400	-1.55500400	-4.36364500
H	0.53822200	-2.38925800	3.06177400
H	4.71198800	-1.70111000	2.85145300
H	3.00012100	1.06108300	-3.71925900
H	2.18206500	-0.49485500	-3.98204700
H	5.73362600	-1.46375000	-3.09484500
H	5.16983400	-2.80555800	1.52419500
H	1.87682500	0.42452700	-2.49588200
H	1.95310600	-4.83927400	-2.39685900
H	2.50251500	-3.94832700	3.61615800
H	3.19357100	1.99914300	4.92951800
H	5.29259000	-0.01422300	-4.01879200
H	4.32161100	3.90507900	-0.75573300
H	6.02412200	-1.86903300	-0.67452100
B	-0.90990300	1.29177400	2.55655800
H	-0.07549300	0.58612300	1.92131300
H	-0.94270700	0.85645200	3.67805100
H	-2.03350400	1.30924900	2.05123900
N	-0.36052800	2.78683200	2.54905700
H	-0.99641100	3.38856900	3.07220300
H	0.54354400	2.87140200	3.01457100
H	-0.26143600	3.21173700	1.60975300
B	0.28320400	4.59337300	-1.18581700
N	1.67717400	5.46636300	-1.08360900
H	1.50763600	6.39441600	-0.69733700
H	2.36049500	5.00425400	-0.48455900
H	2.11053400	5.59781900	-1.99761100
O	0.74820200	3.28342300	-1.74283300
H	0.38300500	2.21955700	-1.11897000
H	0.54797200	3.21840400	-2.68607500
O	-0.52378700	5.34105000	-2.06329800
H	-1.45615600	5.14147000	-1.94583100
O	-0.19440100	4.33392000	0.13539600
H	-0.68226400	5.09344800	0.46971700

INT2-a

E_{solv} = -2305.255812 a.u.

Zero-point energy correction = 1.031043 a.u.

Cu	1.85385800	1.61757500	0.21965100
N	3.95766900	-0.35699000	0.05518600
C	2.29754000	-2.09544900	0.59500900
C	3.06253200	-1.41077900	-0.36623400
C	4.79308800	1.68817200	0.71852300
C	2.07275600	-1.56051600	1.99445200
C	3.02681600	-1.74655800	-1.73095200
C	5.98814800	0.72267100	0.58534800
C	4.51892700	2.08162100	2.18867600
C	3.60757500	0.88133000	0.25366500
C	5.41073700	-0.68608400	0.40607700
C	3.60843100	-0.84247000	-2.79808000
C	1.66289700	-3.66095700	-1.14602600
C	2.31959400	-2.89246600	-2.09759500
C	4.93916800	2.94647700	-0.15393000
C	1.62019200	-3.24204700	0.17698800
C	2.14433200	-2.62470300	3.08363600
C	5.43475400	-1.50710700	1.68865600
C	2.49081700	0.02789700	-3.37808800
C	4.91841900	2.69257200	-1.65406800
C	6.10119500	-1.46556200	-0.69830200
C	4.33486700	-1.59210600	-3.90902900
C	0.71611700	-0.84787400	2.04048000
C	5.57093800	2.98977500	2.80550800
H	2.84220200	-0.80932900	2.21144500
H	4.42899500	1.16436300	2.79001500
H	5.88022700	3.44101500	0.12299100
H	-0.11100000	-1.56107800	1.91872500
H	2.27512600	-3.18177900	-3.14567900
H	3.53606500	2.57514200	2.24307100
H	6.64779000	0.76092900	1.45975300
H	3.08711800	-3.18257200	3.04846100
H	7.13444100	-1.65362800	-0.38647500
H	6.47657000	-1.73438800	1.93881000
H	6.60200300	0.98557900	-0.28461200
H	5.70084200	1.98881000	-1.96696500
H	6.57946100	2.56775800	2.71847600
H	4.32794300	-0.16256700	-2.32502100
H	0.62182000	-0.11228900	1.22461200
H	6.13748700	-0.90733900	-1.63962000
H	3.95343300	2.28466400	-1.98500800
H	5.58097900	3.97906500	2.33585800
H	1.32095700	-3.34523800	3.00038300
H	4.13246300	3.64873600	0.11095800
H	1.03493300	-3.80619200	0.90006700
H	3.64229800	-2.18836200	-4.51545800
H	0.58116400	-0.32123100	2.99372900
H	4.99754400	-0.97002200	2.53752500
H	2.89420100	0.72774300	-4.12020700
H	1.73195000	-0.59378800	-3.87192600
H	5.10210800	-2.26732800	-3.51302800
H	4.90727200	-2.46003900	1.56134800

H	1.98539300	0.61132900	-2.59428900
H	1.14419000	-4.56993400	-1.44526400
H	2.06290800	-2.15508600	4.07024400
H	5.36691700	3.13394600	3.87093800
H	4.82242400	-0.87921300	-4.58347800
H	5.08482000	3.62256900	-2.20636900
H	5.62393600	-2.43682000	-0.87324000
B	0.02536600	2.75769300	0.46826400
H	0.12753900	1.88965100	-0.42444700
H	0.96834900	2.77963100	1.26116300
H	-0.91195200	2.57441200	1.26699200
N	-0.10700000	4.17554600	-0.22200500
H	-0.32646100	4.90990900	0.45308400
H	0.75877700	4.45772400	-0.68595100
H	-0.83872900	4.20763300	-0.93466900
Cu	-1.84698200	1.58773600	0.27189800
N	-3.95237200	-0.32085200	-0.18460800
C	-2.38445600	-2.19697100	-0.38951400
C	-3.18226200	-1.37986800	0.43200900
C	-4.51048000	1.72846900	-1.08079100
C	-2.07540700	-1.84267200	-1.83067500
C	-3.26022400	-1.56092000	1.82332100
C	-5.77436000	0.84537500	-1.14722000
C	-3.88590700	1.96118500	-2.47749500
C	-3.50903800	0.89341400	-0.33307400
C	-5.37288400	-0.56896700	-0.69820600
C	-3.89923300	-0.54921300	2.75201100
C	-1.91111700	-3.55808800	1.56263000
C	-2.61475300	-2.67387100	2.36724200
C	-4.74259500	3.06707400	-0.36384700
C	-1.77476100	-3.30258200	0.20411200
C	-1.93407200	-3.05484400	-2.74442600
C	-5.37550100	-1.57493200	-1.84003600
C	-2.80324600	0.25692300	3.45305200
C	-5.07687300	2.95050300	1.11578500
C	-6.25043900	-1.09079200	0.42749800
C	-4.84012700	-1.17707100	3.77548100
C	-0.80885500	-0.98414100	-1.88801100
C	-4.70077700	2.86269600	-3.39062700
H	-2.89320400	-1.22895600	-2.22274000
H	-3.73455100	0.98310800	-2.96062800
H	-5.55319200	3.59486300	-0.88437400
H	0.03203800	-1.48608700	-1.39121800
H	-2.65884700	-2.84308300	3.44127400
H	-2.87969100	2.39007200	-2.34243900
H	-6.19921200	0.82116900	-2.15723200
H	-2.78505300	-3.73979300	-2.65166300
H	-7.26749100	-1.21728100	0.04095800
H	-6.41570200	-1.76440400	-2.12633700
H	-6.55675500	1.23867000	-0.48756100
H	-5.96153000	2.32486600	1.29231400
H	-5.73222300	2.50735500	-3.50328700
H	-4.48423600	0.15857300	2.15173900
H	-0.96129100	-0.01268200	-1.39571500
H	-6.30045700	-0.39051800	1.26848500
H	-4.24478400	2.51796800	1.68926000
H	-4.74051000	3.89107200	-3.01613700
H	-1.01709500	-3.61893300	-2.53101700
H	-3.84055000	3.68836600	-0.48906700
H	-1.17109200	-3.96868700	-0.40743800
H	-4.29935200	-1.81541400	4.48451000
H	-0.52513000	-0.78656500	-2.92961500
H	-4.85467800	-1.20283400	-2.72840300
H	-3.24288700	1.03746000	4.08575100
H	-2.18359400	-0.38983400	4.08780000
H	-5.61361100	-1.78794500	3.29645100
H	-4.93537700	-2.53256000	-1.53751500
H	-2.13279900	0.74411500	2.72791500
H	-1.43365500	-4.43174300	2.00185200
H	-1.87113100	-2.72640600	-3.78759300
H	-4.25352000	2.89294000	-4.38890000
H	-5.33704200	-0.39299800	4.35797000
H	-5.28812400	3.93473300	1.54489900
H	-5.90734000	-2.06667300	0.79093500

INT2-b

E_{solv} = -2305.257094 a.u.

Zero-point energy correction = 1.03239 a.u.

Cu	1.40783100	-0.60042900	-0.76162300
N	3.81748400	0.51125900	0.04074200
C	3.32085800	-0.71753500	2.10726500
C	3.87405200	-0.71978700	0.81184800
C	2.81671400	2.11329700	-1.28552900
C	2.74040800	0.51634600	2.76900500
C	4.31395200	-1.90320000	0.19025500
C	4.20376100	2.66123700	-0.87068000
C	1.66089100	2.89329700	-0.61376100
C	2.75689600	0.74465700	-0.68262900
C	4.89974600	1.58805200	-0.00946700
C	4.81228400	-1.97252700	-1.23903600
C	3.71024700	-3.11041500	2.21210300
C	4.22697200	-3.09114600	0.92307600
C	2.61207400	2.04076400	-2.80610300
C	3.25592300	-1.93260200	2.79081900
C	3.39056700	0.79622000	4.12217300
C	5.26458200	2.08602200	1.37957800
C	3.87689900	-2.80729900	-2.11348200
C	3.55648300	1.09867500	-3.53495000
C	6.15325000	1.02988700	-0.66649800
C	6.23837200	-2.51421200	-1.31611600
C	1.22389000	0.41568300	2.91524800
C	1.45205200	4.30118200	-1.14502500
H	2.92762100	1.37805400	2.12054000
H	1.85165200	2.92863900	0.47241700
H	2.71806100	3.05575200	-3.21177100
H	0.92123700	-0.46288700	3.50098600
H	4.56730100	-4.01960800	0.46813900
H	0.73141600	2.31458400	-0.73736000
H	4.09749900	3.59031800	-0.29794800
H	4.48294500	0.84066500	4.04931700
H	6.90752000	1.82328200	-0.70055100
H	6.08591100	2.80375400	1.27982200
H	4.81732800	2.90269100	-1.74611700
H	4.60862300	1.37502500	-3.39037900
H	2.37375300	4.89501700	-1.10875100
H	4.81430800	-0.95905400	-1.65449100
H	0.73356600	0.35167100	1.93409800
H	5.97666300	0.69793500	-1.69484900
H	3.43252000	0.05921300	-3.20082400
H	1.09720400	4.29418600	-2.18162600
H	3.13613400	0.02163300	4.85585700
H	1.57290500	1.73513200	-3.00008100
H	2.83008200	-1.95663400	3.79190400
H	6.28354500	-3.56336700	-0.99901300
H	0.83885900	1.31015600	3.42176800
H	4.43855700	2.60479000	1.87558400
H	4.24097700	-2.82639400	-3.14742900
H	3.81016400	-3.84420600	-1.76068100
H	6.92723100	-1.94511900	-0.68173500
H	5.61756400	1.26829400	2.01942000
H	2.85884900	-2.39280300	-2.12750400
H	3.65422200	-4.04608200	2.76278500
H	3.03555800	1.75428200	4.51881600
H	0.69887600	4.82323700	-0.54554100
H	6.60517700	-2.46454400	-2.34764400
H	3.36535000	1.11638700	-4.61221800
H	6.57286700	0.19887900	-0.08718400
B	0.01200000	-2.23949400	-0.32083900
H	0.24700800	-1.40599900	0.59749300
H	0.56613000	-1.96232700	-1.40064300

H	-1.17891700	-2.33199800	-0.60663300
N	0.56301500	-3.60960700	0.22986200
H	0.51623200	-4.35031300	-0.47189500
H	1.54147600	-3.55263200	0.53318200
H	0.02726200	-3.93756000	1.03581700
Cu	-1.43136000	-0.82090400	0.48274400
N	-3.82935700	0.52779800	0.06929900
C	-3.43341400	-0.13551200	-2.26141800
C	-3.97790700	-0.44141700	-1.00047700
C	-2.76963900	1.66329400	1.77313000
C	-2.67189400	1.14238900	-2.54933700
C	-4.53550300	-1.69941200	-0.71119200
C	-4.16352000	2.30861400	1.58891400
C	-1.62829600	2.59736300	1.30399000
C	-2.75795900	0.51314300	0.81164000
C	-4.85252100	1.60986500	0.40220400
C	-4.95132900	-2.13080100	0.68081800
C	-4.12557600	-2.33301700	-3.01771000
C	-4.61051400	-2.62765500	-1.75163800
C	-2.51762500	1.17027300	3.20590000
C	-3.52849700	-1.10386800	-3.26149700
C	-3.15675800	1.84530300	-3.81424800
C	-5.07479800	2.53747400	-0.78265900
C	-3.97703600	-3.17442000	1.23039100
C	-3.42245300	0.03291900	3.65336500
C	-6.17982900	0.97363900	0.78266700
C	-6.38256900	-2.65926800	0.72680700
C	-1.16920400	0.87580600	-2.62648100
C	-1.38532500	3.79997000	2.20036900
H	-2.81704100	1.83103000	-1.71138700
H	-1.85155100	2.93723800	0.27865200
H	-2.63524300	2.02601900	3.88438100
H	-0.91857000	0.13559500	-3.39823900
H	-5.03919100	-3.60877200	-1.55660600
H	-0.70166800	2.00588700	1.22901000
H	-4.07962700	3.38502300	1.39874200
H	-4.23891800	2.01741700	-3.79301700
H	-6.89301200	1.77202600	1.01393200
H	-5.85802100	3.25443400	-0.51421200
H	-4.76999400	2.19852100	2.49531300
H	-4.48609900	0.29438600	3.57763800
H	-2.29523600	4.39511200	2.34543700
H	-4.89458400	-1.26286800	1.34698300
H	-0.78537300	0.50121900	-1.66225400
H	-6.09793200	0.33709300	1.67001200
H	-3.25857200	-0.87457400	3.05593000
H	-1.01936800	3.50203900	3.18900400
H	-2.92822500	1.26209200	-4.71445900
H	-1.46689500	0.85349800	3.28567700
H	-3.11262000	-0.89468000	-4.24517300
H	-6.48688700	-3.58922500	0.15463000
H	-0.63460900	1.80750800	-2.85407100
H	-4.18045300	3.11361400	-1.04076900
H	-4.26754000	-3.46989100	2.24576300
H	-3.96096300	-4.07593100	0.60511200
H	-7.09725000	-1.93493700	0.32008800
H	-5.41909500	1.98603900	-1.66566200
H	-2.94816200	-2.78594100	1.27717100
H	-4.19326300	-3.07210800	-3.81204300
H	-2.65896900	2.81605100	-3.91837700
H	-0.62995700	4.45664500	1.75600900
H	-6.67009600	-2.87698400	1.76173500
H	-3.22983600	-0.22887200	4.69823200
H	-6.59430000	0.38655400	-0.04571300

INT2-c

E_{solv} = -2305.258475 a.u.

Zero-point energy correction = 1.032036 a.u.

Cu	1.63692700	-0.77472400	-1.25503300
N	3.93302100	0.10182300	0.30890400
C	3.46225000	2.41687500	-0.40339900
C	3.36567600	1.40734700	0.56970700
C	4.18292800	-2.05968600	-0.46128400
C	3.97199100	2.17651600	-1.81002800
C	2.72052800	1.61498800	1.80299300
C	5.38387000	-1.75345800	0.45634800
C	4.59716300	-2.20120300	-1.94414400
C	3.31748700	-0.82920800	-0.36288800
C	5.35960500	-0.24751400	0.74240900
C	2.39917800	0.48546900	2.75975800
C	2.40111300	3.93291700	1.16745500
C	2.26147500	2.90123200	2.08652300
C	3.38580200	-3.29630300	-0.00719900
C	2.97175100	3.68243100	-0.07116300
C	5.04387700	3.17718900	-2.23373100
C	6.34508000	0.53647300	-0.11367100
C	0.93328100	0.08023500	2.60638900
C	2.65343100	-3.14592600	1.31882800
C	5.61417800	0.07655200	2.20346500
C	2.71221700	0.81464900	4.21550100
C	2.80445100	2.19780600	-2.79785900
C	5.38957100	-3.45969800	-2.25995300
H	4.41401700	1.17421500	-1.85681700
H	5.18302900	-1.31623000	-2.23434000
H	4.08527500	-4.14115500	0.05390800
H	2.31025600	3.17770400	-2.80826100
H	1.76767000	3.09221700	3.03791100
H	3.68904500	-2.17602700	-2.56756600
H	6.33665300	-2.04517700	-0.00006600
H	5.88067400	3.20642700	-1.52675500
H	6.65231700	-0.18779900	2.43259400
H	7.36220200	0.26914300	0.19197300
H	5.30092200	-2.31078300	1.39740400
H	3.33010800	-2.86960600	2.13827300
H	6.27513100	-3.55717300	-1.62036100
H	2.99310000	-0.39154400	2.47779500
H	2.04364300	1.44805400	-2.53708800
H	4.97356900	-0.49928300	2.87876500
H	1.86474600	-2.38190400	1.26771500
H	4.78508300	-4.36409200	-2.13327900
H	4.63802100	4.19299300	-2.31303200
H	2.66262000	-3.55620300	-0.79734400
H	3.03065100	4.48312800	-0.80575200
H	2.05046500	1.59785400	4.60481800
H	3.15627800	1.98306700	-3.81371600
H	6.24804100	0.31118700	-1.18107800
H	0.70711300	-0.77513900	3.25616300
H	0.26130400	0.90506400	2.88678600
H	3.74626800	1.15386700	4.34427500
H	6.22640200	1.61611000	0.03476800
H	0.69758300	-0.20870400	1.57051600
H	2.03269600	4.92765600	1.40711200
H	5.44066400	2.90670500	-3.21883700
H	5.73563400	-3.43779100	-3.29783400
H	2.56373900	-0.07387700	4.83960900
H	2.17288200	-4.08716800	1.60389100
H	5.49129800	1.14593800	2.41126000
B	-0.13141400	-1.43260700	-2.36838900
H	-0.01153500	-1.78874100	-1.17563100
H	0.68034400	-0.56173400	-2.71420500
H	-1.22065100	-0.89457100	-2.63822200
N	0.03317600	-2.71368600	-3.27685300
H	-0.04337700	-2.49150200	-4.27070100
H	0.93788600	-3.17181700	-3.15238700
H	-0.67837500	-3.41996900	-3.08030800
Cu	-1.84347000	-1.13415700	-1.05328400
N	-3.74383700	0.13078800	0.61931000
C	-2.83440000	2.23609300	-0.30008700
C	-3.80570300	1.22030800	-0.33428300
C	-3.17380000	-1.89468200	1.56929100
C	-1.58258800	2.17537900	0.55056500

C	-4.82876100	1.19973900	-1.30022700
C	-4.27285500	-1.26296000	2.44925700
C	-1.80081900	-1.92779200	2.27397200
C	-3.03170000	-0.94076400	0.41514500
C	-4.47667400	0.17778000	1.95795500
C	-5.73854100	0.00711800	-1.51258500
C	-4.02329000	3.34124400	-2.10374400
C	-4.92192900	2.28566800	-2.17118300
C	-3.54115200	-3.29578600	1.05399200
C	-2.97843400	3.30028800	-1.19302600
C	-1.36699300	3.43180400	1.38970600
C	-3.81009400	1.20864900	2.85831900
C	-5.28657100	-0.76381100	-2.75468600
C	-4.71986900	-3.34135400	0.09398900
C	-5.94004200	0.54054300	1.78198200
C	-7.21251000	0.38539900	-1.62125600
C	-0.37102400	1.92195900	-0.34982800
C	-1.68682300	-2.92423700	3.41544400
H	-1.65980900	1.32100900	1.23535000
H	-1.57599100	-0.91700300	2.64665200
H	-3.75100300	-3.92988200	1.92619600
H	-0.21185900	2.74930400	-1.05357600
H	-5.70515100	2.29496300	-2.92653500
H	-1.02780200	-2.15070000	1.52037000
H	-4.00245700	-1.27303700	3.51148800
H	-2.24529000	3.67444900	1.99802500
H	-6.41107700	0.55734700	2.77084500
H	-4.33139100	1.22014100	3.82150500
H	-5.21101600	-1.82330300	2.35742300
H	-5.63029700	-2.91111500	0.53159300
H	-2.46724200	-2.77453000	4.17135500
H	-5.63041900	-0.67304800	-0.65931200
H	-0.51118300	1.00899400	-0.95117000
H	-6.47856800	-0.19264800	1.17255100
H	-4.50744400	-2.79624400	-0.83566300
H	-1.75454500	-3.95857800	3.06219300
H	-1.14291200	4.30190200	0.75976700
H	-2.65281900	-3.72608400	0.56504700
H	-2.24334900	4.10275100	-1.18340800
H	-7.41419900	0.97353300	-2.52469200
H	0.54296600	1.81174200	0.24746400
H	-2.75609300	0.97764700	3.05229600
H	-5.90071400	-1.66208500	-2.89375500
H	-5.37908600	-0.14543000	-3.65654600
H	-7.54788100	0.97161700	-0.75808900
H	-3.88161800	2.21485400	2.42928500
H	-4.23560700	-1.07721900	-2.67334100
H	-4.11932500	4.18286600	-2.78515600
H	-0.51236200	3.29412700	2.06273800
H	-0.71854900	-2.81332000	3.91620900
H	-7.82792100	-0.51970200	-1.67894500
H	-4.95454500	-4.37411700	-0.18161300
H	-6.06051300	1.53598300	1.33846800

TS6-a

E_{solv} = -2381.660471 a.u.

Zero-point energy correction = 1.046402 a.u.

Cu	1.31927200	1.19563300	-0.26553600
N	3.72794500	-0.37402800	0.10753900
C	2.41231000	-2.35948000	0.70400500
C	3.04708300	-1.58839400	-0.28583500
C	4.11868100	1.81921800	0.68557300
C	2.18245500	-1.83495100	2.10682900
C	3.05543500	-1.96216300	-1.64026700
C	5.48643700	1.10905900	0.63321000
C	3.67930100	2.13250400	2.13640600
C	3.14391400	0.78830300	0.17804500
C	5.21146400	-0.39311800	0.48822000
C	3.48322900	-1.01893400	-2.74620300
C	1.98673500	-4.03983700	-0.99252700
C	2.53106600	-3.21438200	-1.96662900
C	4.07764400	3.08808800	-0.18006800
C	1.89436300	-3.59826200	0.32124700
C	2.20682100	-2.91904900	3.17845000
C	5.42697700	-1.16427900	1.78384900
C	2.23979300	-0.42272200	-3.41066300
C	4.13587100	2.83809000	-1.68018500
C	6.04498400	-1.03334500	-0.60891900
C	4.38546300	-1.67252800	-3.78761900
C	0.85641000	-1.07497300	2.16225900
C	4.46500500	3.24934500	2.80446500
H	2.97582800	-1.11968500	2.34589000
H	3.76268000	1.21351600	2.73633200
H	4.91791300	3.72880500	0.12058900
H	0.03218600	-1.70170600	1.80089500
H	2.52872000	-3.53646000	-3.00614900
H	2.60870900	2.39040200	2.13258300
H	6.08866500	1.31020600	1.52669900
H	3.09944000	-3.55107000	3.10146500
H	7.09782500	-0.98260100	-0.31056300
H	6.50265400	-1.19738500	1.98827100
H	6.06897700	1.46368600	-0.22593100
H	5.02142500	2.25791000	-1.97072100
H	5.54537000	3.06179500	2.78020400
H	4.03521400	-0.18208500	-2.30012600
H	0.88052500	-0.16295100	1.54365700
H	5.94778500	-0.50696900	-1.56414800
H	3.25081700	2.28950500	-2.03447200
H	4.28282800	4.21729800	2.32529100
H	1.32308900	-3.56734800	3.11936400
H	3.16511300	3.65482300	0.06489700
H	1.40712100	-4.22669000	1.06338900
H	3.85068000	-2.43784800	-4.36314900
H	0.62984300	-0.76813000	3.19133800
H	4.94482000	-0.68720800	2.64332700
H	2.52660400	0.30231100	-4.18221900
H	1.63482500	-1.20670400	-3.88529800
H	5.26035100	-2.14769600	-3.32930500
H	5.07328300	-2.19899200	1.70188700
H	1.59843600	0.09265300	-2.67884100
H	1.58941500	-5.01501400	-1.26565000
H	2.19867400	-2.45765500	4.17192700
H	4.17159500	3.34163500	3.85468300
H	4.74015700	-0.92011700	-4.50115100
H	4.17469000	3.78309200	-2.23115800
H	5.78942700	-2.08986500	-0.75169500
B	-0.15970200	3.46308700	0.20130600
H	0.02945900	1.88218100	-0.90973300
H	0.81500200	3.26685600	0.85018000
H	-1.26672900	3.20949400	0.55582800
N	-0.00052500	4.28869700	-1.10690300
H	-0.05865000	5.27447800	-0.82456600
H	0.89554700	4.15359300	-1.57829300
H	-0.73619400	4.11922300	-1.79536900
Cu	-1.32374400	1.16075000	-0.44293800
N	-3.69881600	-0.48626400	-0.04067900
C	-2.31537500	-2.51611500	-0.06084800
C	-2.95526200	-1.50195500	0.67277100
C	-4.19060500	1.41756800	-1.24234200
C	-2.15577800	-2.45220700	-1.56612600
C	-2.90682000	-1.44324100	2.07637300
C	-5.52077900	0.66667300	-1.01917000
C	-3.74172800	1.39511200	-2.72197100
C	-3.16273900	0.61033500	-0.49280700
C	-5.18772200	-0.67159200	-0.34303500
C	-3.34771700	-0.21828700	2.85154500
C	-1.75858000	-3.57810700	2.04771400
C	-2.31533800	-2.51518900	2.74672700
C	-4.22639700	2.86020900	-0.71402700
C	-1.72418200	-3.55640500	0.65946600
C	-2.32768400	-3.80159600	-2.25538800

C	-5.39791200	-1.86245000	-1.26755400
C	-2.12276200	0.62665400	3.21172700
C	-4.38274300	2.98692800	0.79349500
C	-5.97796000	-0.89250800	0.93607000
C	-4.15782300	-0.54475000	4.10122700
C	-0.79322900	-1.85239300	-1.91182400
C	-4.61311600	2.21344300	-3.66103700
H	-2.91652300	-1.77512400	-1.96878700
H	-3.71061500	0.34778100	-3.06239600
H	-5.05179900	3.38466300	-1.21429200
H	0.01921200	-2.46103600	-1.49685300
H	-2.26734800	-2.50341500	3.83388300
H	-2.70298500	1.76170100	-2.77486000
H	-6.05025900	0.49480500	-1.96337600
H	-3.26400300	-4.29356200	-1.96715500
H	-7.03458200	-1.00623400	0.67039100
H	-6.47418100	-1.98413900	-1.43050000
H	-6.19707600	1.25066400	-0.38418700
H	-5.31159100	2.52580000	1.15302500
H	-5.66945500	1.92580100	-3.59573100
H	-3.97580100	0.39954300	2.19888600
H	-0.68259000	-0.83453800	-1.50501400
H	-5.90096600	-0.04391100	1.62400400
H	-3.54933700	2.51538600	1.33265000
H	-4.54524800	3.28559500	-3.44734100
H	-1.50079300	-4.48403200	-2.02099800
H	-3.30402100	3.37100100	-1.03370300
H	-1.22285200	-4.35930000	0.12229000
H	-3.54942500	-1.05651900	4.85686800
H	-0.65811500	-1.79387300	-2.99956700
H	-4.93202300	-1.71816300	-2.24817100
H	-2.43014700	1.56059200	3.69847300
H	-1.46377000	0.08438800	3.90247500
H	-5.01875300	-1.18365100	3.87370800
H	-5.02224300	-2.79131500	-0.82236000
H	-1.52930400	0.88373900	2.32035000
H	-1.30842800	-4.40824300	2.58814800
H	-2.33370100	-3.66597900	-3.34264900
H	-4.29633400	2.06420500	-4.69782700
H	-4.53015300	0.37944200	4.55756000
H	-4.40927000	4.03936100	1.09355800
H	-5.66468600	-1.80647500	1.45430900
O	-0.37549400	5.51128400	1.21199100
H	-1.23006300	5.59465200	1.65163300
H	0.28189100	5.62153700	1.90919500

TS6-b

E_{solv} = -2381.668786 a.u.

Zero-point energy correction = 1.052189 a.u.

Cu	1.22914900	-0.71155200	-0.19636300
N	3.79868500	0.43579900	0.22672000
C	3.64099500	-0.38676800	2.53668700
C	4.02666200	-0.61010900	1.20304300
C	2.67966000	1.74337400	-1.30672100
C	2.85981000	0.83391800	2.97724800
C	4.56671700	-1.83534100	0.77512000
C	4.09216900	2.34885600	-1.13702600
C	1.57589300	2.65714700	-0.72627300
C	2.67867800	0.52129200	-0.43332000
C	4.83710500	1.51196100	-0.08217300
C	4.77574100	-2.17649000	-0.68567800
C	4.49528200	-2.59084600	3.07856100
C	4.80340000	-2.81237500	1.74353200
C	2.35757200	1.36222700	-2.76048400
C	3.90043600	-1.39755500	3.46359400
C	3.44395300	1.50899700	4.21430400
C	5.17449300	2.31223500	1.16623500
C	3.64710400	-3.09221600	-1.16321200
C	3.23775800	0.27123900	-3.34896400
C	6.10964200	0.87684500	-0.62045600
C	6.13738300	-2.80062000	-0.97214100
C	1.39769900	0.45716500	3.21240800
C	1.34914800	3.95493400	-1.48265400
H	2.86531700	1.56640200	2.16223900
H	1.82408200	2.88087700	0.32539400
H	2.43730400	2.27028500	-3.37362700
H	1.29426200	-0.26374800	4.03379800
H	5.22237300	-3.77002600	1.44107900
H	0.63618200	2.08311500	-0.69626100
H	4.03577400	3.39549900	-0.81576500
H	4.50199600	1.76148900	4.08147700
H	6.83756700	1.67161800	-0.81581900
H	5.94046700	3.04998700	0.90406800
H	4.64268500	2.34308300	-2.08484300
H	4.30205200	0.53874600	-3.32696500
H	2.26633500	4.55094100	-1.56295800
H	4.70402000	-1.25507400	-1.27383200
H	0.95191300	0.00310300	2.31291700
H	5.94345800	0.34269300	-1.56195400
H	3.12103800	-0.67989800	-2.81161400
H	0.97860300	3.77682200	-2.49848600
H	3.36107000	0.86858100	5.10077800
H	1.30544700	1.04518900	-2.81213900
H	3.61523400	-1.25107300	4.50357600
H	6.23877200	-3.78857500	-0.50691400
H	0.81511700	1.35156600	3.46952800
H	4.31092400	2.86064500	1.55651300
H	3.74831000	-3.31049100	-2.23337400
H	3.64798000	-4.04314000	-0.61527900
H	6.95605500	-2.17077800	-0.60550600
H	5.58574700	1.67330700	1.95665400
H	2.66678400	-2.61358100	-1.00568200
H	4.69423900	-3.36268500	3.81791100
H	2.89745500	2.43443300	4.42919500
H	0.60276400	4.56620300	-0.96427000
H	6.26805600	-2.93447000	-2.05195800
H	2.97544600	0.08516000	-4.39505000
H	6.55527200	0.18891600	0.10821600
B	-0.47815700	-2.27313900	-1.68921200
H	0.04042700	-1.78352600	0.11177300
H	0.46069600	-1.76207800	-2.21064200
H	-1.56115700	-1.78355300	-1.59062700
N	-0.35272700	-3.76875000	-1.28537000
H	-0.61824800	-4.30538800	-2.11920900
H	0.58901000	-4.05982500	-1.01894900
H	-0.98261800	-4.04944300	-0.53222100
Cu	-1.20664000	-0.73772400	0.29091900
N	-3.75578000	0.52165500	0.04549800
C	-3.60819400	0.13216900	-2.37319300
C	-3.98521200	-0.33335300	-1.10186700
C	-2.63222600	1.51455400	1.79607600
C	-2.86518800	1.43457400	-2.58619900
C	-4.49843700	-1.62745100	-0.90081600
C	-4.02485600	2.18169000	1.71227200
C	-1.49325000	2.48384100	1.40227300
C	-2.64146600	0.46585700	0.72118300
C	-4.79187500	1.52638200	0.54990200
C	-4.72972600	-2.22411600	0.47202800
C	-4.41216100	-1.96131200	-3.30279900
C	-4.70792300	-2.42481900	-2.02722600
C	-2.34677900	0.87880300	3.16585600
C	-3.84637100	-0.70281300	-3.46808700
C	-3.43592100	2.27102300	-3.72666700
C	-5.17444800	2.52258800	-0.53378800
C	-3.63573200	-3.24402900	0.79162800
C	-3.26621000	-0.26956200	3.54835800
C	-6.04525100	0.79326800	1.00342300
C	-6.11148400	-2.85391800	0.62194600
C	-1.37856500	1.16036800	-2.80539300
C	-1.25818000	3.62994700	2.37154800
H	-2.93630400	2.02840100	-1.66938400

H	-1.70954600	2.88705400	0.39790100
H	-2.41206000	1.67073400	3.92432000
H	-1.20785400	0.51380400	-3.67764400
H	-5.10637700	-3.42940000	-1.90172600
H	-0.56530200	1.89867400	1.29750000
H	-3.93134900	3.26003900	1.53800100
H	-4.51262200	2.43861200	-3.60917700
H	-6.77026100	1.53389400	1.35752300
H	-5.95449400	3.17853300	-0.13245000
H	-4.58049500	2.06429700	2.64974800
H	-4.32301800	0.02698500	3.54643800
H	-2.16428100	4.22655100	2.53284700
H	-4.64610200	-1.42601300	1.21745500
H	-0.93490000	0.66434100	-1.92784600
H	-5.85013000	0.10103600	1.82929300
H	-3.15463300	-1.12362500	2.86644400
H	-0.91498600	3.27445500	3.34967500
H	-3.27402200	1.79418700	-4.70098400
H	-1.30522400	0.52620400	3.17385300
H	-3.57800700	-0.36073800	-4.46613600
H	-6.22489900	-3.74084400	-0.01303100
H	-0.84087700	2.10340700	-2.96768600
H	-4.33640200	3.15971200	-0.83382300
H	-3.78577700	-3.67292300	1.78942000
H	-3.63592500	-4.06642100	0.06397900
H	-6.90912200	-2.14961400	0.35991700
H	-5.58646900	2.02253500	-1.41840700
H	-2.63963300	-2.77154600	0.78170300
H	-4.60735800	-2.58987600	-4.16921000
H	-2.93990000	3.24761600	-3.75707200
H	-0.48703200	4.30109500	1.97853900
H	-6.26617700	-3.17305800	1.65874200
H	-3.03607300	-0.62980300	4.55569000
H	-6.50955100	0.24354800	0.17574600
O	-1.20190500	-3.01816900	-3.70299900
H	-0.64368600	-2.70449200	-4.42483800
H	-2.04720500	-2.55864300	-3.81222200

TS6-c

E_{solv} = -2381.668786 a.u.

Zero-point energy correction = 1.052189 a.u.

Cu	1.04758700	-0.45671500	-1.30804900
N	3.54028800	0.03756900	0.10890600
C	3.26802200	2.37906300	-0.62799200
C	3.19568300	1.41498100	0.39288400
C	3.41531000	-2.14719100	-0.63014300
C	3.48440800	2.04298700	-2.09002100
C	2.79731800	1.74392800	1.70220400
C	4.73782300	-1.99499600	0.14832400
C	3.64823800	-2.41212500	-2.13434400
C	2.74715400	-0.80138400	-0.49640200
C	4.95296300	-0.49420700	0.37200100
C	2.47017300	0.69370100	2.74335100
C	2.71533600	4.06986100	1.02491100
C	2.57709300	3.08931500	1.99808800
C	2.47986500	-3.21939700	-0.04112500
C	3.02914100	3.71051100	-0.27689100
C	4.61979400	2.84167300	-2.72443000
C	5.89408800	0.13140700	-0.64985700
C	0.95496700	0.51029200	2.82306400
C	1.98381100	-2.93918700	1.36940500
C	5.46171300	-0.17314800	1.76476800
C	3.04482300	0.99825700	4.12239800
C	2.18224200	2.26261600	-2.86412700
C	4.24138800	-3.77495400	-2.45506800
H	3.73811300	0.97837100	-2.17631300
H	4.30007700	-1.62305800	-2.53850900
H	3.00461600	-4.18395400	-0.06189000
H	1.88855400	3.31997200	-2.85312500
H	2.26795400	3.36954100	3.00333400
H	2.68863100	-2.30474200	-2.66150100
H	5.58766600	-2.42904700	-0.39048000
H	5.56180500	2.71760900	-2.17855700
H	6.47998200	-0.56811400	1.85017700
H	6.90105800	-0.27016100	-0.49400800
H	4.68059400	-2.50943400	1.11522400
H	2.79930400	-2.91176800	2.10309200
H	5.16924500	-3.96125400	-1.90121200
H	2.87982900	-0.26703100	2.40989800
H	1.34772900	1.69232200	-2.42650600
H	4.86246400	-0.64190900	2.55103900
H	1.45472000	-1.97741500	1.42853900
H	3.54466500	-4.58720100	-2.22194300
H	4.38989000	3.91357500	-2.75506600
H	1.61360100	-3.32319700	-0.71645200
H	3.08104600	4.47832000	-1.04639000
H	2.56876400	1.87753000	4.57313100
H	2.29532600	1.95066400	-3.90946900
H	5.60084200	-0.09006600	-1.68181900
H	0.70757100	-0.30838900	3.51149500
H	0.46133100	1.42075200	3.19164600
H	4.12430800	1.18292900	4.08584800
H	5.94567100	1.21925100	-0.52251800
H	0.52818600	0.27243500	1.83761200
H	2.54287800	5.11364200	1.27523700
H	4.78002200	2.51190300	-3.75727100
H	4.47791100	-3.84159500	-3.52148600
H	2.86563700	0.15285600	4.79650900
H	1.28434700	-3.71761800	1.69359000
H	5.51093200	0.90758200	1.94169100
B	0.11380600	-0.81700300	-3.82522100
H	-0.34822100	-0.30503200	-2.14500900
H	1.28127200	-0.74776700	-3.59279100
H	-0.55807600	0.07034800	-4.22443900
N	-0.52854000	-2.23610900	-3.76006600
H	-0.31676700	-2.67549500	-4.66384400
H	-0.15394100	-2.84115500	-3.02676000
H	-1.54493000	-2.22790200	-3.66220300
Cu	-1.39854600	-0.51027000	-0.93961700
N	-3.65529700	0.15757700	0.63866500
C	-3.06594000	2.50635000	0.14361000
C	-3.82353500	1.35939100	-0.15141100
C	-2.82155600	-1.85890000	1.38907700
C	-1.86483700	2.49936800	1.06721200
C	-4.74128500	1.32497800	-1.21749400
C	-4.13667300	-1.58527000	2.14716500
C	-1.57912200	-1.74062400	2.29548900
C	-2.73245800	-0.72969600	0.39946500
C	-4.52213800	-0.12692000	1.86260400
C	-5.35447900	0.03583800	-1.72423900
C	-4.31343300	3.68352700	-1.57391800
C	-4.97831700	2.51211300	-1.91016800
C	-2.80017000	-3.20941000	0.65356700
C	-3.34880400	3.66873200	-0.57776700
C	-1.88022100	3.61562400	2.10635300
C	-4.12411500	0.82987200	2.97888400
C	-4.58923900	-0.42152600	-2.96863500
C	-3.77435200	-3.33282800	-0.50766100
C	-6.00020700	0.04347700	1.56289200
C	-6.84718100	0.14225900	-2.01735400
C	-0.59355300	2.58203200	0.21840900
C	-1.41473300	-2.85634400	3.31337200
H	-1.83660500	1.54239700	1.60490900
H	-1.60797300	-0.77221700	2.81673300
H	-3.00352900	-3.99814400	1.39060100
H	-0.53096000	3.54037300	-0.31415700
H	-5.68454000	2.51376200	-2.73791300
H	-0.69058700	-1.70607600	1.64531900
H	-4.03658300	-1.75825400	3.22491200
H	-2.77282200	3.57368400	2.74087300
H	-6.56246600	-0.18217600	2.47565800

H	-4.73055900	0.61068400	3.86435800
H	-4.93157800	-2.25224700	1.79088800
H	-4.81293100	-3.15380300	-0.20012700
H	-2.29272600	-2.95270900	3.96344200
H	-5.21880600	-0.74179700	-0.96255000
H	-0.56251600	1.78468400	-0.54111200
H	-6.34774000	-0.64285300	0.78384900
H	-3.53901000	-2.62259500	-1.31252600
H	-1.24426600	-3.82661700	2.83410700
H	-1.84726100	4.60612800	1.63666800
H	-1.77228700	-3.38395700	0.29150500
H	-2.78222700	4.57371600	-0.36746000
H	-7.04962100	0.81742900	-2.85753000
H	0.30205000	2.48649600	0.84392900
H	-3.06971900	0.73144200	3.26130600
H	-4.95827800	-1.39457600	-3.31553700
H	-4.70397100	0.30061200	-3.78699500
H	-7.40677700	0.50969400	-1.14947900
H	-4.31698100	1.87054900	2.69184600
H	-3.51227700	-0.51439600	-2.75985400
H	-4.52101400	4.60242100	-2.11662600
H	-0.99828400	3.53672600	2.75437200
H	-0.55051100	-2.65321800	3.95582100
H	-7.24609900	-0.84159500	-2.28925900
H	-3.73646900	-4.33794000	-0.93913100
H	-6.24045800	1.07229900	1.27002300
O	0.66482600	-1.39474400	-5.96802000
H	1.61834700	-1.33166300	-6.09912500
H	0.28001100	-0.76667100	-6.59076300

Cl-INT1

E_{solv} = -1571.398586 a.u.

Zero-point energy correction = 0.465795 a.u.

Cu	-0.55693200	1.40315500	-1.29049100
N	-0.12277400	-0.63549700	0.61979000
C	1.84734000	-1.27861600	-0.70691200
C	1.29230000	-0.51933800	0.33871900
C	-2.39195700	-0.28659800	0.45017400
C	1.01368300	-2.10379000	-1.66648000
C	2.05598700	0.39929700	1.08078500
C	-2.15909900	-1.23368300	1.64630900
C	-3.03312900	-1.01448600	-0.75469100
C	-1.00821900	0.10122500	0.00240300
C	-0.67745200	-1.63792900	1.62377900
C	1.44613400	1.39067600	2.05109700
C	4.00979800	-0.32465400	-0.16047800
C	3.42509300	0.46685400	0.81792600
C	-3.20758100	0.96117800	0.81993600
C	3.22163400	-1.17058600	-0.92756200
C	1.53860800	-3.52565900	-1.84255700
C	-0.46285900	-3.06223100	1.13100200
C	1.45976800	2.79089500	1.43466000
C	-2.51985600	1.90959100	1.79045600
C	-0.00598300	-1.47932600	2.97737100
C	2.13702100	1.39620900	3.41164400
C	0.91927800	-1.39321700	-3.01777700
C	-4.48682200	-1.41115500	-0.55257600
H	-0.00589600	-2.17121300	-1.27209000
H	-2.43568600	-1.91105600	-0.98185900
H	-4.16500600	0.62887600	1.24471300
H	1.90912500	-1.29160700	-3.48088900
H	4.03944100	1.16885200	1.37872200
H	-2.94826200	-0.36318700	-1.63818700
H	-2.80246200	-2.12017200	1.59897600
H	1.64135700	-4.04683400	-0.88353400
H	-0.45017900	-2.20111100	3.67168200
H	-0.84942700	-3.75350600	1.88781500
H	-2.39169500	-0.72686800	2.59060600
H	-2.25244800	1.41753900	2.73487400
H	-4.62622900	-2.00965200	0.35621300
H	0.39419200	1.12257200	2.20888800
H	0.49478400	-0.38452600	-2.91072200
H	-0.15549000	-0.47947700	3.39825600
H	-1.59937300	2.32785700	1.36064400
H	-5.14029800	-0.53528600	-0.47879400
H	2.51886400	-3.53600500	-2.33483100
H	-3.45040700	1.50136600	-0.10844200
H	3.67734800	-1.74774200	-1.73000300
H	3.17129700	1.75406800	3.33734600
H	0.27980900	-1.96072900	-3.70456500
H	-0.99296800	-3.26691300	0.19455000
H	0.96759800	3.50855000	2.10258800
H	2.48725700	3.13635600	1.26348000
H	2.16063400	0.39756700	3.86263800
H	0.60280800	-3.28087600	0.99439500
H	0.93666400	2.80860600	0.46732700
H	5.07917500	-0.25962400	-0.34628600
H	0.85240800	-4.10432600	-2.47168900
H	-4.83696300	-2.01197700	-1.39777100
H	1.60913500	2.06791400	4.09854100
H	-3.17369600	2.75098300	2.04058600
H	1.06921700	-1.68784300	2.92098500
Cl	-0.06390200	2.89226300	-2.73951900

Cl-TS1

E_{solv} = -1654.525328 a.u.

Zero-point energy correction = 0.529752 a.u.

Cu	0.28645700	-1.31422000	-1.55416400
N	0.57351000	0.78363400	0.50848700
C	-1.33771200	1.84529500	-0.64789900
C	-0.84209200	1.07427500	0.42127100
C	2.56702800	-0.31441600	0.17251700
C	-0.46942700	2.44793900	-1.73487900
C	-1.70617400	0.50053800	1.37850700
C	2.78820900	0.72062300	1.29401200
C	3.33502600	0.04471500	-1.11968900
C	1.08955400	-0.23375400	-0.14908300
C	1.56111600	1.63606800	1.30177100
C	-1.23860200	-0.37777200	2.52395500
C	-3.58504200	1.51014800	0.21200100
C	-3.07818100	0.74089600	1.25302800
C	2.92255900	-1.74391800	0.61609200
C	-2.71831100	2.04918400	-0.72577800
C	-0.60962000	3.97018900	-1.77678400
C	1.82476000	2.95451100	0.58429700
C	-1.75768000	-1.80893800	2.39820900
C	2.04014300	-2.31801400	1.71465600
C	1.06921300	1.95004800	2.70301800
C	-1.64574400	0.20048600	3.87951600
C	-0.78158900	1.85949800	-3.11041500
C	4.84906800	-0.04785300	-1.01286900
H	0.57520500	2.20295600	-1.51567500
H	3.05012800	1.06184500	-1.43069200
H	3.97166000	-1.74558100	0.94535400
H	-1.82961400	2.02737500	-3.39145600
H	-3.76083300	0.31672900	1.98804600
H	2.98120200	-0.62085100	-1.92104500
H	3.70503700	1.30397900	1.14879000
H	-0.46771600	4.43155000	-0.79269700
H	1.81732000	2.57898100	3.19832300
H	2.56391400	3.52157200	1.16118100
H	2.88387600	0.22129700	2.26634400
H	2.03262500	-1.68927700	2.61538800
H	5.24376000	0.55649300	-0.18661500
H	-0.14503900	-0.43708300	2.48295600
H	-0.58223000	0.78068800	-3.13750700
H	0.94102200	1.05126700	3.31335500
H	1.00471200	-2.43561700	1.36928600
H	5.18358800	-1.07968500	-0.85948300
H	-1.60368500	4.26452400	-2.13661200
H	2.87228600	-2.39978300	-0.26789500
H	-3.11926500	2.63771600	-1.54892300

H	-2.73285800	0.15011900	4.01891900
H	-0.15364600	2.34092800	-3.87004600
H	2.22933100	2.81360000	-0.42355000
H	-1.38409700	-2.41354700	3.23396500
H	-2.85525600	-1.84401500	2.43774500
H	-1.34486300	1.24718600	3.99458300
H	0.91730400	3.56501300	0.52166300
H	-1.41952500	-2.28719800	1.46989800
H	-4.65550000	1.68249400	0.13164300
H	0.12879200	4.39899000	-2.46446300
H	5.31732600	0.31386300	-1.93400200
H	-1.18537100	-0.37843300	4.68895700
H	2.39803100	-3.30737700	2.01875800
H	0.12702900	2.51153400	2.68308800
B	-2.34549400	-1.69709700	-2.15124700
H	-2.47048600	-2.52760900	-2.98110200
H	0.15858500	-1.57973100	-3.09820400
H	-2.06812600	-0.56301800	-2.34491300
N	-3.19213400	-1.90975300	-0.86677600
H	-4.18874100	-1.94163100	-1.09833500
H	-2.92610100	-2.80300000	-0.43503600
H	-3.06544700	-1.16094000	-0.17494200
Cl	-0.70898500	-3.54377100	-0.72898600

Cl-INT2

E_{solv} = -2682.437316 a.u.

Zero-point energy correction = 0.957405 a.u.

Cu	-1.32968500	-0.66486100	-0.31858400
N	-3.75921600	0.60606000	0.01405600
C	-4.57664800	-1.48537200	-0.97906300
C	-4.22901800	-0.75701200	0.17392900
C	-2.25707000	2.28815700	-0.45249800
C	-4.44552200	-0.93231900	-2.38462100
C	-4.18666400	-1.34843400	1.44915800
C	-3.61945700	2.96053600	-0.16270000
C	-1.85387000	2.41793500	-1.93789100
C	-2.49641400	0.82815900	-0.22815100
C	-4.65044000	1.84058100	0.07676900
C	-3.62912800	-0.65329200	2.67492100
C	-4.98988600	-3.40552800	0.44439200
C	-4.58891100	-2.68102100	1.55778100
C	-1.12615700	2.76537200	0.46620800
C	-4.96763400	-2.81451300	-0.81136800
C	-5.71836900	-1.11501500	-3.20678000
C	-5.72566800	1.78870900	-0.99839300
C	-2.28976800	-1.27227600	3.07967900
C	-1.34726300	2.48128900	1.94260000
C	-5.32157900	1.94007000	1.43735900
C	-4.60366300	-0.66891000	3.84955700
C	-3.24659000	-1.55665900	-3.10026300
C	-1.40102300	3.80915100	-2.34869900
H	-4.24541700	0.14200500	-2.31738100
H	-2.70996200	2.10578700	-2.55699000
H	-0.99111600	3.84584400	0.31653300
H	-3.34558500	-2.64764400	-3.16852500
H	-4.56630200	-3.16426000	2.53278400
H	-1.05183600	1.69251800	-2.14370900
H	-3.93355800	3.59184500	-1.00233500
H	-6.59678900	-0.70457900	-2.69548400
H	-5.96136400	2.82913300	1.44482100
H	-6.36859800	2.66834800	-0.88579200
H	-3.56163500	3.61463900	0.71484600
H	-2.27568000	2.93057400	2.31840000
H	-2.14085400	4.57578900	-2.08629600
H	-3.42898900	0.39352300	2.42068600
H	-2.30512800	-1.33926400	-2.57465700
H	-4.59786700	2.04712200	2.25241800
H	-1.39049900	1.40231000	2.14807500
H	-0.45331300	4.08322100	-1.86859200
H	-5.91636000	-2.17381100	-3.41407600
H	-0.18771000	2.29011300	0.13375000
H	-5.24134700	-3.40209300	-1.68559600
H	-4.77408100	-1.68830000	4.21698400
H	-3.16153300	-1.15748400	-4.11813900
H	-5.30926600	1.81489600	-2.01066100
H	-1.87920700	-0.75100400	3.95355200
H	-2.40139900	-2.33258800	3.33931900
H	-5.57710200	-0.24480800	3.57772200
H	-6.35786900	0.89910100	-0.89074100
H	-1.55020700	-1.20587300	2.26773100
H	-5.29866000	-4.44239400	0.55222500
H	-5.61807000	-0.60701300	-4.17282300
H	-1.24578500	3.85517100	-3.43157100
H	-4.19821500	-0.08373200	4.68305600
H	-0.52578500	2.89267000	2.53943300
H	-5.95861800	1.06922300	1.63401200
Cu	1.51232600	-1.49357500	-0.29243300
N	3.88273300	0.14173900	0.09607700
C	2.86121800	2.19785800	-0.77700100
C	3.14064400	1.36189000	0.31862700
C	4.40887000	-2.04008000	-0.42601200
C	3.02002000	1.73577600	-2.21082700
C	2.75854000	1.69080300	1.63038500
C	5.71315700	-1.35120400	0.02167900
C	4.38606500	-2.31689300	-1.94839400
C	3.33722500	-1.00740500	-0.18363600
C	5.41161700	0.14734200	0.15527700
C	2.80851000	0.68997200	2.76646100
C	2.02199600	3.84412500	0.79301500
C	2.21283700	2.95784400	1.84431100
C	4.11038600	-3.32640200	0.35978900
C	2.30867300	3.45120300	-0.50762200
C	3.63025600	2.78730600	-3.13085500
C	5.98650200	0.96991400	-0.98885300
C	1.40857300	0.11284000	2.99085000
C	3.81306600	-3.11848500	1.83736700
C	5.89841900	0.72265900	1.47449000
C	3.36402900	1.26649800	4.06411300
C	1.66145500	1.28192000	-2.74797000
C	5.33480700	-3.41370300	-2.40513400
H	3.67695600	0.85935200	-2.22373600
H	4.62376300	-1.38212900	-2.47907800
H	4.97221300	-3.99861300	0.24883000
H	0.96609100	2.13100600	-2.79837200
H	1.92608100	3.25051500	2.85288600
H	3.35669500	-2.57704800	-2.24091600
H	6.53068400	-1.51968900	-0.68872300
H	4.58471600	3.16518300	-2.74647800
H	6.99241100	0.66637700	1.48972600
H	7.07803700	0.97158400	-0.89710600
H	6.04783600	-1.75019000	0.98673500
H	4.63343900	-2.60726200	2.35750600
H	6.36563600	-3.22552800	-2.08080700
H	3.45402100	-0.14554800	2.46784800
H	1.20730000	0.51195600	-2.10404200
H	5.52620900	0.15557800	2.33455500
H	2.90121500	-2.52340600	1.98904700
H	5.03734200	-4.39544600	-2.02155600
H	2.95916100	3.64445400	-3.26686500
H	3.25841500	-3.83666100	-0.11747600
H	2.09227300	4.12742300	-1.33297600
H	2.69834400	2.02942300	4.48586400
H	1.76228400	0.86583400	-3.75743800
H	5.73846800	0.55434800	-1.97148400
H	1.43137100	-0.67832700	3.75056000
H	0.71354800	0.89180700	3.33140200
H	4.34964100	1.72336600	3.91829100
H	5.64805200	2.01165600	-0.94304600
H	0.99576200	-0.31621700	2.06371500
H	1.60553200	4.83095300	0.98321900
H	3.80939000	2.35714000	-4.12265400

H	5.34115500	-3.47616000	-3.49772500
H	3.46278900	0.47340000	4.81392200
H	3.66048500	-4.07793200	2.34118600
H	5.61663300	1.77592000	1.58936500
Cl	-0.35389400	-2.60978700	-0.38944200

Cl-INT3

E_{solv} = -2765.652275 a.u.

Zero-point energy correction = 1.02507 a.u.

Cu	-1.46544700	0.98935000	0.74604200
N	-3.91936800	-0.05544100	-0.48489000
C	-3.07987800	-2.35916500	-0.55264500
C	-3.75119300	-1.34365700	0.15134900
C	-3.46864300	2.07398400	-1.22202200
C	-2.38475600	-2.11973400	-1.87825400
C	-4.23290200	-1.53411600	1.45751600
C	-4.83686500	1.67547000	-1.81581100
C	-2.37113000	2.16729800	-2.30364800
C	-3.05233200	0.91435000	-0.34825300
C	-5.13952200	0.24221200	-1.35397900
C	-4.78694500	-0.40986100	2.30953800
C	-3.50420300	-3.84417700	1.31679800
C	-4.10651200	-2.80790400	2.01600200
C	-3.53765000	3.37466400	-0.40987500
C	-2.98001800	-3.61325300	0.05207400
C	-2.70216100	-3.18425600	-2.92413100
C	-5.25498700	-0.73123900	-2.51739700
C	-3.77167400	-0.00843400	3.38076200
C	-4.37891400	3.29806600	0.85383300
C	-6.41078200	0.15345900	-0.52275900
C	-6.12961100	-0.75363300	2.94868100
C	-0.87499900	-2.00891700	-1.67196000
C	-2.52118900	3.31416100	-3.28838400
H	-2.71387300	-1.15208800	-2.27155100
H	-2.33655100	1.20952500	-2.85013600
H	-3.92447900	4.16714200	-1.06524100
H	-0.46510600	-2.93897900	-1.25048300
H	-4.47321300	-2.98401200	3.02562200
H	-1.40121400	2.25153800	-1.79234100
H	-4.82232400	1.72580700	-2.91118700
H	-3.78145500	-3.31598700	-3.06253500
H	-7.26475600	0.38493700	-1.16880400
H	-6.16913000	-0.49337300	-3.07236500
H	-5.62883500	2.35714700	-1.48392700
H	-5.41923400	3.02160100	0.63871500
H	-3.49027200	3.29583800	-3.80212100
H	-4.93532100	0.46808600	1.67033800
H	-0.62737700	-1.19405600	-0.97689100
H	-6.41809300	0.86979100	0.30578300
H	-3.97543700	2.56107900	1.56189000
H	-2.42223900	4.28765000	-2.79528300
H	-2.27858100	-4.15826700	-2.64971400
H	-2.51199800	3.67224300	-0.14421000
H	-2.46786300	-4.41797500	-0.47224200
H	-6.03026200	-1.55661400	3.68950400
H	-0.37111400	-1.81186000	-2.62781900
H	-4.41740000	-0.65058600	-3.21767800
H	-4.15935000	0.82546400	3.97947400
H	-3.56141100	-0.84567100	4.05935200
H	-6.86838100	-1.07472100	2.20523500
H	-5.33841500	-1.76805600	-2.17084300
H	-2.81815100	0.30241300	2.93234100
H	-3.42184600	-4.83003000	1.76826000
H	-2.26703000	-2.90251400	-3.89006600
H	-1.74043400	3.25444800	-4.05458400
H	-6.53188400	0.12226000	3.47104300
H	-4.40269300	4.26529200	1.36568100
H	-6.55899400	-0.85692200	-0.12320000
Cu	1.40167400	-0.91034900	0.74182100
N	3.98256800	-0.22175700	-0.32798000
C	3.23979700	2.02610700	-0.97962300
C	3.77778100	1.17171700	-0.00139400
C	3.55435400	-2.45720500	-0.66105100
C	2.69338100	1.53071000	-2.30376400
C	4.09443400	1.62071500	1.29374700
C	5.05979600	-2.23785000	-0.90650500
C	2.78278400	-2.70067300	-1.97957400
C	3.06133200	-1.12991300	-0.14297000
C	5.29607500	-0.72174500	-0.92713600
C	4.48371500	0.68716200	2.42253200
C	3.50952100	3.86489500	0.58215700
C	3.95423100	2.98355700	1.55925900
C	3.25979100	-3.57830100	0.34627900
C	3.13021800	3.38291000	-0.66502400
C	3.18665300	2.34068900	-3.49892300
C	5.49997400	-0.17035200	-2.33150000
C	3.32346500	0.54389700	3.40835400
C	3.72175600	-3.29989600	1.76911600
C	6.47539600	-0.30686600	-0.06376700
C	5.75062900	1.13043300	3.14899400
C	1.16598000	1.51762600	-2.25969300
C	3.04002600	-4.05293800	-2.62473600
H	3.01499900	0.49401600	-2.44635800
H	3.03585700	-1.90046800	-2.69170100
H	3.73267400	-4.49969700	-0.02077800
H	0.77355200	2.53079400	-2.08754000
H	4.19510700	3.36017400	2.55133900
H	1.70831000	-2.59202000	-1.77544500
H	5.39589400	-2.69709600	-1.84340400
H	4.28012200	2.41240200	-3.52428900
H	7.38967900	-0.70948100	-0.51345300
H	6.46381000	-0.53138600	-2.70646800
H	5.65078800	-2.69292500	-0.10245900
H	4.79888200	-3.09537700	1.82452100
H	4.10944100	-4.23487400	-2.78800900
H	4.66755300	-0.30926600	2.00207500
H	0.79356500	0.87296700	-1.45034900
H	6.40367300	-0.70752200	0.95275000
H	3.19701200	-2.43667200	2.20351200
H	2.65024800	-4.87469200	-2.01443700
H	2.78447500	3.36126500	-3.49018800
H	2.17340200	-3.76594200	0.34396200
H	2.73670500	4.07217300	-1.41053300
H	5.59625400	2.07281500	3.68875100
H	0.75083600	1.15022100	-3.20752100
H	4.72859000	-0.50195300	-3.03435700
H	3.58158500	-0.17439300	4.19632300
H	3.08917200	1.50448100	3.88540000
H	6.59111900	1.27307200	2.46033300
H	5.53560700	0.92537200	-2.32953900
H	2.40953600	0.19340300	2.90780300
H	3.44264000	4.92952900	0.79917300
H	2.85496600	1.86996800	-4.43139200
H	2.54571800	-4.10542000	-3.59989600
H	6.04084000	0.37605200	3.88939700
H	3.52270600	-4.15962200	2.41664500
H	6.58004200	0.78369600	-0.01596900
Cl	-0.37616700	-0.97322100	1.97267500
B	0.03697600	2.37715200	1.62726800
H	-1.09380300	2.21279000	2.11346600
H	0.88705600	2.17560300	2.45737700
H	0.25429000	1.68889200	0.61614700
N	0.15093200	3.90304900	1.13985400
H	-0.03623000	4.56689800	1.89022600
H	1.10526300	4.07867700	0.81474400
H	-0.47210400	4.14004200	0.36811700

Cl-TS2

E_{solv} = -2842.046493 a.u.

Zero-point energy correction = 1.05146 a.u.

Cu	1.15096000	0.85251900	-0.40677000

N	3.69393100	-0.20176600	0.42480000
C	2.54605500	-2.33669300	0.89692100
C	3.20586900	-1.49451200	-0.01533600
C	3.68319200	2.06143800	0.84745300
C	2.28370300	-1.97190500	2.34422300
C	3.32553200	-1.81605700	-1.38078000
C	5.13345800	1.56613300	1.02057400
C	3.00911100	2.41490500	2.19333800
C	2.93733000	0.85852900	0.32244400
C	5.09669000	0.03319900	0.98135500
C	3.94214800	-0.88182500	-2.40435600
C	2.16190800	-3.89582300	-0.92429200
C	2.79416500	-3.03341500	-1.80959800
C	3.57385200	3.24929400	-0.11966300
C	2.04333800	-3.54662500	0.41324800
C	2.88592600	-2.98364200	3.31769400
C	5.24735300	-0.58139900	2.36514300
C	2.88134900	-0.29500000	-3.33333800
C	3.95771900	2.95196500	-1.56084700
C	6.15638800	-0.56366600	0.07035400
C	5.04371300	-1.56172000	-3.21439200
C	0.78552900	-1.84208300	2.60518700
C	3.57895200	3.63693900	2.89524400
H	2.72870600	-0.99017300	2.54153700
H	3.07145500	1.54292300	2.86319500
H	4.20637000	4.06078700	0.26606300
H	0.29077400	-2.81779100	2.52988600
H	2.85988300	-3.29889900	-2.86317200
H	1.93624400	2.57103400	2.00263600
H	5.58097400	1.91886300	1.95678500
H	3.95404300	-3.15210500	3.14297300
H	7.13948400	-0.37849000	0.51687200
H	6.25819800	-0.36430200	2.72720100
H	5.76677300	1.94282600	0.20839100
H	5.00665200	2.64502500	-1.65851400
H	4.65997700	3.55177100	3.05940900
H	4.39516200	-0.03728000	-1.87270200
H	0.30791200	-1.16485700	1.88284600
H	6.15685400	-0.10994900	-0.92560800
H	3.33736400	2.15407600	-1.99077100
H	3.39898100	4.55518600	2.32585200
H	2.38219500	-3.95476600	3.23274700
H	2.53902100	3.62699500	-0.08465200
H	1.53176600	-4.21992700	1.09945000
H	4.63910100	-2.35518400	-3.85465100
H	0.60282700	-1.45735700	3.61738200
H	4.54044200	-0.16742500	3.09220700
H	3.34270100	0.41812500	-4.02872100
H	2.38193200	-1.07562000	-3.91974500
H	5.80858100	-2.00969700	-2.56957700
H	5.13555900	-1.67008600	2.33305500
H	2.08859800	0.22501800	-2.77444400
H	1.74964700	-4.83779800	-1.27918000
H	2.75990200	-2.63726800	4.35027700
H	3.10835500	3.76138000	3.87562000
H	5.53396500	-0.83180500	-3.86938800
H	3.82185000	3.84073300	-2.18680800
H	6.03523400	-1.64911100	-0.02950900
Cu	-1.11715200	-0.37871900	-1.14685000
N	-3.43906500	-0.46700400	0.65660500
C	-2.79676900	1.58338300	1.89146100
C	-3.43866200	0.97279300	0.79664400
C	-2.88988500	-2.59704900	-0.01292600
C	-1.86158200	0.86067600	2.84281200
C	-4.10591000	1.73753200	-0.18282300
C	-4.21801900	-2.69878000	0.76505900
C	-1.72425100	-3.22869600	0.77206400
C	-2.57193600	-1.11975900	-0.08168600
C	-4.52783100	-1.30476900	1.32470500
C	-4.64831500	1.14643200	-1.46813100
C	-3.64912300	3.72914800	1.12973200
C	-4.19624300	3.11919800	0.00730300
C	-2.98424000	-3.21218500	-1.41666600
C	-2.93884100	2.96659000	2.04456600
C	-2.23891400	1.02357800	4.31398000
C	-4.39439700	-1.24819000	2.83723300
C	-3.71425000	1.49030200	-2.62909600
C	-3.95271700	-2.51875300	-2.36087000
C	-5.91190500	-0.81540500	0.93002400
C	-6.07568100	1.58839200	-1.77789000
C	-0.43569500	1.37281200	2.63154600
C	-1.73353600	-4.74646100	0.84484700
H	-1.86758600	-0.20909600	2.59426000
H	-1.74140700	-2.81017100	1.79067900
H	-3.27856200	-4.26468400	-1.29693400
H	-0.36732100	2.44842500	2.84369700
H	-4.70950100	3.72575500	-0.73637800
H	-0.77626400	-2.89204800	0.32168500
H	-4.15241600	-3.43237400	1.57772300
H	-3.27230200	0.72909900	4.52160000
H	-6.65666900	-1.45662200	1.41468400
H	-5.16084400	-1.89439400	3.27920000
H	-5.03289900	-3.02968700	0.11046100
H	-4.97465800	-2.47760700	-1.95997300
H	-2.69931500	-5.13853300	1.18842900
H	-4.64988000	0.05514600	-1.37326000
H	-0.10201600	1.20347300	1.59614100
H	-6.07723100	-0.87595700	-0.15125400
H	-3.62773300	-1.49330500	-2.57697200
H	-1.51379600	-5.19939600	-0.12862800
H	-2.11623000	2.06324700	4.64187500
H	-1.98069400	-3.20517500	-1.86673600
H	-2.46523800	3.45617400	2.89335000
H	-6.12821000	2.65746500	-2.01753800
H	0.26981100	0.85933800	3.29679800
H	-3.41676200	-1.60616100	3.18032900
H	-4.06690100	1.02577400	-3.55856800
H	-3.66740200	2.57619700	-2.79247700
H	-6.75459000	1.39876700	-0.93867700
H	-4.56082900	-0.23329200	3.21479600
H	-2.69307400	1.12661200	-2.44173500
H	-3.74835500	4.80239500	1.27171000
H	-1.57926300	0.40549600	4.93503000
H	-0.97002300	-5.09748000	1.54884400
H	-6.45171400	1.04195700	-2.65051700
H	-4.00376500	-3.04878500	-3.31800400
H	-6.09169900	0.21388800	1.26324600
Cl	-0.57066600	-1.19375300	-3.24463100
B	-0.06113500	2.84709600	-1.96034200
H	1.12065500	2.82701300	-1.84895400
H	-0.67849000	2.36231600	-2.84553300
H	-0.29055900	1.11430700	-1.01310100
N	-0.87225000	3.50962700	-0.79872000
H	-0.99520300	4.50222800	-1.01954600
H	-1.80852100	3.10779800	-0.67363900
H	-0.39481200	3.45321200	0.10273400
O	0.02794700	4.74416400	-2.93137500
H	-0.34306900	4.66025200	-3.81877400
H	0.95507800	4.97942800	-3.06417500

Table S1. The thermal correction to free energy/au, electronic energies/au, gibbs free energies (G/au), entropies (S/[cal/(mol·K)]) and enthalpies (H/au]) for the overall catalytic cycle.

Species	Electronic Energy (au)	Thermal Correction to Free Energy/au	G/au	S/[cal/(mol·K)]	H/au
1	-1110.987245	0.466617	-1110.520628	178.22	-1110.435949
INT1	-1194.222687	0.535892	-1193.686795	196.24	-1193.593555
NH_3BH_3	-83.196393	0.04633	-83.150063	59.548	-83.12177
H_2O	-76.431298	0.004028	-76.42727	45.1	-76.405842
TS1	-1270.604187	0.55373	-1270.050457	209.719	-1269.950813
TS2	-1270.615174	0.55335	-1270.061824	211.344	-1269.961408
TS3	-1270.614578	0.558674	-1270.055904	202.753	-1269.959569
TS4	-1194.134085	0.528421	-1193.605664	201.099	-1193.510116
TS5	-1194.141054	0.53753	-1193.603524	185.457	-1193.515407
INT2	-2305.25595	1.029203	-2304.226747	323.892	-2304.072855
INT2-a	-2305.255812	1.031043	-2304.224769	319.498	-2304.072965
INT2-b	-2305.257094	1.03239	-2304.224704	318.97	-2304.073151
INT2-c	-2305.258475	1.032036	-2304.226439	318.579	-2304.075072
TS6	-2381.669121	1.048957	-2380.620164	334.353	-2380.461302
TS6-a	-2381.660471	1.046402	-2380.614069	339.258	-2380.452876
TS6-b	-2381.668786	1.052189	-2380.616597	330.541	-2380.459547
TS6-c	-2381.661593	1.050972	-2380.610621	331.427	-2380.453149
INT3	-2222.771288	0.966997	-2221.804291	306.595	-2221.658618
$NH_3BH_2(H_2O)$	-158.901811	0.061332	-158.840479	72.325	-158.806115
INT4	-2305.98365	1.035723	-2304.947927	322.852	-2304.794529
INT5	-2464.908956	1.124383	-2463.784573	344.154	-2463.621054
INT5-a	-2464.903921	1.126777	-2463.777144	340.968	-2463.61514
TS7	-2464.904311	1.116938	-2463.787373	347.567	-2463.622233
TS7-a	-2464.878561	1.117697	-2463.760864	345.252	-2463.596823
NH_3BH_2OH	-158.467008	0.050257	-158.416751	66.57	-158.385121
H_2	-1.167911	-0.001365	-1.169276	31.13	-1.154485
INT6	-2380.524526	1.036285	-2379.488241	325.241	-2379.333708
INT7	-2380.523607	1.035521	-2379.488086	324.716	-2379.333803
TS8	-2456.964011	1.055095	-2455.908916	337.885	-2455.748376
$NH_3BH(OH)(H_2O)$	-234.182694	0.067221	-234.115473	74.227	-234.080205
TS9	-2540.184903	1.123077	-2539.061826	350.101	-2538.895481

$NH_3BH(OH)_2$	-233.747267	0.05327	-233.693997	74.266	-233.658711
INT8	-2455.813249	1.04309	-2454.770159	326.439	-2454.615057
INT9	-2455.816647	1.039098	-2454.777549	331.773	-2454.619912
TS9	-2532.253882	1.062268	-2531.191614	339.205	-2531.030446
$NH_3B(OH)_2(H_2O)$	-309.465657	0.068703	-309.396954	83.565	-309.357249
TS11	-2615.470962	1.128644	-2614.342318	351.608	-2614.175258
$NH_3B(OH)_3$	-309.031998	0.057366	-308.974632	80.347	-308.936457
Cl-INT1	-1571.398586	0.465795	-1570.932791	186.559	0.554436
Cl-TS1	-1654.525328	0.529752	-1653.995576	203.517	0.62645
Cl-INT2	-2682.437316	0.957405	-2681.479911	316.618	1.10784
Cl^-	-460.364255	-0.015023	-460.379278	36.586	0.00236
Cl-INT3	-2765.652275	1.02507	-2764.627205	336.649	1.185023
Cl-TS2	-2842.046493	1.05146	-2840.995033	336.377	1.211283