ELECTRONIC SUPPLEMENTARY INFORMATION

Catalytic Cross-Coupling of Diazo compounds with Coinage Metal-Based Catalysts: An Experimental and Theoretical Study

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S1. Conformational analysis of transition states

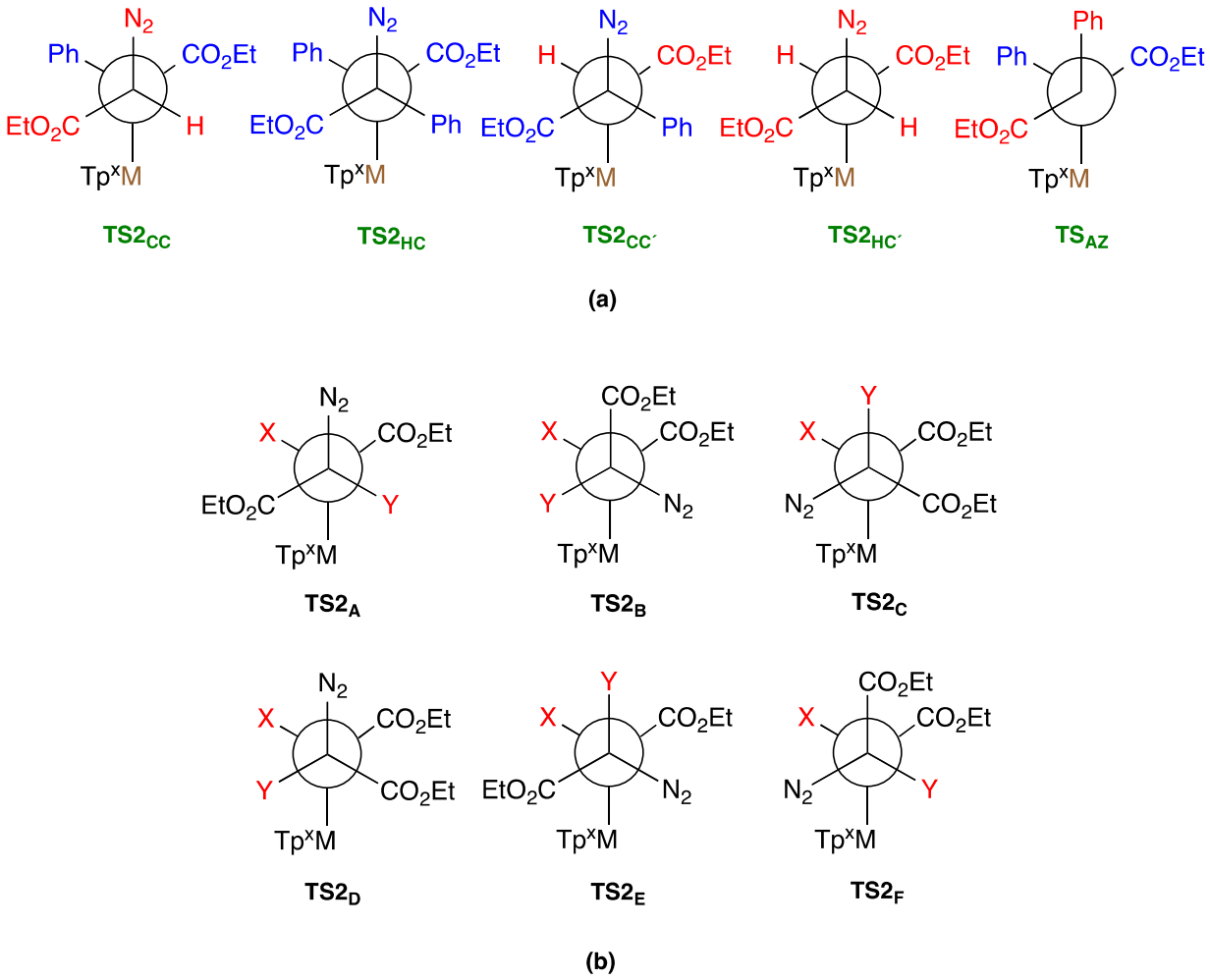

Figure S1. (a) The cross-coupling product, **3**, can be formed through $\mathbf{TS2_{CC}}$ and $\mathbf{TS2_{CC'}}$, and $\mathbf{TS2_{HH}}$ and $\mathbf{TS2_{HH'}}$ leading to the homo-coupling products, (**1** and **2**), while the azine formation undergoes through ($\mathbf{TS_{AZ}}$). (b) Different possible conformations that we considered for the cross-coupling and homo-coupling transition states.

Table S1. Total energies of different possible conformations for the transition state structures
TpBr3Ag system

	$\mathbf{TS2_{CC}}$	$\mathbf{TS2_{HC}}$	$\mathbf{TS2_{CC'}}$	$\mathbf{TS2_{HC'}}$
$\mathbf{TS2_A}$	-1914.018668	-2144.903669	-1913.994968	-1683.097734
$\mathbf{TS2_B}$	-1914.014843	-2144.902066	-1913.995384	-1683.100714
$\mathbf{TS2_C}$	-1914.014616	-2144.898601	-1913.994712	-1683.099687
$\mathbf{TS2_D}$	-1914.018572	-2144.901419	-1913.996121	-1683.098707
$\mathbf{TS2_E}$	-1914.015168	-2144.901697	-1914.000231	-1683.099755
$\mathbf{TS2_F}$	-1914.015434	-2144.898193	-1913.997827	-1683.097986

TpBr3Cu system

	$\mathbf{TS2_{CC}}$	$\mathbf{TS2_{HC}}$	$\mathbf{TS2_{CC'}}$	$\mathbf{TS2_{HC'}}$

$TS2_A$	-1964.413903	-2195.300232	-1964.402543	-1733.514453
$TS2_B$	-1964.415174	-2195.294730	-1964.400171	-1733.509902
$TS2_C$	-1964.414543	-2195.300365	-1964.400887	-1733.509670
$TS2_D$	-1964.413894	-2195.296992	-1964.396052	-1733.501309
$TS2_E$	-1964.408719	-2195.295163	-1964.400685	-1733.509468
$TS2_F$	-1964.416811	-2195.295945	-1964.401057	-1733.510231

$IPrAg^+$ system

	$TS2_{CC}$	**$TS2_{HC}$**	**$TS2_{CC'}$**	**$TS2_{HC'}$**
$TS2_A$	-2258.715121	-2489.595558	-2258.684340	-2027.784762
$TS2_B$	-2258.708340	-2489.594057	-2258.682140	-2027.785462
$TS2_C$	-2258.710558	-2489.591812	-2258.682742	-2027.782029
$TS2_D$	-2258.707711	-2489.598399	-2258.686156	-2027.784943
$TS2_E$	-2258.706665	-2489.592552	-2258.681738	-2027.783942
$TS2_F$	-2258.707434	-2489.588835	-2258.682290	-2027.781923

$IPrCu^+$ system

	$TS2_{CC}$	**$TS2_{HC}$**	**$TS2_{CC'}$**	**$TS2_{HC'}$**
$TS2_A$	-2309.115109	-2539.994653	-2309.096730	-2078.193152
$TS2_B$	-2309.110393	-2539.995106	-2309.089495	-2078.193524
$TS2_C$	-2309.107818	-2539.992289	-2309.092884	-2078.187621
$TS2_D$	-2309.108466	-2539.997647	-2309.085163	-2078.190171
$TS2_E$	-2309.108815	-2539.994875	-2309.091289	-2078.192084
$TS2_F$	-2309.113604	-2539.995693	-2309.094239	-2078.192557

S2 Electronic *vs* steric effects of phenyl substituent

The comparison of full QM and ONIOM(QM:MM) calculations can be used to evaluate the relative importance of electronic and steric contributions of a given substituents. The idea is that the QM calculation contains all the effects of the substituent, while the QM/MM calculation contains only the steric effects, but neglects the electronic ones. We used this approach to evaluate the role of the phenyl substituent in $N_2C(Ph)CO_2Et$ (**6a**) in the reaction with $Tp^{Br3}Ag$. The results are summarized in Figure S2. No solvation effects are introduced, as their introduction is not trivial in the QM/MM calculation, and they do not seem critical for this particular problem.

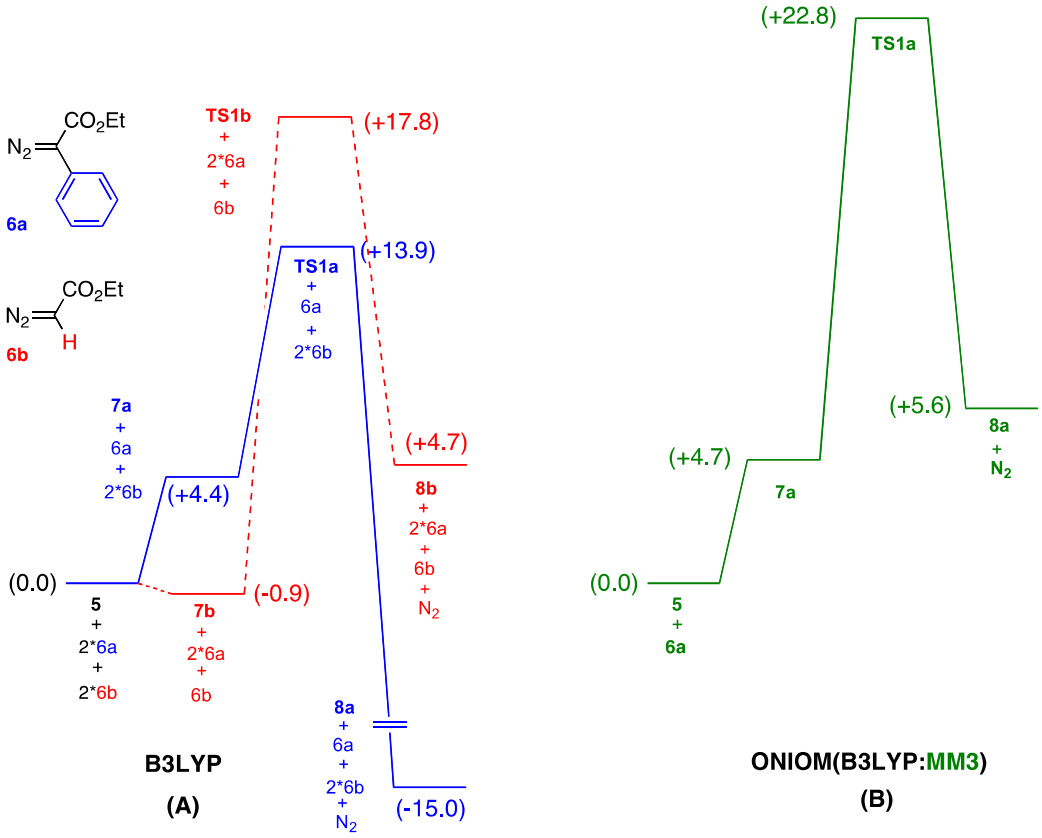

Figure S2. (A) Calculated gas phase free energy (kcal mol^{-1}) profiles generated with DFT for the reaction of $N_2C(Ph)CO_2Et$ (**6a**) and $N_2C(H)CO_2Et$ (**6b**) catalyzed by $Tp^{Br3}Ag$. (B) Gas phase free energy profiles (kcal mol^{-1}) generated with ONIOM(B3LYP:MM3) for the reaction of $N_2C(Ph)CO_2Et$ (**6a**) with $Tp^{Br3}Ag$, where the phenyl group of **6a** was described with MM3, and the other atoms were treated with DFT.

The left part of Figure S2 reports the full B3LYP profiles for the reactions of the metal complex with $N_2C(Ph)CO_2Et$ (**6a**) (in red) and $N_2C(H)CO_2Et$ (**6b**) (in blue). The ONIOM(B3LYP:MM3) profile for the reaction of $N_2C(Ph)CO_2Et$ (**6a**) results is shown in the right part of the Figure. It is clear that the agreement between the blue and green profiles is poor, although they correspond to the same system. This means that the ONIOM(B3LYP:MM3) description is not appropriate for this system, and that the electronic effects of the phenyl group are critical.

These energy results are confirmed by the computed structures for intermediates **8**. The bonds around the metal for the ONIOM(B3LYP:MM3) calculation of **8a** are more similar to those of the B3LYP calculation of **8b** than to those of the B3LYP calculation of **8a.** The difference between 8a and **8b** is in the electronic effects of the phenyl, and these electronic effects are neglected in the ONIOM calculation.

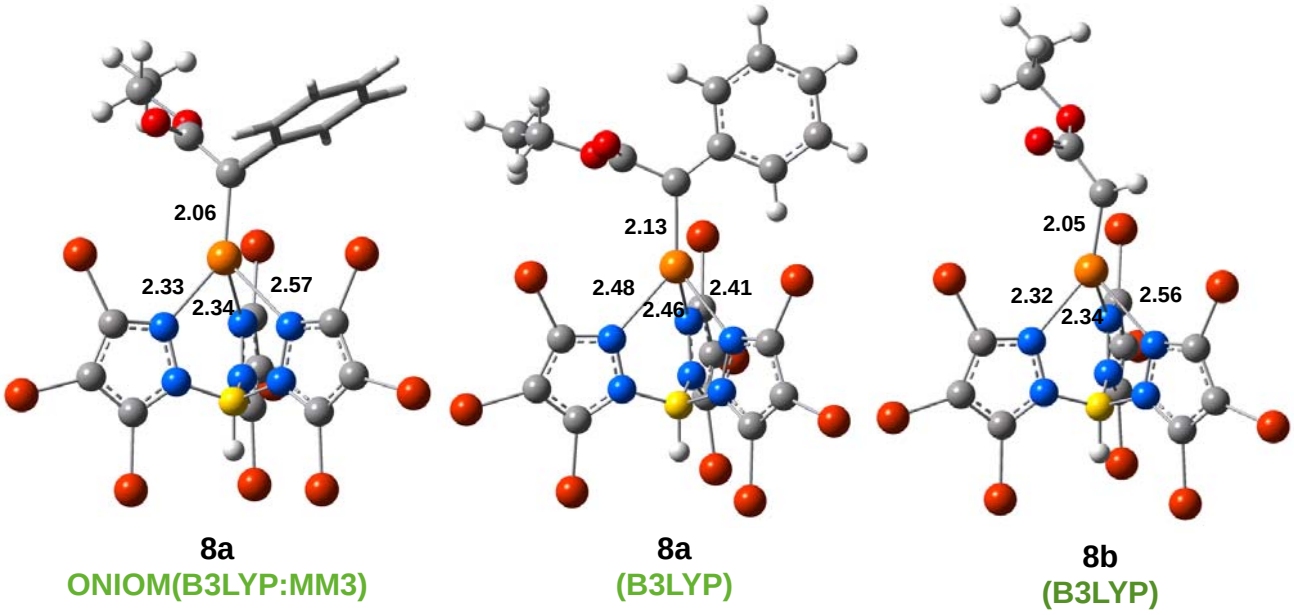

Figure S3. Computed structures for intermediate **8a** with the ONIOM(B3LYP:MM3) and B3LYP methods, and of intermediate **8b** with the B3LYP methods. Selected bond distances are indicated in Å.

S3. Energies, imaginary frequencies and Cartesian coordinates of optimized structures

N_2
Electronic energy = -415.940812
Zero-point correction = 0.005609
Thermal correction to Energy = 0.007969
Thermal correction to Enthalpy = 0.008913
Thermal correction to Gibbs Free Energy = -0.012840

N	0.046306000	-1.383735000	5.341555000
N	0.281906000	-2.256811000	5.976302000

6a
Electronic energy = -415.940812
Zero-point correction = 0.105499
Thermal correction to Energy = 0.113901
Thermal correction to Enthalpy = 0.114846
Thermal correction to Gibbs Free Energy = 0.071841

C	3.214678000	-0.074521000	2.533599000
C	4.548983000	0.481843000	2.349891000
O	4.799253000	1.669150000	2.477588000
O	5.455759000	-0.464590000	2.026299000
C	6.818963000	-0.008669000	1.829700000
H	6.824555000	0.759257000	1.049952000
H	7.175093000	0.446114000	2.759614000
C	7.647552000	-1.215270000	1.438350000
H	7.630552000	-1.977353000	2.225133000
H	7.276729000	-1.663041000	0.509948000
H	8.687212000	-0.907160000	1.280326000
N	3.002571000	-1.354632000	2.388662000
N	2.824829000	-2.471265000	2.261672000
H	2.363939000	0.540633000	2.792962000

6b
Electronic energy = -647.000167
Zero-point correction = 0.187184
Thermal correction to Energy = 0.200049
Thermal correction to Enthalpy = 0.200994
Thermal correction to Gibbs Free Energy = 0.146919

C	4.612529000	-0.265665000	2.801483000
C	4.718132000	1.083696000	3.382133000
O	4.379648000	1.382238000	4.515696000
O	5.236894000	1.960252000	2.498020000
C	5.388221000	3.328963000	2.959441000
H	4.411321000	3.697730000	3.286334000
H	6.062484000	3.334022000	3.821431000
C	4.058510000	-1.476963000	3.444146000
C	3.701628000	-1.480137000	4.806030000
C	3.879656000	-2.660655000	2.700649000
H	3.829221000	-0.580497000	5.392999000
H	4.139989000	-2.691824000	1.646137000
C	3.181048000	-2.633575000	5.394372000
C	3.361737000	-3.806983000	3.299490000
H	2.912210000	-2.612143000	6.447466000
H	3.232697000	-4.706134000	2.702757000
C	3.007468000	-3.802522000	4.651319000
H	2.602042000	-4.696740000	5.116571000
C	5.940813000	4.138479000	1.804240000
H	6.068246000	5.179716000	2.120933000
H	6.915387000	3.755537000	1.482551000
H	5.257886000	4.121244000	0.948111000
N	5.047344000	-0.369472000	1.562827000
N	5.421015000	-0.478421000	0.494072000

$NaBPh_4$
Electronic energy = -1113.810394
Zero-point correction = 0.368526
Thermal correction to Energy = 0.389946
Thermal correction to Enthalpy = 0.390890
Thermal correction to Gibbs Free Energy = 0.316577

C	-0.667347000	0.458072000	1.335516000
B	0.199469000	0.002852000	-0.020436000
C	-1.405886000	1.663095000	1.427116000
H	-1.349429000	2.382951000	0.612363000
C	-2.202584000	1.986938000	2.538247000
H	-2.743170000	2.930982000	2.556166000
C	-2.280535000	1.112926000	3.623537000
H	-2.887804000	1.359287000	4.490774000
C	-1.545945000	-0.077077000	3.583848000
H	-1.579082000	-0.763905000	4.426952000
C	-0.764161000	-0.388213000	2.467489000
H	-0.194385000	-1.314418000	2.483010000
C	1.644905000	-0.651544000	0.448896000
C	2.269503000	-1.715494000	-0.232608000
H	1.767411000	-2.171216000	-1.083232000
C	3.521523000	-2.218624000	0.139724000
H	3.960016000	-3.043733000	-0.418777000
C	4.207252000	-1.668221000	1.224670000
H	5.179756000	-2.055574000	1.520140000
C	3.621100000	-0.610761000	1.925801000
H	4.137765000	-0.166440000	2.774610000
C	2.368745000	-0.122820000	1.541121000
H	1.939334000	0.698629000	2.111512000
C	0.451734000	1.343966000	-0.965051000
C	-0.539057000	1.860635000	-1.830198000
H	-1.473786000	1.315294000	-1.966514000
C	-0.376580000	3.041601000	-2.562527000
H	-1.176297000	3.391032000	-3.213000000
C	0.813410000	3.766321000	-2.463396000
H	0.951916000	4.684001000	-3.030369000
C	1.823707000	3.285077000	-1.628247000
H	2.762417000	3.829064000	-1.540610000
C	1.638346000	2.103534000	-0.902221000
H	2.449821000	1.762754000	-0.264502000
C	-0.659812000	-1.157773000	-0.871798000
C	-0.532825000	-1.293705000	-2.274637000
H	0.102421000	-0.597142000	-2.814879000
C	-1.182540000	-2.294492000	-3.002593000
H	-1.039566000	-2.354700000	-4.079533000
C	-2.013963000	-3.215131000	-2.357476000
H	-2.524851000	-3.990923000	-2.922085000
C	-2.163503000	-3.127482000	-0.973316000
H	-2.786833000	-3.844226000	-0.442683000
C	-1.489845000	-2.126812000	-0.255547000
H	-1.598903000	-2.127469000	0.828846000
Na	-2.918905000	0.030672000	0.041443000

BPh_4^-
Electronic energy = -951.582745
Zero-point correction = 0.367367
Thermal correction to Energy = 0.387509
Thermal correction to Enthalpy = 0.388453
Thermal correction to Gibbs Free Energy = 0.317688

C	-1.000336000	1.258141000	0.418329000
B	-0.001060000	-0.000414000	-0.000337000
C	-0.995170000	1.911498000	1.666441000
H	-0.276806000	1.603944000	2.422406000
C	-1.885522000	2.946273000	1.984400000
H	-1.840712000	3.413690000	2.966880000
C	-2.828628000	3.376094000	1.050164000
H	-3.522019000	4.179236000	1.290387000
C	-2.869718000	2.749781000	-0.200562000
H	-3.601739000	3.063784000	-0.942942000

C	-1.979011000	1.715131000	-0.495483000
H	-2.049921000	1.236428000	-1.471232000
C	-1.006442000	-1.253552000	-0.419897000
C	-1.003435000	-1.907425000	-1.667847000
H	-0.283064000	-1.603592000	-2.423368000
C	-1.898869000	-2.937581000	-1.986489000
H	-1.855540000	-3.405319000	-2.968870000
C	-2.845220000	-3.362219000	-1.053118000
H	-3.542517000	-4.161803000	-1.293861000
C	-2.884576000	-2.735110000	0.197190000
H	-3.619018000	-3.044933000	0.938918000
C	-1.988642000	-1.705176000	0.492848000
H	-2.058292000	-1.225674000	1.468310000
C	1.000069000	-0.422142000	1.256044000
C	1.984295000	0.488059000	1.708444000
H	2.057572000	1.462868000	1.228296000
C	2.877765000	0.190433000	2.739849000
H	3.614059000	0.930065000	3.050316000
C	2.833774000	-1.059455000	3.367684000
H	3.529350000	-1.301701000	4.168326000
C	1.885183000	-1.990165000	2.942447000
H	1.838139000	-2.972062000	3.410849000
C	0.992255000	-1.669540000	1.910627000
H	0.270171000	-2.423215000	1.606066000
C	1.003733000	0.416297000	-1.255078000
C	1.980531000	-0.500219000	-1.710830000
H	2.046023000	-1.477445000	-1.234353000
C	2.876437000	-0.205940000	-2.741143000
H	3.606626000	-0.950388000	-3.054498000
C	2.842827000	1.046682000	-3.364105000
H	3.540331000	1.286302000	-4.163847000
C	1.902130000	1.983690000	-2.935076000
H	1.863318000	2.967796000	-3.399583000
C	1.006436000	1.666386000	-1.904686000
H	0.290157000	2.424447000	-1.597439000

NaCl

Electronic energy = -622.587885
Zero-point correction = 0.000661
Thermal correction to Energy = 0.003454
Thermal correction to Enthalpy = 0.004398
Thermal correction to Gibbs Free Energy = -0.021905

Na	0.000000000	0.000000000	-1.500378000
Cl	0.000000000	0.000000000	0.970833000

Ag systems with Tp^{Br3} ligand

5

Electronic energy = -961.273809
Zero-point correction = 0.106951
Thermal correction to Energy = 0.135872
Thermal correction to Enthalpy = 0.136816
Thermal correction to Gibbs Free Energy = 0.036000

Ag	1.620418000	0.175824000	1.222037000
N	-0.674225000	-0.300146000	1.822101000
N	-1.558716000	-0.355244000	0.781846000
N	0.547579000	1.762605000	-0.240076000
N	-0.559538000	1.314198000	-0.901753000
N	1.138398000	-1.332134000	-0.584803000
N	-0.093402000	-1.205680000	-1.161171000
B	-1.123916000	-0.127234000	-0.700824000
C	-1.366695000	-0.511178000	2.933650000
C	-2.729643000	-0.714259000	2.655292000
C	-2.803629000	-0.605272000	1.270789000
C	0.748917000	3.017085000	-0.619147000
C	-0.223852000	3.431621000	-1.545781000
C	-1.036343000	2.312225000	-1.694056000
C	1.756773000	-2.332161000	-1.198626000
C	0.946111000	-2.893923000	-2.200282000
C	-0.222989000	-2.142501000	-2.139220000
H	-2.086376000	-0.234225000	-1.379196000
Br	-4.356252000	-0.772437000	0.217419000
Br	-4.128384000	-1.052458000	3.867715000
Br	-0.524137000	-0.507158000	4.624910000
Br	-1.748362000	-2.356833000	-3.223226000
Br	1.344114000	-4.325104000	-3.355147000
Br	3.506855000	-2.842710000	-0.703174000
Br	-2.554643000	2.169693000	-2.799443000
Br	-0.395333000	5.106016000	-2.386830000
Br	2.193005000	4.016496000	0.076556000

7a

Electronic energy = -1608.274796
Zero-point correction = 0.293961
Thermal correction to Energy = 0.338351
Thermal correction to Enthalpy = 0.339296
Thermal correction to Gibbs Free Energy = 0.199121

Ag	1.836514000	0.087128000	1.231688000
C	4.141665000	-0.190988000	2.521939000
N	-0.468653000	-0.382133000	1.922908000
N	-1.421610000	-0.193328000	0.961028000
N	0.640938000	1.749839000	-0.134405000
N	-0.393089000	1.256129000	-0.878311000
N	1.204634000	-1.259564000	-0.809848000
N	-0.150130000	-1.287092000	-0.991461000
B	-1.068463000	-0.107388000	-0.550583000
C	-1.101858000	-0.387103000	3.091815000
C	-2.485889000	-0.202577000	2.925586000
C	-2.640900000	-0.081618000	1.549922000
C	0.955047000	2.930462000	-0.654004000
C	0.138566000	3.242268000	-1.755340000
C	-0.705147000	2.142287000	-1.859791000
C	1.688472000	-2.338877000	-1.415511000
C	0.666067000	-3.108006000	-1.998351000
C	-0.489537000	-2.394941000	-1.700355000
H	-2.078149000	-0.175870000	-1.166231000
C	4.203891000	1.178430000	3.108310000
O	3.601525000	1.512279000	4.111266000
O	5.015624000	1.982410000	2.401016000
C	5.196141000	3.334520000	2.908923000
H	4.238985000	3.860483000	2.843811000
H	5.480036000	3.272505000	3.962900000
Br	-4.255131000	0.200610000	0.620607000
Br	-3.820610000	-0.138290000	4.250669000
Br	-0.177035000	-0.621634000	4.718826000
Br	-2.254004000	-2.856119000	-2.169951000
Br	0.817250000	-4.712954000	-2.969025000
Br	3.547018000	-2.684488000	-1.487137000
Br	-2.059111000	1.879747000	-3.142329000
Br	0.165839000	4.785740000	-2.831178000
Br	2.335185000	3.989070000	0.079204000
C	3.827439000	-1.428130000	3.309408000
C	3.859035000	-1.419629000	4.713404000
C	3.550746000	-2.633641000	2.642221000
H	4.070049000	-0.500433000	5.245094000
H	3.523657000	-2.659702000	1.556656000
C	3.605357000	-2.593320000	5.424827000
C	3.310550000	-3.804654000	3.359927000
H	3.631068000	-2.570032000	6.511076000
H	3.100851000	-4.725965000	2.823432000
C	3.333735000	-3.789261000	4.756419000
H	3.141139000	-4.699556000	5.317343000
C	6.272368000	3.994815000	2.072413000
H	6.421190000	5.021953000	2.423421000
H	7.223391000	3.459334000	2.163003000
H	5.992868000	4.030576000	1.013932000
N	4.972540000	-0.371993000	1.488211000
N	5.652275000	-0.539854000	0.600256000

7b

Electronic energy = -1377.227569
Zero-point correction = 0.213430
Thermal correction to Energy = 0.252660
Thermal correction to Enthalpy = 0.253604
Thermal correction to Gibbs Free Energy = 0.127734

Ag	1.757655000	0.022162000	0.979435000
C	3.728355000	-0.278798000	2.286214000
N	-0.579499000	-0.388455000	1.633977000
N	-1.546010000	-0.196975000	0.687992000
N	0.654515000	1.709440000	-0.398586000
N	-0.487423000	1.357559000	-1.060191000
N	0.978236000	-1.338002000	-0.948536000
N	-0.321265000	-1.183517000	-1.336540000
B	-1.199905000	-0.006208000	-0.817877000
C	-1.203974000	-0.548144000	2.794420000
C	-2.599438000	-0.464669000	2.641698000
C	-2.769009000	-0.239291000	1.280356000
C	0.999702000	2.912263000	-0.840684000
C	0.091517000	3.385274000	-1.804168000
C	-0.838490000	2.357454000	-1.911945000
C	1.441379000	-2.409903000	-1.577844000
C	0.457491000	-2.991879000	-2.396416000
C	-0.650760000	-2.173353000	-2.208448000
H	-2.213033000	-0.005524000	-1.429120000
C	3.958084000	0.969451000	3.071128000
O	3.332659000	1.229029000	4.078356000
O	4.913202000	1.736423000	2.526953000
C	5.221788000	2.976247000	3.229335000
H	4.318898000	3.593364000	3.251442000
H	5.494914000	2.729115000	4.258996000
Br	-4.405958000	-0.019678000	0.373239000
Br	-3.928493000	-0.628406000	3.963674000
Br	-0.244089000	-0.849562000	4.392457000
Br	-2.344478000	-2.375238000	-3.008163000
Br	0.599325000	-4.515704000	-3.491309000
Br	3.226066000	-2.986689000	-1.342550000
Br	-2.344933000	2.321677000	-3.042491000
Br	0.120621000	5.023885000	-2.729074000
Br	2.543514000	3.788633000	-0.196246000
C	6.356160000	3.651418000	2.488597000
H	6.607872000	4.588640000	2.997088000
H	7.250392000	3.019141000	2.472175000
H	6.075379000	3.886585000	1.456279000
N	4.713393000	-0.617360000	1.436730000
N	5.522491000	-0.877745000	0.699289000
H	3.343373000	-1.140637000	2.827420000

TS1a

Electronic energy = -1608.253880
Zero-point correction = 0.291462
Thermal correction to Energy = 0.335886
Thermal correction to Enthalpy = 0.336830
Thermal correction to Gibbs Free Energy = 0.196984

Ag	1.729038000	0.154303000	1.264763000
C	3.546882000	-0.095043000	2.553971000
N	-0.660736000	-0.281614000	1.767958000
N	-1.572008000	-0.061172000	0.774961000
N	0.643849000	1.682710000	-0.308355000
N	-0.380409000	1.222193000	-1.084511000
N	1.046218000	-1.352027000	-0.793646000
N	-0.294453000	-1.323651000	-1.051483000
B	-1.161120000	-0.073678000	-0.724210000
C	-1.326913000	-0.220730000	2.916196000
C	-2.692282000	0.042639000	2.704526000
C	-2.798743000	0.139230000	1.321733000
C	1.079965000	2.800613000	-0.877513000
C	0.354707000	3.101407000	-2.043799000
C	-0.564889000	2.062725000	-2.134930000
C	1.494167000	-2.508056000	-1.269279000
C	0.459957000	-3.272143000	-1.840600000
C	-0.664399000	-2.471807000	-1.675926000
H	-2.147138000	-0.113370000	-1.380804000
C	3.864266000	1.168127000	3.279861000
O	3.275681000	1.413086000	4.319008000
O	4.745833000	1.984289000	2.689179000
C	5.002019000	3.250051000	3.367018000
H	4.082523000	3.842666000	3.350114000
H	5.254420000	3.037108000	4.409332000
Br	-4.360471000	0.500031000	0.331060000
Br	-4.060258000	0.216055000	3.985464000
Br	-0.459415000	-0.474013000	4.573648000
Br	-2.429291000	-2.874223000	-2.198991000
Br	0.564158000	-4.966986000	-2.653215000
Br	3.328611000	-2.966923000	-1.185739000
Br	-1.859875000	1.815725000	-3.480457000
Br	0.569433000	4.564878000	-3.206948000
Br	2.501675000	3.793006000	-0.132023000
C	3.775531000	-1.361716000	3.280179000
C	4.724297000	-1.454023000	4.322626000
C	3.034718000	-2.509015000	2.935846000
H	5.311817000	-0.583062000	4.598344000
H	2.303249000	-2.447313000	2.135839000
C	4.911113000	-2.651613000	5.004065000
C	3.225353000	-3.709072000	3.617247000
H	5.640380000	-2.709661000	5.806883000
H	2.642765000	-4.584267000	3.345091000
C	4.162014000	-3.780863000	4.651677000
H	4.310080000	-4.715911000	5.184961000
C	6.138615000	3.937629000	2.640529000
H	6.348351000	4.895361000	3.129556000
H	7.050221000	3.331026000	2.668999000
H	5.884751000	4.136906000	1.593911000
N	4.829958000	-0.122494000	1.282241000
N	5.388122000	-0.355875000	0.353289000

TS1b -1376.859335 AU

Electronic energy = -1377.191879
Zero-point correction = 0.210033
Thermal correction to Energy = 0.249900
Thermal correction to Enthalpy = 0.250844
Thermal correction to Gibbs Free Energy = 0.122511

Ag	1.663561000	0.009293000	1.131802000
C	3.521443000	-0.127032000	2.174833000
N	-0.680094000	-0.144397000	1.641705000
N	-1.628654000	-0.160696000	0.660150000
N	0.677774000	1.583878000	-0.510739000
N	-0.506268000	1.292020000	-1.122469000
N	0.816707000	-1.517628000	-0.703548000
N	-0.388295000	-1.258500000	-1.288089000
B	-1.255291000	-0.043513000	-0.848507000
C	-1.317118000	-0.280426000	2.798720000
C	-2.705367000	-0.390498000	2.606714000
C	-2.855226000	-0.309017000	1.226537000
C	1.047733000	2.782175000	-0.942492000
C	0.115290000	3.310857000	-1.853122000
C	-0.858786000	2.322166000	-1.936750000
C	1.296220000	-2.608356000	-1.285150000
C	0.418645000	-3.096386000	-2.270459000
C	-0.643965000	-2.200526000	-2.234553000
H	-2.256097000	-0.047567000	-1.479963000
C	4.052324000	0.940458000	3.030993000
O	3.547813000	0.939474000	4.146092000
O	4.918599000	1.810956000	2.544829000
C	5.320936000	2.901783000	3.439023000
H	4.441470000	3.526055000	3.620117000
H	5.646220000	2.465167000	4.386574000
Br	-4.473951000	-0.389680000	0.265820000
Br	-4.047495000	-0.601314000	3.908262000
Br	-0.374881000	-0.308016000	4.433070000
Br	-2.194817000	-2.249695000	-3.303826000

Br	0.625818000	-4.605933000	-3.375337000
Br	2.962955000	-3.340119000	-0.772653000
Br	-2.415080000	2.362235000	-2.998452000
Br	0.170778000	4.964859000	-2.749338000
Br	2.648972000	3.584595000	-0.341832000
C	6.432132000	3.662702000	2.749972000
H	6.749421000	4.491045000	3.392925000
H	7.298175000	3.017665000	2.567894000
H	6.095496000	4.079607000	1.794948000
N	4.890310000	-0.157591000	0.631173000
N	5.402109000	-0.077496000	-0.344395000
H	3.870706000	-1.110582000	2.496585000

8a

Electronic energy =	-1498.765584
Zero-point correction =	0.284763
Thermal correction to Energy =	0.326758
Thermal correction to Enthalpy =	0.327702
Thermal correction to Gibbs Free Energy =	0.195279

Ag	1.483185000	0.160637000	1.576291000
C	3.087163000	0.047691000	2.991001000
N	-0.935361000	-0.489886000	1.698092000
N	-1.730613000	-0.364551000	0.595656000
N	0.284055000	1.877283000	0.197067000
N	-0.582822000	1.459487000	-0.771346000
N	1.199789000	-0.983622000	-0.596661000
N	-0.020599000	-0.992972000	-1.206531000
B	-1.140322000	0.007144000	-0.794782000
C	-1.738030000	-0.766642000	2.717955000
C	-3.082934000	-0.834115000	2.311177000
C	-3.027449000	-0.568692000	0.947902000
C	0.528379000	3.160141000	-0.038214000
C	-0.166865000	3.618121000	-1.172015000
C	-0.862079000	2.495227000	-1.605737000
C	1.938247000	-1.905153000	-1.203472000
C	1.218222000	-2.547554000	-2.226751000
C	-0.027256000	-1.930386000	-2.189608000
H	-2.007899000	-0.050537000	-1.598793000
C	3.817296000	1.308752000	3.212257000
O	3.461722000	2.087601000	4.083657000
O	4.818611000	1.504370000	2.351514000
C	5.542376000	2.767922000	2.454121000
H	4.823162000	3.586025000	2.360806000
H	6.001701000	2.824402000	3.445371000
Br	-4.484671000	-0.495042000	-0.244552000
Br	-4.601477000	-1.203574000	3.359715000
Br	-1.065384000	-1.008839000	4.467131000
Br	-1.506137000	-2.307377000	-3.294037000
Br	1.798763000	-3.914081000	-3.383469000
Br	3.729279000	-2.222850000	-0.693672000
Br	-1.997997000	2.381891000	-3.105254000
Br	-0.167848000	5.343916000	-1.923441000
Br	1.665466000	4.161965000	1.088422000
C	3.476668000	-1.086769000	3.744444000
C	4.565579000	-1.057530000	4.671682000
C	2.783195000	-2.320611000	3.559619000
H	5.103780000	-0.129683000	4.839228000
H	1.955734000	-2.347781000	2.857721000
C	4.928581000	-2.195591000	5.369326000
C	3.159647000	-3.458822000	4.252920000
H	5.751979000	-2.166023000	6.076028000
H	2.630097000	-4.394092000	4.101780000
C	4.228990000	-3.394523000	5.157333000
H	4.520386000	-4.286289000	5.705591000
C	6.574965000	2.791330000	1.347389000
H	7.134927000	3.731841000	1.397748000
H	7.284646000	1.963324000	1.449470000
H	6.099252000	2.726718000	0.363076000

8b

Electronic energy =	-1267.676616
Zero-point correction =	0.202770
Thermal correction to Energy =	0.239924
Thermal correction to Enthalpy =	0.240868
Thermal correction to Gibbs Free Energy =	0.120272

Ag	1.717590000	0.071274000	1.164339000
C	3.232218000	0.032849000	2.578615000
N	-0.795349000	-0.311949000	1.772156000
N	-1.690678000	-0.328705000	0.742743000
N	0.580570000	1.621225000	-0.235452000
N	-0.568539000	1.287690000	-0.891531000
N	0.966844000	-1.399913000	-0.536779000
N	-0.236814000	-1.234006000	-1.156292000
B	-1.231298000	-0.112948000	-0.725111000
C	-1.488414000	-0.525597000	2.881326000
C	-2.860257000	-0.689792000	2.611241000
C	-2.940032000	-0.555284000	1.230188000
C	0.880578000	2.867434000	-0.583500000
C	-0.069393000	3.386623000	-1.480152000
C	-0.973856000	2.342971000	-1.645427000
C	1.566579000	-2.432527000	-1.117912000
C	0.766863000	-2.974876000	-2.138738000
C	-0.372857000	-2.176567000	-2.125338000
H	-2.179730000	-0.163651000	-1.430723000
H	3.017781000	-0.184395000	3.630655000
C	4.614993000	0.398584000	2.398134000
O	4.706881000	1.588794000	2.705752000
O	5.537214000	-0.406874000	1.942486000
C	6.892488000	0.151868000	1.781732000
H	6.859521000	0.853974000	0.944477000
H	7.145447000	0.694912000	2.695313000
Br	-4.496652000	-0.661093000	0.173065000
Br	-4.260330000	-1.014220000	3.827169000
Br	-0.641915000	-0.582976000	4.571930000
Br	-1.874978000	-2.341104000	-3.249561000
Br	1.147238000	-4.433823000	-3.264672000
Br	3.277873000	-3.004022000	-0.564359000
Br	-2.516833000	2.353540000	-2.725330000
Br	-0.110153000	5.091036000	-2.275976000
Br	2.412998000	3.730185000	0.099331000
C	7.827725000	-1.007528000	1.525355000
H	7.829185000	-1.707233000	2.367584000
H	7.549620000	-1.548442000	0.614872000
H	8.844428000	-0.619651000	1.397936000

$TS2_{CC}$ (*E*)

Electronic energy =	-1914.69668744
Zero-point correction =	0.391174
Thermal correction to Energy =	0.442404
Thermal correction to Enthalpy =	0.443348
Thermal correction to Gibbs Free Energy =	0.290671

Ag	1.212993000	0.842188000	-0.711249000
C	3.171258000	0.000222000	-1.232838000
N	-0.858801000	-0.311736000	-2.119930000
N	-1.776604000	-0.639827000	-1.164479000
N	-0.654374000	2.333634000	-0.595942000
N	-1.924737000	1.827989000	-0.580432000
N	-0.167590000	-0.148472000	1.296675000
N	-1.504300000	0.120655000	1.261679000
B	-2.229787000	0.386069000	-0.086345000
C	-0.779293000	-1.358075000	-2.933629000
C	-1.631864000	-2.401404000	-2.526769000
C	-2.248214000	-1.891020000	-1.389929000
C	-0.751503000	3.589123000	-1.025237000
C	-2.084262000	3.934905000	-1.305759000
C	-2.794004000	2.777224000	-1.008754000
C	0.146098000	-0.314196000	2.575073000
C	-0.973323000	-0.153432000	3.412070000
C	-2.004907000	0.126786000	2.523902000
H	-3.401062000	0.285534000	0.089093000

C	3.307689000	-1.396422000	-0.735309000
O	4.269052000	-1.644381000	0.164940000
O	2.530497000	-2.238427000	-1.156928000
C	4.371275000	-3.018737000	0.649796000
H	4.553603000	-3.671562000	-0.208192000
H	3.415629000	-3.299688000	1.099909000
C	4.675810000	1.151609000	0.306467000
C	4.473925000	2.602411000	0.100866000
O	3.601165000	3.228663000	0.667552000
O	5.351336000	3.101562000	-0.782480000
C	5.279623000	4.531436000	-1.047670000
H	5.343715000	5.063424000	-0.094436000
H	4.309134000	4.749253000	-1.501963000
N	5.812795000	0.631686000	-0.132888000
N	6.722714000	0.176444000	-0.625187000
Br	1.907806000	-0.740236000	3.115014000
Br	-1.065998000	-0.301871000	5.286471000
Br	-3.807738000	0.470266000	2.951754000
Br	-3.531736000	-2.733143000	-0.296063000
Br	-1.899278000	-4.083165000	-3.331075000
Br	0.327226000	-1.320535000	-4.466796000
Br	-4.653644000	2.524144000	-1.170720000
Br	-2.756833000	5.579979000	-1.923980000
Br	0.761754000	4.702179000	-1.185321000
C	6.426679000	4.877016000	-1.973670000
H	7.391375000	4.646643000	-1.509291000
H	6.350731000	4.326754000	-2.917510000
H	6.399802000	5.949285000	-2.196928000
C	5.511259000	-3.061069000	1.645904000
H	5.318842000	-2.405391000	2.502126000
H	5.625898000	-4.084552000	2.019434000
H	6.454594000	-2.758039000	1.178797000
C	3.840711000	0.287642000	-2.480555000
C	3.516465000	1.471512000	-3.195215000
C	4.823993000	-0.578988000	-3.036079000
H	2.768510000	2.138353000	-2.776550000
H	5.089969000	-1.497114000	-2.521365000
C	4.125306000	1.764349000	-4.406667000
C	5.427651000	-0.283563000	-4.253325000
H	3.858093000	2.667409000	-4.947437000
H	6.165463000	-0.961901000	-4.671136000
C	5.080917000	0.885706000	-4.937631000
H	5.553217000	1.113455000	-5.889283000
H	4.243642000	0.660925000	1.166527000
O	4.714972000	-1.514869000	0.469167000
O	3.240681000	-2.637288000	-0.837618000
C	5.244142000	-2.774362000	0.981878000
H	5.322111000	-3.483252000	0.154491000
H	4.530523000	-3.171269000	1.710384000
C	4.161085000	1.354694000	0.513798000
C	3.729749000	1.101676000	1.907469000
O	2.573532000	1.241977000	2.255267000
O	4.742730000	0.736790000	2.704954000
C	4.411597000	0.528208000	4.109186000
H	3.723223000	-0.318661000	4.179193000
H	3.897550000	1.420586000	4.476655000
N	5.446404000	1.245472000	0.212694000
N	6.509569000	1.051824000	-0.119847000
Br	1.045919000	-2.499045000	2.643553000
Br	-1.713615000	-1.582517000	4.956627000
Br	-3.926596000	0.560617000	2.936786000
Br	-4.848425000	-1.376193000	-1.467869000
Br	-3.153477000	-2.914438000	-4.350045000
Br	0.313667000	-1.594353000	-4.203646000
Br	-4.217246000	3.320379000	-0.870266000
Br	-1.653666000	5.948539000	-1.098753000
Br	1.531914000	4.220706000	-0.409097000
C	5.705672000	0.275146000	4.853324000
H	6.211227000	-0.621744000	4.480341000
H	6.388299000	1.126638000	4.760758000
H	5.484500000	0.126203000	5.916080000
C	6.590332000	-2.480372000	1.609965000
H	6.498183000	-1.744433000	2.414846000
H	7.001986000	-3.404840000	2.030266000
H	7.296523000	-2.097021000	0.865341000
C	3.822766000	0.134806000	-2.207923000
C	3.208149000	1.170839000	-2.958853000
C	5.036293000	-0.417951000	-2.704144000
H	2.278634000	1.594658000	-2.590553000
H	5.533908000	-1.213287000	-2.157607000
C	3.766970000	1.625435000	-4.144342000
C	5.587884000	0.033424000	-3.898109000
H	3.279428000	2.414740000	-4.708703000
H	6.508089000	-0.406155000	-4.271326000
C	4.957315000	1.055076000	-4.616563000
H	5.391306000	1.407179000	-5.548380000
H	3.625390000	2.091833000	-0.067695000

TS2$_{CC}$ (*Z*)

Electronic energy =	-1914.697456
Zero-point correction =	0.390723
Thermal correction to Energy =	0.442212
Thermal correction to Enthalpy =	0.443156
Thermal correction to Gibbs Free Energy =	0.288161

Ag	1.107241000	0.101659000	-0.479637000
C	3.206270000	-0.314399000	-0.976439000
N	-0.955224000	-0.399228000	-1.985489000
N	-2.165296000	-0.339990000	-1.355511000
N	-0.395487000	2.151924000	-0.227946000
N	-1.742745000	1.952648000	-0.326686000
N	-0.605651000	-0.823062000	1.091823000
N	-1.781532000	-0.132251000	1.153698000
B	-2.383290000	0.553402000	-0.105082000
C	-1.107529000	-1.224716000	-3.014045000
C	-2.419082000	-1.730824000	-3.083023000
C	-3.055756000	-1.137507000	-1.999629000
C	-0.192617000	3.444177000	-0.459155000
C	-1.396483000	4.122437000	-0.721036000
C	-2.359042000	3.125149000	-0.624794000
C	-0.429859000	-1.376472000	2.286672000
C	-1.478645000	-1.051847000	3.165720000
C	-2.316327000	-0.253921000	2.394729000
H	-3.548937000	0.695400000	0.063513000
C	3.729524000	-1.593236000	-0.433508000

TS2$_{HC}$

Electronic energy =	-2145.741993
Zero-point correction =	0.471910
Thermal correction to Energy =	0.527724
Thermal correction to Enthalpy =	0.528668
Thermal correction to Gibbs Free Energy =	0.366415

Ag	1.164233000	0.963779000	-0.343983000
C	3.230706000	0.306372000	-0.809325000
N	-0.905523000	-0.103170000	-2.276747000
N	-1.881026000	-0.521654000	-1.419641000
N	-0.750225000	2.325086000	-0.252740000
N	-2.006605000	1.852931000	-0.508978000
N	-0.546985000	-0.620622000	1.188954000
N	-1.813134000	-0.116628000	1.098093000
B	-2.395200000	0.368661000	-0.257658000
C	-0.785445000	-1.059837000	-3.189600000
C	-1.668299000	-2.130222000	-2.949543000
C	-2.348414000	-1.735144000	-1.804566000
C	-0.782561000	3.637847000	-0.481019000
C	-2.056420000	4.052142000	-0.901154000
C	-2.800880000	2.877371000	-0.904632000
C	-0.397329000	-1.015603000	2.448168000
C	-1.550730000	-0.766108000	3.216067000
C	-2.427391000	-0.188731000	2.306503000
H	-3.581992000	0.298470000	-0.202091000
C	3.375657000	-1.116055000	-0.378138000
O	4.338314000	-1.424295000	0.499212000

O	2.599026000	-1.934740000	-0.846857000
C	4.449383000	-2.834341000	0.862898000
H	4.669591000	-3.404006000	-0.044680000
H	3.484152000	-3.169830000	1.249009000
C	4.680520000	1.479902000	0.477813000
C	4.654823000	2.858114000	-0.156733000
O	3.876391000	3.722063000	0.179676000
O	5.590420000	2.980980000	-1.100653000
C	5.692227000	4.278523000	-1.765110000
H	5.760755000	5.050742000	-0.994529000
H	4.776622000	4.438190000	-2.340463000
N	5.798086000	0.811859000	0.102603000
N	6.658761000	0.226930000	-0.324994000
Br	1.187849000	-1.851374000	3.047984000
Br	-1.855105000	-1.141329000	5.036671000
Br	-4.178740000	0.422396000	2.644475000
Br	-3.702525000	-2.668303000	-0.882049000
Br	-1.897681000	-3.714122000	-3.943247000
Br	0.412044000	-0.886482000	-4.644429000
Br	-4.611334000	2.692386000	-1.389211000
Br	-2.629830000	5.789334000	-1.341444000
Br	0.745445000	4.708800000	-0.230121000
C	6.922694000	4.237668000	-2.644898000
H	7.826718000	4.069549000	-2.050013000
H	6.844932000	3.447769000	-3.399134000
H	7.024778000	5.198454000	-3.161493000
C	5.554294000	-2.961743000	1.890363000
H	5.320139000	-2.397727000	2.798798000
H	5.669910000	-4.017206000	2.161261000
H	6.510277000	-2.605825000	1.490613000
C	3.734792000	0.559065000	-2.160800000
C	3.282090000	1.687497000	-2.886871000
C	4.667319000	-0.304003000	-2.793964000
H	2.565739000	2.355762000	-2.417934000
H	5.024387000	-1.190045000	-2.278037000
C	3.722688000	1.933612000	-4.181805000
C	5.109366000	-0.054516000	-4.089736000
H	3.348645000	2.795321000	-4.727097000
H	5.813164000	-0.734543000	-4.560905000
C	4.638611000	1.062948000	-4.786141000
H	4.976889000	1.251269000	-5.801427000
C	4.326234000	1.365893000	1.930357000
C	5.193722000	0.743268000	2.841773000
C	3.137740000	1.944058000	2.402872000
H	6.128016000	0.305686000	2.503376000
H	2.466894000	2.442686000	1.715451000
C	4.876555000	0.697344000	4.198949000
C	2.831266000	1.899303000	3.763567000
H	5.563160000	0.217238000	4.890738000
H	1.909047000	2.354467000	4.114302000
C	3.695049000	1.276971000	4.666436000
H	3.451672000	1.246350000	5.724829000

TS2$_{CC'}$
Electronic energy = -1914.676026
Zero-point correction = 0.390412
Thermal correction to Energy = 0.441671
Thermal correction to Enthalpy = 0.442615
Thermal correction to Gibbs Free Energy = 0.289600

Ag	1.545204000	-0.622327000	-0.077854000
C	3.490947000	-1.162292000	-0.652035000
N	-0.650531000	-1.396612000	-0.883939000
N	-1.755767000	-0.612341000	-0.724263000
N	0.330274000	1.543534000	-0.932081000
N	-0.913296000	1.774600000	-0.420097000
N	0.142982000	-0.102134000	1.770249000
N	-1.169094000	0.236479000	1.606880000
B	-1.745664000	0.626959000	0.214747000
C	-0.981564000	-2.358073000	-1.737991000
C	-2.315057000	-2.226181000	-2.164699000
C	-2.766736000	-1.096690000	-1.491215000
C	0.748356000	2.694557000	-1.441246000
C	-0.207428000	3.714092000	-1.272234000
C	-1.251733000	3.076547000	-0.613026000
C	0.314940000	-0.370994000	3.060820000
C	-0.883236000	-0.212621000	3.777837000
C	-1.801134000	0.174294000	2.807071000
H	-2.859315000	1.000972000	0.363184000
H	4.098437000	-0.498010000	-1.268630000
C	3.913880000	-2.549309000	-0.790228000
O	4.343317000	-3.231851000	0.250485000
O	3.689952000	-2.975046000	-1.921169000
C	4.616142000	-4.660792000	0.045799000
H	5.560982000	-4.741713000	-0.499506000
H	3.815238000	-5.077771000	-0.568155000
C	5.553996000	0.094301000	0.952585000
C	6.454461000	-0.000342000	-0.223604000
O	7.409118000	-0.751264000	-0.283402000
O	6.078844000	0.833976000	-1.212225000
C	6.928552000	0.842509000	-2.399294000
H	7.004426000	-0.180339000	-2.777580000
H	7.925698000	1.176257000	-2.098271000
N	4.688939000	1.102937000	0.926275000
N	3.933638000	1.946814000	0.920432000
Br	2.001127000	-0.878822000	3.732982000
Br	-1.178812000	-0.459863000	5.619788000
Br	-3.627296000	0.552825000	3.071678000
Br	2.430211000	2.837417000	-2.291354000
Br	-0.110092000	5.513157000	-1.818179000
Br	-2.876073000	3.849212000	-0.050502000
Br	0.263503000	-3.681293000	-2.241961000
Br	-3.268999000	-3.322070000	-3.360731000
Br	-4.482662000	-0.325998000	-1.599873000
C	6.299099000	1.776811000	-3.409806000
H	6.194571000	2.788778000	-3.004017000
H	6.941409000	1.829308000	-4.295943000
H	5.315514000	1.413527000	-3.726668000
C	4.682568000	-5.310992000	1.410351000
H	3.726325000	-5.217612000	1.935896000
H	4.904874000	-6.376689000	1.285687000
H	5.467939000	-4.863995000	2.027573000
C	5.856197000	-0.507255000	2.275136000
C	6.525211000	-1.741361000	2.357770000
C	5.503853000	0.156211000	3.464848000
H	6.806566000	-2.262179000	1.452914000
H	5.004396000	1.120347000	3.431345000
C	6.835387000	-2.287738000	3.603181000
C	5.810875000	-0.402789000	4.705248000
H	7.359036000	-3.238837000	3.649213000
H	5.536517000	0.129509000	5.611783000
C	6.480066000	-1.626636000	4.781102000
H	6.724190000	-2.058746000	5.747520000

TS2$_{HC'}$
Electronic energy = -1683.620399
Zero-point correction = 0.308586
Thermal correction to Energy = 0.355644
Thermal correction to Enthalpy = 0.356588
Thermal correction to Gibbs Free Energy = 0.211099

Ag	1.027510000	-0.390170000	-0.871886000
C	3.030631000	-0.265822000	-1.403779000
N	-1.068360000	-0.918879000	-1.829024000
N	-2.242076000	-0.573845000	-1.224361000
N	-0.376034000	1.638831000	-0.188515000
N	-1.648300000	1.427770000	0.255299000
N	-0.191483000	-1.160363000	1.097022000
N	-1.533742000	-0.938404000	1.203868000
B	-2.282046000	0.009434000	0.219913000
C	-1.374635000	-1.400257000	-3.028869000
C	-2.763531000	-1.382598000	-3.243018000
C	-3.273644000	-0.847153000	-2.064831000
C	-0.115053000	2.925476000	-0.003311000

C	-1.212339000	3.596156000	0.568916000
C	-2.167254000	2.596347000	0.717082000
C	0.145143000	-1.974907000	2.089943000
C	-0.970991000	-2.309815000	2.877098000
C	-2.018870000	-1.624655000	2.271514000
H	-3.412862000	0.087750000	0.560188000
H	3.494922000	0.691128000	-1.666731000
C	3.946201000	-1.359031000	-1.619526000
O	4.653840000	-1.910024000	-0.666644000
O	3.888763000	-1.658978000	-2.813038000
C	5.513385000	-3.048448000	-1.034910000
H	6.090266000	-2.768157000	-1.919366000
H	4.857964000	-3.886556000	-1.285690000
C	5.307300000	0.864965000	1.307580000
C	5.937338000	1.218607000	0.044336000
O	5.380668000	1.891150000	-0.812967000
O	7.185977000	0.723814000	-0.067314000
C	7.890115000	1.022550000	-1.303063000
H	7.915492000	2.107763000	-1.438071000
H	7.331546000	0.586895000	-2.137479000
N	5.910483000	0.058634000	2.140052000
N	6.443132000	-0.649315000	2.852492000
Br	1.928507000	-2.549557000	2.322081000
Br	-1.036666000	-3.416625000	4.397501000
Br	-3.823693000	-1.624599000	2.810465000
Br	-5.086829000	-0.533993000	-1.664135000
Br	-3.713920000	-1.952594000	-4.763294000
Br	-0.034749000	-2.008979000	-4.208261000
Br	-3.899276000	2.782690000	1.436579000
Br	-1.358190000	5.416712000	1.025797000
Br	1.562772000	3.655004000	-0.477120000
C	9.282197000	0.436915000	-1.187162000
H	9.828328000	0.882723000	-0.348926000
H	9.246206000	-0.648518000	-1.043729000
H	9.838892000	0.642508000	-2.108385000
C	6.395928000	-3.341790000	0.157243000
H	5.799503000	-3.600323000	1.038303000
H	7.043015000	-4.192908000	-0.082003000
H	7.029440000	-2.482239000	0.398363000
H	4.327183000	1.224906000	1.589102000

TS2$_{AZ}$

Electronic energy =	-2145.754498
Zero-point correction =	0.472184
Thermal correction to Energy =	0.528270
Thermal correction to Enthalpy =	0.529215
Thermal correction to Gibbs Free Energy =	0.361737

Ag	2.106438000	-0.177485000	1.198926000
C	3.798082000	-0.610137000	2.553045000
N	-0.418791000	-0.387051000	1.795273000
N	-1.301676000	-0.010648000	0.823902000
N	1.027280000	1.597059000	-0.150908000
N	-0.006589000	1.247018000	-0.972339000
N	1.163867000	-1.494306000	-0.795180000
N	-0.162127000	-1.305612000	-1.060583000
B	-0.898291000	0.006954000	-0.675727000
C	-1.066299000	-0.285596000	2.950393000
C	-2.387747000	0.162317000	2.766383000
C	-2.488885000	0.327109000	1.390434000
C	1.488153000	2.760319000	-0.598301000
C	0.777155000	3.196854000	-1.730397000
C	-0.166820000	2.196092000	-1.930076000
C	1.477367000	-2.690837000	-1.281138000
C	0.364062000	-3.319599000	-1.867914000
C	-0.659660000	-2.394668000	-1.700860000
H	-1.883963000	0.091903000	-1.328939000
C	4.405909000	0.629878000	3.089906000
O	3.945675000	1.110591000	4.116638000
O	5.363204000	1.211541000	2.355733000
C	5.855892000	2.488640000	2.859787000
H	5.006126000	3.169348000	2.959588000
H	6.278759000	2.326605000	3.855608000
Br	-3.994667000	0.928659000	0.429053000
Br	-3.716073000	0.456755000	4.067908000
Br	-0.239560000	-0.723172000	4.591468000
Br	-2.455685000	-2.581600000	-2.240425000
Br	0.273754000	-5.009396000	-2.692628000
Br	3.235871000	-3.372371000	-1.173610000
Br	-1.457096000	2.118139000	-3.300704000
Br	1.029948000	4.768471000	-2.734796000
Br	2.905455000	3.660997000	0.264103000
C	3.801775000	-1.792478000	3.416338000
C	4.653816000	-1.902340000	4.541840000
C	2.961529000	-2.884438000	3.107298000
H	5.305606000	-1.075627000	4.806835000
H	2.304677000	-2.809196000	2.246139000
C	4.646097000	-3.047393000	5.331062000
C	2.967105000	-4.036706000	3.887103000
H	5.296749000	-3.111163000	6.198563000
H	2.313709000	-4.866482000	3.633514000
C	3.807863000	-4.119269000	5.001995000
H	3.808503000	-5.015858000	5.615873000
C	6.893038000	3.012943000	1.889045000
H	7.256528000	3.982194000	2.249006000
H	7.748875000	2.335393000	1.812176000
H	6.470753000	3.158406000	0.889188000
C	7.124315000	-0.343101000	0.232154000
O	5.702464000	0.349769000	-1.491121000
C	5.384662000	1.133596000	-2.680414000
H	5.341266000	2.187332000	-2.388845000
H	6.195999000	1.006759000	-3.401788000
N	6.042024000	-0.866517000	0.721759000
N	5.093498000	-1.369763000	1.146216000
C	6.930840000	0.501488000	-0.986325000
O	7.793139000	1.223944000	-1.447025000
C	8.414020000	-0.605521000	0.899023000
C	8.443894000	-1.144516000	2.201011000
C	9.631995000	-0.358422000	0.236523000
H	7.519930000	-1.337659000	2.737665000
H	9.629966000	0.053911000	-0.763599000
C	9.657600000	-1.428145000	2.820457000
C	10.841656000	-0.642545000	0.869242000
H	9.660017000	-1.841042000	3.825214000
H	11.772112000	-0.446726000	0.343536000
C	10.863451000	-1.178132000	2.158558000
H	11.809481000	-1.397545000	2.645436000
C	4.061851000	0.633243000	-3.219027000
H	3.266473000	0.723017000	-2.472000000
H	3.783268000	1.231493000	-4.093738000
H	4.133367000	-0.414732000	-3.527986000

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Electronic energy =	-2260.514216
Zero-point correction =	0.882027
Thermal correction to Energy =	0.938696
Thermal correction to Enthalpy =	0.939640
Thermal correction to Gibbs Free Energy =	0.782814

Ag	0.741813000	-0.374937000	-0.391957000
C	4.395202000	0.820332000	-0.803148000
N	-1.050557000	-0.798783000	-1.987256000
N	-2.328899000	-0.661271000	-1.529122000
N	-0.600252000	1.628087000	0.048261000
N	-1.934940000	1.510125000	-0.221799000
N	-1.054975000	-1.380588000	1.076548000
N	-2.240421000	-0.704428000	1.022451000
B	-2.652482000	0.128059000	-0.227368000
C	-1.114390000	-1.534422000	-3.090517000
C	-2.439791000	-1.899058000	-3.387093000
C	-3.177857000	-1.319836000	-2.360455000
C	-0.319369000	2.927519000	0.037178000
C	-1.463978000	3.694352000	-0.245706000
C	-2.467847000	2.745724000	-0.404911000

C	-1.037460000	-2.021301000	2.239014000
C	-2.206960000	-1.777827000	2.981742000
C	-2.943820000	-0.929950000	2.162349000
H	-3.822190000	0.313229000	-0.184105000
C	4.029900000	-0.416973000	-0.032520000
O	4.959313000	-0.781971000	0.837889000
O	2.974902000	-1.032303000	-0.184875000
C	4.668994000	-1.929281000	1.698197000
H	4.435329000	-2.783741000	1.057818000
H	3.785679000	-1.685888000	2.294627000
C	4.813472000	1.875387000	-0.076511000
C	5.119538000	3.248239000	-0.571459000
O	4.640516000	4.242102000	-0.050660000
O	5.986634000	3.267044000	-1.587191000
C	6.309873000	4.573801000	-2.142523000
H	6.762811000	5.182108000	-1.353814000
H	5.378769000	5.055721000	-2.455239000
N	8.265408000	0.413330000	1.393876000
N	8.023822000	0.135220000	0.352286000
Br	0.416079000	-3.125734000	2.727560000
Br	-2.676563000	-2.447848000	4.676788000
Br	-4.632320000	-0.180047000	2.532964000
Br	-5.043827000	-1.413748000	-2.117521000
Br	-3.070840000	-2.922913000	-4.834942000
Br	0.446089000	-1.973657000	-4.057751000
Br	-4.275136000	3.072056000	-0.826103000
Br	-1.609813000	5.567179000	-0.373082000
Br	1.431567000	3.557344000	0.356741000
C	7.253191000	4.351335000	-3.305961000
H	8.177350000	3.863456000	-2.977896000
H	6.784742000	3.731925000	-4.078190000
H	7.513922000	5.318313000	-3.750427000
C	5.890610000	-2.173156000	2.557684000
H	6.117590000	-1.302748000	3.182112000
H	5.695184000	-3.026786000	3.216092000
H	6.766775000	-2.406476000	1.944129000
C	4.163019000	0.779139000	-2.269165000
C	3.519686000	1.830799000	-2.943145000
C	4.607144000	-0.330596000	-3.009791000
H	3.136676000	2.678799000	-2.383574000
H	5.105969000	-1.153557000	-2.504085000
C	3.346425000	1.783873000	-4.326614000
C	4.440301000	-0.371110000	-4.393620000
H	2.841942000	2.602712000	-4.832032000
H	4.802521000	-1.228800000	-4.953789000
C	3.811100000	0.686524000	-5.056221000
H	3.676903000	0.652350000	-6.133917000
H	4.862138000	1.790981000	1.005602000

Cu systems with Tp^{Br3} ligand

5

Electronic energy =	-1011.679933
Zero-point correction=	0.107502
Thermal correction to Energy=	0.135916
Thermal correction to Enthalpy=	0.136860
Thermal correction to Gibbs Free Energy=	0.038924

Cu	1.257921000	0.172624000	0.978219000
N	-0.672347000	-0.240718000	1.781673000
N	-1.587737000	-0.334723000	0.767566000
N	0.555478000	1.711628000	-0.281098000
N	-0.591377000	1.321263000	-0.917280000
N	1.068860000	-1.319162000	-0.509431000
N	-0.129254000	-1.188243000	-1.158548000
B	-1.175014000	-0.113385000	-0.721855000
C	-1.321564000	-0.493806000	2.913727000
C	-2.680934000	-0.759416000	2.670400000
C	-2.802466000	-0.646386000	1.289694000
C	0.800583000	2.963311000	-0.653292000
C	-0.183180000	3.428073000	-1.544134000
C	-1.048142000	2.347354000	-1.681155000
C	1.724724000	-2.312012000	-1.101029000
C	0.972846000	-2.857701000	-2.156700000
C	-0.199560000	-2.109187000	-2.154503000
H	-2.136682000	-0.224437000	-1.401428000
Br	-4.370420000	-0.875865000	0.272770000
Br	-4.027998000	-1.167881000	3.919081000
Br	-0.445658000	-0.475372000	4.587568000
Br	-1.665003000	-2.303597000	-3.320293000
Br	1.437308000	-4.271842000	-3.308036000
Br	3.438932000	-2.846554000	-0.517514000
Br	-2.604752000	2.273713000	-2.737157000
Br	-0.307445000	5.116609000	-2.364772000
Br	2.308619000	3.900818000	-0.012911000

7a

Electronic energy =	-1658.675340
Zero-point correction=	0.295329
Thermal correction to Energy=	0.338670
Thermal correction to Enthalpy=	0.339614
Thermal correction to Gibbs Free Energy=	0.207423

Cu	1.712255000	0.117570000	1.183104000
C	3.621776000	-0.159891000	2.282720000
N	-0.308451000	-0.063109000	1.928011000
N	-1.277360000	-0.065617000	0.961060000
N	0.999726000	1.601543000	-0.306299000
N	-0.160806000	1.229423000	-0.930911000
N	1.239704000	-1.435234000	-0.477375000
N	-0.053624000	-1.315847000	-0.907094000
B	-0.916252000	-0.074228000	-0.549048000
C	-0.941419000	-0.030708000	3.100519000
C	-2.336446000	-0.012162000	2.924566000
C	-2.501805000	-0.034382000	1.545518000
C	1.377210000	2.747967000	-0.868825000
C	0.477176000	3.150467000	-1.871126000
C	-0.485867000	2.150110000	-1.874204000
C	1.708843000	-2.559036000	-1.014404000
C	0.733851000	-3.206047000	-1.794643000
C	-0.373645000	-2.373587000	-1.696285000
H	-1.920530000	-0.122575000	-1.172218000
C	3.755283000	1.119880000	3.065488000
O	3.259442000	1.271486000	4.162638000
O	4.503006000	2.034269000	2.425110000
C	4.719508000	3.297888000	3.115059000
H	3.797009000	3.883207000	3.052168000
H	4.922048000	3.087359000	4.167732000
Br	-4.134168000	-0.022619000	0.605623000
Br	-3.674662000	0.035700000	4.246849000
Br	-0.021715000	-0.004947000	4.743216000
Br	-2.056164000	-2.637941000	-2.501106000
Br	0.886869000	-4.815987000	-2.756835000
Br	3.487605000	-3.144032000	-0.758766000
Br	-2.003798000	2.055512000	-2.985096000
Br	0.548735000	4.687132000	-2.954645000
Br	2.935049000	3.675133000	-0.346394000
C	3.622784000	-1.455201000	3.076373000
C	4.649574000	-1.679804000	4.007938000
C	2.630518000	-2.426229000	2.902935000
H	5.427623000	-0.933451000	4.146264000
H	1.831891000	-2.253657000	2.188313000
C	4.670837000	-2.851569000	4.763482000
C	2.655559000	-3.601684000	3.657317000
H	5.465930000	-3.011761000	5.486444000
H	1.876196000	-4.345867000	3.518334000
C	3.672934000	-3.815326000	4.588904000
H	3.688856000	-4.728169000	5.178217000
C	5.886959000	3.994993000	2.447463000
H	6.062964000	4.956347000	2.942624000
H	6.800088000	3.395181000	2.526344000
H	5.691871000	4.188921000	1.387123000
N	4.480496000	-0.198780000	1.226491000
N	5.158881000	-0.249195000	0.328975000

7b

Electronic energy = -1427.630911
Zero-point correction = 0.213886
Thermal correction to Energy = 0.252570
Thermal correction to Enthalpy = 0.253515
Thermal correction to Gibbs Free Energy= 0.131098

Cu	1.574833000	0.023762000	0.845385000
C	3.184639000	-0.075239000	2.267606000
N	-0.436712000	-0.397550000	1.662015000
N	-1.440857000	-0.248568000	0.746187000
N	0.772420000	1.635251000	-0.351222000
N	-0.423747000	1.362478000	-0.954447000
N	1.068031000	-1.309217000	-0.840504000
N	-0.210586000	-1.149631000	-1.298869000
B	-1.125149000	-0.011931000	-0.757298000
C	-1.023316000	-0.634449000	2.831435000
C	-2.424406000	-0.637192000	2.712244000
C	-2.642424000	-0.386426000	1.362584000
C	1.124710000	2.857159000	-0.738702000
C	0.166282000	3.416736000	-1.601628000
C	-0.801528000	2.424722000	-1.710737000
C	1.596897000	-2.313512000	-1.531986000
C	0.677539000	-2.841209000	-2.455746000
C	-0.461311000	-2.066475000	-2.268620000
H	-2.139569000	-0.014260000	-1.366624000
C	3.492072000	1.271583000	2.840711000
O	2.748975000	1.839053000	3.613784000
O	4.668239000	1.744519000	2.402503000
C	5.099122000	3.025961000	2.943673000
H	4.339885000	3.777039000	2.708673000
H	5.165104000	2.935099000	4.031839000
Br	-4.307069000	-0.245821000	0.493402000
Br	-3.707851000	-0.917156000	4.059358000
Br	-0.031491000	-0.950506000	4.407424000
Br	-2.102954000	-2.235596000	-3.175419000
Br	0.926232000	-4.259773000	-3.666416000
Br	3.377119000	-2.879774000	-1.256868000
Br	-2.382429000	2.495771000	-2.731866000
Br	0.188498000	5.110417000	-2.420829000
Br	2.738823000	3.651788000	-0.175174000
C	6.440649000	3.351311000	2.320935000
H	6.793783000	4.314665000	2.705281000
H	7.185561000	2.588069000	2.570045000
H	6.366550000	3.423718000	1.230358000
N	4.243638000	-0.698817000	1.708267000
N	5.115679000	-1.200231000	1.205513000
H	2.636342000	-0.753745000	2.920787000

TS1a

Electronic energy = -1658.658887
Zero-point correction= 0.292302
Thermal correction to Energy= 0.336039
Thermal correction to Enthalpy= 0.336984
Thermal correction to Gibbs Free Energy= 0.203102

Cu	1.605792000	0.193008000	1.260714000
C	3.281044000	0.017943000	2.377357000
N	-0.453190000	-0.066738000	1.867695000
N	-1.402030000	-0.173310000	0.887831000
N	0.926423000	1.494002000	-0.329313000
N	-0.262707000	1.197672000	-0.935006000
N	1.069630000	-1.553042000	-0.443103000
N	-0.156026000	-1.343790000	-1.011263000
B	-1.026273000	-0.118937000	-0.618358000
C	-1.095004000	-0.154171000	3.031551000
C	-2.477205000	-0.324865000	2.838500000
C	-2.624153000	-0.330177000	1.456799000
C	1.342193000	2.645315000	-0.850414000
C	0.435613000	3.130635000	-1.808469000
C	-0.571249000	2.172531000	-1.827508000
C	1.563258000	-2.643988000	-1.019076000
C	0.675577000	-3.178128000	-1.971683000
C	-0.408443000	-2.311057000	-1.931882000
H	-2.023013000	-0.139407000	-1.255437000
C	3.653371000	1.286797000	3.079624000
O	3.040946000	1.612649000	4.080602000
O	4.639557000	2.006940000	2.523412000
C	4.975424000	3.260928000	3.186648000
H	4.151804000	3.964578000	3.031664000
H	5.065744000	3.070245000	4.258954000
Br	-4.233750000	-0.519874000	0.496562000
Br	-3.820260000	-0.506042000	4.143753000
Br	-0.197545000	-0.036497000	4.682497000
Br	-1.978946000	-2.421723000	-2.968338000
Br	0.897810000	-4.706579000	-3.047800000
Br	3.265420000	-3.340145000	-0.576760000
Br	-2.119597000	2.187955000	-2.899176000
Br	0.550554000	4.706048000	-2.830572000
Br	2.963906000	3.446733000	-0.319800000
C	3.512403000	-1.228187000	3.159964000
C	4.570101000	-1.338648000	4.086584000
C	2.639009000	-2.316584000	2.993921000
H	5.261459000	-0.510580000	4.221318000
H	1.823606000	-2.227961000	2.282877000
C	4.742133000	-2.504493000	4.826160000
C	2.806563000	-3.481808000	3.741649000
H	5.560552000	-2.579920000	5.536512000
H	2.118875000	-4.312370000	3.610816000
C	3.857836000	-3.576786000	4.656138000
H	3.991282000	-4.485271000	5.237341000
C	6.276199000	3.760918000	2.592980000
H	6.549945000	4.705967000	3.075050000
H	7.086193000	3.042955000	2.760626000
H	6.187915000	3.940615000	1.516142000
N	4.515744000	-0.071952000	1.106975000
N	5.037848000	-0.289958000	0.152388000

TS1b

Electronic energy = -1427.603423
Zero-point correction= 0.211111
Thermal correction to Energy= 0.250257
Thermal correction to Enthalpy= 0.251201
Thermal correction to Gibbs Free Energy= 0.126476

Cu	1.570254000	0.219971000	1.162771000
C	3.270576000	0.096871000	2.076363000
N	-0.432660000	-0.015160000	1.789121000
N	-1.410659000	-0.093760000	0.837115000
N	0.862827000	1.528173000	-0.441408000
N	-0.302751000	1.182922000	-1.064665000
N	1.058333000	-1.492647000	-0.404076000
N	-0.167331000	-1.355142000	-0.989793000
B	-1.056778000	-0.119978000	-0.678184000
C	-1.039450000	-0.073592000	2.972924000
C	-2.432252000	-0.186938000	2.821347000
C	-2.619780000	-0.196260000	1.443423000
C	1.269675000	2.666458000	-0.995932000
C	0.379829000	3.093172000	-1.997264000
C	-0.607121000	2.113861000	-2.003712000
C	1.568870000	-2.628621000	-0.862524000
C	0.691849000	-3.265581000	-1.760044000
C	-0.404611000	-2.412616000	-1.808307000
H	-2.057553000	-0.190730000	-1.305883000
C	3.806915000	1.111543000	3.013937000
O	3.399409000	1.055269000	4.162944000
O	4.631076000	2.033712000	2.521647000
C	5.092249000	3.057913000	3.456480000
H	4.238153000	3.692774000	3.710447000
H	5.442694000	2.563871000	4.366192000
Br	-4.259756000	-0.323923000	0.527416000
Br	-3.742465000	-0.301158000	4.166147000

Br	-0.066773000	-0.013597000	4.583723000
Br	-1.974437000	-2.641467000	-2.824336000
Br	0.938374000	-4.888702000	-2.680074000
Br	3.276419000	-3.241305000	-0.327895000
Br	-2.130395000	2.051658000	-3.108348000
Br	0.488160000	4.631180000	-3.075041000
Br	2.853104000	3.529265000	-0.442416000
C	6.196392000	3.834762000	2.771853000
H	6.560265000	4.614858000	3.449663000
H	7.038010000	3.181812000	2.516984000
H	5.836513000	4.318028000	1.857329000
N	4.552761000	0.171437000	0.620154000
N	5.006707000	0.298027000	-0.380354000
H	3.608868000	-0.901899000	2.365051000

8a

Electronic energy =	-1318.094575
Zero-point correction =	0.203742
Thermal correction to Energy =	0.240247
Thermal correction to Enthalpy =	0.241191
Thermal correction to Gibbs Free Energy =	0.123713

Cu	1.392321000	0.156373000	1.511960000
C	2.820478000	0.108687000	2.804977000
N	-0.730276000	-0.390073000	1.816207000
N	-1.536242000	-0.430892000	0.714080000
N	0.433660000	1.840867000	0.258943000
N	-0.500895000	1.434487000	-0.651570000
N	1.366563000	-0.940272000	-0.345517000
N	0.207880000	-0.965934000	-1.067886000
B	-0.982326000	-0.042154000	-0.684996000
C	-1.498954000	-0.681902000	2.862089000
C	-2.826787000	-0.925483000	2.466798000
C	-2.800814000	-0.750803000	1.087869000
C	0.595466000	3.146517000	0.076266000
C	-0.222907000	3.626673000	-0.962906000
C	-0.904513000	2.495881000	-1.395794000
C	2.222048000	-1.751543000	-0.962943000
C	1.637042000	-2.334670000	-2.100901000
C	0.352873000	-1.801455000	-2.126398000
H	-1.839934000	-0.160429000	-1.492262000
C	3.634440000	1.326334000	3.002151000
O	3.386832000	2.121070000	3.896094000
O	4.610110000	1.460831000	2.096867000
C	5.472797000	2.628009000	2.224819000
H	4.856292000	3.529153000	2.168548000
H	5.949370000	2.599860000	3.209435000
Br	-4.251604000	-0.918565000	-0.101353000
Br	-4.299530000	-1.382095000	3.545287000
Br	-0.822007000	-0.725912000	4.623189000
Br	-0.994635000	-2.152675000	-3.393721000
Br	2.408969000	-3.550104000	-3.311931000
Br	3.984425000	-2.004103000	-0.343974000
Br	-2.180225000	2.401782000	-2.778788000
Br	-0.368646000	5.386377000	-1.613263000
Br	1.772410000	4.159182000	1.147098000
C	3.181683000	-1.026672000	3.595711000
C	4.275769000	-1.022285000	4.510456000
C	2.441057000	-2.232939000	3.445474000
H	4.850749000	-0.113325000	4.657872000
H	1.603767000	-2.237208000	2.754958000
C	4.603924000	-2.161885000	5.227415000
C	2.779946000	-3.374292000	4.155893000
H	5.435881000	-2.147681000	5.924946000
H	2.211098000	-4.289965000	4.026907000
C	3.860483000	-3.337821000	5.047218000
H	4.124350000	-4.230061000	5.608565000
C	6.488297000	2.566539000	1.103063000
H	7.166056000	3.424168000	1.179393000
H	7.085845000	1.650504000	1.162192000
H	5.997512000	2.602105000	0.124618000

8b

Electronic energy =	-1549.176019
Zero-point correction =	0.285206
Thermal correction to Energy =	0.326854
Thermal correction to Enthalpy =	0.327799
Thermal correction to Gibbs Free Energy =	0.196120

Cu	1.626832000	0.050799000	0.984249000
C	2.909748000	0.016632000	2.335107000
N	-0.678418000	-0.297107000	1.763736000
N	-1.586757000	-0.316877000	0.745808000
N	0.729677000	1.548065000	-0.182621000
N	-0.421461000	1.268796000	-0.862142000
N	1.080806000	-1.371201000	-0.435981000
N	-0.105293000	-1.240229000	-1.099433000
B	-1.115902000	-0.116116000	-0.717490000
C	-1.360953000	-0.505152000	2.881344000
C	-2.736540000	-0.666635000	2.625273000
C	-2.830891000	-0.537922000	1.244656000
C	1.074252000	2.796067000	-0.493779000
C	0.149094000	3.364236000	-1.385892000
C	-0.785143000	2.353480000	-1.589962000
C	1.694928000	-2.441677000	-0.936776000
C	0.920487000	-3.035893000	-1.947214000
C	-0.216326000	-2.235382000	-2.013576000
H	-2.046571000	-0.165974000	-1.446893000
H	2.632491000	-0.281926000	3.353895000
C	4.297558000	0.464702000	2.308344000
O	4.453126000	1.611157000	2.714515000
O	5.225291000	-0.344866000	1.831807000
C	6.598488000	0.169746000	1.807030000
H	6.608507000	1.082930000	1.206364000
H	6.886658000	0.419328000	2.832023000
Br	-4.391821000	-0.640909000	0.195032000
Br	-4.124959000	-0.982140000	3.856173000
Br	-0.505659000	-0.564375000	4.566975000
Br	-1.686886000	-2.453854000	-3.166722000
Br	1.323316000	-4.556670000	-2.977288000
Br	3.375453000	-3.003492000	-0.299599000
Br	-2.314485000	2.428982000	-2.68336900
Br	0.169609000	5.087952000	-2.137265000
Br	2.621690000	3.597562000	0.217492000
C	7.475362000	-0.911777000	1.215271000
H	7.438892000	-1.825254000	1.818122000
H	7.170509000	-1.151823000	0.191223000
H	8.511846000	-0.557400000	1.191113000

$TS2_{CC}$

Electronic energy =	-1965.101404
Zero-point correction =	0.391923
Thermal correction to Energy =	0.442495
Thermal correction to Enthalpy =	0.443440
Thermal correction to Gibbs Free Energy =	0.295046

Cu	1.062892000	-0.897217000	-0.702242000
C	2.934390000	-0.995825000	-1.307409000
N	-0.764054000	-0.744340000	-1.898752000
N	-1.861263000	-0.212607000	-1.277988000
N	0.393784000	2.150265000	0.322098000
N	-0.742199000	1.934881000	-0.403659000
N	-0.189208000	-0.977910000	1.012757000
N	-1.175542000	-0.039732000	1.151215000
B	-1.708569000	0.753729000	-0.070593000
C	-1.222262000	-1.534756000	-2.868015000
C	-2.627636000	-1.545464000	-2.896904000
C	-2.988861000	-0.693022000	-1.859814000
C	0.839601000	3.346125000	-0.044059000
C	0.021615000	3.940825000	-1.023628000
C	-0.982298000	2.999470000	-1.212838000
C	-0.099862000	-1.609700000	2.183330000
C	-1.004239000	-1.080403000	3.119226000

C	-1.666720000	-0.082513000	2.413352000
H	-2.785933000	1.185346000	0.192253000
C	3.583923000	-2.264684000	-0.888032000
O	4.298751000	-2.236939000	0.245710000
O	3.379635000	-3.280880000	-1.538578000
C	4.829086000	-3.513449000	0.703431000
H	5.535408000	-3.883944000	-0.045826000
H	4.006410000	-4.230513000	0.775904000
C	3.839303000	0.626560000	0.100440000
C	5.303265000	0.768889000	-0.091195000
O	5.768920000	1.255140000	-1.103386000
O	6.011404000	0.316032000	0.952608000
C	7.459455000	0.449521000	0.855022000
H	7.690812000	1.457639000	0.501490000
H	7.818234000	-0.268360000	0.110804000
N	3.418240000	0.265148000	1.314665000
N	3.044775000	-0.126982000	2.301051000
Br	1.055580000	-3.075564000	2.451917000
Br	-1.273895000	-1.606057000	4.904736000
Br	-3.015009000	1.058607000	3.063043000
Br	-4.739889000	-0.262498000	-1.316802000
Br	-3.761792000	-2.484391000	-4.068635000
Br	-0.067414000	-2.483056000	-4.018434000
Br	-2.471532000	3.121920000	-2.360067000
Br	0.217119000	5.611793000	-1.869227000
Br	2.381009000	4.103805000	0.760546000
C	8.041314000	0.185228000	2.227906000
H	7.666098000	0.908519000	2.959802000
H	7.801179000	-0.824314000	2.577537000
H	9.131890000	0.280384000	2.178574000
C	5.500142000	-3.277441000	2.040355000
H	4.787951000	-2.895814000	2.779837000
H	5.908338000	-4.223962000	2.411935000
H	6.320936000	-2.559503000	1.946840000
C	3.393952000	-0.416431000	-2.563437000
C	2.626275000	0.599363000	-3.182561000
C	4.579579000	-0.841284000	-3.212841000
H	1.714138000	0.933318000	-2.697351000
H	5.192823000	-1.614880000	-2.761569000
C	3.015781000	1.156114000	-4.394262000
C	4.956447000	-0.300396000	-4.437123000
H	2.412602000	1.933081000	-4.855071000
H	5.859674000	-0.650093000	-4.928741000
C	4.179176000	0.701635000	-5.027739000
H	4.478736000	1.127799000	-5.981387000
H	3.195371000	1.357305000	-0.368024000

TS2$_{HC}$

Electronic energy =	-2196.142971
Zero-point correction=	0.472824
Thermal correction to Energy=	0.527947
Thermal correction to Enthalpy=	0.528891
Thermal correction to Gibbs Free Energy=	0.369915

Cu	1.314163000	1.227364000	-0.391952000
C	3.071202000	0.460895000	-0.901936000
N	-0.821303000	-0.288150000	-2.287588000
N	-1.589928000	-0.699068000	-1.239488000
N	-0.428288000	2.292888000	-0.323548000
N	-1.670020000	1.749650000	-0.538260000
N	-0.375999000	-0.920955000	1.369307000
N	-1.438109000	-0.076104000	1.245191000
B	-2.048209000	0.288422000	-0.138714000
C	-0.739823000	-1.323279000	-3.111829000
C	-1.451589000	-2.438402000	-2.627531000
C	-1.983761000	-1.983404000	-1.427804000
C	-0.532182000	3.597116000	-0.607233000
C	-1.824107000	3.924750000	-1.037968000
C	-2.508881000	2.715775000	-0.981544000
C	-0.232707000	-1.142010000	2.668646000
C	-1.186145000	-0.440322000	3.432640000
C	-1.937343000	0.224240000	2.472955000
H	-3.237222000	0.248782000	-0.035911000
C	3.146246000	-0.998728000	-0.587317000
O	3.964941000	-1.397577000	0.395082000
O	2.438314000	-1.762202000	-1.225688000
C	4.012129000	-2.836225000	0.637343000
H	4.205867000	-3.338123000	-0.314497000
H	3.031983000	-3.155744000	0.99885300
C	4.581623000	1.426683000	0.447855000
C	4.702500000	2.827778000	-0.122455000
O	3.994385000	3.742523000	0.233984000
O	5.672445000	2.905481000	-1.035810000
C	5.901583000	4.215347000	-1.642266000
H	6.041585000	4.941400000	-0.837139000
H	5.007339000	4.487390000	-2.208791000
N	5.652756000	0.677966000	0.085242000
N	6.480297000	0.034384000	-0.321669000
Br	1.086740000	-2.330025000	3.328017000
Br	-1.416563000	-0.417333000	5.302469000
Br	-3.402232000	1.377254000	2.758499000
Br	-3.101401000	-2.912803000	-0.227212000
Br	-1.658714000	-4.139092000	-3.411389000
Br	0.197334000	-1.191192000	-4.753365000
Br	-4.304113000	2.430306000	-1.468698000
Br	-2.486887000	5.607443000	-1.553282000
Br	0.911795000	4.782891000	-0.390244000
C	7.125167000	4.097649000	-2.524753000
H	8.007982000	3.816449000	-1.940761000
H	6.974109000	3.355987000	-3.315914000
H	7.319281000	5.067825000	-2.995518000
C	5.109081000	-3.103861000	1.646675000
H	4.908540000	-2.603743000	2.599566000
H	5.167054000	-4.182471000	1.831891000
H	6.082762000	-2.769791000	1.271255000
C	3.572785000	0.800154000	-2.241930000
C	3.141027000	1.993910000	-2.867596000
C	4.463592000	-0.035979000	-2.961426000
H	2.458792000	2.646158000	-2.330340000
H	4.803173000	-0.970787000	-2.525806000
C	3.559616000	2.329542000	-4.150602000
C	4.886543000	0.303012000	-4.243446000
H	3.199313000	3.242257000	-4.616603000
H	5.559924000	-0.357705000	-4.782059000
C	4.434917000	1.483770000	-4.842185000
H	4.756729000	1.740545000	-5.847770000
C	4.170851000	1.288369000	1.884610000
C	4.984666000	0.622515000	2.813447000
C	2.979501000	1.885930000	2.322216000
H	5.921298000	0.169352000	2.502121000
H	2.351225000	2.417706000	1.618728000
C	4.609765000	0.550586000	4.155002000
C	2.615096000	1.816660000	3.667559000
H	5.254000000	0.034402000	4.861370000
H	1.691821000	2.288457000	3.992301000
C	3.424435000	1.148102000	4.588137000
H	3.135670000	1.095861000	5.634095000

TS2$_{CC'}$

Electronic energy =	-1965.087112
Zero-point correction =	0.391307
Thermal correction to Energy =	0.441971
Thermal correction to Enthalpy =	0.442915
Thermal correction to Gibbs Free Energy =	0.293263

Cu	1.278503000	1.165976000	0.035923000
C	3.169654000	0.843119000	0.078526000
N	0.372402000	0.203248000	-1.731136000
N	-0.956100000	-0.105163000	-1.658732000
N	-0.460486000	2.428456000	0.009604000
N	-1.676303000	1.831466000	-0.188942000
N	-0.079733000	-0.231042000	1.352420000
N	-1.325969000	-0.458892000	0.844735000
B	-1.803797000	0.297503000	-0.419553000

C	0.798669000	-0.216177000	-2.919259000
C	-0.242094000	-0.816402000	-3.650103000
C	-1.341196000	-0.721156000	-2.804675000
C	-0.691566000	3.735393000	0.127364000
C	-2.062906000	4.021236000	0.017817000
C	-2.648691000	2.777177000	-0.184127000
C	0.007647000	-0.944348000	2.469251000
C	-1.177173000	-1.662953000	2.715825000
C	-2.000109000	-1.318720000	1.650559000
H	-2.937987000	0.032315000	-0.627854000
C	3.675883000	-0.469255000	0.519580000
O	4.539846000	-0.545348000	1.527175000
O	3.236833000	-1.428024000	-0.103285000
C	5.035619000	-1.884022000	1.847003000
H	5.518819000	-2.289882000	0.953715000
H	4.181169000	-2.518160000	2.095840000
C	4.845323000	2.520936000	1.134662000
C	4.516207000	3.639048000	0.201237000
O	3.920379000	4.641083000	0.537414000
O	4.966285000	3.388249000	-1.039285000
C	4.755908000	4.436995000	-2.030856000
H	5.161885000	5.371430000	-1.633663000
H	3.678754000	4.560038000	-2.174663000
N	5.878593000	1.784086000	0.728347000
N	6.735837000	1.133447000	0.381029000
Br	1.550526000	-0.909289000	3.553659000
Br	-1.563910000	-2.818220000	4.150448000
Br	-3.758203000	-1.917396000	1.334334000
Br	-3.088880000	-1.330431000	-3.150989000
Br	-0.173018000	-1.570619000	-5.372577000
Br	2.575634000	0.028430000	-3.503936000
Br	-4.482764000	2.419597000	-0.415482000
Br	-2.911800000	5.697011000	0.118892000
Br	0.711563000	4.963737000	0.371627000
C	5.456535000	4.007524000	-3.302073000
H	6.529897000	3.869785000	-3.133410000
H	5.038835000	3.072444000	-3.690604000
H	5.325415000	4.783785000	-4.064100000
C	6.003974000	-1.754492000	3.002892000
H	5.516087000	-1.332999000	3.887869000
H	6.382582000	-2.749734000	3.261603000
H	6.858247000	-1.122733000	2.736703000
C	4.598150000	2.599525000	2.598794000
C	3.363584000	3.079592000	3.064609000
C	5.576381000	2.209949000	3.527362000
H	2.599753000	3.378109000	2.357224000
H	6.543980000	1.849644000	3.189365000
C	3.121589000	3.172457000	4.434592000
C	5.322346000	2.295767000	4.896554000
H	2.162142000	3.547425000	4.780631000
H	6.091147000	1.991714000	5.601596000
C	4.095490000	2.779266000	5.356294000
H	3.899318000	2.848770000	6.422689000
H	3.731920000	1.164052000	-0.804148000

$TS2_{HC'}$

Electronic energy =	-1734.036195
Zero-point correction =	0.309411
Thermal correction to Energy =	0.355952
Thermal correction to Enthalpy =	0.356896
Thermal correction to Gibbs Free Energy =	0.212331

Cu	1.166704000	0.881978000	-0.079797000
C	3.044422000	0.595605000	-0.081574000
N	0.152476000	-0.012683000	-1.799677000
N	-1.193663000	-0.221662000	-1.705084000
N	-0.473474000	2.201656000	0.056199000
N	-1.734188000	1.720515000	-0.161828000
N	-0.233040000	-0.464135000	1.268709000
N	-1.505010000	-0.612228000	0.796606000
B	-1.978227000	0.206316000	-0.433098000
C	0.524329000	-0.443232000	-3.002724000
C	-0.572292000	-0.951260000	-3.721029000
C	-1.645018000	-0.788365000	-2.851648000
C	-0.587361000	3.508291000	0.283903000
C	-1.931579000	3.913233000	0.219806000
C	-2.623173000	2.740479000	-0.065704000
C	-0.161248000	-1.175098000	2.387071000
C	-1.380389000	-1.820212000	2.667851000
C	-2.208705000	-1.427538000	1.623474000
H	-3.134030000	0.021220000	-0.609298000
C	3.653074000	-0.600868000	0.520339000
O	4.431937000	-0.465365000	1.590084000
O	3.365309000	-1.660832000	-0.019735000
C	5.079920000	-1.682103000	2.082126000
H	5.638151000	-2.129043000	1.254863000
H	4.303813000	-2.384859000	2.395599000
C	4.823497000	2.443115000	0.780195000
C	4.644534000	3.671254000	-0.015521000
O	4.025331000	4.639745000	0.382935000
O	5.242440000	3.574438000	-1.215226000
C	5.168154000	4.746007000	-2.076447000
H	5.634207000	5.588071000	-1.555984000
H	4.114310000	4.984438000	-2.245787000
N	5.855110000	1.675676000	0.480563000
N	6.715760000	1.000831000	0.189880000
Br	1.405114000	-1.210551000	3.439690000
Br	-1.800405000	-2.944947000	4.116910000
Br	-4.006493000	-1.920491000	1.352998000
Br	-3.438183000	-1.266258000	-3.168024000
Br	-0.593071000	-1.682985000	-5.454101000
Br	2.306219000	-0.328370000	-3.612702000
Br	-4.482374000	2.550891000	-0.293818000
Br	-2.633616000	5.642483000	0.456826000
Br	0.938679000	4.555036000	0.612802000
C	5.887675000	4.404692000	-3.364379000
H	6.938041000	4.157745000	-3.176216000
H	5.412295000	3.556776000	-3.869416000
H	5.853351000	5.267933000	-4.038166000
C	5.987091000	-1.282319000	3.226235000
H	5.419893000	-0.824579000	4.043783000
H	6.487885000	-2.176110000	3.614419000
H	6.755806000	-0.576635000	2.893250000
H	3.601241000	0.883111000	-0.978294000
H	4.466534000	2.376197000	1.799228000

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Electronic energy =	-1734.189323
Zero-point correction =	0.311915
Thermal correction to Energy =	0.358256
Thermal correction to Enthalpy =	0.359200
Thermal correction to Gibbs Free Energy =	0.220331

Cu	0.784877000	0.499203000	0.246581000
C	2.655184000	1.646353000	0.576995000
N	0.300712000	-0.567982000	-1.576355000
N	-1.040613000	-0.782846000	-1.753115000
N	-0.903139000	1.930548000	-0.519783000
N	-2.082102000	1.249474000	-0.642347000
N	-0.553546000	-0.804757000	1.250646000
N	-1.783253000	-0.944885000	0.668671000
B	-2.094899000	-0.301313000	-0.711231000
C	0.914425000	-1.097535000	-2.632741000
C	-0.009124000	-1.667589000	-3.525762000
C	-1.240449000	-1.441919000	-2.922363000
C	-1.189872000	3.214735000	-0.709785000
C	-2.565160000	3.408156000	-0.936230000
C	-3.092320000	2.123959000	-0.886598000
C	-0.559088000	-1.563727000	2.345901000
C	-1.797461000	-2.207531000	2.509300000
C	-2.543011000	-1.784405000	1.415419000
H	-3.167625000	-0.657070000	-1.060119000
C	3.837478000	0.888711000	0.068751000
O	4.065413000	-0.250729000	0.739637000

O	4.545813000	1.318474000	-0.822513000
C	5.276529000	-0.976217000	0.389879000
H	6.119138000	-0.280539000	0.427512000
H	5.177452000	-1.338085000	-0.637859000
C	2.044199000	1.366065000	1.772382000
C	1.195502000	2.325271000	2.555244000
O	0.304149000	1.970406000	3.303024000
O	1.592123000	3.592587000	2.388492000
C	0.890833000	4.599347000	3.173762000
H	0.844990000	4.255287000	4.210590000
H	-0.132099000	4.681183000	2.793958000
N	4.930422000	2.273587000	3.402048000
N	5.590486000	1.432737000	3.122715000
Br	0.944766000	-1.768114000	3.464203000
Br	-2.326454000	-3.380583000	3.880480000
Br	-4.311267000	-2.276922000	1.002827000
Br	-2.928011000	-1.947013000	-3.585759000
Br	0.336822000	-2.535197000	-5.158075000
Br	2.786372000	-1.045278000	-2.837828000
Br	-4.897433000	1.632650000	-1.100921000
Br	-3.479013000	5.022532000	-1.249842000
Br	0.142316000	4.555254000	-0.747227000
C	1.655635000	5.899490000	3.041915000
H	2.676259000	5.796116000	3.425609000
H	1.706018000	6.230066000	1.999098000
H	1.146956000	6.676834000	3.622936000
C	5.434268000	-2.114253000	1.375258000
H	4.579574000	-2.798137000	1.333500000
H	6.338946000	-2.681190000	1.128167000
H	5.534165000	-1.736770000	2.398652000
H	2.492303000	2.594824000	0.075414000
H	2.328663000	0.476944000	2.326187000

Ag systems with IPr ligand

IPrAgCl

Electronic energy = -1767.346662
Zero-point correction= 0.597378
Thermal correction to Energy = 0.632526
Thermal correction to Enthalpy = 0.633471
Thermal correction to Gibbs Free Energy = 0.528103

Ag	1.614490000	2.591432000	10.294132000
Cl	-0.738523000	3.120799000	10.125837000
C	3.685569000	2.124983000	10.444482000
N	4.313393000	1.711948000	11.555503000
C	5.769702000	1.504713000	11.356886000
H	6.040792000	0.475415000	11.608382000
H	6.333962000	2.180955000	12.006368000
C	5.950077000	1.823071000	9.860743000
H	6.645700000	2.647690000	9.681315000
H	6.280440000	0.956903000	9.279406000
N	4.578920000	2.214735000	9.447829000
C	3.693066000	1.497976000	12.836017000
C	3.619337000	2.570898000	13.752827000
C	3.010778000	2.334284000	14.992957000
H	2.932334000	3.145820000	15.711289000
C	2.507877000	1.077140000	15.319984000
H	2.037690000	0.914570000	16.286467000
C	2.610532000	0.026952000	14.410476000
H	2.221235000	-0.951713000	14.677013000
C	3.207716000	0.209947000	13.155990000
C	4.175279000	3.957628000	13.442211000
H	4.618140000	3.927975000	12.442546000
C	5.291484000	4.354388000	14.427764000
H	5.722024000	5.322049000	14.142812000
H	6.100109000	3.614099000	14.439463000
H	4.910609000	4.448810000	15.451605000
C	3.062798000	5.023158000	13.415726000
H	3.478703000	6.001190000	13.144112000
H	2.579913000	5.126021000	14.394895000
H	2.286603000	4.770210000	12.683710000
C	3.308558000	-0.969291000	12.191928000
H	3.833954000	-0.627971000	11.295056000
C	4.129951000	-2.125730000	12.794098000
H	4.250913000	-2.929513000	12.057595000
H	3.637420000	-2.555247000	13.674739000
H	5.129600000	-1.794378000	13.099494000
C	1.916902000	-1.459146000	11.746797000
H	2.014393000	-2.270749000	11.015092000
H	1.339026000	-0.652348000	11.280745000
H	1.336213000	-1.842184000	12.594460000
C	4.286925000	2.602084000	8.093261000
C	3.912867000	1.609234000	7.159934000
C	3.640162000	2.013302000	5.846059000
H	3.341360000	1.269758000	5.112267000
C	3.744373000	3.349648000	5.467032000
C	4.132049000	4.310359000	6.398402000
H	4.212335000	5.349849000	6.092687000
C	4.415646000	3.960450000	7.725367000
C	3.804320000	0.132437000	7.527875000
H	4.071253000	0.026054000	8.583475000
C	4.792526000	-0.725932000	6.714060000
C	2.363734000	-0.388923000	7.364040000
H	1.657260000	0.191316000	7.969175000
H	2.034019000	-0.335064000	6.319626000
H	2.299846000	-1.437282000	7.680608000
H	4.555795000	-0.705928000	5.643513000
H	4.749807000	-1.771006000	7.044405000
H	5.824595000	-0.375329000	6.833739000
C	4.840613000	5.042881000	8.713862000
H	5.050853000	4.559662000	9.672530000
C	3.711067000	6.063966000	8.952400000
C	6.132718000	5.752112000	8.264406000
H	6.951363000	5.039020000	8.110195000
H	5.987286000	6.302075000	7.326911000
H	6.452467000	6.474075000	9.025705000
H	3.453834000	6.599947000	8.030922000
H	4.020840000	6.807929000	9.696658000
H	2.801252000	5.575727000	9.320785000
H	3.525944000	3.642490000	4.443247000

IPrAgBPh$_4$

Electronic energy = -2258.550615
Zero-point correction = 0.965301
Thermal correction to Energy = 1.020327
Thermal correction to Enthalpy = 1.021271
Thermal correction to Gibbs Free Energy = 0.871604

Ag	-2.079227000	5.703863000	11.046154000
C	-0.732788000	6.954929000	12.145410000
N	-0.652215000	7.025338000	13.485641000
C	0.194269000	8.148509000	13.952825000
H	0.931993000	7.798667000	14.680119000
H	-0.431059000	8.906203000	14.437780000
C	0.823761000	8.650944000	12.645448000
H	0.717385000	9.729372000	12.507536000
H	1.887860000	8.399369000	12.560218000
N	0.052391000	7.912623000	11.616138000
C	-1.259528000	6.120781000	14.430526000
C	-2.552646000	6.388569000	14.932682000
C	-3.080196000	5.498835000	15.876746000
H	-4.074710000	5.672859000	16.274339000
C	-2.356619000	4.395048000	16.315540000
H	-2.791324000	3.715820000	17.043683000
C	-1.078921000	4.158624000	15.819556000
H	-0.521374000	3.294826000	16.169926000
C	-0.499498000	5.015982000	14.877496000
C	-3.356395000	7.623458000	14.534467000
H	-2.899401000	8.050551000	13.635749000
C	-3.294808000	8.691014000	15.647756000
H	-3.814250000	9.604480000	15.334066000
H	-2.264634000	8.960962000	15.909015000
H	-3.777815000	8.331334000	16.564316000

C	-4.821772000	7.301524000	14.192310000
H	-5.336308000	8.210525000	13.861258000
H	-5.372917000	6.922455000	15.060488000
H	-4.898957000	6.557820000	13.395344000
C	0.926251000	4.744915000	14.403297000
H	1.209504000	5.539325000	13.706129000
C	1.925544000	4.787484000	15.576268000
H	2.953469000	4.684722000	15.208022000
H	1.748875000	3.972836000	16.287914000
H	1.859014000	5.729289000	16.133824000
C	1.042306000	3.415384000	13.635552000
H	2.079235000	3.246528000	13.320042000
H	0.413451000	3.414614000	12.740110000
H	0.746016000	2.562558000	14.256780000
C	0.389410000	8.072732000	10.222771000
C	1.323523000	7.189455000	9.633786000
C	1.677163000	7.407486000	8.296669000
H	2.378186000	6.732637000	7.814398000
C	1.152472000	8.474398000	7.575685000
C	0.246140000	9.340649000	8.178471000
H	-0.161531000	10.167260000	7.604588000
C	-0.159733000	9.159887000	9.505884000
C	1.965341000	6.026708000	10.386146000
H	1.637921000	6.070255000	11.428881000
C	3.503083000	6.126075000	10.389984000
C	1.503440000	4.668695000	9.826269000
H	0.417764000	4.556912000	9.912349000
H	1.769793000	4.557295000	8.769121000
H	1.972454000	3.844093000	10.375633000
H	3.922960000	6.014242000	9.383911000
H	3.933853000	5.332564000	11.012328000
H	3.848001000	7.089004000	10.784885000
C	-1.151324000	10.141901000	10.123098000
H	-1.465868000	9.738270000	11.091090000
C	-2.419063000	10.311072000	9.265138000
C	-0.494040000	11.515312000	10.370595000
H	0.405033000	11.439712000	10.993747000
H	-0.193394000	11.984324000	9.426012000
H	-1.195049000	12.194964000	10.869870000
H	-2.201109000	10.799546000	8.308453000
H	-3.147629000	10.940789000	9.788665000
H	-2.893334000	9.351141000	9.045029000
H	1.443846000	8.626433000	6.540056000
C	-2.859033000	4.914521000	8.871314000
B	-4.154855000	4.717799000	9.910361000
C	-2.595681000	6.142523000	8.228017000
H	-3.207850000	7.011802000	8.394330000
C	-1.565141000	6.254078000	7.291686000
H	-1.379300000	7.202723000	6.806090000
C	-0.798100000	5.140291000	6.955223000
H	-0.001638000	5.230197000	6.228006000
C	-1.083547000	3.903065000	7.529511000
H	-0.513220000	3.029658000	7.240992000
C	-2.116644000	3.785348000	8.462675000
H	-2.356278000	2.799644000	8.839717000
C	-5.098431000	3.706417000	9.018855000
C	-5.406037000	2.385307000	9.415277000
H	-5.035789000	1.965609000	10.338837000
C	-6.194362000	1.563940000	8.604528000
H	-6.424970000	0.554683000	8.920871000
C	-6.679431000	2.036055000	7.385398000
H	-7.288423000	1.395849000	6.760289000
C	-6.372898000	3.330460000	6.968601000
H	-6.744080000	3.694355000	6.019172000
C	-5.585672000	4.157638000	7.772585000
H	-5.361112000	5.158115000	7.423315000
C	-5.007495000	6.118514000	10.214429000
C	-4.383916000	7.313023000	10.643901000
H	-3.318580000	7.407378000	10.726538000
C	-5.133554000	8.454836000	10.939292000
H	-4.634503000	9.360769000	11.257761000
C	-6.521330000	8.429517000	10.839344000
H	-7.098555000	9.314067000	11.075617000
C	-7.165091000	7.259285000	10.448674000
H	-8.245678000	7.232796000	10.390225000
C	-6.422410000	6.115198000	10.147619000
H	-6.974352000	5.220925000	9.894872000
C	-3.848148000	3.966544000	11.372233000
C	-4.882209000	3.913865000	12.332666000
H	-5.832065000	4.397291000	12.156467000
C	-4.722392000	3.206892000	13.526213000
H	-5.525828000	3.180873000	14.251024000
C	-3.539239000	2.516870000	13.776974000
H	-3.422018000	1.957887000	14.696224000
C	-2.505932000	2.548777000	12.843604000
H	-1.590279000	2.008110000	13.041125000
C	-2.652020000	3.267474000	11.653593000
H	-1.815407000	3.276546000	10.976116000

5

Electronic energy = -2258.55061510

Zero-point correction =	0.965301
Thermal correction to Energy =	1.020327
Thermal correction to Enthalpy =	1.021271
Thermal correction to Gibbs Free Energy =	0.871604

Ag	1.624738000	2.626934000	10.294258000
C	3.700262000	2.119665000	10.444086000
N	4.313771000	1.688774000	11.551794000
C	5.771500000	1.478829000	11.350611000
H	6.040389000	0.450928000	11.607372000
H	6.334058000	2.159418000	11.996611000
C	5.950285000	1.789873000	9.851611000
H	6.661767000	2.598533000	9.665466000
H	6.254333000	0.915099000	9.269319000
N	4.584283000	2.211905000	9.444388000
C	3.684970000	1.485717000	12.830432000
C	3.591791000	2.571028000	13.731107000
C	2.964895000	2.347315000	14.964617000
H	2.871738000	3.167797000	15.670833000
C	2.467760000	1.090444000	15.301830000
H	1.985673000	0.937171000	16.263833000
C	2.595143000	0.027510000	14.410271000
H	2.215006000	-0.951724000	14.687050000
C	3.210626000	0.196657000	13.162656000
C	4.148426000	3.955487000	13.412863000
H	4.616034000	3.913996000	12.425009000
C	5.241023000	4.370860000	14.417199000
H	5.674292000	5.335457000	14.126670000
H	6.051063000	3.633429000	14.456290000
H	4.838136000	4.478946000	15.430954000
C	3.032651000	5.015740000	13.347500000
H	3.450067000	5.992608000	13.075056000
H	2.525862000	5.126785000	14.313513000
H	2.273798000	4.752180000	12.599711000
C	3.351234000	-0.999647000	12.224698000
H	3.874248000	-0.664420000	11.323949000
C	4.200913000	-2.116693000	12.861157000
H	4.350343000	-2.934090000	12.145362000
H	3.713302000	-2.537227000	13.748775000
H	5.187636000	-1.748250000	13.165384000
C	1.979205000	-1.542778000	11.781719000
H	2.107821000	-2.368803000	11.071818000
H	1.379758000	-0.766610000	11.290226000
H	1.403802000	-1.922997000	12.634013000
C	4.285299000	2.612891000	8.094874000
C	3.890007000	1.631282000	7.158051000
C	3.608177000	2.049871000	5.850596000
H	3.295197000	1.315430000	5.113674000
C	3.725642000	3.387991000	5.481482000
C	4.135747000	4.336421000	6.415895000
H	4.228991000	5.376737000	6.116932000
C	4.429860000	3.972467000	7.736922000
C	3.769661000	0.152322000	7.513841000
H	4.048545000	0.031434000	8.564774000

C	4.738727000	-0.708501000	6.680022000
C	2.321990000	-0.352562000	7.359825000
H	1.626430000	0.227078000	7.979535000
H	1.981325000	-0.282491000	6.320064000
H	2.250152000	-1.403644000	7.664362000
H	4.492232000	-0.671774000	5.612311000
H	4.685344000	-1.756569000	6.998525000
H	5.775818000	-0.372245000	6.794967000
C	4.882352000	5.041381000	8.727619000
H	5.097443000	4.550188000	9.681250000
C	3.770548000	6.077678000	8.982840000
C	6.179019000	5.734601000	8.266848000
H	6.984287000	5.009953000	8.098548000
H	6.030282000	6.292417000	7.334738000
H	6.518441000	6.446467000	9.028913000
H	3.511384000	6.620787000	8.066288000
H	4.097945000	6.814115000	9.726678000
H	2.856505000	5.601296000	9.358791000
H	3.502566000	3.691274000	4.461823000

7a

Electronic energy =	-1953.948527
Zero-point correction =	0.784727
Thermal correction to Energy =	0.832417
Thermal correction to Enthalpy =	0.833361
Thermal correction to Gibbs Free Energy =	0.699349

Ag	1.622531000	2.784504000	10.128798000
C	3.705476000	2.336316000	10.324853000
N	4.319883000	1.992563000	11.463774000
C	5.752368000	1.651678000	11.262114000
H	5.920771000	0.600423000	11.514966000
H	6.380778000	2.270218000	11.907816000
C	5.956542000	1.944975000	9.763645000
H	6.637246000	2.782176000	9.581880000
H	6.315190000	1.076303000	9.205423000
N	4.586581000	2.307050000	9.316911000
C	3.696614000	1.919756000	12.758932000
C	3.793643000	3.033117000	13.623972000
C	3.181544000	2.941381000	14.881238000
H	3.239049000	3.785238000	15.563079000
C	2.499089000	1.789979000	15.267998000
H	2.028867000	1.740423000	16.246680000
C	2.425670000	0.698958000	14.404622000
H	1.896387000	-0.196562000	14.717582000
C	3.028268000	0.734006000	13.139410000
C	4.528043000	4.313916000	13.237701000
H	4.914400000	4.190549000	12.221629000
C	5.732734000	4.573668000	14.162783000
H	6.276631000	5.468393000	13.836425000
H	6.434033000	3.730937000	14.157928000
H	5.413796000	4.737613000	15.199074000
C	3.580515000	5.529079000	13.221940000
H	4.116323000	6.424060000	12.883268000
H	3.180086000	5.739233000	14.220768000
H	2.731350000	5.367597000	12.547434000
C	2.924897000	-0.482942000	12.224119000
H	3.553363000	-0.301532000	11.347110000
C	3.445056000	-1.765389000	12.899772000
H	3.417066000	-2.601084000	12.190424000
H	2.834236000	-2.046384000	13.765456000
H	4.479587000	-1.648422000	13.242948000
C	1.479675000	-0.678336000	11.724355000
H	1.424267000	-1.523093000	11.026859000
H	1.117538000	0.217163000	11.201392000
H	0.794499000	-0.882542000	12.555843000
C	4.304409000	2.656836000	7.949528000
C	3.944018000	1.636120000	7.041543000
C	3.672715000	2.003226000	5.716206000
H	3.388633000	1.236848000	5.000334000
C	3.764835000	3.330846000	5.303435000
C	4.142916000	4.318925000	6.210044000
H	4.218765000	5.350161000	5.876961000
C	4.427550000	4.006220000	7.546233000
C	3.845989000	0.169385000	7.450023000
H	4.107664000	0.094943000	8.509810000
C	4.844720000	-0.704566000	6.666622000
C	2.410578000	-0.368443000	7.290042000
H	1.690361000	0.233441000	7.857672000
H	2.097925000	-0.362954000	6.239066000
H	2.347660000	-1.402276000	7.650973000
H	4.615276000	-0.713919000	5.594487000
H	4.805139000	-1.740445000	7.024647000
H	5.873349000	-0.344300000	6.784643000
C	4.853550000	5.115964000	8.503453000
H	5.071965000	4.660994000	9.473990000
C	3.723237000	6.140803000	8.720297000
C	6.141588000	5.815139000	8.027047000
H	6.958604000	5.098354000	7.882966000
H	5.988615000	6.343105000	7.078363000
H	6.467020000	6.554229000	8.769061000
H	3.459480000	6.650013000	7.785762000
H	4.035225000	6.905167000	9.442292000
H	2.815599000	5.661259000	9.106756000
C	-0.730413000	3.140640000	9.832644000
O	-1.038240000	2.206644000	7.700164000
C	-1.015503000	2.257392000	6.240567000
H	-1.632453000	3.099545000	5.917453000
H	0.016415000	2.435876000	5.924403000
N	-1.259388000	1.954797000	10.204076000
N	-1.674547000	0.964482000	10.545755000
C	-0.719078000	3.336210000	8.346102000
O	-0.432090000	4.390470000	7.812047000
C	-1.547409000	0.934156000	5.733757000
H	-1.541848000	0.942912000	4.638115000
H	-0.925645000	0.099179000	6.073756000
H	-2.576219000	0.767636000	6.070094000
C	-0.934313000	4.249262000	10.832653000
C	-0.739404000	3.990958000	12.202112000
C	-1.339320000	5.531087000	10.427851000
H	-0.421318000	3.004269000	12.530998000
H	-1.497428000	5.745422000	9.378651000
C	-0.947371000	4.994893000	13.146847000
C	-1.530328000	6.533103000	11.381137000
H	-0.794762000	4.776572000	14.199989000
H	-1.841603000	7.521382000	11.053996000
C	-1.339422000	6.272746000	12.739718000
H	-1.494382000	7.057383000	13.474726000
H	3.549585000	3.595082000	4.271325000

7b

Electronic energy =	-1722.898345
Zero-point correction =	0.703512
Thermal correction to Energy =	0.746518
Thermal correction to Enthalpy =	0.747463
Thermal correction to Gibbs Free Energy =	0.622776

Ag	1.654103000	2.722308000	-10.299480000
C	3.713494000	2.172246000	-10.455064000
N	4.329774000	1.754887000	-11.568133000
C	5.778570000	1.498609000	-11.362129000
H	6.019993000	0.467561000	-11.634017000
H	6.366581000	2.171917000	-11.993019000
C	5.956661000	1.780088000	-9.857558000
H	6.680322000	2.574220000	-9.654912000
H	6.246330000	0.890836000	-9.289989000
N	4.596473000	2.215955000	-9.448860000
C	3.710047000	1.594428000	-12.856722000
C	3.681087000	2.692609000	-13.746255000
C	3.074762000	2.508157000	-14.996352000
H	3.035804000	3.338152000	-15.696485000
C	2.532009000	1.277311000	-15.358794000
H	2.068567000	1.154287000	-16.334257000
C	2.589889000	0.201849000	-14.475055000

H	2.171701000	-0.756464000	-14.769693000
C	3.183374000	0.331959000	-13.211952000
C	4.287247000	4.049114000	-13.398778000
H	4.722581000	3.979687000	-12.397633000
C	5.424922000	4.424664000	-14.367953000
H	5.891743000	5.366857000	-14.056494000
H	6.202595000	3.652502000	-14.391964000
H	5.054464000	4.558666000	-15.391034000
C	3.218055000	5.157897000	-13.357255000
H	3.671052000	6.112753000	-13.064086000
H	2.746368000	5.299065000	-14.337032000
H	2.425508000	4.924473000	-12.635194000
C	3.242885000	-0.877521000	-12.282829000
H	3.721945000	-0.565846000	-11.349884000
C	4.100683000	-2.006507000	-12.887223000
H	4.186035000	-2.839862000	-12.179426000
H	3.655435000	-2.397517000	-13.810016000
H	5.113106000	-1.659922000	-13.125465000
C	1.835939000	-1.394283000	-11.926167000
H	1.904490000	-2.216880000	-11.204021000
H	1.217018000	-0.606298000	-11.480327000
H	1.311053000	-1.772239000	-12.811498000
C	4.299341000	2.598124000	-8.093535000
C	3.890685000	1.606135000	-7.173687000
C	3.604918000	2.007031000	-5.861435000
H	3.281044000	1.264232000	-5.137669000
C	3.731124000	3.338429000	-5.471242000
C	4.156221000	4.297173000	-6.388540000
H	4.257880000	5.331708000	-6.072615000
C	4.456072000	3.950315000	-7.712963000
C	3.757194000	0.134472000	-7.554392000
H	4.044838000	0.027784000	-8.604526000
C	4.707928000	-0.751146000	-6.725566000
C	2.302289000	-0.356253000	-7.423920000
H	1.620533000	0.242186000	-8.040561000
H	1.951678000	-0.301349000	-6.386462000
H	2.221555000	-1.400692000	-7.748562000
H	4.452166000	-0.728135000	-5.659643000
H	4.644113000	-1.793336000	-7.061071000
H	5.750255000	-0.426518000	-6.825940000
C	4.928993000	5.028725000	-8.683646000
H	5.153694000	4.548160000	-9.640450000
C	3.828171000	6.075928000	-8.941325000
C	6.223968000	5.706795000	-8.196272000
H	7.020351000	4.973791000	-8.022236000
H	6.065989000	6.257331000	-7.261308000
H	6.581471000	6.422857000	-8.946106000
H	3.558868000	6.608029000	-8.021169000
H	4.171150000	6.820239000	-9.670243000
H	2.917462000	5.609667000	-9.337648000
C	-0.542009000	3.310419000	-10.067313000
H	-0.621512000	3.239269000	-8.983192000
O	-1.658196000	2.768410000	-12.065470000
C	-2.387212000	1.850828000	-12.938080000
H	-3.314125000	1.565120000	-12.433366000
H	-1.774767000	0.955782000	-13.078567000
N	-0.675684000	4.591916000	-10.481797000
N	-0.759723000	5.648596000	-10.849634000
C	-1.315193000	2.302571000	-10.860661000
O	-1.556361000	1.193638000	-10.429420000
C	-2.646404000	2.575313000	-14.241042000
H	-3.203618000	1.913514000	-14.913290000
H	-1.708207000	2.853686000	-14.733045000
H	-3.242260000	3.479666000	-14.078492000
H	3.504225000	3.628283000	-4.448518000

TS1a

Electronic energy =	-1953.928932
Zero-point correction =	0.781830
Thermal correction to Energy =	0.829964
Thermal correction to Enthalpy =	0.830909
Thermal correction to Gibbs Free Energy =	0.694635

Ag	1.708824000	2.823376000	10.154237000
C	3.775917000	2.294005000	10.331017000
N	4.397623000	1.944765000	11.465982000
C	5.820690000	1.573977000	11.255790000
H	5.973106000	0.523405000	11.521729000
H	6.467357000	2.190058000	11.885978000
C	6.014470000	1.842344000	9.751538000
H	6.714348000	2.659287000	9.551139000
H	6.345088000	0.957603000	9.200948000
N	4.649343000	2.233038000	9.315959000
C	3.780642000	1.891623000	12.764881000
C	3.883479000	3.015237000	13.615988000
C	3.261580000	2.946306000	14.870121000
H	3.324312000	3.797963000	15.541800000
C	2.566220000	1.806211000	15.267781000
H	2.087600000	1.774841000	16.243166000
C	2.494381000	0.701714000	14.421364000
H	1.958677000	-0.186318000	14.744685000
C	3.106210000	0.714357000	13.160302000
C	4.647143000	4.277556000	13.223972000
H	5.029142000	4.141504000	12.207850000
C	5.859666000	4.505817000	14.147669000
H	6.427089000	5.385622000	13.820661000
H	6.538488000	3.644877000	14.142678000
H	5.546116000	4.678295000	15.184212000
C	3.735691000	5.519600000	13.207205000
H	4.301423000	6.400703000	12.881132000
H	3.330172000	5.735346000	14.202844000
H	2.891198000	5.389650000	12.520271000
C	3.015710000	-0.519878000	12.266542000
H	3.662599000	-0.356367000	11.399395000
C	3.520154000	-1.788354000	12.979552000
H	3.509505000	-2.638094000	12.286618000
H	2.889216000	-2.053134000	13.835940000
H	4.546153000	-1.663689000	13.344981000
C	1.581982000	-0.723220000	11.738594000
H	1.536380000	-1.596766000	11.076609000
H	1.245479000	0.151823000	11.168014000
H	0.873494000	-0.885591000	12.559856000
C	4.366145000	2.578707000	7.947721000
C	3.970341000	1.561202000	7.050763000
C	3.697782000	1.924680000	5.724744000
H	3.384796000	1.161001000	5.018054000
C	3.826590000	3.245085000	5.299012000
C	4.241471000	4.229099000	6.193826000
H	4.347133000	5.254379000	5.850793000
C	4.525452000	3.920031000	7.530928000
C	3.837514000	0.100719000	7.471672000
H	4.106177000	0.027661000	8.529686000
C	4.808139000	-0.803803000	6.687496000
C	2.388070000	-0.402581000	7.328685000
H	1.689091000	0.219872000	7.900547000
H	2.063464000	-0.395677000	6.281247000
H	2.303622000	-1.432551000	7.696403000
H	4.572254000	-0.813460000	5.616781000
H	4.743918000	-1.836215000	7.052121000
H	5.846561000	-0.469934000	6.797406000
C	4.994614000	5.024488000	8.473602000
H	5.165995000	4.579033000	9.457922000
C	3.924604000	6.119530000	8.644577000
C	6.329734000	5.636324000	8.006357000
H	7.108038000	4.871812000	7.898134000
H	6.223195000	6.144679000	7.040609000
H	6.682672000	6.377004000	8.734252000
H	3.723745000	6.634933000	7.697992000
H	4.262212000	6.871069000	9.368615000
H	2.977096000	5.701773000	9.005779000
C	-0.385679000	3.439863000	9.871036000
O	-0.991230000	2.565740000	7.727248000
C	-1.036295000	2.692578000	6.272741000
H	-1.636599000	3.570822000	6.021891000
H	-0.014496000	2.852865000	5.915759000

N	-1.237456000	1.875848000	10.157224000
N	-1.568042000	0.922489000	10.615180000
C	-0.596208000	3.644924000	8.408412000
O	-0.312076000	4.722826000	7.913641000
C	-1.637996000	1.415523000	5.726554000
H	-1.680735000	1.477427000	4.633543000
H	-1.031360000	0.544458000	5.996765000
H	-2.655942000	1.266778000	6.102202000
C	-1.034922000	4.356523000	10.823036000
C	-0.515786000	4.476283000	12.129098000
C	-2.167912000	5.121140000	10.466853000
H	0.349783000	3.883212000	12.411322000
H	-2.588152000	5.037243000	9.469484000
C	-1.100798000	5.343146000	13.048073000
C	-2.741612000	5.995934000	11.383245000
H	-0.690442000	5.429268000	14.049731000
H	-3.605898000	6.588126000	11.097555000
C	-2.211119000	6.106202000	12.674044000
H	-2.664516000	6.788267000	13.387898000
H	3.611408000	3.506495000	4.266137000

TS1b

Electronic energy =	-1722.863346
Zero-point correction =	0.700424
Thermal correction to Energy =	0.744036
Thermal correction to Enthalpy =	0.744980
Thermal correction to Gibbs Free Energy =	0.618689

Ag	1.685555000	2.629336000	-10.362177000
C	3.769687000	2.155861000	-10.467689000
N	4.426402000	1.745641000	-11.561036000
C	5.872745000	1.515837000	-11.314116000
H	6.138682000	0.487065000	-11.571793000
H	6.467331000	2.194133000	-11.933308000
C	6.004919000	1.810144000	-9.807770000
H	6.708716000	2.618363000	-9.591513000
H	6.295542000	0.929577000	-9.227251000
N	4.626541000	2.223090000	-9.439255000
C	3.845553000	1.561858000	-12.865060000
C	3.825186000	2.649789000	-13.767038000
C	3.256169000	2.443412000	-15.031163000
H	3.224230000	3.265834000	-15.740605000
C	2.741487000	1.201055000	-15.395151000
H	2.307879000	1.060992000	-16.381986000
C	2.789770000	0.136067000	-14.498184000
H	2.394038000	-0.831546000	-14.794004000
C	3.344048000	0.288896000	-13.219899000
C	4.403210000	4.018610000	-13.419526000
H	4.808036000	3.968427000	-12.404578000
C	5.565325000	4.395199000	-14.359024000
H	6.011916000	5.346739000	-14.046307000
H	6.351924000	3.631804000	-14.350018000
H	5.224178000	4.511662000	-15.394449000
C	3.319837000	5.114344000	-13.426347000
H	3.751796000	6.078295000	-13.131048000
H	2.878910000	5.237978000	-14.422650000
H	2.507221000	4.880436000	-12.727324000
C	3.381367000	-0.905606000	-12.270249000
H	3.868542000	-0.586916000	-11.343910000
C	4.212037000	-2.066619000	-12.850439000
H	4.278422000	-2.885050000	-12.123509000
H	3.758357000	-2.469869000	-13.763661000
H	5.232347000	-1.749805000	-13.096318000
C	1.962751000	-1.382222000	-11.901537000
H	2.013883000	-2.202561000	-11.175254000
H	1.369123000	-0.575109000	-11.455311000
H	1.421444000	-1.749335000	-12.781651000
C	4.286032000	2.601655000	-8.092794000
C	3.872121000	1.603269000	-7.181972000
C	3.543318000	2.000089000	-5.878662000
H	3.213684000	1.252015000	-5.162905000
C	3.633948000	3.333994000	-5.487161000
C	4.066613000	4.299180000	-6.394002000
H	4.142490000	5.335592000	-6.077027000
C	4.407865000	3.956641000	-7.709589000
C	3.780405000	0.128415000	-7.562033000
H	4.096422000	0.026110000	-8.604325000
C	4.730066000	-0.733723000	-6.707551000
C	2.334314000	-0.395358000	-7.467237000
H	1.654162000	0.189925000	-8.097927000
H	1.958226000	-0.351745000	-6.438150000
H	2.285514000	-1.440358000	-7.796663000
H	4.447562000	-0.714149000	-5.648317000
H	4.698164000	-1.777947000	-7.041336000
H	5.767023000	-0.385777000	-6.783113000
C	4.893629000	5.042277000	-8.665831000
H	5.133012000	4.568302000	-9.622338000
C	3.798800000	6.093005000	-8.933762000
C	6.181106000	5.715502000	-8.151913000
H	6.975543000	4.981209000	-7.974294000
H	6.008340000	6.254652000	-7.212841000
H	6.549592000	6.440619000	-8.887718000
H	3.520559000	6.624803000	-8.016106000
H	4.153264000	6.837739000	-9.656819000
H	2.891273000	5.631094000	-9.341438000
C	-0.393947000	3.019458000	-10.188039000
H	-0.811430000	3.364022000	-9.238674000
O	-1.899626000	2.846561000	-12.084327000
C	-2.831311000	2.005844000	-12.854868000
H	-3.626656000	1.680959000	-12.179661000
H	-2.277476000	1.130482000	-13.203624000
N	-0.521402000	5.006385000	-10.918601000
N	-0.363387000	5.992672000	-11.388989000
C	-1.385473000	2.316998000	-10.999326000
O	-1.572687000	1.195526000	-10.538816000
C	-3.354782000	2.849214000	-13.995335000
H	-4.051902000	2.248442000	-14.589572000
H	-2.541242000	3.178712000	-14.650135000
H	-3.889823000	3.728814000	-13.622687000
H	3.373934000	3.620684000	-4.471450000

8b

Electronic energy =	-1844.439319
Zero-point correction =	0.774433
Thermal correction to Energy =	0.820596
Thermal correction to Enthalpy =	0.821540
Thermal correction to Gibbs Free Energy =	0.688622

Ag	1.869320000	3.196831000	10.038817000
C	3.864478000	2.448447000	10.277364000
N	4.413426000	2.035359000	11.429019000
C	5.781140000	1.484253000	11.252409000
H	5.780781000	0.415061000	11.487471000
H	6.482867000	1.988052000	11.921989000
C	6.061544000	1.767259000	9.765311000
H	6.837912000	2.524620000	9.617233000
H	6.337875000	0.870446000	9.205200000
N	4.755706000	2.289394000	9.288525000
C	3.752584000	2.017043000	12.706694000
C	3.961930000	3.093816000	13.598259000
C	3.310529000	3.055020000	14.838472000
H	3.452397000	3.873229000	15.538915000
C	2.491566000	1.983808000	15.189690000
H	1.996350000	1.972681000	16.157189000
C	2.316013000	0.922004000	14.305112000
H	1.686004000	0.084096000	14.590900000
C	2.946430000	0.908943000	13.053237000
C	4.867116000	4.276056000	13.263201000
H	5.303821000	4.099480000	12.275919000
C	6.030129000	4.395959000	14.267028000
H	6.703774000	5.209359000	13.971729000
H	6.616533000	3.470804000	14.315578000
H	5.668203000	4.615094000	15.278566000
C	4.076391000	5.595862000	13.182702000

H	4.744967000	6.423051000	12.914448000
H	3.608440000	5.844503000	14.142745000
H	3.285161000	5.543573000	12.425132000
C	2.752726000	-0.291662000	12.130758000
H	3.324179000	-0.113112000	11.215116000
C	3.298275000	-1.583823000	12.769514000
H	3.204411000	-2.421728000	12.068143000
H	2.745884000	-1.847687000	13.679107000
H	4.356481000	-1.484534000	13.038488000
C	1.278340000	-0.467416000	11.719770000
H	1.174794000	-1.315109000	11.031542000
H	0.895178000	0.427088000	11.212975000
H	0.638003000	-0.663066000	12.588131000
C	4.547299000	2.655999000	7.912958000
C	4.103162000	1.670345000	7.002461000
C	3.904575000	2.051722000	5.668491000
H	3.556752000	1.314743000	4.949912000
C	4.146387000	3.358154000	5.249224000
C	4.604724000	4.308866000	6.158343000
H	4.799440000	5.322831000	5.820098000
C	4.824234000	3.979806000	7.502945000
C	3.835172000	0.226734000	7.419789000
H	4.078556000	0.130332000	8.482117000
C	4.733255000	-0.761572000	6.651411000
C	2.348642000	-0.144637000	7.255402000
H	1.702477000	0.527664000	7.832523000
H	2.036787000	-0.092733000	6.205387000
H	2.170783000	-1.168671000	7.605781000
H	4.512453000	-0.755986000	5.577485000
H	4.573665000	-1.782832000	7.018024000
H	5.795304000	-0.519663000	6.776101000
C	5.358264000	5.044486000	8.457409000
H	5.467772000	4.590875000	9.446870000
C	4.379192000	6.225557000	8.601107000
C	6.751892000	5.538552000	8.022409000
H	7.467468000	4.710886000	7.951739000
H	6.716777000	6.034626000	7.045338000
H	7.142063000	6.261580000	8.749026000
H	4.233856000	6.745566000	7.646797000
H	4.766605000	6.955041000	9.322930000
H	3.396088000	5.889693000	8.953665000
C	-0.122074000	3.877616000	9.739911000
O	-1.060224000	2.653006000	7.962885000
C	-1.363440000	2.472932000	6.542229000
H	-2.039069000	3.273327000	6.229388000
H	-0.428127000	2.564491000	5.982584000
C	-0.529024000	3.820002000	8.323454000
O	-0.300594000	4.765098000	7.583640000
C	-1.990441000	1.104475000	6.386238000
H	-2.227418000	0.935530000	5.329922000
H	-1.304596000	0.316204000	6.714418000
H	-2.918509000	1.027307000	6.962843000
C	-1.013956000	4.409475000	10.692161000
C	-0.593801000	4.517097000	12.055012000
C	-2.340345000	4.831783000	10.353997000
H	0.411925000	4.197669000	12.311926000
H	-2.679842000	4.764952000	9.324796000
C	-1.451241000	5.010734000	13.022524000
C	-3.187470000	5.328423000	11.326381000
H	-1.130023000	5.087348000	14.056233000
H	-4.191670000	5.648683000	11.068166000
C	-2.743400000	5.416587000	12.656789000
H	-3.415140000	5.807097000	13.416306000
H	3.983976000	3.634174000	4.210485000

8b

Electronic energy =	-1613.345625
Zero-point correction =	0.693085
Thermal correction to Energy =	0.734098
Thermal correction to Enthalpy =	0.735042
Thermal correction to Gibbs Free Energy =	0.615997

Ag	1.661885000	2.530728000	-10.334291000
C	3.758388000	2.109826000	-10.454580000
N	4.414325000	1.711102000	-11.553123000
C	5.868135000	1.517027000	-11.320204000
H	6.153381000	0.491102000	-11.568877000
H	6.440616000	2.200663000	-11.954154000
C	6.009938000	1.831624000	-9.818649000
H	6.691178000	2.663428000	-9.619968000
H	6.334870000	0.966738000	-9.232840000
N	4.624430000	2.206337000	-9.436491000
C	3.822887000	1.509630000	-12.849913000
C	3.759711000	2.595875000	-13.752109000
C	3.171662000	2.375233000	-15.005181000
H	3.105323000	3.196551000	-15.713673000
C	2.679378000	1.120837000	-15.358549000
H	2.228001000	0.969994000	-16.335805000
C	2.773569000	0.057251000	-14.463553000
H	2.397392000	-0.920081000	-14.752674000
C	3.351665000	0.223223000	-13.197490000
C	4.309675000	3.978903000	-13.415513000
H	4.733543000	3.938844000	-12.408080000
C	5.445159000	4.384209000	-14.375297000
H	5.871402000	5.348007000	-14.071853000
H	6.252203000	3.642430000	-14.378742000
H	5.083710000	4.489361000	-15.404971000
C	3.198335000	5.045939000	-13.401583000
H	3.610005000	6.020807000	-13.113270000
H	2.735750000	5.158642000	-14.389367000
H	2.406205000	4.789350000	-12.687300000
C	3.455521000	-0.974031000	-12.255835000
H	3.955680000	-0.642470000	-11.340922000
C	4.312612000	-2.099505000	-12.867096000
H	4.437258000	-2.916080000	-12.145635000
H	3.844528000	-2.519173000	-13.765620000
H	5.309796000	-1.740119000	-13.146995000
C	2.066533000	-1.504819000	-11.851863000
H	2.167214000	-2.329935000	-11.136302000
H	1.458998000	-0.722970000	-11.379778000
H	1.513526000	-1.882779000	-12.720004000
C	4.287215000	2.589260000	-8.090460000
C	3.893942000	1.591487000	-7.170094000
C	3.563255000	1.993260000	-5.868775000
H	3.249196000	1.245597000	-5.145607000
C	3.633698000	3.331486000	-5.488155000
C	4.047897000	4.296172000	-6.404084000
H	4.108624000	5.336144000	-6.095562000
C	4.388485000	3.948936000	-7.718523000
C	3.831898000	0.111698000	-7.536091000
H	4.142740000	0.006789000	-8.579721000
C	4.807861000	-0.719317000	-6.680240000
C	2.399434000	-0.444736000	-7.424473000
H	1.700776000	0.115389000	-8.057919000
H	2.029415000	-0.395939000	-6.393448000
H	2.373674000	-1.495085000	-7.739151000
H	4.531059000	-0.697835000	-5.619530000
H	4.800468000	-1.766841000	-7.004941000
H	5.835191000	-0.345767000	-6.764974000
C	4.852060000	5.034717000	-8.685512000
H	5.088640000	4.557792000	-9.641240000
C	3.742415000	6.070742000	-8.950066000
C	6.136349000	5.725708000	-8.187355000
H	6.941132000	5.001657000	-8.013946000
H	5.966136000	6.267279000	-7.249181000
H	6.488999000	6.451508000	-8.930206000
H	3.465665000	6.604967000	-8.033363000
H	4.082237000	6.815201000	-9.680352000
H	2.837012000	5.596230000	-9.347660000
C	-0.383262000	3.003069000	-10.215196000
H	-0.820607000	3.518687000	-9.354441000
O	-1.836444000	3.042560000	-12.224588000
C	-2.852261000	2.245901000	-12.961054000
H	-3.712225000	2.126415000	-12.298578000
H	-2.410213000	1.269374000	-13.170452000
C	-1.384445000	2.548080000	-11.121725000

O	-1.648256000	1.483250000	-10.537242000
C	-3.188074000	3.012688000	-14.217448000
H	-3.940727000	2.448885000	-14.779279000
H	-2.305112000	3.137244000	-14.852329000
H	-3.602199000	3.998048000	-13.981142000
H	3.372827000	3.622001000	-4.473747000

$TS2_{CC}$ (*E*)

Electronic energy = -2260.38054197

Zero-point correction =	0.881495
Thermal correction to Energy =	0.936431
Thermal correction to Enthalpy =	0.937375
Thermal correction to Gibbs Free Energy =	0.787344

Ag	2.146731000	3.980701000	-10.467759000
C	4.226946000	4.207299000	-10.967104000
N	4.811993000	3.739052000	-12.080284000
C	6.278522000	3.971040000	-12.109146000
H	6.805814000	3.019463000	-12.218730000
H	6.537962000	4.611942000	-12.956918000
C	6.535886000	4.644499000	-10.749127000
H	6.989060000	5.635032000	-10.842637000
H	7.161438000	4.038191000	-10.086963000
N	5.167557000	4.757202000	-10.183615000
C	4.137665000	3.084978000	-13.170623000
C	3.665788000	3.862344000	-14.253299000
C	3.017420000	3.198282000	-15.303731000
H	2.644970000	3.772811000	-16.147269000
C	2.854816000	1.814649000	-15.291523000
H	2.351168000	1.319719000	-16.117947000
C	3.353304000	1.063553000	-14.229151000
H	3.239472000	-0.016939000	-14.237862000
C	4.010433000	1.676577000	-13.153351000
C	3.877565000	5.372050000	-14.338325000
H	4.340129000	5.702156000	-13.403911000
C	4.846321000	5.723573000	-15.485766000
H	5.053900000	6.800570000	-15.492203000
H	5.801251000	5.194634000	-15.384911000
H	4.420442000	5.459398000	-16.461218000
C	2.556496000	6.148592000	-14.488712000
H	2.759296000	7.225716000	-14.533830000
H	2.025317000	5.874622000	-15.408152000
H	1.885718000	5.974542000	-13.640566000
C	4.589607000	0.811698000	-12.036897000
H	4.999533000	1.476703000	-11.271181000
C	5.749965000	-0.058789000	-12.559889000
H	6.203209000	-0.623445000	-11.736035000
H	5.401781000	-0.781179000	-13.307883000
H	6.533896000	0.550347000	-13.024843000
C	3.520027000	-0.064372000	-11.358550000
H	3.966383000	-0.630999000	-10.532321000
H	2.699870000	0.536199000	-10.949023000
H	3.088001000	-0.789077000	-12.058974000
C	4.940897000	5.338987000	-8.887822000
C	4.908290000	4.499621000	-7.750714000
C	4.670626000	5.094489000	-6.503849000
H	4.629494000	4.470507000	-5.615576000
C	4.498928000	6.471852000	-6.383278000
C	4.571629000	7.285324000	-7.512215000
H	4.456783000	8.360698000	-7.406614000
C	4.798935000	6.741697000	-8.783803000
C	5.136595000	2.992267000	-7.832493000
H	5.378778000	2.741473000	-8.869597000
C	6.332946000	2.554591000	-6.965080000
C	3.869162000	2.202277000	-7.455068000
H	3.031079000	2.457144000	-8.115644000
H	3.561808000	2.408233000	-6.422563000
H	4.051359000	1.124005000	-7.541656000
H	6.140647000	2.717537000	-5.898176000
H	6.531215000	1.485248000	-7.106384000
H	7.243558000	3.105223000	-7.229253000
C	4.908858000	7.672056000	-9.989306000
H	5.063860000	7.055929000	-10.879775000
C	3.619892000	8.482405000	-10.218448000
C	6.125552000	8.609429000	-9.857272000
H	7.057162000	8.046703000	-9.724599000
H	6.018665000	9.285077000	-9.000115000
H	6.228934000	9.226576000	-10.758016000
H	3.397709000	9.136321000	-9.366432000
H	3.729872000	9.119802000	-11.104486000
H	2.756199000	7.829216000	-10.382720000
C	0.121887000	3.465594000	-9.908303000
O	-0.889338000	2.185606000	-11.686392000
C	-1.133323000	0.892333000	-12.322256000
H	-1.749141000	0.288082000	-11.650279000
H	-0.171028000	0.391703000	-12.459201000
C	-0.267516000	2.163845000	-10.504223000
O	0.086089000	1.143480000	-9.927529000
C	-1.826674000	1.162713000	-13.640373000
H	-2.031164000	0.209845000	-14.140972000
H	-1.196766000	1.768452000	-14.300947000
H	-2.779726000	1.680548000	-13.487697000
H	4.320946000	6.913528000	-5.406089000
C	-0.516722000	3.859864000	-8.683366000
C	-1.715352000	3.250477000	-8.212901000
C	0.063985000	4.893365000	-7.897820000
H	-2.173391000	2.450535000	-8.785556000
H	0.976687000	5.364438000	-8.252094000
C	-2.286137000	3.646653000	-7.010138000
C	-0.510998000	5.283514000	-6.697578000
H	-3.193855000	3.168026000	-6.655473000
H	-0.049914000	6.063978000	-6.099974000
C	-1.686095000	4.660038000	-6.253286000
H	-2.132386000	4.963192000	-5.310246000
C	-1.003291000	5.039906000	-11.479179000
O	-1.365232000	6.974655000	-10.224384000
C	-0.989211000	8.301320000	-9.746958000
H	-0.789000000	8.933550000	-10.616365000
H	-0.069084000	8.209024000	-9.163487000
N	-2.247302000	4.710810000	-11.171333000
N	-3.270792000	4.402155000	-10.803076000
C	-0.513878000	6.365009000	-11.056782000
O	0.560642000	6.807321000	-11.423608000
C	-2.140625000	8.824436000	-8.914757000
H	-1.888267000	9.823237000	-8.541911000
H	-2.333578000	8.174535000	-8.054653000
H	-3.056138000	8.901172000	-9.510894000
H	-0.584641000	4.541206000	-12.341047000

$TS2_{CC}$ (*Z*)

Electronic energy =	-1914.696305
Zero-point correction =	0.391030
Thermal correction to Energy =	0.442326
Thermal correction to Enthalpy =	0.443271
Thermal correction to Gibbs Free Energy =	0.290659

Ag	1.226377000	0.614793000	-0.330876000
C	3.323175000	0.115581000	-0.806214000
N	-0.793234000	-0.243916000	-1.902959000
N	-1.952588000	-0.364250000	-1.191212000
N	-0.513723000	2.424936000	-0.301332000
N	-1.824750000	2.057904000	-0.420559000
N	-0.416816000	-0.327163000	1.332533000
N	-1.689781000	0.162138000	1.286147000
B	-2.317534000	0.630296000	-0.056335000
C	-0.810069000	-1.216992000	-2.806982000
C	-1.972308000	-2.004403000	-2.703549000
C	-2.669689000	-1.419425000	-1.653757000
C	-0.445971000	3.697552000	-0.681975000
C	-1.705594000	4.193064000	-1.062343000
C	-2.552963000	3.107168000	-0.879652000
C	-0.209954000	-0.721841000	2.584154000
C	-1.338550000	-0.491121000	3.391636000
C	-2.257268000	0.075971000	2.515629000

H	-3.497610000	0.658150000	0.069328000
C	3.699282000	-1.248347000	-0.335304000
O	4.773930000	-1.361816000	0.452501000
O	3.008981000	-2.191424000	-0.691108000
C	5.080557000	-2.694862000	0.956786000
H	5.258697000	-3.355250000	0.103393000
H	4.208822000	-3.067130000	1.502176000
C	4.661210000	1.414507000	0.610761000
C	4.111564000	1.400573000	1.995146000
O	4.505065000	0.631176000	2.846378000
O	3.158663000	2.327712000	2.159350000
C	2.614314000	2.460088000	3.506982000
H	3.434491000	2.738363000	4.175711000
H	2.228748000	1.486982000	3.819805000
N	4.577960000	2.563422000	-0.055529000
N	4.438751000	3.459710000	-0.726262000
Br	1.428011000	-1.498288000	3.109876000
Br	-1.566847000	-0.867618000	5.222011000
Br	-4.002397000	0.658774000	2.921264000
Br	-4.327811000	-1.962505000	-0.939349000
Br	-2.480858000	-3.486261000	-3.748217000
Br	0.576605000	-1.415972000	-4.075697000
Br	-4.406666000	3.053830000	-1.212181000
Br	-2.151420000	5.921271000	-1.660067000
Br	1.179553000	4.659608000	-0.675952000
C	1.529495000	3.514332000	3.467353000
H	1.923887000	4.479592000	3.133278000
H	0.714387000	3.216217000	2.799773000
H	1.119319000	3.640748000	4.475653000
C	6.298868000	-2.568302000	1.846743000
H	6.106720000	-1.874091000	2.670899000
H	6.545833000	-3.549968000	2.266068000
H	7.165714000	-2.209959000	1.280451000
C	3.896458000	0.498939000	-2.089336000
C	3.314012000	1.559215000	-2.829650000
C	5.030524000	-0.153442000	-2.646315000
H	2.435333000	2.053458000	-2.428153000
H	5.512933000	-0.957014000	-2.097911000
C	3.824830000	1.938263000	-4.069045000
C	5.534378000	0.224426000	-3.882329000
H	3.356157000	2.745723000	-4.623645000
H	6.396486000	-0.289667000	-4.297417000
C	4.932488000	1.271757000	-4.596353000
H	5.329855000	1.563238000	-5.564742000
H	5.583128000	0.876721000	0.427531000

TS2$_{HC}$

Electronic energy =	-2145.741993
Zero-point correction =	0.471910
Thermal correction to Energy =	0.527724
Thermal correction to Enthalpy =	0.528668
Thermal correction to Gibbs Free Energy =	0.366415

Ag	1.869965000	3.964300000	-10.617768000
C	3.972523000	4.239834000	-11.059774000
N	4.645867000	3.809567000	-12.138822000
C	6.110947000	4.034491000	-12.043085000
H	6.634220000	3.074586000	-12.074946000
H	6.451668000	4.645673000	-12.883351000
C	6.251440000	4.747255000	-10.688716000
H	6.641826000	5.764895000	-10.781683000
H	6.878585000	4.198372000	-9.980436000
N	4.850162000	4.784571000	-10.199952000
C	4.082298000	3.185444000	-13.305736000
C	3.726219000	3.995785000	-14.408432000
C	3.193781000	3.364099000	-15.541160000
H	2.909679000	3.964286000	-16.401119000
C	3.037897000	1.980191000	-15.588276000
H	2.623905000	1.510094000	-16.476655000
C	3.431681000	1.196940000	-14.505569000
H	3.330986000	0.116927000	-14.562739000
C	3.972437000	1.776399000	-13.349500000
C	3.939387000	5.508023000	-14.425033000
H	4.375185000	5.799396000	-13.465194000
C	4.940439000	5.913221000	-15.525456000
H	5.142878000	6.990102000	-15.476367000
H	5.894472000	5.383809000	-15.418665000
H	4.547379000	5.694377000	-16.525477000
C	2.619583000	6.286438000	-14.578229000
H	2.814558000	7.365809000	-14.559847000
H	2.122334000	6.057140000	-15.528460000
H	1.919645000	6.059048000	-13.766676000
C	4.477055000	0.878506000	-12.222920000
H	4.759284000	1.517838000	-11.381150000
C	5.740663000	0.113632000	-12.669552000
H	6.141393000	-0.480909000	-11.839435000
H	5.515473000	-0.572511000	-13.495024000
H	6.528829000	0.795874000	-13.009449000
C	3.405571000	-0.103377000	-11.715050000
H	3.802977000	-0.687752000	-10.876027000
H	2.508229000	0.417689000	-11.364152000
H	3.105099000	-0.813157000	-12.495045000
C	4.533388000	5.393716000	-8.936280000
C	4.559834000	4.602657000	-7.765289000
C	4.254639000	5.224758000	-6.546794000
H	4.260522000	4.636784000	-5.633188000
C	3.958529000	6.584828000	-6.486211000
C	3.974458000	7.354648000	-7.647699000
H	3.768111000	8.419606000	-7.587476000
C	4.268447000	6.782190000	-8.892878000
C	4.942274000	3.124902000	-7.779092000
H	5.142031000	2.836644000	-8.815414000
C	6.235080000	2.878233000	-6.976110000
C	3.803350000	2.225938000	-7.263599000
H	2.893812000	2.349359000	-7.861745000
H	3.553772000	2.450076000	-6.219657000
H	4.100030000	1.171222000	-7.315443000
H	6.097383000	3.105528000	-5.912203000
H	6.534647000	1.826085000	-7.055218000
H	7.063731000	3.494421000	-7.344525000
C	4.337653000	7.673798000	-10.130333000
H	4.545154000	7.038076000	-10.995971000
C	3.008591000	8.400616000	-10.407670000
C	5.495036000	8.685760000	-10.010060000
H	6.453909000	8.183766000	-9.835732000
H	5.328721000	9.384062000	-9.180883000
H	5.583831000	9.275047000	-10.930828000
H	2.736541000	9.071902000	-9.584209000
H	3.096223000	9.010481000	-11.315199000
H	2.185177000	7.694273000	-10.560879000
C	-0.113161000	3.420856000	-9.848672000
O	-1.678749000	1.759256000	-10.661514000
C	-2.010151000	0.368211000	-10.979444000
H	-3.098397000	0.341425000	-10.898993000
H	-1.577012000	-0.271326000	-10.207508000
C	-0.448578000	2.009262000	-10.202668000
O	0.408073000	1.154379000	-10.021365000
C	-1.542039000	-0.028218000	-12.367195000
H	-1.857156000	-1.059784000	-12.564548000
H	-0.451944000	0.015659000	-12.447567000
H	-1.982254000	0.616737000	-13.133677000
H	3.731322000	7.049321000	-5.529954000
C	-0.448210000	3.777664000	-8.475859000
C	-1.343769000	3.009915000	-7.680049000
C	0.142447000	4.924706000	-7.882123000
H	-1.814631000	2.123921000	-8.093061000
H	0.826438000	5.523763000	-8.475350000
C	-1.602882000	3.356251000	-6.356422000
C	-0.126753000	5.271489000	-6.565827000
H	-2.275550000	2.746503000	-5.760553000
H	0.346075000	6.144860000	-6.126796000
C	-0.998372000	4.485254000	-5.798734000
H	-1.200880000	4.753387000	-4.765491000
C	-1.615909000	4.660749000	-11.089299000
O	-1.657594000	6.667410000	-9.862096000

C	-1.203898000	8.019702000	-9.540285000
H	-1.180754000	8.599138000	-10.466546000
H	-0.187795000	7.951006000	-9.143417000
N	-2.673258000	4.405062000	-10.291485000
N	-3.445685000	4.136431000	-9.516145000
C	-1.035331000	6.033406000	-10.856332000
O	-0.110267000	6.470768000	-11.509342000
C	-2.175225000	8.591976000	-8.530480000
H	-1.860980000	9.608439000	-8.269106000
H	-2.195787000	7.992067000	-7.614663000
H	-3.188683000	8.641320000	-8.942160000
C	-1.737416000	4.140817000	-12.487590000
C	-0.607702000	4.068621000	-13.314954000
C	-2.988514000	3.754169000	-12.996203000
H	0.363032000	4.366082000	-12.937662000
H	-3.878674000	3.818984000	-12.376721000
C	-0.734805000	3.615863000	-14.629060000
C	-3.105972000	3.299240000	-14.308732000
H	0.148466000	3.561846000	-15.258052000
H	-4.081973000	3.009424000	-14.687706000
C	-1.978933000	3.228723000	-15.131484000
H	-2.070038000	2.878280000	-16.155725000

$TS2_{CC'}$

Electronic energy = -1844.16524839

Zero-point correction =	0.537394
Thermal correction to Energy =	0.585464
Thermal correction to Enthalpy =	0.586408
Thermal correction to Gibbs Free Energy =	0.443671

Ag	2.188172000	4.027519000	-10.694669000
C	4.300198000	4.192367000	-11.034543000
N	4.963736000	3.702559000	-12.090950000
C	6.427230000	3.943802000	-12.017513000
H	6.968623000	2.996790000	-12.089761000
H	6.738661000	4.586961000	-12.846193000
C	6.583723000	4.622296000	-10.644162000
H	7.050649000	5.608249000	-10.707046000
H	7.148432000	4.014019000	-9.930790000
N	5.175997000	4.750375000	-10.187116000
C	4.363658000	3.052403000	-13.225965000
C	3.937569000	3.836821000	-14.321731000
C	3.351298000	3.177617000	-15.410994000
H	3.004225000	3.758673000	-16.261062000
C	3.210997000	1.791624000	-15.423788000
H	2.756418000	1.300117000	-16.280104000
C	3.660659000	1.034740000	-14.343898000
H	3.557099000	-0.046593000	-14.367592000
C	4.247809000	1.643823000	-13.226484000
C	4.092796000	5.354833000	-14.355861000
H	4.613080000	5.663151000	-13.444486000
C	4.953266000	5.812127000	-15.549456000
H	5.103601000	6.897933000	-15.513079000
H	5.939782000	5.333936000	-15.539905000
H	4.476115000	5.575305000	-16.507691000
C	2.724648000	6.062596000	-14.361823000
H	2.857996000	7.150945000	-14.340216000
H	2.147792000	5.814226000	-15.260329000
H	2.124503000	5.778897000	-13.488922000
C	4.740414000	0.777017000	-12.071068000
H	5.146446000	1.438540000	-11.299900000
C	5.877188000	-0.163546000	-12.516840000
H	6.254602000	-0.734856000	-11.660144000
H	5.532173000	-0.881645000	-13.270087000
H	6.716922000	0.394318000	-12.947360000
C	3.592263000	-0.024334000	-11.427873000
H	3.964741000	-0.602010000	-10.573261000
H	2.794277000	0.635279000	-11.066038000
H	3.147557000	-0.731682000	-12.137964000
C	4.849367000	5.341605000	-8.916471000
C	4.734777000	4.509957000	-7.779052000
C	4.423738000	5.115698000	-6.553653000
H	4.323394000	4.498322000	-5.665467000
C	4.252515000	6.494490000	-6.454160000
C	4.393399000	7.298841000	-7.583319000
H	4.270907000	8.374180000	-7.492042000
C	4.694632000	6.744942000	-8.834891000
C	4.956665000	3.000305000	-7.832567000
H	5.214413000	2.729656000	-8.861102000
C	6.137443000	2.576875000	-6.936527000
C	3.682167000	2.219421000	-7.459251000
H	2.849116000	2.468023000	-8.128655000
H	3.365352000	2.435636000	-6.431916000
H	3.862447000	1.139899000	-7.532123000
H	5.927791000	2.768865000	-5.877625000
H	6.332737000	1.503386000	-7.047418000
H	7.054735000	3.116991000	-7.199094000
C	4.878487000	7.660327000	-10.042165000
H	4.961676000	7.029339000	-10.932083000
C	3.679305000	8.602044000	-10.258933000
C	6.184968000	8.470908000	-9.923486000
H	7.056367000	7.818659000	-9.793650000
H	6.149348000	9.155221000	-9.067062000
H	6.343649000	9.073153000	-10.826400000
H	3.572663000	9.319386000	-9.436533000
H	3.820254000	9.180033000	-11.180426000
H	2.735616000	8.052335000	-10.347503000
C	0.168723000	3.693085000	-10.214433000
O	-1.365768000	2.341929000	-11.599838000
C	-1.957523000	0.988607000	-11.749415000
H	-2.422655000	0.724701000	-10.797302000
H	-1.133772000	0.302421000	-11.957430000
C	-0.580466000	2.531277000	-10.587944000
O	-0.223656000	1.749558000	-9.694370000
C	-2.955301000	1.058375000	-12.880613000
H	-3.388001000	0.062185000	-13.024357000
H	-2.474493000	1.362746000	-13.815751000
H	-3.768116000	1.754512000	-12.649920000
H	4.017790000	6.944752000	-5.493067000
C	-1.665156000	6.276307000	-11.416144000
O	-1.231140000	6.602471000	-9.143902000
C	-0.529273000	7.248451000	-8.042426000
H	-0.604874000	8.331181000	-8.174681000
H	0.527329000	6.967948000	-8.089580000
N	-2.615812000	5.487328000	-10.951978000
N	-3.434734000	4.795954000	-10.573300000
C	-0.854147000	6.957160000	-10.390868000
O	0.052471000	7.735312000	-10.634562000
C	-1.183025000	6.786282000	-6.757082000
H	-0.681227000	7.262371000	-5.907503000
H	-1.102542000	5.700132000	-6.637549000
H	-2.241917000	7.064207000	-6.730994000
C	-1.581738000	6.462240000	-12.883042000
C	-0.913608000	7.568978000	-13.438646000
C	-2.202713000	5.541748000	-13.749155000
H	-0.432506000	8.287780000	-12.788586000
H	-2.719179000	4.674767000	-13.346287000
C	-0.871703000	7.739550000	-14.823387000
C	-2.159536000	5.725144000	-15.129724000
H	-0.354351000	8.602767000	-15.233644000
H	-2.646975000	5.002336000	-15.778338000
C	-1.493122000	6.825059000	-15.676453000
H	-1.460650000	6.967666000	-16.752896000
H	-0.341957000	4.262629000	-9.431948000

$TS2_{HC'}$

Electronic energy =	-1683.620399
Zero-point correction =	0.308586
Thermal correction to Energy =	0.355644
Thermal correction to Enthalp y=	0.356588
Thermal correction to Gibbs Free Energy =	0.211099

Ag	1.027510000	-0.390170000	-0.871886000
C	3.030631000	-0.265822000	-1.403779000

N	-1.068360000	-0.918879000	-1.829024000
N	-2.242076000	-0.573845000	-1.224361000
N	-0.376034000	1.638831000	-0.188515000
N	-1.648300000	1.427770000	0.255299000
N	-0.191483000	-1.160363000	1.097022000
N	-1.533742000	-0.938404000	1.203868000
B	-2.282046000	0.009434000	0.219913000
C	-1.374635000	-1.400257000	-3.028869000
C	-2.763531000	-1.382598000	-3.243018000
C	-3.273644000	-0.847153000	-2.064831000
C	-0.115053000	2.925476000	-0.003311000
C	-1.212339000	3.596156000	0.568916000
C	-2.167254000	2.596347000	0.717082000
C	0.145143000	-1.974907000	2.089943000
C	-0.970991000	-2.309815000	2.877098000
C	-2.018870000	-1.624655000	2.271514000
H	-3.412862000	0.087750000	0.560188000
H	3.494922000	0.691128000	-1.666731000
C	3.946201000	-1.359031000	-1.619526000
O	4.653840000	-1.910024000	-0.666644000
O	3.888763000	-1.658978000	-2.813038000
C	5.513385000	-3.048448000	-1.034910000
H	6.090266000	-2.768157000	-1.919366000
H	4.857964000	-3.886556000	-1.285690000
C	5.307300000	0.864965000	1.307580000
C	5.937338000	1.218607000	0.044336000
O	5.380668000	1.891150000	-0.812967000
O	7.185977000	0.723814000	-0.067314000
C	7.890115000	1.022550000	-1.303063000
H	7.915492000	2.107763000	-1.438071000
H	7.331546000	0.586895000	-2.137479000
N	5.910483000	0.058634000	2.140052000
N	6.443132000	-0.649315000	2.852492000
Br	1.928507000	-2.549557000	2.322081000
Br	-1.036666000	-3.416625000	4.397501000
Br	-3.823693000	-1.624599000	2.810465000
Br	-5.086829000	-0.533993000	-1.664135000
Br	-3.713920000	-1.952594000	-4.763294000
Br	-0.034749000	-2.008979000	-4.208261000
Br	-3.899276000	2.782690000	1.436579000
Br	-1.358190000	5.416712000	1.025797000
Br	1.562772000	3.655004000	-0.477120000
C	9.282197000	0.436915000	-1.187162000
H	9.828328000	0.882723000	-0.348926000
H	9.246206000	-0.648518000	-1.043729000
H	9.838892000	0.642508000	-2.108385000
C	6.395928000	-3.341790000	0.157243000
H	5.799503000	-3.600323000	1.038303000
H	7.043015000	-4.192908000	-0.082003000
H	7.029440000	-2.482239000	0.398363000
H	4.327183000	1.224906000	1.589102000

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Electronic energy = -2260.514216
Zero-point correction = 0.882027
Thermal correction to Energy = 0.938696
Thermal correction to Enthalpy = 0.939640
Thermal correction to Gibbs Free Energy = 0.782814

Ag	2.112379000	4.549758000	-11.459359000
C	4.170170000	4.266454000	-11.014173000
N	5.015151000	3.605628000	-11.818592000
C	6.394440000	3.539305000	-11.271448000
H	6.730673000	2.500637000	-11.221911000
H	7.075931000	4.096403000	-11.922173000
C	6.231817000	4.183490000	-9.883002000
H	6.903554000	5.030464000	-9.722922000
H	6.368756000	3.468851000	-9.065511000
N	4.819847000	4.646815000	-9.907277000
C	4.702416000	3.102374000	-13.130726000
C	4.822509000	3.964159000	-14.244809000
C	4.514415000	3.445682000	-15.509827000
H	4.592911000	4.089824000	-16.381202000
C	4.115067000	2.120566000	-15.668576000
H	3.881469000	1.738880000	-16.659090000
C	4.024652000	1.282239000	-14.559605000
H	3.721755000	0.247481000	-14.692718000
C	4.320052000	1.749580000	-13.271879000
C	5.281063000	5.414722000	-14.122352000
H	5.475702000	5.623564000	-13.066287000
C	6.598165000	5.655627000	-14.885566000
H	6.938896000	6.687485000	-14.737107000
H	7.391689000	4.984005000	-14.537433000
H	6.475041000	5.497203000	-15.963393000
C	4.190779000	6.397657000	-14.590368000
H	4.521960000	7.432602000	-14.441505000
H	3.964674000	6.270173000	-15.655686000
H	3.257934000	6.256807000	-14.030434000
C	4.224245000	0.793255000	-12.086393000
H	4.521088000	1.338838000	-11.185542000
C	5.190839000	-0.396658000	-12.243097000
H	5.163228000	-1.029745000	-11.347912000
H	4.922573000	-1.023996000	-13.101381000
H	6.223834000	-0.058317000	-12.386188000
C	2.780607000	0.301131000	-11.868755000
H	2.729520000	-0.355086000	-10.991334000
H	2.092859000	1.139577000	-11.703217000
H	2.415937000	-0.266837000	-12.732857000
C	4.259994000	5.388758000	-8.809239000
C	3.608681000	4.694715000	-7.764910000
C	3.095166000	5.447903000	-6.700006000
H	2.581493000	4.941929000	-5.888049000
C	3.236532000	6.833460000	-6.663131000
C	3.897007000	7.495941000	-7.695691000
H	4.008231000	8.575816000	-7.654740000
C	4.425560000	6.792111000	-8.786034000
C	3.434523000	3.178266000	-7.771065000
H	4.022713000	2.773523000	-8.600319000
C	3.961101000	2.526763000	-6.478819000
C	1.963247000	2.788943000	-8.016855000
H	1.599787000	3.189260000	-8.972517000
H	1.311854000	3.172130000	-7.222399000
H	1.855231000	1.697643000	-8.044267000
H	3.375068000	2.826660000	-5.602358000
H	3.900164000	1.434660000	-6.556915000
H	5.007697000	2.793448000	-6.290742000
C	5.149807000	7.552635000	-9.893772000
H	5.511864000	6.823662000	-10.625131000
C	4.198264000	8.508754000	-10.637722000
C	6.376240000	8.314102000	-9.354720000
H	7.077397000	7.641369000	-8.847284000
H	6.084479000	9.093377000	-8.640954000
H	6.911691000	8.801944000	-10.178195000
H	3.816668000	9.291737000	-9.971637000
H	4.723602000	9.002560000	-11.464400000
H	3.337868000	7.972289000	-11.055662000
C	-1.104197000	6.536860000	-11.516445000
O	-1.939054000	5.030383000	-13.142136000
C	-1.859367000	3.803296000	-13.935264000
H	-1.829935000	2.956694000	-13.243435000
H	-0.926786000	3.825845000	-14.505637000
C	-0.960984000	5.293509000	-12.299681000
O	0.035082000	4.560623000	-12.206953000
C	-3.079769000	3.770270000	-14.829307000
H	-3.056473000	2.853649000	-15.428933000
H	-3.093282000	4.627067000	-15.511141000
H	-4.001789000	3.773207000	-14.238989000
H	2.835575000	7.397470000	-5.824956000
C	-2.253921000	7.130526000	-11.125975000
O	-0.980682000	8.664020000	-9.828137000
C	-0.810753000	9.936476000	-9.139012000
H	-1.674845000	10.093517000	-8.488268000
H	-0.795423000	10.732838000	-9.889645000
N	-1.351960000	6.184468000	-7.811217000
N	-0.499342000	5.685553000	-7.316323000

C	-2.163974000	8.466950000	-10.424085000
O	-3.075327000	9.272062000	-10.408418000
C	0.483555000	9.861556000	-8.358290000
H	0.638730000	10.806219000	-7.825316000
H	1.338248000	9.697508000	-9.022861000
H	0.450407000	9.051400000	-7.621890000
C	-3.618414000	6.566144000	-11.287956000
C	-4.644769000	7.282968000	-11.925367000
C	-3.899267000	5.293375000	-10.761483000
H	-4.443088000	8.267664000	-12.330304000
H	-3.115389000	4.743468000	-10.247313000
C	-5.916588000	6.723473000	-12.052028000
C	-5.175948000	4.744674000	-10.877010000
H	-6.698695000	7.281415000	-12.559656000
H	-5.380925000	3.764186000	-10.455883000
C	-6.187582000	5.456980000	-11.527110000
H	-7.182566000	5.029968000	-11.618786000
H	-0.154320000	6.980234000	-11.236806000

Cu systems with IPr ligand

IPrCuCl

Electronic energy =	-1817.749375
Zero-point correction =	0.597569
Thermal correction to Energy =	0.632536
Thermal correction to Enthalpy =	0.633480
Thermal correction to Gibbs Free Energy =	0.528653

Cu	0.000073000	-0.000180000	1.685735000
C	-0.000038000	0.000029000	-0.256995000
N	-1.091343000	0.003760000	-1.041992000
C	-0.770139000	-0.021758000	-2.489606000
H	-1.219438000	0.839366000	-2.992634000
H	-1.166920000	-0.934482000	-2.945199000
C	0.769955000	0.022059000	-2.489647000
H	1.219244000	-0.839007000	-2.992782000
H	1.166707000	0.934838000	-2.945152000
N	1.091224000	-0.003623000	-1.042043000
C	-2.450765000	-0.002926000	-0.570518000
C	-3.100893000	-1.240229000	-0.359775000
C	-4.424747000	-1.218004000	0.098876000
H	-4.941658000	-2.156826000	0.277844000
C	-5.086144000	-0.014621000	0.333200000
H	-6.112360000	-0.019125000	0.691521000
C	-4.433519000	1.194505000	0.104080000
H	-4.957505000	2.128599000	0.287202000
C	-3.110092000	1.228717000	-0.355405000
C	-2.414437000	-2.581598000	-0.602430000
H	-1.415319000	-2.382418000	-1.000679000
C	-3.165277000	-3.426922000	-1.649101000
H	-2.618430000	-4.356623000	-1.848336000
H	-3.273913000	-2.889031000	-2.598427000
H	-4.169008000	-3.701391000	-1.303472000
C	-2.237027000	-3.368226000	0.710848000
H	-1.697456000	-4.305224000	0.525005000
H	-3.205199000	-3.622746000	1.158468000
H	-1.668009000	-2.790417000	1.448570000
C	-2.434949000	2.576433000	-0.594798000
H	-1.435735000	2.386794000	-0.997711000
C	-3.196353000	3.420103000	-1.635091000
H	-2.657123000	4.354496000	-1.833103000
H	-4.200731000	3.685959000	-1.284739000
H	-3.304520000	2.884724000	-2.585910000
C	-2.258973000	3.358546000	0.721338000
H	-1.729122000	4.301509000	0.537673000
H	-1.681172000	2.782586000	1.453669000
H	-3.227508000	3.601596000	1.174593000
C	2.450695000	0.003006000	-0.570691000
C	3.100857000	1.240289000	-0.359892000
C	4.424746000	1.217997000	0.098669000
H	4.941657000	2.156797000	0.277743000
C	5.086136000	0.014584000	0.332854000
C	4.433475000	-1.194509000	0.103678000
H	4.957463000	-2.128622000	0.286697000
C	3.110020000	-1.228663000	-0.355726000
C	2.414400000	2.581710000	-0.602291000
H	1.415209000	2.382616000	-1.000394000
C	3.165051000	3.427130000	-1.649024000
C	2.237247000	3.368214000	0.711095000
H	1.668290000	2.790381000	1.448843000
H	3.205515000	3.622590000	1.158589000
H	1.697735000	4.305281000	0.525425000
H	4.168819000	3.701637000	-1.303545000
H	2.618135000	4.356819000	-1.848133000
H	3.273562000	2.889297000	-2.598399000
C	2.434801000	-2.576344000	-0.595076000
H	1.435623000	-2.386653000	-0.99806100
C	2.258743000	-3.358308000	0.721164000
C	3.196128000	-3.420226000	-1.635228000
H	3.304482000	-2.884954000	-2.586086000
H	4.200423000	-3.686308000	-1.284803000
H	2.656694000	-4.354509000	-1.833198000
H	3.227282000	-3.601247000	1.174475000
H	1.728936000	-4.301318000	0.537612000
H	1.680907000	-2.782280000	1.453408000
H	6.112373000	0.019025000	0.691116000
Cl	0.000434000	-0.000201000	3.905128000

IPrCuBPh$_4$

Electronic energy =	-2308.952603
Zero-point correction =	0.966143
Thermal correction to Energy =	1.020586
Thermal correction to Enthalpy =	1.021531
Thermal correction to Gibbs Free Energy =	0.874070

Cu	0.612604000	-0.288220000	-0.620169000
C	2.316059000	0.268644000	0.203452000
N	3.340558000	-0.560331000	0.480114000
C	4.490265000	0.125897000	1.118984000
H	5.419318000	-0.125074000	0.601484000
H	4.575049000	-0.192821000	2.163523000
C	4.103383000	1.603447000	0.979355000
H	4.181703000	2.156487000	1.917748000
H	4.692894000	2.125397000	0.217126000
N	2.688032000	1.520333000	0.536782000
C	3.385602000	-1.975777000	0.229556000
C	2.935635000	-2.875627000	1.222403000
C	3.022944000	-4.248353000	0.951656000
H	2.682500000	-4.961190000	1.696988000
C	3.549858000	-4.714810000	-0.250451000
H	3.608386000	-5.783639000	-0.439594000
C	4.015724000	-3.812191000	-1.203914000
H	4.442368000	-4.184971000	-2.131019000
C	3.952542000	-2.429648000	-0.984446000
C	2.420468000	-2.406276000	2.580493000
H	2.293063000	-1.320523000	2.537169000
C	3.453243000	-2.707691000	3.686206000
H	3.108067000	-2.314016000	4.650100000
H	4.426460000	-2.254384000	3.464395000
H	3.607105000	-3.787617000	3.801063000
C	1.051738000	-3.011196000	2.941282000
H	0.694860000	-2.592591000	3.889983000
H	1.103407000	-4.099468000	3.063500000
H	0.299891000	-2.794633000	2.174653000
C	4.514898000	-1.479110000	-2.038760000
H	4.375510000	-0.454940000	-1.680076000
C	6.028083000	-1.695662000	-2.236934000
H	6.428147000	-0.958647000	-2.943945000
H	6.242440000	-2.693025000	-2.639189000
H	6.576174000	-1.591353000	-1.293064000
C	3.767246000	-1.597105000	-3.380372000
H	4.174913000	-0.883187000	-4.106639000
H	2.698961000	-1.384074000	-3.261282000
H	3.864098000	-2.600817000	-3.811425000

C	1.947704000	2.728316000	0.285243000
C	1.931445000	3.278445000	-1.018251000
C	1.229631000	4.475449000	-1.217032000
H	1.194806000	4.911317000	-2.211452000
C	0.593106000	5.123113000	-0.161652000
C	0.651577000	4.584391000	1.121432000
H	0.166550000	5.105203000	1.941909000
C	1.328494000	3.384316000	1.374472000
C	2.674357000	2.652844000	-2.196219000
H	3.164594000	1.739185000	-1.847557000
C	3.779900000	3.591522000	-2.719200000
C	1.716688000	2.251379000	-3.333699000
H	0.952622000	1.549844000	-2.978857000
H	1.201468000	3.122350000	-3.755521000
H	2.272454000	1.766664000	-4.145821000
H	3.360978000	4.517079000	-3.131292000
H	4.349129000	3.099281000	-3.517355000
H	4.481510000	3.867814000	-1.923282000
C	1.408878000	2.859420000	2.805301000
H	1.885980000	1.875203000	2.778052000
C	0.019828000	2.677600000	3.443369000
C	2.286489000	3.778773000	3.679231000
H	3.288369000	3.907893000	3.253442000
H	1.837562000	4.774188000	3.782182000
H	2.398167000	3.356981000	4.685654000
H	-0.504894000	3.633775000	3.555506000
H	0.120372000	2.239446000	4.443883000
H	-0.615780000	2.016814000	2.844794000
H	0.058541000	6.053033000	-0.337248000
C	-3.455787000	1.177923000	-0.580401000
B	-3.531208000	-0.429277000	-0.182783000
C	-3.282216000	2.220364000	0.351249000
H	-3.187490000	1.977479000	1.406645000
C	-3.244248000	3.570591000	-0.021478000
H	-3.116139000	4.336938000	0.740895000
C	-3.376104000	3.935207000	-1.362240000
H	-3.348508000	4.981725000	-1.657627000
C	-3.558293000	2.930357000	-2.318438000
H	-3.677514000	3.192700000	-3.368310000
C	-3.603941000	1.590086000	-1.925996000
H	-3.778354000	0.835553000	-2.691628000
C	-4.904714000	-1.045741000	-0.890245000
C	-4.978549000	-2.264462000	-1.592800000
H	-4.079426000	-2.861961000	-1.722897000
C	-6.171843000	-2.752912000	-2.141170000
H	-6.170472000	-3.700719000	-2.676900000
C	-7.357411000	-2.030152000	-2.004415000
H	-8.287611000	-2.404436000	-2.426137000
C	-7.325845000	-0.811758000	-1.317974000
H	-8.237786000	-0.228708000	-1.201261000
C	-6.124882000	-0.337718000	-0.784442000
H	-6.134529000	0.618690000	-0.264723000
C	-3.588581000	-0.636731000	1.462322000
C	-2.442106000	-0.406870000	2.256941000
H	-1.513842000	-0.109646000	1.769510000
C	-2.440158000	-0.545880000	3.647767000
H	-1.530501000	-0.348276000	4.211886000
C	-3.604947000	-0.937807000	4.315113000
H	-3.611701000	-1.051260000	5.396882000
C	-4.755733000	-1.184868000	3.565392000
H	-5.672341000	-1.497786000	4.062494000
C	-4.738577000	-1.034855000	2.172697000
H	-5.655223000	-1.238891000	1.625498000
C	-2.204794000	-1.254265000	-0.751593000
C	-1.963994000	-2.579953000	-0.327313000
H	-2.605170000	-3.005548000	0.441286000
C	-0.961313000	-3.390199000	-0.873284000
H	-0.842025000	-4.412085000	-0.520077000
C	-0.123148000	-2.900452000	-1.875387000
H	0.645264000	-3.529108000	-2.315959000
C	-0.296464000	-1.577632000	-2.312590000
H	0.300395000	-1.195158000	-3.137933000
C	-1.311863000	-0.768502000	-1.745538000
H	-1.475993000	0.220939000	-2.165738000

5

Electronic energy =	-1357.338816
Zero-point correction =	0.597480
Thermal correction to Energy =	0.630053
Thermal correction to Enthalpy =	0.630998
Thermal correction to Gibbs Free Energy =	0.533177

Cu	1.824108000	2.499892000	10.270431000
C	3.700780000	2.101539000	10.434441000
N	4.321087000	1.685557000	11.549092000
C	5.782017000	1.500532000	11.360502000
H	6.067834000	0.477571000	11.619745000
H	6.330004000	2.190462000	12.009512000
C	5.967921000	1.812742000	9.862435000
H	6.666752000	2.634013000	9.682025000
H	6.296360000	0.942560000	9.285855000
N	4.599240000	2.206409000	9.443226000
C	3.686113000	1.483190000	12.824384000
C	3.581470000	2.570386000	13.721901000
C	2.948519000	2.347710000	14.952478000
H	2.846252000	3.170251000	15.655040000
C	2.455536000	1.089534000	15.291130000
H	1.968566000	0.936941000	16.250798000
C	2.592808000	0.024727000	14.403290000
H	2.215002000	-0.955277000	14.680766000
C	3.215345000	0.193220000	13.158976000
C	4.128617000	3.958013000	13.400715000
H	4.605873000	3.914282000	12.417627000
C	5.207361000	4.390642000	14.412608000
H	5.635723000	5.356399000	14.118581000
H	6.023008000	3.660266000	14.465832000
H	4.793720000	4.503877000	15.421496000
C	3.002741000	5.006376000	13.316950000
H	3.412768000	5.986271000	13.044028000
H	2.483788000	5.116901000	14.276531000
H	2.256202000	4.730564000	12.561758000
C	3.362563000	-1.003710000	12.222848000
H	3.906093000	-0.672266000	11.333008000
C	4.187575000	-2.131818000	12.871863000
H	4.342036000	-2.948102000	12.155834000
H	3.678984000	-2.550864000	13.748182000
H	5.172258000	-1.775059000	13.195941000
C	1.992838000	-1.530512000	11.752710000
H	2.124829000	-2.358571000	11.045744000
H	1.413417000	-0.746936000	11.248924000
H	1.395771000	-1.902415000	12.593765000
C	4.301445000	2.607180000	8.093613000
C	3.904243000	1.627022000	7.156023000
C	3.616213000	2.046896000	5.850257000
H	3.297916000	1.314275000	5.113944000
C	3.733210000	3.385264000	5.481572000
C	4.145861000	4.332697000	6.415977000
H	4.236968000	5.373527000	6.117949000
C	4.442221000	3.967382000	7.736105000
C	3.773326000	0.150257000	7.517334000
H	4.113944000	0.022806000	8.549181000
C	4.663854000	-0.739083000	6.628854000
C	2.304797000	-0.313519000	7.457941000
H	1.669977000	0.288697000	8.120342000
H	1.900214000	-0.232298000	6.441887000
H	2.220702000	-1.361695000	7.769539000
H	4.349850000	-0.707208000	5.579010000
H	4.605534000	-1.782766000	6.960603000
H	5.714088000	-0.428246000	6.673860000
C	4.885527000	5.036978000	8.730270000
H	5.108735000	4.543241000	9.680616000
C	3.760406000	6.056961000	8.994453000
C	6.172395000	5.748699000	8.270877000
H	6.986181000	5.034719000	8.097927000
H	6.015820000	6.309403000	7.341779000

H	6.504214000	6.460877000	9.035989000
H	3.490081000	6.600879000	8.081551000
H	4.080117000	6.794194000	9.740853000
H	2.854801000	5.565892000	9.371578000
H	3.506572000	3.689532000	4.463020000

7a

Electronic energy =	-1894.847454
Zero-point correction =	0.775225
Thermal correction to Energy =	0.820891
Thermal correction to Enthalpy =	0.821835
Thermal correction to Gibbs Free Energy =	0.692183

Cu	1.662122000	2.767968000	-10.039707000
C	3.555236000	2.360142000	-10.261800000
N	4.169028000	2.149417000	-11.436868000
C	5.622814000	1.883774000	-11.294189000
H	5.868899000	0.906554000	-11.719148000
H	6.195744000	2.648532000	-11.826764000
C	5.823937000	1.942292000	-9.768117000
H	6.525681000	2.722714000	-9.461033000
H	6.157246000	0.989811000	-9.345349000
N	4.460495000	2.263030000	-9.275956000
C	3.520675000	2.131689000	-12.721115000
C	3.498231000	3.312215000	-13.498223000
C	2.855183000	3.265699000	-14.742532000
H	2.814671000	4.162833000	-15.353762000
C	2.274220000	2.089309000	-15.210841000
H	1.782346000	2.075077000	-16.179955000
C	2.332538000	0.928811000	-14.442167000
H	1.889031000	0.012152000	-14.821319000
C	2.962796000	0.919792000	-13.190288000
C	4.147208000	4.614618000	-13.036595000
H	4.631103000	4.429761000	-12.073009000
C	5.240593000	5.079676000	-14.018066000
H	5.740672000	5.975112000	-13.629740000
H	6.001795000	4.305530000	-14.170233000
H	4.820892000	5.333143000	-14.998689000
C	3.103370000	5.726040000	-12.817343000
H	3.591392000	6.640530000	-12.458577000
H	2.575889000	5.971239000	-13.746778000
H	2.352834000	5.429842000	-12.075445000
C	3.040890000	-0.384456000	-12.400450000
H	3.593120000	-0.188996000	-11.476346000
C	3.815483000	-1.465676000	-13.179161000
H	3.926997000	-2.368336000	-12.566320000
H	3.292079000	-1.751453000	-14.099055000
H	4.817314000	-1.119609000	-13.458897000
C	1.644856000	-0.899335000	-12.000069000
H	1.732344000	-1.825461000	-11.419183000
H	1.107143000	-0.166490000	-11.385660000
H	1.029074000	-1.116063000	-12.880901000
C	4.189153000	2.381571000	-7.868591000
C	3.792091000	1.233138000	-7.145023000
C	3.573357000	1.368837000	-5.767125000
H	3.267567000	0.501112000	-5.188943000
C	3.753036000	2.592712000	-5.125718000
C	4.157671000	3.709126000	-5.854711000
H	4.303859000	4.657499000	-5.345224000
C	4.389857000	3.628876000	-7.234690000
C	3.602567000	-0.131900000	-7.800569000
H	3.842350000	-0.036054000	-8.863665000
C	4.559944000	-1.183488000	-7.207142000
C	2.141387000	-0.612260000	-7.701666000
H	1.448099000	0.104553000	-8.159565000
H	1.834169000	-0.752914000	-6.658594000
H	2.020936000	-1.573029000	-8.216746000
H	4.349069000	-1.366862000	-6.147102000
H	4.451000000	-2.137206000	-7.737447000
H	5.606291000	-0.867528000	-7.290402000
C	4.851232000	4.871130000	-7.991417000
H	4.970502000	4.600896000	-9.044639000
C	3.806123000	6.001352000	-7.920780000
C	6.219693000	5.363922000	-7.482214000
H	6.981148000	4.577832000	-7.545985000
H	6.163653000	5.690337000	-6.436928000
H	6.562472000	6.217660000	-8.079165000
H	3.670408000	6.358458000	-6.892860000
H	4.129172000	6.855416000	-8.528361000
H	2.828141000	5.672349000	-8.291228000
C	-0.426342000	3.236984000	-9.782020000
O	-0.513950000	3.330859000	-7.438013000
C	-0.378625000	4.013976000	-6.153157000
H	-1.073382000	4.857859000	-6.142060000
H	0.642514000	4.397353000	-6.077870000
N	-0.931418000	2.005645000	-9.529419000
N	-1.333557000	0.970542000	-9.341892000
C	-0.301231000	4.066395000	-8.535910000
O	-0.017780000	5.249906000	-8.536525000
C	-0.689158000	3.004355000	-5.069296000
H	-0.602662000	3.492640000	-4.092384000
H	0.015401000	2.166416000	-5.096125000
H	-1.707882000	2.615294000	-5.169769000
C	-0.776471000	3.779640000	-11.143860000
C	-1.019680000	2.891611000	-12.207895000
C	-0.870778000	5.162394000	-11.375199000
H	-0.948858000	1.817703000	-12.057466000
H	-0.685880000	5.860117000	-10.569608000
C	-1.359005000	3.375784000	-13.469727000
C	-1.205650000	5.635238000	-12.645907000
H	-1.548230000	2.672212000	-14.275377000
H	-1.278170000	6.707481000	-12.806096000
C	-1.452998000	4.751072000	-13.696871000
H	-1.717407000	5.127055000	-14.681018000
H	3.584097000	2.674607000	-4.055123000

7b

Electronic energy =	-1663.755813
Zero-point correction =	0.692649
Thermal correction to Energy =	0.733774
Thermal correction to Enthalpy =	0.734718
Thermal correction to Gibbs Free Energy =	0.614292

Cu	1.929190000	2.940659000	-10.048888000
C	3.775389000	2.332586000	-10.266301000
N	4.334340000	1.914212000	-11.412528000
C	5.748116000	1.491210000	-11.248131000
H	5.851523000	0.430962000	-11.498794000
H	6.393636000	2.070491000	-11.914051000
C	6.011529000	1.780144000	-9.757767000
H	6.766051000	2.557348000	-9.602795000
H	6.309572000	0.889450000	-9.197841000
N	4.688831000	2.260614000	-9.285999000
C	3.669543000	1.856412000	-12.687398000
C	3.751911000	2.971058000	-13.553155000
C	3.100693000	2.889765000	-14.791503000
H	3.144068000	3.735368000	-15.472205000
C	2.399132000	1.744842000	-15.163252000
H	1.901393000	1.702590000	-16.128559000
C	2.340665000	0.652174000	-14.301148000
H	1.794990000	-0.238209000	-14.600905000
C	2.975372000	0.680170000	-13.051688000
C	4.503818000	4.246249000	-13.181248000
H	4.970145000	4.091527000	-12.203620000
C	5.629241000	4.562223000	-14.184751000
H	6.189518000	5.446853000	-13.858790000
H	6.335688000	3.728806000	-14.274089000
H	5.230696000	4.772326000	-15.184309000
C	3.544082000	5.445063000	-13.045967000
H	4.092999000	6.339947000	-12.728511000
H	3.053335000	5.675001000	-13.999218000
H	2.760264000	5.249892000	-12.303625000
C	2.884907000	-0.538976000	-12.138138000
H	3.479401000	-0.335751000	-11.242512000

C	3.473846000	-1.797839000	-12.802710000
H	3.451846000	-2.640762000	-12.101639000
H	2.902798000	-2.090340000	-13.691578000
H	4.514442000	-1.640648000	-13.109643000
C	1.434204000	-0.792375000	-11.682174000
H	1.396044000	-1.633658000	-10.979444000
H	1.010627000	0.086962000	-11.180016000
H	0.784436000	-1.035659000	-12.531133000
C	4.464548000	2.640660000	-7.916787000
C	4.053689000	1.655125000	-6.990687000
C	3.836053000	2.050906000	-5.663941000
H	3.512840000	1.313583000	-4.934299000
C	4.030644000	3.371795000	-5.265803000
C	4.457406000	4.323268000	-6.189430000
H	4.612531000	5.349182000	-5.867523000
C	4.690616000	3.980605000	-7.528302000
C	3.840481000	0.196310000	-7.385459000
H	4.100903000	0.090594000	-8.442752000
C	4.761806000	-0.748018000	-6.589842000
C	2.365470000	-0.222756000	-7.231287000
H	1.703084000	0.416279000	-7.827882000
H	2.039422000	-0.161981000	-6.186147000
H	2.225401000	-1.258332000	-7.564442000
H	4.528763000	-0.731281000	-5.518674000
H	4.640091000	-1.780036000	-6.940459000
H	5.816453000	-0.472991000	-6.707477000
C	5.170284000	5.050484000	-8.505327000
H	5.324896000	4.576213000	-9.479244000
C	4.114962000	6.157117000	-8.694766000
C	6.519131000	5.654118000	-8.068736000
H	7.286112000	4.880256000	-7.947677000
H	6.431181000	6.190542000	-7.116574000
H	6.875545000	6.368732000	-8.820485000
H	3.923380000	6.691281000	-7.756760000
H	4.459688000	6.890900000	-9.433590000
H	3.160829000	5.745158000	-9.045495000
C	-0.027347000	3.588645000	-9.815025000
O	-0.871583000	2.412732000	-7.959781000
C	-1.124350000	2.250586000	-6.529816000
H	-1.691084000	3.118114000	-6.181864000
H	-0.159219000	2.233670000	-6.015795000
N	-0.804522000	2.749844000	-10.546158000
N	-1.417762000	2.028553000	-11.147625000
C	-0.269843000	3.546471000	-8.337118000
O	0.085821000	4.442878000	-7.600349000
C	-1.892338000	0.958886000	-6.349571000
H	-2.101640000	0.812020000	-5.284250000
H	-1.314778000	0.099472000	-6.706706000
H	-2.847039000	0.989477000	-6.885450000
H	3.855438000	3.658991000	-4.232234000
H	0.012288000	4.577943000	-10.271820000

TS1a

Electronic energy =	-2004.335506
Zero-point correction =	0.782313
Thermal correction to Energy =	0.830095
Thermal correction to Enthalpy =	0.831039
Thermal correction to Gibbs Free Energ y=	0.697208

Cu	1.763212000	2.850388000	-10.153127000
C	3.641845000	2.278341000	-10.308035000
N	4.284868000	1.984741000	-11.450235000
C	5.685167000	1.541922000	-11.235824000
H	5.807606000	0.513934000	-11.590073000
H	6.372943000	2.185036000	-11.791939000
C	5.843845000	1.669601000	-9.710088000
H	6.576626000	2.428613000	-9.419928000
H	6.112780000	0.724899000	-9.229506000
N	4.486948000	2.092180000	-9.281071000
C	3.722260000	2.061860000	-12.772099000
C	3.842614000	3.269222000	-13.497778000
C	3.291908000	3.319340000	-14.785793000
H	3.363088000	4.239726000	-15.358761000
C	2.661749000	2.209021000	-15.343674000
H	2.243871000	2.267506000	-16.345376000
C	2.575735000	1.020342000	-14.621679000
H	2.091549000	0.156448000	-15.068400000
C	3.107622000	0.916755000	-13.328844000
C	4.543982000	4.501702000	-12.934033000
H	4.916505000	4.252003000	-11.935928000
C	5.758741000	4.901786000	-13.793272000
H	6.283970000	5.748656000	-13.335312000
H	6.471574000	4.074764000	-13.892052000
H	5.456029000	5.204522000	-14.802646000
C	3.571461000	5.686609000	-12.776928000
H	4.086696000	6.545676000	-12.330319000
H	3.168080000	6.006461000	-13.744997000
H	2.724573000	5.427898000	-12.129799000
C	3.001635000	-0.408268000	-12.578495000
H	3.498426000	-0.291002000	-11.610815000
C	3.719496000	-1.544854000	-13.331527000
H	3.692337000	-2.468578000	-12.740958000
H	3.241483000	-1.753435000	-14.295986000
H	4.769824000	-1.297936000	-13.525416000
C	1.533616000	-0.782537000	-12.296006000
H	1.480623000	-1.716176000	-11.722888000
H	1.025813000	-0.001766000	-11.715954000
H	0.970201000	-0.928654000	-13.225279000
C	4.196699000	2.353844000	-7.896571000
C	3.779880000	1.285941000	-7.069793000
C	3.526996000	1.561247000	-5.719000000
H	3.200659000	0.757987000	-5.064409000
C	3.696227000	2.843930000	-5.201205000
C	4.127433000	3.878925000	-6.028644000
H	4.268653000	4.873245000	-5.614224000
C	4.392774000	3.658053000	-7.387299000
C	3.605508000	-0.136263000	-7.594853000
H	3.900154000	-0.144355000	-8.648558000
C	4.518488000	-1.132230000	-6.854087000
C	2.134669000	-0.590738000	-7.528578000
H	1.481720000	0.079268000	-8.101118000
H	1.767239000	-0.615577000	-6.495711000
H	2.028651000	-1.600206000	-7.944570000
H	4.251713000	-1.212683000	-5.793725000
H	4.426155000	-2.131499000	-7.296509000
H	5.571211000	-0.831797000	-6.911647000
C	4.891278000	4.812617000	-8.251668000
H	5.023655000	4.439449000	-9.271390000
C	3.869303000	5.963839000	-8.314851000
C	6.261591000	5.324673000	-7.766838000
H	7.008673000	4.522396000	-7.751204000
H	6.198485000	5.743233000	-6.755363000
H	6.628887000	6.115708000	-8.431899000
H	3.724169000	6.427780000	-7.331892000
H	4.219701000	6.743825000	-9.001715000
H	2.890445000	5.616812000	-8.666453000
C	-0.139259000	3.414959000	-9.910156000
O	-0.426020000	3.380850000	-7.530863000
C	-0.379617000	4.059807000	-6.238153000
H	-1.096404000	4.885115000	-6.259712000
H	0.624804000	4.471250000	-6.106568000
N	-0.833930000	1.824935000	-9.519889000
N	-1.097083000	0.748619000	-9.564995000
C	-0.213907000	4.141169000	-8.609048000
O	0.007169000	5.341131000	-8.587765000
C	-0.720690000	3.037502000	-5.175166000
H	-0.698290000	3.521854000	-4.192768000
H	0.004497000	2.217040000	-5.168605000
H	-1.722612000	2.623263000	-5.330639000
C	-0.984134000	3.893716000	-11.023595000
C	-0.586132000	3.634383000	-12.349130000
C	-2.182927000	4.603331000	-10.796588000
H	0.333477000	3.085745000	-12.525523000
H	-2.509014000	4.805823000	-9.780654000
C	-1.356696000	4.079089000	-13.421139000

C	-2.947200000	5.052394000	-11.868292000
H	-1.037028000	3.877534000	-14.439242000
H	-3.865191000	5.603060000	-11.684954000
C	-2.536013000	4.789681000	-13.180665000
H	-3.136978000	5.140411000	-14.015166000
H	3.499865000	3.035501000	-4.149501000

TS1b

Electronic energy = -1773.271951
Zero-point correction = 0.700896
Thermal correction to Energy = 0.744105
Thermal correction to Enthalpy = 0.745050
Thermal correction to Gibbs Free Energy = 0.621727

Cu	1.969003000	2.948861000	-9.982159000
C	3.815356000	2.313208000	-10.261078000
N	4.340563000	1.869146000	-11.413002000
C	5.777543000	1.512620000	-11.296620000
H	5.938325000	0.481039000	-11.621093000
H	6.375456000	2.173923000	-11.931454000
C	6.049408000	1.717726000	-9.794544000
H	6.857678000	2.428062000	-9.601226000
H	6.275824000	0.782421000	-9.273363000
N	4.758390000	2.265125000	-9.308361000
C	3.648624000	1.815984000	-12.672639000
C	3.594401000	2.975516000	-13.479949000
C	2.912876000	2.891995000	-14.702010000
H	2.847205000	3.771632000	-15.336632000
C	2.326146000	1.699556000	-15.120299000
H	1.805689000	1.655764000	-16.073501000
C	2.412515000	0.561630000	-14.321031000
H	1.958758000	-0.365975000	-14.659133000
C	3.077893000	0.591696000	-13.087853000
C	4.244078000	4.294269000	-13.069638000
H	4.777616000	4.130738000	-12.128731000
C	5.282375000	4.766800000	-14.105283000
H	5.780020000	5.677551000	-13.751043000
H	6.052522000	4.005861000	-14.277781000
H	4.817478000	4.996886000	-15.070926000
C	3.188912000	5.387857000	-12.812951000
H	3.672530000	6.315150000	-12.482443000
H	2.616263000	5.613591000	-13.720537000
H	2.479361000	5.080860000	-12.034354000
C	3.163652000	-0.680031000	-12.248280000
H	3.735257000	-0.451187000	-11.343812000
C	3.912503000	-1.799783000	-12.996446000
H	4.024145000	-2.679408000	-12.351011000
H	3.370082000	-2.114114000	-13.895797000
H	4.913538000	-1.477307000	-13.305978000
C	1.769922000	-1.160620000	-11.799268000
H	1.860069000	-2.048373000	-11.161636000
H	1.243198000	-0.386440000	-11.227519000
H	1.142141000	-1.428767000	-12.657199000
C	4.564097000	2.644235000	-7.934219000
C	4.089906000	1.683168000	-7.012116000
C	3.913260000	2.082876000	-5.680281000
H	3.545417000	1.364153000	-4.953206000
C	4.202831000	3.383523000	-5.273634000
C	4.684762000	4.310913000	-6.194640000
H	4.912500000	5.321802000	-5.867885000
C	4.884203000	3.962363000	-7.537295000
C	3.765313000	0.246649000	-7.413232000
H	3.980269000	0.134919000	-8.480053000
C	4.648588000	-0.764745000	-6.657880000
C	2.271572000	-0.075528000	-7.210042000
H	1.630583000	0.618472000	-7.768246000
H	1.988778000	-0.015642000	-6.152357000
H	2.050657000	-1.092381000	-7.556581000
H	4.460906000	-0.734887000	-5.578106000
H	4.439626000	-1.784364000	-7.003535000
H	5.714397000	-0.564576000	-6.818618000
C	5.432155000	5.003294000	-8.509559000
H	5.536622000	4.529452000	-9.490238000
C	4.462818000	6.189884000	-8.674587000
C	6.829873000	5.492826000	-8.084106000
H	7.537755000	4.660219000	-7.996999000
H	6.800010000	6.008432000	-7.117064000
H	7.226490000	6.197950000	-8.824621000
H	4.321171000	6.726512000	-7.729030000
H	4.855934000	6.904378000	-9.408265000
H	3.477153000	5.856272000	-9.021579000
C	0.208464000	3.639134000	-9.637441000
O	-1.101897000	2.576337000	-7.906508000
C	-1.557769000	2.573768000	-6.510360000
H	-2.145574000	3.480896000	-6.347122000
H	-0.673752000	2.603704000	-5.868296000
N	-0.909557000	2.270411000	-10.645940000
N	-1.236412000	1.391965000	-11.230811000
C	-0.355463000	3.599763000	-8.279048000
O	0.016582000	4.536570000	-7.585313000
C	-2.374512000	1.317745000	-6.304861000
H	-2.732644000	1.292732000	-5.269883000
H	-1.772492000	0.420181000	-6.481458000
H	-3.244480000	1.297390000	-6.969514000
H	4.057136000	3.673427000	-4.236224000
H	-0.227489000	4.447600000	-10.230078000

8a

Electronic energy = -1894.847454
Zero-point correction = 0.775225
Thermal correction to Energy = 0.820891
Thermal correction to Enthalpy = 0.821835
Thermal correction to Gibbs Free Energy = 0.692183

Cu	1.945162000	3.142504000	-10.055415000
C	3.791131000	2.472699000	-10.298648000
N	4.363232000	2.069906000	-11.444323000
C	5.731354000	1.526529000	-11.250009000
H	5.738927000	0.456274000	-11.481149000
H	6.439365000	2.030671000	-11.912727000
C	5.992410000	1.815409000	-9.760649000
H	6.754752000	2.585859000	-9.605685000
H	6.278642000	0.924039000	-9.196596000
N	4.673734000	2.315887000	-9.299382000
C	3.717215000	2.044132000	-12.729053000
C	3.933919000	3.118167000	-13.622480000
C	3.294738000	3.074912000	-14.868985000
H	3.441288000	3.891622000	-15.570230000
C	2.481101000	2.001152000	-15.225061000
H	1.995345000	1.986393000	-16.197286000
C	2.298963000	0.941489000	-14.339233000
H	1.673760000	0.101372000	-14.629129000
C	2.916976000	0.933121000	-13.081069000
C	4.830580000	4.304559000	-13.278979000
H	5.263534000	4.126320000	-12.290268000
C	5.997363000	4.437064000	-14.276634000
H	6.665193000	5.252280000	-13.973272000
H	6.589139000	3.515515000	-14.327958000
H	5.639444000	4.660596000	-15.288575000
C	4.029778000	5.618200000	-13.195772000
H	4.691134000	6.449864000	-12.923550000
H	3.561450000	5.865781000	-14.155896000
H	3.237444000	5.557449000	-12.439884000
C	2.717513000	-0.266319000	-12.158291000
H	3.279388000	-0.084185000	-11.237407000
C	3.273697000	-1.557948000	-12.788827000
H	3.176000000	-2.394616000	-12.086492000
H	2.730869000	-1.825532000	-13.703011000
H	4.334052000	-1.455475000	-13.047839000
C	1.239394000	-0.446500000	-11.762346000
H	1.131830000	-1.291047000	-11.070939000
H	0.846340000	0.448595000	-11.264747000
H	0.609267000	-0.649192000	-12.636497000
C	4.439287000	2.675217000	-7.926219000

C	3.993105000	1.681106000	-7.025902000
C	3.769746000	2.054950000	-5.693648000
H	3.420177000	1.311231000	-4.982927000
C	3.991496000	3.362309000	-5.265795000
C	4.451563000	4.321964000	-6.164577000
H	4.629017000	5.336790000	-5.819662000
C	4.693571000	4.000775000	-7.507224000
C	3.744373000	0.237817000	-7.455473000
H	4.020826000	0.146470000	-8.510192000
C	4.620918000	-0.751439000	-6.664269000
C	2.254272000	-0.137114000	-7.338558000
H	1.623317000	0.538710000	-7.928402000
H	1.912726000	-0.094096000	-6.297357000
H	2.088106000	-1.158678000	-7.701814000
H	4.364535000	-0.755442000	-5.598288000
H	4.479027000	-1.770620000	-7.043657000
H	5.685215000	-0.503112000	-6.751579000
C	5.223718000	5.075952000	-8.452013000
H	5.344616000	4.628520000	-9.443090000
C	4.233715000	6.247984000	-8.595540000
C	6.608957000	5.582408000	-8.004780000
H	7.332760000	4.762069000	-7.932902000
H	6.561050000	6.073487000	-7.025705000
H	6.996713000	6.312999000	-8.725117000
H	4.084391000	6.766866000	-7.641305000
H	4.613788000	6.980715000	-9.317921000
H	3.253021000	5.903488000	-8.945799000
C	0.141983000	3.749257000	-9.740803000
O	-0.804148000	2.603000000	-7.912228000
C	-1.057354000	2.455091000	-6.478867000
H	-1.621319000	3.326153000	-6.135643000
H	-0.091635000	2.439042000	-5.965372000
C	-0.211556000	3.731094000	-8.307658000
O	0.102883000	4.663969000	-7.583977000
C	-1.829903000	1.167737000	-6.285800000
H	-2.037368000	1.029577000	-5.218815000
H	-1.257555000	0.303187000	-6.638577000
H	-2.785714000	1.198105000	-6.819818000
C	-0.792799000	4.261408000	-10.671829000
C	-0.424011000	4.328188000	-12.049728000
C	-2.100270000	4.702281000	-10.297226000
H	0.568502000	3.991470000	-12.333167000
H	-2.403192000	4.662909000	-9.255236000
C	-1.311937000	4.804058000	-12.999750000
C	-2.979668000	5.181220000	-11.251537000
H	-1.027078000	4.849495000	-14.046044000
H	-3.971167000	5.516459000	-10.964201000
C	-2.586194000	5.231340000	-12.599039000
H	-3.282669000	5.607741000	-13.343215000
H	3.811254000	3.632343000	-4.228450000

8b

Electronic energy =	-1663.755813
Zero-point correction =	0.692649
Thermal correction to Energy =	0.733774
Thermal correction to Enthalpy =	0.734718
Thermal correction to Gibbs Free Energy =	0.614292

Cu	2.053521000	3.105779000	-9.875565000
C	3.889970000	2.435376000	-10.211318000
N	4.367135000	1.996757000	-11.384431000
C	5.770197000	1.518535000	-11.297464000
H	5.817732000	0.456864000	-11.558005000
H	6.400866000	2.076665000	-11.995205000
C	6.123896000	1.789549000	-9.822153000
H	6.922505000	2.528216000	-9.706059000
H	6.405290000	0.883143000	-9.279050000
N	4.851471000	2.331634000	-9.282830000
C	3.623911000	1.943672000	-12.615641000
C	3.688278000	3.042937000	-13.501235000
C	2.964344000	2.963687000	-14.698624000
H	2.992403000	3.797351000	-15.394905000
C	2.213909000	1.832694000	-15.013114000
H	1.662279000	1.790517000	-15.948687000
C	2.175797000	0.753447000	-14.132972000
H	1.591997000	-0.126402000	-14.388980000
C	2.878766000	0.781978000	-12.920852000
C	4.510611000	4.292778000	-13.199761000
H	5.030991000	4.133787000	-12.250543000
C	5.582369000	4.540978000	-14.278307000
H	6.208401000	5.397894000	-14.001479000
H	6.236599000	3.670421000	-14.403751000
H	5.129803000	4.762193000	-15.252050000
C	3.613160000	5.533710000	-13.027347000
H	4.221128000	6.411180000	-12.775468000
H	3.062602000	5.761830000	-13.947731000
H	2.879643000	5.390730000	-12.224188000
C	2.811995000	-0.421324000	-11.984663000
H	3.442951000	-0.209155000	-11.116299000
C	3.362339000	-1.695959000	-12.652495000
H	3.358758000	-2.528510000	-11.938793000
H	2.753871000	-1.994569000	-13.514269000
H	4.391795000	-1.555197000	-13.002159000
C	1.379639000	-0.652984000	-11.464858000
H	1.363413000	-1.486980000	-10.752619000
H	0.990739000	0.236274000	-10.953089000
H	0.690683000	-0.897274000	-12.282056000
C	4.707746000	2.704430000	-7.900337000
C	4.289386000	1.728553000	-6.966909000
C	4.151792000	2.117654000	-5.627496000
H	3.824510000	1.387983000	-4.892049000
C	4.428882000	3.422065000	-5.224127000
C	4.858959000	4.363531000	-6.156348000
H	5.080595000	5.376108000	-5.831212000
C	5.013918000	4.027492000	-7.508328000
C	3.985335000	0.286629000	-7.364508000
H	4.173602000	0.182710000	-8.437191000
C	4.911452000	-0.707602000	-6.638212000
C	2.505870000	-0.069266000	-7.120097000
H	1.834491000	0.607638000	-7.662629000
H	2.250876000	-0.013084000	-6.055127000
H	2.299052000	-1.091805000	-7.458416000
H	4.750352000	-0.689188000	-5.553975000
H	4.717827000	-1.729709000	-6.985409000
H	5.967927000	-0.481600000	-6.824054000
C	5.500563000	5.087270000	-8.493220000
H	5.596041000	4.618837000	-9.477412000
C	4.488541000	6.242137000	-8.627917000
C	6.891421000	5.625651000	-8.105907000
H	7.628399000	4.817755000	-8.029276000
H	6.867469000	6.150227000	-7.143619000
H	7.246181000	6.336197000	-8.862192000
H	4.354253000	6.769968000	-7.676220000
H	4.838666000	6.971559000	-9.368341000
H	3.504557000	5.879362000	-8.950560000
C	0.220715000	3.497040000	-9.693586000
O	-1.195196000	2.181111000	-8.223016000
C	-1.913646000	2.114294000	-6.934040000
H	-2.678980000	2.894280000	-6.941640000
H	-1.193051000	2.323550000	-6.140058000
C	-0.564198000	3.291085000	-8.497602000
O	-0.466588000	4.315516000	-7.820206000
C	-2.505268000	0.727770000	-6.825065000
H	-3.053310000	0.651574000	-5.879568000
H	-1.722734000	-0.038125000	-6.831883000
H	-3.204207000	0.529922000	-7.644171000
H	4.315718000	3.703588000	-4.180388000
H	-0.353077000	4.041589000	-10.453687000

$TS2_{CC}$ (*E*)

Electronic energy =	-2310.786437
Zero-point correction =	0.882205
Thermal correction to Energy =	0.936655
Thermal correction to Enthalpy =	0.937600

Thermal correction to Gibbs Free Energy = 0.790471

Cu	2.173784000	3.834313000	-10.355622000
C	4.054924000	4.154001000	-10.875109000
N	4.620789000	3.775637000	-12.033929000
C	6.053158000	4.150647000	-12.136260000
H	6.659584000	3.269627000	-12.362569000
H	6.188276000	4.881916000	-12.939405000
C	6.340890000	4.737011000	-10.744090000
H	6.751758000	5.748724000	-10.784209000
H	7.015633000	4.111025000	-10.150719000
N	4.994321000	4.750134000	-10.119042000
C	3.955560000	3.078503000	-13.102251000
C	3.384175000	3.818927000	-14.162748000
C	2.749686000	3.108765000	-15.191643000
H	2.301746000	3.654405000	-16.017419000
C	2.696532000	1.716573000	-15.181377000
H	2.202131000	1.185916000	-15.990981000
C	3.295719000	1.004276000	-14.144688000
H	3.271433000	-0.081892000	-14.157195000
C	3.944917000	1.664042000	-13.091983000
C	3.476562000	5.340610000	-14.248411000
H	3.931666000	5.705774000	-13.323287000
C	4.391277000	5.768708000	-15.414524000
H	4.510426000	6.859013000	-15.423187000
H	5.387968000	5.319818000	-15.332497000
H	3.969313000	5.470679000	-16.381919000
C	2.095546000	6.009847000	-14.371919000
H	2.209477000	7.099794000	-14.416865000
H	1.570555000	5.694759000	-15.281355000
H	1.458865000	5.781281000	-13.510323000
C	4.643579000	0.842698000	-12.011225000
H	5.053418000	1.536466000	-11.271155000
C	5.825223000	0.046008000	-12.600121000
H	6.358865000	-0.485788000	-11.802901000
H	5.481741000	-0.699979000	-13.326786000
H	6.542024000	0.701674000	-13.108140000
C	3.673552000	-0.096685000	-11.271958000
H	4.201539000	-0.630955000	-10.472345000
H	2.841743000	0.452287000	-10.817107000
H	3.249647000	-0.850027000	-11.946840000
C	4.805483000	5.227009000	-8.775003000
C	4.867118000	4.310435000	-7.699299000
C	4.668450000	4.805920000	-6.403009000
H	4.703567000	4.120753000	-5.560640000
C	4.443946000	6.161636000	-6.175714000
C	4.428489000	7.054323000	-7.245481000
H	4.276466000	8.113059000	-7.055076000
C	4.615757000	6.612231000	-8.562320000
C	5.181036000	2.828481000	-7.891939000
H	5.273752000	2.636588000	-8.964970000
C	6.531603000	2.464431000	-7.242655000
C	4.058315000	1.917982000	-7.360874000
H	3.101806000	2.134260000	-7.850426000
H	3.917403000	2.034936000	-6.279850000
H	4.302481000	0.865915000	-7.551808000
H	6.502893000	2.600530000	-6.154995000
H	6.778390000	1.414416000	-7.441597000
H	7.346147000	3.084699000	-7.635129000
C	4.655736000	7.631790000	-9.698689000
H	4.700323000	7.083314000	-10.644346000
C	3.398368000	8.518357000	-9.745516000
C	5.926310000	8.501343000	-9.604074000
H	6.836913000	7.890668000	-9.602230000
H	5.927611000	9.103229000	-8.687071000
H	5.980856000	9.189665000	-10.456284000
H	3.284699000	9.110440000	-8.829829000
H	3.468468000	9.222617000	-10.583699000
H	2.489287000	7.924101000	-9.886259000
C	0.377218000	3.305842000	-9.776328000
O	-0.588584000	2.035039000	-11.586299000
C	-0.826869000	0.747567000	-12.234349000
H	-1.443069000	0.135657000	-11.569521000
H	0.135919000	0.248988000	-12.373728000
C	0.018460000	2.003009000	-10.393871000
O	0.377067000	0.974438000	-9.834761000
C	-1.517230000	1.026263000	-13.552437000
H	-1.720218000	0.076468000	-14.059544000
H	-0.885705000	1.636009000	-14.207726000
H	-2.470970000	1.542702000	-13.399057000
H	4.296337000	6.525461000	-5.162089000
C	-0.236175000	3.624430000	-8.506957000
C	-1.383181000	2.941144000	-8.017217000
C	0.321662000	4.656115000	-7.706846000
H	-1.821677000	2.138931000	-8.601952000
H	1.195280000	5.187140000	-8.072645000
C	-1.929287000	3.267176000	-6.781262000
C	-0.228306000	4.977884000	-6.473541000
H	-2.799403000	2.731247000	-6.414081000
H	0.216808000	5.760424000	-5.866344000
C	-1.354120000	4.283297000	-6.009777000
H	-1.780375000	4.532003000	-5.041831000
C	-0.835211000	4.836170000	-11.209468000
O	-1.371630000	6.671048000	-9.869959000
C	-1.133749000	8.009202000	-9.338442000
H	-1.021017000	8.696912000	-10.181053000
H	-0.198177000	7.992304000	-8.772755000
N	-2.060674000	4.406274000	-10.935478000
N	-3.059791000	4.009769000	-10.588130000
C	-0.477147000	6.192060000	-10.740202000
O	0.533431000	6.762694000	-11.108641000
C	-2.318972000	8.363694000	-8.466154000
H	-2.169430000	9.364710000	-8.046703000
H	-2.425292000	7.655705000	-7.637635000
H	-3.248101000	8.369563000	-9.045929000
H	-0.397334000	4.435675000	-12.112504000

$TS2_{CC}$ (*Z*)

Electronic energy = -2310.780374
Zero-point correction = 0.881849
Thermal correction to Energy = 0.936544
Thermal correction to Enthalpy = 0.937489
Thermal correction to Gibbs Free Energy = 0.788132

Cu	2.181681000	3.925676000	-10.547798000
C	4.094014000	4.152584000	-10.971979000
N	4.719670000	3.777006000	-12.100997000
C	6.190855000	3.965035000	-12.048124000
H	6.692402000	2.997003000	-12.143156000
H	6.518473000	4.607616000	-12.870235000
C	6.393999000	4.608191000	-10.664919000
H	6.796814000	5.623917000	-10.722507000
H	7.039415000	4.015597000	-10.010179000
N	5.013481000	4.639729000	-10.120931000
C	4.085472000	3.183127000	-13.246627000
C	3.685620000	4.015981000	-14.316218000
C	3.050476000	3.415669000	-15.412300000
H	2.721823000	4.034785000	-16.242444000
C	2.843810000	2.038418000	-15.459480000
H	2.351286000	1.592504000	-16.319713000
C	3.286702000	1.229965000	-14.414585000
H	3.144803000	0.154329000	-14.472796000
C	3.922879000	1.779548000	-13.292937000
C	3.942981000	5.521534000	-14.325890000
H	4.495922000	5.776672000	-13.416717000
C	4.819535000	5.932434000	-15.525256000
H	5.056661000	7.001873000	-15.471608000
H	5.764000000	5.376157000	-15.541950000
H	4.309164000	5.753281000	-16.478822000
C	2.633339000	6.332354000	-14.306862000
H	2.850760000	7.407400000	-14.316373000
H	2.009090000	6.109913000	-15.180206000
H	2.045115000	6.118837000	-13.406718000
C	4.452055000	0.856855000	-12.198086000
H	4.873170000	1.480780000	-11.404436000

C	5.590497000	-0.035639000	-12.732174000
H	6.013433000	-0.637430000	-11.918637000
H	5.231142000	-0.725835000	-13.504861000
H	6.400068000	0.561153000	-13.168222000
C	3.343159000	-0.002272000	-11.563038000
H	3.761854000	-0.627846000	-10.765363000
H	2.553621000	0.615642000	-11.120885000
H	2.879813000	-0.671998000	-12.297418000
C	4.745049000	5.138481000	-8.798828000
C	4.770365000	4.241568000	-7.706305000
C	4.502258000	4.754385000	-6.429980000
H	4.508164000	4.083420000	-5.575621000
C	4.235536000	6.108241000	-6.238187000
C	4.245087000	6.981329000	-7.324065000
H	4.051269000	8.038357000	-7.163284000
C	4.508624000	6.520911000	-8.621775000
C	5.096729000	2.759079000	-7.866135000
H	5.245528000	2.559156000	-8.931464000
C	6.408150000	2.396888000	-7.140913000
C	3.941945000	1.857953000	-7.389760000
H	3.014254000	2.073441000	-7.932488000
H	3.742803000	1.986205000	-6.319192000
H	4.191592000	0.803090000	-7.557051000
H	6.323989000	2.548675000	-6.058186000
H	6.657768000	1.342586000	-7.311280000
H	7.247273000	3.005411000	-7.498648000
C	4.547630000	7.517375000	-9.778113000
H	4.785794000	6.967205000	-10.693333000
C	3.184109000	8.200215000	-9.996799000
C	5.655187000	8.569144000	-9.570819000
H	6.634486000	8.098550000	-9.425647000
H	5.452958000	9.197038000	-8.695236000
H	5.721978000	9.228041000	-10.445011000
H	2.873583000	8.771376000	-9.113988000
H	3.237598000	8.897183000	-10.842014000
H	2.398999000	7.466220000	-10.215264000
C	0.323014000	3.586679000	-9.988763000
O	-0.761163000	2.053368000	-11.507080000
C	-1.039406000	0.679732000	-11.916027000
H	-1.736925000	0.244417000	-11.194185000
H	-0.106127000	0.112325000	-11.880711000
C	-0.095023000	2.209891000	-10.360535000
O	0.272928000	1.282353000	-9.649200000
C	-1.623830000	0.722733000	-13.312280000
H	-1.863852000	-0.298243000	-13.629797000
H	-0.910845000	1.145276000	-14.028356000
H	-2.543913000	1.315779000	-13.339494000
H	4.030469000	6.485007000	-5.239482000
C	-0.241985000	4.128951000	-8.766410000
C	-1.389130000	3.573608000	-8.143050000
C	0.377513000	5.243524000	-8.148625000
H	-1.892161000	2.726377000	-8.599693000
H	1.254844000	5.677399000	-8.619922000
C	-1.867880000	4.088752000	-6.944981000
C	-0.111424000	5.767298000	-6.958608000
H	-2.739502000	3.644620000	-6.473238000
H	0.380653000	6.617026000	-6.494782000
C	-1.232612000	5.186788000	-6.352697000
H	-1.612184000	5.590464000	-5.418056000
C	-0.761947000	5.001670000	-11.521611000
O	-2.947558000	4.308583000	-12.041623000
C	-4.384906000	4.293084000	-11.795392000
H	-4.733647000	5.326653000	-11.720992000
H	-4.560877000	3.797970000	-10.835631000
N	-0.422980000	4.531063000	-12.724026000
N	-0.117370000	4.062298000	-13.700933000
C	-2.210182000	5.044433000	-11.201655000
O	-2.634299000	5.682256000	-10.257722000
C	-5.037202000	3.555120000	-12.945091000
H	-6.120423000	3.525929000	-12.783235000
H	-4.672822000	2.524512000	-13.014308000
H	-4.846331000	4.060754000	-13.897707000
H	-0.147104000	5.831691000	-11.199081000

$TS2_{HC}$

Electronic energy =	-2541.824004
Zero-point correction =	0.963027
Thermal correction to Energy =	1.022235
Thermal correction to Enthalpy =	1.023179
Thermal correction to Gibbs Free Energy =	0.865872

Cu	1.998878000	4.160989000	-10.230987000
C	3.876369000	4.211219000	-10.886502000
N	4.330914000	3.761092000	-12.070150000
C	5.804288000	3.860161000	-12.213824000
H	6.229173000	2.868246000	-12.392545000
H	6.055496000	4.502999000	-13.062572000
C	6.229574000	4.459091000	-10.863100000
H	6.735556000	5.423335000	-10.965127000
H	6.873112000	3.789684000	-10.284419000
N	4.930679000	4.636664000	-10.167571000
C	3.524815000	3.180394000	-13.109208000
C	3.036964000	4.008352000	-14.145307000
C	2.226389000	3.420885000	-15.126405000
H	1.828284000	4.037111000	-15.927841000
C	1.930320000	2.059791000	-15.095750000
H	1.297152000	1.624792000	-15.864745000
C	2.468450000	1.250535000	-14.096738000
H	2.262257000	0.183715000	-14.103317000
C	3.287627000	1.786664000	-13.093455000
C	3.400446000	5.487764000	-14.253211000
H	4.024957000	5.746347000	-13.392691000
C	4.232112000	5.756773000	-15.523887000
H	4.557669000	6.803802000	-15.550699000
H	5.126042000	5.123258000	-15.561782000
H	3.648387000	5.565411000	-16.432104000
C	2.165197000	6.405133000	-14.211728000
H	2.471122000	7.455724000	-14.287706000
H	1.476296000	6.196967000	-15.038517000
H	1.612512000	6.284824000	-13.273084000
C	3.937445000	0.856012000	-12.071612000
H	4.522648000	1.468523000	-11.378970000
C	4.914768000	-0.114476000	-12.765494000
H	5.441284000	-0.722319000	-12.019619000
H	4.386494000	-0.798617000	-13.440225000
H	5.665764000	0.423841000	-13.355728000
C	2.904560000	0.080520000	-11.235264000
H	3.413647000	-0.573544000	-10.516644000
H	2.255443000	0.755669000	-10.667356000
H	2.270484000	-0.553124000	-11.866706000
C	4.885068000	5.179470000	-8.836545000
C	4.978608000	4.303764000	-7.730381000
C	4.954291000	4.865657000	-6.446520000
H	5.020929000	4.213805000	-5.580033000
C	4.856701000	6.243149000	-6.263087000
C	4.793342000	7.090826000	-7.366976000
H	4.733893000	8.164981000	-7.215437000
C	4.814729000	6.581793000	-8.672732000
C	5.145513000	2.794296000	-7.884966000
H	5.095252000	2.554314000	-8.951222000
C	6.526855000	2.339094000	-7.373090000
C	4.023146000	2.004298000	-7.185638000
H	3.034438000	2.275198000	-7.572009000
H	4.021304000	2.176163000	-6.102765000
H	4.162819000	0.928717000	-7.349326000
H	6.630361000	2.514761000	-6.295630000
H	6.664365000	1.265697000	-7.552060000
H	7.340623000	2.873155000	-7.877581000
C	4.772439000	7.546641000	-9.855223000
H	4.838281000	6.958160000	-10.775261000
C	3.443176000	8.322451000	-9.907071000
C	5.971950000	8.513725000	-9.840883000
H	6.924469000	7.971596000	-9.814196000
H	5.942944000	9.181501000	-8.971804000
H	5.964264000	9.140447000	-10.740968000

H	3.299436000	8.937133000	-9.010417000
H	3.425163000	8.991398000	-10.776424000
H	2.587963000	7.641812000	-9.987679000
C	0.237622000	3.871486000	-9.335256000
O	-0.850017000	2.155047000	-10.615010000
C	-1.106403000	0.746398000	-10.889523000
H	-1.701536000	0.339321000	-10.066321000
H	-0.150325000	0.218816000	-10.915909000
C	-0.116041000	2.439543000	-9.527255000
O	0.355119000	1.578926000	-8.793013000
C	-1.837556000	0.662605000	-12.213366000
H	-2.055571000	-0.387876000	-12.436649000
H	-1.224418000	1.065846000	-13.026924000
H	-2.781565000	1.214662000	-12.179785000
H	4.842143000	6.657373000	-5.258345000
C	0.037415000	4.420214000	-7.999498000
C	-0.817225000	3.824326000	-7.036241000
C	0.750259000	5.582337000	-7.618397000
H	-1.376465000	2.933027000	-7.295848000
H	1.407053000	6.051666000	-8.343698000
C	-0.926188000	4.351696000	-5.755709000
C	0.637367000	6.112638000	-6.336382000
H	-1.575383000	3.874318000	-5.027175000
H	1.204584000	6.997790000	-6.064249000
C	-0.199963000	5.496933000	-5.402042000
H	-0.286705000	5.904435000	-4.398420000
C	-1.370601000	4.982360000	-10.520723000
O	-3.133197000	4.100670000	-9.208647000
C	-4.442825000	3.460078000	-9.056236000
H	-4.378179000	2.458581000	-9.488550000
H	-5.169700000	4.041763000	-9.629502000
N	-0.817602000	4.719158000	-11.733176000
N	-0.290890000	4.422393000	-12.677031000
C	-2.690334000	4.219178000	-10.456425000
O	-3.251884000	3.799864000	-11.447077000
C	-4.773374000	3.425550000	-7.580440000
H	-5.755385000	2.956946000	-7.450990000
H	-4.818140000	4.434393000	-7.157198000
H	-4.039238000	2.838179000	-7.019573000
C	-1.308128000	6.425927000	-10.123317000
C	-2.044942000	6.888678000	-9.019825000
C	-0.516267000	7.341165000	-10.840751000
H	-2.657504000	6.204356000	-8.448112000
H	0.056816000	7.023333000	-11.706573000
C	-1.992570000	8.234745000	-8.653748000
C	-0.470214000	8.683226000	-10.466547000
H	-2.573495000	8.571786000	-7.799869000
H	0.140347000	9.373970000	-11.041111000
C	-1.209005000	9.138499000	-9.371591000
H	-1.175605000	10.185698000	-9.085221000

TS2$_{CC'}$

Electronic energy =	-2310.758704
Zero-point correction =	0.880109
Thermal correction to Energy =	0.935493
Thermal correction to Enthalpy =	0.936438
Thermal correction to Gibbs Free Energy =	0.781866

Cu	2.297564000	4.419771000	-10.748424000
C	4.269855000	4.274739000	-10.948700000
N	4.925899000	3.932557000	-12.066677000
C	6.397817000	3.870834000	-11.880877000
H	6.753882000	2.854364000	-12.073205000
H	6.893448000	4.551035000	-12.579098000
C	6.564728000	4.295031000	-10.409242000
H	7.118902000	5.231790000	-10.296973000
H	7.049292000	3.528327000	-9.798574000
N	5.159737000	4.485094000	-9.968354000
C	4.308338000	3.611123000	-13.326346000
C	4.159663000	4.629932000	-14.295093000
C	3.564501000	4.290246000	-15.517258000
H	3.431801000	5.056976000	-16.275265000
C	3.142302000	2.988038000	-15.775914000
H	2.681404000	2.745880000	-16.729882000
C	3.313055000	1.994952000	-14.814140000
H	2.988000000	0.980648000	-15.028305000
C	3.905412000	2.279242000	-13.576144000
C	4.615082000	6.066434000	-14.053500000
H	5.089571000	6.109591000	-13.068479000
C	5.663602000	6.516114000	-15.08901900
H	6.028193000	7.521251000	-14.845227000
H	6.525815000	5.839422000	-15.109976000
H	5.242517000	6.553058000	-16.100700000
C	3.419881000	7.038337000	-14.027411000
H	3.759903000	8.057519000	-13.806360000
H	2.900313000	7.062222000	-14.992685000
H	2.688369000	6.753354000	-13.262020000
C	4.101377000	1.155180000	-12.562237000
H	4.615968000	1.570703000	-11.690617000
C	4.990922000	0.031630000	-13.128670000
H	5.180755000	-0.726581000	-12.359225000
H	4.513778000	-0.470698000	-13.978316000
H	5.958851000	0.417828000	-13.469013000
C	2.754329000	0.588911000	-12.072556000
H	2.918901000	-0.188064000	-11.315993000
H	2.129686000	1.370587000	-11.622519000
H	2.185832000	0.138785000	-12.894999000
C	4.836557000	4.885559000	-8.624120000
C	4.696649000	3.891873000	-7.628790000
C	4.390064000	4.307243000	-6.325948000
H	4.271783000	3.562977000	-5.543318000
C	4.232694000	5.657044000	-6.018726000
C	4.389256000	6.621792000	-7.011600000
H	4.272571000	7.672401000	-6.760694000
C	4.701931000	6.261312000	-8.329468000
C	4.876630000	2.405767000	-7.923887000
H	5.042513000	2.293038000	-8.999650000
C	6.115823000	1.839399000	-7.203218000
C	3.619003000	1.591893000	-7.564896000
H	2.727693000	1.978745000	-8.072940000
H	3.421383000	1.612766000	-6.486751000
H	3.749660000	0.542746000	-7.857195000
H	5.998186000	1.883579000	-6.113915000
H	6.271890000	0.789525000	-7.479939000
H	7.023112000	2.396924000	-7.464066000
C	4.882089000	7.349585000	-9.384074000
H	5.182050000	6.867189000	-10.319005000
C	3.562165000	8.097889000	-9.655047000
C	6.000748000	8.336813000	-8.999438000
H	6.950461000	7.818626000	-8.822521000
H	5.751348000	8.897658000	-8.090991000
H	6.157963000	9.064263000	-9.805107000
H	3.211688000	8.627414000	-8.760971000
H	3.698810000	8.839344000	-10.451631000
H	2.768885000	7.407784000	-9.968455000
C	0.539424000	4.517309000	-10.089464000
O	-0.902986000	2.577084000	-10.045034000
C	-1.531008000	1.512909000	-9.237073000
H	-2.106298000	1.993118000	-8.441984000
H	-0.728732000	0.919176000	-8.792507000
C	-0.145499000	3.435031000	-9.409454000
O	0.149956000	3.457338000	-8.215173000
C	-2.403334000	0.699039000	-10.164775000
H	-2.875662000	-0.104466000	-9.589071000
H	-1.813786000	0.245625000	-10.968332000
H	-3.193432000	1.316030000	-10.604847000
H	3.992575000	5.957848000	-5.002219000
C	-1.906755000	5.424085000	-12.628524000
O	-1.816102000	7.154864000	-11.062607000
C	-1.389725000	8.475896000	-10.624945000
H	-1.699319000	9.206201000	-11.377942000
H	-0.297477000	8.488045000	-10.561697000
N	-2.731471000	4.903960000	-11.740298000
N	-3.440078000	4.434301000	-10.986120000
C	-1.365015000	6.746033000	-12.268656000

O	-0.598439000	7.395232000	-12.960773000
C	-2.035987000	8.739395000	-9.281050000
H	-1.736897000	9.732146000	-8.926803000
H	-1.719251000	8.000574000	-8.536631000
H	-3.128283000	8.715901000	-9.356177000
C	-1.669157000	4.664499000	-13.876229000
C	-2.248707000	3.391965000	-14.054187000
C	-0.873692000	5.190347000	-14.911987000
H	-2.871113000	2.957688000	-13.277034000
H	-0.423982000	6.167691000	-14.798580000
C	-2.039344000	2.671472000	-15.227933000
C	-0.671551000	4.458995000	-16.083536000
H	-2.500724000	1.693956000	-15.340092000
H	-0.057242000	4.887255000	-16.871228000
C	-1.248809000	3.199256000	-16.252159000
H	-1.088500000	2.637641000	-17.168183000
H	-0.007429000	5.458814000	-9.957892000

$TS2_{HC'}$

Electronic energy = -2079.699942
Zero-point correction = 0.798993
Thermal correction to Energy = 0.849764
Thermal correction to Enthalpy = 0.850708
Thermal correction to Gibbs Free Energy = 0.707426

Cu	2.413621000	3.633956000	-10.425199000
C	4.315304000	3.987954000	-10.859355000
N	4.946884000	3.654662000	-11.994168000
C	6.386406000	4.018985000	-11.985209000
H	6.998653000	3.119098000	-12.094652000
H	6.608370000	4.693639000	-12.816803000
C	6.551863000	4.691241000	-10.608309000
H	6.844453000	5.742680000	-10.682262000
H	7.270661000	4.174756000	-9.965913000
N	5.187287000	4.583874000	-10.033590000
C	4.344599000	2.973116000	-13.109860000
C	3.791794000	3.736144000	-14.163341000
C	3.206787000	3.048510000	-15.235287000
H	2.766253000	3.613035000	-16.052248000
C	3.182895000	1.655935000	-15.271134000
H	2.725145000	1.142336000	-16.112553000
C	3.754490000	0.922252000	-14.233875000
H	3.740423000	-0.163382000	-14.274554000
C	4.352291000	1.559859000	-13.138131000
C	3.805148000	5.262256000	-14.167345000
H	4.352829000	5.597422000	-13.281309000
C	4.536818000	5.823243000	-15.401749000
H	4.600119000	6.916349000	-15.340274000
H	5.556868000	5.429011000	-15.478151000
H	4.010581000	5.573971000	-16.330796000
C	2.378968000	5.838519000	-14.069562000
H	2.411604000	6.934345000	-14.032073000
H	1.770095000	5.551453000	-14.935372000
H	1.868357000	5.484039000	-13.166252000
C	4.983507000	0.716226000	-12.034151000
H	5.392600000	1.394964000	-11.279790000
C	6.153438000	-0.130884000	-12.571292000
H	6.634913000	-0.676149000	-11.750481000
H	5.811811000	-0.869250000	-13.306233000
H	6.913242000	0.494601000	-13.054117000
C	3.941083000	-0.176060000	-11.333608000
H	4.409001000	-0.738720000	-10.516814000
H	3.122464000	0.416777000	-10.907855000
H	3.502531000	-0.901253000	-12.029303000
C	4.874401000	5.066320000	-8.713865000
C	4.985588000	4.184180000	-7.614793000
C	4.666609000	4.678365000	-6.342609000
H	4.735566000	4.017208000	-5.483261000
C	4.266067000	6.000272000	-6.162104000
C	4.183519000	6.859191000	-7.255948000
H	3.877830000	7.890831000	-7.105725000
C	4.488620000	6.415973000	-8.549899000
C	5.438237000	2.734371000	-7.763239000
H	5.668331000	2.556377000	-8.818051000
C	6.724852000	2.456906000	-6.962164000
C	4.323630000	1.749065000	-7.361481000
H	3.411134000	1.912628000	-7.948059000
H	4.061483000	1.850614000	-6.301639000
H	4.650361000	0.715234000	-7.526905000
H	6.563091000	2.575734000	-5.884439000
H	7.063845000	1.428475000	-7.135871000
H	7.535283000	3.134342000	-7.255487000
C	4.395630000	7.393744000	-9.718433000
H	4.696847000	6.865881000	-10.628282000
C	2.951326000	7.885290000	-9.933903000
C	5.358824000	8.582533000	-9.536350000
H	6.392147000	8.243532000	-9.397383000
H	5.087303000	9.192305000	-8.666519000
H	5.331887000	9.233343000	-10.418784000
H	2.579293000	8.434175000	-9.060806000
H	2.902514000	8.558979000	-10.798125000
H	2.267513000	7.047841000	-10.119666000
C	0.575171000	3.350588000	-10.148816000
O	-0.668082000	2.125285000	-11.822855000
C	-1.288588000	0.852626000	-12.237105000
H	-2.151831000	0.679051000	-11.589875000
H	-0.557127000	0.055873000	-12.083074000
C	-0.124444000	2.179724000	-10.633783000
O	-0.051191000	1.298340000	-9.777780000
C	-1.678620000	1.006764000	-13.689625000
H	-2.167068000	0.085723000	-14.025923000
H	-0.798840000	1.180105000	-14.317886000
H	-2.378646000	1.837761000	-13.823110000
H	4.023413000	6.362986000	-5.166680000
C	-1.173914000	5.486075000	-12.493690000
O	-3.232952000	4.551128000	-11.923082000
C	-4.242540000	4.178077000	-10.945619000
H	-4.540874000	5.074416000	-10.394139000
H	-3.799872000	3.471154000	-10.236908000
N	-1.393699000	5.125385000	-13.730444000
N	-1.587853000	4.799722000	-14.802057000
C	-2.124021000	5.143860000	-11.444998000
O	-1.916746000	5.378579000	-10.261586000
C	-5.404202000	3.568970000	-11.702842000
H	-6.187613000	3.281761000	-10.992747000
H	-5.094325000	2.673712000	-12.252713000
H	-5.830738000	4.285423000	-12.413041000
H	-0.264642000	6.036699000	-12.296257000
H	-0.065866000	3.959691000	-9.501881000

TS_{AZ}

Electronic energy = -2541.841113
Zero-point correction = 0.962789
Thermal correction to Energy = 1.022271
Thermal correction to Enthalpy = 1.023216
Thermal correction to Gibbs Free Energy = 0.861459

Cu	2.462129000	4.230479000	-10.643589000
C	4.399139000	4.134426000	-10.999179000
N	4.923463000	3.431655000	-12.019205000
C	6.406737000	3.456212000	-12.044813000
H	6.795741000	2.457462000	-11.819482000
H	6.766518000	3.754868000	-13.032613000
C	6.734644000	4.484306000	-10.951524000
H	7.123736000	5.424190000	-11.357519000
H	7.441339000	4.108780000	-10.207251000
N	5.406938000	4.722391000	-10.330428000
C	4.180463000	2.609444000	-12.937342000
C	3.822638000	3.145434000	-14.195401000
C	3.106468000	2.326207000	-15.078515000
H	2.813624000	2.716851000	-16.049194000
C	2.769769000	1.018386000	-14.735492000
H	2.213422000	0.399261000	-15.434480000
C	3.155872000	0.500207000	-13.501767000

H	2.900641000	-0.524745000	-13.247733000
C	3.874375000	1.275852000	-12.581638000
C	4.189974000	4.566244000	-14.615133000
H	4.796228000	5.006313000	-13.818181000
C	5.040153000	4.579914000	-15.899860000
H	5.347422000	5.605018000	-16.139927000
H	5.945934000	3.972417000	-15.787900000
H	4.481268000	4.192247000	-16.759760000
C	2.938317000	5.450647000	-14.775809000
H	3.226751000	6.479726000	-15.023355000
H	2.290535000	5.084226000	-15.581176000
H	2.348285000	5.477497000	-13.852237000
C	4.312305000	0.652616000	-11.258677000
H	4.850254000	1.413458000	-10.685619000
C	5.284957000	-0.520863000	-11.488686000
H	5.641101000	-0.912425000	-10.528013000
H	4.800217000	-1.345158000	-12.025157000
H	6.159482000	-0.210794000	-12.072746000
C	3.110648000	0.202298000	-10.406161000
H	3.456998000	-0.204580000	-9.448112000
H	2.433632000	1.037806000	-10.193350000
H	2.530314000	-0.579568000	-10.909864000
C	5.285149000	5.575435000	-9.179268000
C	5.472213000	5.013064000	-7.894915000
C	5.386310000	5.864552000	-6.785425000
H	5.519054000	5.454777000	-5.788109000
C	5.148686000	7.228652000	-6.941184000
C	4.991852000	7.767881000	-8.216260000
H	4.824072000	8.835380000	-8.329139000
C	5.063661000	6.959874000	-9.359763000
C	5.783066000	3.533045000	-7.682755000
H	5.853312000	3.058399000	-8.665819000
C	7.140511000	3.336545000	-6.979575000
C	4.660451000	2.816535000	-6.908667000
H	3.703763000	2.884027000	-7.439667000
H	4.523575000	3.245942000	-5.908976000
H	4.901374000	1.753670000	-6.785049000
H	7.127887000	3.736354000	-5.958698000
H	7.380893000	2.268413000	-6.915156000
H	7.952353000	3.833641000	-7.523501000
C	4.925657000	7.601184000	-10.737840000
H	5.046120000	6.816789000	-11.490785000
C	3.531160000	8.224541000	-10.939768000
C	6.028664000	8.649338000	-10.984794000
H	7.029330000	8.217473000	-10.866683000
H	5.944031000	9.493030000	-10.289807000
H	5.950272000	9.048206000	-12.003382000
H	3.348388000	9.037117000	-10.226157000
H	3.443653000	8.642932000	-11.949938000
H	2.735149000	7.480519000	-10.814362000
C	0.502863000	4.151541000	-10.453213000
O	-0.355728000	5.017727000	-12.537208000
C	-0.833616000	4.769867000	-13.891727000
H	-1.735482000	4.153761000	-13.834292000
H	-0.066622000	4.206790000	-14.430708000
C	-0.108470000	3.932261000	-11.792596000
O	-0.269770000	2.784852000	-12.186399000
C	-1.109267000	6.114192000	-14.532343000
H	-1.472001000	5.958579000	-15.554573000
H	-0.202604000	6.726956000	-14.580434000
H	-1.875931000	6.665868000	-13.977785000
H	5.099674000	7.874376000	-6.068228000
C	-0.188051000	3.588947000	-9.301242000
C	-1.564582000	3.249643000	-9.321442000
C	0.531087000	3.385159000	-8.099870000
H	-2.142727000	3.406692000	-10.226925000
H	1.581959000	3.659425000	-8.070616000
C	-2.176171000	2.694392000	-8.202290000
C	-0.083538000	2.835865000	-6.979692000
H	-3.228264000	2.426731000	-8.236481000
H	0.486611000	2.675777000	-6.069327000
C	-1.437070000	2.484280000	-7.032005000
H	-1.917641000	2.048858000	-6.160235000
C	-1.226541000	6.737459000	-8.299964000
O	-2.982882000	6.609047000	-9.847828000
C	-4.396243000	6.646498000	-10.214019000
H	-4.800396000	7.617888000	-9.916189000
H	-4.914018000	5.865703000	-9.649756000
N	-0.489848000	6.477134000	-9.336348000
N	0.154539000	6.183496000	-10.249296000
C	-2.701822000	6.800913000	-8.555836000
O	-3.520419000	7.003198000	-7.682058000
C	-4.485201000	6.425465000	-11.708442000
H	-5.538759000	6.436977000	-12.008631000
H	-4.058652000	5.457294000	-11.991574000
H	-3.963921000	7.217374000	-12.256559000
C	-0.577634000	7.023980000	-7.005968000
C	0.748094000	7.496563000	-6.977274000
C	-1.259011000	6.807549000	-5.794308000
H	1.281149000	7.685481000	-7.905540000
H	-2.277364000	6.442645000	-5.803625000
C	1.377237000	7.747638000	-5.760971000
C	-0.618522000	7.065247000	-4.582540000
H	2.398589000	8.116016000	-5.754685000
H	-1.153877000	6.893382000	-3.652944000
C	0.696928000	7.532980000	-4.558318000
H	1.189395000	7.731999000	-3.610638000

9

Electronic energy =	-2310.919484
Zero-point correction =	0.882465
Thermal correction to Energy =	0.939004
Thermal correction to Enthalpy =	0.939949
Thermal correction to Gibbs Free Energy =	0.783540

Cu	2.504756000	4.902706000	-10.999233000
C	4.273946000	4.135182000	-11.035726000
N	4.785469000	3.411427000	-12.044876000
C	6.200846000	3.025905000	-11.823060000
H	6.310649000	1.939983000	-11.884934000
H	6.834519000	3.483188000	-12.589385000
C	6.478363000	3.577875000	-10.411494000
H	7.306958000	4.291010000	-10.388178000
H	6.676482000	2.789272000	-9.679225000
N	5.206071000	4.265879000	-10.079452000
C	4.093500000	3.087415000	-13.263302000
C	4.116340000	4.007904000	-14.336579000
C	3.420468000	3.669435000	-15.505507000
H	3.413314000	4.364252000	-16.340669000
C	2.747227000	2.454645000	-15.617948000
H	2.217149000	2.210031000	-16.534812000
C	2.762591000	1.548778000	-14.559249000
H	2.246928000	0.597809000	-14.659915000
C	3.439485000	1.838913000	-13.366573000
C	4.867842000	5.334770000	-14.269566000
H	5.354758000	5.400395000	-13.292070000
C	5.976198000	5.410517000	-15.338111000
H	6.543643000	6.342316000	-15.226984000
H	6.678959000	4.573706000	-15.249740000
H	5.562369000	5.392559000	-16.353175000
C	3.914421000	6.539414000	-14.386244000
H	4.474690000	7.478024000	-14.296842000
H	3.395661000	6.551854000	-15.352183000
H	3.153710000	6.525722000	-13.596119000
C	3.453428000	0.806671000	-12.242130000
H	4.049678000	1.209032000	-11.417776000
C	4.119713000	-0.507114000	-12.694934000
H	4.177573000	-1.211369000	-11.856215000
H	3.551112000	-0.992412000	-13.496976000
H	5.137398000	-0.335332000	-13.064501000
C	2.039145000	0.540903000	-11.693282000
H	2.078943000	-0.190003000	-10.876463000
H	1.584279000	1.458443000	-11.301020000
H	1.374924000	0.138425000	-12.467247000
C	5.034627000	4.984783000	-8.845126000

C	4.590472000	4.286671000	-7.699872000
C	4.433018000	5.010989000	-6.510402000
H	4.085626000	4.498979000	-5.617312000
C	4.717251000	6.373877000	-6.454520000
C	5.173293000	7.038978000	-7.590649000
H	5.398766000	8.100270000	-7.535751000
C	5.349440000	6.362140000	-8.805020000
C	4.279710000	2.792368000	-7.718077000
H	4.495798000	2.413822000	-8.721597000
C	5.171132000	2.015078000	-6.730289000
C	2.788997000	2.520732000	-7.437441000
H	2.144929000	3.013731000	-8.175898000
H	2.496279000	2.879877000	-6.443483000
H	2.583773000	1.443863000	-7.476646000
H	4.969361000	2.303950000	-5.692067000
H	4.982984000	0.938044000	-6.816643000
H	6.235603000	2.189951000	-6.925365000
C	5.865867000	7.123894000	-10.022576000
H	5.969070000	6.412800000	-10.847879000
C	4.871719000	8.210645000	-10.475150000
C	7.257755000	7.731873000	-9.764170000
H	7.981945000	6.966077000	-9.462318000
H	7.226148000	8.492897000	-8.975368000
H	7.634531000	8.214034000	-10.674384000
H	4.729453000	8.972389000	-9.699424000
H	5.243796000	8.715289000	-11.375130000
H	3.888958000	7.783415000	-10.708453000
C	-1.320320000	6.828448000	-10.491391000
O	-1.049719000	5.098193000	-12.093621000
C	-0.276306000	4.169393000	-12.916280000
H	0.234225000	3.466919000	-12.252843000
H	0.469002000	4.747374000	-13.469599000
C	-0.437791000	5.843530000	-11.194615000
O	0.768364000	5.766478000	-10.933026000
C	-1.254266000	3.471557000	-13.836045000
H	-0.703764000	2.771536000	-14.473440000
H	-1.771177000	4.190276000	-14.480124000
H	-1.998563000	2.906575000	-13.265473000
H	4.589356000	6.917276000	-5.521844000
C	-0.702279000	7.588441000	-9.370560000
C	-0.124740000	6.922751000	-8.277118000
C	-0.684446000	8.991797000	-9.400900000
H	-0.137078000	5.837341000	-8.237091000
H	-1.114531000	9.514257000	-10.251159000
C	0.441306000	7.648057000	-7.228743000
C	-0.109626000	9.715490000	-8.355179000
H	0.875149000	7.121496000	-6.383120000
H	-0.098859000	10.801314000	-8.394651000
C	0.452729000	9.045739000	-7.265636000
H	0.900155000	9.608662000	-6.450998000
C	-2.571168000	7.012537000	-10.965333000
O	-3.673187000	7.986750000	-9.108125000
C	-4.661080000	8.885628000	-8.529485000
H	-5.655873000	8.550730000	-8.839821000
H	-4.495765000	9.888865000	-8.932932000
N	-1.341662000	3.039700000	-8.597738000
N	-0.573090000	2.949455000	-9.385911000
C	-3.610539000	7.945345000	-10.441845000
O	-4.345578000	8.562928000	-11.192103000
C	-4.486481000	8.841998000	-7.025761000
H	-5.216620000	9.511122000	-6.557125000
H	-3.482249000	9.171175000	-6.738144000
H	-4.648564000	7.830633000	-6.637760000
H	-2.886622000	6.486539000	-11.860232000

Au systems with IPr ligand

IPrAuCl

Electronic energy =	-1757.052186
Zero-point correction =	0.598151
Thermal correction to Energy =	0.633001
Thermal correction to Enthalpy =	0.633945
Thermal correction to Gibbs Free Energy =	0.529213

Au	-0.000091000	-0.000231000	1.606973000
C	0.000043000	0.000017000	-0.397915000
N	-1.096302000	-0.003915000	-1.172891000
C	-0.769687000	0.027095000	-2.617706000
H	-1.160470000	0.945120000	-3.066974000
H	-1.223985000	-0.828590000	-3.124452000
C	0.769781000	-0.026350000	-2.617708000
H	1.160562000	-0.944240000	-3.067251000
H	1.224086000	0.829489000	-3.124191000
N	1.096394000	0.004215000	-1.172883000
C	-2.461698000	0.001484000	-0.714353000
C	-3.121747000	-1.231489000	-0.514298000
C	-4.453147000	-1.198268000	-0.078895000
H	-4.979873000	-2.133128000	0.091521000
C	-5.109889000	0.010313000	0.141037000
H	-6.142255000	0.013695000	0.481135000
C	-4.445731000	1.214607000	-0.080361000
H	-4.966450000	2.153023000	0.089036000
C	-3.113935000	1.238740000	-0.514804000
C	-2.444277000	-2.577832000	-0.753100000
H	-1.427361000	-2.386389000	-1.108105000
C	-3.168583000	-3.390259000	-1.843982000
H	-2.633709000	-4.328174000	-2.037054000
H	-3.228269000	-2.834469000	-2.787438000
H	-4.190994000	-3.647571000	-1.542588000
C	-2.328267000	-3.392021000	0.549612000
H	-1.789192000	-4.329559000	0.365436000
H	-3.315806000	-3.648226000	0.951626000
H	-1.785105000	-2.833769000	1.320902000
C	-2.426396000	2.580137000	-0.752328000
H	-1.409576000	2.381199000	-1.103104000
C	-3.140858000	3.397194000	-1.846231000
H	-2.599068000	4.331562000	-2.037194000
H	-4.162628000	3.661275000	-1.548470000
H	-3.200984000	2.841917000	-2.789942000
C	-2.309408000	3.394824000	0.550062000
H	-1.762075000	4.327785000	0.367001000
H	-1.773955000	2.833250000	1.324289000
H	-3.296537000	3.659512000	0.947504000
C	2.461802000	-0.001204000	-0.714410000
C	3.121715000	1.231777000	-0.513940000
C	4.453109000	1.198560000	-0.078520000
H	4.979731000	2.133422000	0.092207000
C	5.109969000	-0.010023000	0.141050000
C	4.445928000	-1.214317000	-0.080701000
H	4.966730000	-2.152730000	0.088451000
C	3.114146000	-1.238454000	-0.515189000
C	2.444075000	2.578119000	-0.752245000
H	1.427160000	2.386681000	-1.107253000
C	3.168252000	3.390987000	-1.842886000
C	2.328031000	3.391861000	0.550740000
H	1.785025000	2.833267000	1.321894000
H	3.315552000	3.648119000	0.952764000
H	1.788778000	4.329363000	0.366907000
H	4.190665000	3.648253000	-1.541453000
H	2.633304000	4.328935000	-2.035591000
H	3.227932000	2.835539000	-2.786544000
C	2.426729000	-2.579853000	-0.753060000
H	1.409960000	-2.380927000	-1.103989000
C	2.309565000	-3.394755000	0.549178000
C	3.141444000	-3.396684000	-1.846967000
H	3.201734000	-2.841239000	-2.790569000
H	4.163167000	-3.660774000	-1.549053000
H	2.599734000	-4.331041000	-2.038214000
H	3.296647000	-3.659431000	0.946749000
H	1.762336000	-4.327728000	0.365875000
H	1.773933000	-2.833341000	1.323398000
H	6.142327000	-0.013405000	0.481173000
Cl	-0.000247000	-0.000558000	3.990877000

IPrAuBPh$_4$

Electronic energy = -2248.248007
Zero-point correction = 0.965776
Thermal correction to Energy = 1.020708
Thermal correction to Enthalpy = 1.021653
Thermal correction to Gibbs Free Energy = 0.870474

Au	-0.646302000	-0.520597000	-0.799419000
C	-2.469385000	-0.196593000	0.023125000
N	-3.043452000	0.989284000	0.278515000
C	-4.456489000	0.840656000	0.709495000
H	-5.114637000	1.206072000	-0.086270000
H	-4.641371000	1.424107000	1.613276000
C	-4.578845000	-0.672297000	0.935617000
H	-4.612832000	-0.940033000	1.996902000
H	-5.444214000	-1.111514000	0.434679000
N	-3.323859000	-1.185062000	0.336236000
C	-2.510452000	2.300664000	0.014967000
C	-2.044301000	3.067647000	1.106914000
C	-1.594022000	4.368500000	0.849361000
H	-1.228395000	4.977608000	1.670909000
C	-1.606912000	4.892752000	-0.440926000
H	-1.248887000	5.903079000	-0.620542000
C	-2.086675000	4.126250000	-1.499623000
H	-2.105326000	4.548463000	-2.500360000
C	-2.561862000	2.823344000	-1.297612000
C	-2.037086000	2.540260000	2.539395000
H	-2.349306000	1.491875000	2.514971000
C	-3.043284000	3.308264000	3.419364000
H	-3.064039000	2.887724000	4.432210000
H	-4.059961000	3.258016000	3.011428000
H	-2.770031000	4.367033000	3.503775000
C	-0.629907000	2.579436000	3.161921000
H	-0.646391000	2.127433000	4.161229000
H	-0.262219000	3.606508000	3.270286000
H	0.092148000	2.028064000	2.550696000
C	-3.140514000	2.052367000	-2.481590000
H	-3.427690000	1.055208000	-2.135603000
C	-4.413794000	2.733266000	-3.022448000
H	-4.845763000	2.138334000	-3.836434000
H	-4.196199000	3.732411000	-3.418411000
H	-5.176586000	2.841716000	-2.242317000
C	-2.105274000	1.866048000	-3.606401000
H	-2.526491000	1.254710000	-4.413909000
H	-1.202876000	1.366597000	-3.235437000
H	-1.802892000	2.826464000	-4.039908000
C	-3.104942000	-2.599825000	0.178675000
C	-3.554101000	-3.225330000	-1.007083000
C	-3.347628000	-4.604971000	-1.137666000
H	-3.674566000	-5.108235000	-2.043281000
C	-2.737793000	-5.341179000	-0.124355000
C	-2.331718000	-4.709534000	1.048587000
H	-1.871117000	-5.294772000	1.839320000
C	-2.510756000	-3.331216000	1.230923000
C	-4.259182000	-2.465195000	-2.127665000
H	-4.345960000	-1.417017000	-1.825718000
C	-5.687570000	-2.996398000	-2.358180000
C	-3.449013000	-2.497896000	-3.437405000
H	-2.448349000	-2.072945000	-3.297690000
H	-3.331718000	-3.521816000	-3.811708000
H	-3.958728000	-1.915586000	-4.214866000
H	-5.678309000	-4.033850000	-2.712796000
H	-6.198442000	-2.390753000	-3.116554000
H	-6.284637000	-2.962523000	-1.439298000
C	-2.087716000	-2.687603000	2.548197000
H	-2.231098000	-1.606446000	2.460571000
C	-0.598575000	-2.928876000	2.854670000
C	-2.970113000	-3.178950000	3.713791000
H	-4.033225000	-2.988335000	3.525040000
H	-2.848011000	-4.256116000	3.879693000
H	-2.693593000	-2.664895000	4.642415000
H	-0.384002000	-3.993430000	3.005099000
H	-0.310534000	-2.401622000	3.771866000
H	0.041584000	-2.568007000	2.042230000
H	-2.587337000	-6.410892000	-0.245016000
C	2.589812000	-0.827357000	-0.606443000
B	3.676860000	0.264503000	0.019795000
C	2.642269000	-2.179933000	-0.221822000
H	3.323575000	-2.468482000	0.575325000
C	1.894071000	-3.191937000	-0.845766000
H	2.004562000	-4.221976000	-0.514241000
C	1.037551000	-2.893247000	-1.899283000
H	0.482826000	-3.673616000	-2.412265000
C	0.917118000	-1.549025000	-2.310264000
H	0.358131000	-1.306962000	-3.212063000
C	1.667151000	-0.535093000	-1.654026000
H	1.643458000	0.467742000	-2.071343000
C	5.159567000	0.012583000	-0.693050000
C	6.188998000	0.967047000	-0.517074000
H	5.982043000	1.860545000	0.069318000
C	7.463522000	0.818825000	-1.068787000
H	8.219684000	1.583299000	-0.898718000
C	7.766885000	-0.305318000	-1.844386000
H	8.754952000	-0.425042000	-2.283219000
C	6.776301000	-1.266613000	-2.047263000
H	6.987896000	-2.147454000	-2.651167000
C	5.505541000	-1.103846000	-1.479061000
H	4.764974000	-1.878437000	-1.662999000
C	3.766860000	0.006807000	1.654582000
C	2.593523000	-0.004632000	2.442972000
H	1.631161000	0.147549000	1.956233000
C	2.609430000	-0.203551000	3.826201000
H	1.676237000	-0.192757000	4.386807000
C	3.821503000	-0.419275000	4.489777000
H	3.842928000	-0.579608000	5.565451000
C	5.001595000	-0.427679000	3.744858000
H	5.955870000	-0.599832000	4.239835000
C	4.965590000	-0.218208000	2.360056000
H	5.906571000	-0.233212000	1.815904000
C	3.237235000	1.826180000	-0.325778000
C	2.810885000	2.765924000	0.633520000
H	2.749853000	2.468639000	1.677242000
C	2.476914000	4.086215000	0.304287000
H	2.160762000	4.773004000	1.087498000
C	2.552239000	4.524150000	-1.018692000
H	2.293963000	5.547958000	-1.279951000
C	2.978459000	3.624575000	-2.001133000
H	3.058749000	3.946761000	-3.037933000
C	3.317590000	2.314843000	-1.651471000
H	3.678635000	1.652249000	-2.436478000

5

Electronic energy = -1296.628000
Zero-point correction = 0.597734
Thermal correction to Energy = 0.630417
Thermal correction to Enthalpy = 0.631361
Thermal correction to Gibbs Free Energy = 0.531645

Au	1.773477000	2.538812000	10.292121000
C	3.699365000	2.124808000	10.443374000
N	4.299641000	1.720549000	11.565721000
C	5.755848000	1.514765000	11.359970000
H	6.020472000	0.483963000	11.608497000
H	6.315910000	2.189580000	12.012763000
C	5.940197000	1.837180000	9.862931000
H	6.626356000	2.669416000	9.687652000
H	6.275576000	0.974740000	9.280744000
N	4.570842000	2.221163000	9.435666000
C	3.674226000	1.502962000	12.846152000
C	3.608099000	2.574223000	13.764806000
C	3.001923000	2.331954000	15.004856000
H	2.931312000	3.138805000	15.728910000
C	2.497253000	1.074022000	15.326166000
H	2.030836000	0.907500000	16.293615000
C	2.596988000	0.026582000	14.413160000

H	2.211057000	-0.953443000	14.678668000
C	3.192907000	0.212144000	13.158490000
C	4.173048000	3.958927000	13.462448000
H	4.603939000	3.938914000	12.457135000
C	5.306020000	4.330860000	14.438629000
H	5.741893000	5.297900000	14.160648000
H	6.106730000	3.582335000	14.430088000
H	4.938150000	4.414647000	15.467922000
C	3.072111000	5.036743000	13.466727000
H	3.495204000	6.012517000	13.199311000
H	2.608085000	5.134542000	14.455233000
H	2.279555000	4.802280000	12.745444000
C	3.300154000	-0.965713000	12.193466000
H	3.830286000	-0.625318000	11.298677000
C	4.120880000	-2.120533000	12.799637000
H	4.246929000	-2.922758000	12.062641000
H	3.624112000	-2.551368000	13.676918000
H	5.117819000	-1.786662000	13.110336000
C	1.911422000	-1.458832000	11.742819000
H	2.014138000	-2.271762000	11.013750000
H	1.333353000	-0.654368000	11.271599000
H	1.327991000	-1.841387000	12.588562000
C	4.278208000	2.605508000	8.077560000
C	3.914049000	1.605173000	7.149228000
C	3.644487000	2.005814000	5.833813000
H	3.354065000	1.258931000	5.100399000
C	3.744982000	3.341986000	5.452777000
C	4.126604000	4.307455000	6.381811000
H	4.207755000	5.345630000	6.072466000
C	4.406928000	3.963531000	7.710979000
C	3.813015000	0.128982000	7.521043000
H	4.085748000	0.023290000	8.575619000
C	4.800555000	-0.727413000	6.704638000
C	2.373029000	-0.396015000	7.363203000
H	1.667690000	0.183639000	7.971360000
H	2.039502000	-0.342975000	6.320136000
H	2.312815000	-1.444046000	7.680549000
H	4.559524000	-0.709485000	5.635291000
H	4.761335000	-1.771553000	7.037494000
H	5.831574000	-0.373189000	6.820528000
C	4.830163000	5.048734000	8.696840000
H	5.037375000	4.571120000	9.659297000
C	3.702262000	6.074052000	8.924472000
C	6.125331000	5.752658000	8.247887000
H	6.942500000	5.036771000	8.100573000
H	5.983449000	6.297450000	7.307121000
H	6.443209000	6.477616000	9.006774000
H	3.450338000	6.603913000	7.998264000
H	4.011638000	6.822047000	9.664360000
H	2.789135000	5.590942000	9.293190000
H	3.531150000	3.630880000	4.427077000

Gas phase calculations: $Tp^{Br3}Ag$ system

N_2

Electronic energy = -109.520718
Zero-point correction = 0.005600
Thermal correction to Energy = 0.007961
Thermal correction to Enthalpy = 0.008905
Thermal correction to Gibbs Free Energy = -0.012849

N	-2.006398000	-0.148514000	-3.463094000
N	-2.558140000	-1.100957000	-3.563721000

6a

Electronic energy = -646.988655
Zero-point correction = 0.187163
Thermal correction to Energy = 0.200196
Thermal correction to Enthalpy = 0.201140
Thermal correction to Gibbs Free Energy = 0.145842

C	3.151548000	0.268852000	2.554945000
C	4.558239000	0.674079000	2.395462000
O	4.988507000	1.799073000	2.569538000
O	5.333290000	-0.374405000	2.024624000
C	6.737266000	-0.083709000	1.837363000
H	6.838124000	0.672210000	1.051913000
H	7.135307000	0.343865000	2.762887000
C	7.423973000	-1.385234000	1.467709000
H	7.310381000	-2.128179000	2.263691000
H	7.006657000	-1.801029000	0.544965000
H	8.493614000	-1.206908000	1.312584000
N	2.906864000	-1.003163000	2.313072000
N	2.668286000	-2.097615000	2.109656000
C	2.014615000	1.130627000	2.945903000
C	0.708580000	0.607259000	3.001110000
C	2.209184000	2.485456000	3.271891000
H	0.523172000	-0.434359000	2.753321000
H	3.205846000	2.903685000	3.232152000
C	-0.366782000	1.410690000	3.370434000
C	1.123788000	3.280332000	3.639394000
H	-1.364425000	0.981079000	3.404495000
H	1.296839000	4.324446000	3.886846000
C	-0.167430000	2.754515000	3.692519000
H	-1.006895000	3.381194000	3.980141000

6b

Electronic energy = -415.934980
Zero-point correction= 0.105572
Thermal correction to Energy= 0.114069
Thermal correction to Enthalpy= 0.115013
Thermal correction to Gibbs Free Energy= 0.071548

C	3.218239000	-0.079105000	2.542413000
C	4.555536000	0.477367000	2.359812000
O	4.813238000	1.656494000	2.503388000
O	5.457593000	-0.473719000	2.015493000
C	6.811182000	-0.007599000	1.814729000
H	6.809950000	0.750775000	1.025243000
H	7.159593000	0.472318000	2.734854000
C	7.655581000	-1.213290000	1.445705000
H	7.639944000	-1.961458000	2.244767000
H	7.288551000	-1.681963000	0.526946000
H	8.693642000	-0.902921000	1.283901000
N	2.987104000	-1.354828000	2.377165000
N	2.798502000	-2.467965000	2.230340000
H	2.382014000	0.546390000	2.818939000

5

Electronic energy = -961.239375
Zero-point correction = 0.107084
Thermal correction to Energy = 0.136024
Thermal correction to Enthalpy = 0.136968
Thermal correction to Gibbs Free Energy = 0.034570

Ag	2.005800000	0.136780000	1.058540000
N	-0.157649000	-0.213962000	1.944765000
N	-1.167073000	-0.270429000	1.026106000
N	0.888275000	1.676529000	-0.354203000
N	-0.299892000	1.241345000	-0.868635000
N	1.320110000	-1.439678000	-0.556310000
N	0.034970000	-1.307880000	-1.000231000
B	-0.901088000	-0.155832000	-0.510162000
C	-0.708153000	-0.339939000	3.144707000
C	-2.102841000	-0.484259000	3.050759000
C	-2.348712000	-0.433408000	1.681553000
C	1.112417000	2.886911000	-0.847437000
C	0.073125000	3.286188000	-1.705111000
C	-0.803466000	2.204888000	-1.687453000
C	1.838773000	-2.502050000	-1.157339000
C	0.905966000	-3.103369000	-2.019293000
C	-0.228453000	-2.307679000	-1.885326000

H	-1.937071000	-0.262270000	-1.071212000
Br	-4.026507000	-0.564008000	0.841930000
Br	-3.345067000	-0.696832000	4.444093000
Br	0.362726000	-0.310554000	4.697291000
Br	-1.873021000	-2.549039000	-2.765352000
Br	1.133872000	-4.623322000	-3.099650000
Br	3.616043000	-3.026920000	-0.805692000
Br	-2.425010000	2.064180000	-2.630093000
Br	-0.096486000	4.899302000	-2.653098000
Br	2.670456000	3.838736000	-0.373286000

7a

Electronic energy = -1608.234858
Zero-point correction = 0.294454
Thermal correction to Energy = 0.338726
Thermal correction to Enthalpy = 0.339670
Thermal correction to Gibbs Free Energy = 0.200755

Ag	1.904337000	0.030801000	1.215955000
C	4.077488000	-0.225597000	2.492094000
N	-0.364319000	-0.330128000	1.927498000
N	-1.349682000	-0.219393000	0.988021000
N	0.803573000	1.683876000	-0.203225000
N	-0.348336000	1.294484000	-0.825321000
N	1.191477000	-1.331818000	-0.729736000
N	-0.136967000	-1.245634000	-1.036892000
B	-1.032965000	-0.074020000	-0.526697000
C	-0.963630000	-0.421100000	3.109401000
C	-2.362547000	-0.374924000	2.976179000
C	-2.560870000	-0.244126000	1.606358000
C	1.125297000	2.870494000	-0.701433000
C	0.193835000	3.297124000	-1.663208000
C	-0.727447000	2.256601000	-1.709307000
C	1.670148000	-2.372502000	-1.400113000
C	0.670984000	-3.004798000	-2.159059000
C	-0.465935000	-2.248711000	-1.894667000
H	-2.056148000	-0.110652000	-1.120450000
C	4.136363000	1.163371000	3.044398000
O	3.504352000	1.527110000	4.014101000
O	4.979539000	1.943077000	2.341542000
C	5.104354000	3.316784000	2.797957000
H	4.130355000	3.802888000	2.691969000
H	5.364479000	3.305439000	3.860155000
Br	-4.216352000	-0.113608000	0.720624000
Br	-3.662578000	-0.471005000	4.330202000
Br	0.038200000	-0.582893000	4.694993000
Br	-2.191339000	-2.543800000	-2.584322000
Br	0.830126000	-4.508595000	-3.275049000
Br	3.499520000	-2.838731000	-1.313191000
Br	-2.253115000	2.162489000	-2.806707000
Br	0.188561000	4.895336000	-2.651898000
Br	2.675699000	3.781844000	-0.130559000
C	3.768203000	-1.430007000	3.339431000
C	3.802384000	-1.353263000	4.740513000
C	3.484259000	-2.662493000	2.729037000
H	4.007334000	-0.407982000	5.226420000
H	3.448334000	-2.739165000	1.645750000
C	3.545472000	-2.490261000	5.506697000
C	3.240878000	-3.795925000	3.503032000
H	3.570368000	-2.415295000	6.590402000
H	3.021206000	-4.739658000	3.012107000
C	3.266958000	-3.714188000	4.896094000
H	3.068347000	-4.595007000	5.499835000
C	6.175018000	3.978224000	1.951833000
H	6.294736000	5.021734000	2.262179000
H	7.138037000	3.471407000	2.070279000
H	5.905829000	3.962554000	0.890758000
N	4.967989000	-0.450085000	1.508530000
N	5.690530000	-0.658829000	0.665139000

7b

Electronic energy = -1377.191643
Zero-point correction = 0.213286
Thermal correction to Energy = 0.252839
Thermal correction to Enthalpy = 0.253783
Thermal correction to Gibbs Free Energy = 0.121380

Ag	1.992829000	0.222906000	1.135121000
C	3.755440000	0.203550000	2.714325000
N	-0.242259000	-0.409210000	1.910743000
N	-1.243517000	-0.423945000	0.983098000
N	0.715063000	1.710413000	-0.233132000
N	-0.434057000	1.239208000	-0.800724000
N	1.351430000	-1.294343000	-0.630165000
N	0.057812000	-1.262489000	-1.062710000
B	-0.960187000	-0.205238000	-0.533535000
C	-0.804759000	-0.640617000	3.088926000
C	-2.195010000	-0.813425000	2.970725000
C	-2.428234000	-0.665425000	1.607468000
C	0.887151000	2.948738000	-0.676753000
C	-0.147130000	3.329549000	-1.548558000
C	-0.965468000	2.205500000	-1.597359000
C	1.949277000	-2.291205000	-1.268130000
C	1.064113000	-2.946017000	-2.141502000
C	-0.131619000	-2.253784000	-1.975017000
H	-1.976141000	-0.341427000	-1.124909000
C	4.040440000	1.632425000	3.050151000
O	3.351966000	2.269314000	3.813745000
O	5.124180000	2.090022000	2.398841000
C	5.468836000	3.480579000	2.645907000
H	4.598046000	4.097187000	2.406119000
H	5.681832000	3.598012000	3.712774000
Br	-4.093579000	-0.770777000	0.737833000
Br	-3.444992000	-1.163713000	4.329645000
Br	0.230945000	-0.709271000	4.668341000
Br	-1.761443000	-2.606855000	-2.846173000
Br	1.409839000	-4.408433000	-3.269982000
Br	3.770794000	-2.680841000	-0.954994000
Br	-2.551183000	2.019163000	-2.592683000
Br	-0.374692000	4.968198000	-2.439921000
Br	2.380247000	3.973800000	-0.146216000
C	6.668436000	3.811342000	1.779896000
H	6.961162000	4.854072000	1.943013000
H	7.521794000	3.172335000	2.028403000
H	6.434117000	3.681213000	0.718626000
N	4.779987000	-0.500902000	2.205017000
N	5.632435000	-1.074580000	1.741929000
H	3.177396000	-0.362221000	3.441887000

TS1a

Electronic energy = -1658.619687
Zero-point correction = 0.292373
Thermal correction to Energy = 0.336297
Thermal correction to Enthalpy = 0.337241
Thermal correction to Gibbs Free Energy = 0.201075

Cu	1.611576000	0.094477000	1.146451000
C	3.243879000	-0.066246000	2.318331000
N	-0.419161000	-0.093683000	1.825565000
N	-1.393652000	-0.135126000	0.866976000
N	0.949006000	1.479372000	-0.372837000
N	-0.252729000	1.214036000	-0.966482000
N	1.072082000	-1.518178000	-0.464186000
N	-0.161083000	-1.322408000	-1.022863000
B	-1.033115000	-0.092226000	-0.640511000
C	-1.037846000	-0.141667000	3.004337000
C	-2.432712000	-0.218524000	2.841523000
C	-2.610851000	-0.210496000	1.463169000
C	1.385809000	2.622337000	-0.892971000
C	0.481108000	3.136108000	-1.837326000
C	-0.548595000	2.201309000	-1.850182000
C	1.574385000	-2.604610000	-1.044124000
C	0.685391000	-3.149784000	-1.987327000

C	-0.408665000	-2.294582000	-1.938896000
H	-2.031130000	-0.113272000	-1.276583000
C	3.574136000	1.205749000	3.039474000
O	2.984340000	1.489399000	4.062332000
O	4.510718000	1.984222000	2.462629000
C	4.746572000	3.264240000	3.106733000
H	3.847636000	3.877517000	2.992010000
H	4.903733000	3.092202000	4.175008000
Br	-4.246321000	-0.289321000	0.535980000
Br	-3.753533000	-0.309188000	4.175509000
Br	-0.087574000	-0.090909000	4.625124000
Br	-1.987733000	-2.430544000	-2.953307000
Br	0.917021000	-4.673209000	-3.063572000
Br	3.288497000	-3.275416000	-0.618581000
Br	-2.107786000	2.257930000	-2.900571000
Br	0.625559000	4.713664000	-2.848055000
Br	3.036187000	3.369249000	-0.377187000
C	3.476571000	-1.309411000	3.108532000
C	4.504245000	-1.392405000	4.069631000
C	2.641562000	-2.422303000	2.915814000
H	5.157001000	-0.539402000	4.234876000
H	1.840526000	-2.360245000	2.187050000
C	4.688702000	-2.552777000	4.813403000
C	2.821247000	-3.583480000	3.666497000
H	5.484162000	-2.603423000	5.551383000
H	2.161645000	-4.432357000	3.512919000
C	3.845246000	-3.651072000	4.612140000
H	3.986317000	-4.556343000	5.196444000
C	5.957292000	3.893519000	2.443938000
H	6.167450000	4.862908000	2.908446000
H	6.842030000	3.258677000	2.557520000
H	5.785901000	4.057246000	1.374991000
N	4.517307000	-0.127881000	1.088964000
N	5.078297000	-0.317324000	0.149608000

TS1b

Electronic energy = -1377.162725
Zero-point correction = 0.208691
Thermal correction to Energy = 0.250317
Thermal correction to Enthalpy = 0.251261
Thermal correction to Gibbs Free Energy = 0.113077

Ag	1.297735000	0.288642000	1.252998000
C	3.055869000	0.063870000	2.299738000
N	-1.006601000	0.253676000	1.580167000
N	-1.878097000	0.162013000	0.534805000
N	0.609405000	1.549822000	-0.634871000
N	-0.495185000	1.190144000	-1.349821000
N	0.591429000	-1.533060000	-0.396475000
N	-0.580110000	-1.349308000	-1.070329000
B	-1.380502000	-0.024768000	-0.931816000
C	-1.729578000	0.394520000	2.685997000
C	-3.103946000	0.397807000	2.392517000
C	-3.148757000	0.247777000	1.009575000
C	1.133800000	2.611946000	-1.234895000
C	0.385531000	2.978350000	-2.366503000
C	-0.643369000	2.041876000	-2.398759000
C	1.029082000	-2.742061000	-0.715776000
C	0.156439000	-3.389551000	-1.610117000
C	-0.858209000	-2.459338000	-1.806481000
H	-2.323990000	-0.067958000	-1.645568000
C	3.643457000	0.979187000	3.255477000
O	3.306757000	0.657098000	4.391137000
O	4.353692000	2.026354000	2.887983000
C	4.783325000	2.924759000	3.960936000
H	3.891001000	3.272068000	4.488756000
H	5.398125000	2.351731000	4.660951000
Br	-4.693111000	0.173341000	-0.061729000
Br	-4.546089000	0.566596000	3.585182000
Br	-0.901367000	0.563167000	4.369877000
Br	-2.378496000	-2.663150000	-2.897230000
Br	0.319324000	-5.103223000	-2.365290000
Br	2.643234000	-3.418464000	0.000815000
Br	-2.025073000	1.936108000	-3.670376000
Br	0.696277000	4.399464000	-3.556083000
Br	2.684683000	3.446510000	-0.559348000
C	5.550098000	4.060190000	3.314686000
H	5.890427000	4.756044000	4.088823000
H	6.427078000	3.686561000	2.777193000
H	4.916124000	4.609656000	2.612094000
N	5.024331000	0.231125000	0.045827000
N	5.749787000	0.292488000	-0.785018000
H	3.599350000	-0.884485000	2.255431000

8a

Electronic energy = -1498.719144
Zero-point correction = 0.284514
Thermal correction to Energy = 0.326783
Thermal correction to Enthalpy = 0.327728
Thermal correction to Gibbs Free Energy = 0.192029

Ag	1.327888000	0.041431000	1.479496000
C	2.961833000	-0.102798000	2.840080000
N	-1.073104000	-0.614273000	1.543188000
N	-1.859969000	-0.373705000	0.454197000
N	0.178765000	1.882428000	0.310031000
N	-0.707736000	1.595309000	-0.686219000
N	1.040514000	-0.935133000	-0.712104000
N	-0.136292000	-0.798953000	-1.387555000
B	-1.260740000	0.154238000	-0.882731000
C	-1.881274000	-1.009587000	2.518106000
C	-3.222309000	-1.042317000	2.096419000
C	-3.158167000	-0.625514000	0.771367000
C	0.406882000	3.188318000	0.257049000
C	-0.321397000	3.795295000	-0.782051000
C	-1.018026000	2.737309000	-1.355918000
C	1.780526000	-1.800087000	-1.395399000
C	1.106672000	-2.256186000	-2.541757000
C	-0.113403000	-1.589450000	-2.492992000
H	-2.118938000	0.183280000	-1.698474000
C	3.823183000	1.091769000	2.904443000
O	3.705135000	1.891979000	3.817581000
O	4.654900000	1.207819000	1.864451000
C	5.445051000	2.427908000	1.797267000
H	4.756783000	3.275557000	1.736062000
H	6.022822000	2.522481000	2.721862000
Br	-4.606079000	-0.426644000	-0.414701000
Br	-4.744115000	-1.536144000	3.083497000
Br	-1.211471000	-1.443138000	4.230927000
Br	-1.524901000	-1.737544000	-3.728831000
Br	1.707983000	-3.476229000	-3.839570000
Br	3.508660000	-2.286754000	-0.811941000
Br	-2.195878000	2.826950000	-2.821377000
Br	-0.354565000	5.608407000	-1.278033000
Br	1.563312000	4.019954000	1.495068000
C	3.307714000	-1.213356000	3.662493000
C	2.536804000	-2.405871000	3.570651000
C	4.415186000	-1.194431000	4.561630000
H	1.686378000	-2.417443000	2.897228000
H	4.995409000	-0.283826000	4.669078000
C	2.869656000	-3.528369000	4.314904000
C	4.729220000	-2.310639000	5.318425000
H	2.280838000	-4.436088000	4.228066000
H	5.567521000	-2.286139000	6.007970000
C	3.961706000	-3.478372000	5.189311000
H	4.216720000	-4.354080000	5.780379000
C	6.332088000	2.323897000	0.572368000
H	6.939951000	3.230678000	0.481847000
H	7.004814000	1.463322000	0.645038000
H	5.730843000	2.218760000	-0.335876000

8b

Electronic energy = -1267.639689

Zero-point correction =	0.202616
Thermal correction to Energy =	0.239960
Thermal correction to Enthalpy =	0.240904
Thermal correction to Gibbs Free Energy =	0.117134

Ag	1.305271000	0.232376000	1.349236000
C	2.994470000	-0.067337000	2.477440000
N	-0.994457000	0.470915000	1.626176000
N	-1.858463000	0.338628000	0.579119000
N	0.811815000	1.320052000	-0.663980000
N	-0.340234000	1.057962000	-1.345227000
N	0.407477000	-1.682778000	-0.101017000
N	-0.696298000	-1.426003000	-0.860162000
B	-1.356872000	-0.020087000	-0.853418000
C	-1.718984000	0.758088000	2.702334000
C	-3.086939000	0.821444000	2.386498000
C	-3.126120000	0.547243000	1.022508000
C	1.465064000	2.257230000	-1.341953000
C	0.754321000	2.637160000	-2.492912000
C	-0.389755000	1.845270000	-2.451894000
C	0.733711000	-2.948124000	-0.318469000
C	-0.148249000	-3.561467000	-1.227944000
C	-1.045634000	-2.548272000	-1.545942000
H	-2.284572000	-0.024031000	-1.588789000
C	3.569342000	0.815794000	3.470279000
O	3.158204000	0.505715000	4.584478000
O	4.349300000	1.825949000	3.145155000
C	4.776158000	2.696169000	4.242972000
H	3.879760000	3.108083000	4.714510000
H	5.304051000	2.083230000	4.979035000
Br	-4.659801000	0.468824000	-0.063414000
Br	-4.528198000	1.191537000	3.533778000
Br	-0.901138000	1.025337000	4.378600000
Br	-2.510640000	-2.667877000	-2.721614000
Br	-0.123676000	-5.329469000	-1.865723000
Br	2.223467000	-3.734702000	0.540552000
Br	-1.794532000	1.837750000	-3.702201000
Br	1.230820000	3.916012000	-3.784563000
Br	3.126119000	2.915876000	-0.740040000
C	5.659981000	3.771331000	3.645410000
H	5.999030000	4.445285000	4.439260000
H	6.540527000	3.334102000	3.164733000
H	5.112077000	4.360235000	2.903615000
H	3.507386000	-1.034826000	2.447018000

Gas phase ONIOM(DFT:MM3) calculations: $Tp^{Br3}Ag$ system

Following data table summarizes Tinker atom types that we used for **7a**.

Atom number	Atom	Tinker atom type
1	Ag	-
2	C	1
3	N	37
4	N	40
5	N	37
6	N	40
7	N	37
8	N	40
9	B	27
10	C	2
11	C	2
12	C	2
13	C	2
14	C	2
15	C	2
16	C	2
17	C	2
18	C	2
19	H	5
20	C	3
21	O	78
22	O	75
23	C	1
24	H	5
25	H	5
26	Br	13
27	Br	13
28	Br	13
29	Br	13
30	Br	13
31	Br	13
32	Br	13
33	Br	13
34	Br	13
35	C	2
36	C	2
37	C	2
38	H	5
39	H	5
40	C	2
41	C	2
42	H	5
43	H	5
44	C	2
45	H	5
46	C	1
47	H	5
48	H	5
49	H	5
50	N	10
51	N	10

Van der Waal parameters for Ag was obtained from the UFF;

Ag	3.1480	0.0360000

7a

ONIOM: extrapolated energy =	-1377.174064
Zero-point correction =	0.297353
Thermal correction to Energy =	0.341289
Thermal correction to Enthalpy =	0.342233
Thermal correction to Gibbs Free Energy =	0.203300

Ag	1.975655000	0.199781000	1.071236000
C	3.989851000	-0.315617000	2.478204000
N	-0.269948000	-0.258797000	1.864661000
N	-1.270506000	-0.270221000	0.934682000
N	0.808827000	1.761391000	-0.302330000
N	-0.383210000	1.365438000	-0.839006000
N	1.250220000	-1.270204000	-0.762660000
N	-0.054639000	-1.159055000	-1.147826000
B	-0.991649000	-0.049707000	-0.580593000
C	-0.837082000	-0.470557000	3.046105000
C	-2.228831000	-0.629663000	2.923822000
C	-2.458552000	-0.492677000	1.559604000
C	1.037961000	2.994316000	-0.735408000
C	0.001704000	3.447126000	-1.568685000

C	-0.881651000	2.372989000	-1.605608000
C	1.768782000	-2.278792000	-1.449945000
C	0.818706000	-2.863884000	-2.304430000
C	-0.330776000	-2.114804000	-2.076294000
H	-2.022663000	-0.111145000	-1.157674000
C	4.061050000	1.092711000	2.993734000
O	3.367768000	1.516495000	3.891343000
O	4.980538000	1.808901000	2.319303000
C	5.115927000	3.200442000	2.717002000
H	4.151124000	3.694175000	2.571761000
H	5.356900000	3.231332000	3.783536000
Br	-4.124899000	-0.589573000	0.690341000
Br	-3.486723000	-0.949528000	4.283134000
Br	0.182431000	-0.506637000	4.631461000
Br	-2.007374000	-2.361514000	-2.894073000
Br	1.044979000	-4.313011000	-3.479459000
Br	3.581787000	-2.768529000	-1.244853000
Br	-2.504702000	2.295767000	-2.553875000
Br	-0.156806000	5.108834000	-2.431568000
Br	2.604033000	3.923889000	-0.241424000
C	3.680861000	-1.455168000	3.415168000
C	3.966745000	-1.363289000	4.729467000
C	3.152677000	-2.608576000	2.958087000
H	4.422270000	-0.445923000	5.138336000
H	2.932821000	-2.731481000	1.885026000
C	3.707613000	-2.380822000	5.564167000
C	2.893427000	-3.627586000	3.790659000
H	3.942514000	-2.284812000	6.638608000
H	2.458224000	-4.563452000	3.398633000
C	3.166925000	-3.513668000	5.096808000
H	2.954641000	-4.351264000	5.783738000
C	6.210470000	3.809246000	1.862470000
H	6.344012000	4.861931000	2.133760000
H	7.162935000	3.291759000	2.015294000
H	5.954776000	3.756488000	0.799253000
N	4.974908000	-0.650724000	1.631721000
N	5.778289000	-0.930887000	0.892235000

TS1a

ONIOM: extrapolated energy =	-1377.140631
Zero-point correction =	0.293932
Thermal correction to Energy =	0.338425
Thermal correction to Enthalpy =	0.339369
Thermal correction to Gibbs Free Energy =	0.198712

Ag	1.433833000	0.104878000	1.238316000
C	3.187796000	-0.141193000	2.486838000
N	-0.900266000	0.195055000	1.598906000
N	-1.780508000	0.117737000	0.559909000
N	0.774318000	1.494081000	-0.640841000
N	-0.406805000	1.251064000	-1.279017000
N	0.631588000	-1.582896000	-0.447248000
N	-0.504147000	-1.300828000	-1.148882000
B	-1.294580000	0.020408000	-0.916578000
C	-1.615266000	0.256040000	2.715938000
C	-2.992890000	0.220681000	2.437904000
C	-3.048679000	0.132014000	1.050477000
C	1.289324000	2.587196000	-1.187948000
C	0.460813000	3.095247000	-2.202775000
C	-0.610766000	2.207754000	-2.223738000
C	1.064232000	-2.758944000	-0.879071000
C	0.225110000	-3.285268000	-1.877532000
C	-0.763279000	-2.316912000	-2.015928000
H	-2.244317000	0.021778000	-1.623066000
C	3.576007000	1.022632000	3.305532000
O	3.001091000	1.085675000	4.379770000
O	4.411077000	1.925069000	2.799881000
C	4.627739000	3.113253000	3.619027000
H	3.658965000	3.591693000	3.786810000
H	5.024412000	2.793792000	4.587047000
Br	-4.602540000	0.043145000	-0.007309000
Br	-4.425960000	0.281049000	3.652490000
Br	-0.766245000	0.374489000	4.393848000
Br	-2.228720000	-2.369412000	-3.195893000
Br	0.393683000	-4.910771000	-2.806527000
Br	2.632910000	-3.547438000	-0.175015000
Br	-2.111309000	2.290131000	-3.355716000
Br	0.732412000	4.611982000	-3.278874000
Br	2.943679000	3.280303000	-0.595294000
C	3.646717000	-1.440337000	3.108618000
C	4.953288000	-1.680494000	3.341323000
C	2.750253000	-2.374888000	3.481763000
H	5.714695000	-0.927010000	3.076580000
H	1.671519000	-2.201279000	3.333805000
C	5.352321000	-2.830411000	3.904798000
C	3.147399000	-3.525265000	4.045410000
H	6.426185000	-3.012086000	4.085722000
H	2.399058000	-4.280747000	4.342252000
C	4.450023000	-3.756683000	4.254251000
H	4.777601000	-4.702314000	4.720117000
C	5.591687000	4.010166000	2.869085000
H	5.787836000	4.910237000	3.461293000
H	6.544514000	3.502204000	2.689610000
H	5.171920000	4.318529000	1.906443000
N	4.534015000	-0.121036000	1.006592000
N	5.005455000	0.017169000	0.015602000

8a

ONIOM: extrapolated energy =	-1267.629073
Zero-point correction =	0.286988
Thermal correction to Energy =	0.328952
Thermal correction to Enthalp y=	0.329896
Thermal correction to Gibbs Free Energy =	0.194560

Ag	1.399738000	0.014726000	1.382551000
C	3.104243000	-0.205236000	2.525643000
N	-0.884541000	0.355094000	1.691065000
N	-1.761042000	0.342254000	0.646685000
N	0.967360000	1.188340000	-0.597941000
N	-0.213238000	1.045350000	-1.264242000
N	0.373378000	-1.788782000	-0.141333000
N	-0.720650000	-1.426656000	-0.873773000
B	-1.292298000	0.015032000	-0.803710000
C	-1.580619000	0.635384000	2.787667000
C	-2.942027000	0.813653000	2.488200000
C	-3.008052000	0.616938000	1.111733000
C	1.682345000	2.095457000	-1.253913000
C	0.984157000	2.575936000	-2.374448000
C	-0.219253000	1.876720000	-2.339214000
C	0.610420000	-3.063045000	-0.419360000
C	-0.321933000	-3.575076000	-1.341261000
C	-1.152515000	-2.492050000	-1.601903000
H	-2.223049000	0.098386000	-1.530225000
C	3.551115000	0.791571000	3.479875000
O	3.129100000	0.527093000	4.601367000
O	4.252519000	1.841390000	3.104367000
C	4.560276000	2.825990000	4.143216000
H	3.615417000	3.173261000	4.569976000
H	5.132346000	2.324846000	4.929222000
Br	-4.548384000	0.708087000	0.036240000
Br	-4.346633000	1.223874000	3.666949000
Br	-0.731183000	0.754986000	4.465035000
Br	-2.637217000	-2.463793000	-2.758898000
Br	-0.425270000	-5.311138000	-2.054569000
Br	2.049636000	-3.995011000	0.373508000
Br	-1.643199000	2.031374000	-3.557950000
Br	1.539075000	3.862366000	-3.626712000
Br	3.402730000	2.590027000	-0.660809000
C	3.989387000	-1.420581000	2.528845000
C	5.016860000	-1.507415000	1.665521000
C	3.772375000	-2.426679000	3.394334000
H	5.206669000	-0.685583000	0.953474000
H	2.934395000	-2.364297000	4.109817000
C	5.813140000	-2.586793000	1.663940000

C	4.568651000	-3.506081000	3.394216000
H	6.653388000	-2.651457000	0.950838000
H	4.382550000	-4.328166000	4.107074000
C	5.589080000	-3.587275000	2.528133000
H	6.243533000	-4.476263000	2.526936000
C	5.341015000	3.943307000	3.482349000
H	5.588059000	4.705208000	4.229213000
H	6.274169000	3.568325000	3.050711000
H	4.752523000	4.414553000	2.689288000