Theoretical Study on the Concerted Catalysis of Ir/Ni for Amino Radical Transfer for C(sp^2)-C(sp^3) Bond Formation

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Supporting Information

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Table S1. Energies for all stationary points.

Energies calculated at B3LYP(D3)/(6-31g(d), SDD) level in gas phase, and correction solvation energies calculated at M06(D3)/(def-TZVP, SDD) in DMF of reaction pathways. (unit: Hartree)

	E	***G***	G_{corr}	E_{sol}
R	-287.8028913	-287.695458	0.107433	-287.7061508
R`$^{+}$	-287.5231152	-287.416687	0.106428	-287.5051021
R^{+}	-288.1755273	-288.052974	0.122554	-288.1717412
0	-575.3671959	-575.136692	0.230505	-575.2296821
1	-575.3692013	-575.137935	0.231266	-575.234637
R1	-1008.489772	-1008.081172	0.408601	-1008.1204269
R2	-3031.247849	-3031.151246	0.096599	-3033.4466291
N1	-287.1493001	-287.056735	0.092565	-287.0485307
N2	-1295.663886	-1295.135335	0.528551	-1295.1919731
N3	-698.555321	-698.287232	0.268088	-698.3112416
N4	-597.1127123	-596.880385	0.232328	-596.8859236
M1	-5113.503490	-5113.214223	0.289267	-5115.5690968
M2	-2679.387962	-2678.96098	0.426982	-2679.0227102
M3	-5113.570123	-5113.280158	0.289892	-5115.6228686
M4	-5113.555232	-5113.26819	0.287042	-5115.6031401
M5	-5710.679064	-5710.127895	0.551170	-5712.4931601
M6	-5710.733921	-5710.18262	0.551301	-5712.5400395
M7	-4654.010446	-4653.84279	0.167655	-4656.2431403
M8	-2541.763804	-2541.47344	0.290364	-2541.4784329
M9	-3138.969046	-3138.415607	0.553438	-3138.4372937
M10	-3138.962437	-3138.407405	0.555032	-3138.4449602
M11	-3138.968062	-3138.413589	0.554473	-3138.446773
M12	-2082.131341	-2081.959526	0.171815	-2082.0185963
P	-1056.729609	-1056.370545	0.359064	-1056.3440457
PC1	-2942.823398	-2942.225965	0.597433	-2942.1003572
PC2	-2942.723467	-2942.133092	0.590375	-2942.0015622
PC3	-2942.973188	-2942.377078	0.596110	-2942.2043353
TS	-575.365897	-575.138044	0.227853	-575.2289639
TS1-2	-1295.662381	-1295.134985	0.527396	-1295.1870536
TS2a	-5710.673407	-5710.121479	0.551928	-5712.4859657
TS2b	-5113.492204	-5113.205027	0.287177	-5115.5487135
TS2c	-5113.483623	-5113.195156	0.288467	-5115.533617
TS3a	-5710.720194	-5710.170398	0.549795	-5712.5360833

TS3b	-5710.685129	-5710.14048	0.544648	-5712.4884979
TS4a	-3138.919792	-3138.36574	0.554057	-3138.4028228
TS4b	-3138.887632	-3138.340749	0.546882	-3138.3678566

Figure S1. The generation process of amino radicals.

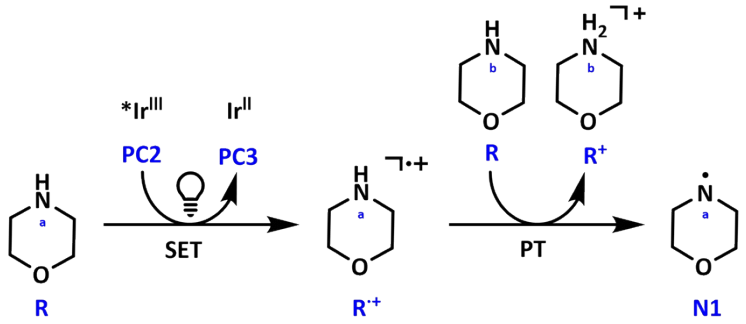
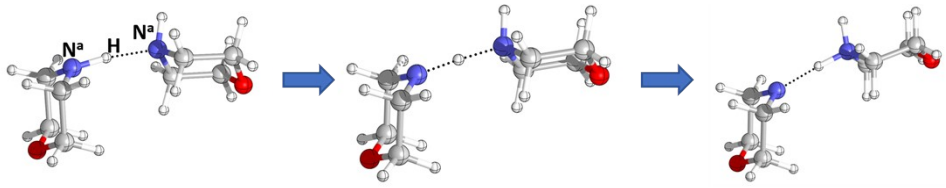


Figure S2. The bond length during the proton transfer transition state.



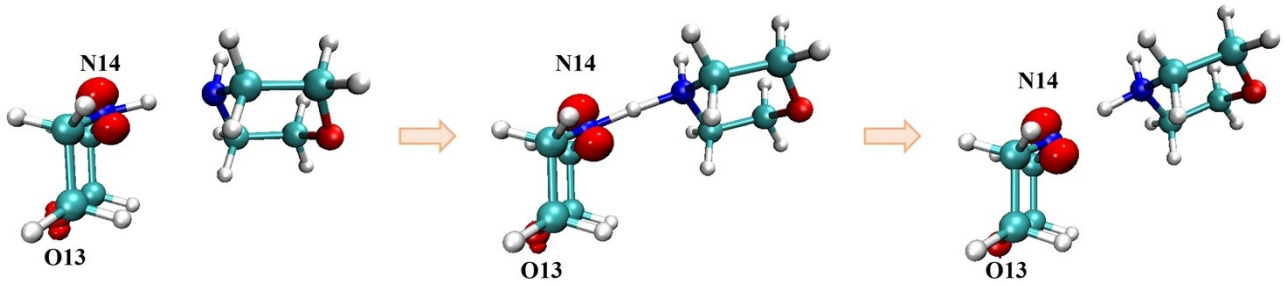
	INT1	TS1-2	INT2
Bond length of Nª-H (Å)	1.10	1.26	1.62
Bond length of Nª-H (Å)	1.63	1.34	1.10

Table S2. Energies for INT1 and TS1-2.

	E	*ΔE*	*H*	*ΔH*	*G*	*ΔG*
0	-575.367196	0	-575.081734	0	-575.136691	0
TS	-575.365897	0.001299	-575.083918	-0.002184	-575.138044	-0.001353

The energy analysis results reveal that the potential energy of transition state TS1-2 exceeds that of INT1, while the Gibbs free energy is marginally lower than that of the transition state. Simultaneously, a negative reaction enthalpy change suggests the presence of an entropy effect in this process.

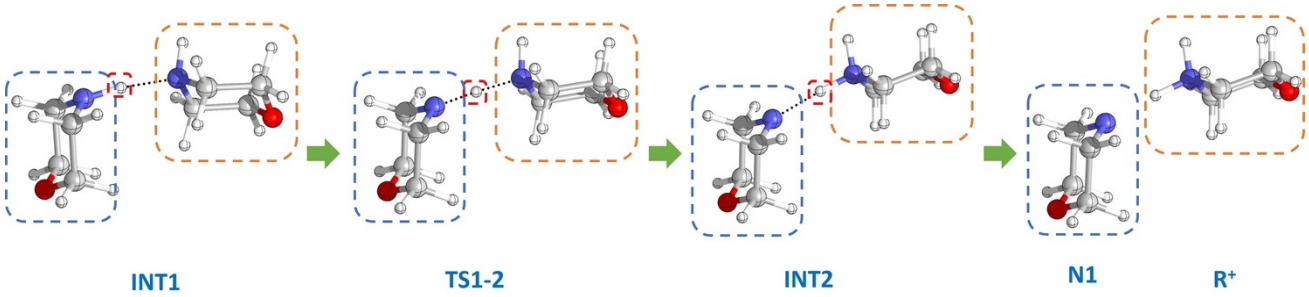
Figure S3. The spin layout during the proton transfer transition state.



INT1 TS1-2 INT2

	0	TS	1	N1
O^{13}	0.103024	0.080085	0.042625	0.014088
N^{14}	0.695452	0.744863	0.830684	0.889923

Figure 4. The NPA charge during the process of proton transfer.



	INT1	TS 1-2	INT2	N1 and R^+
fragment 1 (blue)	0.411	0.304	0.139	0.000
fragment 2 (red)	0.455	0.456	0.475	—
fragment 3 (orange)	0.134	0.240	0.386	1.000

Utilizing Marcus theory for the computation of energy barriers associated with single electron transfer steps.

According to the Marcus-Hush equation, the reorganization energy λ can be decomposed into two components: inner-sphere reorganization energy (λ_i) and outer-sphere solvent reorganization energy (λ_o), as shown in Equation S1. The calculation of inner-sphere reorganization energy (λ_i) can be performed using Equation S2.

$$\lambda = \lambda_i + \lambda_o$$ Equation S1

$$\lambda_i = \left|E^D(Q_P) - E^D(Q_R)\right| + \left|E^{A^-}(Q_P) - E^{A^-}(Q_R)\right|$$ Equation S2

In the Equation S2, *D* represents the recombination energy of the electron-donating substrate, while *A* represents that of the electron-accepting substrate. Q_R and Q_P respectively denote the equilibrium geometries of reactants and products.

The Equation S3 represents for the solvent recombination energy λ_o of an external sphere.

$$\lambda_o = (332\ kcal/mol)\left(\frac{1}{2a_1} + \frac{1}{2a_2} - \frac{1}{R}\right)\left(\frac{1}{\varepsilon_{op}} - \frac{1}{\varepsilon}\right)$$ Equation S3

Among them, a_1 and a_2 represent the radii of reactants, ε_{op} denotes the optical dielectric constant (2.038), ε signifies the static dielectric constant (37.219) of N,N-dimethylformamide solvent, and ΔG_r represents the change in free energy for SET reaction.

The equation S4 represents the calculation formula for the overall activation energy barrier of the SET process, where ΔG_r denotes the change in Gibbs free energy during the reaction.

$$\Delta G_{SET}^{\neq} = \frac{\lambda}{4}\left(1 + \frac{\Delta G_r}{\lambda}\right)^2$$ Equation S4

Table S3. Energy barriers data of single electron transfe.

SET	a_1	a_2	R	λ_o	λ_i	λ	ΔGr	$\Delta G_{SET}^{\neq}$
1	3.624	8.594	12.218	17.591	21.758	39.349	1.886	10.802
2	5.930	8.685	14.615	11.312	19.600	30.912	32.500	32.509
3	8.984	8.685	17.669	8.719	21.936	30.655	-7.297	4.450

The radii of the reactants in the first single electron transfer process were calculated as a_1 equals 3.624 and a_2 equals 8.594, with R equals 12.218 Å. The change in ΔG_r is determined to be 1.886 kcal·mol^{-1}, while λ_i and λ_o are found to be 21.758 kcal·mol^{-1} and 17.591 kcal·mol^{-1} respectively. By substituting these values into equation S1, it can be deduced that λ equals 39.349 kcal·mol^{-1}, thereby indicating an activation energy barrier of 10.802 kcal·mol^{-1} for the SET process.

In the second SET process, the values of a_1, a_2, and R are determined to be 5.930, 8.685, and 14.615 respectively. The change in ΔG_r is calculated as 32.500 kcal·mol^{-1} while λ_i is measured at 19.600 kcal·mol^{-1} and λ_o at 11.312 kcal·mol^{-1}; consequently yielding an overall value of λ equal to 30.912 kcal·mol^{-1}. Consequently, employing the same methodology allows us to determine that the activation energy barrier for this SET process amounts to approximately 32.509 kcal·mol^{-1}.

Similarly for the third SET process with relevant data inputted, suggested that the energy barrier is estimated to be around 4.450 kcal·mol^{-1}.

Calculation details of redox potential.

The correlation between the variation in standard *G* and the standard potential (V).

$$E^0 = \frac{\Delta G_r^0}{nF}$$ Equation S5

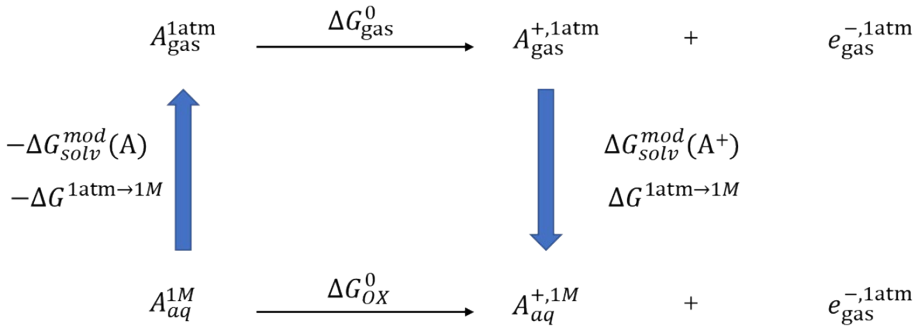
The relationship between the change in *G* of oxidation reaction and the oxidation potential is primarily determined by ionization energy, which is closely associated with $E_{(HOMO)}$. Conversely, the relationship between the change in *G* of reduction reaction and the reduction potential is primarily governed by electron affinity, which is closely linked to $E_{(LUMO)}$.

$$E_{OX}^{\ 0} = \frac{\Delta G_{OX}^{\ 0}}{nF}$$ Equation S6

$$E_{red}^{\ 0} = \frac{\Delta G_{red}^{\ 0}}{nF}$$ Equation S7

$$R + Ir^{III} \rightarrow R^{`+} + Ir^{II}$$ Equation S8

Oxidation potential calculation.



$$\Delta G_{OX}^{\ 0} = \Delta G_{gas}^{\ 0} + \Delta G_{solv}^{mod}(A^+) - \Delta G_{solv}^{mod}(A)$$ Equation S9

$$E_{OX-SHE} = \Delta G_{OX}^{\ 0} - 4.28$$ Equation S10

$$\Delta G_{gas}^{\ 0} = 27.2114 * (-287.416687 + 287.695458) = 7.586\ eV$$

$$E_{OX-SHE} = \Delta G_{OX}^{\ 0} - 4.28$$

Restoration of potential calculation.

$$Ir^{III} + e^- \rightarrow Ir^{II}$$ Equation S11

$$\Delta G_{red}^{\ 0} = \Delta G_{gas}^{\ 0} + \Delta G_{solv}^{mod}(A^-) - \Delta G_{solv}^{mod}(A)$$ Equation S12

$$\Delta G_{gas}^{\ 0} = G_{gas}^{\ 0}(A^-) - G_{gas}^{\ 0}(A) - G_{gas}^{\ 0}(e^-)$$ Equation S13

$$G_{gas}^{0}(e^{-}) = 0$$ Equation S14

$$\Delta G_{gas}^{0} = 27.2114 * (-2942.377078 + 2942.133092) = -6.639\ eV$$

$$E_{red-SHE} = -\Delta G_{red}^{0} - 4.28$$

$$= -\Delta G_{gas}^{0} - \Delta G_{solv}^{mod}(A^{-}) + \Delta G_{solv}^{mod}(A) - 4.2_{8}$$

$$M7 + Ir^{II} \rightarrow M7^{\neg -\cdot} + Ir^{III}$$ Equation S15

Oxidation potential calculation.

$$\Delta G_{OX}^{0} = \Delta G_{gas}^{0} + \Delta G_{solv}^{mod}(A^{+}) - \Delta G_{solv}^{mod}(A)$$

$$E_{OX-SHE} = \Delta G_{OX}^{0} - 4.28$$

$$\Delta G_{gas}^{0} = 27.2114 * (-2942.225965 + 2942.377078) = 4.112\ eV$$

$$E_{OX-SHE} = \Delta G_{OX}^{0} - 4.28$$

$$= \Delta G_{gas}^{0} + \Delta G_{solv}^{mod}(A^{+}) - \Delta G_{solv}^{mod}(A) - 4.2_{8}$$

Restoration of potential calculation.

$$\Delta G_{red}^{0} = \Delta G_{gas}^{0} + \Delta G_{solv}^{mod}(A^{-}) - \Delta G_{solv}^{mod}(A)$$

$$\Delta G_{gas}^{0} = G_{gas}^{0}(A^{-}) - G_{gas}^{0}(A) - G_{gas}^{0}(e^{-}) \qquad G_{gas}^{0}(e^{-}) = 0$$

$$\Delta G_{gas}^{0} = 27.2114 * (-4653.837827 + 4653.842799) = 0.135\ eV$$

$$\Delta G_{solv}^{mod}(A) = 27.2114 * (-4653.7337747 + 4653.7124341) = -0.581\ eV$$

$$\Delta G_{solv}^{mod}(A^{-}) = 27.2114 * (-4653.7391560 + 4653.8190546) = -2.174\ eV$$

$$E_{red-SHE} = -\Delta G_{red}^{0} - 4.28$$

$$= -\Delta G_{gas}^{0} - \Delta G_{solv}^{mod}(A^{-}) + \Delta G_{solv}^{mod}(A) - 4.2_{8}$$

$$= -2.822\ eV$$

$$M4 + Ir^{II} \rightarrow M4^{\neg -\cdot} + Ir^{III}$$ Equation S16

Oxidation potential calculation.

$$\Delta G_{OX}^{0} = \Delta G_{gas}^{0} + \Delta G_{solv}^{mod}(A^{+}) - \Delta G_{solv}^{mod}(A)$$

$$E_{OX-SHE} = \Delta G_{OX}^{0} - 4.28$$

$$\Delta G_{gas}^{0} = 27.2114 * (-2942.225965 + 2942.377078) = 4.112\ eV$$

$$\Delta G_{solv}^{mod}(A) = 27.2114 * (-2942.5554227 + 2942.5251003) = -0.825\ eV$$

$$\Delta G_{solv}^{mod}(A^{+}) = 27.2114 * (-2942.4578226 + 2942.3750722) = -2.252\ eV$$

$$E_{OX-SHE} = \Delta G_{OX}^{0} - 4.28$$

$$= \Delta G_{gas}^{\ 0} + \Delta G_{solv}^{mod}(A^+) - \Delta G_{solv}^{mod}(A) - 4.2_8$$

$$= -1.594\ eV$$

Restoration of potential calculation.

$\Delta G_{red}^{\ 0} = \Delta G_{gas}^{\ 0} + \Delta G_{solv}^{mod}(A^-) - \Delta G_{solv}^{mod}(A)$

$\Delta G_{gas}^{\ 0} = G_{gas}^{\ 0}(A^-) - G_{gas}^{\ 0}(A) - G_{gas}^{\ 0}(e^-)$ $\qquad G_{gas}^{\ 0}(e^-) = 0$

$\Delta G_{gas}^{\ 0} = 27.2114 * (-5113.328034 + 5113.26819) = -1.628\ eV$

$\Delta G_{solv}^{mod}(A) = 27.2114 * (-5113.3003538 + 5113.2535616) = -1.273\ eV$

$\Delta G_{solv}^{mod}(A^-) = 27.2114 * (-5113.3753273 + 5113.2936216) = -2.223\ eV$

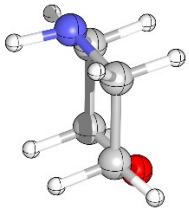
$E_{red-SHE} = -\Delta G_{red}^{\ 0} - 4.28$

$$= -\Delta G_{gas}^{\ 0} - \Delta G_{solv}^{mod}(A^-) + \Delta G_{solv}^{mod}(A) - 4.2_8$$

$$= -1.702\ eV$$

Cartesian coordinates and energies

R



C	-0.01371800	-0.77592900	1.17771400
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C	-0.01371800	-0.77592900	-1.17771400
H	-1.05142500	1.10846200	1.27149800
H	0.52029300	1.12625100	2.09000700
H	1.02678900	-1.14846000	1.22685700
H	-0.56846600	-1.19680100	2.02351000
H	-1.05142500	1.10846200	-1.27149800
H	0.52029300	1.12625100	-2.09000700
H	-0.56846600	-1.19680100	-2.02351000
H	1.02678900	-1.14846000	-1.22685700
O	-0.64918400	-1.26290700	0.00000000
N	0.58339700	1.34550300	0.00000000
H	1.58455400	1.14407200	0.00000000

Zero-point correction= 0.135883 (Hartree/Particle)
Thermal correction to Energy= 0.141169
Thermal correction to Enthalpy= 0.142114
Thermal correction to Gibbs Free Energy= 0.107433
Sum of electronic and zero-point Energies= -287.667008
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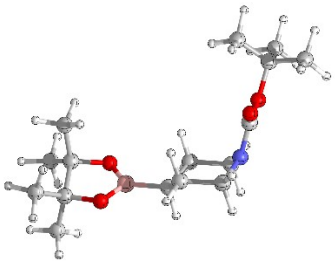
Sum of electronic and thermal Enthalpies= -287.660778
Sum of electronic and thermal Free Energies= -287.695458

R1



B	-2.13006600	-0.47143600	-0.34127700
O	-3.09668500	-1.00329700	0.47841700
O	-2.45135100	0.77921700	-0.80990900
C	-4.26343200	-0.13679700	0.39241200
C	-3.63200400	1.22457800	-0.08284200

C	-4.94056600	-0.09422100	1.75861600
H	-5.77348500	0.61793200	1.75471400
H	-5.33775900	-1.08414000	2.00406000
H	-4.23849800	0.19107200	2.54487600
C	-5.19935800	-0.76518500	-0.64693800
H	-6.13899700	-0.20984100	-0.73273000
H	-4.72352700	-0.80172900	-1.63200000
H	-5.42745500	-1.79094100	-0.34234500
C	-3.12615800	2.09203500	1.07576200
H	-2.49526300	1.50926900	1.75420700
H	-2.52244600	2.90883500	0.66900100
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C	-4.50211800	2.05027800	-1.02472200
H	-4.74735000	1.49672600	-1.93350200
H	-5.43450900	2.34605500	-0.53062600
H	-3.96693700	2.95919200	-1.31692800
C	1.53749300	-1.08441700	-1.69594800
C	0.21426100	-0.34312000	-1.46256300
C	-0.78459300	-1.21532700	-0.67373800
C	-0.12807900	-1.76794700	0.61669700
C	1.20855900	-2.45749400	0.31131700
H	0.42544200	0.57831600	-0.90347400
H	-0.21936000	-0.03598300	-2.42222700
H	1.36452000	-1.97017200	-2.32365200
H	2.27054900	-0.45643300	-2.19961000
H	0.06745000	-0.94627300	1.32007300
H	-0.80907700	-2.46449800	1.11956200
H	1.71746100	-2.77084800	1.22292200
H	1.04023100	-3.34361000	-0.31624800
H	-1.03823000	-2.08934000	-1.30025700
N	2.09710800	-1.55260800	-0.42342400
C	2.99858200	-0.81804500	0.30800300
O	3.27405300	-1.04230200	1.47917500
O	3.55297400	0.16472800	-0.44808800
C	4.54975100	1.07824600	0.11776000
C	3.93399500	1.87767100	1.27069800
H	3.70115600	1.22626400	2.11371700
H	4.63626000	2.65197500	1.59964100
H	3.01353500	2.36877400	0.93551300
C	5.79734400	0.30139900	0.54947200
H	6.58200600	1.00438000	0.85136800
H	5.57123300	-0.36218300	1.38476400
H	6.17520400	-0.29644600	-0.28719300
C	4.86459400	1.99396800	-1.06755600

H	5.61138000	2.74107900	-0.77916300
H	5.25888400	1.41216500	-1.90715400
H	3.96050900	2.51372700	-1.40151700

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Thermal correction to Enthalpy= 0.485992
Thermal correction to Gibbs Free Energy= 0.408601
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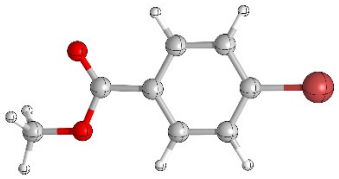
Sum of electronic and thermal Enthalpies= -1008.003780
Sum of electronic and thermal Free Energies= -1008.081172

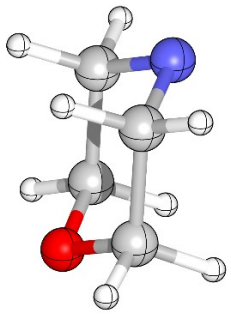
R2



C	-1.35892300	0.19100500	0.00002100
C	-0.73637200	-1.06448400	-0.00007900
C	0.65318000	-1.15950600	-0.00008900
C	1.41398400	0.01023000	0.00002200
C	0.81244200	1.26986800	0.00012400
C	-0.57644900	1.35310500	0.00012500
H	-1.34064100	-1.96454500	-0.00016100
H	1.14242000	-2.12724000	-0.00016900
H	1.42328100	2.16578700	0.00020000
H	-1.07413400	2.31723700	0.00020600
Br	3.32015200	-0.11546200	0.00000400
C	-2.84009700	0.35051200	0.00001400
O	-3.41588200	1.42105700	-0.00000200
O	-3.48643500	-0.83751500	0.00008200
C	-4.92049600	-0.75028100	-0.00017700
H	-5.27221400	-0.21820300	-0.88861200
H	-5.27644000	-1.78106200	-0.00230400
H	-5.27266500	-0.22185800	0.89028700

Zero-point correction= 0.134104 (Hartree/Particle)
Thermal correction to Energy= 0.144280
Thermal correction to Enthalpy= 0.145225
Thermal correction to Gibbs Free Energy= 0.096599
Sum of electronic and zero-point Energies= -3031.113741
Sum of electronic and thermal Energies= -3031.103564
Sum of electronic and thermal Enthalpies= -3031.102620
Sum of electronic and thermal Free Energies= -3031.151246

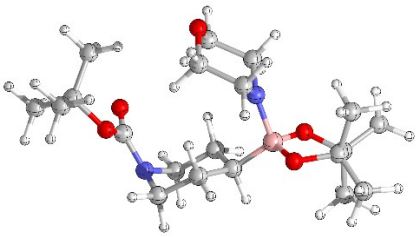
N1



C	0.01061500	-0.74653000	1.17084100
C	0.01061500	0.80316500	1.18073100
C	0.01061500	0.80316500	-1.18073100
C	0.01061500	-0.74653000	-1.17084100
H	-1.04307200	1.13090600	1.20907900
H	0.51584000	1.17250700	2.08104300
H	1.04814000	-1.11226600	1.23371100
H	-0.55272500	-1.13668500	2.02368700
H	-1.04307200	1.13090600	-1.20907900
H	0.51584000	1.17250700	-2.08104300
H	-0.55272500	-1.13668500	-2.02368700
H	1.04814000	-1.11226600	-1.23371100
O	-0.62126200	-1.23426300	0.00000000
N	0.68271100	1.29793700	0.00000000

Zero-point correction= 0.121691 (Hartree/Particle)
Thermal correction to Energy= 0.127005
Thermal correction to Enthalpy= 0.127949
Thermal correction to Gibbs Free Energy= 0.092565
Sum of electronic and zero-point Energies= -287.027609
Sum of electronic and thermal Energies= -287.022295
Sum of electronic and thermal Enthalpies= -287.021351
Sum of electronic and thermal Free Energies= -287.056735

N2



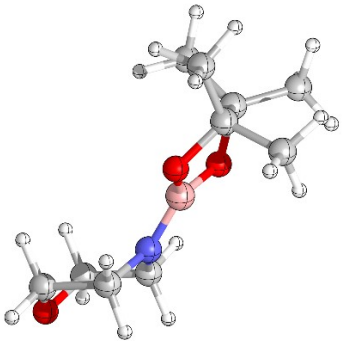
B	1.84365300	-0.24116900	0.06393900
O	2.77143300	-0.39480600	-1.04741300
O	2.61794700	-0.03526400	1.26938100
C	4.08961700	-0.50397200	-0.49818400
C	3.96307500	0.26406400	0.87065900
C	5.08858500	0.10124500	-1.48436100
H	6.09853400	0.12419400	-1.05811700

H	5.11754000	-0.50286400	-2.39744900
H	4.80360000	1.11800000	-1.76599300
C	4.39544800	-1.99778500	-0.29865500
H	5.42809800	-2.16804400	0.02612800
H	3.71939000	-2.43386500	0.44233500
H	4.23890900	-2.51583100	-1.25009500
C	4.11754200	1.78581300	0.70055700
H	3.51111500	2.15623200	-0.13201100
H	3.78337300	2.28052200	1.61873200
H	5.15816100	2.07225300	0.51376000
C	4.90776800	-0.22042600	1.97049300
H	4.71444400	-1.26559700	2.22110600
H	5.95559600	-0.11688200	1.66451900
H	4.75611300	0.37529100	2.87728800
C	-1.46088600	-2.15441400	1.34094300
C	-0.29232400	-1.16083300	1.33837100
C	0.71811800	-1.41400500	0.20009000
C	0.03568900	-1.72616000	-1.14791700
C	-1.13069300	-2.71196100	-1.01189600
H	-0.74068800	-0.16681700	1.24024600
H	0.22959900	-1.17532900	2.30322500
H	-1.11194900	-3.16853400	1.57173600
H	-2.22325200	-1.88548300	2.07297900
H	-0.38586700	-0.81703900	-1.59276800
H	0.78509700	-2.09845400	-1.85595000
H	-1.66922800	-2.83864700	-1.95187900
H	-0.78316700	-3.69569800	-0.67423700
H	1.30167900	-2.30730600	0.47947000
N	-2.06947900	-2.20545000	0.00270400
C	-2.94264600	-1.23594800	-0.42469500
O	-3.23809200	-1.05028900	-1.59956300
O	-3.43290800	-0.50746900	0.61603000
C	-4.62316400	0.33798200	0.44382500
C	-4.37494600	1.46820300	-0.56194500
H	-4.26119200	1.07329300	-1.57102200
H	-5.22674900	2.15794600	-0.54180300
H	-3.47652200	2.03828900	-0.30614600
C	-5.80719700	-0.53958800	0.02881800
H	-6.72347200	0.06038300	0.00222300
H	-5.63909600	-0.96767300	-0.96151700
H	-5.94687500	-1.35248100	0.74955900
C	-4.82393700	0.90363200	1.85119600
H	-5.70714700	1.55023900	1.87662600
H	-4.96058200	0.09427500	2.57547000

H	-3.95261300	1.49431700	2.15413700
C	-0.82742800	2.49544400	0.60855300
C	0.66216700	2.10603800	0.78047700
C	0.75360200	1.63680900	-1.59077900
C	-0.74834100	2.01076900	-1.68472700
H	1.26119700	3.02304600	0.68130400
H	0.87057200	1.65658000	1.75226100
H	-1.47244600	1.63269600	0.82403700
H	-1.07574900	3.30336800	1.30206000
H	1.33397200	2.54859000	-1.79652300
H	1.04574400	0.86773000	-2.30594000
H	-0.95259200	2.46530300	-2.65730400
H	-1.37905600	1.11746600	-1.57543300
O	-1.06888900	2.98172200	-0.69962500
N	1.06391200	1.18427500	-0.25558200

Zero-point correction= 0.586205 (Hartree/Particle)
Thermal correction to Energy= 0.615414
Thermal correction to Enthalpy= 0.616358
Thermal correction to Gibbs Free Energy= 0.528551
Sum of electronic and zero-point Energies= -1295.077681
Sum of electronic and thermal Energies= -1295.048472
Sum of electronic and thermal Enthalpies= -1295.047528
Sum of electronic and thermal Free Energies= -1295.135335

N3

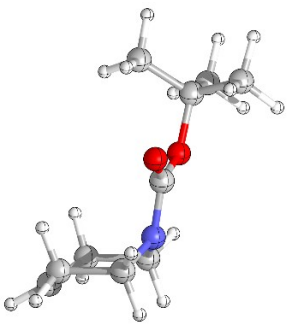


C	-3.33889700	1.22430800	0.23910800
C	-2.23211300	1.08561100	-0.80890500
C	-2.22352500	-1.31316200	-0.38742200
C	-3.32919400	-1.09471600	0.64777300
H	-2.69769400	0.99257200	-1.80262200
H	-1.58749100	1.96873200	-0.81193800
H	-2.88659400	1.44254500	1.22220600
H	-4.02844300	2.03479500	-0.01871200
H	-2.69083100	-1.56567000	-1.35238300
H	-1.57274100	-2.14081100	-0.09255500
H	-4.01199000	-1.94985600	0.68428100

H	-2.87530500	-0.95971200	1.64482400
O	-4.12457300	0.03866200	0.31334800
N	-1.42956600	-0.09811900	-0.52550700
B	-0.04501300	-0.05096200	-0.28513600
O	0.71531200	1.09970100	-0.42529700
O	0.69966400	-1.14994300	0.11425900
C	2.01499600	0.80425600	0.14604300
C	2.09300500	-0.76218200	0.00487700
C	2.88377900	-1.46926000	1.10131600
H	3.92592600	-1.12990200	1.10708500
H	2.44940400	-1.28791000	2.08682700
H	2.87739600	-2.54932700	0.92302200
C	2.57865100	-1.21313000	-1.37856300
H	3.64804000	-1.02168300	-1.51528100
H	2.40108600	-2.28788800	-1.48178100
H	2.02690600	-0.69935200	-2.17204300
C	1.97948200	1.27195800	1.60673500
H	2.95189200	1.15362500	2.09613800
H	1.70461900	2.33087400	1.63078000
H	1.23112500	0.71300400	2.17758100
C	3.07644100	1.57553100	-0.63250400
H	4.08140100	1.30850900	-0.28620300
H	3.00913100	1.37585400	-1.70416500
H	2.93720900	2.65060300	-0.48006200

Zero-point correction= 0.309590 (Hartree/Particle)
Thermal correction to Energy= 0.324594
Thermal correction to Enthalpy= 0.325538
Thermal correction to Gibbs Free Energy= 0.268088
Sum of electronic and zero-point Energies= -698.245731
Sum of electronic and thermal Energies= -698.230727
Sum of electronic and thermal Enthalpies= -698.229783
Sum of electronic and thermal Free Energies= -698.287232

N4

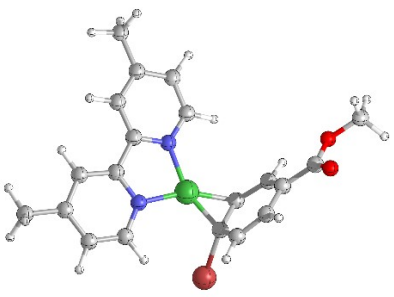


C	-1.49092300	1.08026500	-1.02165600
C	-2.18662200	1.64482500	0.23708600
C	-3.25880300	0.71625300	0.71809700

C	-2.98211400	-0.75551000	0.73859300
C	-2.24449000	-1.20257800	-0.54297300
H	-1.40467000	1.77322300	1.00951600
H	-2.58653900	2.64548800	0.02997200
H	-2.18497500	1.10435600	-1.87087800
H	-0.60870700	1.66089400	-1.28589400
H	-2.32936600	-1.01685600	1.59222400
H	-3.90557400	-1.33443300	0.86409700
H	-1.87404600	-2.22342800	-0.45278300
H	-2.91985700	-1.14691300	-1.40530100
H	-4.12266200	1.11332900	1.24341400
N	-1.10802100	-0.31789900	-0.80850100
C	0.11114700	-0.68044000	-0.28235400
O	0.35790300	-1.79336300	0.16068300
O	0.99233200	0.34889600	-0.34717000
C	2.37103400	0.19197300	0.13069400
C	2.37468100	-0.12209500	1.63001500
H	1.94173700	-1.10403600	1.82402500
H	3.40353400	-0.10486100	2.00653300
H	1.79762400	0.63476600	2.17304000
C	3.09635400	-0.87824600	-0.69036800
H	4.15533300	-0.90118800	-0.40948600
H	2.66058800	-1.86282400	-0.51703500
H	3.02920200	-0.64266000	-1.75810600
C	2.96798700	1.57612700	-0.13322900
H	4.01570000	1.60129000	0.18416500
H	2.92027800	1.81778500	-1.19999400
H	2.41716500	2.34365700	0.42046700

Zero-point correction= 0.273478 (Hartree/Particle)
Thermal correction to Energy= 0.287410
Thermal correction to Enthalpy= 0.288354
Thermal correction to Gibbs Free Energy= 0.232328
Sum of electronic and zero-point Energies= -596.839234
Sum of electronic and thermal Energies= -596.825302
Sum of electronic and thermal Enthalpies= -596.824358
Sum of electronic and thermal Free Energies= -596.880385

M1

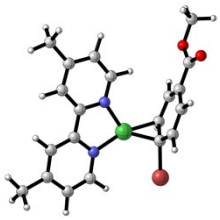


C	-2.07007100	1.66999800	-0.18429400
C	-0.16519600	2.55060100	-1.18135100
C	-0.68878600	3.83498400	-1.14794600
C	-1.96388600	4.05249800	-0.60612200
C	-2.64941200	2.93706500	-0.11849900
C	-2.69340500	0.42478000	0.30890600
C	-2.36171100	-1.85929400	0.58817100
C	-3.63087300	-2.01598200	1.12796200
C	-4.47295400	-0.90444700	1.27091300
C	-3.97919700	0.32956800	0.83984200
H	0.82234400	2.34131700	-1.57668100
H	-0.10426000	4.66251300	-1.53916500
H	-3.63351100	3.06315100	0.32096400
H	-1.69125000	-2.69706900	0.43009900
H	-3.96210900	-3.00470100	1.43176700
H	-4.60440600	1.21330700	0.91637300
N	-0.83267200	1.47871800	-0.71830800
N	-1.88466900	-0.66432000	0.19473500
Ni	-0.16792500	-0.29262000	-0.51191600
C	1.62278100	-0.60472900	-1.15004000
C	2.63544900	-1.04845800	1.46896900
C	2.77294600	0.09828700	-0.67202900
H	1.56221800	-0.73339200	-2.23279900
C	3.23895400	-0.06290600	0.61558500
H	3.03485500	-1.16436200	2.47125900
H	3.30082400	0.76663200	-1.34648700
Br	0.47055000	-3.39397800	-1.15605400
C	1.62013500	-1.84619500	1.02469800
H	1.22338200	-2.63471200	1.65785000
C	1.03063200	-1.64521000	-0.27804400
C	-5.84928100	-1.04069300	1.86911500
H	-5.78568400	-1.26309000	2.94171700
H	-6.43464800	-0.12382700	1.75120100
H	-6.40287300	-1.86281300	1.40159900
C	-2.55623300	5.43666600	-0.54439400
H	-3.57592500	5.42367700	-0.14830000
H	-1.95286100	6.09080600	0.09677000
H	-2.58302600	5.89632800	-1.53939800
C	4.38151100	0.70164700	1.14973100
O	4.85380400	0.56864300	2.26591000
O	4.87798800	1.61047900	0.26043500
C	6.00127500	2.36045100	0.73362300
H	6.27732400	3.02688600	-0.08569100
H	5.73767100	2.93831000	1.62511100

H	6.83557000	1.69810400	0.98483100

Zero-point correction= 0.349665 (Hartree/Particle)
Thermal correction to Energy= 0.375213
Thermal correction to Enthalpy= 0.376157
Thermal correction to Gibbs Free Energy= 0.289267
Sum of electronic and zero-point Energies= -5113.153825
Sum of electronic and thermal Energies= -5113.128277
Sum of electronic and thermal Enthalpies= -5113.127332
Sum of electronic and thermal Free Energies= -5113.214223

^{3}M1

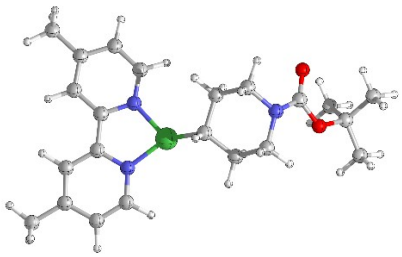


C	1.35820200	-1.59145900	-1.04801000
C	0.66335900	-2.02724800	0.14323900
C	1.26496300	-1.84888300	1.42788800
C	2.43226200	-1.13912200	1.53405300
C	3.10816000	-0.65387700	0.37306900
C	2.59805900	-0.92355500	-0.88527500
Br	-0.54117700	-3.57411800	-0.07263200
H	0.76622600	-2.24936600	2.30354200
H	1.14965900	-2.06281900	-2.00618700
H	3.15368500	-0.62024300	-1.76626400
H	2.87771100	-0.94290400	2.50344100
C	-2.48540200	1.09890200	-0.01099700
C	-3.26122700	-1.11362900	-0.21769400
C	-4.55291000	-0.74883800	0.08132800
C	-4.84502700	0.61748200	0.35501400
C	-3.79840400	1.51610900	0.30875000
C	-1.33875100	1.95860100	-0.08520200
C	0.98126500	2.06691000	-0.44237100
C	0.99627600	3.43573800	-0.30443000
C	-0.22218600	4.12311500	-0.04399900
C	-1.37160200	3.36611200	0.05512900
H	-2.99502900	-2.14764100	-0.40857100
H	-5.33432300	-1.50169600	0.11373900
H	-3.98390500	2.56174200	0.53364600
H	1.89467000	1.51871600	-0.64104100
H	1.93240500	3.97788400	-0.39558400
H	-2.32143000	3.85962500	0.23576000
N	-2.23208500	-0.23600800	-0.28795400

N	-0.13599500	1.31186700	-0.33032100
Ni	-0.37298100	-0.59713400	-0.59129200
C	-0.23288900	5.62128000	0.10413800
H	0.42008600	5.93947300	0.92737200
H	0.14102700	6.11062800	-0.80480300
H	-1.23918600	6.00285500	0.30384000
C	-6.25021400	1.04041600	0.69219700
H	-6.62131600	0.50685500	1.57701300
H	-6.31374000	2.11440300	0.89369400
H	-6.93956600	0.80865100	-0.13038400
C	4.35704900	0.11579300	0.57286800
O	4.81392100	0.67129400	-0.58013800
O	4.91424900	0.26767200	1.64394200
C	6.02721800	1.42713800	-0.44936900
H	5.89002300	2.25673500	0.25019700
H	6.84034000	0.79222800	-0.08556500
H	6.24934000	1.80009900	-1.45000800

Zero-point correction= 0.348516 (Hartree/Particle)
Thermal correction to Energy= 0.374096
Thermal correction to Enthalpy= 0.375040
Thermal correction to Gibbs Free Energy= 0.289037
Sum of electronic and zero-point Energies= -5113.139075
Sum of electronic and thermal Energies= -5113.113495
Sum of electronic and thermal Enthalpies= -5113.112551
Sum of electronic and thermal Free Energies= -5113.198555

M2



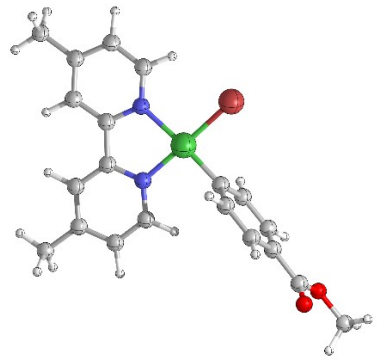
C	-3.73187800	0.58033400	0.20545300
C	-2.80181600	2.72778700	0.35156900
C	-4.03406900	3.32656100	0.22841100
C	-5.18951200	2.51969100	0.05472400
C	-5.01061500	1.14708800	0.04134400
C	-3.44456600	-0.83668500	0.25360200
C	-1.75139300	-2.43263700	0.53296600
C	-2.64915100	-3.47470400	0.45905000
C	-4.02289700	-3.19682200	0.24427900
C	-4.39761800	-1.86745300	0.14035800
H	-1.89397100	3.31546400	0.45505200

H	-4.11433100	4.40916400	0.25489900
H	-5.87016500	0.49751900	-0.09264900
H	-0.68850900	-2.60780900	0.66703800
H	-2.29928900	-4.49796600	0.55621500
H	-5.44052000	-1.61764000	-0.02811300
N	-2.61892600	1.38488200	0.34486900
N	-2.11172900	-1.13277000	0.43333700
Ni	-0.96915800	0.40650300	0.21635300
C	-5.02040500	-4.31974300	0.13143000
H	-6.03736600	-3.94478500	-0.01980600
H	-4.77497700	-4.98098200	-0.70938700
H	-5.01885700	-4.94052800	1.03642800
C	-6.54544200	3.15352100	-0.11149700
H	-6.57360900	3.79913300	-0.99879800
H	-7.33370200	2.40162700	-0.21695700
H	-6.79362300	3.78594200	0.75058100
C	2.90471200	1.28543500	-1.52836600
C	1.66256000	1.43883800	-0.62947800
C	0.56301800	0.42119800	-0.98932400
C	1.15313900	-1.00252600	-1.03279800
C	2.41302900	-1.08897400	-1.91199500
H	1.99339900	1.30408900	0.41164300
H	1.28294800	2.46683500	-0.71005400
H	2.63117500	1.49708100	-2.57146800
H	3.70830200	1.96441900	-1.24424700
H	1.43972200	-1.33524100	-0.02256600
H	0.40230500	-1.71459600	-1.40025600
H	2.87993600	-2.07402100	-1.87037000
H	2.15299200	-0.86743700	-2.95620500
H	0.22073500	0.65900800	-2.01274300
N	3.40051000	-0.09502900	-1.47905100
C	4.37058800	-0.50620900	-0.60216300
O	4.61608800	-1.67882100	-0.34627500
O	5.03773500	0.55756100	-0.07720200
C	6.12927400	0.36216800	0.87742000
C	5.60718600	-0.32914900	2.14168400
H	5.28889100	-1.34867800	1.92194000
H	6.39642200	-0.35479000	2.90166300
H	4.75654900	0.22904600	2.54870400
C	7.27731500	-0.41358700	0.22331900
H	8.13764400	-0.44074900	0.90182700
H	6.97235900	-1.43450800	-0.00884600
H	7.58521300	0.08402700	-0.70285000
C	6.55556600	1.79953600	1.18700700

H	7.37954600	1.80252300	1.90841800
H	6.88731200	2.30596900	0.27469100
H	5.71817600	2.36428800	1.61009900

Zero-point correction= 0.491021 (Hartree/Particle)
Thermal correction to Energy= 0.519855
Thermal correction to Enthalpy= 0.520799
Thermal correction to Gibbs Free Energy= 0.426982
Sum of electronic and zero-point Energies= -2678.896942
Sum of electronic and thermal Energies= -2678.868108
Sum of electronic and thermal Enthalpies= -2678.867163
Sum of electronic and thermal Free Energies= -2678.960980

M3

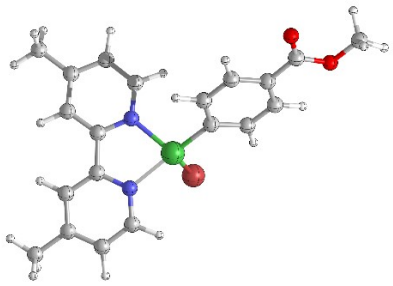


Ni	0.55849900	-0.69386600	0.00409300
C	-1.29557900	-0.51590300	0.07205100
C	-4.08336400	-0.03880800	0.18663000
C	-1.96103000	-0.38528100	1.30387400
C	-2.06873500	-0.43401700	-1.09884400
C	-3.44007700	-0.19405400	-1.05107700
C	-3.33023900	-0.14386200	1.36577300
H	-1.39626600	-0.47990600	2.22881100
H	-1.58795600	-0.56681200	-2.06552000
H	-4.01966100	-0.13029100	-1.96631400
H	-3.84078800	-0.03699600	2.31833700
N	0.85925200	1.18819700	0.00020600
C	1.55361000	3.93386900	-0.01398400
C	-0.08198000	2.15739600	0.00837600
C	2.16368200	1.58676000	-0.01765700
C	2.52577200	2.93419400	-0.02488000
C	0.21951100	3.51017700	0.00179200
N	2.54894800	-0.74497300	-0.03304800
C	5.35116700	-0.48233400	-0.05470500
C	3.34606400	-1.82699800	-0.04678300
C	3.13012400	0.47838200	-0.03113500
C	4.51779000	0.63687500	-0.04130000
C	4.73106800	-1.73826900	-0.05830400

H	-1.10613400	1.81312700	0.02145800
H	3.57446600	3.20968100	-0.04014500
H	-0.59351100	4.22995500	0.00900800
H	2.82013400	-2.77569100	-0.04787800
H	4.95488500	1.62926900	-0.03783900
H	5.32228600	-2.64913400	-0.06951400
Br	0.26208100	-2.94158500	-0.01412200
C	6.85214400	-0.35405500	-0.06150100
H	7.17118300	0.69198400	-0.08794000
H	7.28521300	-0.81913000	0.83211900
H	7.28263300	-0.86450500	-0.93094200
C	1.91240000	5.39631200	-0.01378500
H	1.42720300	5.91775800	-0.84704700
H	1.57180500	5.87897800	0.91029500
H	2.99226600	5.54954800	-0.09762600
C	-5.53595700	0.22674000	0.30719500
O	-6.16103300	0.27756400	-0.90012400
O	-6.13465900	0.38925800	1.35547400
C	-7.57131500	0.52069800	-0.84022300
H	-7.91354700	0.52504600	-1.87639900
H	-8.07700600	-0.26627600	-0.27250300
H	-7.78022700	1.48303600	-0.36265800

Zero-point correction= 0.351089 (Hartree/Particle)
Thermal correction to Energy= 0.376793
Thermal correction to Enthalpy= 0.377737
Thermal correction to Gibbs Free Energy= 0.289892
Sum of electronic and zero-point Energies= -5113.219034
Sum of electronic and thermal Energies= -5113.193330
Sum of electronic and thermal Enthalpies= -5113.192386
Sum of electronic and thermal Free Energies= -5113.280231

M4



C	-3.05759300	0.17542600	0.58045700
C	-2.76474000	-2.04134500	1.19555900
C	-4.10197700	-2.17164900	1.54430800
C	-4.96245300	-1.07504800	1.39601800
C	-4.41518400	0.11190500	0.90213900

C	-2.38537700	1.37490000	0.02501500
C	-0.40952400	2.17901100	-0.89853400
C	-0.96128300	3.43844800	-1.09425600
C	-2.28259400	3.68330800	-0.69791400
C	-2.99289900	2.62215100	-0.12878000
H	-2.06734000	-2.86927000	1.26829000
H	-4.47262600	-3.12145200	1.91757900
H	-5.05555800	0.97501900	0.75517900
H	0.61470900	1.94219800	-1.16543800
H	-0.36369900	4.22250900	-1.54907600
H	-4.01733300	2.77645100	0.19283300
N	-2.24851700	-0.89362900	0.73903800
N	-1.10266100	1.17240000	-0.35027700
Ni	-0.35064000	-0.66583300	-0.04038600
C	2.53780400	-1.16985600	-0.43409400
C	3.37958900	0.95818000	1.15412800
C	3.89986400	-0.94430700	-0.24879100
H	2.21597000	-1.99323000	-1.06690300
C	4.33239300	0.12589400	0.55089700
H	3.72505700	1.78451900	1.76885100
H	4.63520400	-1.58741300	-0.72178200
Br	-0.68186300	-2.17968300	-1.80304200
C	2.02253400	0.71583200	0.95238100
H	1.30412000	1.38563000	1.42783200
C	1.55482500	-0.35478900	0.16053900
C	-2.90266000	5.04636300	-0.86390100
H	-2.70210200	5.44963400	-1.86236100
H	-3.98596100	5.02044700	-0.71416800
H	-2.47933500	5.75198800	-0.13817900
C	-6.42645500	-1.18807400	1.73290700
H	-6.91989500	-0.21178400	1.73268700
H	-6.94002900	-1.82549000	1.00261300
H	-6.56866800	-1.64552400	2.71823600
C	5.76613200	0.42635200	0.78488800
O	6.18768500	1.35309200	1.45410400
O	6.59405500	-0.45477700	0.16402300
C	7.99213900	-0.21008300	0.35597100
H	8.50724700	-0.99718300	-0.19702400
H	8.27062000	0.77541000	-0.03001500
H	8.25185400	-0.25388200	1.41814500

Zero-point correction= 0.350133 (Hartree/Particle)
Thermal correction to Energy= 0.376345
Thermal correction to Enthalpy= 0.377289
Thermal correction to Gibbs Free Energy= 0.287042

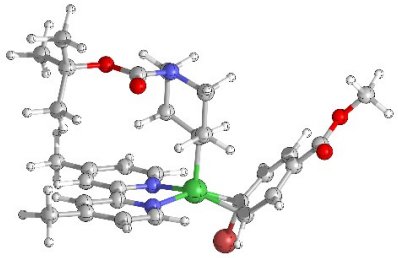
Sum of electronic and zero-point Energies= -5113.205099

Sum of electronic and thermal Energies= -5113.178887

Sum of electronic and thermal Enthalpies= -5113.177943

Sum of electronic and thermal Free Energies= -5113.268190

M5

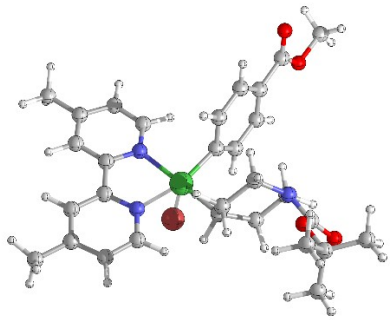


C	-1.42703400	-1.68481600	1.19209500
C	-0.60350400	-0.16753200	2.74949800
C	-1.81631100	-0.10933900	3.41196900
C	-2.89927200	-0.87489400	2.94252800
C	-2.67841900	-1.66977200	1.82090500
C	-1.11688800	-2.45786200	-0.01864100
C	0.49032600	-2.88396000	-1.64433300
C	-0.35692200	-3.73476700	-2.33064400
C	-1.65416400	-3.96968300	-1.83656100
C	-2.01876900	-3.31420600	-0.66472900
H	0.24650100	0.42505800	3.07053600
H	-1.92584000	0.53093800	4.28193000
H	-3.49278000	-2.26689700	1.42421800
H	1.49816700	-2.68291300	-1.98907600
H	-0.01494400	-4.21814000	-3.24105500
H	-3.01095100	-3.46872500	-0.25385600
N	-0.39355800	-0.93179900	1.66043300
N	0.13435300	-2.25455900	-0.51010600
Ni	1.15472900	-0.83840500	0.41311600
C	-2.60075300	-4.89145000	-2.56034400
H	-3.55444100	-4.98882200	-2.03300100
H	-2.80925800	-4.52155700	-3.57184800
H	-2.16759500	-5.89332200	-2.66743800
C	-4.24699700	-0.80106100	3.60960300
H	-4.72466500	0.16345100	3.39746200
H	-4.91759900	-1.59008100	3.25588000
H	-4.15637000	-0.88846700	4.69826900
C	-1.18891800	1.74940300	-2.22778900
C	-0.65122900	0.48374800	-1.52997400
C	0.52371400	0.78909500	-0.60384900
C	0.17581200	1.94389800	0.33616200
C	-0.36490100	3.17029000	-0.42467600

H	-1.48737200	0.05172800	-0.95910400
H	-0.37335100	-0.25346600	-2.29364000
H	-0.41515300	2.17505700	-2.87930700
H	-2.06596200	1.53635000	-2.83940100
H	-0.61601400	1.64999000	1.03653900
H	1.04306700	2.24448500	0.93250800
H	-0.67102900	3.96470600	0.25740200
H	0.39500900	3.56905400	-1.10802500
H	1.39110100	1.07927900	-1.21212500
N	-1.52688800	2.77249300	-1.23065700
C	-2.73670400	2.75661900	-0.58139800
O	-2.96198100	3.33099000	0.47624900
O	-3.65737000	2.03567300	-1.28039700
C	-5.00401500	1.83027000	-0.75231700
C	-4.93502500	1.09245300	0.58967000
H	-4.46521100	1.71691700	1.35074000
H	-5.94585100	0.82224700	0.91642100
H	-4.34736700	0.17465700	0.48163900
C	-5.74580500	3.16598600	-0.64359300
H	-6.79105500	2.98755300	-0.36577100
H	-5.27914300	3.80604400	0.10582800
H	-5.72966000	3.68203900	-1.60965100
C	-5.64346200	0.93888100	-1.82024800
H	-6.67634200	0.69907000	-1.54594800
H	-5.64825800	1.44719700	-2.78978800
H	-5.08127400	0.00465000	-1.92409200
C	3.03465200	-1.03004700	0.06976600
C	3.78747100	1.68597300	0.13292900
C	2.87214000	-0.26103200	1.29604100
C	3.71020300	-0.43980900	-1.05117500
C	4.01835900	0.89200000	-1.03810100
C	3.29163300	1.09559700	1.27806600
H	2.85309300	-0.76850500	2.25961000
H	3.92896200	-1.05419800	-1.91860900
H	4.46342300	1.35886300	-1.90939000
H	3.22419400	1.69495600	2.18124000
Br	3.38323500	-2.97389200	0.32390800
C	4.08414800	3.13479100	0.18292700
O	4.62122200	3.59490900	-0.97694300
O	3.86494100	3.86182400	1.13616800
C	4.90323800	5.00071000	-0.99734800
H	5.31802400	5.20297300	-1.98591300
H	3.98903800	5.58019200	-0.83740300
H	5.62378500	5.26218100	-0.21676900

Zero-point correction= 0.627476 (Hartree/Particle)
Thermal correction to Energy= 0.667478
Thermal correction to Enthalpy= 0.668423
Thermal correction to Gibbs Free Energy= 0.551170
Sum of electronic and zero-point Energies= -5710.051588
Sum of electronic and thermal Energies= -5710.011586
Sum of electronic and thermal Enthalpies= -5710.010642
Sum of electronic and thermal Free Energies= -5710.127895

M6



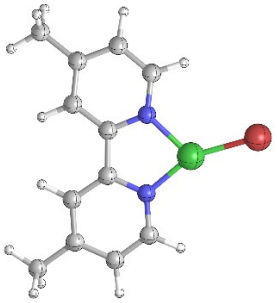
C	2.98015800	-2.26115700	-0.58147900
C	1.07653800	-3.43069500	0.00270500
C	1.68478700	-4.65405800	-0.24136900
C	3.01237000	-4.68507800	-0.68099900
C	3.65247300	-3.45665400	-0.84987700
C	3.61884100	-0.93103600	-0.69419700
C	3.34882400	1.34633200	-0.38113300
C	4.66988800	1.59934400	-0.72268200
C	5.50785100	0.53695800	-1.07926800
C	4.95567000	-0.74471700	-1.05645900
H	0.05314500	-3.38401600	0.35362000
H	1.12649300	-5.57200300	-0.08479600
H	4.68359700	-3.44020200	-1.18359800
H	2.67667000	2.14230800	-0.08661100
H	5.04044400	2.61980100	-0.70578600
H	5.57954700	-1.59380000	-1.31143800
N	1.69243300	-2.25320500	-0.16644700
N	2.82336100	0.11279800	-0.37930800
Ni	0.95010900	-0.34800100	0.30948500
C	0.26237900	2.35207400	1.11280000
C	-0.17570200	3.20139600	-1.50884100
C	-0.02633400	3.69161200	0.85581500
H	0.45209700	2.02727300	2.13090200
C	-0.25478600	4.12651900	-0.45883300
H	-0.34545500	3.54865500	-2.52350900
H	-0.07496000	4.40601700	1.67097100
Br	1.85266500	-0.47868800	2.57840400

C	0.11692900	1.86630300	-1.23982300
H	0.18366100	1.16803500	-2.07325800
C	0.32547200	1.41262800	0.07426100
C	6.94975200	0.77128000	-1.44701100
H	7.42528200	-0.13734800	-1.82775900
H	7.03743600	1.55150400	-2.21140900
H	7.51882100	1.10941700	-0.57245700
C	3.72475100	-5.98801500	-0.93265700
H	4.64047100	-5.84348700	-1.51357200
H	4.00204600	-6.46070300	0.01790400
H	3.08173100	-6.69300800	-1.47028300
C	-0.57034300	5.53773700	-0.79612100
O	-0.74755900	5.96085800	-1.92387400
O	-0.64351000	6.33111400	0.30188000
C	-0.95474900	7.70591500	0.03800700
H	-0.98003500	8.19345000	1.01353100
H	-0.19053300	8.16019500	-0.59986100
H	-1.92424400	7.79338700	-0.46126600
C	-2.54393300	-0.38456800	-1.14545200
C	-1.57661200	-1.41782200	-0.55159700
C	-0.85995100	-0.93800700	0.72928700
C	-1.78846200	-0.15403700	1.66674800
C	-2.77125600	0.79699500	0.97139000
H	-2.17678900	-2.30989300	-0.30785800
H	-0.86119500	-1.73562600	-1.32420300
H	-1.99834700	0.48549200	-1.51937000
H	-3.11091700	-0.81274600	-1.97116700
H	-2.39577900	-0.88475600	2.22363900
H	-1.19428300	0.38132800	2.41298000
H	-3.51829400	1.16126900	1.67661200
H	-2.25745800	1.65624000	0.53546800
H	-0.53657800	-1.80817400	1.31302600
N	-3.46518600	0.09656600	-0.11595000
C	-4.63308700	-0.55418000	0.18954300
O	-5.28465200	-0.35835500	1.20647400
O	-4.97870700	-1.42487100	-0.79958600
C	-6.20803200	-2.21389300	-0.70583400
C	-6.14369500	-3.14543200	0.50940000
H	-6.14845400	-2.57263600	1.43727400
H	-7.00461800	-3.82350700	0.50143500
H	-5.23015700	-3.74973800	0.47012400
C	-7.43189700	-1.29310600	-0.66681600
H	-8.34671500	-1.89337400	-0.73060100
H	-7.44961500	-0.71085000	0.25495800

H	-7.41111200	-0.60592300	-1.51978000
C	-6.17992100	-3.02100000	-2.00625200
H	-7.05727300	-3.67373900	-2.06553800
H	-6.18251300	-2.35182700	-2.87285500
H	-5.27882800	-3.64183800	-2.05192700

Zero-point correction= 0.629840 (Hartree/Particle)
Thermal correction to Energy= 0.670144
Thermal correction to Enthalpy= 0.671088
Thermal correction to Gibbs Free Energy= 0.551301
Sum of electronic and zero-point Energies= -5710.104081
Sum of electronic and thermal Energies= -5710.063777
Sum of electronic and thermal Enthalpies= -5710.062833
Sum of electronic and thermal Free Energies= -5710.182620

M7

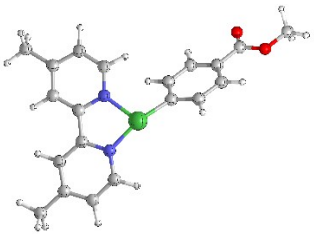


C	-1.54669500	-0.34914100	0.00001500
C	-0.92304800	-2.60065300	-0.00006700
C	-2.23966100	-3.00934000	0.00002400
C	-3.27684600	-2.05042300	0.00010500
C	-2.89750300	-0.71191500	0.00011600
C	-1.04347600	1.02355400	0.00001800
C	0.90723800	2.30386600	-0.00003500
C	0.18766200	3.48620500	-0.00005600
C	-1.22030900	3.44005700	-0.00002000
C	-1.82553800	2.18604000	0.00000100
H	-0.10531400	-3.31415500	-0.00011600
H	-2.47005000	-4.07080100	0.00005300
H	-3.66031800	0.06064100	0.00022700
H	1.99258600	2.27925600	-0.00007400
H	0.71109800	4.43756600	-0.00011400
H	-2.90835600	2.11236100	-0.00001500
N	-0.54898400	-1.29602800	-0.00008200
N	0.31678600	1.09605600	0.00000300
Ni	1.20243100	-0.61874700	-0.00004900
Br	3.43402900	-0.73923400	0.00004300
C	-2.03035900	4.71075000	0.00003000

H	-3.10525500	4.50671700	-0.00087500
H	-1.80103500	5.32060400	0.88239800
H	-1.79969800	5.32157300	-0.88130800
C	-4.72190400	-2.47455300	-0.00003300
H	-5.39612800	-1.61254900	0.00173400
H	-4.95464500	-3.08340800	-0.88281700
H	-4.95393200	-3.08656100	0.88073400

Zero-point correction= 0.215610 (Hartree/Particle)
Thermal correction to Energy= 0.231625
Thermal correction to Enthalpy= 0.232569
Thermal correction to Gibbs Free Energy= 0.167655
Sum of electronic and zero-point Energies= -4653.794836
Sum of electronic and thermal Energies= -4653.778821
Sum of electronic and thermal Enthalpies= -4653.777877
Sum of electronic and thermal Free Energies= -4653.842791

M8

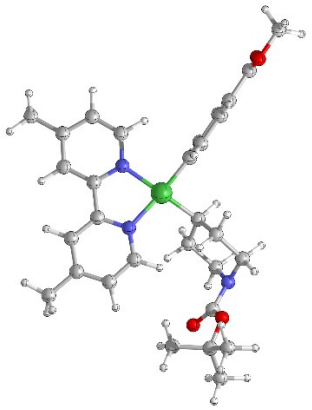


Ni	0.45829200	-0.81766500	-0.49128900
C	-1.43035400	-0.65598500	-0.25246300
C	-4.21766500	-0.21241900	0.22764400
C	-1.89743300	0.25633100	0.72507900
C	-2.43965900	-1.33681200	-0.97087700
C	-3.79976500	-1.12753100	-0.75045600
C	-3.24830800	0.47864000	0.97004300
H	-1.17016200	0.81372300	1.31504800
H	-2.15528900	-2.05876000	-1.73524700
H	-4.54325800	-1.66675700	-1.32914400
H	-3.58020300	1.18291300	1.72774300
N	1.24860400	0.96342400	-0.41561400
C	2.61285300	3.39866100	-0.12014700
C	0.61351500	2.13453700	-0.59405400
C	2.57176700	0.97671500	-0.09864800
C	3.26650900	2.18138100	0.06176300
C	1.24893300	3.35853600	-0.46183600
N	2.25580100	-1.37355900	-0.21439700
C	4.93946100	-1.93959200	0.48400100
C	2.71106700	-2.64668900	-0.12319500
C	3.14951600	-0.36298100	0.03780800
C	4.47565300	-0.63012300	0.39151300

C	4.01221900	-2.96593600	0.20941500
H	-0.44241800	2.05202200	-0.82936500
H	4.31952100	2.17256400	0.32421800
H	0.68947400	4.27620400	-0.61751500
H	1.97335200	-3.41669100	-0.32470500
H	5.15333300	0.19252400	0.59748500
H	4.31098000	-4.00894900	0.26060900
C	6.36059800	-2.26059900	0.86544900
H	6.95437000	-1.35320200	1.01233300
H	6.39726500	-2.84140600	1.79573800
H	6.85037800	-2.86434500	0.09135700
C	3.32829000	4.71492800	0.04303400
H	3.26025900	5.31359700	-0.87325900
H	2.87671800	5.30732100	0.84816700
H	4.38735400	4.57476400	0.27932600
C	-5.64499100	0.06208400	0.51501500
O	-6.48760800	-0.67503000	-0.25881100
O	-6.05460200	0.85437800	1.34512100
C	-7.88087600	-0.44775800	-0.01952900
H	-8.40981900	-1.10719100	-0.70971600
H	-8.14192900	-0.68733400	1.01594400
H	-8.14325400	0.59746000	-0.21068800

Zero-point correction= 0.348023 (Hartree/Particle)
Thermal correction to Energy= 0.371988
Thermal correction to Enthalpy= 0.372932
Thermal correction to Gibbs Free Energy= 0.290364
Sum of electronic and zero-point Energies= -2541.415781
Sum of electronic and thermal Energies= -2541.391816
Sum of electronic and thermal Enthalpies= -2541.390872
Sum of electronic and thermal Free Energies= -2541.473440

M9



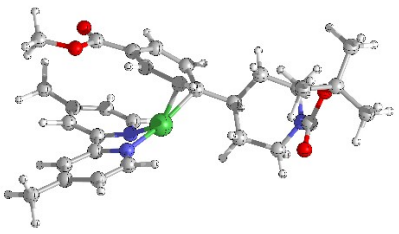
Ni	0.60700900	0.45708900	-0.23686200
C	2.15931700	-0.56601100	-0.17538300
C	4.62655500	-1.96659100	0.09163500

C	2.96069700	-0.88005800	-1.29329400
C	2.63407600	-1.00387100	1.07907000
C	3.83893600	-1.69053800	1.21953200
C	4.17139200	-1.55392100	-1.17085300
H	2.62269000	-0.58729400	-2.28598800
H	2.04862000	-0.79633300	1.97357100
H	4.17805200	-2.01306700	2.19894500
H	4.78300400	-1.77781200	-2.04023400
N	1.55587400	2.15379000	0.00997200
C	2.67428200	4.74723500	-0.11460900
C	2.88981800	2.34319400	-0.04829500
C	0.76770600	3.26031600	0.03511300
C	1.29516300	4.55131600	-0.03773800
C	3.47637300	3.59888700	-0.10504500
N	-0.96783600	1.63694400	0.05787700
C	-2.97541800	3.56661100	0.58098800
C	-2.25581300	1.28984500	0.24676300
C	-0.66617100	2.95912300	0.16368900
C	-1.63926900	3.92909400	0.41656700
C	-3.27025500	2.20066800	0.50168900
H	3.48765900	1.44124900	-0.05409400
H	0.63228600	5.40998700	-0.04435500
H	4.55887300	3.67683400	-0.14605800
H	-2.47993300	0.23646500	0.17540500
H	-1.35391300	4.97204400	0.50063600
H	-4.28474100	1.83831800	0.62706500
C	-4.05470100	4.58695500	0.82985400
H	-3.63886300	5.58364500	1.00503000
H	-4.73092000	4.64949600	-0.03169200
H	-4.66404500	4.31127400	1.69801000
C	3.27675500	6.12368900	-0.22192900
H	4.12761800	6.23580000	0.45918500
H	3.65029700	6.30390400	-1.23790300
H	2.54654300	6.90524400	0.00889100
C	5.92265200	-2.67685000	0.17090200
O	6.24835400	-3.03468800	1.44363700
O	6.64560000	-2.92791000	-0.77724300
C	7.49370400	-3.72921100	1.57492800
H	7.60122100	-3.94270300	2.63977000
H	7.48375800	-4.65823800	0.99666600
H	8.32416200	-3.10966000	1.22224800
C	-1.77014800	-3.10561800	-0.28824700
C	-0.92143200	-1.94138700	0.24926400
C	-0.27755600	-1.12607000	-0.88853600

C	-1.24186700	-0.79388100	-2.04916100
C	-2.09165000	-2.01134100	-2.45427600
H	-1.56998500	-1.33314600	0.89471000
H	-0.12641700	-2.32823500	0.89926400
H	-1.13039200	-3.82762600	-0.81091400
H	-2.30150600	-3.63494200	0.50274200
H	-1.93653700	0.01826500	-1.81801500
H	-0.65876700	-0.45396900	-2.91542200
H	-2.86679800	-1.74489700	-3.17471900
H	-1.45961800	-2.79280800	-2.89424100
H	0.46045800	-1.80932600	-1.33171900
N	-2.73766400	-2.59560900	-1.27141100
C	-3.94169100	-2.06879100	-0.89038800
O	-4.62009300	-1.31467600	-1.57974600
O	-4.29272200	-2.50454400	0.35284800
C	-5.57708600	-2.13830900	0.94513900
C	-5.64765600	-0.62089400	1.15011700
H	-5.65728700	-0.10745100	0.18732000
H	-6.55526300	-0.36068700	1.70625600
H	-4.78097300	-0.28486800	1.73133600
C	-6.73168000	-2.66001000	0.08393800
H	-7.68367700	-2.49046900	0.59978300
H	-6.75323500	-2.15561200	-0.88279000
H	-6.61702400	-3.73676800	-0.08093600
C	-5.53712900	-2.86070500	2.29414000
H	-6.45598100	-2.66427300	2.85685500
H	-5.44208100	-3.94107000	2.14581600
H	-4.68267300	-2.51833400	2.88724000

Zero-point correction= 0.628470 (Hartree/Particle)
Thermal correction to Energy= 0.666676
Thermal correction to Enthalpy= 0.667620
Thermal correction to Gibbs Free Energy= 0.553438
Sum of electronic and zero-point Energies= -3138.340576
Sum of electronic and thermal Energies= -3138.302370
Sum of electronic and thermal Enthalpies= -3138.301426
Sum of electronic and thermal Free Energies= -3138.415607

M10



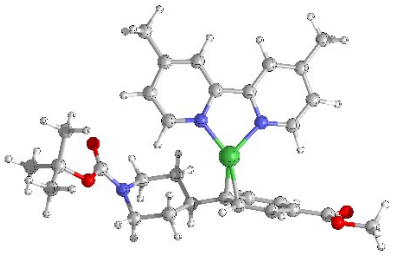
Ni	0.69914900	0.13501400	-0.72940700

C	-0.42836400	-1.39597900	-0.25782300
C	1.76970000	-1.59182000	1.50650400
C	0.27697500	-2.65547000	-0.06772700
C	-0.27975900	-0.39849300	0.80705000
C	0.92446900	-0.48643800	1.57473300
C	1.36123300	-2.74572900	0.75278700
H	-0.04026100	-3.51932500	-0.65113700
H	-1.09518700	0.23705500	1.15611300
H	1.17947600	0.33178400	2.24083400
H	1.95645200	-3.64905700	0.82929500
N	2.33718700	-0.39271400	-1.57017000
C	4.91072600	-1.44963500	-1.04493600
C	2.68022100	-1.64199300	-1.94684400
C	3.32301100	0.37862900	-1.01312500
C	4.59300100	-0.12584800	-0.73609400
C	3.92906700	-2.19494800	-1.71152600
N	1.54160500	1.86834900	-0.54195700
C	3.24205800	4.06329500	-0.07654400
C	1.04425500	3.08147400	-0.23970600
C	2.89097700	1.73589500	-0.64354800
C	3.75423600	2.80965100	-0.40864400
C	1.84489800	4.18814600	-0.00129100
H	1.88693400	-2.22246800	-2.40138100
H	5.31332500	0.49276500	-0.20954200
H	4.12025300	-3.22339700	-2.00305000
H	-0.03769400	3.13891000	-0.17089700
H	4.82620000	2.67009700	-0.50648500
H	1.38601500	5.14108700	0.24590600
C	4.14097200	5.24331700	0.18962900
H	3.88006100	6.09109200	-0.45491500
H	4.03923700	5.58448400	1.22735500
H	5.19302500	4.99687600	0.01786500
C	6.19969800	-2.07484100	-0.58772900
H	6.03657300	-2.52505200	0.40007400
H	6.53228200	-2.86542800	-1.26854900
H	7.00227600	-1.33494300	-0.49620700
C	3.11991600	-1.58258300	2.07451600
O	3.45268100	-0.38299900	2.64609600
O	3.92096800	-2.50636700	2.02064700
C	4.78424900	-0.31038700	3.15686600
H	4.87735300	0.68285400	3.60055600
H	4.96293300	-1.08400100	3.90995000
H	5.51681700	-0.43646500	2.35198200
C	-4.23764500	-2.02477000	-0.84057000

C	-2.89502700	-1.98927200	-0.09918600
C	-1.75601700	-1.46950000	-1.00458900
C	-2.16263900	-0.13173000	-1.65713000
C	-3.52664600	-0.23431600	-2.35227600
H	-2.99405900	-1.33021500	0.77365000
H	-2.64114900	-2.98723000	0.27935800
H	-4.18832300	-2.73691400	-1.67569300
H	-5.05289900	-2.33244100	-0.18766700
H	-2.22671400	0.65772000	-0.89768000
H	-1.39466500	0.17690300	-2.37985600
H	-3.84749600	0.72762100	-2.75155700
H	-3.47821700	-0.95552700	-3.17911300
H	-1.63456300	-2.19703400	-1.82421200
N	-4.54395300	-0.70662300	-1.40910800
C	-5.24022300	0.25147700	-0.71107700
O	-5.25246600	1.43915400	-1.00699500
O	-5.92296700	-0.30058900	0.32405100
C	-6.73724500	0.52881200	1.21736400
C	-5.85264800	1.55681200	1.93060500
H	-5.45419200	2.28473900	1.22287500
H	-6.43947100	2.08253100	2.69226600
H	-5.01787000	1.05132400	2.42909800
C	-7.87910800	1.18610000	0.43635900
H	-8.55102800	1.70204100	1.13176800
H	-7.49178300	1.90574700	-0.28569900
H	-8.45672800	0.42356300	-0.09746100
C	-7.28124200	-0.49875500	2.21251900
H	-7.91778300	-0.00552200	2.95461900
H	-7.87432600	-1.25853300	1.69326500
H	-6.45917700	-0.99931800	2.73449900

Zero-point correction= 0.627966 (Hartree/Particle)
Thermal correction to Energy= 0.665563
Thermal correction to Enthalpy= 0.666507
Thermal correction to Gibbs Free Energy= 0.555032
Sum of electronic and zero-point Energies= -3138.334471
Sum of electronic and thermal Energies= -3138.296875
Sum of electronic and thermal Enthalpies= -3138.295930
Sum of electronic and thermal Free Energies= -3138.407405

M11



Ni	0.96447200	-0.07345800	0.27992500
C	0.96365000	-1.92821700	-0.59872000
C	3.73581100	-2.22581700	0.07553900
C	1.99048000	-2.01079400	-1.60161500
C	1.40401400	-2.02075200	0.77315900
C	2.78030200	-2.16878100	1.07834700
C	3.31834400	-2.14562100	-1.28564800
H	1.69102600	-1.98820300	-2.64628700
H	0.69641300	-2.25047000	1.56696300
H	3.08438900	-2.25501300	2.11568200
H	4.07646700	-2.20401900	-2.05928700
N	2.25263800	1.35173800	-0.07192800
C	3.84023500	3.65172100	-0.50564100
C	3.58001200	1.25924300	-0.31437100
C	1.68544100	2.61546400	-0.04126300
C	2.48642200	3.76058700	-0.25644800
C	4.39798500	2.34450900	-0.53418500
N	-0.29725000	1.38754500	0.43979700
C	-1.89294700	3.72876600	0.43480000
C	-1.63686600	1.33875200	0.65205500
C	0.27253600	2.63449500	0.21172500
C	-0.53246500	3.79681100	0.21724300
C	-2.45690500	2.44077500	0.65793300
H	3.97630600	0.25212400	-0.33315000
H	2.02886400	4.74451800	-0.22260200
H	5.45577800	2.19295200	-0.72624400
H	-2.05075800	0.34706000	0.81095400
H	-0.07098000	4.76153200	0.03068200
H	-3.52177000	2.32049300	0.81369800
C	-2.77240400	4.95030800	0.42856800
H	-3.54932900	4.87156300	-0.34327300
H	-3.29089500	5.06940300	1.38924000
H	-2.19834300	5.86302400	0.23917200
C	4.71159100	4.85737900	-0.74009000
H	5.19171100	4.81098700	-1.72639100
H	4.13890700	5.78881800	-0.68670100
H	5.51822500	4.91272700	0.00273000

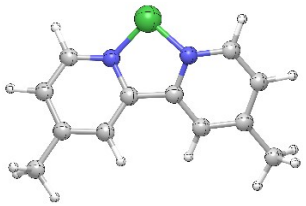
C	5.18366800	-2.33450500	0.35601700
O	5.45524400	-2.46867200	1.67952200
O	6.05517700	-2.29808800	-0.49528600
C	6.84943200	-2.54866600	2.00686600
H	6.89059600	-2.64683200	3.09250100
H	7.31087900	-3.41516900	1.52408900
H	7.37487800	-1.64562900	1.68215500
C	-2.82944400	-2.90470900	-0.36386200
C	-1.41379900	-2.59119800	0.13285200
C	-0.46483300	-2.27980600	-1.03766800
C	-1.07941500	-1.19307800	-1.94998800
C	-2.51793400	-1.52200100	-2.36456300
H	-1.46075800	-1.73015900	0.81310300
H	-1.03688900	-3.44207100	0.71293900
H	-2.80825400	-3.81793400	-0.97727100
H	-3.51062100	-3.07528400	0.46702900
H	-1.06984600	-0.23969900	-1.41502700
H	-0.46158700	-1.05654200	-2.84566400
H	-2.97407600	-0.68817900	-2.89791900
H	-2.53339600	-2.40328200	-3.02284500
H	-0.38533000	-3.20401000	-1.63298100
N	-3.33874000	-1.81580500	-1.19192800
C	-4.31134100	-0.93164600	-0.80287500
O	-4.65930400	0.03920200	-1.45962400
O	-4.83235300	-1.28712200	0.40213700
C	-6.07042400	-0.67497800	0.89868900
C	-5.84030600	0.80442500	1.21679500
H	-5.61881700	1.36214900	0.30613100
H	-6.73659700	1.22503900	1.68647100
H	-5.00506200	0.91282600	1.91727000
C	-7.20104300	-0.87894000	-0.11410900
H	-8.14797000	-0.53892700	0.31942100
H	-7.00977200	-0.31898400	-1.03061500
H	-7.29824200	-1.94197600	-0.36045300
C	-6.33815000	-1.46833800	2.17959100
H	-7.24514300	-1.09861800	2.66894500
H	-6.47217500	-2.53116100	1.95310400
H	-5.49957400	-1.36545100	2.87615100

Zero-point correction= 0.627852 (Hartree/Particle)
Thermal correction to Energy= 0.665783
Thermal correction to Enthalpy= 0.666728
Thermal correction to Gibbs Free Energy= 0.554473
Sum of electronic and zero-point Energies= -3138.340211
Sum of electronic and thermal Energies= -3138.302279

Sum of electronic and thermal Enthalpies= -3138.301335

Sum of electronic and thermal Free Energies= -3138.413589

M12



0 1

C	-0.72467800	0.31661700	0.06807800
C	-2.62207400	-1.02318600	0.38232300
C	-3.46236800	0.04504600	0.14366500
C	-2.92846400	1.32919200	-0.09775000
C	-1.54053600	1.43123200	-0.13860800
C	0.72471300	0.31663800	-0.06811000
C	2.62209900	-1.02330300	-0.38196400
C	3.46241200	0.04501100	-0.14372100
C	2.92850800	1.32922000	0.09735700
C	1.54058800	1.43130900	0.13820900
H	-3.01513400	-2.00045700	0.64042600
H	-4.53806500	-0.10598400	0.17961800
H	-1.07710600	2.38021300	-0.39419200
H	3.01510600	-2.00065700	-0.63981700
H	4.53811000	-0.10598200	-0.17979400
H	1.07719100	2.38040400	0.39343800
N	-1.26168600	-0.92039600	0.41739400
N	1.26173000	-0.92045100	-0.41702900
Ni	-0.00007700	-2.14215600	-0.00008900
C	3.82807400	2.51449800	0.33272900
H	3.25150100	3.43230000	0.48686500
H	4.46391900	2.36649500	1.21554900
H	4.49977700	2.67967700	-0.51977100
C	-3.82801600	2.51460300	-0.33246700
H	-4.49226400	2.68587500	0.52471700
H	-3.25123500	3.43054900	-0.49654400
H	-4.47149700	2.36260100	-1.20899900

Zero-point correction= 0.213724 (Hartree/Particle)

Thermal correction to Energy= 0.227603

Thermal correction to Enthalpy= 0.228548

Thermal correction to Gibbs Free Energy= 0.171815

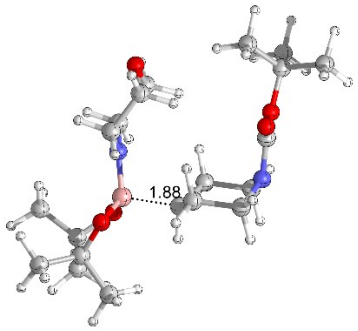
Sum of electronic and zero-point Energies= -2081.917617

Sum of electronic and thermal Energies= -2081.903738

Sum of electronic and thermal Enthalpies= -2081.902794

Sum of electronic and thermal Free Energies= -2081.959526

TS1-2

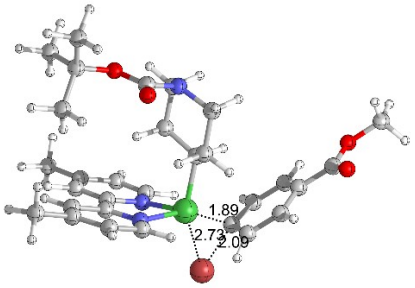


B	1.93649500	0.13524800	-0.00300200
O	2.79614300	-0.25991000	-1.07863700
O	2.65896500	0.11374100	1.23378900
C	4.07180100	-0.60339000	-0.50791200
C	4.05117100	0.16084600	0.87038500
C	5.16377800	-0.14660000	-1.47590700
H	6.15999800	-0.29284900	-1.04196000
H	5.10469400	-0.73188300	-2.39967000
H	5.04478700	0.90679800	-1.73893500
C	4.14183700	-2.12893200	-0.33964700
H	5.14105900	-2.45775800	-0.03365500
H	3.42357400	-2.47996200	0.40588600
H	3.90005900	-2.59932000	-1.29805200
C	4.44646200	1.64011200	0.72616300
H	3.88080500	2.11762600	-0.08008300
H	4.20942000	2.15757100	1.66120300
H	5.51550900	1.76323600	0.52208800
C	4.86907600	-0.49266700	1.98140400
H	4.49994700	-1.49568000	2.20732500
H	5.92677600	-0.56100800	1.70127200
H	4.79574100	0.10624000	2.89529600
C	-1.39917800	-2.08828100	1.35848500
C	-0.32220800	-0.98067800	1.30603500
C	0.65693000	-1.23587200	0.17461900
C	0.02015100	-1.57513800	-1.16032800
C	-1.05924800	-2.66917300	-0.98322900
H	-0.85871600	-0.04282800	1.15179400
H	0.20917000	-0.90743400	2.26162400
H	-0.95324700	-3.05528900	1.61950200
H	-2.16599100	-1.85653300	2.09778000
H	-0.49283600	-0.70945300	-1.58936100
H	0.78666000	-1.89057100	-1.87532100

H	-1.59311200	-2.84617700	-1.91730800
H	-0.61451300	-3.61268300	-0.64718100
H	1.38287900	-2.00230100	0.46068200
N	-2.01990100	-2.23544900	0.03764400
C	-2.98363200	-1.34596800	-0.39806300
O	-3.31620200	-1.23081400	-1.56927300
O	-3.49816600	-0.63201400	0.63199500
C	-4.66467400	0.24520100	0.43678100
C	-4.35640300	1.36560800	-0.56246300
H	-4.20260400	0.96415300	-1.56403700
H	-5.20108800	2.06355900	-0.58573500
H	-3.46552200	1.92907300	-0.26800000
C	-5.86442200	-0.59904000	-0.00079400
H	-6.76336300	0.02618100	-0.03496800
H	-5.69494400	-1.02677900	-0.99054400
H	-6.03595300	-1.41102400	0.71413400
C	-4.87561600	0.81705700	1.83981400
H	-5.73582300	1.49432200	1.84470600
H	-5.05813400	0.01353700	2.56069000
H	-3.99095900	1.37696700	2.16134300
C	-0.81032200	2.63194600	0.64302000
C	0.66557300	2.23786000	0.78400100
C	0.69644300	1.74213700	-1.59922200
C	-0.79157400	2.10724000	-1.65064600
H	1.27129100	3.15719000	0.71028400
H	0.87122900	1.78524700	1.75620200
H	-1.46529100	1.78299200	0.89062000
H	-1.04743300	3.45607600	1.32296800
H	1.27763800	2.63841400	-1.87475800
H	0.94851200	0.95512600	-2.31245000
H	-1.04757700	2.54419600	-2.62019600
H	-1.41752900	1.21476900	-1.49810900
O	-1.10161000	3.09569200	-0.67039400
N	1.09471900	1.33014200	-0.26548500

Zero-point correction= 0.585214 (Hartree/Particle)
Thermal correction to Energy= 0.614272
Thermal correction to Enthalpy= 0.615217
Thermal correction to Gibbs Free Energy= 0.527396
Sum of electronic and zero-point Energies= -1295.077167
Sum of electronic and thermal Energies= -1295.048109
Sum of electronic and thermal Enthalpies= -1295.047165
Sum of electronic and thermal Free Energies= -1295.134985

TS2a



C	-1.74844300	-1.73573100	0.90326900
C	-0.98916000	-0.52194700	2.73134500
C	-2.25819200	-0.44893900	3.27910600
C	-3.33621900	-1.04770200	2.60510200
C	-3.05540600	-1.69591300	1.40444500
C	-1.37471500	-2.36645400	-0.37451600
C	0.35574600	-2.74093300	-1.87563400
C	-0.48388200	-3.39140400	-2.76306000
C	-1.84504000	-3.54392500	-2.44117300
C	-2.27677200	-3.01792900	-1.22710400
H	-0.13990500	-0.05404300	3.21825600
H	-2.41117100	0.07322300	4.21855400
H	-3.86444100	-2.16174500	0.85193000
H	1.41065900	-2.60194500	-2.08640300
H	-0.08750400	-3.78168800	-3.69578900
H	-3.32041600	-3.11323000	-0.94698600
N	-0.71998500	-1.14861300	1.57092500
N	-0.06698300	-2.23615800	-0.70603600
Ni	0.97537500	-0.99886600	0.48613100
C	-2.78843200	-4.24297000	-3.38534100
H	-3.79783200	-4.31625000	-2.96965100
H	-2.85362500	-3.70644100	-4.33994500
H	-2.43830900	-5.25763000	-3.60992100
C	-4.73724900	-0.95501700	3.14813400
H	-5.11793600	0.06834500	3.04436100
H	-5.42255800	-1.62222100	2.61673000
H	-4.76627500	-1.20852900	4.21387100
C	-0.92154100	2.08690300	-1.96307500
C	-0.56981000	0.69147300	-1.41025800
C	0.58207800	0.74686100	-0.40893400
C	0.31087700	1.80774300	0.65993700
C	-0.04865800	3.17260900	0.04385800
H	-1.47958200	0.29832200	-0.93086600
H	-0.33615100	0.02207100	-2.24834100
H	-0.06811900	2.49453300	-2.51955700
H	-1.78040100	2.05847800	-2.63411500
H	-0.54461500	1.51844900	1.28429600

H	1.17503500	1.92059300	1.32417900
H	-0.30644200	3.90851300	0.80676800
H	0.78790900	3.56061400	-0.54969500
H	1.50054200	1.02167600	-0.94709900
N	-1.19971800	3.01160000	-0.85669400
C	-2.43924400	3.06209700	-0.26949900
O	-2.65977000	3.52082100	0.84432400
O	-3.39440200	2.55484000	-1.09845900
C	-4.78595400	2.45974400	-0.66477900
C	-4.88994900	1.55096500	0.56519400
H	-4.39229300	2.00413100	1.42375400
H	-5.94418300	1.37555300	0.80882600
H	-4.41582500	0.58589500	0.35684400
C	-5.36554100	3.85442500	-0.40778800
H	-6.44031500	3.77701800	-0.20657000
H	-4.87427000	4.32646800	0.44356900
H	-5.22575600	4.48585600	-1.29183200
C	-5.46270600	1.80540600	-1.87207300
H	-6.53155600	1.66511800	-1.67861900
H	-5.34772300	2.43326400	-2.76142400
H	-5.01157300	0.82912500	-2.07962500
C	2.85153300	-1.11265200	0.24694000
C	4.24844800	1.31630600	0.10592000
C	3.00627900	-0.30627600	1.42505900
C	3.60957300	-0.79846600	-0.91954500
C	4.24160600	0.41791200	-0.99900700
C	3.66395100	0.91931700	1.31124500
H	2.73407900	-0.68355000	2.40552800
H	3.60807200	-1.48351600	-1.76087800
H	4.74783100	0.70693600	-1.91369400
H	3.76087500	1.57490900	2.17131800
Br	2.66745100	-3.13033400	0.75268800
C	4.89895700	2.63714100	0.05529300
O	5.45556700	2.89799600	-1.16063500
O	4.94318000	3.43544400	0.97670800
C	6.09273400	4.17627000	-1.26990300
H	6.47492100	4.22854800	-2.29069700
H	5.37742600	4.98367600	-1.08576000
H	6.91112900	4.26532500	-0.54891400

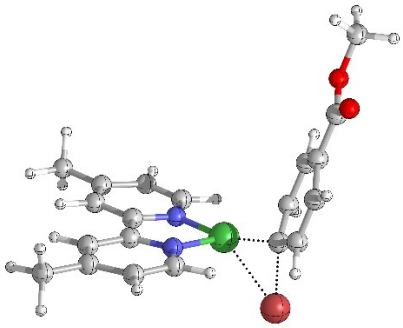
Zero-point correction= 0.626970 (Hartree/Particle)
Thermal correction to Energy= 0.666511
Thermal correction to Enthalpy= 0.667455
Thermal correction to Gibbs Free Energy= 0.551928
Sum of electronic and zero-point Energies= -5710.046438

Sum of electronic and thermal Energies= -5710.006896

Sum of electronic and thermal Enthalpies= -5710.005952

Sum of electronic and thermal Free Energies= -5710.121479

TS2b

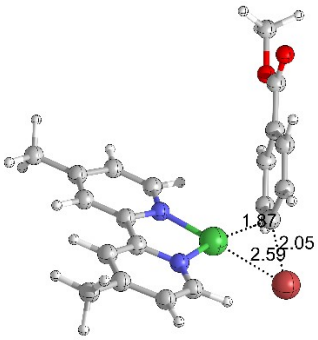


C	-2.53935300	0.86717400	0.37785700
C	-1.64412600	2.49237600	-1.02378100
C	-2.65173100	3.38763300	-0.70826900
C	-3.65784900	3.01110600	0.19795300
C	-3.58243900	1.72764800	0.73542400
C	-2.35718100	-0.49701000	0.89562300
C	-0.94970800	-2.34218800	0.90574100
C	-1.79012300	-3.03544300	1.76032800
C	-2.97931900	-2.43651600	2.20912000
C	-3.24677900	-1.14543600	1.75773300
H	-0.85305300	2.74719800	-1.72098700
H	-2.65739500	4.37319300	-1.16454800
H	-4.33738700	1.39914400	1.44224900
H	-0.01773200	-2.76869900	0.55253300
H	-1.52171200	-4.03896800	2.07799200
H	-4.15636100	-0.64579700	2.07541700
N	-1.57056000	1.25343000	-0.49865700
N	-1.20930100	-1.09523400	0.46767800
Ni	-0.19055200	-0.04501800	-0.78934700
C	1.74563500	0.63619700	-1.13611900
C	3.23075600	-1.26667200	0.35523500
C	2.77541600	1.04895200	-0.26216100
H	1.56486500	1.25234500	-2.01377700
C	3.47567800	0.12922700	0.51419900
H	3.84464300	-1.95700000	0.92530700
H	3.08307600	2.09012100	-0.24980800
Br	0.31782400	-1.28311600	-2.94848100
C	2.24245500	-1.72982900	-0.48053600
H	2.05938300	-2.79131100	-0.61301800
C	1.39245300	-0.77271500	-1.08740400
C	-3.91006000	-3.16154000	3.14643600
H	-3.43828200	-3.31433100	4.12527700

H	-4.83885100	-2.60509000	3.30491300
H	-4.16927800	-4.15267200	2.75604700
C	-4.76190300	3.96632700	0.57094800
H	-5.49970200	3.49554800	1.22751600
H	-4.35982200	4.84497100	1.09040500
H	-5.28409300	4.33111600	-0.32155000
C	4.55075600	0.52998700	1.44246200
O	5.22683500	-0.23878000	2.10517100
O	4.72174900	1.88036500	1.50238600
C	5.75973200	2.31689100	2.38688700
H	5.76770000	3.40597100	2.31671800
H	5.55420800	2.00046500	3.41415900
H	6.72791900	1.90629300	2.08404000

Zero-point correction= 0.348673 (Hartree/Particle)
Thermal correction to Energy= 0.373765
Thermal correction to Enthalpy= 0.374709
Thermal correction to Gibbs Free Energy= 0.287177
Sum of electronic and zero-point Energies= -5113.143531
Sum of electronic and thermal Energies= -5113.118440
Sum of electronic and thermal Enthalpies= -5113.117495
Sum of electronic and thermal Free Energies= -5113.205027

TS2c

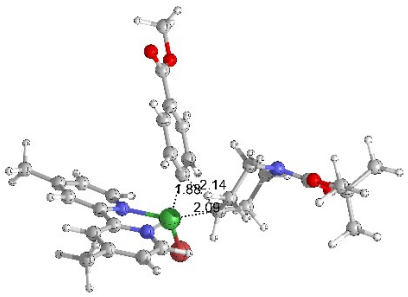


C	1.75432200	-1.19668700	-1.11554700
C	0.89312500	-1.83987700	-0.17766900
C	1.24637600	-1.95248200	1.18975100
C	2.32923000	-1.23343900	1.64208700
C	3.13650900	-0.47736900	0.75058300
C	2.85917200	-0.49107500	-0.61524700
Br	-0.31836600	-3.25178700	-1.03305800
H	0.61166800	-2.51524700	1.86443300
H	1.66732300	-1.37110600	-2.18368500
H	3.52447300	0.02193400	-1.30105700
H	2.58880800	-1.22757200	2.69568400
C	-2.47927500	0.84730800	0.26452000
C	-2.94755000	-1.43558100	0.57148300

C	-4.09651200	-1.16526700	1.28013200
C	-4.47064200	0.18928200	1.50435600
C	-3.64860800	1.17253100	0.99243500
C	-1.56792300	1.80055800	-0.30017300
C	0.48049900	2.08680800	-1.42442000
C	0.34700900	3.45524500	-1.44458300
C	-0.81639500	4.04663900	-0.87185900
C	-1.75136300	3.20358400	-0.30646400
H	-2.62595900	-2.45484000	0.38439900
H	-4.70417000	-1.98058000	1.66035800
H	-3.89546300	2.21603500	1.16171800
H	1.35675900	1.59916800	-1.84047300
H	1.12337600	4.07136400	-1.88738500
H	-2.64951900	3.62383600	0.13559300
N	-2.14104200	-0.48154500	0.05752900
N	-0.43435000	1.25165500	-0.88256300
Ni	-0.41969000	-0.67388600	-0.81241700
C	-0.99623800	5.54123600	-0.89684400
H	-0.16429100	6.04696500	-0.38919600
H	-1.01579800	5.91947100	-1.92750200
H	-1.92658400	5.84654300	-0.40759300
C	-5.71833800	0.51331400	2.28278800
H	-5.67365500	0.08978800	3.29470400
H	-5.87063800	1.59333300	2.37497300
H	-6.60635400	0.08591600	1.79885400
C	4.28200400	0.26622900	1.32213200
O	4.97563100	0.95851500	0.38239100
O	4.58250700	0.27396900	2.50227100
C	6.09620200	1.70183100	0.88282900
H	5.76917300	2.44558400	1.61534900
H	6.82037200	1.03479400	1.35964600
H	6.53762900	2.18859600	0.01212000

Zero-point correction= 0.347484 (Hartree/Particle)
Thermal correction to Energy= 0.372613
Thermal correction to Enthalpy= 0.373557
Thermal correction to Gibbs Free Energy= 0.288467
Sum of electronic and zero-point Energies= -5113.136140
Sum of electronic and thermal Energies= -5113.111011
Sum of electronic and thermal Enthalpies= -5113.110067
Sum of electronic and thermal Free Energies= -5113.195156

TS3a



C	2.53347200	-2.24509900	-1.00096400
C	0.42432300	-3.19945400	-0.98381900
C	0.76810800	-4.10727000	-1.97515600
C	2.06050300	-4.07746500	-2.51671200
C	2.94540700	-3.12813200	-2.00326500
C	3.42242200	-1.24563500	-0.36739200
C	3.60651200	0.27250500	1.37427900
C	4.88692700	0.63598900	0.98021700
C	5.46267400	0.03433100	-0.14756300
C	4.70443400	-0.92489300	-0.82210200
H	-0.56668800	-3.20025300	-0.54291600
H	0.03707300	-4.83304100	-2.31852500
H	3.96365500	-3.09145500	-2.37501500
H	3.11126800	0.71672600	2.23121600
H	5.43134900	1.38713000	1.54476800
H	5.11151900	-1.40470200	-1.70577000
N	1.27200700	-2.27426400	-0.50930900
N	2.88978800	-0.64421100	0.71376100
Ni	0.90771100	-0.92146400	1.01200300
C	0.51747300	1.83756000	1.03142100
C	0.91909600	2.12944600	-1.70800800
C	0.83203600	3.08838000	0.50897700
H	0.37275400	1.73014300	2.10238100
C	1.03512500	3.25029400	-0.87025600
H	1.08887200	2.25837900	-2.77276500
H	0.92310400	3.94558500	1.16778700
Br	1.01488700	-1.22297100	3.37419300
C	0.60271700	0.88548500	-1.17975600
H	0.53457500	0.03196500	-1.84818600
C	0.40616700	0.70125700	0.20429500
C	6.84396500	0.41979300	-0.61037900
H	7.14728500	-0.14366100	-1.49767300
H	6.88755600	1.48770400	-0.85476000
H	7.58373200	0.23800800	0.17817600
C	2.47081300	-5.03986000	-3.60053700
H	3.53141800	-4.94248200	-3.84932500

H	2.28459200	-6.07567400	-3.29441200
H	1.89057700	-4.86370900	-4.51443400
C	1.37708500	4.55171400	-1.48815400
O	1.58712000	4.72632200	-2.67557500
O	1.43801600	5.56003400	-0.58027300
C	1.75820900	6.84733900	-1.12402400
H	1.75742800	7.53308400	-0.27555500
H	2.74104500	6.83152400	-1.60489500
H	1.01219000	7.15090200	-1.86446000
C	-2.68140200	0.51058300	-0.94318100
C	-1.92161900	-0.76379700	-0.54420800
C	-1.15282400	-0.63995900	0.77847400
C	-1.95003600	0.09651000	1.86136600
C	-2.73045800	1.31794700	1.35613700
H	-2.67358300	-1.56085600	-0.42984900
H	-1.26302700	-1.07359000	-1.36215700
H	-1.98072000	1.31521600	-1.18475000
H	-3.30631200	0.33083200	-1.81663800
H	-2.68334000	-0.61322400	2.27224100
H	-1.29632900	0.36431100	2.69537800
H	-3.41310200	1.67946900	2.12503200
H	-2.05397600	2.13161600	1.07854600
H	-0.98392200	-1.66137700	1.15908600
N	-3.51497900	0.96946700	0.16808100
C	-4.80804500	0.54985700	0.35251500
O	-5.43863400	0.70323300	1.38956800
O	-5.29551000	-0.03311600	-0.77673900
C	-6.67986000	-0.50754500	-0.83832000
C	-6.89814400	-1.62766500	0.18404800
H	-6.81551000	-1.24503500	1.20178800
H	-7.89286700	-2.06608200	0.04514800
H	-6.15186400	-2.41729700	0.04027400
C	-7.65164000	0.65963200	-0.63744100
H	-8.67809100	0.31903700	-0.81515400
H	-7.57713100	1.05594400	0.37571100
H	-7.42744500	1.46114200	-1.34984500
C	-6.77627500	-1.05150800	-2.26585900
H	-7.77835100	-1.45248500	-2.45105300
H	-6.57782400	-0.25720000	-2.99289300
H	-6.04549900	-1.85236100	-2.42074800

Zero-point correction= 0.628203 (Hartree/Particle)
Thermal correction to Energy= 0.668146
Thermal correction to Enthalpy= 0.669090
Thermal correction to Gibbs Free Energy= 0.549795

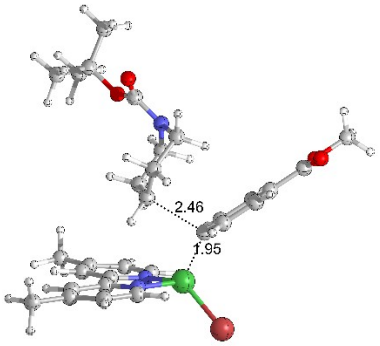
Sum of electronic and zero-point Energies= -5710.091991

Sum of electronic and thermal Energies= -5710.052047

Sum of electronic and thermal Enthalpies= -5710.051103

Sum of electronic and thermal Free Energies= -5710.170398

TS3b



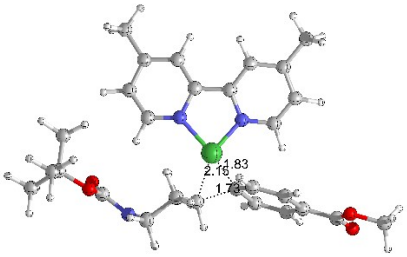
Ni	-2.50712600	0.32331500	0.33554600
C	-0.89267700	1.36624300	-0.00956800
C	0.28396500	3.96476800	-0.08735600
C	-0.91473700	2.16647200	-1.17976800
C	-0.26638100	1.94166100	1.12038500
C	0.30743500	3.20974200	1.09544600
C	-0.34258800	3.42802700	-1.22757700
H	-1.40809600	1.78347600	-2.07192700
H	-0.20633200	1.36938600	2.04489900
H	0.77954200	3.62126100	1.98183000
H	-0.36941700	4.02759400	-2.13257600
N	-1.91653700	-1.15607400	1.56803400
C	-0.83646900	-3.32784000	2.97990100
C	-1.49528700	-1.01464300	2.83381100
C	-1.84493700	-2.38012300	0.99066100
C	-1.30133600	-3.47187200	1.67119000
C	-0.95689300	-2.06110600	3.56890300
N	-2.73573600	-1.23674400	-0.89371900
C	-3.02319200	-3.55016600	-2.43947200
C	-3.23351000	-1.16717600	-2.13595100
C	-2.37803600	-2.43881800	-0.38878100
C	-2.51658100	-3.60897900	-1.13966700
C	-3.38413000	-2.28923200	-2.93784400
H	-1.59674200	-0.01872300	3.25227700
H	-1.23035400	-4.43752100	1.18221300
H	-0.62932100	-1.88961500	4.58971500
H	-3.51597500	-0.17312800	-2.46700900
H	-2.23832300	-4.56836700	-0.71689900
H	-3.78685700	-2.18494600	-3.94072200
Br	-4.48940600	1.51544800	0.23730400

C	-3.18862100	-4.78923100	-3.28039200
H	-4.24311900	-4.94578700	-3.53702800
H	-2.63720200	-4.69619300	-4.22326800
H	-2.82928200	-5.68304500	-2.76237000
C	-0.21216300	-4.47705700	3.72705600
H	0.87690400	-4.35351700	3.77905200
H	-0.58255300	-4.52671900	4.75665000
H	-0.41679000	-5.43537000	3.24079800
C	2.58343100	0.14273100	0.75289100
C	1.41148400	-0.83582500	0.55601000
C	0.57059700	-0.50279200	-0.64778400
C	1.28579800	-0.02561900	-1.88241000
C	2.42752200	0.94637400	-1.54798400
H	1.84033100	-1.84863700	0.43503400
H	0.79899200	-0.86843200	1.46454700
H	2.20478000	1.11433800	1.08085300
H	3.28460900	-0.22535700	1.50024100
H	1.73063600	-0.88940100	-2.40986300
H	0.58384100	0.44120200	-2.58273800
H	3.03642100	1.16181100	-2.42549600
H	2.02267700	1.88450000	-1.15692300
H	-0.26500900	-1.16620100	-0.82904400
N	3.28735400	0.35958500	-0.51333600
C	4.31782200	-0.44388100	-0.93118300
O	4.72874700	-0.49133400	-2.08296000
O	4.83147800	-1.15746000	0.10829500
C	5.97021600	-2.05585000	-0.08895700
C	5.59422900	-3.17719100	-1.06370900
H	5.42077300	-2.77939800	-2.06409400
H	6.40243100	-3.91602600	-1.10596700
H	4.68445700	-3.68243400	-0.71950200
C	7.19689300	-1.26627600	-0.55667100
H	8.07309100	-1.92424600	-0.57818100
H	7.03536400	-0.85366700	-1.55305500
H	7.40061000	-0.44482100	0.13878600
C	6.19247800	-2.61705900	1.31783100
H	7.02934700	-3.32339100	1.31556500
H	6.41811600	-1.80933900	2.02167100
H	5.29546200	-3.13929700	1.66765700
C	0.89370600	5.30976500	-0.19271400
O	0.90971400	5.99269600	-1.20108300
O	1.45604500	5.72208800	0.97511200
C	2.06246700	7.01949000	0.92729400
H	2.45898600	7.19601500	1.92843600

H	2.86663200	7.04465000	0.18557700
H	1.32366300	7.78331800	0.66658500

Zero-point correction= 0.625737 (Hartree/Particle)
Thermal correction to Energy= 0.666527
Thermal correction to Enthalpy= 0.667471
Thermal correction to Gibbs Free Energy= 0.544648
Sum of electronic and zero-point Energies= -5710.059392
Sum of electronic and thermal Energies= -5710.018602
Sum of electronic and thermal Enthalpies= -5710.017658
Sum of electronic and thermal Free Energies= -5710.140480

TS4a



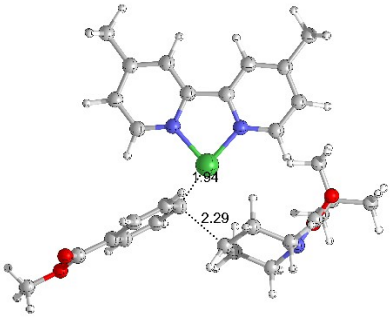
Ni	0.44254000	0.20263800	-0.51067800
C	1.59389700	-1.21191200	-0.36989900
C	4.38888500	-1.83727300	-0.00325400
C	2.45422500	-1.59729900	-1.46341500
C	2.21786500	-1.25982600	0.93020800
C	3.56189800	-1.52887300	1.09777300
C	3.78971600	-1.87619300	-1.28717300
H	2.03650600	-1.63556800	-2.46706200
H	1.61856700	-1.02997600	1.80718200
H	3.99735200	-1.50057700	2.09188500
H	4.42057100	-2.12295100	-2.13660900
N	1.57148400	1.70255100	-0.43952200
C	3.08197800	3.94969800	0.35859300
C	2.92275000	1.68327000	-0.46537100
C	0.95813200	2.85235500	-0.03609300
C	1.68930400	3.96818000	0.38460100
C	3.69612000	2.77172400	-0.10289300
N	-1.01446900	1.54728700	-0.31067900
C	-2.71444100	3.80414300	-0.18220100
C	-2.34997200	1.43644100	-0.46056600
C	-0.50764700	2.79963800	-0.12038900
C	-1.33270600	3.92737500	-0.05310200
C	-3.22093000	2.51270400	-0.39587800
H	3.36729800	0.75011400	-0.79151300
H	1.17044600	4.84968000	0.74833200
H	4.77789500	2.69950300	-0.16833300

H	-2.73395500	0.43962100	-0.64796100
H	-0.89073500	4.91026900	0.07363200
H	-4.28584000	2.34389500	-0.51584400
C	-3.63165000	4.99735700	-0.11566300
H	-4.20840600	5.10076000	-1.04269100
H	-4.35482900	4.88851700	0.70188100
H	-3.07688800	5.92675800	0.04414900
C	3.90420300	5.12946600	0.80802200
H	4.52081500	4.86995900	1.67754100
H	4.58902600	5.45498700	0.01552200
H	3.27453400	5.98107400	1.08365800
C	5.81839200	-2.11520100	0.11194100
O	6.26920900	-2.05211300	1.40581500
O	6.57297300	-2.37408300	-0.81591400
C	7.66360200	-2.31829000	1.56521700
H	7.86093900	-2.23480800	2.63604200
H	7.91563700	-3.32227800	1.20856500
H	8.26869900	-1.59487600	1.00866000
C	-1.98406500	-3.00061000	0.65621600
C	-0.86866900	-1.95855400	0.83743200
C	0.00382500	-1.89947600	-0.43379400
C	-0.84453800	-1.64443500	-1.70841800
C	-2.00461200	-2.65433500	-1.77736300
H	-1.34076600	-0.99281300	1.05574800
H	-0.24976500	-2.22246000	1.70134400
H	-1.54671800	-3.99678200	0.50406300
H	-2.64019100	-3.04812700	1.52349900
H	-1.27904300	-0.64074700	-1.75400800
H	-0.22297000	-1.75493600	-2.60290100
H	-2.68272300	-2.42383600	-2.59919000
H	-1.60102200	-3.66460100	-1.92850100
H	0.38499500	-2.91777500	-0.56064800
N	-2.77695400	-2.67121700	-0.53336100
C	-3.93031400	-1.93337200	-0.47170700
O	-4.42497700	-1.35147000	-1.43173600
O	-4.44946300	-1.94240900	0.78121300
C	-5.75568700	-1.33825200	1.06642900
C	-5.71986700	0.16724500	0.78829800
H	-5.63497300	0.35895600	-0.28201600
H	-6.63792300	0.63256800	1.16434000
H	-4.86659400	0.62380800	1.30112800
C	-6.84584600	-2.05065200	0.26125100
H	-7.83028200	-1.67236500	0.55854900
H	-6.70987300	-1.88331700	-0.80829500

H	-6.81718500	-3.12748400	0.45950500
C	-5.91840400	-1.60642900	2.56411200
H	-6.87643000	-1.21051900	2.91672200
H	-5.88966000	-2.68200100	2.76538300
H	-5.11265700	-1.12694800	3.12966800

Zero-point correction= 0.626801 (Hartree/Particle)
Thermal correction to Energy= 0.664444
Thermal correction to Enthalpy= 0.665388
Thermal correction to Gibbs Free Energy= 0.554057
Sum of electronic and zero-point Energies= -3138.292992
Sum of electronic and thermal Energies= -3138.255349
Sum of electronic and thermal Enthalpies= -3138.254404
Sum of electronic and thermal Free Energies= -3138.365735

TS4b



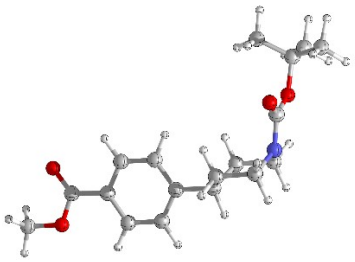
Ni	-0.21073400	0.49209600	-0.06474600
C	-1.62118000	-0.82377000	0.13507700
C	-4.41143000	-1.56328000	0.19804500
C	-2.46233600	-0.60724100	1.27656900
C	-2.29849500	-1.40832000	-0.98191000
C	-3.63553000	-1.77600000	-0.95946300
C	-3.79629500	-0.97017700	1.32006100
H	-2.02272100	-0.15423400	2.16461300
H	-1.73463400	-1.59199300	-1.89545400
H	-4.10120500	-2.21793400	-1.83525600
H	-4.40172100	-0.79588700	2.20533100
N	-1.19330900	2.15262100	-0.43232700
C	-2.38028200	4.67244800	-0.76624200
C	-2.47892400	2.26222700	-0.80734200
C	-0.47340400	3.28370900	-0.22036600
C	-1.04709300	4.54985200	-0.37486100
C	-3.10221500	3.48798700	-0.98725400
N	1.21859700	1.69375300	0.29911900
C	3.14095600	3.67869200	0.90078800
C	2.46693400	1.36754400	0.70694400
C	0.91348800	3.02461300	0.19519800
C	1.85176900	4.01638300	0.48963400

C	3.43421600	2.30860300	1.01022300
H	-3.00054400	1.32115200	-0.94821400
H	-0.45892400	5.44285300	-0.18959500
H	-4.14403100	3.52195400	-1.29202100
H	2.68438900	0.31149100	0.80266900
H	1.57651300	5.06241800	0.39969900
H	4.41330300	1.96773400	1.33367100
C	4.17473400	4.72493700	1.22611400
H	4.49165900	4.65114400	2.27383000
H	5.07286600	4.59490000	0.61001800
H	3.79344300	5.73710000	1.05961600
C	-3.03375700	6.01941300	-0.93958400
H	-3.86992800	6.13961000	-0.24004300
H	-2.32838300	6.83790700	-0.76746300
H	-3.44274100	6.12886700	-1.95110800
C	-5.83851600	-1.91676000	0.28618900
O	-6.31300000	-2.48521900	-0.86104000
O	-6.55310300	-1.73641600	1.25925700
C	-7.69590500	-2.84927800	-0.82365300
H	-7.91329100	-3.28494500	-1.80065200
H	-7.88674600	-3.57756700	-0.02909400
H	-8.32680900	-1.97225600	-0.64696700
C	1.65812500	-3.82796200	0.00416200
C	0.41145700	-2.99280000	-0.35932700
C	-0.31540700	-2.54788400	0.87901400
C	0.54942900	-1.92232400	1.94156600
C	1.84052100	-2.73356400	2.19669700
H	0.75989300	-2.10766000	-0.91807400
H	-0.24709100	-3.55948200	-1.02654800
H	1.36128300	-4.75397100	0.51291800
H	2.23920900	-4.09572500	-0.87715900
H	0.83276200	-0.91062500	1.61017800
H	-0.00241300	-1.79380200	2.87978300
H	2.54528200	-2.17980200	2.81820700
H	1.59826500	-3.67812600	2.69999100
H	-1.12766800	-3.18526800	1.21937800
N	2.50280200	-3.06488300	0.93076200
C	3.53189500	-2.27071200	0.50485900
O	4.08145100	-1.41921600	1.20125000
O	3.87517600	-2.55695000	-0.77485700
C	4.99418600	-1.88005400	-1.43691300
C	4.73097800	-0.37358000	-1.52811800
H	4.80395000	0.09952900	-0.54937700
H	5.46334900	0.08699200	-2.20070900

H	3.72939300	-0.18916800	-1.93234200
C	6.30304000	-2.19793500	-0.70861800
H	7.14734800	-1.77868700	-1.26736500
H	6.29752800	-1.77627900	0.29752000
H	6.44140800	-3.28223400	-0.63877600
C	4.97599400	-2.51339700	-2.83019200
H	5.78636600	-2.10377700	-3.44214200
H	5.10532700	-3.59808600	-2.75910900
H	4.02333400	-2.31108100	-3.33059900

Zero-point correction= 0.623614 (Hartree/Particle)
Thermal correction to Energy= 0.662242
Thermal correction to Enthalpy= 0.663186
Thermal correction to Gibbs Free Energy= 0.546882
Sum of electronic and zero-point Energies= -3138.264018
Sum of electronic and thermal Energies= -3138.225390
Sum of electronic and thermal Enthalpies= -3138.224446
Sum of electronic and thermal Free Energies= -3138.340749

P

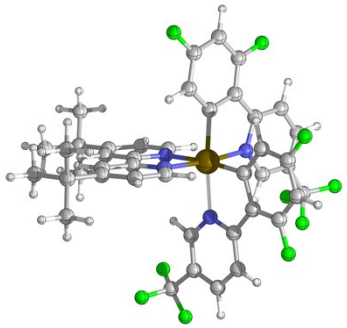


C	1.67865700	0.40324600	-0.32155900
C	3.95916500	-1.01465600	0.42965900
C	2.92889000	1.00210800	-0.41905600
H	0.79616100	0.96361700	-0.61860400
C	4.08128700	0.29760900	-0.04367700
H	4.84692100	-1.56472400	0.72132200
H	3.03702400	2.01791200	-0.78515900
C	2.70116800	-1.60577800	0.52382200
H	2.61648500	-2.62519800	0.89310900
C	1.54203600	-0.91196900	0.15235100
C	-2.12174200	-1.48306200	1.34195600
C	-0.73312800	-0.83179900	1.27766900
C	0.17817400	-1.56418500	0.26465700
C	-0.52957400	-1.68486200	-1.10551100
C	-1.92586000	-2.30477800	-0.95594200
H	-0.85472500	0.21778900	0.98024100
H	-0.26559300	-0.83473700	2.27008300
H	-2.03627800	-2.51360900	1.71334900
H	-2.78562100	-0.94067800	2.01280000

H	-0.64076000	-0.69212100	-1.55951600
H	0.08206700	-2.28607600	-1.78925500
H	-2.45682200	-2.31868100	-1.90746200
H	-1.84732400	-3.33646900	-0.58722900
H	0.32429600	-2.58693800	0.64432300
N	-2.72375900	-1.54384900	0.00775600
C	-3.52156600	-0.53747700	-0.48978900
O	-3.80026200	-0.41324800	-1.67395600
O	-3.96320500	0.26849800	0.50702000
C	-4.83838200	1.41257900	0.22091500
C	-4.11460300	2.40916300	-0.68962700
H	-3.94561200	1.98094000	-1.67823000
H	-4.71723900	3.31838200	-0.79246100
H	-3.14924300	2.68589300	-0.25103900
C	-6.16151200	0.92901500	-0.37950100
H	-6.85444600	1.77335500	-0.46669500
H	-6.00412900	0.49308700	-1.36658700
H	-6.61745600	0.17647200	0.27301500
C	-5.05857900	2.01038700	1.61215100
H	-5.70465900	2.89181400	1.54530100
H	-5.53349600	1.27860800	2.27370300
H	-4.10380200	2.31033100	2.05653000
C	5.39337500	0.98822900	-0.16864900
O	5.53948100	2.12628700	-0.57187600
O	6.42980600	0.20671500	0.21955700
C	7.72382800	0.82045100	0.12006700
H	8.43298800	0.06631100	0.46349900
H	7.93546500	1.10662400	-0.91424700
H	7.77574300	1.71370600	0.74934500

Zero-point correction= 0.412978 (Hartree/Particle)
Thermal correction to Energy= 0.435648
Thermal correction to Enthalpy= 0.436592
Thermal correction to Gibbs Free Energy= 0.359064
Sum of electronic and zero-point Energies= -1056.316631
Sum of electronic and thermal Energies= -1056.293961
Sum of electronic and thermal Enthalpies= -1056.293017
Sum of electronic and thermal Free Energies= -1056.370545

PC1



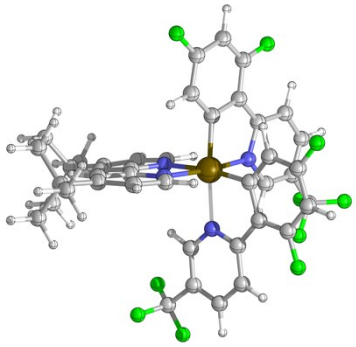
Ir	0.38406600	-0.54457600	0.06296300
C	0.11778600	2.10018000	-1.59808300
C	1.38911200	0.40158400	-2.61648900
C	0.30839800	2.96536600	-2.66526700
H	-0.45883400	2.39846600	-0.73007800
C	1.61888100	1.24545300	-3.72064800
C	1.07892100	2.52349900	-3.74465500
H	2.21697500	0.89534500	-4.54783100
H	1.25806300	3.17971900	-4.58999700
C	-2.26300300	0.56747300	0.89926700
C	-0.60099000	1.56374800	2.18342900
C	-3.24087600	1.31812200	1.55833800
C	-1.52861400	2.33388100	2.86666500
H	0.45991500	1.62415600	2.40175900
C	-2.89746500	2.22779700	2.56408600
H	-4.27780900	1.19176500	1.28168500
H	-1.17616600	3.01311800	3.63432800
C	-1.67853000	-1.94072100	-1.69614500
C	-2.55619900	-0.40824600	-0.17418200
C	-2.94152200	-2.25594700	-2.16792000
H	-0.78843600	-2.41707300	-2.08753200
C	-3.84840200	-0.69606600	-0.61982000
C	-4.08059900	-1.63241900	-1.63195000
H	-3.02550000	-2.99588400	-2.95539700
H	-4.68235500	-0.18239200	-0.16360700
C	2.44137300	-0.84611600	2.14622600
C	2.96935700	0.91023900	0.66219900
C	3.63436500	-0.59924600	2.84932800
C	4.15091200	1.18892200	1.32962300
H	2.67593900	1.47094500	-0.21517900
C	4.48788300	0.41560200	2.44449500
H	3.88153500	-1.21332100	3.70212400
H	5.41419100	0.60234700	2.97764000
C	1.50482800	-1.64533800	-1.23379100
C	1.93084400	-2.96262300	-1.03731300
C	1.87239800	-0.96974500	-2.44170700

C	2.70213000	-3.59616500	-2.00858100
H	1.67572900	-3.51005800	-0.13724600
C	2.65518000	-1.66636400	-3.38144200
C	3.07979900	-2.97006900	-3.19241000
H	3.68169700	-3.47441700	-3.93785500
C	0.33616500	-1.93072700	1.53852700
C	1.44546300	-1.86983800	2.43482700
C	-0.65072700	-2.89822600	1.74691200
C	1.50426700	-2.78876500	3.49723000
C	-0.53609800	-3.78274400	2.81610300
H	-1.50781200	-2.99233300	1.08934900
C	0.53200900	-3.75119100	3.70898100
H	0.60464700	-4.44773800	4.53461400
N	-1.47635700	-1.03632900	-0.71669100
N	-0.95172900	0.70130100	1.21442900
N	0.64164300	0.86758400	-1.56868700
N	2.13711800	-0.06876900	1.05460000
F	3.09877700	-4.85931500	-1.80181300
F	3.02607200	-1.07019700	-4.53577300
F	-1.49136200	-4.70651800	2.99904900
F	2.53762800	-2.75829100	4.36597300
C	-5.47933100	-1.98228500	-2.14688900
C	-3.92868700	3.08076600	3.30911900
C	-6.58339700	-1.19217100	-1.42079500
H	-7.55999300	-1.47897900	-1.82247500
H	-6.59815500	-1.40396700	-0.34517900
H	-6.47618900	-0.11070400	-1.56543100
C	-5.54958800	-1.65766300	-3.65886700
H	-5.37209900	-0.59229200	-3.84302400
H	-4.81662100	-2.22980100	-4.23696300
H	-6.54366600	-1.90890800	-4.04362900
C	-3.61637900	4.57452500	3.04796100
H	-3.68003300	4.81097900	1.97992000
H	-4.34061700	5.20151100	3.57876200
H	-2.61716600	4.85253600	3.39877600
C	-5.36888100	2.79075300	2.84834500
H	-5.65420000	1.74777800	3.02971100
H	-6.06442400	3.42162100	3.41013900
H	-5.51224500	3.01548800	1.78496700
C	-3.82588800	2.78380700	4.82478900
H	-4.02840200	1.72798500	5.03565500
H	-2.83698900	3.02765800	5.22618800
H	-4.56062200	3.38658100	5.36896600
C	-0.36167300	4.31191400	-2.66445300

F	0.33248400	5.20785800	-3.38712100
F	-1.60386700	4.23569100	-3.19048100
F	-0.49233500	4.79018100	-1.40574700
C	5.00499600	2.34318800	0.87883600
F	4.64871300	3.48321900	1.50990300
F	4.86980500	2.56150700	-0.44763700
F	6.30474200	2.12116300	1.14154300
C	-5.72728500	-3.49468600	-1.92681300
H	-5.00068800	-4.11339100	-2.46336800
H	-5.67494800	-3.75343000	-0.86346800
H	-6.72401600	-3.76185400	-2.29347300

Zero-point correction= 0.687686 (Hartree/Particle)
Thermal correction to Energy= 0.738582
Thermal correction to Enthalpy= 0.739527
Thermal correction to Gibbs Free Energy= 0.597433
Sum of electronic and zero-point Energies= -2942.135712
Sum of electronic and thermal Energies= -2942.084815
Sum of electronic and thermal Enthalpies= -2942.083871
Sum of electronic and thermal Free Energies= -2942.225965

PC2



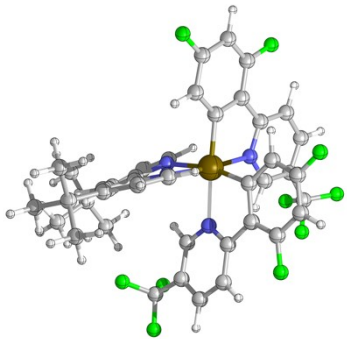
Ir	0.43040700	-0.56569600	0.04393500
C	-0.10589400	2.12439800	-1.49212900
C	1.26614300	0.58095500	-2.61975000
C	-0.02417800	3.04382200	-2.52694900
H	-0.67473800	2.34082800	-0.59569700
C	1.39080800	1.48526400	-3.69250600
C	0.74595700	2.71298800	-3.64567200
H	1.98936100	1.22106900	-4.55062000
H	0.84315600	3.41576200	-4.46670800
C	-2.24255500	0.42933400	0.96563100
C	-0.58769000	1.47091200	2.22693400
C	-3.21941900	1.20087900	1.59178400
C	-1.52225400	2.25939100	2.88870000
H	0.47339500	1.54434100	2.44188600

C	-2.88343500	2.14703200	2.57298300
H	-4.25627600	1.07976900	1.30551500
H	-1.17056400	2.95662400	3.63816100
C	-1.63756200	-2.04140200	-1.66431400
C	-2.52796800	-0.57122900	-0.08814700
C	-2.90447300	-2.43311400	-2.07945000
H	-0.74116400	-2.46239000	-2.10381100
C	-3.81575600	-0.93948900	-0.46807500
C	-4.04482200	-1.88660100	-1.47707700
H	-2.97803000	-3.17110400	-2.86792500
H	-4.66050500	-0.48992000	0.03730000
C	2.54863000	-0.81566700	2.08979600
C	2.91263500	1.04484000	0.63145600
C	3.75556000	-0.47543200	2.78936800
C	4.08843700	1.38092900	1.29286200
H	2.57923100	1.62449800	-0.21952100
C	4.51420200	0.59756000	2.41455300
H	4.05698100	-1.09315100	3.62319700
H	5.42802100	0.85173500	2.93902200
C	1.58168800	-1.51261100	-1.33863400
C	2.11628200	-2.79883300	-1.21509500
C	1.85957700	-0.75424000	-2.52104900
C	2.91216600	-3.32178800	-2.23104900
H	1.92643300	-3.40751900	-0.33873400
C	2.67199200	-1.34136900	-3.50886700
C	3.20650800	-2.61296600	-3.39125100
H	3.82731700	-3.03121200	-4.17357100
C	0.51614000	-2.02012100	1.41984600
C	1.69244400	-1.90130000	2.31474500
C	-0.37727400	-3.06795400	1.60681400
C	1.84718800	-2.91171200	3.33036600
C	-0.15770600	-4.00346600	2.61657300
H	-1.24777100	-3.19109900	0.97176700
C	0.95930600	-3.93618200	3.48811200
H	1.10301700	-4.68215900	4.26074900
N	-1.44026300	-1.13736700	-0.68935500
N	-0.93014800	0.58418900	1.28256800
N	0.51946700	0.94060900	-1.53144600
N	2.13855900	0.02256900	0.99679800
F	3.41457200	-4.55576600	-2.09229200
F	2.96312400	-0.66512400	-4.64088100
F	-1.01934800	-5.01392500	2.78779400
F	2.90843800	-2.85001000	4.16149700
C	-5.47621500	-2.27144800	-1.86249500

C	-3.97613500	2.99642900	3.23026500
C	-6.21715600	-1.00583400	-2.35879200
H	-7.24406800	-1.26488100	-2.63741500
H	-6.26950900	-0.22954800	-1.58760100
H	-5.72372800	-0.57783700	-3.23835800
C	-5.50891200	-3.33202000	-2.97783900
H	-5.03385900	-2.97290000	-3.89780600
H	-5.01820100	-4.26245700	-2.67047800
H	-6.54835000	-3.57429600	-3.21975000
C	-4.70662800	3.80704300	2.13179900
H	-5.18712000	3.15918200	1.39069300
H	-5.48905900	4.42335300	2.58694800
H	-4.01327700	4.47152500	1.60452400
C	-4.98048700	2.05832900	3.94254300
H	-4.48625500	1.47235200	4.72517800
H	-5.77232700	2.65250400	4.41079600
H	-5.45878900	1.36066900	3.24664700
C	-3.40108900	3.98006100	4.26551900
H	-2.89099900	3.46078700	5.08469700
H	-2.70086200	4.68923400	3.80968200
H	-4.21645600	4.56230600	4.70534000
C	-0.80616700	4.32649500	-2.45204500
F	-0.19515600	5.31498200	-3.12711900
F	-2.04051800	4.17240700	-2.97951900
F	-0.96971000	4.72449700	-1.16926000
C	4.88638000	2.57294800	0.86413400
F	4.87520200	3.53158500	1.81809300
F	4.40280700	3.12411400	-0.27292100
F	6.17655900	2.24410900	0.65076400
C	-6.19581000	-2.84157500	-0.61596900
H	-5.68264300	-3.73207500	-0.23677800
H	-6.25546600	-2.11106700	0.19811600
H	-7.22003200	-3.12566500	-0.87959900

Zero-point correction= 0.683264 (Hartree/Particle)
Thermal correction to Energy= 0.734907
Thermal correction to Enthalpy= 0.735851
Thermal correction to Gibbs Free Energy= 0.590375
Sum of electronic and zero-point Energies= -2942.040203
Sum of electronic and thermal Energies= -2941.988560
Sum of electronic and thermal Enthalpies= -2941.987616
Sum of electronic and thermal Free Energies= -2942.133092

PC3



Ir	0.69573000	-0.51496200	0.17899900
C	-1.07626100	1.58252300	-1.34905300
C	0.10581700	0.07917400	-2.71518800
C	-1.80323100	2.08148000	-2.42311000
H	-1.22565300	1.96890500	-0.34899000
C	-0.58938700	0.56545800	-3.84093800
C	-1.55373300	1.55380300	-3.69171900
H	-0.38251100	0.15387100	-4.81680200
H	-2.10755500	1.91613700	-4.55132200
C	-1.93907300	0.15258400	1.32167100
C	-0.34729000	1.65858000	2.18991100
C	-2.97279700	1.04743800	1.71885800
C	-1.32264700	2.52938700	2.62874500
H	0.70752900	1.87038500	2.34372400
C	-2.69544000	2.25129900	2.33044300
H	-3.99004700	0.79088600	1.45448900
H	-1.02997400	3.43014300	3.15474600
C	-1.15202900	-2.83905200	-0.59037700
C	-2.15038100	-1.06874200	0.61633900
C	-2.35419100	-3.49771400	-0.72390800
H	-0.23436500	-3.24561000	-1.00084300
C	-3.40766400	-1.71910200	0.48300600
C	-3.54280100	-2.92225900	-0.17630600
H	-2.37439700	-4.44633400	-1.24692300
H	-4.26463000	-1.25100700	0.94915000
C	3.24838400	0.17509700	1.47173600
C	2.63912500	1.78234200	-0.14252600
C	4.41731900	0.90886200	1.75074300
C	3.77538800	2.53722100	0.10400400
H	1.91096400	2.07789700	-0.88728800
C	4.68029500	2.08717500	1.07186100
H	5.10517500	0.54088900	2.49695600
H	5.58292800	2.65314900	1.27741000
C	1.60906300	-1.39927000	-1.41236500
C	2.61445800	-2.37546000	-1.36380400

C	1.12984800	-0.96960600	-2.69522300
C	3.11857900	-2.91807700	-2.53901100
H	3.00190300	-2.72894800	-0.41455100
C	1.68149800	-1.56174900	-3.84464300
C	2.66762900	-2.53190400	-3.79857600
H	3.07099600	-2.96195900	-4.70652100
C	1.57808700	-1.60363000	1.61604100
C	2.81919200	-1.06904100	2.09083900
C	1.10276600	-2.79820900	2.17603900
C	3.51604000	-1.76457300	3.09398700
C	1.83948500	-3.43633600	3.16341000
H	0.16530100	-3.23605000	1.85292800
C	3.05447100	-2.94542300	3.64433600
H	3.61210600	-3.46167200	4.41522300
N	-1.02562700	-1.65379200	0.04260000
N	-0.61365000	0.52354900	1.51559100
N	-0.17275500	0.60799100	-1.48464300
N	2.37819400	0.64305700	0.51704400
F	4.07871100	-3.86056500	-2.47163900
F	1.26188600	-1.18769500	-5.07987500
F	1.37443600	-4.58425200	3.69231000
F	4.69578800	-1.28662500	3.56410400
C	-4.87888500	-3.65765000	-0.32197600
C	-3.76824800	3.29783600	2.64642400
C	-6.04840600	-2.88590900	0.31560000
H	-6.98042900	-3.44476400	0.17581700
H	-5.90353800	-2.74857000	1.39324100
H	-6.17978900	-1.89925100	-0.14344400
C	-5.18927300	-3.85355800	-1.82506600
H	-5.27421800	-2.88637000	-2.33359100
H	-4.40889500	-4.43120900	-2.33095700
H	-6.13711100	-4.39112300	-1.94936700
C	-5.15789800	2.88402800	2.12899000
H	-5.50797100	1.95611400	2.59584300
H	-5.88764800	3.66674400	2.36424000
H	-5.15007700	2.74737900	1.04171700
C	-3.84561300	3.50537300	4.17635900
H	-2.88240400	3.82128000	4.59128000
H	-4.58558500	4.27772400	4.41928000
H	-4.14019100	2.57768000	4.68022900
C	-3.38494400	4.63226600	1.96016700
H	-2.43424100	5.02683400	2.33342400
H	-3.29184900	4.50106500	0.87696400
H	-4.15568000	5.38874900	2.15131600

C	-2.85613800	3.11231300	-2.14602100
F	-3.42822000	3.57286800	-3.27604100
F	-3.84385600	2.61017300	-1.36210900
F	-2.34584300	4.17524000	-1.47651400
C	3.98287900	3.83884500	-0.61328700
F	3.48699400	4.87927000	0.09613200
F	3.36772600	3.85036600	-1.81617400
F	5.29491400	4.08732200	-0.81362300
C	-4.77483100	-5.03971300	0.36574600
H	-3.98018200	-5.65298500	-0.07148600
H	-4.56154900	-4.92644800	1.43467900
H	-5.71857100	-5.58860400	0.26029900

Zero-point correction= 0.684431 (Hartree/Particle)
Thermal correction to Energy= 0.735319
Thermal correction to Enthalpy= 0.736263
Thermal correction to Gibbs Free Energy= 0.596110
Sum of electronic and zero-point Energies= -2942.288757
Sum of electronic and thermal Energies= -2942.237869
Sum of electronic and thermal Enthalpies= -2942.236925
Sum of electronic and thermal Free Energies= -2942.377078