Supporting Information

On The Nature of Csp^3)-C(sp^2) Bond Formation in Nickel-Catalyzed Tertiary Radical Cross-Couplings: A Case Study of Ni/Photoredox Catalytic Cross-Coupling of Alkyl Radicals and Aryl Halides

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A. Computational Details and Details on Quasi-Classical Direct-Dynamics Simulations

All geometry optimizations of intermediates and transition states were achieved using spin-unrestricted UB3LYP[1]-D3[2]/def2-SVP[3] method, in THF solvent using the CPCM solvent model[4] with "opt=noeigen" and "guess=mix" keywords as implemented in Gaussian09[5]. Frequency calculations were also conducted at the same level of theory to obtain vibrational frequencies to determine the identity of stationary points as intermediates (no imaginary frequencies) or transition states (only one imaginary frequency), as well as obtaining the thermal corrections to enthalpy ($H_{correction}$) and free energy ($G_{correction}$) at the temperature of 298 K. Energies were refined by computing single point energies in implicit solvent with UB3LYP-D3/def2-TZVPP[3] method using larger basis set compared to optimization method. To explore the effect of DMA solvent in Ni-TMHD catalytic system, single point energy was also calculated in implicit DMA solvent as labeled as UB3LYP-D3/def2-TZVPP-CPCM(DMA)//UB3LYP-D3/def2-SVP-CPCM(THF). For comparison, single point energies were also computed using UM06[6]/def2-TZVPP method using Gaussian 09[5]. Moreover, domain-based local pair-natural orbital coupled-cluster calculations using single and double excitations with perturbative triple excitations (DLPNO-CCSD(T))[7] were performed with def2-TZVPP as basis set and def2-TZVPP/C as auxiliary basis set using ORCA software[8]. This method was used to obtain energy with high accuracy at affordable computational cost compared to DFT calculations.[9] Free energies obtained with each method was calculated generally as $G^{method\text{-}solvent} = E^{method\text{-}solvent} + G_{correction}$. In part **E**, single point energies obtained directly with each method ($E^{method\text{-}solvent}$ computed with UB3LYP-D3 and UM06 methods, and $E^{DLPNO\text{-}CCSD(T)\text{-}gas}$ computed with DLPNO-CCSD(T) method) would be shown. All structural figures were generated with CYLview.[10] Distances in structural figures are shown in Å and energies are in kcal/mol.

Molecular dynamics (MD) simulations were performed in the gas phase on the truncated doublet transition states **^{2}I'-TS** (shown in Figure S7) and **^{2}K-TS** (shown in Figure S20). The truncated **^{2}I'-TS** and **^{2}K-TS** were located at the UB3LYP-D3/def2-SVP level of theory using Gaussian 09 with HOMO−LUMO mixing for the initial guess in both transition state optimization and dynamics simulation. Quasi-classical direct-dynamics simulations were then initialized within the region of the potential energy surface near **^{2}I'-TS** and **^{2}K-TS**, adding zero-point energy for each real normal mode in corresponding transition states, plus a Boltzmann sampling of thermal energy available at 298.15 K with a random phase. The trajectories were propagated backward on **^{2}I'-TS** and forward on **^{2}K-TS** (settings are made on "searchdir" keyword line as shown in Section B), with focus on observing possible radical dissociation or C(sp^2)-C(sp^3) bond formation within the lifetime of Ni(III) intermediate. Parameters of radical dissociation concomitant with generation of Ni(II) intermediate were set as **^{1}G/^{1}G'** (C_{Ph}–$C_{t\text{Bu}}$ > 3.00 Å and Ni–$C_{t\text{Bu}}$ > 2.70 Å) for **^{2}K-TS** and **^{1}G/^{1}G'** (C_{Ph}–$C_{t\text{Bu}}$ > 3.00 Å and Ni–$C_{t\text{Bu}}$ > 3.50 Å) for **^{2}I'-TS** or product formation as **$^2\mathbf{P_B}$ + *t*Bu-Ph** (C_{Ph}–$C_{t\text{Bu}}$ < 1.70 Å and Ni–$C_{t\text{Bu}}$ > 5.00 Å) based on corresponding distances at the transition states. The classical equations of motion were integrated with a velocity-Verlet algorithm using Singleton's program Progdyn[11], with the energies and derivatives computed using the UB3LYP-D3/def2-SVP method with Gaussian 09. The step length for integration was 1 fs.

B. Input Parameters on Progdyn

The configuration file progdyn.conf for trajectory initialization for the doublet reduction elimination transition state **^{2}I'-TS** is given below as an example.

```
/#This is the configuration file for PROGDYN.  This file is read by progdynstarterHP and
# the awk programs proggenHP, prog1stpoint, prog2ndpoint, and progdynb.
#The programs won't read anything past the first blank line,
#and this file must end with a blank line.
#The program has a number of default values but they are unlikely to be what you want.
#Do not delete lines - rather, comment out lines for unwanted options.
#The values here are read repeatedly and most can be changed in the middle of running jobs
#***The keywords are case sensitive.  The following keywords should always be defined:***
#***method, charge, multiplicity, memory, processors, title
#*** method --The following word is copied exactly to the gaussian input file.
method ub3lyp/def2svp
#To do a nonstandard route, make nonstandard 1.  For normal calcs, use nonstandard 0 or else leave it out.
#Then make a file called "nonstandard" containing the nonstandard route with no extra lines.
nonstandard 0
# NMRoptions As is NMR=1 will add a section for an NMR calc at every NMRevery intervals. If you want to combine the two use nonstandard
#NMRtype 1
#NMRmethod B3LYP/cc-pvtz
#NMRevery 4
#geometry linear
rotationmode 1
#*** method2 --The options here are restricted, unrestricted, and read. restricted is the default
#If the method is U..., put unrestricted here and the .com files will have in them guess=mix.
#If you put read here, the .com files will contain guess=tcheck, which sometimes makes things faster, sometimes not.
#The use of read requires a specifically defined checkpoint file name using the keyword checkpoint.
method2 unrestricted
charge 0
multiplicity 2
processors 32
#*** memory --The following "word" is copied exactly to the gaussian input file after %mem=.
memory 64gb
#*** killcheck and checkpoint -- You can use a specifically defined checkpoint file name by putting
```

#the name after the keyword checkpoint. This is necessary if you use the read option with method2.
#Defined checkpoint names are an unnecessary modest hastle and if you do not want to bother, use killcheck 1
killcheck 1
#checkpoint g09.chk
#*** diagnostics -- 0 prints out nothing extra, 1 (default) prints out extra stuff to a
#file "diagnostics", 2 adds more stuff, 3 adds velocities to a file "vellist"
#4 adds the apparent temperature to vellist, but this is meaningless with quasiclassical calculations
diagnostics 1
#*** title -- the title keyword must be followed by exactly four words
title j j j Ni-trun-TS-RE-r2-g
#*** initialdis -- 0 (default) turns off displacement of the normal modes, so that all trajectories start from the same place
and only the energies and signs of the motion in the modes are randomized
1 gives a flat distribution of displacements where all of the possible values are equally likely
2 (recommended) gives a QM-like gaussian distribution of displacements, so that displacements in the middle are more likely that
those at the end by 1/e
initialdis 2
#*** timestep -- this is the time bet*-ween points in the trajectory. Typical values would be 1E-15 or 0.5E-15 or 0.25E-15
timestep 1E-15
#*** scaling -- this lets you scale the gaussian frequencies by a constant
scaling 1.0
temperature 298.15
#*** method3, method4, method5, and method6 -- These keywords let you add extra lines to the gaussian input file.
#method3 and method4 add lines at the top of the input after the lines defining the method, and
#this is useful to implement things like the iop for mPW1k
#method5 and method6 add lines after the geometry, after a blank line of course
#only a single term with no spaces can be added, one per method line. Here are some examples to uncomment if needed
#add the line below with big structures to get it to put out the distance matrix and the input orientation
#method3 iop(2/9=2000)
#method4 iop(3/124=3)
#method5 eps=32.63
#method6 rsolv=1.329
#*** methodfile -- This keyword lets you add more complicated endings to gaussian input files
#such as a gen basis set. Put after the keyword the number of lines in a file you create called

#methodfile that contains the test you want to add to the end of the gaussian input
methodfile 0
#*** numimag --This tells the program the number of imaginary frequencies in the starting structure.
#if 0, treats as ground state and direction of all modes is random
#if 1, motion along the reaction coordinate will start out in the direction defined by searchdir
#if 2, only lowest freq will go direction of searchdir and other imag mode will go in random direction
numimag 2
#*** searchdir -- This keyword says what direction to follow the mode associated with the imaginary frequency.
#The choices are "negative" and "positive". Positive moves in the direction defined in the gaussian frequency calculation
#for the imaginary frequency, while negative moves in the opposite direction. The correct choice can be made either
#by a careful inspection of the normal modes and standard orientation geometry, or by trial and error.
searchdir positive
#*** classical -- for quassiclassical dynamics, the default, use 0. for classical dynamics, use 1
#if there are no normal modes and the velocities are to be generated from scratch, use classical 2
classical 0
#*** DRP, saddlepoint, and maxAtomMove --to run a DRP use 'DRP 1' in the line below, otherwise leave it at 0 or comment it out
#the treatment of starting saddlepoints is not yet implemented so use saddlepoint no
#if DRP shows oscillations then decrease maxAtomMove
#DRP 1
#saddlepoint no
#maxAtomMove 0.01
#*** cannonball -- The program can "fire" a trajectory from a starting position toward a particular target, such as toward
#a ts. To use this, make a file cannontraj with numAtom lines and three numbers per line that defines the vector
#for firing the trajectory, relative to the starting geometry's standard orientation. The number following cannonball sets
#the extra energy being put into the structure in kcal/mol
#cannonball 10
#*** keepevery --This tells the program how often to write the gaussian output file to file dyn, after the first two points.
#Use 1 for most dynamics to start with, but use a higher number to save on disk space or molden loading time.
keepevery 1
#*** highlevel --For ONIOM jobs, the following line states the number of highlevel atoms,

#which must come before the medium level atoms. Use some high value such as 999 if not using ONIOM
highlevel 999
#*** fixedatom1, fixedatom2, fixedatom3, and fixedatom4 - These fix atoms in space.
#Fixing one atom serves no useful purpose and messes things up, while fixing two atoms
#fixes one distance and fixing three has the effect of fixing three distances, not just two
#in current form fixed atoms only are meant to work with no displacements, that is, initialdis=0
#fixedatom1 2
#fixedatom2 3
#fixedatom3 19
#*** boxon and boxsize - With boxon 1, a cubic box is set such that atoms that reach the edge
#are reflected back toward the middle. Useful for dynamics with solvent molecules. This is a crude
#implementation that is ok for a few thousand femtoseconds but will not conserve energy long term.
#Set the box size so as to fit the entire initial molecule but not have too much extra room.
#The dimensions of the box are two times the boxsize, e.g. boxsize 7.5 leads to a box that is 15 x 15 x 15 angstroms
boxon 0
boxsize 7.5
#*** displacements -- This keyword lets you set the initialdis of particular modes by using a series of lines of the format
displacements NumberOfMode InitialDisForThatMode, as in the example below. You should be able to do as many of these as you like
you might consider this for rotations where a straight-line displacement goes wrong at large displacements
The choices for InitialDisForThatMode are 0, 1, 2, and 10, where 10 does the same thing as 0 but is maintained for now because
a previous version of the program had a bug that made 0 not work.
#displacements 2 0
#displacements 3 0
#*** etolerance --This sets the allowable difference between the desired energy in a trajectory and the actual
#energy, known after point 1 from the potential energy + the kinetic energy in the initial velocities.
#The unit is kcal/mol and 1 is a normal value for mid-sized organic systems. For very large and floppy molecules, a larger value
#may be needed, but the value must stay way below the average thermal energy in the molecule (not counting zpe).
#If initialdis is not 0 and few trajectories are being rejected, decrease the value.
etolerance 0.5
#*** controlphase --It is sometimes useful to set the phase of particular modes in the initialization of trajectories.

#The format is controlphase numberOfModeToControl positive or controlphase numberOfModeToControl negative.
#controlphase 2 positive
#*** damping -- The damping keyword lets you add or subtract energy from the system at each point, by multiplying the velocities
#by the damping factor. A damping of 1 has no effect, and since you mostly want to change the energy slowly, normal values range
#from 0.95 to 1.05. The use of damping lets one do simulated annealing - you add energy until the structure is moving enough
#to sample the kinds of possibilities you are interested in, then you take away the energy slowly.
damping 1
#*** reversetraj --This keyword sets the trajectories so that both directions from a transition state are explored.
reversetraj true

#updated Aug 9, 2007 to include the possibility of classical dynamics by the keyword classical
#updated Jan 2008 to include fixed atoms, ONIOM jobs, keepevery, and box size
#update Feb 2008 to include methodfile parameter
updated Nov 2008 to allow for start without an initial freq calc using classical = 2
update Aug 2010 to include etolerance, damping controlphase and reversetraj

C. Energetics with Different Methods and Conformational Search

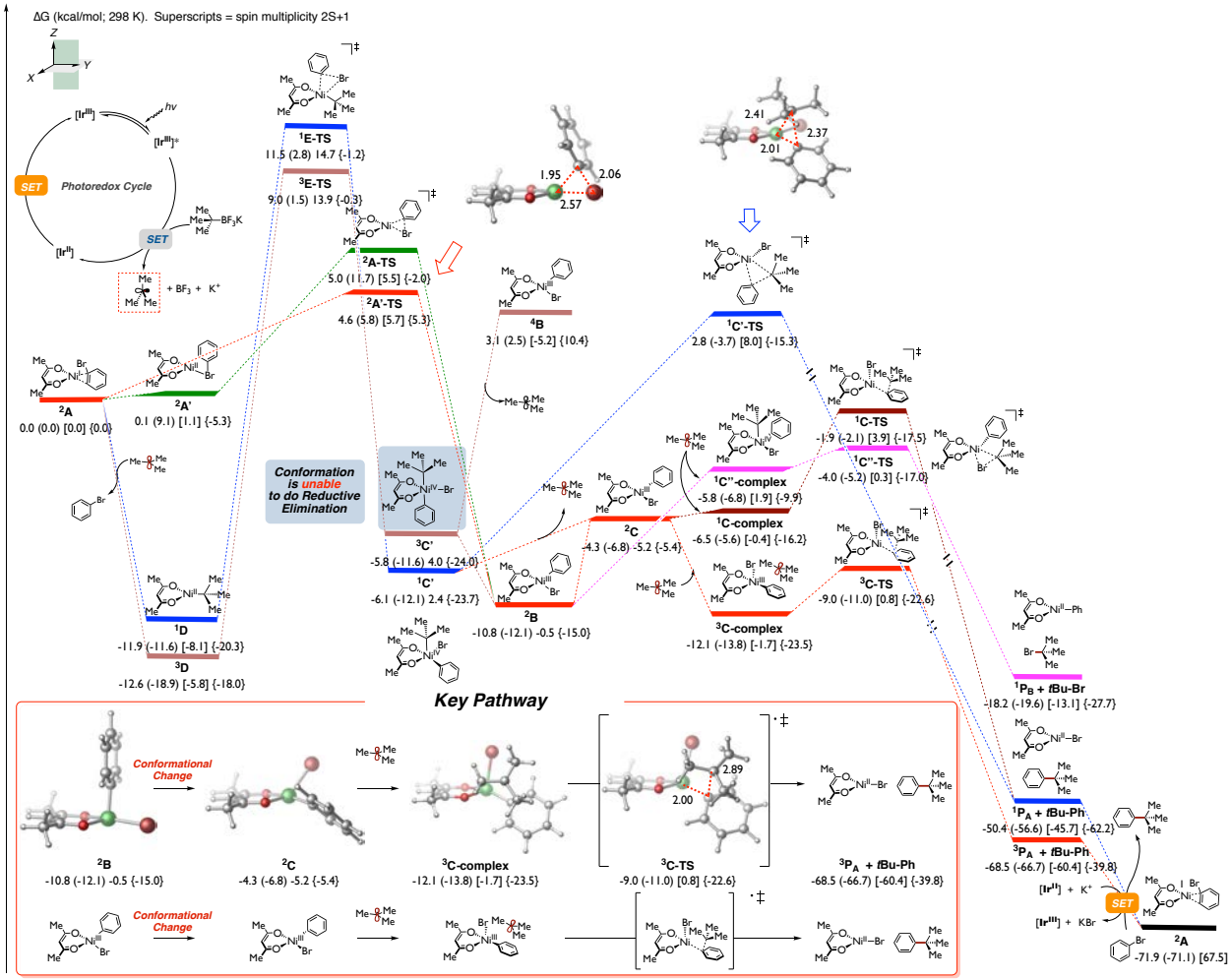


Figure S1. Calculated energetics of the Ni-catalyzed cross-coupling between *tert*-butyl radical and phenyl bromide using anionic TMHD as ligand. Free energies (kcal/mol) were computed at the UB3LYP-D3/def2-TZVPP-CPCM(DMA)//UB3LYP-D3/def2-SVP-CPCM(THF), UB3LYP-D3/def2-SVP-CPCM(THF) (in parenthesis), UM06/def2-TZVPP-CPCM(DMA)//UB3LYP-D3/def2-SVP-CPCM(THF) (in bracket), and DLPNO-CCSD(T)/def2-TZVPP-gas//UB3LYP-D3/def2-SVP-CPCM(THF) (in brace) levels of theory. Energetics of the last SET step was calculated in UB3LYP-D3/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF), UB3LYP-D3/def2-SVP-CPCM(THF) (in parenthesis), UM06/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF) (in bracket) levels of theory for better comparison with the Ni-bipyridine system.

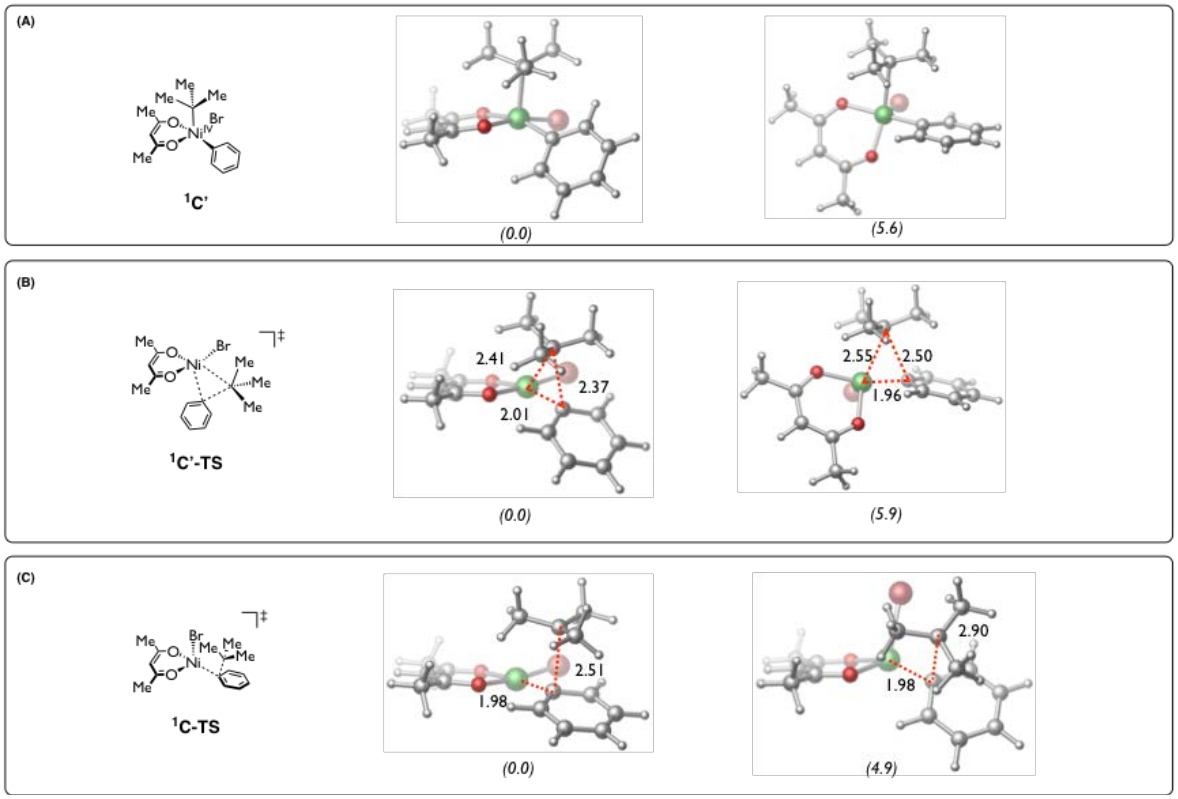


Figure S2. Conformational search of key intermediates and transition states of Ni-catalyzed cross-coupling between *tert*-butyl radical and phenyl bromide using anionic TMHD as ligand. Relative free energies (kcal/mol) were calculated with respect to corresponding lowest-energy level structure at the UB3LYP-D3/def2-SVP-CPCM(THF) (in parenthesis) level of theory.

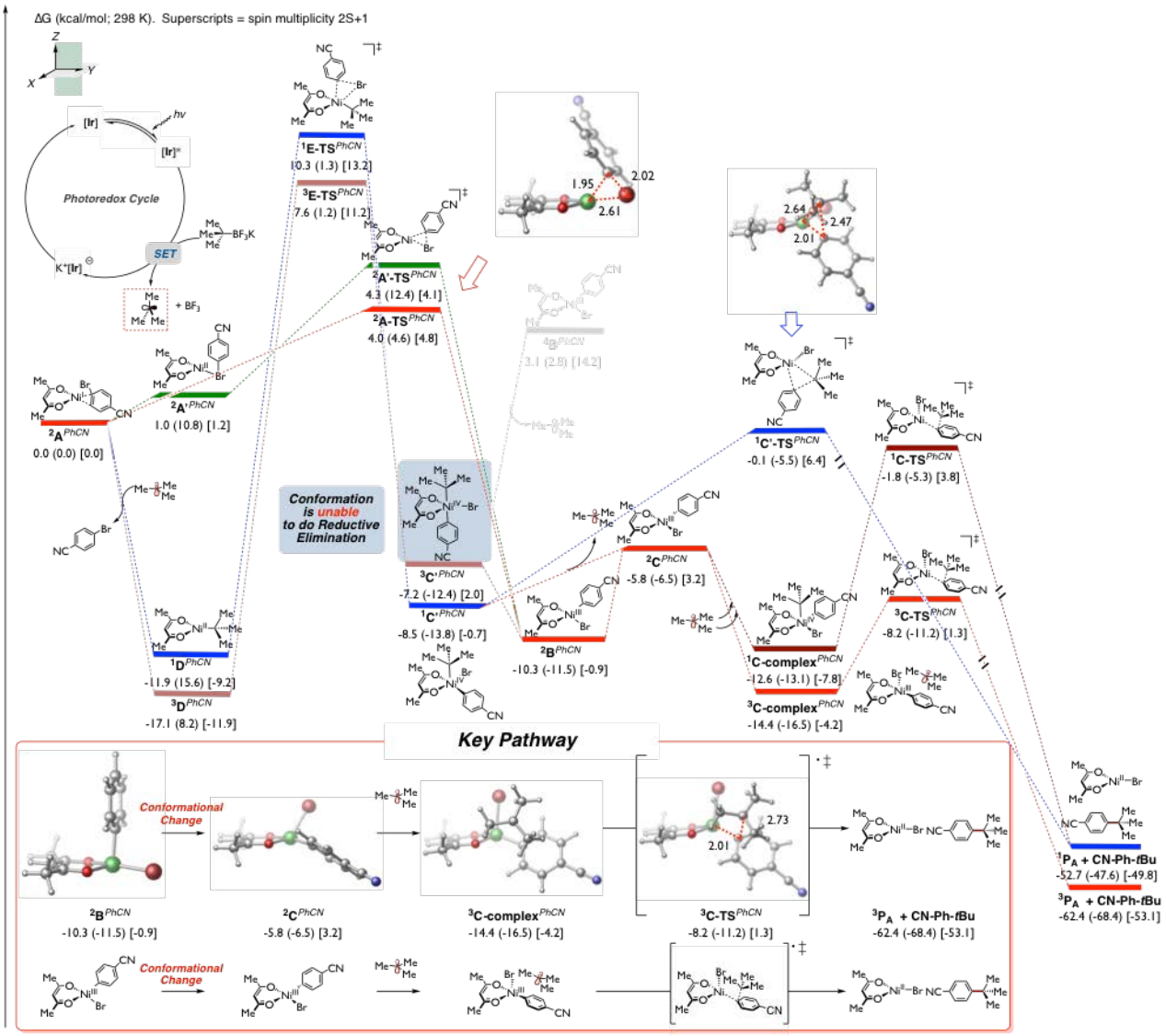


Figure S3. Calculated energetics of the Ni-catalyzed cross-coupling between *tert*-butyl radical and 4-bromobenzonitrile using anionic acac as ligand. Free energies (kcal/mol) were computed at the UB3LYP-D3/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF), UB3LYP-D3/def2-SVP-CPCM(THF) (in parenthesis) and UM06/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF) (in bracket) levels of theory.

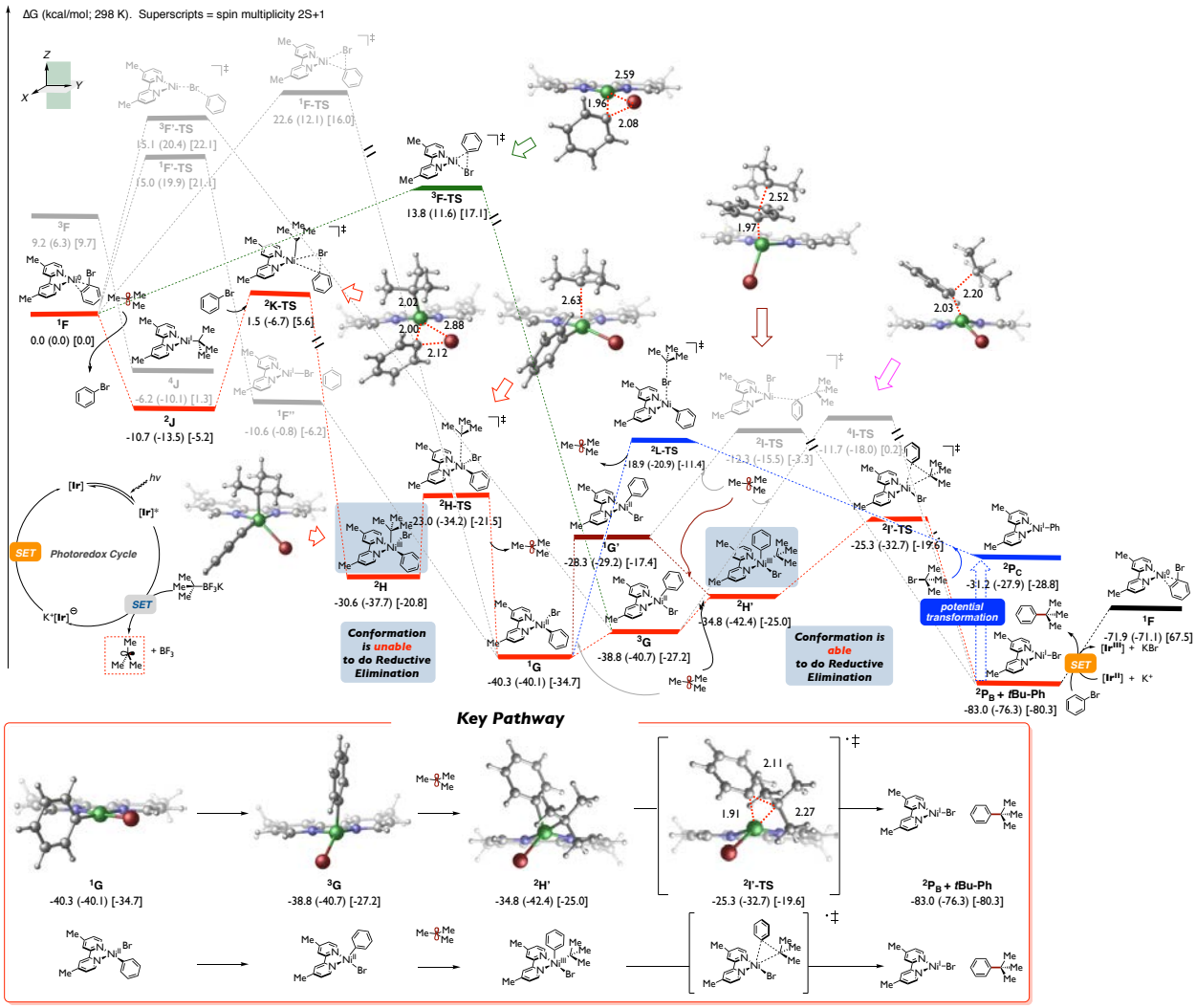


Figure S4. Calculated energetics of the Ni-catalyzed cross-coupling between *tert*-butyl radical and phenyl bromide using neutral bipyridine as ligand. Free energies (kcal/mol) were computed at the UB3LYP-D3/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF), UB3LYP-D3/def2-SVP-CPCM(THF) (in parenthesis), and UM06/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF) (in bracket) levels of theory.

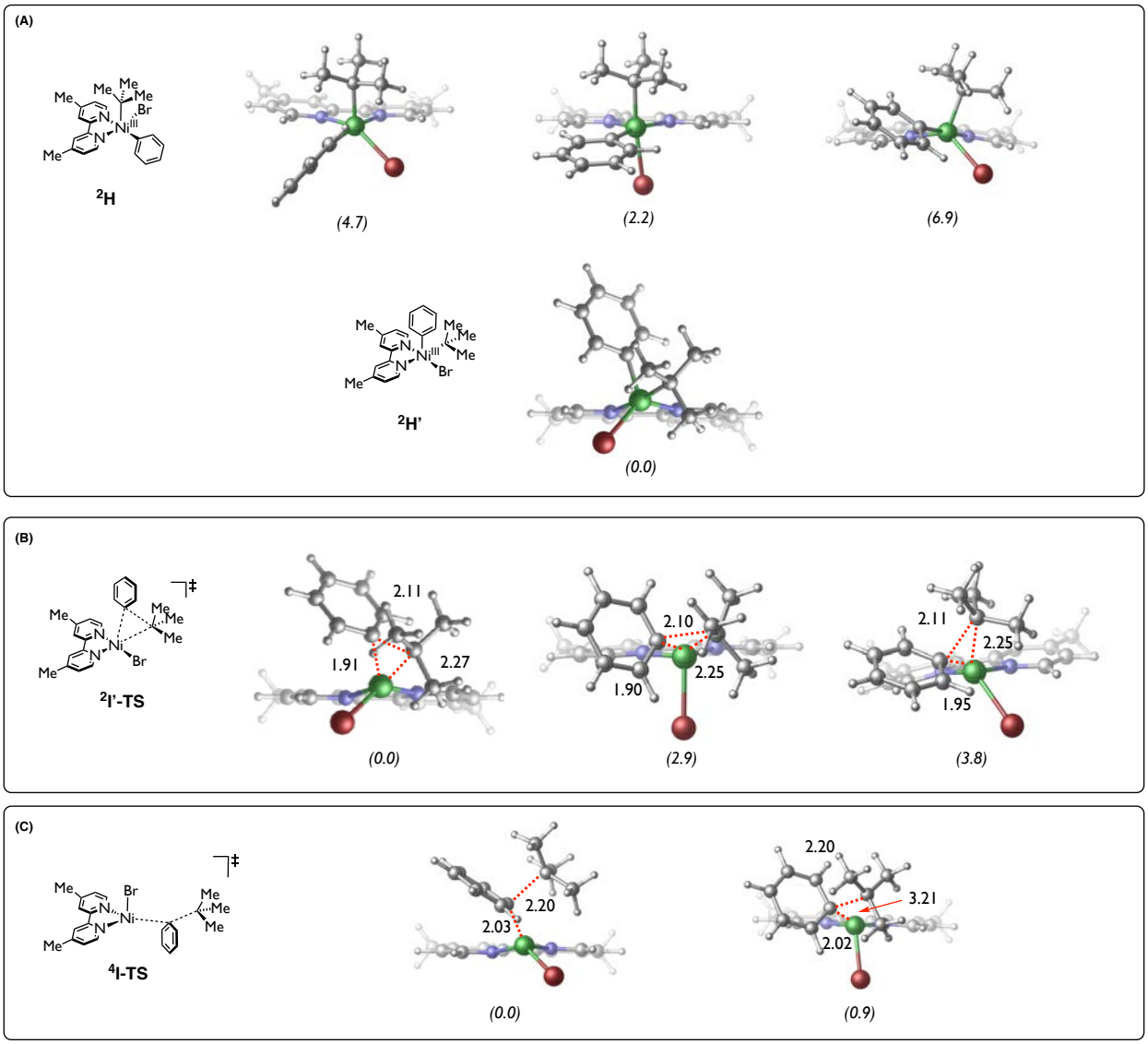


Figure S5. Conformational search of key intermediates and transition states of Ni-catalyzed cross-coupling between *tert*-butyl radical and phenyl bromide using neutral bipyridine as ligand. Relative free energies (kcal/mol) were calculated with respect to corresponding lowest-energy level structure at the UB3LYP-D3/def2-SVP-CPCM(THF) (in parenthesis) level of theory.

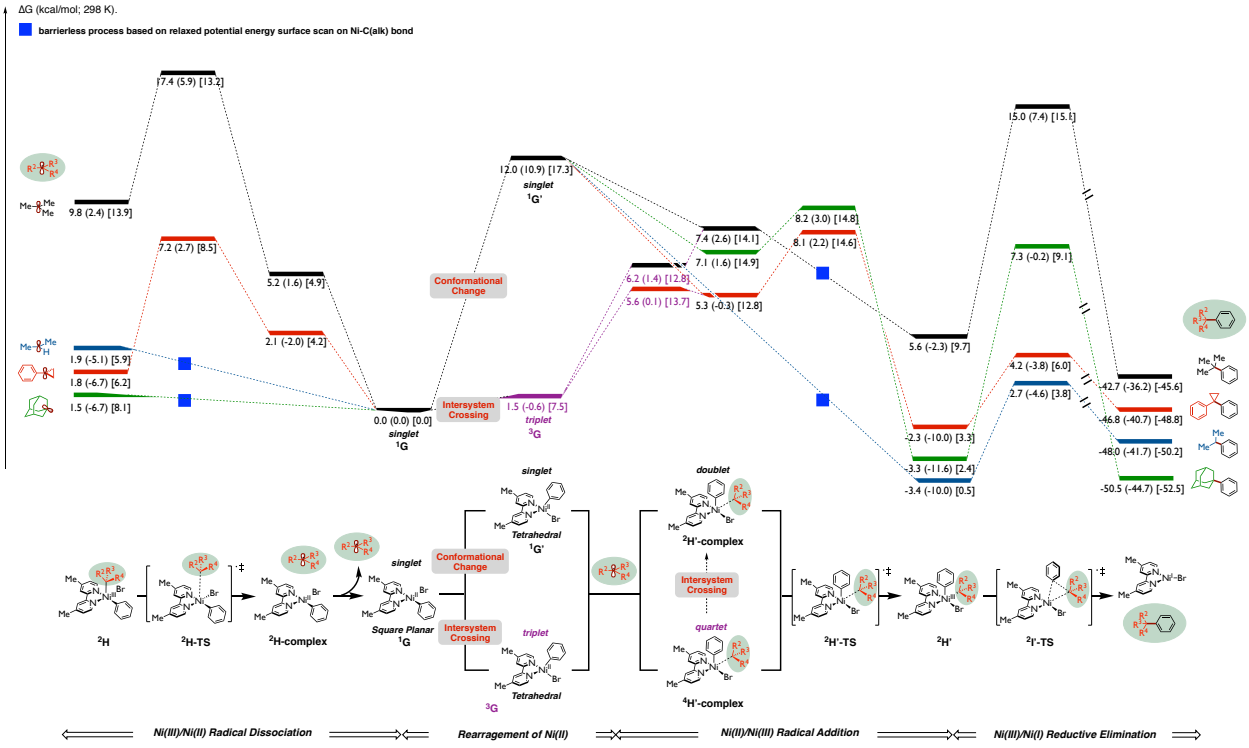
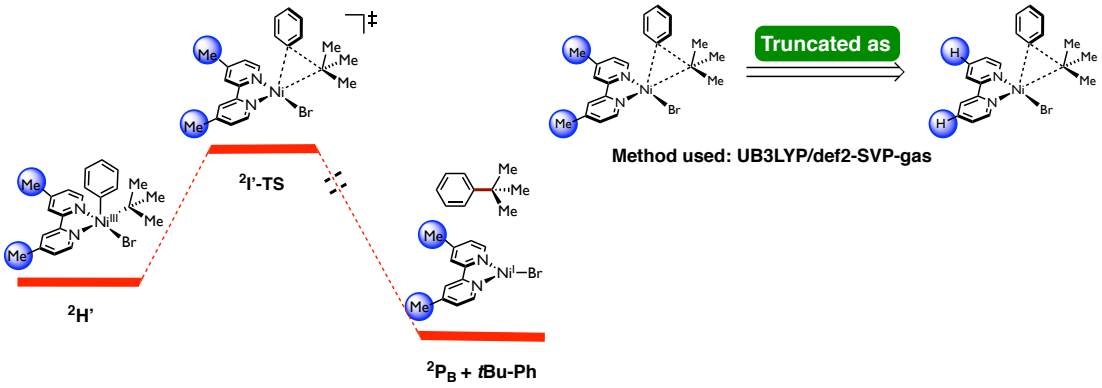
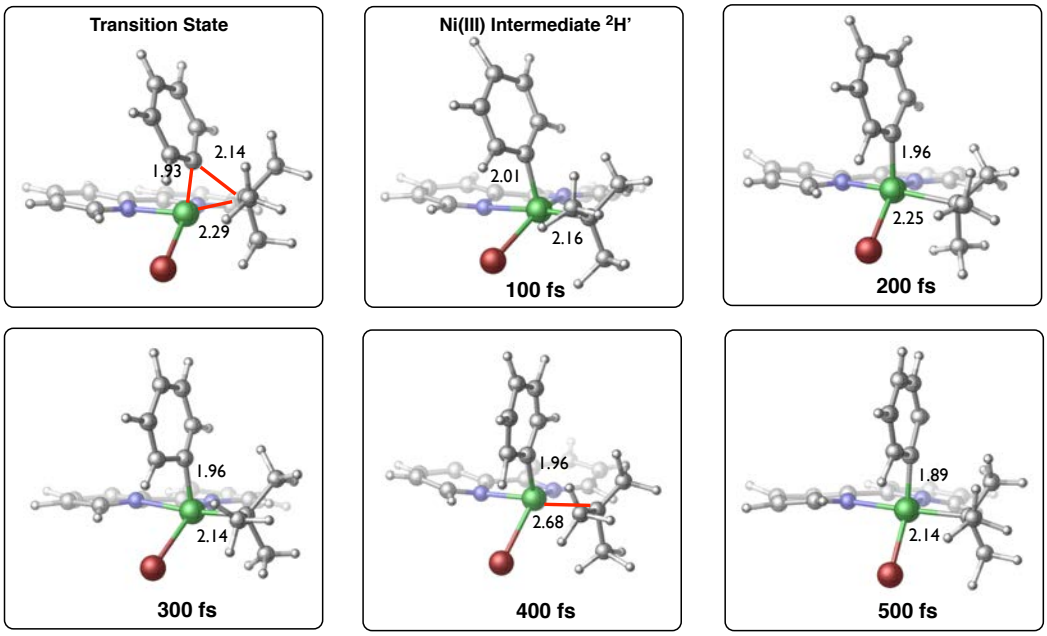


Figure S6. Calculated energetics of the key pathway using neutral bipyridine as ligand and *tert*-butyl radical (black), *iso*-propyl radical (blue), 1-phenylcyclopropyl radical (red) and adamantly radical (green) as radical substrates. Free energies (kcal/mol) were computed at the UB3LYP-D3/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF), UB3LYP-D3/def2-SVP-CPCM(THF) (in parenthesis), and UM06/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF) (in bracket) levels of theory.

Starting from *singlet spin square planar* Ni(II) species **^{1}G**, *tert*-butyl radical can undergo radical addition from axial position via **^{2}H-TS** to generate the endergonic Ni(III) intermediate **^{2}H**, which is a reversible process so *tert*-butyl radical is less favorable to be bound to Ni center. Alternatively, **^{1}G** could undergo conformational change or intersystem crossing to generate *singlet spin tetrahedral* Ni(II) species **^{1}G'** and *triplet spin tetrahedral* **^{3}G**, respectively. Upon interaction with *tert*-butyl radical, Ni species can form doublet or quartet (purple energy values) complex, then after barrierless radical addition (blue squares, based on relaxed potential energy surface scan on Ni-C bond) Ni(III) species **^{2}H'** could be formed. More importantly, the barrier of reductive elimination step of *tert*-butyl radical (15.0 kcal/mol with respect to **^{1}G**) is much higher than those with other alkyl radicals. This might explain the observed failure with *tert*-butyl radical substrate and the success of adamantly and 1-phenylcyclopropyl radicals in experiment.[13]



(A) example of reverse direction from ^{2}**I'-TS**



(B) example of forward direction from ^{2}**I'-TS**

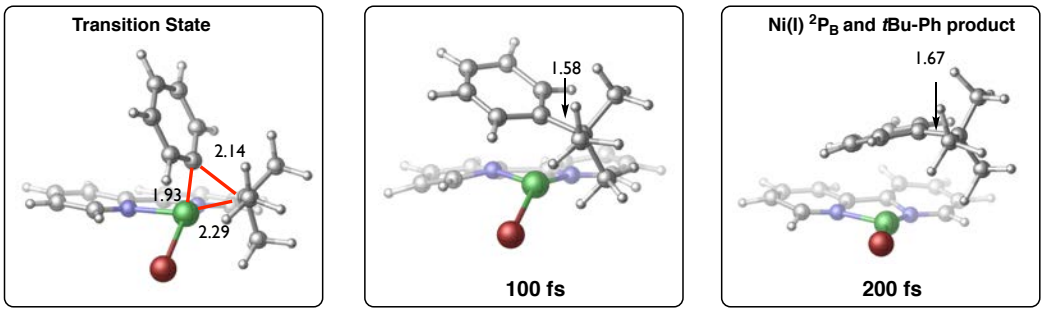


Figure S7. Snapshots of representative examples of quasi-classical dynamic calculation of truncated system from reductive elimination transition state **^{2}I'-TS** in both forward and backward directions of Ni-catalyzed cross-coupling between *tert*-butyl radical and phenyl bromide in Ni-bipyridine system.

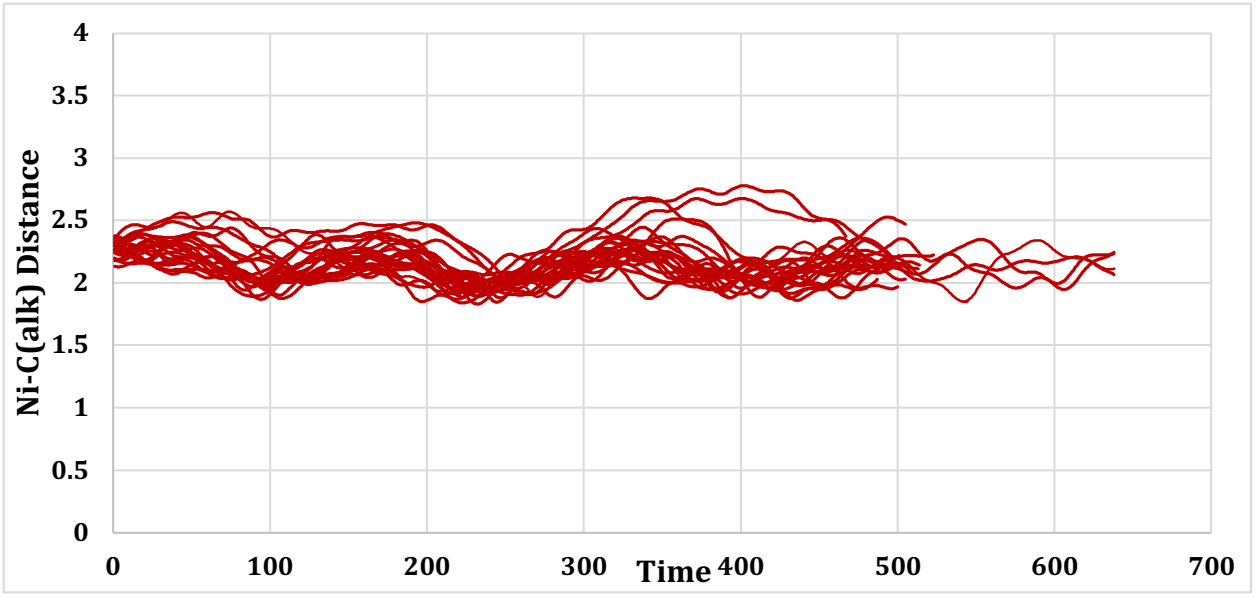


Figure S8. Time (fs) plot of trajectories versus Ni-C(alkyl radical) bond length (Å) of truncated system initiated at the reductive elimination transition state **^{2}I'-TS** in the reverse direction.

The red lines represent the results of more than 20 trajectories (ran for 500 to 700 fs) obtained, all of which show that the Ni-C(alk) bond length lies in the range of 1.8 to 2.8 Å. These results suggest that after initiated in the reverse direction at **^{2}I'-TS**, Ni(III) intermediate **^{2}H'** was formed and maintained until the end of trajectory, without the observation of *tert*-butyl radical dissociating from Ni center and generating corresponding Ni(II) intermediate (as shown in Figure S7). Overall, the results of quasi-classical dynamic calculation is consistent with the proposed pathway that the dissociation of *tert*-butyl radical from Ni(III) intermediate **^{2}H'** is uphill in energy. Also, the radical addition process of *tert*-butyl radical to Ni center occurs on *singlet spin tetrahedral* Ni species **^{1}G'** or *triplet spin tetrahedral* Ni species **^{3}G** rather than *singlet spin square planar* Ni species **^{1}G**, because the former Ni(II) species is either higher in energy level (**^{1}G'**) than Ni(III) intermediate **^{2}H'** while the latter Ni(II) is lower, and the dynamic simulations operate on single-spin state potential energy surface thus cannot reveal the performances of system when spin state is changed. The exploration in which intermediate does the alkyl radical add to is ongoing in our group.

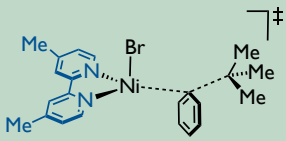
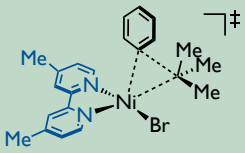
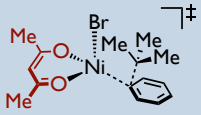
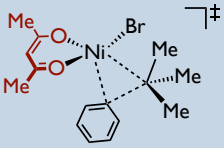
			$\Delta E_{activation}$ (kcal/mol)	$\Delta E_{distortion}$ (kcal/mol)	$\Delta E_{interaction}$ (kcal/mol)
Outer-Sphere		^{2}I-TS	15.0 (11.6) [18.3]	24.6 (24.8) [29.9]	-9.6 (-13.2) [-11.6]
		^{4}I-TS	13.6 (7.1) [19.8]	27.6 (25.4) [33.1]	-14.0 (-18.3) [-13.3]
Inner-Sphere		^{2}I'-TS	-3.5 (-11.2) [-3.4]	37.1 (35.7) [42.6]	-40.6 (-46.9) [-46.0]
Outer-Sphere		^{1}C-TS	-14.5 (-11.1) [-18.2]	16.0 (16.4) [18.3]	-30.5 (-27.6) [-36.5]
		^{3}C-TS	-17.4 (-19.2) [-17.1]	17.4 (18.0) [19.8]	-34.8 (-37.2) [-36.9]
Inner-Sphere		^{1}C'-TS	-12.3 (-17.7) [-16.6]	18.6 (19.2) [19.6]	-30.9 (-36.9) [-36.2]

Table S1. Activation Strain-Distortion/Interaction analysis of C(sp^2)-C(sp^3) bond formation step. Relative electronic energy values were computed with respect to separate corresponding phenyl-bromo-Ni-ligand species and *tert*-butyl radical at the UB3LYP-D3/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF), UB3LYP-D3/def2-SVP-CPCM(THF) (in parenthesis) and UM06/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF) (in bracket) levels of theory.

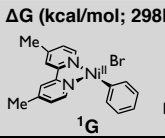
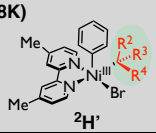
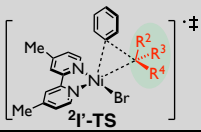
	ΔG (kcal/mol; 298K)  ^{1}G	 ^{2}H'	 ^{2}I'-TS	Ni-C(sp^3) Bond Dissociation Energy (ΔE; kcal/mol)	$\Delta E_{activation}$ (kcal/mol)	$\Delta E_{distortion}$ (kcal/mol)	$\Delta E_{interaction}$ (kcal/mol)
		5.6 (-2.3) [9.7]	15.0 (7.4) [15.1]	12.8 (20.7) [8.7]	-3.5 (-11.2) [-3.4]	37.1 (35.7) [42.6]	-40.6 (-46.9) [-46.0]
		-2.3 (-10.0) [3.3]	4.2 (-3.8) [6.0]	20.1 (27.8) [14.5]	-13.2 (-21.2) [-11.4]	33.6 (32.7) [53.4]	-46.8 (-53.9) [-64.8]
	0.0 (0.0) [0.0]	-3.4 (-10.0) [0.5]	2.7 (-4.6) [3.8]	21.5 (28.1) [17.6]	-14.6 (-22.0) [-13.6]	29.8 (28.1) [35.4]	-44.4 (-50.1) [-49.0]
		-3.3 (-11.6) [2.4]	7.3 (-0.2) [9.1]	19.2 (27.5) [13.5]	-8.7 (-16.2) [-6.8]	28.2 (27.3) [48.0]	-36.9 (-43.5) [-54.8]

Table S2. Grey: calculated energetics on inner-sphere reductive elimination step with different alkyl radicals; Green: related analysis on bond dissociation energy of Ni(III) intermediate; Yellow: activation strain-distortion/interaction analysis on reductive elimination transition state (relative electronic energy values was calculated with respect to separate corresponding Ni(II) species and *tert*-butyl radical). All relative energy values were computed with respect to Ni(II) species at the UB3LYP-D3/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF), UB3LYP-D3/def2-SVP-CPCM(THF) (in parenthesis) and UM06/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF) (in bracket) levels of theory.

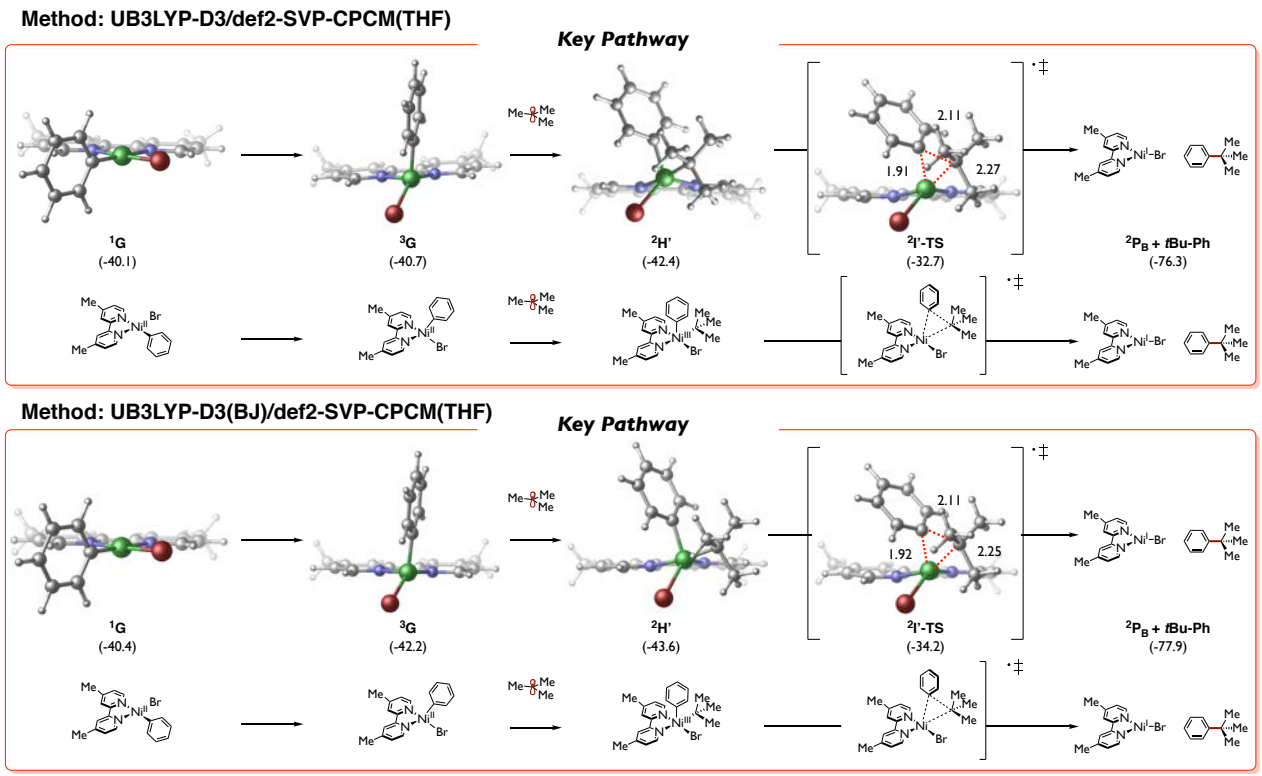


Figure S9. Comparison of key pathway in Ni-bipyridine system with original zero damping and Becke-Johnson damping of Grimme's dispersion correction. Relative Gibbs free energy values were computed at the UB3LYP-D3/def2-SVP-CPCM(THF) (in parenthesis) level of theory.

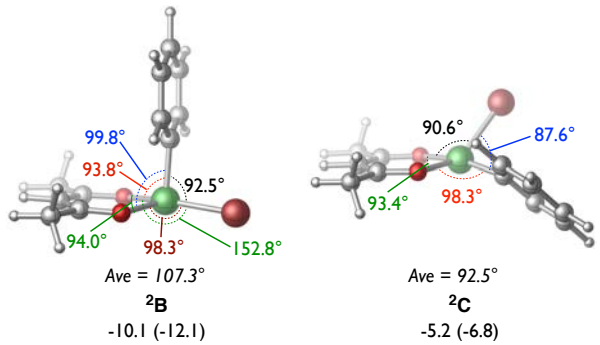


Figure S10. Structural parameters of **^{2}B** and **^{2}C**.

We have described "distorted tetrahedral" and "distorted square planar" as defined by the average angle deviations from a true tetrahedral geometry (109°) and square planar (90°).[12] As shown above, the average angle of the "distorted tetrahedral" structure **^{2}B** is 107.3° which is close to the angle of standard tetrahedral structure (109°). Also, the average angle of the "distorted square planar" structure **^{2}C** is 92.5° which is close to the angle of standard square planar structure (90°).

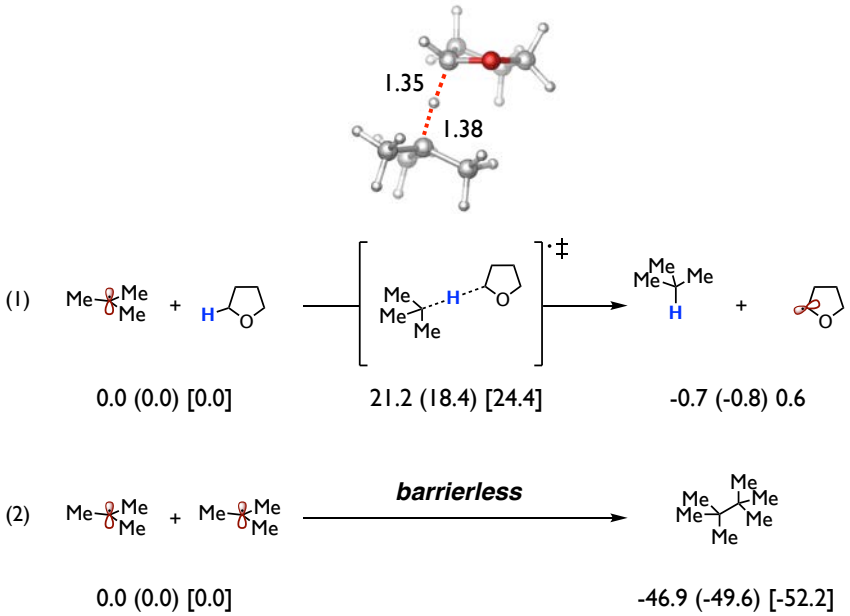


Figure S11. Calculated energetics of (1) HAT reaction between *tert*-butyl radical and THF, and (2) dimerization of two tert-butyl radicals. Relative Gibbs free energy values were computed at the UB3LYP-D3/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF), UB3LYP-D3/def2-SVP-CPCM(THF) (in parenthesis) and UM06/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF) (in bracket) levels of theory.

We computed the HAT pathways between the presumably formed *t*Bu radical and THF solvent (eq.1) and found that the HAT of *t*Bu• from THF is 0.7 kcal/mol downhill in energy with barrier of 21.1 kcal/mol. In comparison, the barrier of HAT of *t*Bu• from THF is only slightly higher than that of radical addition of *t*Bu• to Ni(II)(bpy) intermediate **^{1}G** (17.3 kcal/mol at **^{2}H-TS**), thus HAT pathway is feasible and stays competitive to the radical addition pathway. This could explain the observed experimental results[13] that both Ar-H (3-15% yield) and THF-Ar were observed in the stoichiometric studies using (bpy)Ni(Ar)(Br) complex and *t*Bu-BF_3K reagent. Moreover, we considered possible dimerization between two *tert*-butyl radicals (eq.2) and found that the dimerization process was barrierless based on relaxed potential energy surface scan on the newly formed C-C bond, resulting in the formation of 2,2-4,4-tetramethylbutane which is 46.9 kcal/mol downhill. This suggests that under higher concentration of *t*Bu radical, as expected, these radicals will likely lead to dimerization instead of undergoing radical addition to Ni(II) intermediate to generate Ni(III) intermediate, which is uphill in energy. Given the efficiency of the system, these calculations support low concentration of *t*Bu radical which lead to the desired cross-coupling product and only minor formation of side products such as HAT from solvent (due to higher barrier) or dimerization (due to low radical concentration).

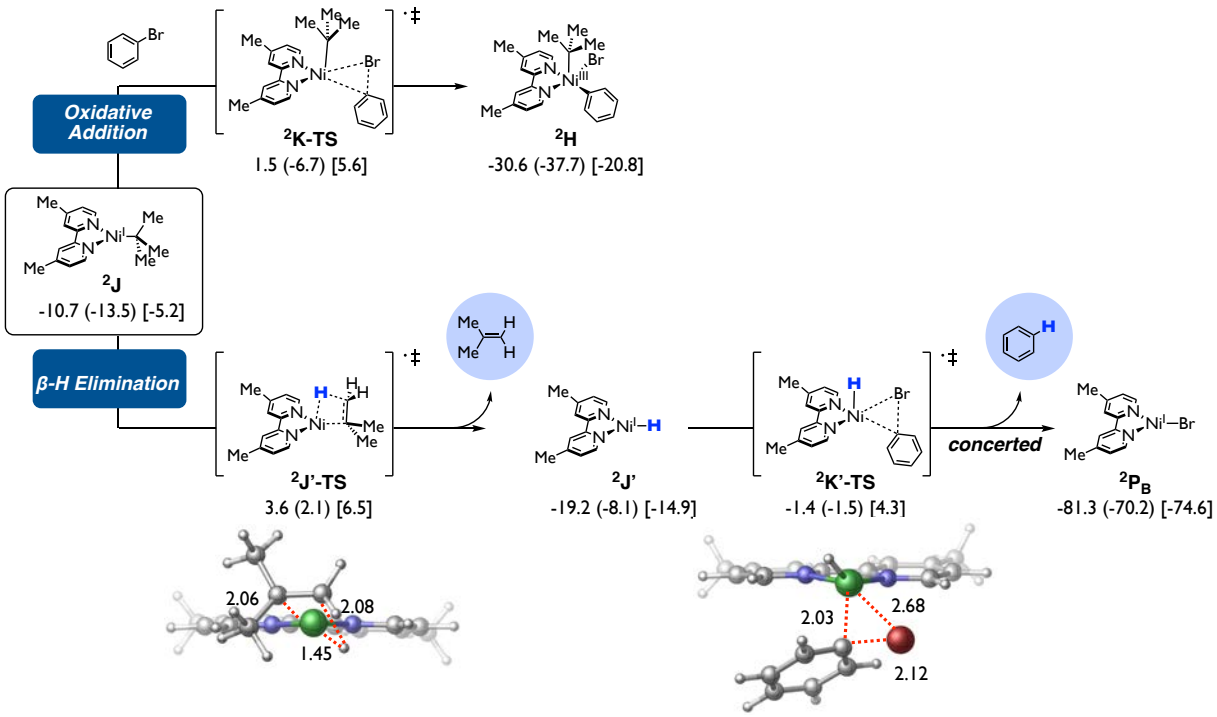


Figure S12. Calculated energetics of oxidative addition and β-H elimination pathways from Ni(I)-tBu intermediate **²J**. Relative Gibbs free energy values were computed at the UB3LYP-D3/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF), UB3LYP-D3/def2-SVP-CPCM(THF) (in parenthesis) and UM06/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF) (in bracket) levels of theory.

We also performed calculation on possible β-H elimination pathways (*vide infra*) from (bpy)Ni(*t*Bu) intermediate **²J**, and found that oxidative addition to PhBr (via **²K-TS**, with barrier of 12.2 kcal/mol with respect to **²J**) is comparable with the β-H elimination pathway (via **²J'-TS**, with barrier of 14.3 kcal/mol). Moreover, since the difference between barrier of oxidative addition pathway (12.2 kcal/mol) and that of β-H elimination pathway (14.3 kcal/mol) is only 2.1 kcal/mol, the β-H elimination pathway from (bpy)Ni(*t*Bu) intermediate **²J** is a possible side reaction pathway in this reaction system leading to the generation of metal hydride species (bpy)Ni(H) and isobutylene as side products. Unfortunately, isobutylene has a low boiling point (-7.9 ºC) and it is highly volatile thus challenging to assess experimentally. Nonetheless, the newly formed (bpy)Ni(H) species **²J'** can undergo oxidative addition with phenyl bromide (via **²K'-TS**), followed by concerted Ph-H bond formation (observed via intrinsic reaction coordinate at **²K'-TS**) to generate the experimentally observed side product *benzene* (Ph-H). Taken together, these computational and experimental results provide strong support for the formation of observed side products in experiment (i.e., THF-Ar adduct and Ar-H)[13] due to H atom transfer of *t*Bu radical from THF solvent followed by C-C bond formation and β-H elimination followed by Ar-H bond formation, respectively.

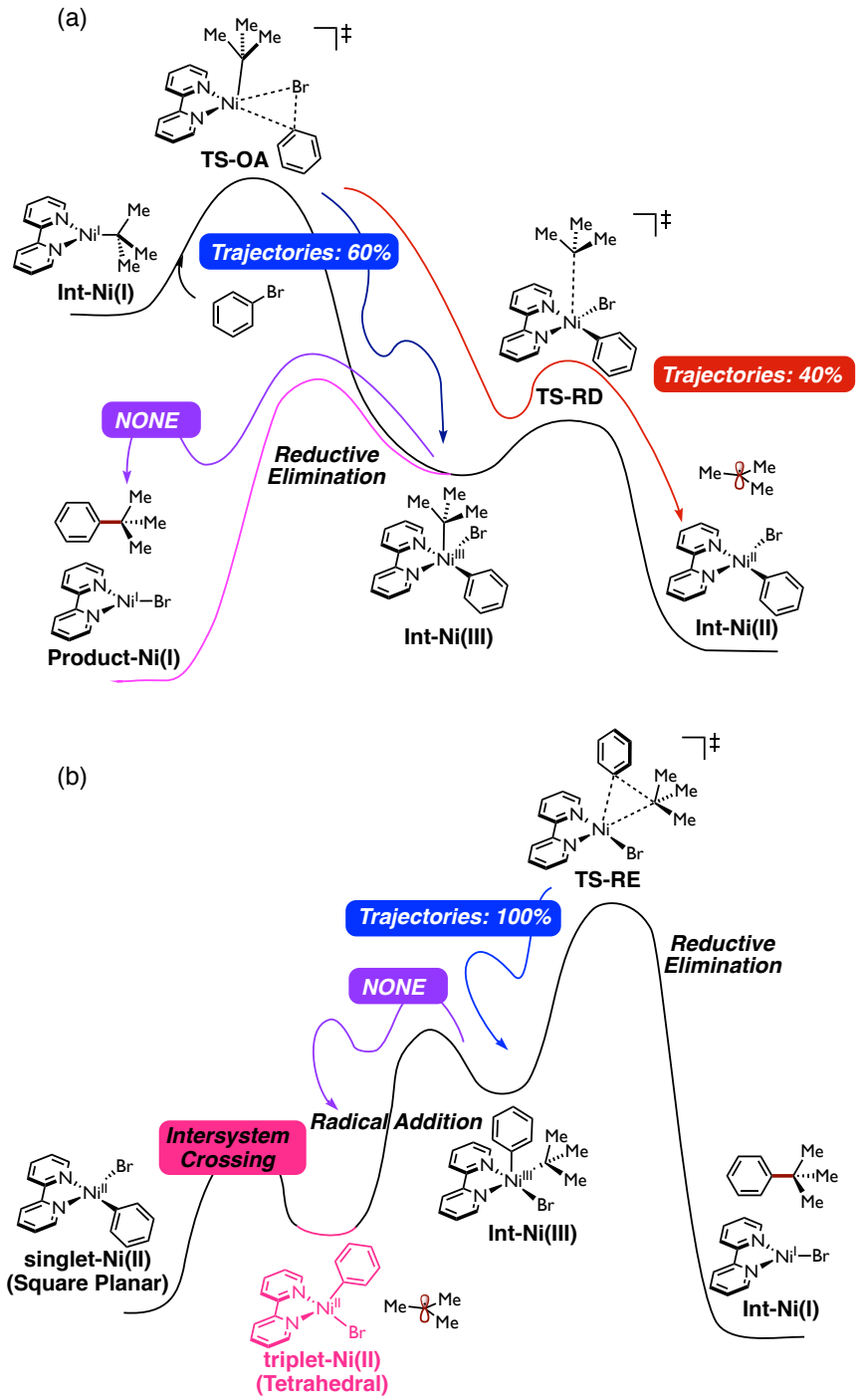


Figure S13. Preliminary results of quasi-classical dynamic simulations starting from (a) **^{2}K-TS** in forward direction and (b) **^{2}I'-TS** in reverse direction.

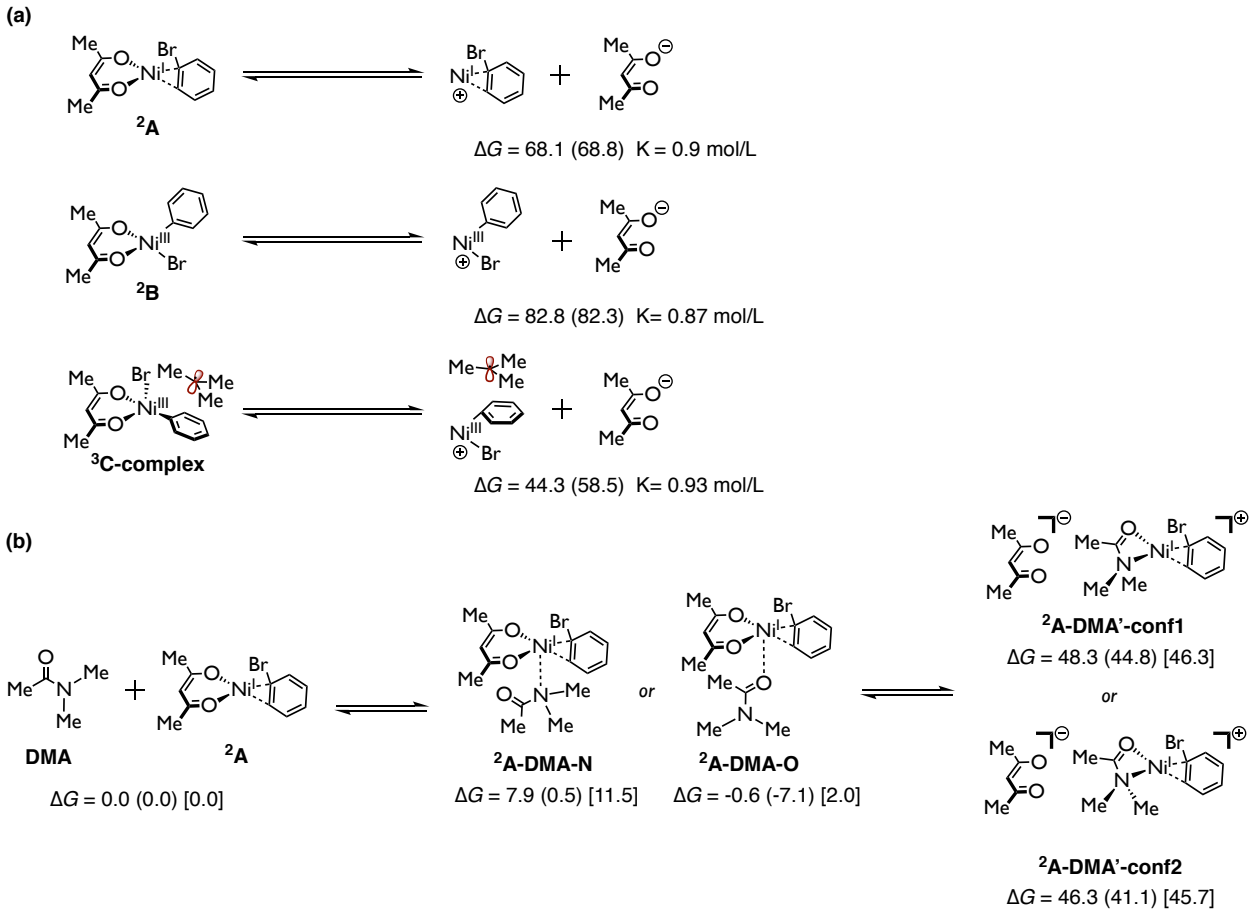


Figure S14. Calculated energetics of (a) ligand dissociation from key Ni(acac) species and (b) displacement and coordination of DMA solvent on key Ni(acac) species. Relative Gibbs free energy values were computed at the UB3LYP-D3/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF), UB3LYP-D3/def2-SVP-CPCM(THF) (in parenthesis) and UM06/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF) (in bracket) levels of theory.

To assess the likelihood of ligand dissociation, we have performed addition calculations to estimate the energy associated with ligand dissociation (shown above, Figure S14a), which showed there is an extremely energy uphill if the ligand dissociates from the Ni atom and the equilibrium constant for ligand dissociation is small. As a result, ligand dissociation pathways are unlikely. We also performed computations to gain insight at the propensity of DMA solvent to coordinate to the nickel active species and displace the acac (TMHD) ligand. As shown above (Figure S14b), the coordination of DMA to the nickel active species (prior to substrate activation) is energetically disfavored via N-mode coordination, but only weakly (dependent on the method) favorable via O-mode coordination. However, displacement of THMD ligand (here modeled as acac) is found highly unfavorable (> 40 kcal/mol). Based on these results, TMHD ligand is likely to stay coordinated to the Ni center during the whole catalytic process, and the coordination of DMA solvent to Ni center is possible via O-mode but it could not displace TMHD ligand of key Ni catalytic species.

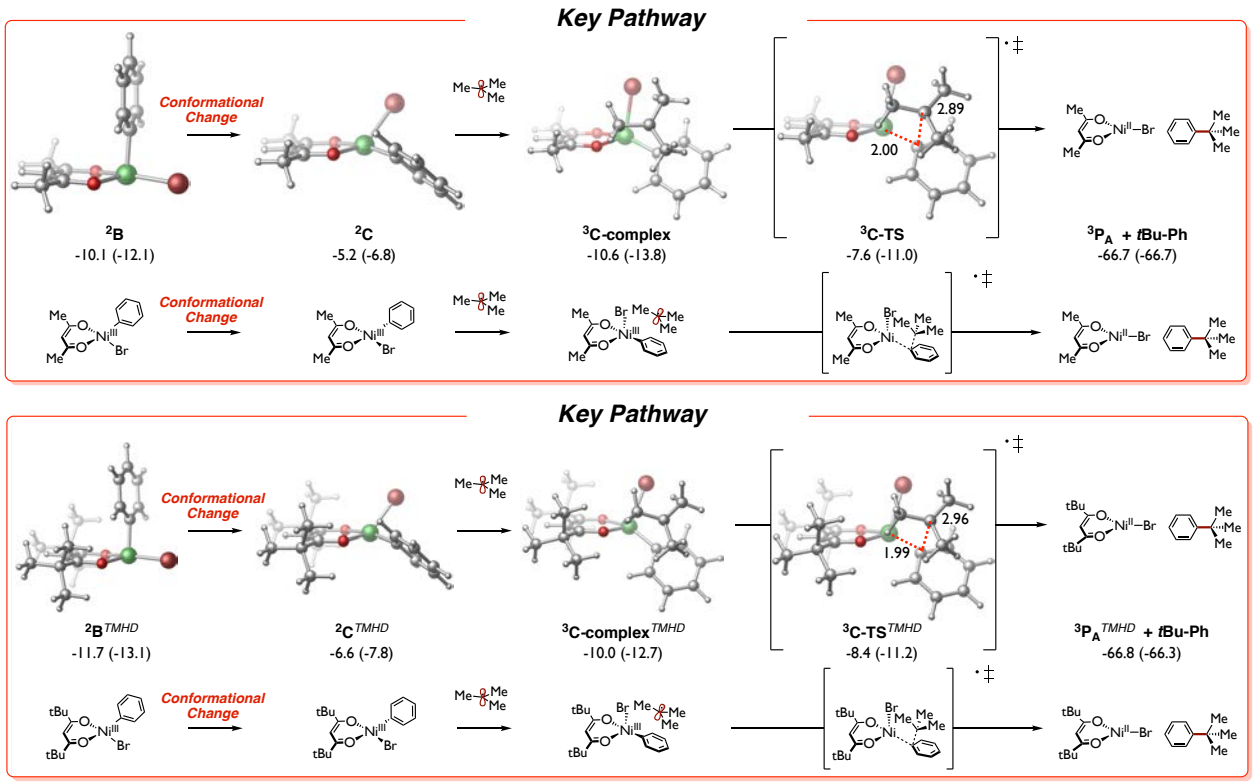


Figure S15. Comparison of energetics of the key pathways using truncated and full anionic TMHD as ligands. Relative Gibbs free energy values were computed at the UB3LYP-D3/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF) and UB3LYP-D3/def2-SVP-CPCM(THF) (in parenthesis) levels of theory.

We also computed the lowest energy pathway using the full TMHD ligand and found that the results of the full system are consistent with the pathway with truncated ligand (see below). Therefore, using acac ligand as computational model is a reasonable strategy.

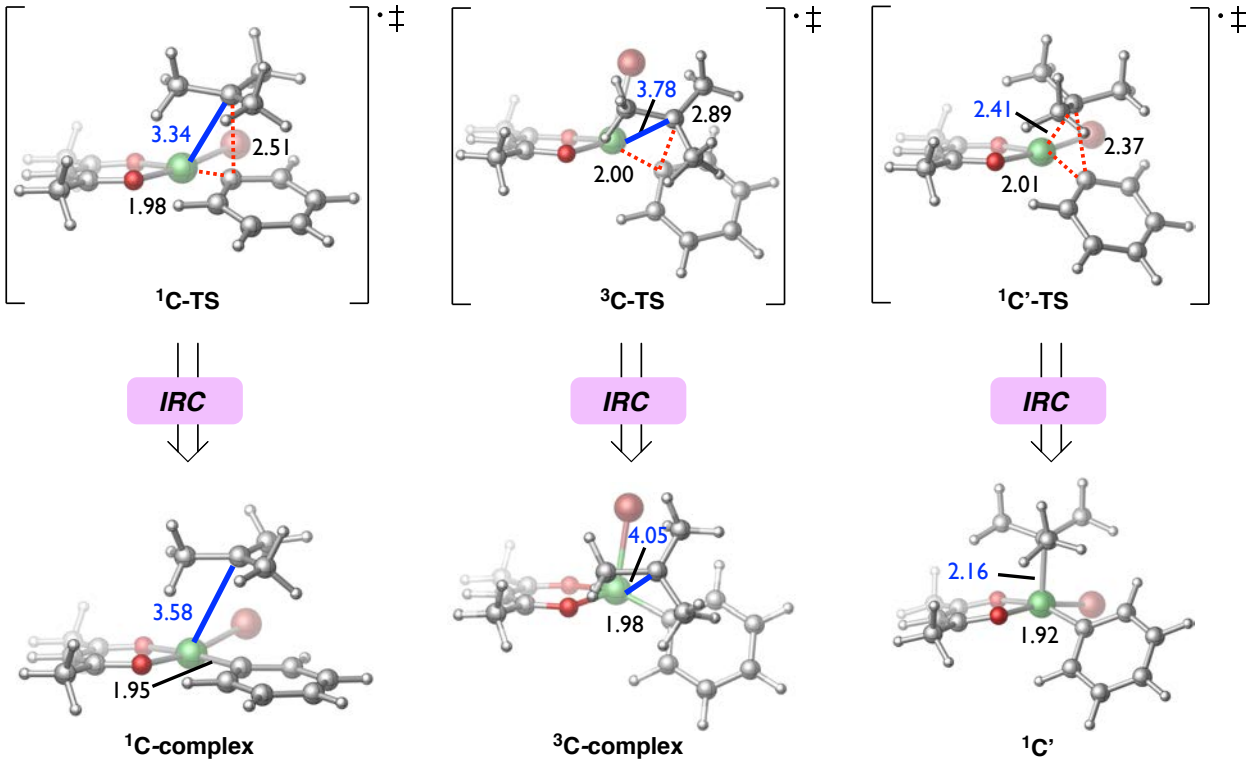


Figure S16. Comparison of three transition states of C-C formation in Ni(acac) system and their corresponding intermediates obtained from intrinsic reaction coordinate calculations (Unit: Å).

The distance between the *tert*-butyl and the Ni atom (in blue) in the *outer-sphere* transition states **¹C-TS** and **³C-TS** are relative long (3.34 and 3.78 Å, respectively). Thus, based on these distances, there is no Ni-*tert*-butyl interaction in the *outer sphere* transition states. However, for the *inner-sphere* TS **¹C'-TS**, the Ni-*t*Bu distance is much shorter, 2.41 Å, than that in the outer-sphere transition states. Moreover, the intrinsic reaction coordinate calculations of **¹C-TS**, **³C-TS** and **¹C'-TS** showed that the *outer-sphere* transition states **¹C-TS** and **³C-TS** lead to Ni•••*t*Bu radical complexes (**¹C-complex** and **³C-complex**) rather than Ni-alkyl intermediates (**¹C'**) as determined by examining the corresponding distances between Ni-*t*Bu and the hybridization of the optimized intermediates (from the IRCs), respectively.

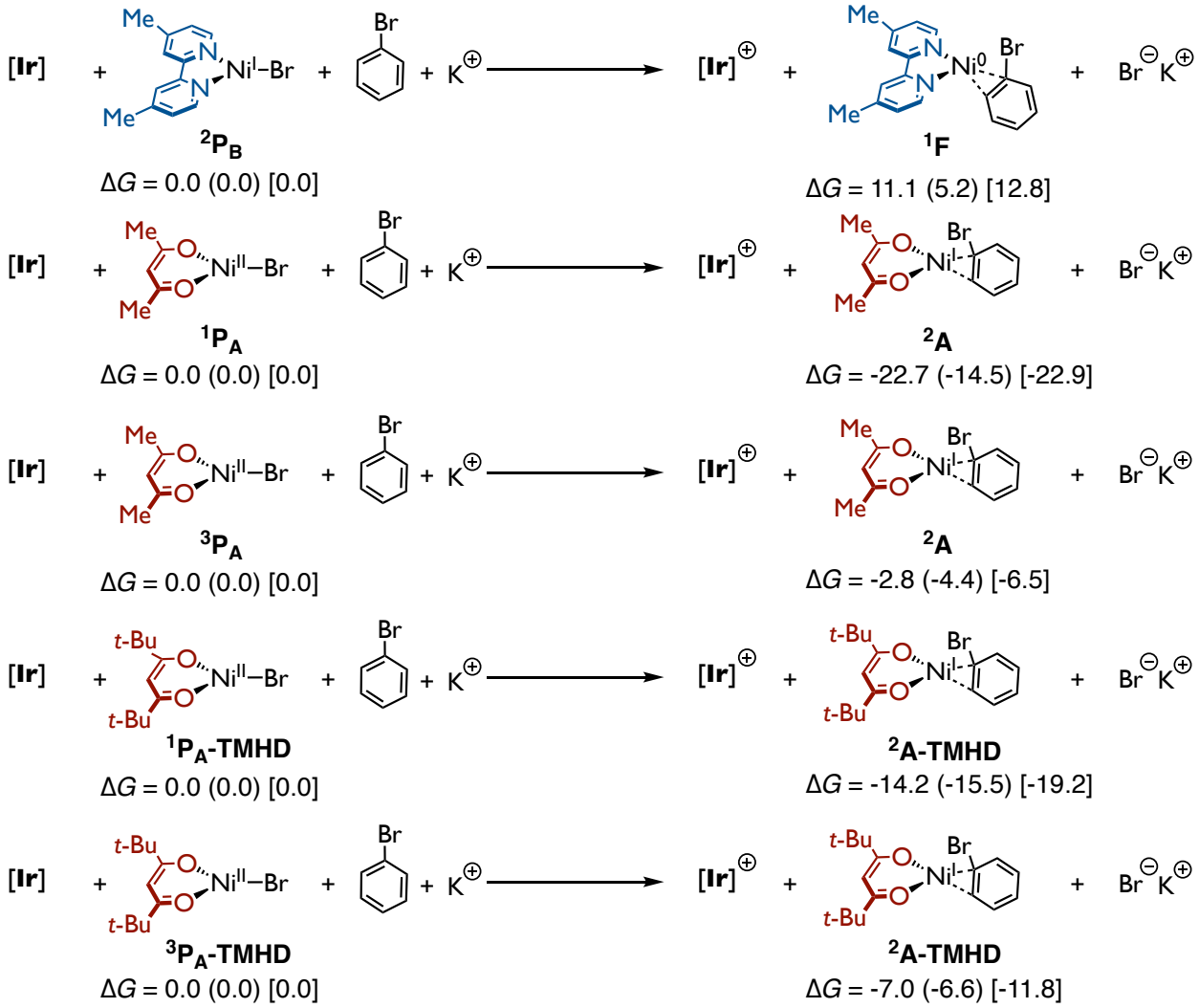


Figure S17. Calculation of single electron transfer steps between bromo Ni-ligand species and Ir photocatalyst to regenerate corresponding starting Ni species. Relative Gibbs free energy values were computed at the UB3LYP-D3/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF), UB3LYP-D3/def2-SVP-CPCM(THF) (in parenthesis) and UM06/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF) (in bracket) levels of theory.

Based on the calculated thermodynamic data of SET of bromo-Ni-ligand species with reduced Ir(II) photocatalyst , the single electron transfer steps should be not problematic. Specifically, for the Ni(bpy) system, while this process is slightly uphill in energy, based on free energy span model[14] the reaction can still progress with turnover of catalytic cycle since the following steps from Ni(0) **^{1}F** have great thermodynamic drive with low barrier. As for Ni(acac) system, the SET steps between (acac)Ni-Br and photocatalyst are downhill in energy for both singlet and triplet spin states of (acac)Ni-Br, thus should be energetically feasible. Calculated results of full Ni-TMHD system are similar with those of the truncated Ni-acac system, both of which are downhill in energy. Therefore, in the absence of any direct experimental evidence (reduction potentials) for any of these mono-ligand bromo Ni

species to the best of our knowledge, computations predict that this step should not be problematic for both (acac)Ni(II)-Br and (bpy)Ni(I)-Br to retrieve (acac)Ni(I) complex **^{2}A** and (bpy)Ni(0) complex **^{1}F**, respectively.

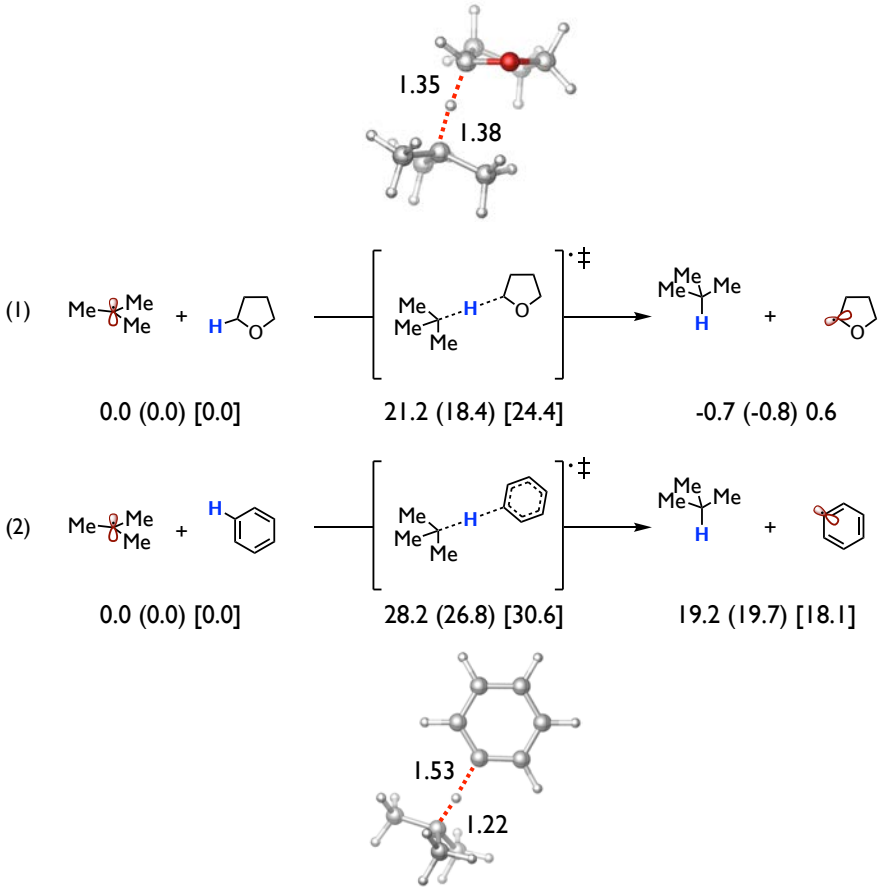


Figure S18. Calculated energetics of (1) HAT reaction between *tert*-butyl radical and THF, and (2) benzene. Relative Gibbs free energy values were computed at the UB3LYP-D3/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF), UB3LYP-D3/def2-SVP-CPCM(THF) (in parenthesis) and UM06/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF) (in bracket) levels of theory.

Calculations of HAT reactions between *tert*-butyl radical and different solvent molecules (i.e., THF and benzene) here were intended to show that the mechanism of this type of reaction might differ depending on the nature of solvent, electrophile, nucleophile even though the same *tert*-butyl radical was presumed to exist in the Ni-bipyridine system reported by Fu.[15]

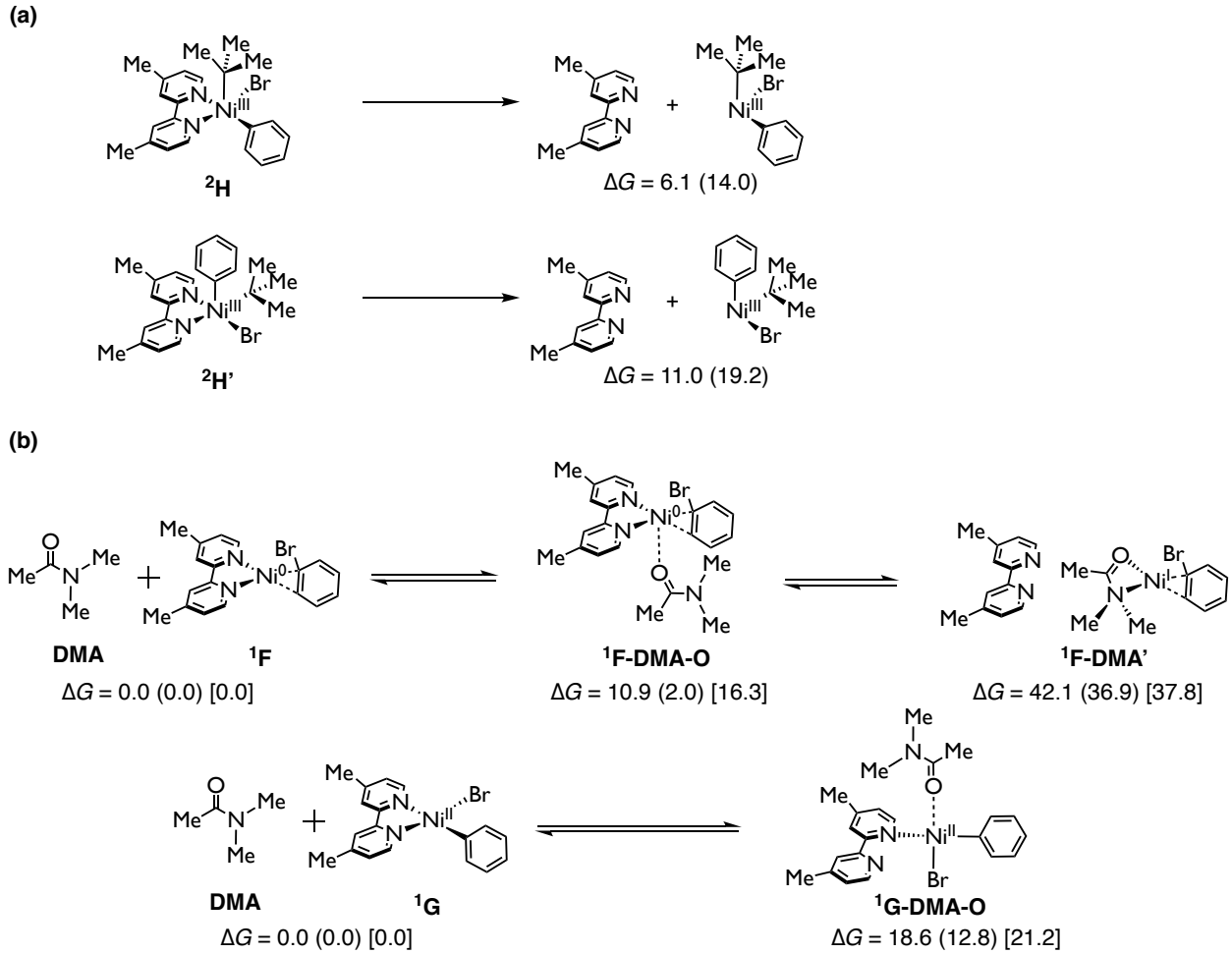


Figure S19. Energetics of (a) complete ligand dissociation from key Ni(III) intermediates **²H** and **²H'**, and (b) coordination and displacement with DMA solvent. Relative Gibbs free energy values were computed at the UB3LYP-D3/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF), UB3LYP-D3/def2-SVP-CPCM(THF) (in parenthesis) and UM06/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF) (in bracket) levels of theory.

These results show that complete ligand dissociation from Ni(III) intermediates is unlikely to occur since it's uphill in energy level from **²H** and **²H'** by 6.1 and 11.0 kcal/mol, respectively. Moreover, we explored the tendency of displacement or coordination with DMA solvent for the byp-nickel system, and found that DMA coordination to Ni(0) or Ni(II) is found energetically unfavorable (**¹F-DMA-O** and **¹G-DMA-O**) and, like the TMHD ligand, highly unfavorable to cause the dissociation of bipyridine ligand (**¹F-DMA'**).

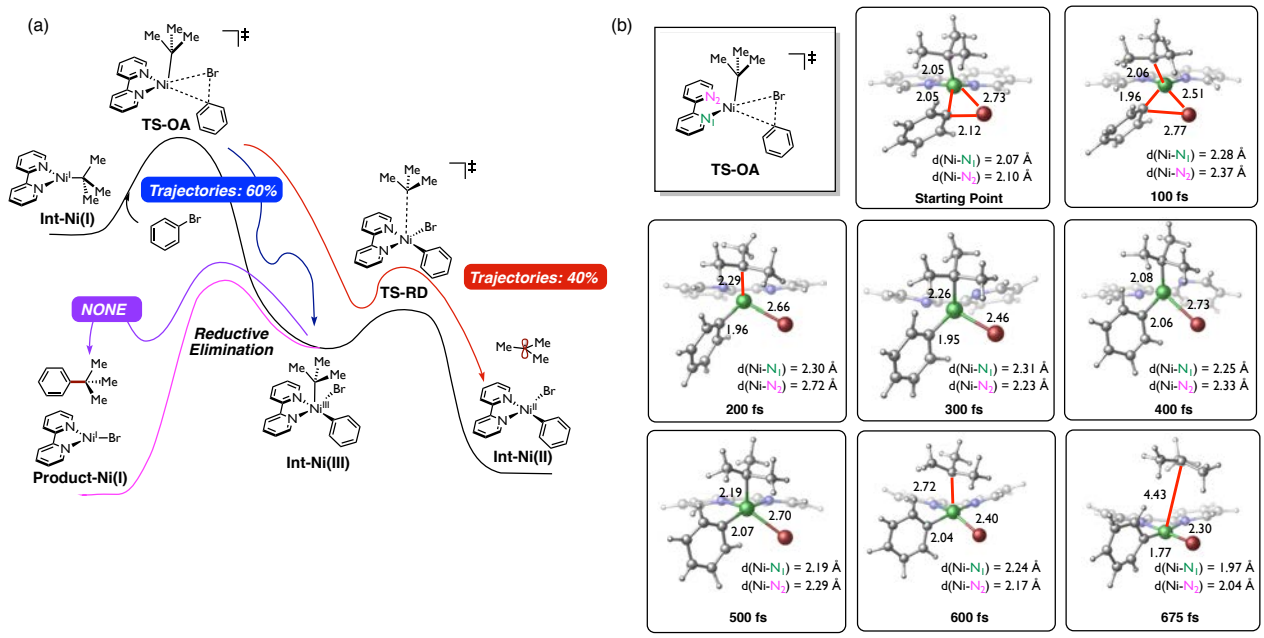


Figure S20. (a) Preliminary results of quasi-classical dynamic simulations starting from **^{2}K-TS** in forward direction and (b) snapshots of one example trajectory undergoing radical dissociation.

To explore the likelihood of transient ligand dissociation during the reaction, we also performed quasi-classical dynamic calculations which allow us to "see" if ligand dissociation occurs, and if so, at what time step (Figure S20). Dynamic calculations starting from TS-Oxidative Addition from Ni(I) showed that complete ligand dissociation is unlikely to happen within the lifetime of Ni(III) intermediate. In addition, although transient decoordination of one of the pyridine ligands was observed during some simulated trajectories (see Figure S20(b) for an example trajectory), *the Ni(III) intermediate doesn't undergo any structural rearrangement*. Rather, Ni(III) intermediate either stayed the same conformation until the end of simulation (60% of trajectories) or underwent radical dissociation of *t*Bu radical from axial position of Ni center (40% of trajectories).

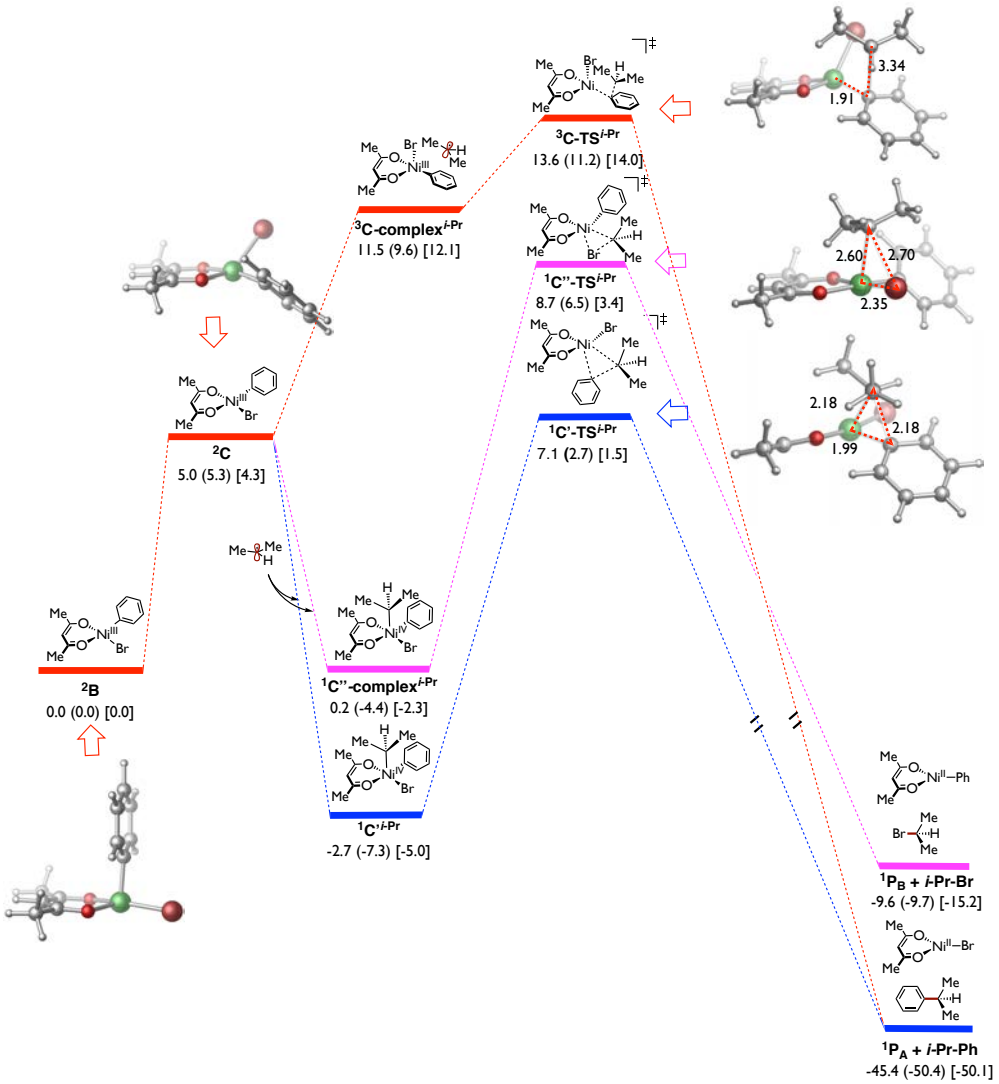


Figure S21. Calculated energetics of the Ni-catalyzed cross-coupling between *iso*-propyl radical and phenyl bromide using anionic acac as ligand. Free energies (kcal/mol) were computed at the UB3LYP-D3/def2-TZVPP-CPCM(DMA)//UB3LYP-D3/def2-SVP-CPCM(THF), UB3LYP-D3/def2-SVP-CPCM(THF) (in parenthesis) and UM06/def2-TZVPP-CPCM(DMA)//UB3LYP-D3/def2-SVP-CPCM(THF) (in bracket) levels of theory.

We performed computations to investigate the effect of secondary radical in the reaction pathway and found that the favored pathway is via inner-sphere C-C bond formation with overall barriers for C-C bond formation of ~9 kcal/mol. Thus, the cross-coupling of secondary alkyl radical is also applicable in Ni-TMHD system, which is shown in the experiment results (see part D, Page S31). Presumably, the less sterically hindered secondary alkyl radical (in contrast to the tertiary alkyl radical) does not pay a penalty to form the LNi-alkyl-Ar-Br species and can quickly undergo inner sphere C-C bond formation. Thus, from these results, we hypothesize that for acac/TMHD-Ni systems, sterics more than electronics influence the nature of the C-C bond formation and whether inner- or outer-sphere $C(sp^2)$-$C(sp^3)$ is operative.

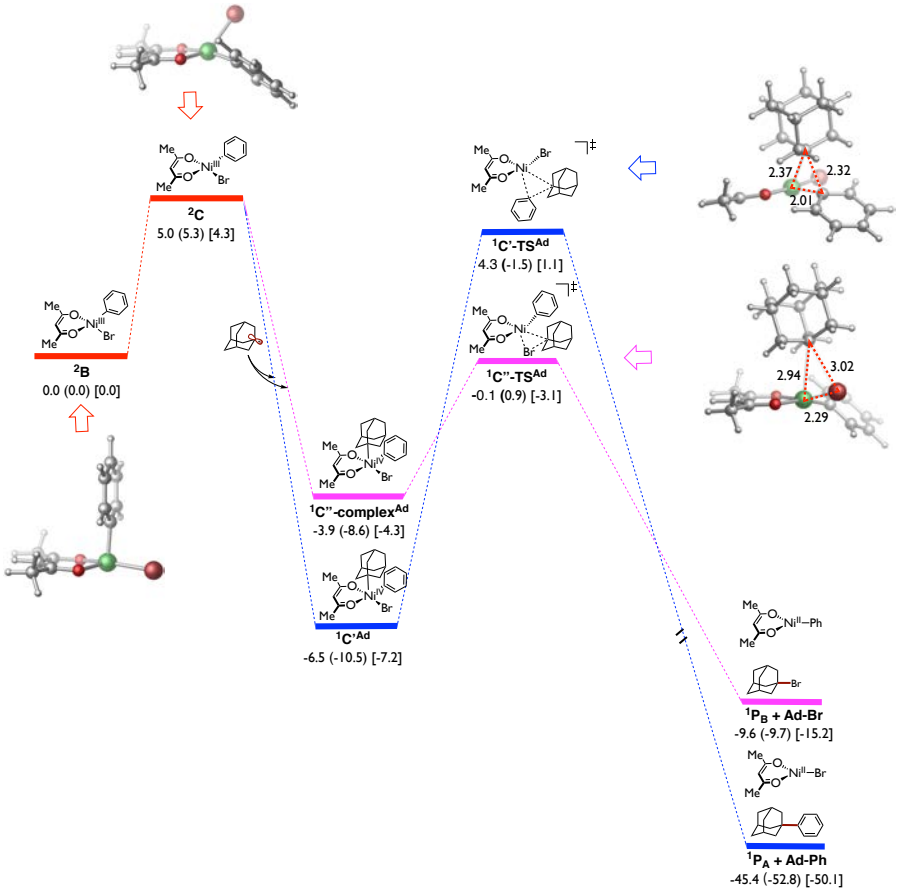


Figure S22. Calculated energetics of the Ni-catalyzed cross-coupling between adamantyl radical and phenyl bromide using anionic acac as ligand. Free energies (kcal/mol) were computed at the UB3LYP-D3/def2-TZVPP-CPCM(DMA)//UB3LYP-D3/def2-SVP-CPCM(THF), UB3LYP-D3/def2-SVP-CPCM(THF) (in parenthesis) and UM06/def2-TZVPP-CPCM(DMA)//UB3LYP-D3/def2-SVP-CPCM(THF) (in bracket) levels of theory.

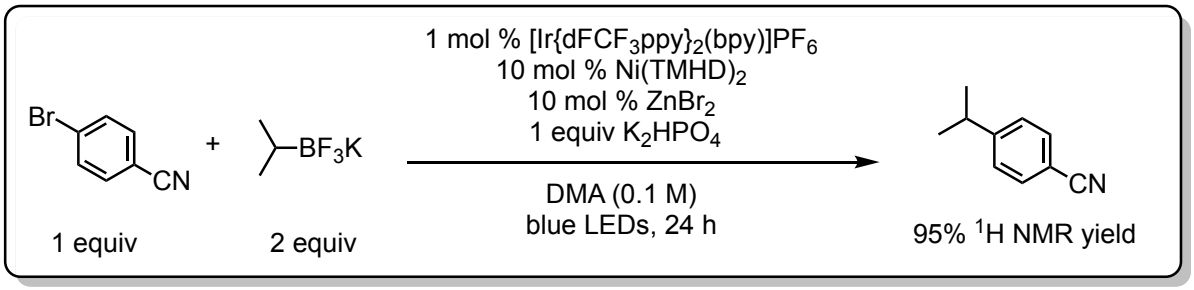
We performed computations to investigate the effect of cyclic tertiary radical in the reaction pathway, showing that, if the cyclic radical were to engage with the nickel in the cross-coupling cycle, formation of 1-bromoadamantane via inner-sphere C-Br bond formation is favored over C-C bond formation. However, since this step is reversible with only 5.7 kcal/mol in thermodynamic drive with low barrier of 3.8 kcal/mol, the acac-Ni species is likely to also undergo other pathways in this system. Presumably, the sterically hindered cyclic adamantyl radical (compared with the acyclic tertiary radical and acyclic secondary radical) needs to pay a penalty to undergo inner-sphere C-C bond formation to form the desired product 1-phenyladamantane. As a result, we assume that sterics plays an important role in the C-C bond formation step and have a significant effect on the final product. Compared with the experimental results (see part D, Page S33) where no cross-coupling product was observed and aryl bromide was recovered, our calculations suggest that *if the aryl halide substrate were activated*, the reactions of adamantyl radical should be feasible to form many possible products, including 1-bromoadamantane and phenyladamantane. While regarding the failure of activating aryl bromide substrate in this system, more exploration of its properties in the Ni-TMHD system is ongoing in our group.

D. Experimental Details

General: All chemical transformations were carried out under an inert atmosphere of argon unless otherwise noted. Standard Schlenk line techniques with a 4- or 5-port dual-bank manifold were used for the manipulation of solvents and reagents. LED irradiation was accomplished as described in our previous reports.[16] Reactions were monitored by GC/MS and ^{1}H NMR.

Chemicals: DMA was purchased as 99.9%, extra dry. K_2HPO_4 and Na_2CO_3 were stored and dispensed in a dry glovebox. Deuterated NMR solvents were purchased and stored over 4Å molecular sieves. $IrCl_3 \cdot xH_2O$, and $Ni(TMHD)_2$ were purchased from commercial sources. The iridium photocatalyst $Ir[dFCF_3ppy]_2(bpy)]PF_6$ was prepared in-house by the procedure outlined in our previous publication.[17] Organotrifluoroborates were used as purchased without further purification.

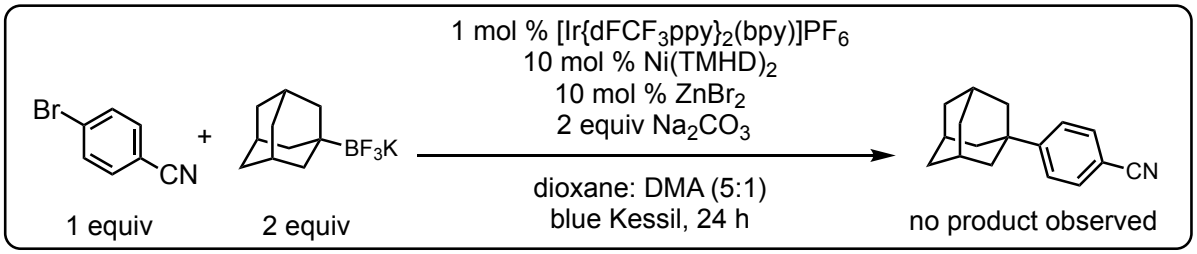
General Procedure I: Cross-Coupling of Secondary Trifluoroborates[18]



To an 8 mL reaction vial equipped with a Teflon-coated magnetic stir bar were added $Ir[dFCF_3ppy]_2(bpy)]PF_6$ (3.0 mg, 0.003 mmol, 1 mol %), isopropyltrifluoroborate (90 mg, 0.6 mmol, 2.0 equiv), and 4-bromobenzonitrile (55 mg, 0.3 mmol, 1.0 equiv). The vial was then transferred into a glove box where $Ni(TMHD)_2$ (12.8 mg, 0.03 mmol, 10 mol %), $ZnBr_2$ (6.8 mg, 0.03 mmol, 10 mol %), and anhydrous K_2HPO_4 (52 mg, 0.3 mmol, 1.0 equiv) were added. The vial was then capped and removed from the glovebox. Anhydrous DMA (3 mL) was added to the vial via syringe under inert atmosphere. The vial was subsequently sparged with argon for 10 min. The vial was sealed with parafilm and stirred for 24 h approximately 1 cm away from a ring of blue LED lights strips (see below). A fan was used to maintain the reaction at temperature. After completion, the crude reaction mixture was diluted with ether, and ^{1}H NMR yield was determined using 1,3,5-trimethoxybenzene as internal standard (95% yield).

Figure S23. Reaction set-up using blue LEDs.

General Procedure II: Cross-Coupling of Adamantyltrifluoroborate[16a]



To an 8 mL reaction vial equipped with a Teflon-coated magnetic stir bar were added $Ir[dFCF_3ppy]_2(bpy)]PF_6$ (3.0 mg, 0.003 mmol, 1 mol %), adamantyltrifluoroborate (145 mg, 0.6 mmol, 2.0 equiv), and 4-bromobenzonitrile (55 mg, 0.3 mmol, 1.0 equiv). The vial was then transferred into a glove box where $Ni(TMHD)_2$ (12.8 mg, 0.03 mmol, 10 mol %), $ZnBr_2$ (6.8 mg, 0.03 mmol, 10 mol %), and anhydrous Na_2CO_3 (64 mg, 0.6 mmol, 2.0 equiv) were added. A mixture of anhydrous DMA and dioxane (5:1, 3 mL) was then added to the vial via syringe under inert atmosphere. The vial was then capped, removed from the glovebox, and sealed with parafilm. The reaction was stirred for 24 h using blue Kessil lamps (see below). A fan was used to maintain the reaction around 40 °C. After completion, the crude reaction mixture was diluted with ether, and ^1H NMR yield was determined using 1,3,5-trimethoxybenzene as internal standard (no product observed, recovery of aryl bromide was detected).

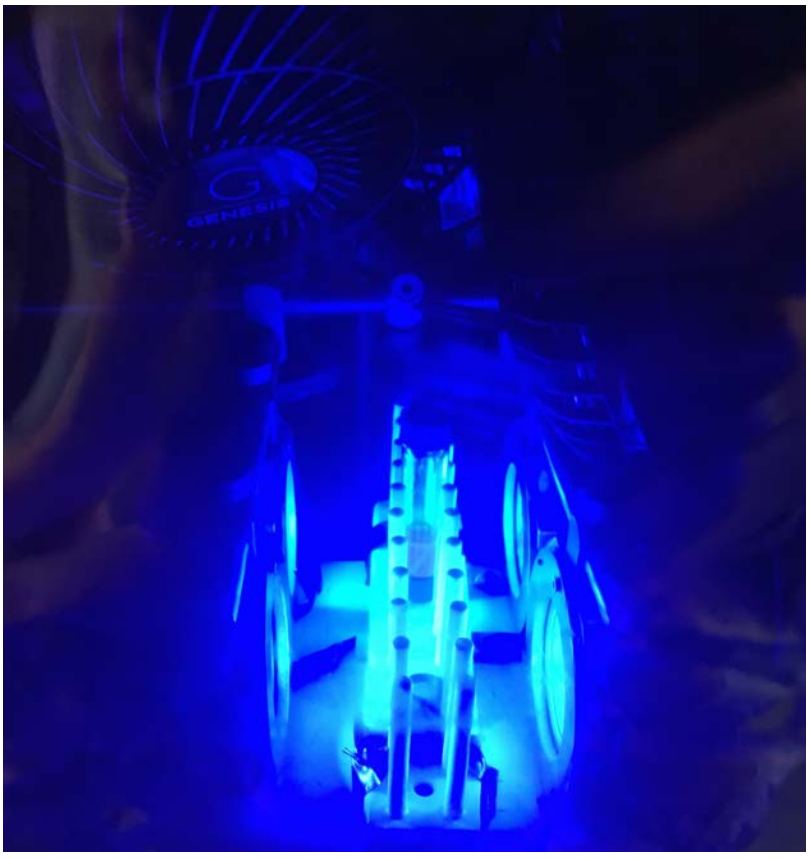
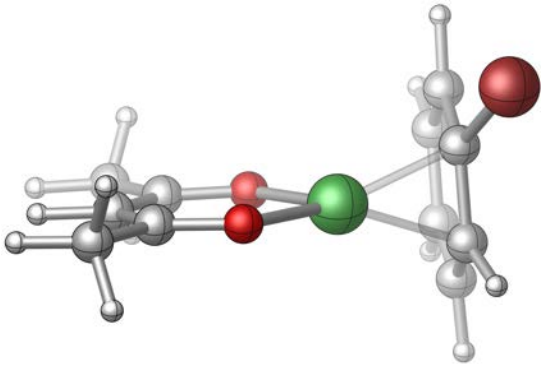


Figure S24. Reaction set-up using blue Kessil lamps.

E. Coordinates and Energies of Optimized Structures in Computation

Figure S1

^{2}A



UB3LYP-D3/def2-SVP-CPCM(THF)
Zero-point correction= 0.202379 (Hartree/Particle)
Thermal correction to Energy= 0.219143
Thermal correction to Enthalpy= 0.220087
Thermal correction to Gibbs Free Energy= 0.154245
Sum of electronic and zero-point Energies= -4658.354829
Sum of electronic and thermal Energies= -4658.338065
Sum of electronic and thermal Enthalpies= -4658.337121
Sum of electronic and thermal Free Energies= -4658.402963

C	-2.53178800	-0.43393100	1.44289900
C	-2.49128200	-0.70770400	0.04310200
C	-2.82017300	0.30666700	-0.89855000
C	-3.12620200	1.57753200	-0.44707400
C	-3.16201600	1.86786400	0.93761200
C	-2.88072000	0.87951200	1.86361900
Br	-2.54192800	-2.55709300	-0.56147600
H	-2.81567400	0.07267600	-1.96415900
H	-2.52967100	-1.25152100	2.17009600
H	-2.94103100	1.08783300	2.93438200
H	-3.42275400	2.87405900	1.27307400
H	-3.35065300	2.36310200	-1.17251700
Ni	-0.56734700	-0.47208200	0.70356300
O	1.21828000	-1.16628900	0.90826800
O	0.02037900	1.33193300	0.22988800
C	1.23370500	1.69364400	0.14842900
C	2.29158200	-0.49781500	0.74328500
C	3.57343000	-1.27103100	0.96263700
H	3.59819100	-2.13082300	0.27315600
H	4.47667500	-0.66388700	0.81587100
H	3.57522100	-1.68356600	1.98485100
C	1.45377000	3.14181900	-0.23613100
H	0.94702500	3.78917700	0.49802400
H	2.51434800	3.42083000	-0.29455600

H	0.97410500	3.33085400	-1.21040400
C	2.35582500	0.86357500	0.38303500
H	3.34439500	1.31082700	0.27594500

$\Delta G_{solvation}^{UM06}$= -0.01015289

UB3LYP-D3/def2-TZVPP-CPCM(DMA)// UB3LYP-D3/def2-SVP-CPCM(THF)

HF= -4659.7324910

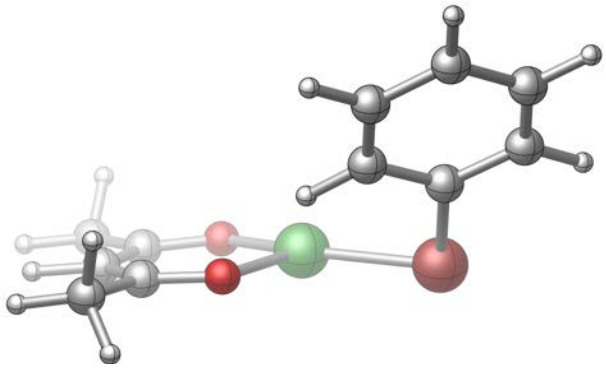
UM06/def2-TZVPP-CPCM(DMA)// UB3LYP-D3/def2-SVP-CPCM(THF)

HF= -4659.08046134

DLPNO-CCSD(T)/def2-TZVPP-gas// UB3LYP-D3/def2-SVP-CPCM(THF)

HF= -4656.139208237236

^{2}A'

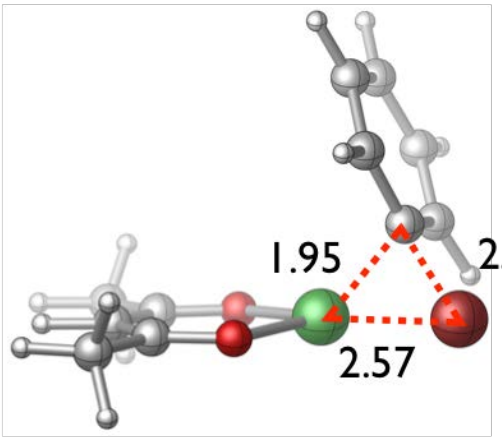


UB3LYP-D3/def2-SVP-CPCM(THF)
Zero-point correction= 0.202973 (Hartree/Particle)
Thermal correction to Energy= 0.219947
Thermal correction to Enthalpy= 0.220891
Thermal correction to Gibbs Free Energy= 0.153592
Sum of electronic and zero-point Energies= -4658.339107
Sum of electronic and thermal Energies= -4658.322134
Sum of electronic and thermal Enthalpies= -4658.321189
Sum of electronic and thermal Free Energies= -4658.388488

C	-2.39558900	-1.29660400	1.46528600
O	-3.01344300	-0.46132500	2.20271700
C	-2.62407300	-1.50135300	0.08499500
H	-2.00279700	-2.24497400	-0.41559300
C	-3.57722900	-0.82185700	-0.70626700
O	-4.39832100	0.05707200	-0.28385800
C	-3.65895500	-1.12503700	-2.18735400
H	-3.36882900	-0.22458200	-2.75493600
H	-3.01600500	-1.96028300	-2.49641100
H	-4.70403500	-1.34785900	-2.45572700
C	-1.33179000	-2.11378000	2.16762300
H	-1.79735200	-2.68589100	2.98713700
H	-0.80630300	-2.80818600	1.49836800
H	-0.59918600	-1.43325400	2.63169000
Ni	-4.40417900	0.65782000	1.56899600
C	-5.84502100	3.55560900	0.40545300
C	-5.11523300	3.21248800	-0.73216100
C	-6.31983600	4.84551300	0.63839800
C	-4.85440300	4.21613700	-1.67210700
H	-4.76971000	2.18660000	-0.87699500
C	-6.04643900	5.83341500	-0.31547300
H	-6.88723200	5.08057900	1.54072600
C	-5.31538900	5.52154900	-1.46676400
H	-4.28514800	3.96951900	-2.57183700
H	-6.40818700	6.85128500	-0.15063500
H	-5.10506800	6.29799200	-2.20597100

Br -6.22832200 2.16943000 1.71547300
$\Delta G_{solvation}^{UM06}$= -0.01025185
UB3LYP-D3/def2-TZVPP-CPCM(DMA)// UB3LYP-D3/def2-SVP-CPCM(THF)
HF= -4659.7317488
UM06/def2-TZVPP-CPCM(DMA)// UB3LYP-D3/def2-SVP-CPCM(THF)
HF= -4659.07809925
DLPNO-CCSD(T)/def2-TZVPP-gas// UB3LYP-D3/def2-SVP-CPCM(THF)
HF= -4656.147502274090

^{2}A-TS



UB3LYP-D3/def2-SVP-CPCM(THF)
Zero-point correction= 0.201937 (Hartree/Particle)
Thermal correction to Energy= 0.218204
Thermal correction to Enthalpy= 0.219148
Thermal correction to Gibbs Free Energy= 0.154635
Sum of electronic and zero-point Energies= -4658.347249
Sum of electronic and thermal Energies= -4658.330981
Sum of electronic and thermal Enthalpies= -4658.330037
Sum of electronic and thermal Free Energies= -4658.394550

C	-2.97553100	0.34941000	1.52032600
C	-2.28096300	-0.59136300	0.72958800
C	-2.22260500	-0.47104200	-0.67640700
C	-2.76148000	0.66671600	-1.26751200
C	-3.39786600	1.65092700	-0.48816400
C	-3.50377600	1.48785900	0.89375700
Br	-1.98440100	-2.44446100	1.57505900
H	-1.71192700	-1.23486700	-1.26342300
H	-3.09258000	0.19415400	2.59402000
H	-4.01492600	2.23971400	1.50025600
H	-3.82107400	2.53564400	-0.96881000
H	-2.68434600	0.79329200	-2.35040300
Ni	-0.52357700	-0.33275800	1.52376600
O	1.01536800	-1.09755800	0.59651700
O	0.21836200	1.44706400	1.68152500
C	1.32888400	1.80411800	1.16900400
C	2.01888200	-0.41530700	0.21813600
C	3.08153200	-1.19043800	-0.53120500
H	2.61808300	-1.68999300	-1.39733500
H	3.91530000	-0.56422100	-0.87564500
H	3.47357700	-1.98682000	0.12262600
C	1.69846700	3.25582900	1.38174300
H	1.77581900	3.45268200	2.46373500
H	2.64190000	3.53881800	0.89617300

H	0.88502700	3.89360000	0.99959700
C	2.20761400	0.96722700	0.44827700
H	3.12192600	1.41793300	0.06166900

$\Delta G_{solvation}^{UM06}$= -0.01048663

UB3LYP-D3/def2-TZVPP-CPCM(DMA)// UB3LYP-D3/def2-SVP-CPCM(THF)

HF= -4659.7254964

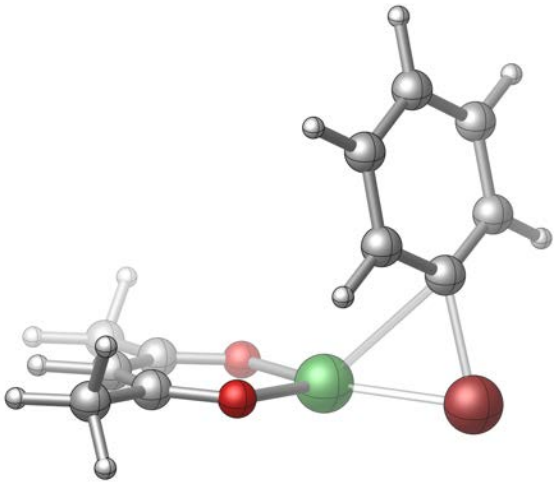
UM06/def2-TZVPP-CPCM(DMA)// UB3LYP-D3/def2-SVP-CPCM(THF)

HF= -4659.07173765

DLPNO-CCSD(T)/def2-TZVPP-gas// UB3LYP-D3/def2-SVP-CPCM(THF)

HF= -4656.13047753174

^{2}A'-TS



UB3LYP-D3/def2-SVP-CPCM(THF)
Zero-point correction= 0.202302 (Hartree/Particle)
Thermal correction to Energy= 0.218638
Thermal correction to Enthalpy= 0.219582
Thermal correction to Gibbs Free Energy= 0.154463
Sum of electronic and zero-point Energies= -4658.336430
Sum of electronic and thermal Energies= -4658.320094
Sum of electronic and thermal Enthalpies= -4658.319150
Sum of electronic and thermal Free Energies= -4658.384269

C	-2.66543400	-0.54021800	1.31203400
O	-3.54977000	0.16165100	1.90193600
C	-2.75745500	-1.04436600	-0.00579100
H	-1.90838400	-1.62150400	-0.37388500
C	-3.85190100	-0.88199200	-0.88726100
O	-4.92957500	-0.25548300	-0.62718400
C	-3.77392900	-1.48775300	-2.27347800
H	-3.80891100	-0.67890700	-3.02257300
H	-2.86623300	-2.08441200	-2.43690400
H	-4.66111800	-2.11855300	-2.44475900
C	-1.42598100	-0.83438100	2.13127200
H	-1.71780700	-1.37441000	3.04723200
H	-0.67674900	-1.42635100	1.58862700
H	-0.97157900	0.11643800	2.45493400
Ni	-5.19980300	0.62850900	1.07948300
C	-6.10163200	2.98309900	0.22911100
C	-5.54528100	2.78780600	-1.03909300
C	-5.83997500	4.12340300	0.99130100
C	-4.67424300	3.75969200	-1.53660500
H	-5.75086700	1.87337400	-1.59511700
C	-4.96455900	5.08430900	0.47191200
H	-6.29762700	4.25476200	1.97282800

C	-4.38118000	4.90613300	-0.78654100
H	-4.21726900	3.61269900	-2.51828900
H	-4.74398900	5.97824200	1.06040800
H	-3.69838300	5.66021300	-1.18447700
Br	-7.38844100	1.67802400	0.90565300

$\Delta G_{solvation}^{UM06}$= -0.01078544

UB3LYP-D3/def2-TZVPP-CPCM(DMA)// UB3LYP-D3/def2-SVP-CPCM(THF)

HF= -4659.7247785

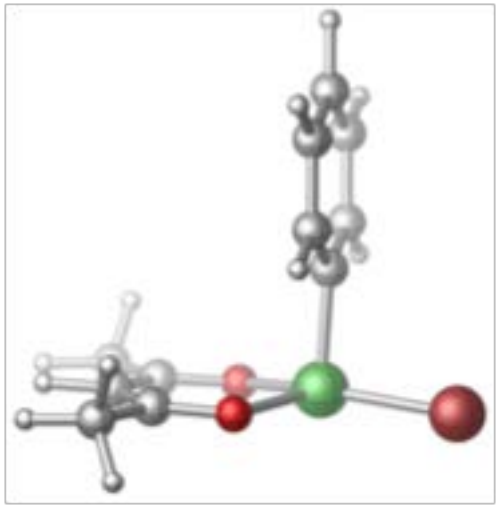
UM06/def2-TZVPP-CPCM(DMA)// UB3LYP-D3/def2-SVP-CPCM(THF)

HF= -4659.07196787

DLPNO-CCSD(T)/def2-TZVPP-gas// UB3LYP-D3/def2-SVP-CPCM(THF)

HF= -4656.14180760118

^{2}B



UB3LYP-D3/def2-SVP-CPCM(THF)
Zero-point correction= 0.202983 (Hartree/Particle)
Thermal correction to Energy= 0.219779
Thermal correction to Enthalpy= 0.220724
Thermal correction to Gibbs Free Energy= 0.154827
Sum of electronic and zero-point Energies= -4658.374184
Sum of electronic and thermal Energies= -4658.357387
Sum of electronic and thermal Enthalpies= -4658.356443
Sum of electronic and thermal Free Energies= -4658.422339

C	-3.02059400	-0.20232900	1.26979400
O	-4.07185600	0.32063600	1.77961800
C	-2.95186100	-0.78793100	-0.00600300
H	-1.99375400	-1.19622900	-0.32547500
C	-4.04737800	-0.91164300	-0.88740700
O	-5.22036900	-0.47009500	-0.65790600
C	-3.86952100	-1.60621900	-2.21422100
H	-4.05556200	-0.87921700	-3.02177500
H	-2.86939100	-2.04016200	-2.34084500
H	-4.63093300	-2.39592900	-2.31225800
C	-1.80066000	-0.15896100	2.15343300
H	-2.04085200	-0.61999500	3.12457700
H	-0.93424800	-0.66604800	1.71000300
H	-1.54579800	0.89479300	2.35266900
Ni	-5.71248500	0.61864700	0.87298400
C	-5.19472900	2.32978100	0.23203000
C	-5.19034500	2.57300000	-1.13601600
C	-4.75413100	3.25115500	1.17378500
C	-4.69931500	3.80998800	-1.57972800
H	-5.55481400	1.82299900	-1.83842000
C	-4.26938600	4.48369700	0.71022200
H	-4.76930400	3.02260600	2.24103100

C	-4.24174700	4.76093100	-0.66091600
H	-4.68212400	4.02467100	-2.65162900
H	-3.91042100	5.22314300	1.43107900
H	-3.86301800	5.72289400	-1.01479200
Br	-7.96348000	1.16584000	0.81094000

$\Delta G_{solvation}^{UM06}$= -0.01656274

UB3LYP-D3/def2-TZVPP-CPCM(THF)// UB3LYP-D3/def2-SVP-CPCM(THF)

HF= -4659.7503056

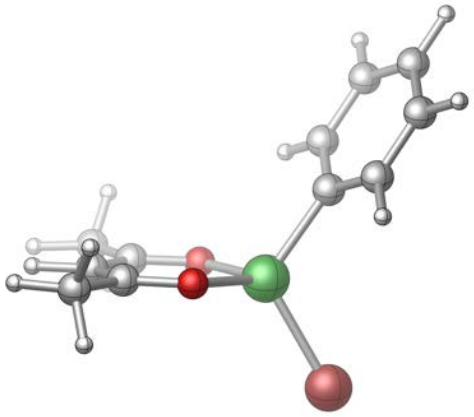
UM06/def2-TZVPP-CPCM(THF)// UB3LYP-D3/def2-SVP-CPCM(THF)

HF= -4659.08182533

DLPNO-CCSD(T)/def2-TZVPP-gas// UB3LYP-D3/def2-SVP-CPCM(THF)

HF= -4656.15666595836

^{4}B



UB3LYP-D3/def2-SVP-CPCM(THF)
Zero-point correction= 0.202208 (Hartree/Particle)
Thermal correction to Energy= 0.219348
Thermal correction to Enthalpy= 0.220292
Thermal correction to Gibbs Free Energy= 0.151895
Sum of electronic and zero-point Energies= -4658.348616
Sum of electronic and thermal Energies= -4658.331476
Sum of electronic and thermal Enthalpies= -4658.330532
Sum of electronic and thermal Free Energies= -4658.398929

C	-2.53491700	-0.04438600	0.44720700
O	-3.45994600	0.83791000	0.44218300
C	-2.67146600	-1.36031800	-0.03946100
H	-1.80695100	-2.01811300	0.03895100
C	-3.83428900	-1.88275600	-0.63716800
O	-4.92384800	-1.23471600	-0.81410200
C	-3.86040600	-3.30632900	-1.12795900
H	-2.89759000	-3.81763200	-1.00407400
H	-4.64043000	-3.85609300	-0.57657600
H	-4.15140600	-3.31515500	-2.19015100
C	-1.21873800	0.41733700	1.01577600
H	-1.38537500	0.82720900	2.02416700
H	-0.46996900	-0.38341500	1.05983800
H	-0.83424800	1.24120400	0.39257500
Ni	-5.22881600	0.54852000	-0.23443600
C	-5.46095600	1.86181000	-1.72835600
C	-6.55428600	1.78500400	-2.59514300
C	-4.48140700	2.84937200	-1.87097100
C	-6.66247600	2.71521700	-3.63763400
H	-7.32014100	1.01517300	-2.46594800
C	-4.59858000	3.77508300	-2.91779300
H	-3.63388100	2.89464700	-1.18267100
C	-5.68550100	3.70639500	-3.79706900
H	-7.51247100	2.66496400	-4.32370400

H	-3.83656200	4.54916800	-3.04445300
H	-5.77334100	4.43004600	-4.61156800
Br	-6.84790200	0.65981100	1.44015000

$\Delta G_{solvation}^{UM06}$= -0.01265173

UB3LYP-D3/def2-TZVPP-CPCM(DMA)// UB3LYP-D3/def2-SVP-CPCM(THF)

HF= -4659.7252207

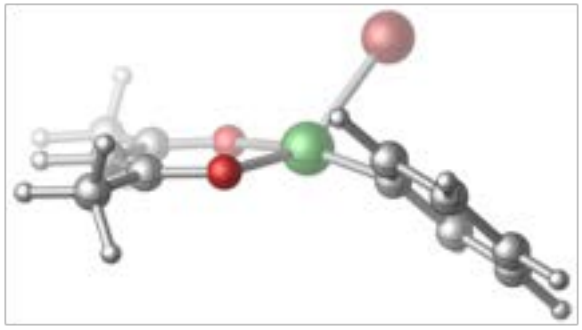
UM06/def2-TZVPP-CPCM(DMA)// UB3LYP-D3/def2-SVP-CPCM(THF)

HF= -4659.05442964

DLPNO-CCSD(T)/def2-TZVPP-gas// UB3LYP-D3/def2-SVP-CPCM(THF)

HF= -4656.12009381385

^{2}C

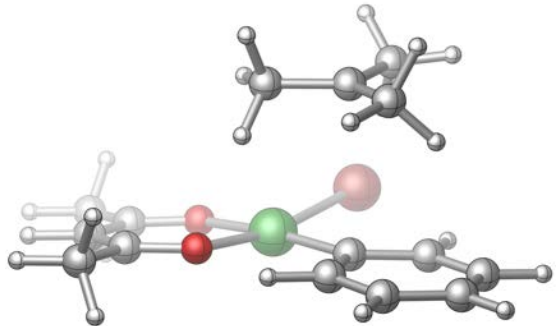


UB3LYP-D3/def2-SVP-CPCM(THF)
Zero-point correction= 0.203033 (Hartree/Particle)
Thermal correction to Energy= 0.219788
Thermal correction to Enthalpy= 0.220732
Thermal correction to Gibbs Free Energy= 0.154904
Sum of electronic and zero-point Energies= -4658.365732
Sum of electronic and thermal Energies= -4658.348977
Sum of electronic and thermal Enthalpies= -4658.348033
Sum of electronic and thermal Free Energies= -4658.413861

C	-3.04514500	-1.46216400	-1.03628300
O	-3.57397700	-0.29461400	-1.12691700
C	-3.74079000	-2.67377400	-0.94109100
H	-3.15807600	-3.59216900	-0.88087600
C	-5.15014200	-2.77270900	-0.87397300
O	-5.94095200	-1.78133000	-0.92750100
C	-5.80154400	-4.12411100	-0.71697400
H	-6.48528600	-4.29041600	-1.56490200
H	-5.07672100	-4.94657800	-0.66475800
H	-6.41865100	-4.12034900	0.19580100
C	-1.53706500	-1.45059300	-1.03019100
H	-1.10420300	-2.45547900	-0.94566500
H	-1.17843300	-0.97177500	-1.95544400
H	-1.18747700	-0.82794600	-0.19108900
Ni	-5.43346800	0.08164600	-1.20696600
C	-5.08026700	1.95510000	-1.05476400
C	-3.99209900	2.54261800	-1.69347000
C	-5.86831600	2.65173300	-0.14046100
C	-3.66331500	3.86730200	-1.37849400
H	-3.39494400	1.96999400	-2.40527500
C	-5.52134000	3.97451900	0.17688300
H	-6.74517300	2.18891100	0.31987700
C	-4.42433500	4.58064000	-0.44321000
H	-2.80610100	4.34068800	-1.86514000
H	-6.12317000	4.52971300	0.90150700
H	-4.16500000	5.61492900	-0.20352600
Br	-6.96918100	0.60457500	-2.86262600

$\Delta G_{solvation}^{UM06}$= -0.01550038
UB3LYP-D3/def2-TZVPP-CPCM(DMA)// UB3LYP-D3/def2-SVP-CPCM(THF)
HF= -4659.7424670
UM06/def2-TZVPP-CPCM(DMA)// UB3LYP-D3/def2-SVP-CPCM(THF)
HF= -4659.07503520
DLPNO-CCSD(T)/def2-TZVPP-gas// UB3LYP-D3/def2-SVP-CPCM(THF)
HF= -4656.14246856537

^{1}C-Complex



UB3LYP-D3/def2-SVP-CPCM(THF)
<S^2> = 0.0000
Zero-point correction= 0.321793 (Hartree/Particle)
Thermal correction to Energy= 0.345372
Thermal correction to Enthalpy= 0.346316
Thermal correction to Gibbs Free Energy= 0.266666
Sum of electronic and zero-point Energies= -4815.961361
Sum of electronic and thermal Energies= -4815.937782
Sum of electronic and thermal Enthalpies= -4815.936838
Sum of electronic and thermal Free Energies= -4816.016488

C	-2.39389900	-0.51158900	0.85223300
O	-3.16522000	0.50574200	0.78907600
C	-2.71944800	-1.79987800	0.41085300
H	-1.98340700	-2.59607000	0.51874000
C	-3.97684100	-2.09793400	-0.15803300
O	-4.89931000	-1.24925400	-0.33500800
C	-4.29154200	-3.50971500	-0.59734200
H	-5.16367100	-3.87591700	-0.03156700
H	-4.58235000	-3.49963100	-1.66004200
H	-3.45120300	-4.20207400	-0.45432900
C	-1.03817200	-0.23166100	1.45705400
H	-1.17136600	0.17955600	2.47068300
H	-0.40097400	-1.12445700	1.50836900
H	-0.52952400	0.54356600	0.86098000
Ni	-4.91195500	0.64605000	0.07844800
C	-4.99953900	2.50811500	0.65906200
C	-6.12341400	3.35603800	0.49553300
C	-3.91788700	3.08391300	1.37120400
C	-6.15450200	4.67390600	0.96723000
H	-7.00179300	2.98136900	-0.02977600
C	-3.93725600	4.39577400	1.85616400
H	-3.02687800	2.48050200	1.54351300
C	-5.05541000	5.21046400	1.64826300
H	-7.04731600	5.28507700	0.80167100
H	-3.06751200	4.78736500	2.39322600

H	-5.07368500	6.24054700	2.01495700
Br	-6.93045800	0.69849500	-1.24748000
C	-3.78836200	3.27854900	-2.07598600
C	-2.83200500	2.16456600	-1.96954600
H	-3.23484300	1.21227300	-2.33469500
H	-1.94892600	2.45282100	-2.57626200
H	-2.47887700	2.05448900	-0.93337400
C	-3.44417400	4.59300800	-1.51780700
H	-4.29727800	5.00047100	-0.94601400
H	-2.54094700	4.58697700	-0.89899700
H	-3.31618400	5.27966000	-2.37812800
C	-5.01093400	3.10074300	-2.82892700
H	-5.63665200	2.37048200	-2.23075300
H	-5.58515500	4.01886200	-2.99881900
H	-4.82514200	2.53406000	-3.75685000

$\Delta G_{solvation}^{UM06}$= -0.02574488

UB3LYP-D3/def2-TZVPP-CPCM(DMA)// UB3LYP-D3/def2-SVP-CPCM(THF)

HF= -4817.6391478

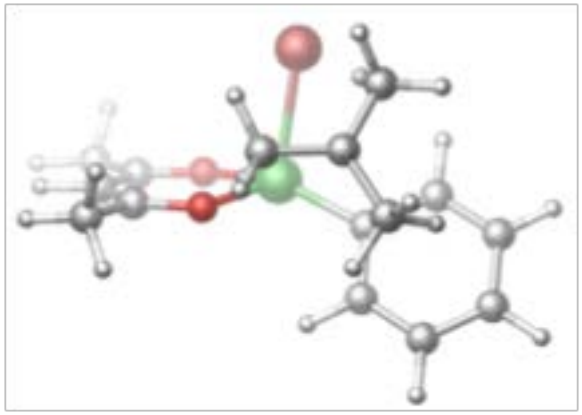
UM06/def2-TZVPP-CPCM(DMA)// UB3LYP-D3/def2-SVP-CPCM(THF)

HF= -4816.82739558

DLPNO-CCSD(T)/def2-TZVPP-gas// UB3LYP-D3/def2-SVP-CPCM(THF)

HF= -4813.64164587687

^{3}C-Complex



UB3LYP-D3/def2-SVP-CPCM(THF)
Zero-point correction= 0.319982 (Hartree/Particle)
Thermal correction to Energy= 0.344022
Thermal correction to Enthalpy= 0.344966
Thermal correction to Gibbs Free Energy= 0.262848
Sum of electronic and zero-point Energies= -4815.972389
Sum of electronic and thermal Energies= -4815.948349
Sum of electronic and thermal Enthalpies= -4815.947405
Sum of electronic and thermal Free Energies= -4816.029523

C	-4.15367600	-1.41276300	2.26173000
O	-4.35116300	-0.19214200	2.52854000
C	-3.73006500	-1.91348600	1.00408200
H	-3.60922400	-2.99215100	0.90413100
C	-3.43197400	-1.12180400	-0.11561500
O	-3.50121800	0.15626900	-0.15480400
C	-2.99001800	-1.78044500	-1.40201000
H	-3.75492200	-1.60320000	-2.17660300
H	-2.06059400	-1.30531600	-1.75349600
H	-2.83458800	-2.86246800	-1.30039500
C	-4.40031600	-2.38362100	3.39540800
H	-3.77611000	-2.09581800	4.25669500
H	-5.45031300	-2.29249200	3.71819700
H	-4.19265200	-3.42806000	3.12751500
Ni	-4.26902900	1.34948400	1.25137300
C	-3.56788700	3.12039600	0.70705800
C	-4.28449200	4.33358900	0.78157700
C	-2.21259500	3.21856100	0.32091500
C	-3.69088500	5.57106100	0.49728400
H	-5.34321100	4.30433700	1.06194300
C	-1.59909800	4.44647300	0.04030500
H	-1.61930500	2.30107200	0.22867700
C	-2.34013100	5.63197100	0.12702100
H	-4.27959300	6.49178900	0.56253000

H	-0.54563900	4.48189000	-0.25554800
H	-1.87154100	6.59461500	-0.09671300
Br	-6.71638600	1.45750200	0.76756600
C	-4.65053800	2.79903500	-2.50779300
C	-3.54389200	3.74091800	-2.71956500
H	-2.55928900	3.26066300	-2.75496800
H	-3.75079400	4.19638600	-3.71156300
H	-3.56377800	4.56803800	-1.99440600
C	-5.95245700	3.28546600	-2.08653800
H	-6.12663400	2.82740200	-1.06818200
H	-6.02785300	4.37627600	-2.01441200
H	-6.76080600	2.84453600	-2.69183100
C	-4.43574000	1.37782900	-2.69432000
H	-4.00735400	1.03277100	-1.70193000
H	-5.35326300	0.79746600	-2.85305000
H	-3.65027900	1.15190900	-3.42980100

$\Delta G_{solvation}^{UM06}$= -0.02679875

UB3LYP-D3/def2-TZVPP-CPCM(DMA)// UB3LYP-D3/def2-SVP-CPCM(THF)

HF= -4817.6442305

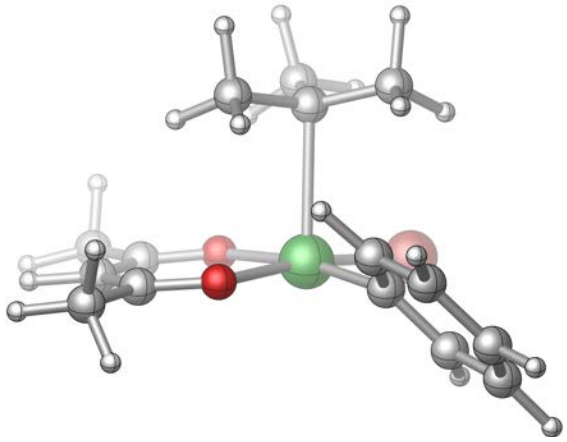
UM06/def2-TZVPP-CPCM(DMA)// UB3LYP-D3/def2-SVP-CPCM(THF)

HF= -4816.82575635

DLPNO-CCSD(T)/def2-TZVPP-gas// UB3LYP-D3/def2-SVP-CPCM(THF)

HF= -4813.65211594193

^{1}C''-Complex



UB3LYP-D3/def2-SVP-CPCM(THF)
$<S^2>$ = 0.0000
Zero-point correction= 0.324614 (Hartree/Particle)
Thermal correction to Energy= 0.347556
Thermal correction to Enthalpy= 0.348500
Thermal correction to Gibbs Free Energy= 0.272116
Sum of electronic and zero-point Energies= -4815.971390
Sum of electronic and thermal Energies= -4815.948448
Sum of electronic and thermal Enthalpies= -4815.947503
Sum of electronic and thermal Free Energies= -4816.023888

C	-2.56409800	-0.05189600	1.57097900
O	-3.24509600	1.01608200	1.52880700
C	-2.66238000	-1.10373900	0.63246700
H	-2.02670000	-1.97852900	0.76495400
C	-3.53212100	-1.07621300	-0.46587900
O	-4.34521900	-0.13186300	-0.75350300
C	-3.58261900	-2.24368800	-1.42137600
H	-2.83716500	-3.01577200	-1.19078700
H	-4.59053800	-2.68868300	-1.38594200
H	-3.43024800	-1.87715000	-2.44866900
C	-1.61501700	-0.17841800	2.73942100
H	-2.20639500	-0.29521500	3.66331200
H	-0.93160100	-1.03275600	2.64636500
H	-1.03796200	0.75312900	2.84200900
Ni	-4.64120100	1.52916100	0.15583700
C	-5.73390400	2.01241500	-1.36217900
C	-6.62198700	1.07590000	-1.91342500
C	-5.52757900	3.21485500	-2.05731600
C	-7.32192500	1.34630500	-3.09518700
H	-6.75783100	0.10436400	-1.43632300
C	-6.21143900	3.48070700	-3.25325500
H	-4.83534000	3.96122800	-1.66685400
H	-8.01675100	0.60121800	-3.49385500

H	-6.03070100	4.42495700	-3.77559300
C	-6.40956000	0.77147400	1.74155100
C	-5.86660600	1.18283900	3.07146000
H	-4.81572200	0.90108400	3.19701600
H	-5.98730400	2.25399300	3.26155500
H	-6.45979300	0.61732700	3.81893900
C	-7.62285400	1.49747100	1.27064300
H	-7.48049900	2.58460200	1.29571500
H	-7.96088300	1.18106700	0.27916400
H	-8.41877000	1.24568600	2.00229500
C	-6.28906000	-0.67665700	1.40965800
H	-6.53065400	-0.89919400	0.36531800
H	-5.30444800	-1.08750700	1.66770200
H	-7.03971500	-1.19230200	2.04333800
C	-7.12004700	2.55461800	-3.77175500
H	-7.66094000	2.76739300	-4.69778500
Br	-4.74380600	3.68847500	1.10334400

$\Delta G_{solvation}^{UM06}$= -0.01640250

UB3LYP-D3/def2-TZVPP-CPCM(THF)// UB3LYP-D3/def2-SVP-CPCM(THF)

HF= -4817.64084424

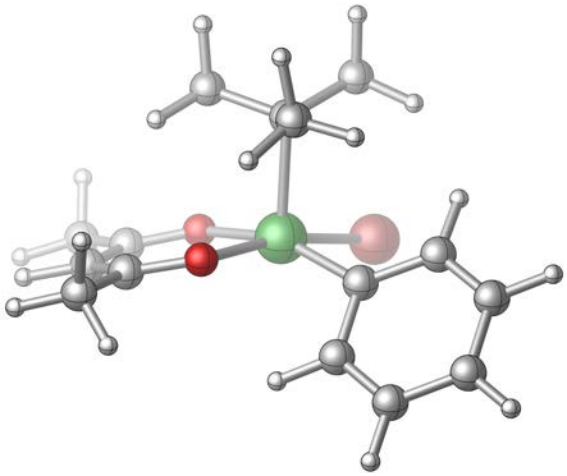
UM06/def2-TZVPP-CPCM(THF)// UB3LYP-D3/def2-SVP-CPCM(THF)

HF= -4816.82646240

DLPNO-CCSD(T)/def2-TZVPP-gas// UB3LYP-D3/def2-SVP-CPCM(THF)

HF= -4813.63811608447

^{1}C'



UB3LYP-D3/def2-SVP-CPCM(THF)
$<S^2>$ = 0.0000
Zero-point correction= 0.325423 (Hartree/Particle)
Thermal correction to Energy= 0.347952
Thermal correction to Enthalpy= 0.348896
Thermal correction to Gibbs Free Energy= 0.273698
Sum of electronic and zero-point Energies= -4815.975127
Sum of electronic and thermal Energies= -4815.952597
Sum of electronic and thermal Enthalpies= -4815.951653
Sum of electronic and thermal Free Energies= -4816.026851

C	-4.30533800	-0.34406200	0.82260900
O	-5.46671300	0.16780700	0.64013700
C	-3.50074900	-0.92262900	-0.16399200
H	-2.52904700	-1.31736900	0.12959100
C	-3.88626900	-1.00908500	-1.52163100
O	-4.98712200	-0.58324800	-1.97837200
C	-2.94568800	-1.61997800	-2.53197800
H	-3.48526700	-2.38441400	-3.11230700
H	-2.63518100	-0.83676300	-3.24324500
H	-2.05215600	-2.06364000	-2.07366200
C	-3.82097100	-0.25596200	2.24854800
H	-2.85698700	-0.75844500	2.39998400
H	-3.72549700	0.80600700	2.52813200
H	-4.57859300	-0.69714900	2.91499900
Ni	-6.50227900	0.19844700	-0.94819300
C	-8.09615900	0.31863700	0.12195900
C	-9.22403100	1.12080100	-0.08108500
C	-8.10532000	-0.61378400	1.16896200
C	-10.32913100	1.02564200	0.77250400
H	-9.26388400	1.81980500	-0.91581100
C	-9.22086600	-0.72184300	2.01314400
H	-7.24535900	-1.26051000	1.34753700

C	-10.33225000	0.10288000	1.82498600
H	-11.19653700	1.66954700	0.60193500
H	-9.20915400	-1.45434300	2.82537700
H	-11.19751200	0.02494000	2.48836200
Br	-7.85869200	-0.23305700	-2.81430900
C	-6.12142100	2.32226000	-1.09046200
C	-4.65707600	2.26823100	-1.45419300
H	-4.03287600	1.80718900	-0.68059400
H	-4.48784900	1.76506300	-2.41280300
H	-4.32700000	3.31993900	-1.56103000
C	-6.39950500	2.92315200	0.26541100
H	-7.47184500	3.01331100	0.47024700
H	-5.92118600	2.35653400	1.07135600
H	-5.96755000	3.94255300	0.25597000
C	-6.97276700	2.88665500	-2.19907600
H	-6.73225300	2.45386700	-3.17629900
H	-8.04707600	2.78417000	-2.01539400
H	-6.75013600	3.97167700	-2.23111000

$\Delta G_{solvation}^{UM06}$=-0.01592820

UB3LYP-D3/def2-TZVPP-CPCM(DMA)// UB3LYP-D3/def2-SVP-CPCM(THF)

HF= -4817.64556732

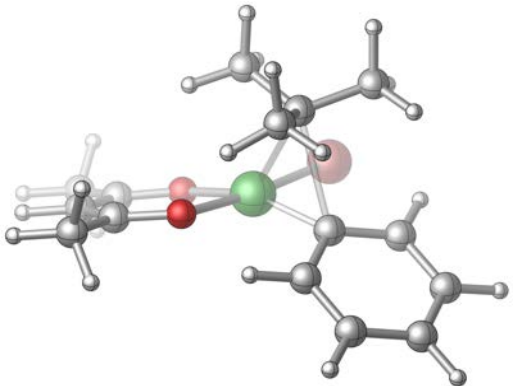
UM06/def2-TZVPP-CPCM(DMA)// UB3LYP-D3/def2-SVP-CPCM(THF)

HF= -4816.82999570

DLPNO-CCSD(T)/def2-TZVPP-gas// UB3LYP-D3/def2-SVP-CPCM(THF)

HF= -4813.66328229734

^{1}C'-TS



UB3LYP-D3/def2-SVP-CPCM(THF)
Zero-point correction= 0.325398 (Hartree/Particle)
Thermal correction to Energy= 0.347305
Thermal correction to Enthalpy= 0.348249
Thermal correction to Gibbs Free Energy= 0.274271
Sum of electronic and zero-point Energies= -4815.962361
Sum of electronic and thermal Energies= -4815.940454
Sum of electronic and thermal Enthalpies= -4815.939510
Sum of electronic and thermal Free Energies= -4816.013487

C	-4.07305100	-0.47179400	0.72299900
O	-5.21739300	0.05547100	0.50807100
C	-3.31981100	-1.16659600	-0.23020200
H	-2.35284000	-1.57653600	0.05776300
C	-3.79081300	-1.37457500	-1.54133500
O	-4.89846000	-0.94266300	-1.98728700
C	-2.96580700	-2.16396700	-2.52823400
H	-3.54296700	-3.04484700	-2.85257600
H	-2.79267100	-1.54729000	-3.42439100
H	-2.00315300	-2.49127900	-2.11454000
C	-3.55362000	-0.28675400	2.12694000
H	-2.57966800	-0.76748100	2.28527800
H	-3.46679600	0.79119100	2.33909100
H	-4.28610700	-0.69772300	2.83994900
Ni	-6.24064000	0.13838100	-1.10969200
C	-7.89699300	0.65210700	-0.09676100
C	-9.14944900	0.79710000	-0.71833000
C	-7.87409500	0.28009600	1.26002400
C	-10.33457300	0.54289500	-0.02069300
H	-9.20968600	1.09428200	-1.76283400
C	-9.05935700	0.02313200	1.95769500
H	-6.92269700	0.18118000	1.77724700
C	-10.29717800	0.15377400	1.32188800
H	-11.29244300	0.65356700	-0.53631500
H	-9.00771500	-0.27860500	3.00751500

H	-11.22395300	-0.04056900	1.86803200
Br	-7.25628200	0.20116400	-3.31752100
C	-6.49527800	2.48171500	-0.62929300
C	-5.17178100	2.47401100	-1.38310800
H	-4.37219700	1.92770600	-0.86779100
H	-5.26263500	2.13048600	-2.42187300
H	-4.85246400	3.53388100	-1.42398900
C	-6.33285300	2.87239800	0.81735300
H	-7.29265800	2.95925100	1.33988000
H	-5.67778800	2.17634200	1.35265400
H	-5.84606500	3.86603400	0.82104900
C	-7.56261900	3.24373600	-1.37123800
H	-7.76831100	2.80584400	-2.35563500
H	-8.49221000	3.33671100	-0.79839800
H	-7.16021300	4.26105800	-1.53518800

$\Delta G_{solvation}^{UM06}$= -0.01578531

UB3LYP-D3/def2-TZVPP-CPCM(DMA)// UB3LYP-D3/def2-SVP-CPCM(THF)

HF= -4817.63196236

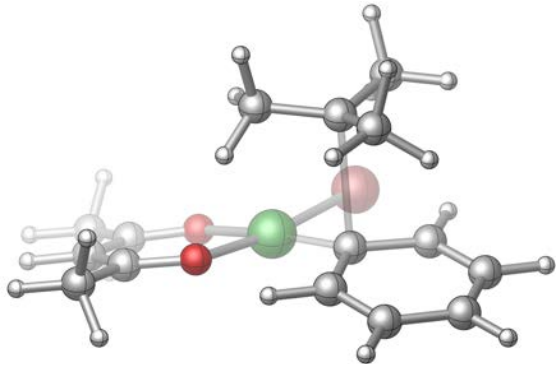
UM06/def2-TZVPP-CPCM(DMA)// UB3LYP-D3/def2-SVP-CPCM(THF)

HF= -4816.82172077

DLPNO-CCSD(T)/def2-TZVPP-gas// UB3LYP-D3/def2-SVP-CPCM(THF)

HF= -4813.65006456835

^{1}C-TS



UB3LYP-D3/def2-SVP-CPCM(THF)
Zero-point correction= 0.323859 (Hartree/Particle)
Thermal correction to Energy= 0.346214
Thermal correction to Enthalpy= 0.347158
Thermal correction to Gibbs Free Energy= 0.271504
Sum of electronic and zero-point Energies= -4815.958572
Sum of electronic and thermal Energies= -4815.936217
Sum of electronic and thermal Enthalpies= -4815.935273
Sum of electronic and thermal Free Energies= -4816.010927

C	-2.31677600	-0.52043500	0.71526300
O	-3.09316900	0.48973200	0.61191500
C	-2.66193400	-1.83578400	0.38478000
H	-1.92370800	-2.62590900	0.51776900
C	-3.94469700	-2.16533600	-0.10222400
O	-4.87180500	-1.32585600	-0.30197000
C	-4.28888000	-3.60301700	-0.41523600
H	-5.11266400	-3.92526100	0.24255800
H	-4.66226100	-3.66774500	-1.44950100
H	-3.43791500	-4.28519100	-0.28750900
C	-0.93617200	-0.19863500	1.23552200
H	-1.02328100	0.29140100	2.21861600
H	-0.29783400	-1.08722100	1.32771500
H	-0.45437600	0.52495600	0.55767100
Ni	-4.86499600	0.58582400	-0.04958400
C	-4.90608600	2.52000300	0.35886900
C	-6.04267300	3.35988500	0.18257800
C	-3.91875200	3.02813100	1.25252500
C	-6.18028700	4.59194300	0.82211500
H	-6.83748700	3.03000000	-0.48546600
C	-4.04636800	4.25246500	1.90523600
H	-3.02458700	2.43032400	1.42612500
C	-5.17815400	5.04973800	1.68712100
H	-7.07112600	5.20082000	0.64448300
H	-3.25862500	4.59507100	2.58225300
H	-5.27734800	6.01794800	2.18550100

Br	-7.00945500	0.52068600	-1.13207000
C	-3.84272600	3.24560100	-1.79453200
C	-2.85038500	2.14864400	-1.92283300
H	-3.29711300	1.20688400	-2.26338500
H	-2.12888200	2.49671900	-2.69059600
H	-2.29171800	1.98245100	-0.99492400
C	-3.34809200	4.57349000	-1.35644300
H	-4.12468400	5.16280300	-0.84725200
H	-2.44764300	4.51311700	-0.73492000
H	-3.10468400	5.12032300	-2.28966100
C	-5.02868200	3.20251600	-2.68368200
H	-5.59850300	2.27022600	-2.55158300
H	-5.68496100	4.07287000	-2.56557700
H	-4.62680000	3.19333100	-3.71704800

$\Delta G_{solvation}^{UM06}$= -0.02375768

UB3LYP-D3/def2-TZVPP-CPCM(DMA)// UB3LYP-D3/def2-SVP-CPCM(THF)

HF=-4817.63659718

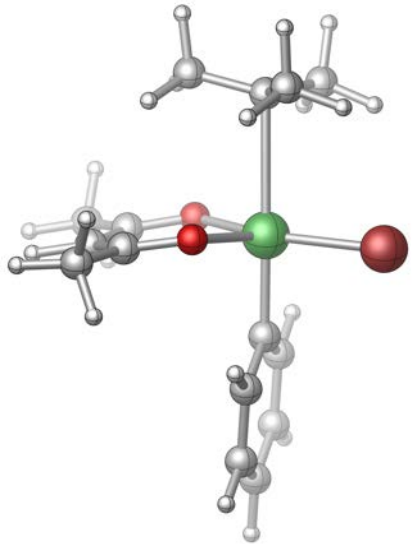
UM06/def2-TZVPP-CPCM(DMA)// UB3LYP-D3/def2-SVP-CPCM(THF)

HF= -4816.82544584

DLPNO-CCSD(T)/def2-TZVPP-gas// UB3LYP-D3/def2-SVP-CPCM(THF)

HF= -4816.801688160

^{3}C'



Zero-point correction= 0.322394 (Hartree/Particle)
Thermal correction to Energy= 0.346206
Thermal correction to Enthalpy= 0.347150
Thermal correction to Gibbs Free Energy= 0.265944
Sum of electronic and zero-point Energies= -4815.969566
Sum of electronic and thermal Energies= -4815.945754
Sum of electronic and thermal Enthalpies= -4815.944810
Sum of electronic and thermal Free Energies= -4816.026016

C	-2.71674100	0.15818900	0.46731300
O	-3.68961800	0.76472700	1.01871000
C	-2.84124300	-0.89722800	-0.46363200
H	-1.92410400	-1.32440800	-0.86729900
C	-4.05853200	-1.47163300	-0.87047100
O	-5.21790200	-1.08617400	-0.49479200
C	-4.06055500	-2.65359500	-1.80629400
H	-3.05063800	-2.96868500	-2.09848800
H	-4.58026500	-3.49553100	-1.32115400
H	-4.64035000	-2.39382100	-2.70661200
C	-1.34435300	0.63578500	0.87462200
H	-1.27105600	0.62861200	1.97340500
H	-0.53425200	0.03103100	0.44706900
H	-1.22480200	1.68294100	0.55117000
Ni	-5.57704200	0.53911500	0.46401600
C	-5.46032000	1.54197700	-1.17637500
C	-6.30204000	1.16259200	-2.21934600
C	-4.51593300	2.55468800	-1.32304700
C	-6.18500300	1.81631800	-3.45483700
H	-7.03210300	0.36077100	-2.08662300
C	-4.40562300	3.19862400	-2.56419000
H	-3.87784800	2.84052900	-0.48566300

C	-5.23777300	2.83176700	-3.62770800
H	-6.83712900	1.52338800	-4.28243800
H	-3.66636900	3.99430900	-2.69264000
H	-5.14927800	3.33860400	-4.59196600
Br	-6.88502600	2.24706700	1.39887900
C	-5.85136200	-1.03027400	2.56522100
C	-5.44340900	-0.08607000	3.65131700
H	-4.42897300	0.30321700	3.47266700
H	-6.13525600	0.75959600	3.75236300
H	-5.41939200	-0.63468600	4.61627100
C	-7.30547000	-1.27937200	2.31401200
H	-7.90724800	-0.36629700	2.41787800
H	-7.47114900	-1.71116400	1.31364800
H	-7.68088500	-2.02395000	3.04851200
C	-4.90689700	-2.15583500	2.28389100
H	-5.21957800	-2.75774100	1.42086700
H	-3.87937800	-1.79936300	2.11999200
H	-4.87840500	-2.82348200	3.16979100

$\Delta G_{solvation}^{UM06}$= -0.01168905

UB3LYP-D3/def2-TZVPP-CPCM(DMA)// UB3LYP-D3/def2-SVP-CPCM(THF)

HF= -4817.63659718

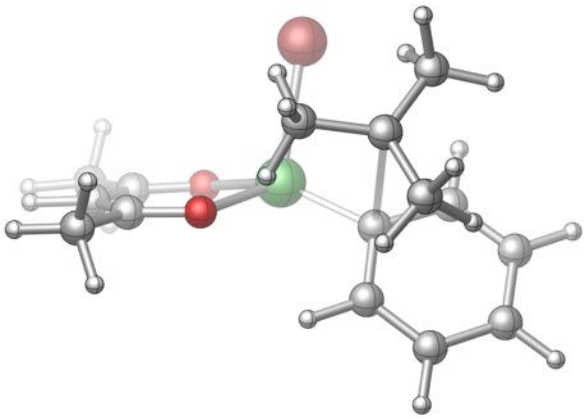
UM06/def2-TZVPP-CPCM(DMA)// UB3LYP-D3/def2-SVP-CPCM(THF)

HF= -4816.82544584

DLPNO-CCSD(T)/def2-TZVPP-gas// UB3LYP-D3/def2-SVP-CPCM(THF)

HF= -4813.66623270917

^{3}C-TS



UB3LYP-D3/def2-SVP-CPCM(THF)
Zero-point correction= 0.320766 (Hartree/Particle)
Thermal correction to Energy= 0.344184
Thermal correction to Enthalpy= 0.345128
Thermal correction to Gibbs Free Energy= 0.264977
Sum of electronic and zero-point Energies= -4815.969306
Sum of electronic and thermal Energies= -4815.945888
Sum of electronic and thermal Enthalpies= -4815.944944
Sum of electronic and thermal Free Energies= -4816.025095

C	-4.17569500	-1.41235000	2.26028700
O	-4.45944600	-0.18562600	2.40579100
C	-3.60900800	-1.98301900	1.09566100
H	-3.41889300	-3.05637000	1.09739000
C	-3.22444000	-1.25305200	-0.04437100
O	-3.37533000	0.00339800	-0.20266800
C	-2.56208900	-1.96938400	-1.20010100
H	-3.17651000	-1.83288600	-2.10524300
H	-1.58602000	-1.49942100	-1.40242800
H	-2.41819300	-3.04292200	-1.01976200
C	-4.47673300	-2.30100600	3.44709800
H	-3.95559700	-1.90616400	4.33410100
H	-5.55654600	-2.25081300	3.66312500
H	-4.18688000	-3.34853900	3.29038100
Ni	-4.38550600	1.22748000	0.99835600
C	-3.69264400	2.99837000	0.39281200
C	-4.33254400	4.23459000	0.63232500
C	-2.31962000	3.05650300	0.05320800
C	-3.65690000	5.45632800	0.53510600
H	-5.39649800	4.23584400	0.89250400
C	-1.62390700	4.26538500	-0.03657000
H	-1.78874700	2.11986800	-0.15035700
C	-2.29683700	5.47446400	0.19508000
H	-4.18578800	6.39627300	0.71990000

H	-0.56153800	4.27464600	-0.29885800
H	-1.76414900	6.42571200	0.11003600
Br	-6.83441500	1.24573900	0.56164400
C	-4.70877100	3.03216600	-2.30928500
C	-3.59189600	3.87447000	-2.76245400
H	-2.66149900	3.31955800	-2.92536100
H	-3.92879800	4.32085900	-3.72098200
H	-3.42884100	4.72688000	-2.08357800
C	-5.99990900	3.64971600	-1.99038000
H	-6.44553000	3.14142100	-1.11290700
H	-5.95342000	4.73686700	-1.86120500
H	-6.67907700	3.39382200	-2.82949800
C	-4.64388000	1.57410500	-2.48245000
H	-3.72960500	1.15204300	-2.03797500
H	-5.52063200	1.05891000	-2.07283800
H	-4.57697000	1.40007400	-3.57653100

$\Delta G_{solvation}^{UM06}$= -0.02583388

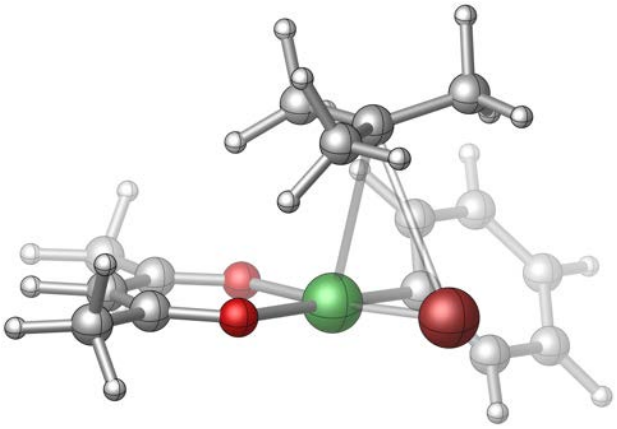
UB3LYP-D3/def2-TZVPP-CPCM(DMA)// UB3LYP-D3/def2-SVP-CPCM(THF)

HF= -4817.64143428

UM06/def2-TZVPP-CPCM(DMA)// UB3LYP-D3/def2-SVP-CPCM(THF)

HF= -4816.82379643

^{1}C''-TS



UB3LYP-D3/def2-SVP-CPCM(THF)
Zero-point correction= 0.323194 (Hartree/Particle)
Thermal correction to Energy= 0.345704
Thermal correction to Enthalpy= 0.346648
Thermal correction to Gibbs Free Energy= 0.270392
Sum of electronic and zero-point Energies= -4815.963060
Sum of electronic and thermal Energies= -4815.940550
Sum of electronic and thermal Enthalpies= -4815.939606
Sum of electronic and thermal Free Energies= -4816.015862

C	-2.61804000	-0.11587600	1.50279400
O	-3.28107000	0.96028700	1.36471500
C	-2.62710600	-1.17982700	0.57954600
H	-2.02814200	-2.06374500	0.79722900
C	-3.36956400	-1.15248000	-0.61512500
O	-4.10550200	-0.18872600	-1.00732800
C	-3.33683000	-2.33974000	-1.54909400
H	-2.68961400	-3.15038800	-1.18927200
H	-4.36200100	-2.72257200	-1.67947400
H	-2.99105500	-2.00886900	-2.54157800
C	-1.81107900	-0.22777000	2.77527900
H	-2.50250600	-0.29135000	3.63256000
H	-1.14990300	-1.10450300	2.78907900
H	-1.21601900	0.68866400	2.91009200
Ni	-4.45396200	1.44872600	-0.12523600
C	-5.56794100	1.92570100	-1.58861800
C	-6.50501600	1.00619300	-2.09445700
C	-5.46396400	3.16350700	-2.25127500
C	-7.32553600	1.31348300	-3.18889900
H	-6.57766400	0.01011700	-1.64810500
C	-6.26175600	3.47232000	-3.36084400
H	-4.75242000	3.90936400	-1.88744500
H	-8.05176700	0.57764300	-3.54881400
H	-6.14997500	4.44165400	-3.85710400

C	-6.55526900	1.09284500	2.13554300
C	-5.84629700	1.32869700	3.40960500
H	-4.76541100	1.18169700	3.26734700
H	-6.05186700	2.31252100	3.84399600
H	-6.18952900	0.53314900	4.10327300
C	-7.78354200	1.83570800	1.78339100
H	-7.82823400	2.83379700	2.23076800
H	-7.92518800	1.88416200	0.69458200
H	-8.61811200	1.22308900	2.18706900
C	-6.34665000	-0.21996800	1.47810200
H	-6.65932400	-0.22871800	0.42893000
H	-5.33118700	-0.61240300	1.59721400
H	-7.03180800	-0.90144800	2.02842400
C	-7.20594000	2.55126300	-3.83021700
H	-7.83821100	2.79415900	-4.68894100
Br	-5.03147700	3.39640500	1.07445000

$\Delta G_{solvation}^{UM06}$= -0.02358562

UB3LYP-D3/def2-TZVPP-CPCM(DMA)// UB3LYP-D3/def2-SVP-CPCM(THF)

HF= -4817.63883416

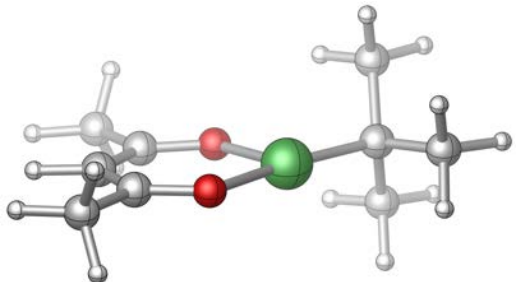
UM06/def2-TZVPP-CPCM(DMA)// UB3LYP-D3/def2-SVP-CPCM(THF)

HF= -4816.82668057

DLPNO-CCSD(T)/def2-TZVPP-gas// UB3LYP-D3/def2-SVP-CPCM(THF)

HF= -4813.64502028160

^{1}D



UB3LYP-D3/def2-SVP-CPCM(THF)
$<S^2>$ = 0.0000
Zero-point correction= 0.231479 (Hartree/Particle)
Thermal correction to Energy= 0.247258
Thermal correction to Enthalpy= 0.248202
Thermal correction to Gibbs Free Energy= 0.187876
Sum of electronic and zero-point Energies= -2010.679481
Sum of electronic and thermal Energies= -2010.663702
Sum of electronic and thermal Enthalpies= -2010.662758
Sum of electronic and thermal Free Energies= -2010.723084

C	-3.04816600	-1.58856000	-0.57249400
O	-3.60656400	-1.11182600	0.47582600
C	-3.70755300	-2.17290100	-1.66924000
H	-3.09228100	-2.53376600	-2.49332400
C	-5.10941900	-2.32678100	-1.77738000
O	-5.94271900	-1.95284300	-0.89416000
C	-5.69777000	-2.97457500	-3.00927000
H	-6.40228000	-2.27226900	-3.48390600
H	-4.93822100	-3.27644600	-3.74245500
H	-6.28308000	-3.85839000	-2.70744500
C	-1.54066400	-1.48285400	-0.57486500
H	-1.08171800	-1.90585300	-1.47800800
H	-1.25437500	-0.42241300	-0.48396900
H	-1.14133700	-1.99867100	0.31328800
Ni	-5.45834700	-1.07899900	0.75321600
C	-5.36148700	-0.20184800	2.44527100
C	-6.85048200	-0.01437400	2.74608700
H	-7.34072500	0.64322600	2.00600100
H	-7.39456400	-0.97745200	2.75785000
H	-7.01234600	0.44873200	3.74164700
C	-4.68369100	-1.13415500	3.43934400
H	-5.21201700	-2.10018300	3.51694800
H	-3.64852000	-1.34277500	3.12473100
H	-4.64536400	-0.69906200	4.46062000
C	-4.62877300	1.12534200	2.32230600
H	-3.59170500	0.96134600	1.99039200
H	-5.11526600	1.79012400	1.58796800

H -4.59442700 1.67192500 3.28840700

$\Delta G_{solvation}^{UM06}$= -0.01003141

UB3LYP-D3/def2-TZVPP-CPCM(DMA)// UB3LYP-D3/def2-SVP-CPCM(THF)

HF= -2011.69926554

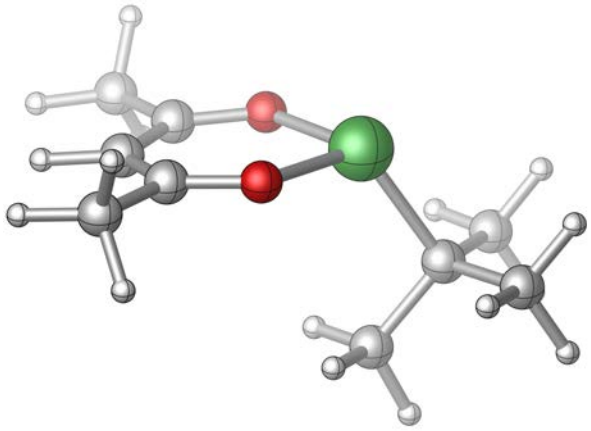
UM06/def2-TZVPP-CPCM(DMA)// UB3LYP-D3/def2-SVP-CPCM(THF)

HF= -2011.20902185

DLPNO-CCSD(T)/def2-TZVPP-gas// UB3LYP-D3/def2-SVP-CPCM(THF)

HF= -2009.74405799902

^{3}D



UB3LYP-D3/def2-SVP-CPCM(THF)
Zero-point correction= 0.230992 (Hartree/Particle)
Thermal correction to Energy= 0.246945
Thermal correction to Enthalpy= 0.247889
Thermal correction to Gibbs Free Energy= 0.185693
Sum of electronic and zero-point Energies= -2010.689470
Sum of electronic and thermal Energies= -2010.673517
Sum of electronic and thermal Enthalpies= -2010.672573
Sum of electronic and thermal Free Energies= -2010.734769

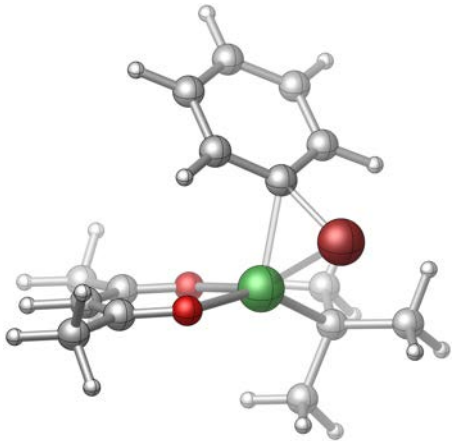
C	2.88294900	-0.62000300	-0.03246900
O	1.91881300	-0.10380500	0.62159600
C	2.75216000	-1.55531800	-1.08246100
H	3.67019200	-1.91116500	-1.55012700
C	1.53232200	-2.03671200	-1.60597800
O	0.37074000	-1.73345800	-1.17690700
C	1.55555100	-2.98975900	-2.77931900
H	2.57087600	-3.24883400	-3.10707900
H	1.01343900	-3.90930400	-2.50563400
H	1.00744700	-2.53559800	-3.62102700
C	4.26177700	-0.15780400	0.38065000
H	4.40134800	-0.36319800	1.45430900
H	5.06838900	-0.63674200	-0.18980100
H	4.32697900	0.93529300	0.25450700
Ni	0.04955000	-0.57161400	0.34993800
C	-0.70065700	-1.48494200	1.93145700
C	-0.49386500	-0.56712600	3.13475300
H	0.57087200	-0.30870000	3.26301700
H	-1.05574900	0.37752100	3.03218300
H	-0.83381100	-1.04675900	4.07922700
C	-2.18021400	-1.78639700	1.70272400
H	-2.77245400	-0.86448100	1.57134700
H	-2.33162400	-2.41077700	0.80525400
H	-2.62238800	-2.33825000	2.56176600

C	0.10745800	-2.77042800	2.07677300
H	-0.00376700	-3.41607400	1.18970100
H	1.18320200	-2.55750200	2.19646200
H	-0.21282800	-3.36266100	2.96191300

$\Delta G_{solvation}^{UM06}$=-0.01003141

UB3LYP-D3/def2-TZVPP-CPCM(DMA)// UB3LYP-D3/def2-SVP-CPCM(THF)
HF=-2011.69926554
UM06/def2-TZVPP-CPCM(DMA)// UB3LYP-D3/def2-SVP-CPCM(THF)
HF=-2011.20902185
DLPNO-CCSD(T)/def2-TZVPP-gas// UB3LYP-D3/def2-SVP-CPCM(THF)
HF=-2009.74405799902

^{1}E-TS



UB3LYP-D3/def2-SVP-CPCM(THF)
Zero-point correction= 0.322368 (Hartree/Particle)
Thermal correction to Energy= 0.345098
Thermal correction to Enthalpy= 0.346042
Thermal correction to Gibbs Free Energy= 0.269644
Sum of electronic and zero-point Energies= -4815.950397
Sum of electronic and thermal Energies= -4815.927667
Sum of electronic and thermal Enthalpies= -4815.926723
Sum of electronic and thermal Free Energies= -4816.003121

C	-3.00307000	-1.22231000	-0.44759300
O	-3.69710000	-0.57016400	0.39855700
C	-3.50532800	-2.02518000	-1.48790600
H	-2.78502000	-2.54792500	-2.11693700
C	-4.87949500	-2.24543200	-1.72767000
O	-5.82153700	-1.67147400	-1.10282900
C	-5.30048000	-3.21663400	-2.80853300
H	-5.92334300	-2.68493600	-3.54627500
H	-4.45170200	-3.68744000	-3.32225900
H	-5.93451400	-3.99931100	-2.36133900
C	-1.50734100	-1.09884400	-0.25894100
H	-0.93093600	-1.64707800	-1.01580000
H	-1.23129700	-0.03259200	-0.29008900
H	-1.23818200	-1.47080900	0.74304300
Ni	-5.61982400	-0.35771600	0.40848800
C	-5.90709600	1.45818600	-0.58928400
C	-5.36013200	1.26412600	-1.87017900
C	-5.64389400	2.63195200	0.13258700
C	-4.43037100	2.18592200	-2.35379000
H	-5.63258900	0.38379100	-2.44920300
C	-4.70978600	3.54169800	-0.36896500
H	-6.14351500	2.81977400	1.08192500
C	-4.09048700	3.32024600	-1.60481400
H	-3.97233200	2.01315200	-3.33120000

H	-4.47578700	4.43687400	0.21312900
H	-3.36454500	4.03843500	-1.99252600
Br	-7.80850500	0.56785400	-0.21395000
C	-5.56419400	0.00627800	2.42335200
C	-6.89048000	0.51468900	2.95920100
H	-7.12606700	1.52936500	2.60747500
H	-7.72918200	-0.14284500	2.69049600
H	-6.83591200	0.55586700	4.06544200
C	-5.32913200	-1.45368400	2.79451400
H	-6.12726000	-2.11848900	2.42136800
H	-4.36071200	-1.82387700	2.43036800
H	-5.33366500	-1.55297300	3.89912500
C	-4.40834300	0.90721100	2.80702900
H	-3.47282800	0.58559900	2.33408300
H	-4.59640300	1.95486700	2.53150400
H	-4.27091300	0.87836700	3.90643200

$\Delta G_{solvation}^{UM06}$= -0.00708735

UB3LYP-D3/def2-TZVPP-CPCM(DMA)// UB3LYP-D3/def2-SVP-CPCM(THF)

HF=-4817.61341725

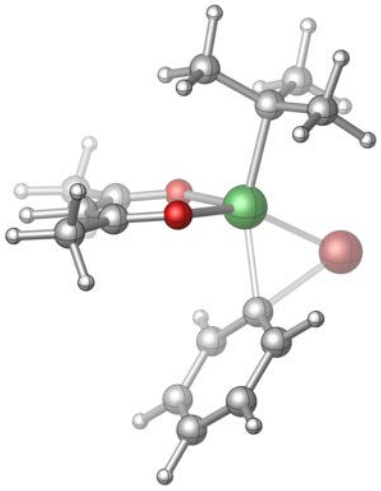
UM06/def2-TZVPP-CPCM(DMA)// UB3LYP-D3/def2-SVP-CPCM(THF)

HF= -4816.80636293

DLPNO-CCSD(T)/def2-TZVPP-gas// UB3LYP-D3/def2-SVP-CPCM(THF)

HF= -4813.63643423474

^{3}E-TS



UB3LYP-D3/def2-SVP-CPCM(THF)
Zero-point correction= 0.321470 (Hartree/Particle)
Thermal correction to Energy= 0.344473
Thermal correction to Enthalpy= 0.345417
Thermal correction to Gibbs Free Energy= 0.266848
Sum of electronic and zero-point Energies= -4815.950515
Sum of electronic and thermal Energies= -4815.927512
Sum of electronic and thermal Enthalpies= -4815.926568
Sum of electronic and thermal Free Energies= -4816.005138

C	-2.61196700	0.18283800	0.53402100
O	-3.57685300	0.71560400	1.16547700
C	-2.73328900	-0.77010100	-0.50178800
H	-1.81115800	-1.12268900	-0.96317200
C	-3.94146300	-1.31825200	-0.98262700
O	-5.10643500	-1.03825600	-0.55492800
C	-3.90068300	-2.33891400	-2.09702900
H	-2.88247200	-2.56208300	-2.44168100
H	-4.38065000	-3.26873200	-1.75113200
H	-4.49871500	-1.96485800	-2.94377800
C	-1.23439700	0.65037500	0.94795600
H	-1.12598000	0.53442400	2.03789200
H	-0.42350700	0.11249100	0.43932800
H	-1.14444000	1.72759400	0.73009000
Ni	-5.46981700	0.36182000	0.73736900
C	-5.74173500	1.86079900	-0.71154500
C	-6.72503600	1.46517500	-1.62506000
C	-4.55920600	2.48765400	-1.11722800
C	-6.45737200	1.59675900	-2.99090900
H	-7.66105800	1.02595800	-1.27433300
C	-4.31227400	2.61389600	-2.48716200
H	-3.83302600	2.81934500	-0.37499100

C	-5.25373500	2.16734500	-3.42426800
H	-7.19999000	1.25695800	-3.71758300
H	-3.37438700	3.06516200	-2.82153700
H	-5.05435000	2.27606500	-4.49283900
Br	-6.55256900	2.46067300	1.30294000
C	-5.88803100	-0.89029700	2.36315000
C	-5.63925700	-0.06327600	3.60582300
H	-4.60750700	0.32183800	3.62181300
H	-6.32698500	0.79121100	3.68432400
H	-5.77669800	-0.68835000	4.51294200
C	-7.34150600	-1.22579900	2.09787500
H	-7.98078500	-0.32864200	2.11583400
H	-7.46946400	-1.72707100	1.12416200
H	-7.72628600	-1.92120900	2.87410300
C	-4.95430600	-2.07471900	2.25267900
H	-5.13629500	-2.65515100	1.33788500
H	-3.90021200	-1.75808000	2.25673300
H	-5.09940500	-2.75296700	3.11923200

$\Delta G_{solvation}^{UM06}$= -0.00793865

UB3LYP-D3/def2-TZVPP-CPCM(DMA)// UB3LYP-D3/def2-SVP-CPCM(THF)

HF= -4817.61456950

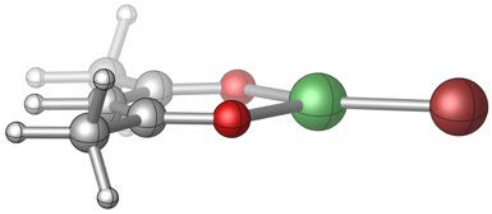
UM06/def2-TZVPP-CPCM(DMA)// UB3LYP-D3/def2-SVP-CPCM(THF)

HF= -4816.80487186

DLPNO-CCSD(T)/def2-TZVPP-gas// UB3LYP-D3/def2-SVP-CPCM(THF)

HF= -4813.63413962550

^1P_A

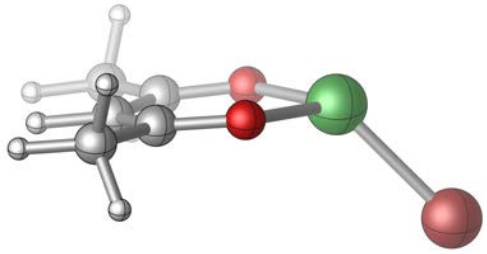


UB3LYP-D3/def2-SVP-CPCM(THF)
$<S^2>$ = 0.0000
Zero-point correction= 0.113187 (Hartree/Particle)
Thermal correction to Energy= 0.124416
Thermal correction to Enthalpy= 0.125360
Thermal correction to Gibbs Free Energy= 0.073570
Sum of electronic and zero-point Energies= -4426.989320
Sum of electronic and thermal Energies= -4426.978091
Sum of electronic and thermal Enthalpies= -4426.977147
Sum of electronic and thermal Free Energies= -4427.028936

C	-2.69078700	-0.69335300	0.04535900
O	-3.10573800	0.05502500	-0.90451100
C	-3.52303100	-1.49102600	0.85184900
H	-3.05780900	-2.09108800	1.63271400
C	-4.92182300	-1.55970500	0.70982100
O	-5.60859700	-0.91850000	-0.15687200
C	-5.73285500	-2.44487400	1.62186500
H	-6.27668200	-3.18374600	1.01159500
H	-5.11746100	-2.96656100	2.36552200
H	-6.49134400	-1.83242700	2.13483000
C	-1.20113200	-0.67764400	0.26909300
H	-0.69442000	-0.97056400	-0.66433700
H	-0.88303500	0.35244000	0.49720500
H	-0.88699300	-1.34500100	1.08144700
Ni	-4.89234400	0.25158000	-1.44258200
Br	-6.68390100	1.00741000	-2.74760800

$\Delta G_{solvation}^{UM06}$= -0.01991587
UB3LYP-D3/def2-TZVPP-CPCM(DMA)// UB3LYP-D3/def2-SVP-CPCM(THF)
HF=-4427.55542114
UM06/def2-TZVPP-CPCM(DMA)// UB3LYP-D3/def2-SVP-CPCM(THF)
HF= -4428.01914375
DLPNO-CCSD(T)/def2-TZVPP-gas// UB3LYP-D3/def2-SVP-CPCM(THF)
HF= -4424.94554428170

^3P_B

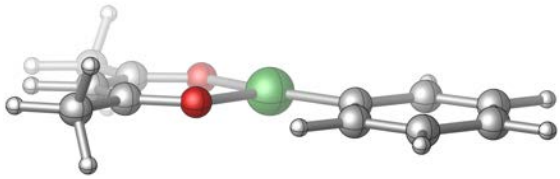


UB3LYP-D3/def2-SVP-CPCM(THF)
Zero-point correction= 0.112925 (Hartree/Particle)
Thermal correction to Energy= 0.124251
Thermal correction to Enthalpy= 0.125196
Thermal correction to Gibbs Free Energy= 0.071801
Sum of electronic and zero-point Energies= -4427.003874
Sum of electronic and thermal Energies= -4426.992547
Sum of electronic and thermal Enthalpies= -4426.991603
Sum of electronic and thermal Free Energies= -4427.044998

C	-4.20757300	-0.40855400	2.63898700
O	-5.19577900	0.33291600	2.31336500
C	-3.26815500	-0.95076300	1.73918100
H	-2.47361500	-1.57001100	2.15421500
C	-3.24996600	-0.71386500	0.34959900
O	-4.10948800	-0.01850100	-0.29141900
C	-2.14189100	-1.29426900	-0.49341100
H	-2.58428600	-1.91486600	-1.28911500
H	-1.60283000	-0.47216300	-0.99154900
H	-1.43116100	-1.89547600	0.08788200
C	-4.07828000	-0.68320200	4.11637000
H	-3.22289600	-1.32584400	4.36080800
H	-3.98111300	0.27525500	4.65145700
H	-5.00727100	-1.15576500	4.47399700
Ni	-5.66814500	0.76594500	0.50679800
Br	-7.78070400	0.13913100	-0.29285100

$\Delta G_{solvation}^{UM06}$= -0.02500545
UB3LYP-D3/def2-TZVPP-CPCM(DMA)// UB3LYP-D3/def2-SVP-CPCM(THF)
HF= -4428.04619084
UM06/def2-TZVPP-CPCM(DMA)// UB3LYP-D3/def2-SVP-CPCM(THF)
HF= -4427.57712008
DLPNO-CCSD(T)/def2-TZVPP-gas// UB3LYP-D3/def2-SVP-CPCM(THF)
HF= -4424.90484789000

^1P_B



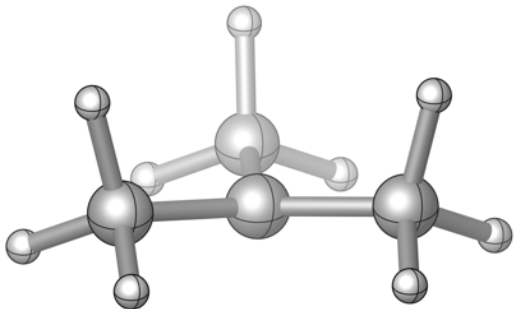
UB3LYP-D3/def2-SVP-CPCM(THF)
Zero-point correction= 0.202049 (Hartree/Particle)
Thermal correction to Energy= 0.216762
Thermal correction to Enthalpy= 0.217706
Thermal correction to Gibbs Free Energy= 0.158091
Sum of electronic and zero-point Energies= -2084.454886
Sum of electronic and thermal Energies= -2084.440173
Sum of electronic and thermal Enthalpies= -2084.439229
Sum of electronic and thermal Free Energies= -2084.498844

C	-3.48194900	-1.13581000	-0.48983600
O	-4.33939100	-0.48231100	-1.17667500
C	-3.70619700	-1.71587200	0.77299500
H	-2.87856800	-2.24759800	1.24151500
C	-4.93100400	-1.65226000	1.47069500
O	-5.97348900	-1.06389700	1.03670900
C	-5.06421500	-2.30948900	2.82250600
H	-5.87443900	-3.05549000	2.78090800
H	-4.13886900	-2.79642700	3.15644800
H	-5.36615700	-1.55135400	3.56309700
C	-2.12617400	-1.26197300	-1.14288800
H	-2.24489600	-1.74270900	-2.12716400
H	-1.72101800	-0.25367500	-1.32600300
H	-1.41193800	-1.83698000	-0.53957300
Ni	-6.12012700	-0.15017800	-0.63501200
C	-6.64257400	0.84499400	-2.17224800
C	-7.98622500	1.26568400	-2.23167400
C	-5.80052100	1.20696400	-3.23827300
C	-8.47194300	2.02031700	-3.30933100
H	-8.67812600	1.00321400	-1.42072400
C	-6.27457400	1.96044600	-4.31967100
H	-4.75447400	0.88763800	-3.21292900
C	-7.61378000	2.37016400	-4.35809600
H	-9.52006300	2.33493900	-3.33048000
H	-5.59874200	2.23079900	-5.13727500
H	-7.98651200	2.95857200	-5.20135600

$\Delta G_{solvation}^{UM06}$= -0.01662909
UB3LYP-D3/def2-TZVPP-CPCM(DMA)// UB3LYP-D3/def2-SVP-CPCM(THF)
HF= -2085.51525078
UM06/def2-TZVPP-CPCM(DMA)// UB3LYP-D3/def2-SVP-CPCM(THF)
HF= -2084.97451907

DLPNO-CCSD(T)/def2-TZVPP-gas// UB3LYP-D3/def2-SVP-CPCM(THF)
HF= -2083.39540036421

***tert*-Butyl radical**

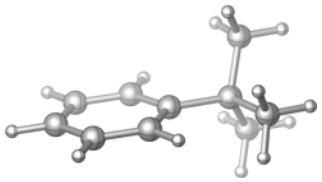


UB3LYP-D3/def2-SVP-CPCM(THF)
Zero-point correction= 0.115524 (Hartree/Particle)
Thermal correction to Energy= 0.121853
Thermal correction to Enthalpy= 0.122797
Thermal correction to Gibbs Free Energy= 0.086138
Sum of electronic and zero-point Energies= -157.575218
Sum of electronic and thermal Energies= -157.568888
Sum of electronic and thermal Enthalpies= -157.567944
Sum of electronic and thermal Free Energies= -157.604604

C	0.05439000	1.47296400	1.28749000
H	1.15371300	1.47939600	1.19271400
H	-0.30833600	2.51095700	1.19567200
H	-0.16750400	1.15507600	2.33125000
C	-2.04795000	0.72978000	0.00109100
H	-2.34155300	1.79222600	-0.04829300
H	-2.34037500	0.24384600	-0.94544000
H	-2.67577200	0.26835000	0.79647700
C	0.05291600	-0.75676200	0.00135100
H	-0.30729100	-1.19427100	-0.94544200
H	1.15254900	-0.68014400	-0.04738600
H	-0.17378700	-1.50250000	0.79647000
C	-0.58858200	0.56453700	0.28731600

$\Delta G_{solvation}^{UM06}$= -0.00051217
UB3LYP-D3/def2-TZVPP-CPCM(DMA)// UB3LYP-D3/def2-SVP-CPCM(THF)
HF= -157.86998506
UM06/def2-TZVPP-CPCM(DMA)// UB3LYP-D3/def2-SVP-CPCM(THF)
HF= -157.72008051
DLPNO-CCSD(T)/def2-TZVPP-gas// UB3LYP-D3/def2-SVP-CPCM(THF)
HF= -157.49166663063

***t*Bu-Ph**

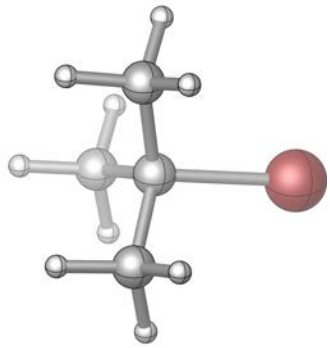


Zero-point correction= 0.212567 (Hartree/Particle)
Thermal correction to Energy= 0.222196
Thermal correction to Enthalpy= 0.223140
Thermal correction to Gibbs Free Energy= 0.178263
Sum of electronic and zero-point Energies= -389.034497
Sum of electronic and thermal Energies= -389.024869
Sum of electronic and thermal Enthalpies= -389.023924
Sum of electronic and thermal Free Energies= -389.068801

C	-2.58176900	1.21472200	0.38690900
C	-1.22824900	1.17869200	-0.00409700
C	-0.63158200	2.39658000	-0.37075900
C	-1.35282800	3.59764200	-0.34863500
C	-2.69310700	3.61187300	0.04204300
C	-3.30571500	2.40859500	0.41120700
H	-3.08621700	0.29102200	0.68019000
H	0.41272100	2.42820900	-0.68195400
H	-0.85703000	4.52750500	-0.64054300
H	-3.25607900	4.54860800	0.05950800
H	-4.35445400	2.39895700	0.72043100
C	-0.47089600	-0.16262400	-0.01661400
C	-0.47838100	-0.76833300	1.40543100
H	0.05896700	-1.73089600	1.41423100
H	0.01717500	-0.09334900	2.12156900
H	-1.50102700	-0.95357000	1.76740000
C	0.99279300	-0.00337300	-0.46382900
H	1.49247000	-0.98475200	-0.45386700
H	1.06693700	0.39712100	-1.48696000
H	1.55563000	0.66298200	0.20845000
C	-1.17186700	-1.13447600	-0.99315200
H	-2.21471300	-1.32907300	-0.69996500
H	-1.17865300	-0.72448000	-2.01584700
H	-0.64427600	-2.10218800	-1.01578600

$\Delta G_{solvation}^{UM06}$= -0.00210233
UB3LYP-D3/def2-TZVPP-CPCM(DMA)// UB3LYP-D3/def2-SVP-CPCM(THF)
HF= -389.32908106
UM06/def2-TZVPP-CPCM(DMA)// UB3LYP-D3/def2-SVP-CPCM(THF)
HF= -389.32942074
DLPNO-CCSD(T)/def2-TZVPP-gas// UB3LYP-D3/def2-SVP-CPCM(THF)
HF= -388.77305156643

***t*Bu-Br**

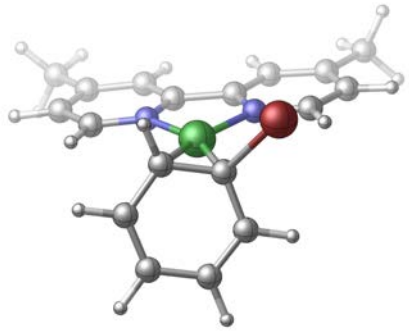


UB3LYP-D3/def2-SVP-CPCM(THF)
Zero-point correction= 0.121383 (Hartree/Particle)
Thermal correction to Energy= 0.127998
Thermal correction to Enthalpy= 0.128942
Thermal correction to Gibbs Free Energy= 0.090831
Sum of electronic and zero-point Energies= -2731.509375
Sum of electronic and thermal Energies= -2731.502760
Sum of electronic and thermal Enthalpies= -2731.501816
Sum of electronic and thermal Free Energies= -2731.539927

C	-0.80126600	0.79228800	-0.05867000
C	-2.32358400	0.83072300	0.00721800
H	-2.69950800	1.86412100	0.00978500
H	-2.72789300	0.31834600	-0.88296400
H	-2.70045000	0.31407300	0.90179900
C	-0.25779100	-0.63025600	0.00764600
H	-0.60744900	-1.18347300	-0.88130800
H	0.84182700	-0.64079900	0.00849400
H	-0.61779200	-1.15675100	0.90345100
C	-0.25801100	1.56088200	-1.25757100
H	-0.62018200	2.59917700	-1.26690400
H	0.84159800	1.56916000	-1.26547000
H	-0.60583300	1.06605800	-2.18093300
Br	-0.11938200	1.75722800	1.61166300

$\Delta G_{solvation}^{UM06}$= -0.00339442shang
UB3LYP-D3/def2-TZVPP-CPCM(THF)// UB3LYP-D3/def2-SVP-CPCM(THF)
HF= -2732.12476199
UM06/def2-TZVPP-CPCM(THF)// UB3LYP-D3/def2-SVP-CPCM(THF)
HF= -2731.85678123
DLPNO-CCSD(T)/def2-TZVPP-gas// UB3LYP-D3/def2-SVP-CPCM(THF)
HF= -2730.27021223902

Figure S4
^{1}F



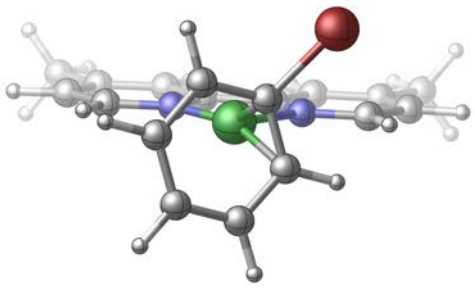
UB3LYP-D3/def2-SVP-CPCM(THF)
$<S^2>$ = 0.0000
Zero-point correction= 0.303924 (Hartree/Particle)
Thermal correction to Energy= 0.325242
Thermal correction to Enthalpy= 0.326187
Thermal correction to Gibbs Free Energy= 0.250047
Sum of electronic and zero-point Energies= -4886.916607
Sum of electronic and thermal Energies= -4886.895289
Sum of electronic and thermal Enthalpies= -4886.894345
Sum of electronic and thermal Free Energies= -4886.970485

C	-2.35713200	0.66818000	1.26433000
C	-2.03043400	-0.65370700	0.71070300
C	-2.62076800	-1.02021400	-0.55416500
C	-3.44410600	-0.14832400	-1.22864300
C	-3.81708500	1.11177900	-0.66154400
C	-3.31437600	1.48551300	0.56283800
Br	-1.96632800	-2.28793700	2.02852200
H	-2.38920200	-2.00165300	-0.97713300
H	-2.27581600	0.83379700	2.34714300
H	-3.66010700	2.41098000	1.03589400
H	-4.52466100	1.75435400	-1.19237200
H	-3.83293100	-0.43097800	-2.21173200
C	2.21375300	0.23800000	0.02640300
C	1.28434400	-1.89145700	0.08627200
C	2.50108900	-2.47921900	-0.24527300
C	3.63211900	-1.67205600	-0.45328500
C	3.46510300	-0.28824000	-0.30866900
C	1.93080300	1.68321100	0.20974400
C	0.27895400	3.23495100	0.72077800
C	1.17039700	4.29550300	0.59312500
C	2.51051000	4.03996100	0.25709500
C	2.87800700	2.70142300	0.06452300
H	0.38679600	-2.48706000	0.26939100

H	2.56598100	-3.56530600	-0.34084200
H	4.31685000	0.37601000	-0.45956400
H	-0.77124200	3.39503000	0.97473900
H	0.82053000	5.31726600	0.75559100
H	3.90785100	2.45862100	-0.19952300
N	1.13741300	-0.56421400	0.21612900
N	0.64473000	1.95767100	0.53838200
Ni	-0.50805500	0.38037200	0.64864600
C	3.49880600	5.16258500	0.09922700
H	4.52387400	4.78948200	-0.03455000
H	3.24147300	5.78012500	-0.77752400
H	3.47932900	5.82800300	0.97684100
C	4.96407200	-2.27782300	-0.80119200
H	5.70898400	-1.51094000	-1.05612000
H	5.35276300	-2.86437800	0.04800500
H	4.86880100	-2.97073500	-1.65217600

UM06/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF)
HF=-4887.748303
UB3LYP-D3/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF)
HF=-4888.625241

^{3}F



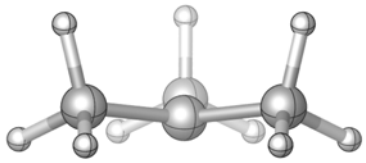
UB3LYP-D3/def2-SVP-CPCM(THF)
Zero-point correction= 0.303037 (Hartree/Particle)
Thermal correction to Energy= 0.324280
Thermal correction to Enthalpy= 0.325224
Thermal correction to Gibbs Free Energy= 0.249695
Sum of electronic and zero-point Energies= -4886.907048
Sum of electronic and thermal Energies= -4886.885805
Sum of electronic and thermal Enthalpies= -4886.884861
Sum of electronic and thermal Free Energies= -4886.960390

C	-2.86004700	0.53399500	1.63679200
C	-2.15805200	-0.57910400	1.08878500
C	-2.26351900	-0.85908500	-0.30596100
C	-3.10501400	-0.04467300	-1.10984200
C	-3.79390400	1.02973300	-0.56253900
C	-3.64814000	1.32896700	0.81157400
Br	-1.52628800	-1.94341300	2.30708200
H	-1.85251500	-1.78191100	-0.71809400
H	-2.77869900	0.74475100	2.70382100
H	-4.16773000	2.18873400	1.24078100
H	-4.43714500	1.64913600	-1.19054800
H	-3.21198200	-0.28990300	-2.16894500
C	2.15628700	0.25623200	-0.12325500
C	1.20467500	-1.89164300	-0.22112200
C	2.43029100	-2.49963900	-0.42579900
C	3.60169000	-1.68391100	-0.48870600
C	3.44226400	-0.31924600	-0.33446200
C	1.90132600	1.65745700	0.05116200
C	0.24662700	3.29745600	0.41826600
C	1.16875300	4.32630100	0.40858600
C	2.55027900	4.01179700	0.20563700
C	2.88970500	2.68307500	0.03207200
H	0.29296100	-2.49250900	-0.15567100
H	2.49366400	-3.58438700	-0.53297200
H	4.31863800	0.33053900	-0.37358800

H	-0.81895300	3.49727300	0.57204000
H	0.84330100	5.35821500	0.55466200
H	3.93614900	2.41393200	-0.12380200
N	1.03958100	-0.56588900	-0.07685900
N	0.57121700	2.00171800	0.24642200
Ni	-0.64075000	0.46304200	0.21118700
C	3.57627900	5.11229600	0.18684700
H	4.59281000	4.72480500	0.02373200
H	3.35484800	5.84380100	-0.60967300
H	3.57029400	5.67354700	1.13742000
C	4.94888900	-2.31570000	-0.71341400
H	5.75680500	-1.56926700	-0.72674000
H	5.17458600	-3.05339200	0.07598500
H	4.97190800	-2.86455500	-1.67084600

UM06/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF)
HF=-4887.7324304
UB3LYP-D3/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF)
HF=-4888.61024

***tert*-butyl radical**

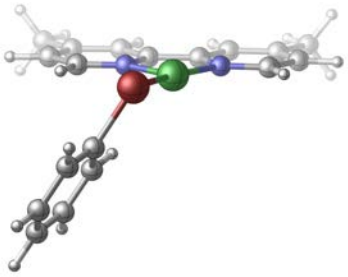


UB3LYP-D3/def2-SVP-CPCM(THF)
Zero-point correction= 0.115524 (Hartree/Particle)
Thermal correction to Energy= 0.121853
Thermal correction to Enthalpy= 0.122797
Thermal correction to Gibbs Free Energy= 0.086138
Sum of electronic and zero-point Energies= -157.575218
Sum of electronic and thermal Energies= -157.568888
Sum of electronic and thermal Enthalpies= -157.567944
Sum of electronic and thermal Free Energies= -157.604604

C	-1.40592600	-5.80885900	-0.81665200
C	-0.76293300	-4.90023200	-1.81663000
H	0.33639100	-4.89385900	-1.72186500
H	-0.98485100	-5.21787700	-2.86045900
H	-1.12562200	-3.86224700	-1.72457600
C	-2.86529500	-5.64365300	-0.53040600
H	-3.49311600	-6.10490200	-1.32589700
H	-3.15773800	-6.12978300	0.41601800
H	-3.15888000	-4.58121200	-0.48079900
C	-0.76445100	-7.13022500	-0.53094900
H	0.33518400	-7.05363400	-0.48219000
H	-1.12467000	-7.56791800	0.41575500
H	-0.99116000	-7.87580100	-1.32621900

UM06/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF)
HF=-157.7200251
UB3LYP-D3/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF)
HF=-157.8699418

^{1}F'



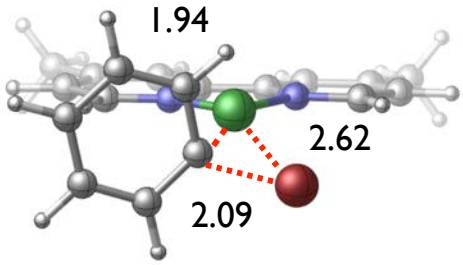
UB3LYP-D3/def2-SVP-CPCM(THF)
<S^2> = 1.0136 (before annihilation, 0.1453 after)
Zero-point correction= 0.303179 (Hartree/Particle)
Thermal correction to Energy= 0.324700
Thermal correction to Enthalpy= 0.325644
Thermal correction to Gibbs Free Energy= 0.249331
Sum of electronic and zero-point Energies= -4886.889735
Sum of electronic and thermal Energies= -4886.868214
Sum of electronic and thermal Enthalpies= -4886.867270
Sum of electronic and thermal Free Energies= -4886.943582

Ni	0.45097900	0.75422500	-0.51615600
C	-2.61923300	1.79943100	0.69437800
C	-3.80753400	2.52186400	0.78846000
C	-2.19830900	0.91052900	1.68156500
C	-4.60388600	2.33902600	1.92544600
H	-4.11043300	3.21117600	-0.00201500
C	-3.00841600	0.74202800	2.80967800
H	-1.26345000	0.35964700	1.56075100
C	-4.20732800	1.45287100	2.93326100
H	-5.53949000	2.89587200	2.01842400
H	-2.69559000	0.04769500	3.59335200
H	-4.83495500	1.31567000	3.81678000
Br	-1.50765300	2.03093300	-0.89197600
N	2.28718000	0.21033200	-0.31399000
C	4.84792900	-0.93207900	0.03142900
C	3.39401500	0.97541600	-0.30108000
C	2.41655000	-1.16425800	-0.14525500
C	3.71534600	-1.72516400	0.02368700
C	4.67452600	0.47726100	-0.13626800
N	0.03521700	-1.16120900	-0.33288500
C	-0.13784100	-3.96464000	-0.05814400
C	-1.15006500	-1.78968900	-0.37876300
C	1.19027000	-1.91125100	-0.16131900

C	1.08842900	-3.32614300	-0.02063400
C	-1.30380400	-3.15959400	-0.24831900
H	3.22394300	2.04850100	-0.43475300
H	3.81785500	-2.80464900	0.15126000
H	5.53174800	1.15357700	-0.13713000
H	-2.01951200	-1.13964800	-0.52399200
H	1.99565600	-3.91758100	0.11796900
H	-2.29792000	-3.60929800	-0.28986200
C	-0.27003300	-5.45646000	0.09238600
H	0.70641800	-5.94504900	0.22688500
H	-0.90393100	-5.71038000	0.95979200
H	-0.75831100	-5.90086800	-0.79227800
C	6.22827000	-1.50473400	0.20983000
H	6.72258100	-1.07366300	1.09787100
H	6.20833200	-2.59852100	0.32607300
H	6.87116100	-1.26235900	-0.65425100

UM06/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF)
HF=-4887.7258715
UB3LYP-D3/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF)
HF=-4888.6064849

^{1}F-TS



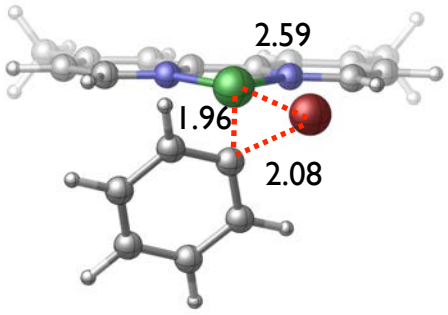
UB3LYP-D3/def2-SVP-CPCM(THF)
Zero-point correction= 0.301918 (Hartree/Particle)
Thermal correction to Energy= 0.322858
Thermal correction to Enthalpy= 0.323802
Thermal correction to Gibbs Free Energy= 0.249700
Sum of electronic and zero-point Energies= -4886.898920
Sum of electronic and thermal Energies= -4886.877980
Sum of electronic and thermal Enthalpies= -4886.877036
Sum of electronic and thermal Free Energies= -4886.951138

C	-2.70242500	-0.07554900	1.35175300
C	-2.48593000	-0.39023000	-0.01498100
C	-3.05621300	0.39728800	-1.04546700
C	-3.73353300	1.55588600	-0.69934200
C	-3.89777500	1.92626000	0.65600600
C	-3.38781700	1.11697300	1.66513800
Br	-2.12202100	-2.41383100	-0.41069800
H	-2.92249600	0.10757100	-2.08902100
H	-2.45280700	-0.78360900	2.14542300
H	-3.54905800	1.37642100	2.71467400
H	-4.44490500	2.83755500	0.90673400
H	-4.13919000	2.19419300	-1.48866800
C	2.19635700	-0.18511600	0.13256200
C	1.61021300	-2.43581700	0.48578500
C	2.91959700	-2.85802600	0.37086400
C	3.94211800	-1.89307300	0.11678500
C	3.55615000	-0.56848700	-0.00168500
C	1.69785800	1.16386500	0.02495300
C	-0.22368200	2.51283400	0.03841500
C	0.51265500	3.67144500	-0.13362700
C	1.93122600	3.58101900	-0.23607400
C	2.50121600	2.32069200	-0.14974900
H	0.79904300	-3.14721000	0.66887500
H	3.16380100	-3.91739100	0.47412500
H	4.30957700	0.19363200	-0.20966200
H	-1.31199400	2.54355600	0.12135900
H	0.00621600	4.63712200	-0.19221500

H	3.58624200	2.21663100	-0.20901400
N	1.23237700	-1.14498000	0.38190200
N	0.32544800	1.28692800	0.10394600
Ni	-0.59521100	-0.44560400	0.41120500
C	2.75756800	4.82441400	-0.42441900
H	3.83290500	4.59969700	-0.47785000
H	2.46931800	5.35042400	-1.35077400
H	2.59448200	5.53480400	0.40408600
C	5.37543700	-2.32903300	-0.02113200
H	6.04717400	-1.47871200	-0.20990800
H	5.72017300	-2.84371400	0.89234900
H	5.49120200	-3.04913900	-0.84959000

UM06/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF)
HF=-4887.7224721
UB3LYP-D3/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF)
HF=-4888.5888467

^{3}F-TS



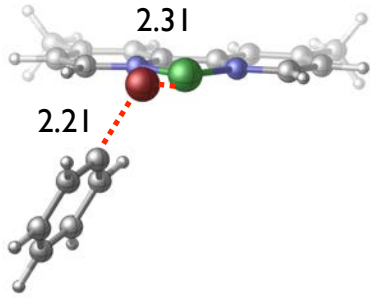
UB3LYP-D3/def2-SVP-CPCM(THF)
Zero-point correction= 0.302378 (Hartree/Particle)
Thermal correction to Energy= 0.323155
Thermal correction to Enthalpy= 0.324099
Thermal correction to Gibbs Free Energy= 0.249623
Sum of electronic and zero-point Energies= -4886.899261
Sum of electronic and thermal Energies= -4886.878484
Sum of electronic and thermal Enthalpies= -4886.877540
Sum of electronic and thermal Free Energies= -4886.952015

C	-2.98196100	0.53763500	1.38884700
C	-2.33565200	-0.52608900	0.72079200
C	-2.36186400	-0.63350000	-0.68707300
C	-2.91143900	0.41192200	-1.42107900
C	-3.48624400	1.52278900	-0.77458900
C	-3.52523800	1.57702300	0.61953700
Br	-2.08238700	-2.26280700	1.84526800
H	-1.90111900	-1.49363900	-1.17414800
H	-3.04337300	0.55394600	2.47831900
H	-3.99362100	2.42496800	1.12564600
H	-3.91880800	2.33250400	-1.36618300
H	-2.89098200	0.36639800	-2.51298700
C	2.05129500	-0.07640600	0.27065900
C	1.46030100	-2.33969800	0.54765700
C	2.64594000	-2.78631300	-0.00664700
C	3.60420100	-1.82406500	-0.45249700
C	3.28789500	-0.48615500	-0.30556800
C	1.64408500	1.28764500	0.46008000
C	-0.06051900	2.71784700	1.23765500
C	0.65030600	3.85620700	0.90591100
C	1.94513700	3.71219100	0.31631600
C	2.41633100	2.43014600	0.10215400
H	0.70141500	-3.04605900	0.89799400
H	2.84014600	-3.85685000	-0.09874500
H	3.99931200	0.27131700	-0.63996600
H	-1.05796400	2.78637800	1.68256700

H	0.22330000	4.84404900	1.09008300
H	3.39904400	2.29004700	-0.35189200
N	1.14828700	-1.03991000	0.69664600
N	0.39751300	1.46825400	1.04211400
Ni	-0.52639600	-0.24001900	1.41846100
C	2.74293800	4.93376200	-0.05191900
H	3.71690200	4.67299800	-0.49169400
H	2.19380200	5.55869000	-0.77748000
H	2.92340600	5.56765700	0.83347900
C	4.90367700	-2.28019500	-1.05894700
H	5.54204100	-1.43300400	-1.35015000
H	5.46934000	-2.91019800	-0.35082700
H	4.72425000	-2.89977300	-1.95472800

UM06/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF)
HF=-4887.7206594
UB3LYP-D3/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF)
HF=-4888.6028485

^{1}F'-TS



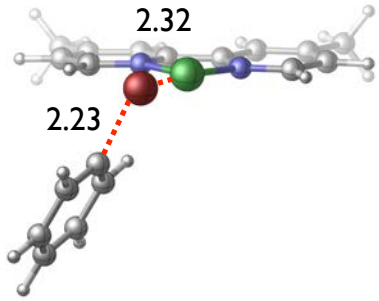
UB3LYP-D3/def2-SVP-CPCM(THF)
Zero-point correction= 0.302070 (Hartree/Particle)
Thermal correction to Energy= 0.323321
Thermal correction to Enthalpy= 0.324265
Thermal correction to Gibbs Free Energy= 0.248135
Sum of electronic and zero-point Energies= -4886.884886
Sum of electronic and thermal Energies= -4886.863635
Sum of electronic and thermal Enthalpies= -4886.862690
Sum of electronic and thermal Free Energies= -4886.938820

Ni	-3.25440100	1.69922200	-0.86461000
C	-6.35073000	2.74589100	0.53308000
C	-7.53839400	3.44711300	0.67417300
C	-5.86220800	1.86132000	1.48043900
C	-8.28028700	3.24455700	1.84917500
H	-7.88972100	4.13539600	-0.10011600
C	-6.61321900	1.66746500	2.64876800
H	-4.91949200	1.33067400	1.30643200
C	-7.81837600	2.35839500	2.83071200
H	-9.22162300	3.78253300	1.99505000
H	-6.25559300	0.97493500	3.41641200
H	-8.40158400	2.20507500	3.74213700
Br	-5.14157500	2.96186900	-1.30211900
N	-1.43673700	1.14855000	-0.56103500
C	1.13037600	0.04417700	-0.13811000
C	-0.33715600	1.93142800	-0.52312200
C	-1.28515500	-0.21011700	-0.37455300
C	0.00054600	-0.76171700	-0.17187300
C	0.93910900	1.44332600	-0.31648700
N	-3.65142800	-0.21949300	-0.60653600
C	-3.85403800	-3.00901400	-0.27941300
C	-4.84620800	-0.83417400	-0.65249500
C	-2.52059100	-0.97139200	-0.40358000
C	-2.61976500	-2.37340400	-0.23952300
C	-5.00368800	-2.20043400	-0.49558900
H	-0.51503800	3.00012000	-0.67276100

H	0.10638300	-1.83949400	-0.03613000
H	1.78764300	2.13053100	-0.29576000
H	-5.70475700	-0.17691700	-0.81941800
H	-1.71623100	-2.96410700	-0.07912700
H	-6.00041000	-2.64452600	-0.53793000
C	-3.99416700	-4.49675500	-0.10296000
H	-3.02112100	-4.98599000	0.04915400
H	-4.63647800	-4.72965900	0.76334700
H	-4.47599200	-4.95299000	-0.98434100
C	2.51010400	-0.51465700	0.07923900
H	2.97467100	-0.07668900	0.97929200
H	2.49559500	-1.60786000	0.19844700
H	3.17260700	-0.26945500	-0.76839500

UM06/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF)
HF=-4887.712787
UB3LYP-D3/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF)
HF=-4888.5994182

^{3}F'-TS



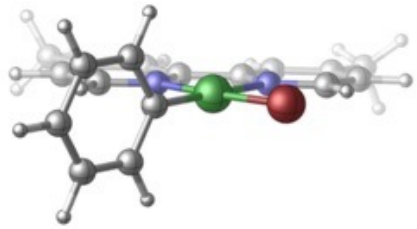
UB3LYP-D3/def2-SVP-CPCM(THF)
Zero-point correction= 0.301975 (Hartree/Particle)
Thermal correction to Energy= 0.323268
Thermal correction to Enthalpy= 0.324212
Thermal correction to Gibbs Free Energy= 0.246893
Sum of electronic and zero-point Energies= -4886.882832
Sum of electronic and thermal Energies= -4886.861540
Sum of electronic and thermal Enthalpies= -4886.860596
Sum of electronic and thermal Free Energies= -4886.937914

Ni	-3.25263800	1.70106100	-0.95983300
C	-6.35184300	2.70762400	0.47578100
C	-7.55100900	3.38369900	0.63666300
C	-5.83505700	1.82269900	1.40707900
C	-8.27458100	3.15564700	1.81877700
H	-7.92568500	4.07211900	-0.12667200
C	-6.56771500	1.60345900	2.58285800
H	-4.88479500	1.31169300	1.21578400
C	-7.78363000	2.26932300	2.78604100
H	-9.22429000	3.67396400	1.98147500
H	-6.18755400	0.91068700	3.33952800
H	-8.35277500	2.09594900	3.70278900
Br	-5.16984200	2.93988300	-1.39971200
N	-1.44440100	1.16785800	-0.57589000
C	1.12337200	0.07844800	-0.12970900
C	-0.34815200	1.95332000	-0.55288900
C	-1.28934600	-0.18483900	-0.37268100
C	-0.00578600	-0.73140600	-0.15506900
C	0.93004300	1.47088600	-0.33441100
N	-3.64223100	-0.21697000	-0.71040900
C	-3.86427200	-2.97683700	-0.19545900
C	-4.83578800	-0.83350300	-0.75824100
C	-2.52536900	-0.95129400	-0.40433400
C	-2.63166100	-2.33606400	-0.14348800
C	-5.00027300	-2.18742000	-0.51776000
H	-0.52837500	3.01905900	-0.71892100

H	0.10223800	-1.80749000	-0.00874000
H	1.77655600	2.16077100	-0.32147800
H	-5.68585400	-0.18916700	-1.00093400
H	-1.73827800	-2.90972000	0.10926100
H	-5.99455300	-2.63537700	-0.57555400
C	-4.01310800	-4.44828300	0.08160900
H	-3.04713800	-4.92357100	0.30576000
H	-4.68840300	-4.61997400	0.93698100
H	-4.46063000	-4.96689600	-0.78309200
C	2.50309700	-0.47512700	0.10090000
H	2.48847200	-1.56499400	0.24673500
H	3.16503000	-0.25058400	-0.75271500
H	2.96709300	-0.01490200	0.98984600

UM06/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF)
HF=-4887.710583
UB3LYP-D3/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF)
HF=-4888.5980175

^{1}G



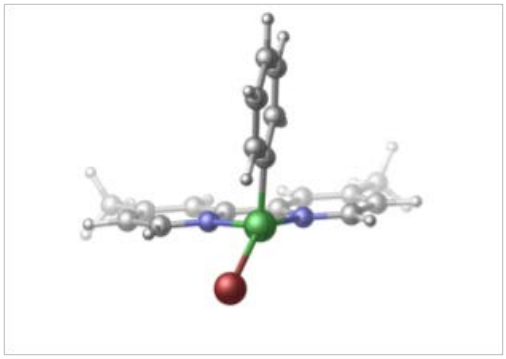
UB3LYP-D3/def2-SVP-CPCM(THF)
<S^2> = 0.0000
Zero-point correction= 0.306236 (Hartree/Particle)
Thermal correction to Energy= 0.327471
Thermal correction to Enthalpy= 0.328416
Thermal correction to Gibbs Free Energy= 0.251298
Sum of electronic and zero-point Energies= -4886.979456
Sum of electronic and thermal Energies= -4886.958220
Sum of electronic and thermal Enthalpies= -4886.957276
Sum of electronic and thermal Free Energies= -4887.034393

Ni	-4.62164100	0.37276900	-0.35551800
C	-6.48961200	0.30741100	-0.60607900
C	-7.09110200	0.71952100	-1.80860200
C	-7.32438700	-0.22393800	0.39359000
C	-8.47025500	0.58409600	-2.01712600
H	-6.47263100	1.15269500	-2.60117700
C	-8.70484800	-0.36076100	0.19395800
H	-6.89063800	-0.54663600	1.34577600
C	-9.28439000	0.04067100	-1.01568600
H	-8.91247300	0.90753700	-2.96479400
H	-9.33112800	-0.78186000	0.98683500
H	-10.36102100	-0.06552000	-1.17536300
Br	-4.86562300	2.59801700	0.38673300
C	-2.08305200	-0.93380400	-0.43222200
C	-0.71910400	-1.20423500	-0.28347300
C	0.14074900	-0.22825800	0.23592100
C	-0.43238600	1.00444300	0.58288700
C	-1.79853600	1.20493800	0.40952800
C	-3.06402100	-1.89823600	-0.97117700
C	-2.72086900	-3.17719700	-1.42003300
C	-3.69785200	-4.04180700	-1.92546000
C	-5.01382400	-3.55700200	-1.95217400
C	-5.29150600	-2.27595300	-1.49150600
H	-0.31683100	-2.17600900	-0.56937000
H	0.18079400	1.81192400	0.98842400
H	-2.28181300	2.14944200	0.66877300
H	-1.68270700	-3.50593000	-1.37942800

H	-5.83107600	-4.17356900	-2.33189100
H	-6.30644800	-1.88304700	-1.50502500
N	-2.61180200	0.26140400	-0.08511500
N	-4.34639000	-1.44945200	-1.00598000
C	1.60662000	-0.49444200	0.43630000
H	1.81183200	-0.69302500	1.50204700
H	1.94610500	-1.36673200	-0.14000000
H	2.21068100	0.37926600	0.14824900
C	-3.36195400	-5.41711900	-2.42902400
H	-3.53113800	-5.47644100	-3.51705900
H	-2.31471700	-5.68322400	-2.22918800
H	-4.01304700	-6.17284000	-1.96195100

UM06/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF)
HF=-4887.8048777
UB3LYP-D3/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF)
HF=-4888.6907597

^{3}G



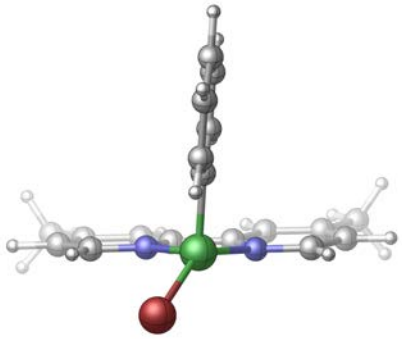
UB3LYP-D3/def2-SVP-CPCM(THF)
Zero-point correction= 0.305000 (Hartree/Particle)
Thermal correction to Energy= 0.326820
Thermal correction to Enthalpy= 0.327764
Thermal correction to Gibbs Free Energy= 0.248330
Sum of electronic and zero-point Energies= -4886.978664
Sum of electronic and thermal Energies= -4886.956844
Sum of electronic and thermal Enthalpies= -4886.955900
Sum of electronic and thermal Free Energies= -4887.035334

C	-1.73044200	0.93421700	-0.63476400
C	-1.87312800	0.01418300	0.42272300
C	-3.09150000	-0.69213400	0.48577300
C	-4.11710000	-0.48980600	-0.44888000
C	-3.94577100	0.43216300	-1.48845600
C	-2.74396600	1.14515500	-1.57994400
Br	-0.88450500	-2.21177200	3.23222000
H	-3.23786100	-1.42479400	1.28704600
H	-0.80136700	1.50807000	-0.73169700
H	-2.59751400	1.86676900	-2.39048300
H	-4.74106900	0.59286600	-2.22222600
H	-5.05158000	-1.05493100	-0.36868500
C	2.01065800	0.06705500	0.27402200
C	1.37737300	-2.16886900	0.19169000
C	2.45861300	-2.49492100	-0.62011900
C	3.36180300	-1.48973000	-1.00624600
C	3.11900900	-0.19089800	-0.54028200
C	1.66580800	1.40468700	0.82149200
C	0.17929400	2.58600300	2.15870500
C	0.84043600	3.78607700	1.92081700
C	1.97024400	3.79875800	1.08551300
C	2.37512800	2.57640700	0.53376900
H	0.65416600	-2.91549900	0.52937300
H	2.59867200	-3.52731600	-0.94686900
H	3.80224600	0.61390500	-0.81193400

H	-0.71171300	2.54155000	2.79011400
H	0.47461800	4.70615700	2.38100800
H	3.24287400	2.54531600	-0.12525700
N	1.16153900	-0.92126200	0.62231300
N	0.58416900	1.42588700	1.62949600
Ni	-0.43901900	-0.35359100	1.74233300
C	2.69511000	5.08093000	0.78436100
H	3.65064800	4.90126000	0.27232000
H	2.07555700	5.72408100	0.13705800
H	2.88953100	5.64723300	1.70840800
C	4.53562400	-1.80355900	-1.89196600
H	5.22460800	-0.95168800	-1.97632800
H	5.09354100	-2.67194100	-1.50816100
H	4.18856300	-2.06632300	-2.90518900

UM06/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF)
HF=-4887.7899161
UB3LYP-D3/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF)
HF=-4888.6853609

^{1}G'



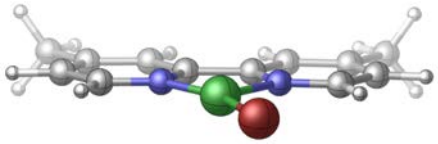
UB3LYP-D3/def2-SVP-CPCM(THF)
<S^2> = 0.9508 (before annihilation, 0.0349 after)
Zero-point correction= 0.304833 (Hartree/Particle)
Thermal correction to Energy= 0.326760
Thermal correction to Enthalpy= 0.327704
Thermal correction to Gibbs Free Energy= 0.247505
Sum of electronic and zero-point Energies= -4886.959643
Sum of electronic and thermal Energies= -4886.937717
Sum of electronic and thermal Enthalpies= -4886.936773
Sum of electronic and thermal Free Energies= -4887.016971

Ni	1.09190800	0.85609700	-1.70045300
C	2.38443500	0.71457900	-0.24778600
C	4.32361600	0.52823400	1.82293400
C	2.00852900	0.65376700	1.10673000
C	3.76251500	0.67514900	-0.53491700
C	4.72335100	0.58681800	0.48277100
C	2.95825500	0.55992200	2.13304300
H	0.94689300	0.67949200	1.37739800
H	4.09105500	0.70806600	-1.57887300
H	5.78794100	0.56005200	0.22846600
H	2.63351000	0.51232000	3.17757600
N	-0.25402700	2.12891000	-0.78486400
C	-2.03722900	3.59640700	0.80378900
C	-0.08589800	3.44506300	-0.61045800
C	-1.28901800	1.50693000	-0.18117900
C	-2.19373900	2.21728500	0.61705300
C	-0.94786200	4.21283200	0.16501000
N	-0.34638900	-0.47557600	-1.12802500
C	-2.39020200	-2.15220500	-0.22052400
C	-0.31543500	-1.78422300	-1.40004300
C	-1.36863100	0.04049700	-0.41723000
C	-2.40540200	-0.77721600	0.04796700
C	-1.30952600	-2.65450600	-0.96577900
H	0.77765700	3.88987600	-1.11133800

H	-3.01999300	1.69972700	1.10459300
H	-0.76936800	5.28462200	0.27348500
H	0.53822100	-2.12410100	-1.99223700
H	-3.23277300	-0.34994300	0.61481500
H	-1.24475100	-3.71689000	-1.20969400
Br	1.96750300	0.21137900	-3.84444000
H	5.06948400	0.45680800	2.61980200
C	-3.48105700	-3.06467300	0.26779900
H	-3.89910200	-3.65146300	-0.56545100
H	-3.07828400	-3.78603900	0.99785100
H	-4.29730700	-2.50768600	0.74835000
C	-2.98421500	4.39357400	1.65712600
H	-3.78647000	3.76897300	2.07386900
H	-2.44347800	4.86833200	2.49191800
H	-3.44307200	5.20520200	1.06971000

UM06/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF)
HF=-4887.7735251
UB3LYP-D3/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF)
HF=-4888.6678698

^{1}F'' (Ni-bromo species)



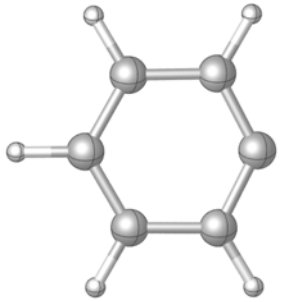
UB3LYP-D3/def2-SVP-CPCM(THF)
Zero-point correction= 0.214708 (Hartree/Particle)
Thermal correction to Energy= 0.230876
Thermal correction to Enthalpy= 0.231820
Thermal correction to Gibbs Free Energy= 0.166322
Sum of electronic and zero-point Energies= -4655.579462
Sum of electronic and thermal Energies= -4655.563294
Sum of electronic and thermal Enthalpies= -4655.562349
Sum of electronic and thermal Free Energies= -4655.627848

Ni	-3.99183200	1.30009300	-1.54653000
C	-1.87359800	-0.39708200	-0.83451100
C	-0.60463100	-0.81497600	-0.41773600
C	0.38038200	0.12429500	-0.09164500
C	0.02971800	1.48282700	-0.20377800
C	-1.24637600	1.83242200	-0.62458000
C	-2.97912600	-1.31121800	-1.19958100
C	-2.90514100	-2.70937500	-1.17420400
C	-4.01531200	-3.47922700	-1.54213400
C	-5.17917400	-2.78948900	-1.92940000
C	-5.18373000	-1.39947400	-1.93172800
H	-0.37768600	-1.87943400	-0.34653600
H	0.75171100	2.26661600	0.03582700
H	-1.54668200	2.87837300	-0.72245500
H	-1.98301600	-3.20525100	-0.86858000
H	-6.07708900	-3.33486700	-2.22820500
H	-6.06484300	-0.82279400	-2.22618200
N	-2.18757800	0.92199600	-0.93709400
N	-4.11313300	-0.67488700	-1.57617200
C	1.75486100	-0.28579000	0.36089600
H	1.95781900	0.09097300	1.37696900
H	1.87445700	-1.37835300	0.36807700
H	2.52660300	0.14347000	-0.29878000
C	-3.97959500	-4.98297800	-1.52479800
H	-2.98906900	-5.36658100	-1.24261000
H	-4.71990400	-5.37924000	-0.81035300
H	-4.24149600	-5.38984900	-2.51492300
Br	-5.83964900	2.56755300	-2.20535500

UM06/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF)
HF=-4656.2756634

UB3LYP-D3/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF)
HF=-4656.9610627

[1]F'' (phenyl radical)

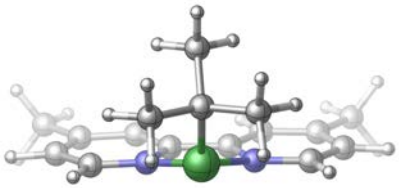


UB3LYP-D3/def2-SVP-CPCM(THF)
Zero-point correction= 0.087289 (Hartree/Particle)
Thermal correction to Energy= 0.091650
Thermal correction to Enthalpy= 0.092595
Thermal correction to Gibbs Free Energy= 0.059244
Sum of electronic and zero-point Energies= -231.315888
Sum of electronic and thermal Energies= -231.311527
Sum of electronic and thermal Enthalpies= -231.310583
Sum of electronic and thermal Free Energies= -231.343933

C	-0.29103800	0.26151900	0.00004900
C	1.08781900	0.18926900	0.00053500
C	1.78056300	1.41499000	-0.00004200
C	1.07310400	2.62406400	-0.00104400
C	-0.32767200	2.63227200	-0.00149100
C	-1.04299800	1.41956500	-0.00093600
H	1.62938100	-0.76109600	0.00131300
H	2.87438700	1.41756800	0.00029600
H	1.61954800	3.57046000	-0.00149000
H	-0.87218400	3.58094900	-0.00227600
H	-2.13682400	1.41357900	-0.00127400

UM06/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF)
HF=-231.4580093
UB3LYP-D3/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF)
HF=-231.6566083

^{2}J



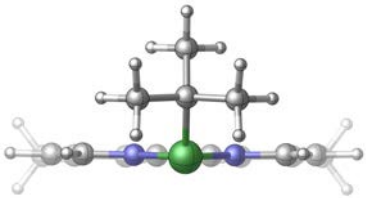
UB3LYP-D3/def2-SVP-CPCM(THF)
Zero-point correction= 0.331279 (Hartree/Particle)
Thermal correction to Energy= 0.351894
Thermal correction to Enthalpy= 0.352838
Thermal correction to Gibbs Free Energy= 0.280022
Sum of electronic and zero-point Energies= -2239.242341
Sum of electronic and thermal Energies= -2239.221726
Sum of electronic and thermal Enthalpies= -2239.220782
Sum of electronic and thermal Free Energies= -2239.293598

Ni	-4.10779300	1.25373400	-1.32019600
C	-5.28347400	2.10080600	0.03079000
C	-5.03401900	1.38406500	1.35564100
H	-5.25906000	0.30620400	1.28131900
H	-3.98154200	1.47642200	1.67430500
H	-5.66375000	1.79496700	2.17789100
C	-6.74299800	1.93257600	-0.39703800
H	-6.94980400	2.42389700	-1.36397600
H	-7.01521500	0.86793600	-0.50344000
H	-7.44565000	2.37383100	0.34714100
C	-4.92890800	3.58415100	0.15262900
H	-3.87438700	3.72864900	0.44643000
H	-5.08315600	4.12523800	-0.79738700
H	-5.55196400	4.09679500	0.92164600
C	-1.89191700	-0.41456100	-0.88502500
C	-0.61814100	-0.81574800	-0.41270300
C	0.35899600	0.12005500	-0.11030600
C	0.02631300	1.49591800	-0.28126800
C	-1.23753900	1.83555500	-0.71914600
C	-2.96893100	-1.31088500	-1.24418800
C	-2.91389500	-2.72433300	-1.16927600
C	-3.99501600	-3.50287200	-1.55282100
C	-5.16206000	-2.82501300	-2.01248100
C	-5.17490100	-1.44531200	-2.04011900
H	-0.40127800	-1.87823200	-0.28847900
H	0.75671600	2.27789200	-0.06274800
H	-1.53394200	2.88224600	-0.83746600
H	-2.00592900	-3.20789700	-0.80444100
H	-6.04307800	-3.38544700	-2.33253800

H	-6.06335400	-0.89367900	-2.36210800
N	-2.18708600	0.92479600	-1.02438100
N	-4.11948700	-0.68522600	-1.67555800
C	1.72370800	-0.27320800	0.38598300
H	1.91667200	0.15250000	1.38561100
H	1.83814000	-1.36510800	0.45040600
H	2.51186200	0.11755900	-0.28004500
C	-3.96763700	-5.00572600	-1.48791700
H	-2.99793700	-5.38363700	-1.13244600
H	-4.75292300	-5.38446500	-0.81138900
H	-4.16727900	-5.44621100	-2.47965200

UM06/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF)
HF=-2239.8687984
UB3LYP-D3/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF)
HF=-2240.5868708

^{4}J



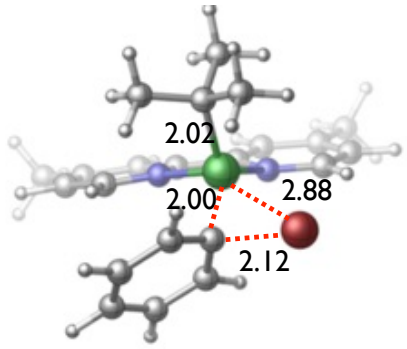
UB3LYP-D3/def2-SVP-CPCM(THF)
Zero-point correction= 0.331122 (Hartree/Particle)
Thermal correction to Energy= 0.351753
Thermal correction to Enthalpy= 0.352697
Thermal correction to Gibbs Free Energy= 0.279075
Sum of electronic and zero-point Energies= -2239.236155
Sum of electronic and thermal Energies= -2239.215524
Sum of electronic and thermal Enthalpies= -2239.214580
Sum of electronic and thermal Free Energies= -2239.288203

Ni	-4.11364400	1.25171300	-1.35136700
C	-5.30943000	2.15278900	-0.05189500
C	-5.12379100	1.41771900	1.27095000
H	-5.39083100	0.35173000	1.17915700
H	-4.07610200	1.46491900	1.61216600
H	-5.75620800	1.85139700	2.07662700
C	-6.75210500	2.03935200	-0.54491100
H	-6.89621400	2.53596100	-1.51987700
H	-7.06181300	0.98624900	-0.65716300
H	-7.46358700	2.51074500	0.16894000
C	-4.88469300	3.61585700	0.07013500
H	-3.83618700	3.70884700	0.40156800
H	-4.98128000	4.15545000	-0.88780900
H	-5.50788100	4.15995300	0.81427700
C	-1.91951800	-0.43473700	-0.77691700
C	-0.59133900	-0.83128600	-0.44384100
C	0.37256900	0.10003800	-0.10652300
C	-0.00177800	1.48126100	-0.10583800
C	-1.29654900	1.81858100	-0.45309700
C	-2.98536800	-1.32921200	-1.12487800
C	-2.87841100	-2.74941200	-1.18917800
C	-3.96492000	-3.53686600	-1.52063800
C	-5.20546100	-2.88212200	-1.80354600
C	-5.25574700	-1.50197000	-1.74635900
H	-0.33246100	-1.89167700	-0.45113800
H	0.71715700	2.25835400	0.16045200
H	-1.61984100	2.86445500	-0.47338200
H	-1.92065000	-3.22417300	-0.96819200
H	-6.09774700	-3.45525900	-2.06244500

H	-6.18319900	-0.96266000	-1.96463600
N	-2.23720000	0.91623900	-0.78353100
N	-4.20098500	-0.73186300	-1.42625700
C	1.77899500	-0.29547500	0.25316800
H	2.03975500	0.05842200	1.26556500
H	1.92119900	-1.38575800	0.22253200
H	2.50625700	0.16658900	-0.43672600
C	-3.87769300	-5.03726600	-1.58960400
H	-2.86973500	-5.40369900	-1.34554800
H	-4.59329800	-5.50453600	-0.89112100
H	-4.14191300	-5.40041900	-2.59786800

UM06/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF)
HF=-2239.8575927
UB3LYP-D3/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF)
HF=-2240.5786207

^{2}K-TS



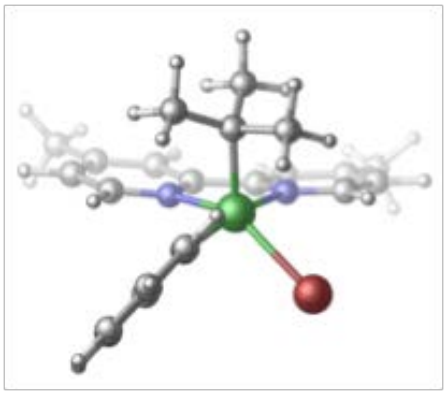
UB3LYP-D3/def2-SVP-CPCM(THF)
Zero-point correction= 0.422956 (Hartree/Particle)
Thermal correction to Energy= 0.450436
Thermal correction to Enthalpy= 0.451380
Thermal correction to Gibbs Free Energy= 0.361910
Sum of electronic and zero-point Energies= -5044.524684
Sum of electronic and thermal Energies= -5044.497204
Sum of electronic and thermal Enthalpies= -5044.496260
Sum of electronic and thermal Free Energies= -5044.585730

Ni	-0.56887500	-0.10884500	0.03179700
C	-2.00773300	0.73061800	-1.07367400
C	-1.81809100	3.47023400	-1.69584400
C	-2.92075100	1.65519000	-0.50062400
C	-1.11674800	1.17633300	-2.09208400
C	-1.00348100	2.54641200	-2.35490100
C	-2.78829100	3.00870100	-0.78061000
H	-3.67843900	1.30166500	0.19970900
H	-0.51865100	0.45366200	-2.64898900
H	-0.27773300	2.88665100	-3.09898500
H	-3.44890000	3.72264300	-0.28033800
N	0.96824900	1.25462800	0.18035100
C	3.21273000	2.93003500	0.37307900
C	0.83008500	2.54873000	0.50132000
C	2.20297300	0.76608600	-0.07367600
C	3.34015400	1.58115100	0.02500900
C	1.91223300	3.41398800	0.60596400
N	1.02235400	-1.20962300	-0.72080700
C	3.36186200	-2.72388100	-1.08916100
C	0.95766700	-2.48795200	-1.12680000
C	2.23627000	-0.65439000	-0.49338800
C	3.41657000	-1.39275300	-0.66507600
C	2.08643100	-3.27123000	-1.32808200
H	-0.19249800	2.89070500	0.66852000
H	4.32833000	1.17240700	-0.18817700

H	1.74447000	4.46123100	0.86657200
H	-0.04933300	-2.87875200	-1.29817400
H	4.38455800	-0.93335800	-0.46190100
H	1.97710300	-4.30344700	-1.66790300
Br	-2.75469400	-1.21241800	-1.48193200
C	-1.25942500	-0.30913100	1.91997700
H	-1.73267300	4.53737400	-1.91319300
C	4.60421000	-3.55062400	-1.27741800
H	5.51773900	-2.95597000	-1.13619400
H	4.62398100	-4.38736500	-0.55940500
H	4.62857200	-3.99435000	-2.28578400
C	4.40757900	3.83624900	0.49373300
H	4.53584500	4.16752900	1.53775800
H	5.33438400	3.33736200	0.17694300
H	4.27328200	4.74427900	-0.11569700
C	-0.10593600	-1.08166100	2.57143300
H	-0.28871200	-1.26294300	3.65582700
H	0.04439400	-2.07046200	2.10401900
H	0.85066700	-0.53464100	2.49801600
C	-2.54257900	-1.12746400	2.00560400
H	-3.39265400	-0.61222000	1.52877500
H	-2.44129500	-2.10488300	1.50598200
H	-2.83192800	-1.32398200	3.06326500
C	-1.44613300	1.02819800	2.62310500
H	-0.50872100	1.60684200	2.65959400
H	-2.20175500	1.65594800	2.12145600
H	-1.78013400	0.89735600	3.67747900

UM06/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF)
HF=-5045.4850601
UB3LYP-D3/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF)
HF=-5046.5185177

^{2}H



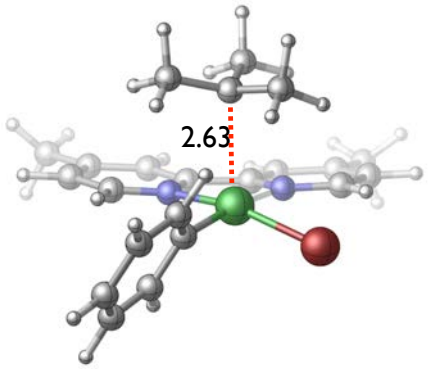
UB3LYP-D3/def2-SVP-CPCM(THF)
Zero-point correction= 0.427053 (Hartree/Particle)
Thermal correction to Energy= 0.454642
Thermal correction to Enthalpy= 0.455586
Thermal correction to Gibbs Free Energy= 0.366581
Sum of electronic and zero-point Energies= -5044.574659
Sum of electronic and thermal Energies= -5044.547070
Sum of electronic and thermal Enthalpies= -5044.546126
Sum of electronic and thermal Free Energies= -5044.635131

Ni	-0.56337000	-0.04631900	0.09841600
C	-1.85804600	1.35728300	-0.24505500
C	-3.52873200	3.40894600	-1.28522000
C	-3.21390200	1.44004700	0.10238600
C	-1.36915700	2.30647500	-1.16099100
C	-2.18768500	3.32555400	-1.66969900
C	-4.04026600	2.45236000	-0.40091300
H	-3.65663600	0.70026200	0.77209900
H	-0.33487500	2.25428800	-1.51272900
H	-1.77097400	4.05105900	-2.37504500
H	-5.09288800	2.48722500	-0.10395600
N	1.18278400	1.17021700	0.40025100
C	3.58866200	2.49028000	1.00364600
C	1.18840300	2.46208000	0.75018400
C	2.35080400	0.49932700	0.36745100
C	3.56597200	1.13467400	0.65549500
C	2.35389800	3.15589100	1.05841300
N	0.98567200	-1.44060000	0.01814400
C	3.18735400	-3.15570700	-0.31343600
C	0.81036500	-2.75503700	-0.17462800
C	2.24156800	-0.95071800	0.06963400
C	3.35492100	-1.78141500	-0.10891200
C	1.87055000	-3.64127200	-0.32900300
H	0.21530000	2.95470900	0.77867800

H	4.50024400	0.57419700	0.62972700
H	2.29688100	4.20930500	1.34012000
H	-0.22492700	-3.09449300	-0.22423700
H	4.36042800	-1.36177600	-0.09062700
H	1.66697900	-4.70462200	-0.47039500
Br	-1.71056300	-1.32864000	-1.79047600
C	-1.01599900	-0.24129500	2.08666000
H	-4.17092500	4.20206200	-1.67755800
C	4.35962500	-4.07147500	-0.52983600
H	5.30517400	-3.60717500	-0.21595500
H	4.22852600	-5.01710600	0.01787800
H	4.44652500	-4.32663800	-1.59967900
C	4.87320000	3.21007200	1.30667700
H	4.79438000	3.77049200	2.25134900
H	5.72470600	2.51890000	1.37659300
H	5.09240900	3.94510400	0.51426800
C	0.22707200	-0.77930600	2.79634400
H	-0.00940400	-0.91046400	3.87057900
H	0.55316300	-1.75566600	2.41804000
H	1.07501900	-0.08110100	2.74214300
C	-2.10117100	-1.30721300	2.02841900
H	-2.99088000	-0.97953000	1.47438100
H	-1.73718700	-2.23009000	1.55095900
H	-2.42666400	-1.57395900	3.05447600
C	-1.45739800	1.03009500	2.80018200
H	-0.67484600	1.80304400	2.75646200
H	-2.38075100	1.46045700	2.39947000
H	-1.63209800	0.80641000	3.87152200

UM06/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF)
HF=-5045.5318625
UB3LYP-D3/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF)
HF=-5046.574292

^{2}H-TS



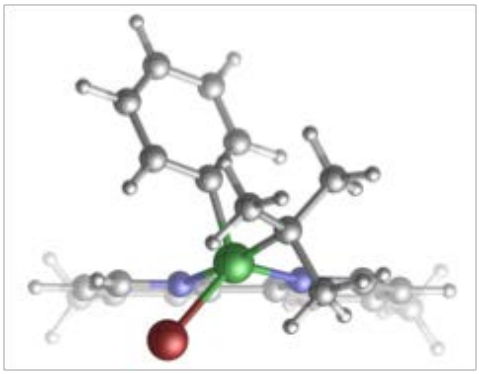
UB3LYP-D3/def2-SVP-CPCM(THF)
Zero-point correction= 0.425172 (Hartree/Particle)
Thermal correction to Energy= 0.452637
Thermal correction to Enthalpy= 0.453581
Thermal correction to Gibbs Free Energy= 0.364426
Sum of electronic and zero-point Energies= -5044.568901
Sum of electronic and thermal Energies= -5044.541436
Sum of electronic and thermal Enthalpies= -5044.540492
Sum of electronic and thermal Free Energies= -5044.629648

Ni	-0.46974300	0.02068700	-0.41675500
C	-1.67999300	1.47643000	-0.71360400
C	-3.33826900	3.67087900	-1.45007500
C	-2.93718800	1.67823500	-0.11874800
C	-1.29229400	2.39258900	-1.71215700
C	-2.10400800	3.47523700	-2.07868300
C	-3.75171000	2.76341500	-0.46731700
H	-3.30482800	0.96789700	0.62514800
H	-0.32764400	2.26819500	-2.21592700
H	-1.76874500	4.16777600	-2.85720600
H	-4.72066300	2.89393800	0.02480100
N	1.12230200	1.19482600	0.05908800
C	3.44215700	2.57769300	0.86492300
C	1.07213100	2.49079000	0.40411800
C	2.31387300	0.55519600	0.12799900
C	3.48031900	1.22225200	0.51855700
C	2.19097300	3.20998100	0.80897500
N	1.02820200	-1.38687300	-0.39265100
C	3.26845500	-3.08892800	-0.43383200
C	0.88870200	-2.70292700	-0.60348100
C	2.26766600	-0.89109600	-0.17997300
C	3.39905200	-1.71348400	-0.20709000
C	1.96801900	-3.58059600	-0.62304700
H	0.09083200	2.95996400	0.35015300

H	4.42582100	0.68308600	0.57120700
H	2.08068200	4.26147400	1.08174800
H	-0.13439700	-3.04380200	-0.77330200
H	4.38996300	-1.28850400	-0.04812700
H	1.79076100	-4.64487400	-0.79103100
Br	-2.06051700	-1.42111000	-1.56489200
C	-0.76489300	-0.35275700	2.17087200
H	-3.97441700	4.51618300	-1.72696000
C	4.46631600	-3.99507300	-0.49511200
H	5.33972900	-3.55120300	0.00358500
H	4.25037000	-4.97063000	-0.03427000
H	4.74108900	-4.18581400	-1.54668100
C	4.68127100	3.32656200	1.26822300
H	4.47905600	3.99892200	2.11576100
H	5.49923900	2.64542300	1.54252400
H	5.03122800	3.95568200	0.43210800
C	0.50842700	-0.98541500	2.66028000
H	0.42913300	-1.17567500	3.75235700
H	0.71453000	-1.95213600	2.17918200
H	1.38256900	-0.32989800	2.52195900
C	-1.93737800	-1.28175200	2.04413200
H	-2.79048300	-0.81209200	1.53520400
H	-1.67886300	-2.18943100	1.47926000
H	-2.28243400	-1.59901300	3.05304200
C	-1.03843600	1.00820600	2.74490500
H	-0.15733500	1.66519500	2.67936800
H	-1.88232000	1.51224100	2.25590000
H	-1.28787500	0.91589500	3.82446800

UM06/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF)
HF=-5045.5308871
UB3LYP-D3/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF)
HF=-5046.5693344

^{2}H'



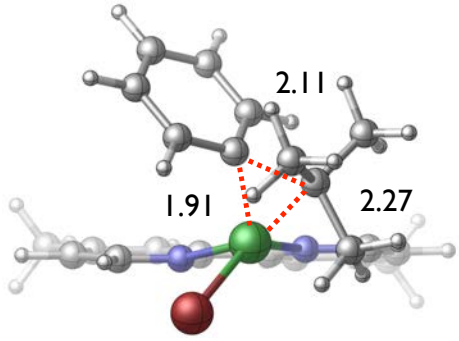
UB3LYP-D3/def2-SVP-CPCM(THF)
Zero-point correction= 0.427088 (Hartree/Particle)
Thermal correction to Energy= 0.454746
Thermal correction to Enthalpy= 0.455691
Thermal correction to Gibbs Free Energy= 0.366759
Sum of electronic and zero-point Energies= -5044.582270
Sum of electronic and thermal Energies= -5044.554611
Sum of electronic and thermal Enthalpies= -5044.553667
Sum of electronic and thermal Free Energies= -5044.642599

C	2.72335600	0.70789700	0.18970800
C	3.75298800	-0.41261300	0.27880000
C	2.97297200	1.55139000	-1.06760500
H	3.70918900	-1.07763500	-0.59404700
H	3.61723800	-1.01751200	1.18615500
H	3.11295700	0.91777900	-1.95212800
H	2.16471200	2.26014100	-1.30123400
C	-1.70961900	1.57648700	-0.04686300
C	-2.65033500	2.60378800	0.11017800
C	-2.24023100	3.93516500	0.23146300
C	-0.85950600	4.17639400	0.18311300
C	0.01525300	3.10655200	0.02942200
C	-2.10728300	0.15486800	-0.20310600
C	-3.43402400	-0.28925800	-0.10788500
C	-3.73664600	-1.64641600	-0.26159800
C	-2.66328500	-2.51620700	-0.51343200
C	-1.37323800	-2.00530300	-0.59468700
H	-3.71474700	2.37279300	0.12957800
H	-0.46145000	5.18998600	0.26278000
H	1.08852400	3.28660900	-0.00950700
H	-4.23973900	0.41575000	0.09379700
H	-2.82910800	-3.58791500	-0.64141200
H	-0.51253300	-2.64608700	-0.79182700
N	-0.38202400	1.83068500	-0.07700800
N	-1.10205500	-0.70319200	-0.44673700

Br	1.50064300	-1.34350900	-2.30830600
Ni	0.86324300	0.01931200	-0.25483600
C	0.82842000	-0.73700000	1.51091600
C	0.23013700	-0.08929800	2.59837300
C	1.21218600	-2.07747200	1.64691200
C	0.02519700	-0.76720800	3.80788300
H	-0.07727800	0.95631400	2.50930000
C	1.00946900	-2.75990800	2.85462700
H	1.67143400	-2.59586100	0.79964700
H	-0.44213800	-0.24725900	4.64978200
H	1.31577900	-3.80640300	2.94602500
C	0.41579000	-2.10526800	3.94016600
H	0.25773600	-2.63455900	4.88374000
C	-3.22289900	5.06030200	0.39531800
H	-3.13734000	5.77041300	-0.44331400
H	-4.25907000	4.69732800	0.43832600
H	-3.01158100	5.62624400	1.31685800
C	-5.14604400	-2.16100000	-0.16329600
H	-5.45402400	-2.62397900	-1.11504700
H	-5.22023800	-2.94123900	0.61121900
H	-5.85899800	-1.36057200	0.07871800
H	4.76852300	0.02874600	0.32310300
H	3.89106400	2.15487300	-0.92408400
C	2.77608100	1.55777200	1.45779800
H	1.92937700	2.24961100	1.55717100
H	2.78584400	0.93211000	2.36012000
H	3.70125000	2.16594700	1.45988300

UM06/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF)
HF=-5045.5387051
UB3LYP-D3/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF)
HF=-5046.5811753

^{2}I'-TS



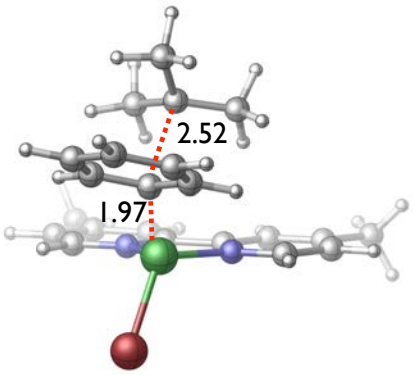
UB3LYP-D3/def2-SVP-CPCM(THF)
Zero-point correction= 0.426807 (Hartree/Particle)
Thermal correction to Energy= 0.453769
Thermal correction to Enthalpy= 0.454713
Thermal correction to Gibbs Free Energy= 0.366959
Sum of electronic and zero-point Energies= -5044.567409
Sum of electronic and thermal Energies= -5044.540447
Sum of electronic and thermal Enthalpies= -5044.539502
Sum of electronic and thermal Free Energies= -5044.627257

C	2.47756700	0.52963500	0.50619500
C	3.59074200	-0.50541300	0.62937500
C	2.69296100	1.27633000	-0.83597600
H	3.50650100	-1.27055700	-0.15537000
H	3.59625100	-0.99952600	1.61104300
H	2.89116500	0.58777800	-1.66519700
H	1.87756200	1.94478300	-1.14710300
C	-2.00954800	1.50230600	-0.13993600
C	-2.94484600	2.52885500	0.05036000
C	-2.53057300	3.85937000	0.16696800
C	-1.15101300	4.10093700	0.08094300
C	-0.28187800	3.03329200	-0.11364300
C	-2.40652900	0.07676900	-0.26387500
C	-3.70782000	-0.38689300	-0.02447700
C	-4.00335400	-1.74934200	-0.14650300
C	-2.94968800	-2.60226100	-0.51360000
C	-1.68261200	-2.07229100	-0.73146100
H	-4.00836400	2.29638700	0.09838000
H	-0.75091100	5.11370200	0.16189500
H	0.79136600	3.21327800	-0.18329100
H	-4.49584300	0.30491700	0.27245700
H	-3.11289100	-3.67649700	-0.62411400
H	-0.83301300	-2.69688500	-1.01558600
N	-0.68378500	1.75827400	-0.22123600
N	-1.41708500	-0.76567600	-0.61231500

Br	1.40168200	-1.60311700	-2.29320600
Ni	0.51705700	-0.02284900	-0.48947000
C	0.89376300	-0.62924200	1.28296600
C	0.15210500	-0.03739800	2.32491800
C	1.14006200	-2.01494600	1.35357400
C	-0.36135300	-0.80750500	3.37237100
H	-0.05846300	1.03243100	2.30102800
C	0.62738700	-2.78433700	2.40279400
H	1.69961200	-2.49969600	0.55288600
H	-0.95334000	-0.32388900	4.15510200
H	0.81577700	-3.86192800	2.42004200
C	-0.12792600	-2.18770600	3.41948900
H	-0.52755500	-2.78946600	4.23983300
C	-3.50767800	4.98413300	0.36577100
H	-3.45621400	5.69224200	-0.47742700
H	-4.54096600	4.61980500	0.44926900
H	-3.26263800	5.55310700	1.27705300
C	-5.38404000	-2.28838400	0.10891100
H	-5.77387800	-2.79393300	-0.78952600
H	-5.36298100	-3.03958400	0.91507700
H	-6.08872000	-1.49437900	0.39309300
H	4.56567300	0.00058500	0.50057000
H	3.58393500	1.92378900	-0.71775000
C	2.55206500	1.54057900	1.64884500
H	1.72780400	2.26708000	1.62507400
H	2.54372100	1.05494100	2.63426500
H	3.49408500	2.11235900	1.56275600

UM06/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF)
HF=-5045.5303702
UB3LYP-D3/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF)
HF=-5046.5662454

^{2}I-TS



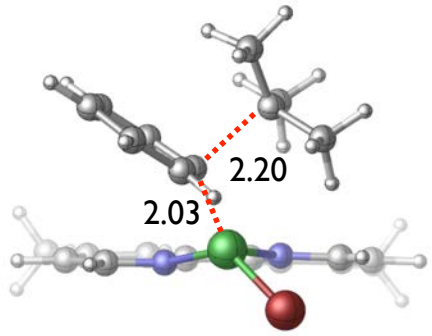
UB3LYP-D3/def2-SVP-CPCM(THF)
Zero-point correction= 0.422563 (Hartree/Particle)
Thermal correction to Energy= 0.451102
Thermal correction to Enthalpy= 0.452046
Thermal correction to Gibbs Free Energy= 0.358259
Sum of electronic and zero-point Energies= -5044.535437
Sum of electronic and thermal Energies= -5044.506898
Sum of electronic and thermal Enthalpies= -5044.505954
Sum of electronic and thermal Free Energies= -5044.599741

Ni	1.15698000	0.80313900	-0.58477500
C	2.32848100	0.33814200	0.92428500
C	5.11920600	0.20086500	1.49479100
C	3.04155200	1.45126300	1.43037300
C	3.07877700	-0.84127500	0.69778300
C	4.44572700	-0.91665100	0.98020600
C	4.40990400	1.38942900	1.71551000
H	2.50862100	2.39036600	1.62008700
H	2.57443100	-1.73002300	0.30029100
H	4.99329200	-1.84687500	0.79755300
H	4.92832600	2.26924700	2.11004400
N	-0.40671000	1.93537300	0.04765400
C	-2.69659900	3.26224200	0.96611900
C	-0.33012700	3.19445800	0.49328600
C	-1.60084200	1.30443100	0.03778200
C	-2.75851900	1.94552700	0.49241800
C	-1.43981300	3.89018500	0.96037900
N	-0.34382800	-0.53554700	-0.82382800
C	-2.55499400	-2.24308600	-1.00356100
C	-0.20010200	-1.78530500	-1.27722900
C	-1.56646500	-0.09342900	-0.46128400
C	-2.68807300	-0.92631400	-0.54461700
C	-1.26934200	-2.66854900	-1.37809500
H	0.66285300	3.65020900	0.47535400

H	-3.71494700	1.42282200	0.48486800
H	-1.32455100	4.91485400	1.31930300
H	0.81230000	-2.07394900	-1.57021900
H	-3.67063500	-0.55699600	-0.25052300
H	-1.10182100	-3.68134400	-1.74991400
Br	2.04109800	1.26858800	-2.81423400
C	0.90892800	-0.32085900	2.89960800
C	2.06565600	-0.62608100	3.80419000
C	0.14137600	0.92248900	3.22797600
H	2.70749700	0.25543600	3.95657700
H	2.69217600	-1.43948000	3.40736200
H	0.79502900	1.81017100	3.24348300
H	-0.67731400	1.10772600	2.52043400
H	6.18789400	0.14581000	1.71989400
C	-3.73205600	-3.17533400	-1.08137800
H	-3.75552200	-3.69814800	-2.05004800
H	-3.65572600	-3.94915500	-0.29912400
H	-4.68451900	-2.64474300	-0.94359900
C	-3.92289200	3.98596800	1.44833600
H	-4.78181200	3.30884900	1.55526400
H	-3.73480200	4.47411400	2.41718100
H	-4.20010800	4.78067500	0.73558800
C	0.14094900	-1.50531600	2.39991100
H	-0.66437500	-1.21879700	1.71091100
H	0.79774500	-2.22523500	1.88452900
H	-0.33165900	-2.05264400	3.24444900
H	-0.31389900	0.84612700	4.23935000
H	1.69877500	-0.94589100	4.80346700

UM06/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF)
HF=-5045.4957062
UB3LYP-D3/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF)
HF=-5046.5367812

^{4}I-TS



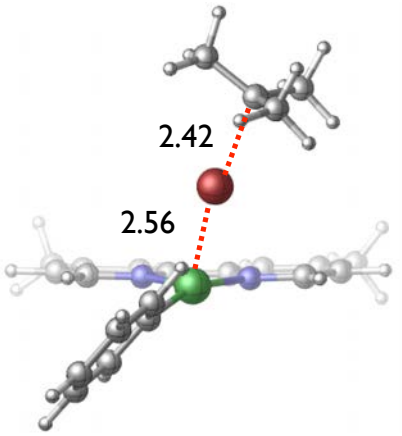
UB3LYP-D3/def2-SVP-CPCM(THF)
Zero-point correction= 0.423090 (Hartree/Particle)
Thermal correction to Energy= 0.450907
Thermal correction to Enthalpy= 0.451851
Thermal correction to Gibbs Free Energy= 0.361396
Sum of electronic and zero-point Energies= -5044.542031
Sum of electronic and thermal Energies= -5044.514215
Sum of electronic and thermal Enthalpies= -5044.513270
Sum of electronic and thermal Free Energies= -5044.603726

Ni	1.00135600	1.42580000	0.04129900
C	2.02000000	0.07814700	1.17453600
C	3.93315500	-2.07728400	1.15319100
C	3.43288500	0.29828400	1.02085000
C	1.63092500	-1.30446900	1.21498900
C	2.55286200	-2.34444500	1.23634800
C	4.35898900	-0.74276500	1.03278300
H	3.79393400	1.32489200	0.90185400
H	0.56512100	-1.55255200	1.24828500
H	2.20252300	-3.38075100	1.29090300
H	5.42643100	-0.52063300	0.92890300
N	-0.89401700	2.03940500	0.51380700
C	-3.56934600	2.63784800	1.09908700
C	-1.21167500	3.15802500	1.18217100
C	-1.87998700	1.21421900	0.09068800
C	-3.22327800	1.48924400	0.38009700
C	-2.52195100	3.49173000	1.49550500
N	-0.09733200	0.04534000	-0.98052000
C	-1.72321000	-2.06579300	-1.84944700
C	0.42587200	-0.97644000	-1.67241200
C	-1.41869300	0.04577700	-0.68977000
C	-2.24981100	-0.99990400	-1.11028500
C	-0.34489300	-2.03680300	-2.13142800
H	-0.37158200	3.79948600	1.45667900
H	-4.00678500	0.81553400	0.03241500

H	-2.72889600	4.41386500	2.04218700
H	1.50289900	-0.93420300	-1.84772000
H	-3.31006400	-0.99346900	-0.85626500
H	0.12601800	-2.84155600	-2.69960600
Br	2.10369000	3.55939100	-0.38470900
C	1.60926300	0.73058300	3.23513900
C	2.54956500	-0.10886100	4.05616600
C	1.93791500	2.19806400	3.21829800
H	3.60092400	0.08623000	3.79444600
H	2.35480700	-1.18411500	3.92224600
H	2.99142400	2.37533000	2.95440400
H	1.32098100	2.75065800	2.49722400
H	4.65885800	-2.89498300	1.15903700
C	-2.58235200	-3.20804900	-2.31633900
H	-3.63844800	-3.06244600	-2.04961600
H	-2.51152600	-3.32503800	-3.40984200
H	-2.23976200	-4.15626900	-1.87026900
C	-4.99807700	2.96615500	1.43148300
H	-5.69656700	2.22517400	1.01846500
H	-5.13933800	3.00560100	2.52409000
H	-5.26879600	3.95941000	1.03818500
C	0.15182100	0.40560400	3.42019600
H	-0.46414900	0.87526500	2.64206100
H	-0.02996500	-0.67959200	3.39789400
H	-0.20509700	0.78000400	4.40156300
H	1.76418400	2.64050000	4.22078000
H	2.42471500	0.12233500	5.13414200

UM06/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF)
HF=-5045.4932847
UB3LYP-D3/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF)
HF=-5046.5389644

^{2}L-TS



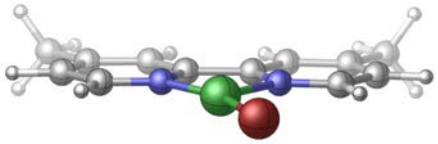
UB3LYP-D3/def2-SVP-CPCM(THF)
Zero-point correction= 0.422923 (Hartree/Particle)
Thermal correction to Energy= 0.451544
Thermal correction to Enthalpy= 0.452488
Thermal correction to Gibbs Free Energy= 0.356259
Sum of electronic and zero-point Energies= -5044.541704
Sum of electronic and thermal Energies= -5044.513083
Sum of electronic and thermal Enthalpies= -5044.512138
Sum of electronic and thermal Free Energies= -5044.608368

Ni	-0.42182000	0.28394900	0.52338800
C	-1.80483100	1.59839400	0.08222800
C	-3.75127500	3.55126000	-0.71046800
C	-3.11085500	1.62512200	0.62313500
C	-1.52534800	2.60154000	-0.87716700
C	-2.46877300	3.56119400	-1.27153000
C	-4.06879200	2.57418800	0.24189900
H	-3.38188200	0.88078600	1.38049600
H	-0.52897400	2.64102100	-1.33505300
H	-2.20361700	4.31984100	-2.01585000
H	-5.06786900	2.55682500	0.69094200
N	1.38089900	1.24846600	0.65316400
C	3.94018900	2.39158400	0.67012700
C	1.53603800	2.56455300	0.83111200
C	2.47049700	0.46895700	0.48739400
C	3.75881600	1.01414900	0.48322500
C	2.78796100	3.17384400	0.85031300
N	0.86296800	-1.29176100	0.35058000
C	2.78615500	-3.31968700	0.11769000
C	0.49414600	-2.57644000	0.27451100
C	2.17591600	-0.98024300	0.33754200
C	3.15617800	-1.97280700	0.21740800
C	1.41223400	-3.61388500	0.15535900

H	0.61307200	3.13688900	0.95197000
H	4.62822500	0.37261300	0.33671800
H	2.86288300	4.25292500	1.00057900
H	-0.58091200	-2.76685800	0.32347700
H	4.21293800	-1.70438900	0.20897700
H	1.05973000	-4.64567000	0.09425500
C	-1.70339200	-1.51724700	4.95922900
H	-4.49368300	4.29747100	-1.00910500
C	3.80773700	-4.41465600	-0.01957800
H	4.83431000	-4.02383000	0.01188900
H	3.69193600	-5.15735300	0.78619000
H	3.67032500	-4.95176500	-0.97237900
C	5.31233900	3.00659900	0.70318300
H	5.61477600	3.20019900	1.74652000
H	6.06663800	2.34633500	0.25205200
H	5.32697200	3.97333400	0.17749400
C	-3.17908900	-1.74559500	4.77101000
H	-3.72436000	-0.79764000	4.64426200
H	-3.38258300	-2.38384100	3.89725400
H	-3.59803200	-2.25610000	5.66316200
C	-0.85347500	-2.75976100	4.94519400
H	0.22032000	-2.51700700	4.94208600
H	-1.05765300	-3.36614900	5.85213700
H	-1.07002500	-3.38925900	4.06831700
C	-1.33700500	-0.49842700	6.00492700
H	-1.58017900	-0.89104400	7.01440800
H	-0.26032500	-0.26896400	5.98909400
H	-1.89570700	0.44068200	5.87117300
Br	-1.07018600	-0.42224200	2.89432600

UM06/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF)
HF=-5045.5065849
UB3LYP-D3/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF)
HF=-5046.5454233

^2P_B



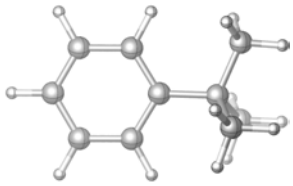
UB3LYP-D3/def2-SVP-CPCM(THF)
Zero-point correction= 0.214708 (Hartree/Particle)
Thermal correction to Energy= 0.230876
Thermal correction to Enthalpy= 0.231820
Thermal correction to Gibbs Free Energy= 0.166322
Sum of electronic and zero-point Energies= -4655.579462
Sum of electronic and thermal Energies= -4655.563294
Sum of electronic and thermal Enthalpies= -4655.562349
Sum of electronic and thermal Free Energies= -4655.627848

Ni	-3.99183200	1.30009300	-1.54653000
C	-1.87359800	-0.39708200	-0.83451100
C	-0.60463100	-0.81497600	-0.41773600
C	0.38038200	0.12429500	-0.09164500
C	0.02971800	1.48282700	-0.20377800
C	-1.24637600	1.83242200	-0.62458000
C	-2.97912600	-1.31121800	-1.19958100
C	-2.90514100	-2.70937500	-1.17420400
C	-4.01531200	-3.47922700	-1.54213400
C	-5.17917400	-2.78948900	-1.92940000
C	-5.18373000	-1.39947400	-1.93172800
H	-0.37768600	-1.87943400	-0.34653600
H	0.75171100	2.26661600	0.03582700
H	-1.54668200	2.87837300	-0.72245500
H	-1.98301600	-3.20525100	-0.86858000
H	-6.07708900	-3.33486700	-2.22820500
H	-6.06484300	-0.82279400	-2.22618200
N	-2.18757800	0.92199600	-0.93709400
N	-4.11313300	-0.67488700	-1.57617200
C	1.75486100	-0.28579000	0.36089600
H	1.95781900	0.09097300	1.37696900
H	1.87445700	-1.37835300	0.36807700
H	2.52660300	0.14347000	-0.29878000
C	-3.97959500	-4.98297800	-1.52479800
H	-2.98906900	-5.36658100	-1.24261000
H	-4.71990400	-5.37924000	-0.81035300
H	-4.24149600	-5.38984900	-2.51492300
Br	-5.83964900	2.56755300	-2.20535500

UM06/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF)
HF=-4656.2756634

UB3LYP-D3/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF)
HF=-4656.9610627

***t*Bu-Ph**

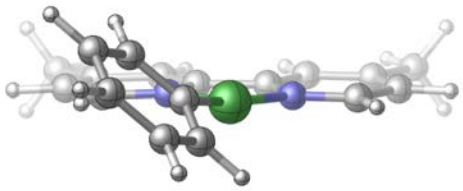


UB3LYP-D3/def2-SVP-CPCM(THF)
Zero-point correction= 0.212552 (Hartree/Particle)
Thermal correction to Energy= 0.222172
Thermal correction to Enthalpy= 0.223116
Thermal correction to Gibbs Free Energy= 0.178247
Sum of electronic and zero-point Energies= -389.034504
Sum of electronic and thermal Energies= -389.024885
Sum of electronic and thermal Enthalpies= -389.023940
Sum of electronic and thermal Free Energies= -389.068810

C	0.04421000	1.70961600	1.14572500
C	1.44490300	1.73358100	1.12055900
C	2.12656700	2.88889000	0.73341700
C	1.38993500	4.02254300	0.37071900
C	-0.00591100	3.99264800	0.39798600
C	-0.71318100	2.83690300	0.78576000
H	-0.45028400	0.78804600	1.45338500
H	2.00284900	0.83794100	1.40728300
H	3.21924500	2.90824800	0.71359200
H	1.90528600	4.93693000	0.06433300
H	-0.55299400	4.89314100	0.10924100
C	-2.25333700	2.84939200	0.79950700
C	-2.74935100	3.94948800	1.76551900
H	-2.40180400	4.94892000	1.46299200
H	-3.85134000	3.97127700	1.78683700
H	-2.39094800	3.76208800	2.79042100
C	-2.84401600	1.50472700	1.25836000
H	-3.94379100	1.56138300	1.25324000
H	-2.55073000	0.67977000	0.59043900
H	-2.52933600	1.24749100	2.28192300
C	-2.77455500	3.14452300	-0.62558100
H	-3.87683800	3.15946900	-0.63495500
H	-2.42445300	4.11964200	-0.99703000
H	-2.43723000	2.37132500	-1.33443100

UM06/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF)
HF=-389.3290308
UB3LYP-D3/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF)
HF=-389.6748001

$^{2}P_{C}$



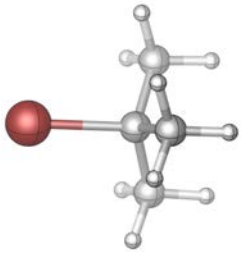
UB3LYP-D3/def2-SVP-CPCM(THF)
Zero-point correction= 0.303134 (Hartree/Particle)
Thermal correction to Energy= 0.322860
Thermal correction to Enthalpy= 0.323805
Thermal correction to Gibbs Free Energy= 0.250611
Sum of electronic and zero-point Energies= -2313.026966
Sum of electronic and thermal Energies= -2313.007240
Sum of electronic and thermal Enthalpies= -2313.006296
Sum of electronic and thermal Free Energies= -2313.079489

Ni	-3.96398300	1.44675100	-1.21509900
C	-1.83575500	-0.36900700	-0.73179300
C	-0.55130400	-0.83036800	-0.42006200
C	0.43164200	0.05760500	0.03112800
C	0.06264200	1.41025300	0.15257000
C	-1.22735300	1.80375600	-0.17808400
C	-2.94328000	-1.23262600	-1.20069300
C	-2.85927000	-2.62301000	-1.34872800
C	-3.97607300	-3.35335800	-1.77274900
C	-5.15577000	-2.63260900	-2.03077500
C	-5.16546600	-1.25120500	-1.86635600
H	-0.31078600	-1.88864300	-0.52848300
H	0.78098300	2.15531600	0.50175800
H	-1.53996000	2.84781500	-0.09948800
H	-1.92710500	-3.14475700	-1.12852900
H	-6.06285900	-3.14566800	-2.35800600
H	-6.06078500	-0.65514500	-2.05962300
N	-2.16615900	0.94343400	-0.61445400
N	-4.08728100	-0.56287300	-1.46861500
C	1.82261900	-0.39985100	0.37491200
H	2.05670900	-0.17550000	1.42863300
H	1.94941500	-1.48000600	0.21584000
H	2.56967500	0.13060300	-0.23804800
C	-3.92851700	-4.84679700	-1.94782400
H	-2.95001600	-5.26161200	-1.66768600
H	-4.70238900	-5.33564400	-1.33408100
H	-4.13207500	-5.11973300	-2.99640100
C	-5.53228400	2.36315800	-1.90331200
C	-6.16411500	3.46923000	-1.27984400

C	-6.13057200	1.95132100	-3.12227500
C	-7.29512300	4.10503900	-1.81103500
H	-5.75841000	3.85373800	-0.33612700
C	-7.25947700	2.57286700	-3.67293800
H	-5.69267000	1.10759400	-3.66945300
C	-7.85243900	3.65805100	-3.01549200
H	-7.74560100	4.95361600	-1.28450500
H	-7.67970900	2.21192800	-4.61812500
H	-8.73512500	4.14906300	-3.43623300

UM06/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF)
HF=-2313.662927
UB3LYP-D3/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF)
HF=-2314.4257224

***t*Bu-Br**

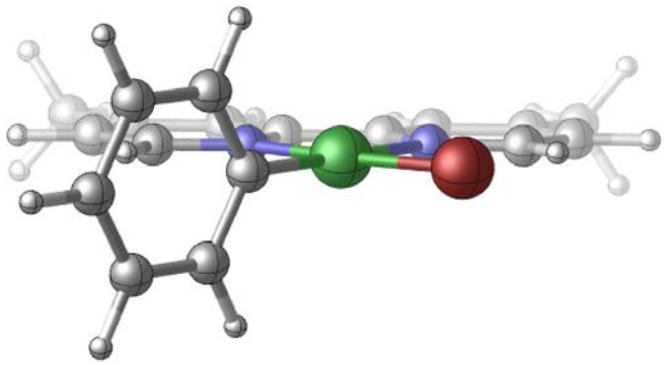


UB3LYP-D3/def2-SVP-CPCM(THF)
Zero-point correction= 0.121249 (Hartree/Particle)
Thermal correction to Energy= 0.127905
Thermal correction to Enthalpy= 0.128849
Thermal correction to Gibbs Free Energy= 0.090653
Sum of electronic and zero-point Energies= -2731.509462
Sum of electronic and thermal Energies= -2731.502806
Sum of electronic and thermal Enthalpies= -2731.501862
Sum of electronic and thermal Free Energies= -2731.540058

Br	0.66845300	-3.32582400	-0.02012300
C	-0.35404100	-1.55353000	-0.02192100
C	0.09890600	-0.79012700	-1.26110700
H	-0.13485200	-1.34337700	-2.18230000
H	-0.43396200	0.17601100	-1.29443400
H	1.17917200	-0.58596100	-1.23527900
C	-1.83589000	-1.90706100	-0.07308600
H	-2.13789300	-2.49998800	0.80239100
H	-2.42204700	-0.97172100	-0.07532100
H	-2.08349000	-2.47031100	-0.98450400
C	0.02110100	-0.83233800	1.26757900
H	-0.51694000	0.13087300	1.30189300
H	-0.26517900	-1.41745400	2.15359400
H	1.10013000	-0.62515900	1.31345500

UM06/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF)
HF=-2731.8563155
UB3LYP-D3/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF)
HF=-2732.1242505

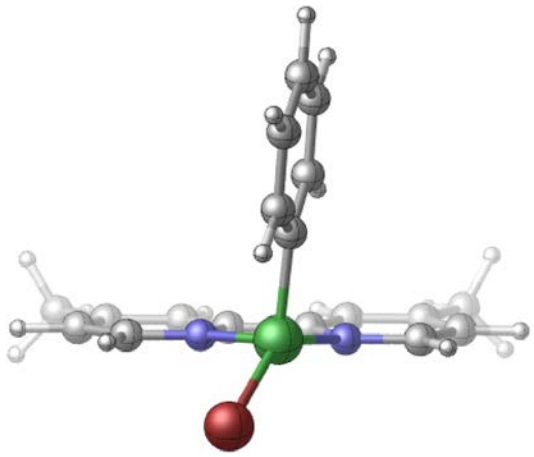
Figure S9 (with Becke-Johnson damping)



UB3LYP-D3BJ/def2-SVP-CPCM(THF)
Zero-point correction= 0.306461 (Hartree/Particle)
Thermal correction to Energy= 0.326798
Thermal correction to Enthalpy= 0.327742
Thermal correction to Gibbs Free Energy= 0.253612
Sum of electronic and zero-point Energies= -4887.034664
Sum of electronic and thermal Energies= -4887.014327
Sum of electronic and thermal Enthalpies= -4887.013383
Sum of electronic and thermal Free Energies= -4887.087513

Ni	-4.61455800	0.39141800	-0.38378100
C	-6.47995100	0.32752600	-0.64642700
C	-7.06929100	0.72563800	-1.85950000
C	-7.32573900	-0.19722300	0.34733000
C	-8.44464000	0.58283800	-2.08288600
H	-6.44788200	1.15381400	-2.65241400
C	-8.70232500	-0.34109800	0.13197000
H	-6.90771400	-0.51094000	1.30937600
C	-9.26861600	0.04583400	-1.08749400
H	-8.87587500	0.89543900	-3.03877400
H	-9.33600100	-0.75704500	0.92114600
H	-10.34235900	-0.06639400	-1.25931300
Br	-4.83954100	2.61489600	0.34890300
C	-2.08006400	-0.92116800	-0.45758300
C	-0.71658600	-1.19386200	-0.31567800
C	0.14713300	-0.21566200	0.18983700
C	-0.42098800	1.02026200	0.53406200
C	-1.78653700	1.22356800	0.36804800
C	-3.06510700	-1.88765800	-0.98117200
C	-2.72565700	-3.17109000	-1.41575200
C	-3.70626600	-4.03929000	-1.90596700
C	-5.02125000	-3.55308100	-1.93323700
C	-5.29618900	-2.26681600	-1.48742800
H	-0.31865600	-2.16867700	-0.59552600

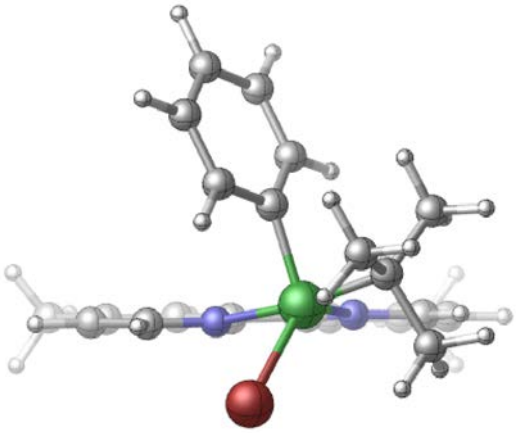
H	0.19699500	1.82707600	0.93279300
H	-2.26735000	2.17027400	0.62492300
H	-1.68801300	-3.50015800	-1.37533500
H	-5.84024600	-4.17312400	-2.30241600
H	-6.31123600	-1.87427200	-1.50210400
N	-2.60198000	0.27710900	-0.11591900
N	-4.34663200	-1.43785100	-1.01661200
C	1.61663500	-0.47344500	0.36269600
H	1.89776400	-0.40195800	1.42590300
H	1.90088100	-1.46896700	-0.00428500
H	2.20936800	0.28185300	-0.17712700
C	-3.37343200	-5.42157500	-2.38792100
H	-3.59867400	-5.51805300	-3.46249700
H	-2.31286900	-5.66220400	-2.23393200
H	-3.98429000	-6.17334000	-1.86370600



UB3LYP-D3BJ/def2-SVP-CPCM(THF)
Zero-point correction= 0.305082 (Hartree/Particle)
Thermal correction to Energy= 0.327019
Thermal correction to Enthalpy= 0.327963
Thermal correction to Gibbs Free Energy= 0.246939
Sum of electronic and zero-point Energies= -4887.032375
Sum of electronic and thermal Energies= -4887.010439
Sum of electronic and thermal Enthalpies= -4887.009494
Sum of electronic and thermal Free Energies= -4887.090519

C	-1.67439600	0.90308300	-0.64637300
C	-1.84605600	0.00921700	0.42800600
C	-3.07766900	-0.67227900	0.49143500
C	-4.08768700	-0.47102500	-0.45923300
C	-3.88787800	0.42453000	-1.51520600
C	-2.67264600	1.11236300	-1.60688000
Br	-0.90109600	-2.16723900	3.30580200
H	-3.25387400	-1.38515300	1.30419200
H	-0.73615300	1.46023800	-0.75016000
H	-2.50304800	1.81374400	-2.43003000
H	-4.67130500	0.58428500	-2.26125500
H	-5.03298000	-1.01689000	-0.37771600
C	1.99355600	0.06542900	0.28566900
C	1.37074100	-2.17251900	0.20732800
C	2.44074900	-2.48947000	-0.62142100
C	3.33200200	-1.47888000	-1.01880900
C	3.08937000	-0.18348100	-0.54637800
C	1.65209400	1.39945800	0.83712100
C	0.17967400	2.57976100	2.18952000
C	0.83585100	3.77934100	1.94024000
C	1.95525000	3.79245000	1.09192400
C	2.35588900	2.57050500	0.53879900
H	0.65892000	-2.92818700	0.54830100

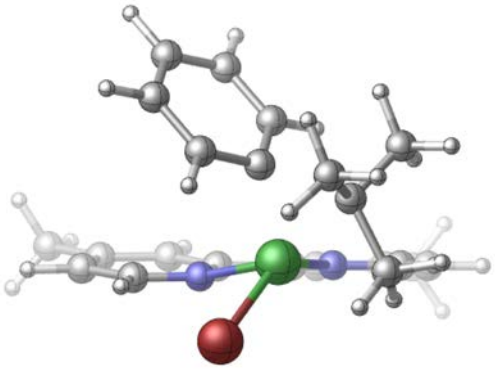
H	2.58098600	-3.51968000	-0.95371900
H	3.76239000	0.62605000	-0.82761700
H	-0.70242300	2.53971100	2.83335800
H	0.47388300	4.69967200	2.40212200
H	3.21583000	2.53874300	-0.12966200
N	1.15583200	-0.92758900	0.64512400
N	0.58069100	1.41995500	1.65742100
Ni	-0.43284100	-0.35400600	1.76916300
C	2.67656200	5.07255000	0.78089400
H	3.61042600	4.89040300	0.23203700
H	2.03937000	5.72984800	0.16640500
H	2.91062900	5.62385500	1.70458600
C	4.49472400	-1.78212000	-1.92015900
H	5.15539700	-0.91255100	-2.03768400
H	5.08551300	-2.62309900	-1.52506400
H	4.13702000	-2.08132800	-2.91901300



UB3LYP-D3BJ/def2-SVP-CPCM(THF)
Zero-point correction= 0.426844 (Hartree/Particle)
Thermal correction to Energy= 0.454721
Thermal correction to Enthalpy= 0.455665
Thermal correction to Gibbs Free Energy= 0.365748
Sum of electronic and zero-point Energies= -5044.644159
Sum of electronic and thermal Energies= -5044.616282
Sum of electronic and thermal Enthalpies= -5044.615338
Sum of electronic and thermal Free Energies= -5044.705255

C	2.71091400	0.70133000	0.17596900
C	3.72349900	-0.43154200	0.28402500
C	2.98998400	1.53526600	-1.08049000
H	3.67687400	-1.10725700	-0.58063800
H	3.57774000	-1.02143400	1.19949200
H	3.15682700	0.89559100	-1.95584100
H	2.18550900	2.23884300	-1.34152700
C	-1.69402700	1.55618600	-0.04726500
C	-2.63173800	2.57677800	0.15141200
C	-2.22064200	3.90684800	0.27641200
C	-0.84314500	4.15306100	0.18713200
C	0.03023000	3.08910500	-0.00498100
C	-2.09021700	0.13838900	-0.21383300
C	-3.41303500	-0.30945800	-0.10707200
C	-3.71271400	-1.66483200	-0.27611500
C	-2.64112400	-2.52694500	-0.55775500
C	-1.35382900	-2.01254400	-0.65025000
H	-3.69370500	2.34105200	0.20160700
H	-0.44643100	5.16687700	0.26539300
H	1.10083200	3.27379300	-0.07558200
H	-4.21723300	0.39093900	0.11374100
H	-2.80673000	-3.59632400	-0.70153300
H	-0.49597000	-2.64747600	-0.87629200
N	-0.36945900	1.81503100	-0.11266300

N	-1.08673700	-0.71263200	-0.48381700
Br	1.50821600	-1.31897800	-2.33001600
Ni	0.85259800	0.02307700	-0.28079500
C	0.79730100	-0.69864000	1.49793900
C	0.19519200	-0.03263100	2.57163300
C	1.17579900	-2.03728600	1.66018800
C	-0.01918000	-0.68997200	3.79003700
H	-0.10878200	1.01265000	2.47201700
C	0.96369600	-2.69875500	2.87698900
H	1.63990400	-2.57691200	0.82945200
H	-0.48937000	-0.15415600	4.61983500
H	1.26665300	-3.74406700	2.98682800
C	0.36551400	-2.02585000	3.94750800
H	0.19984000	-2.53889000	4.89826300
C	-3.20164200	5.02385800	0.48646100
H	-3.13626200	5.75429200	-0.33587700
H	-4.23415500	4.65350500	0.54162900
H	-2.97452000	5.56770700	1.41724000
C	-5.11835800	-2.18248600	-0.16317700
H	-5.43728700	-2.64475300	-1.11124400
H	-5.18275500	-2.96280500	0.61179300
H	-5.82734500	-1.38202800	0.08820300
H	4.74437300	-0.00292000	0.32699200
H	3.90056500	2.14439200	-0.91590400
C	2.76897100	1.55791900	1.43739900
H	1.95083600	2.28612000	1.51619100
H	2.74202400	0.94099800	2.34489300
H	3.71643100	2.13055100	1.44891200

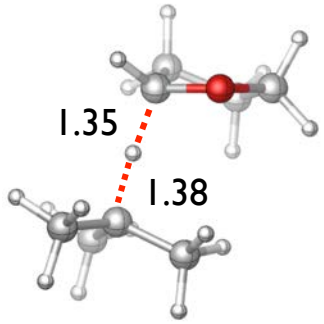


UB3LYP-D3BJ/def2-SVP-CPCM(THF)
Zero-point correction= 0.426726 (Hartree/Particle)
Thermal correction to Energy= 0.453765
Thermal correction to Enthalpy= 0.454709
Thermal correction to Gibbs Free Energy= 0.366635
Sum of electronic and zero-point Energies= -5044.630260
Sum of electronic and thermal Energies= -5044.603220
Sum of electronic and thermal Enthalpies= -5044.602276
Sum of electronic and thermal Free Energies= -5044.690350

C	2.44567300	0.53879700	0.51789700
C	3.55988700	-0.48320800	0.69515100
C	2.69124800	1.26143600	-0.82820000
H	3.51406200	-1.25983000	-0.08110200
H	3.53199200	-0.96353900	1.68286000
H	2.97872300	0.55874900	-1.61770900
H	1.84801100	1.85518400	-1.21171100
C	-1.97392900	1.50906500	-0.14440500
C	-2.90744400	2.53108100	0.06641500
C	-2.49476400	3.86306000	0.16272800
C	-1.11973300	4.10986300	0.03412600
C	-0.25100100	3.04575600	-0.17615500
C	-2.36794500	0.08522200	-0.26140900
C	-3.65266100	-0.38646800	0.03509500
C	-3.94659600	-1.74822600	-0.09126900
C	-2.90999100	-2.58957500	-0.52593500
C	-1.65662000	-2.05212900	-0.79547800
H	-3.96773700	2.29311700	0.14331500
H	-0.72282900	5.12494000	0.09412100
H	0.81856500	3.23114600	-0.27955900
H	-4.42648800	0.29800700	0.38125300
H	-3.07541100	-3.66202900	-0.64685900
H	-0.81926500	-2.66854200	-1.13014400
N	-0.65260300	1.76954400	-0.26060600
N	-1.39242000	-0.74687800	-0.66659600
Br	1.43767500	-1.57408300	-2.31924700

Ni	0.52937800	0.00131100	-0.52962500
C	0.85280700	-0.63865600	1.24830300
C	0.09354700	-0.06193700	2.28413400
C	1.10655300	-2.02232200	1.30784000
C	-0.43862000	-0.84744200	3.31019100
H	-0.11698500	1.00807500	2.27819200
C	0.57567900	-2.80689800	2.33566600
H	1.68758200	-2.49660000	0.51628400
H	-1.04554100	-0.37555300	4.08810000
H	0.76942900	-3.88326900	2.34387300
C	-0.20357300	-2.22681000	3.34286400
H	-0.61848600	-2.84046300	4.14613200
C	-3.47141200	4.98238300	0.38274900
H	-3.43766600	5.69516600	-0.45690500
H	-4.50023900	4.61061200	0.48136200
H	-3.21471500	5.54710100	1.29320600
C	-5.30712300	-2.29630900	0.23476800
H	-5.71999000	-2.85009600	-0.62328000
H	-5.24523600	-3.00657000	1.07528700
H	-6.01222800	-1.49930600	0.50773000
H	4.53399100	0.03065800	0.59548900
H	3.52402500	1.97625100	-0.68136900
C	2.46599700	1.56065500	1.64871200
H	1.63202800	2.27372300	1.59353400
H	2.43495200	1.08311300	2.63716600
H	3.40078300	2.14669100	1.58526300

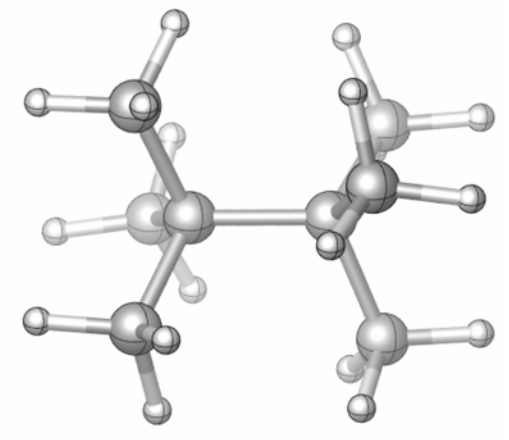
Figure S11



UB3LYP-D3/def2-SVP-CPCM(THF)
Zero-point correction= 0.229357 (Hartree/Particle)
Thermal correction to Energy= 0.240955
Thermal correction to Enthalpy= 0.241899
Thermal correction to Gibbs Free Energy= 0.191011
Sum of electronic and zero-point Energies= -389.737578
Sum of electronic and thermal Energies= -389.725980
Sum of electronic and thermal Enthalpies= -389.725036
Sum of electronic and thermal Free Energies= -389.775924

C	-1.44189600	-5.62124800	-0.67071100
C	-0.61480900	-5.32477500	-1.90511300
H	0.42581800	-5.67253000	-1.79015200
H	-1.03222900	-5.82984500	-2.79962000
H	-0.58926400	-4.24371200	-2.12344100
C	-2.83311600	-5.02126000	-0.70209400
H	-3.44082800	-5.45479900	-1.52205400
H	-3.37638700	-5.20671800	0.23949800
H	-2.79434600	-3.93056700	-0.85593700
C	-1.39181600	-7.06756400	-0.22146500
H	-0.35337000	-7.42058800	-0.10399400
H	-1.91094600	-7.21344800	0.74069000
H	-1.88170500	-7.73489100	-0.95970900
H	-0.81877200	-4.90191300	0.32518700
C	-0.33452700	-4.09984500	1.30392300
O	-1.24547200	-3.04426000	1.45253600
C	-0.33630300	-4.89587900	2.59470000
H	0.63069200	-3.73694500	0.91889100
C	-2.10155200	-3.29099300	2.57721000
C	-1.79547200	-4.71958900	3.04322000
H	0.35604400	-4.45544600	3.33635100
H	-0.04777600	-5.94793800	2.44839100
H	-1.87162600	-2.55110400	3.36634100
H	-3.15091700	-3.14936800	2.27110800
H	-1.94582300	-4.85268400	4.12428800

H -2.44122600 -5.44128100 2.51794600
UB3LYP-D3/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF)
HF= -390.4090221
UM06/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF)
HF= -390.0778207



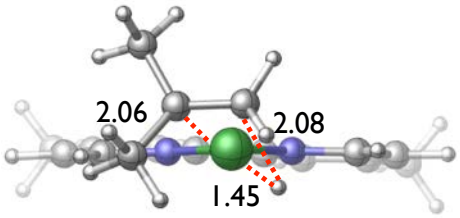
UB3LYP-D3/def2-SVP-CPCM(THF)
Zero-point correction= 0.243588 (Hartree/Particle)
Thermal correction to Energy= 0.253800
Thermal correction to Enthalpy= 0.254744
Thermal correction to Gibbs Free Energy= 0.210503
Sum of electronic and zero-point Energies= -315.255129
Sum of electronic and thermal Energies= -315.244917
Sum of electronic and thermal Enthalpies= -315.243973
Sum of electronic and thermal Free Energies= -315.288214

C	-2.41708000	-0.14457300	0.06622800
C	-0.88402500	-0.24743600	-0.08529400
H	-2.74165800	0.88150100	0.29535000
H	-2.94544800	-0.47308000	-0.84217800
H	-2.75610000	-0.78736300	0.89495100
C	-0.51590700	-1.74621100	-0.13042400
C	-0.24575200	0.35513700	1.18492900
H	0.55546200	-1.90306300	-0.32988500
H	-0.74310900	-2.21871100	0.83915500
H	-1.08705800	-2.28817800	-0.89894500
H	-0.70779400	-0.08687200	2.08277100
H	0.83422400	0.15250100	1.24049600
H	-0.39027400	1.44511100	1.24399800
C	-0.38354500	0.50698200	-1.39515200
C	-1.02342000	1.90725400	-1.51033200
C	1.14931300	0.69016800	-1.38276200
C	-0.75168200	-0.28406100	-2.66911300
H	-2.10296400	1.85183000	-1.71534600
H	-0.88128800	2.50327700	-0.59565000
H	-0.56103700	2.46448200	-2.34135800
H	1.67895000	-0.26049400	-1.21503400
H	1.48707500	1.08812900	-2.35358700
H	1.47371500	1.40115000	-0.60831800
H	-0.52342700	0.31783100	-3.56385600

H	-0.18082000	-1.22083700	-2.75183900
H	-1.82331800	-0.53448200	-2.70559900

UB3LYP-D3/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF)
HF= -315.8529126
UM06/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF)
HF= -315.5614974

Figure S12

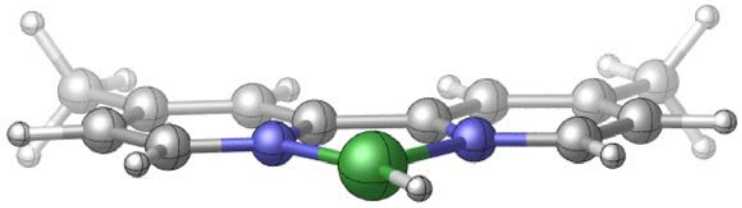


UB3LYP-D3/def2-SVP-CPCM(THF)
Zero-point correction= 0.328127 (Hartree/Particle)
Thermal correction to Energy= 0.347968
Thermal correction to Enthalpy= 0.348913
Thermal correction to Gibbs Free Energy= 0.279623
Sum of electronic and zero-point Energies= -2239.220375
Sum of electronic and thermal Energies= -2239.200534
Sum of electronic and thermal Enthalpies= -2239.199590
Sum of electronic and thermal Free Energies= -2239.268880

Ni	-4.61321300	0.86810700	-0.83470900
C	-5.09920600	2.52182300	0.29792100
C	-4.55216600	2.36939500	1.70282700
H	-4.74404000	1.36415800	2.10736000
H	-3.46927900	2.55485400	1.75648600
H	-5.03615100	3.10331500	2.37489000
C	-6.24127500	1.79571800	-0.07944700
H	-5.62378300	0.94464700	-1.87805000
H	-6.68945700	1.07302700	0.61440600
H	-6.94016700	2.20648100	-0.81286700
C	-4.78498200	3.83112300	-0.39198000
H	-3.70030100	4.01587900	-0.45027500
H	-5.18660100	3.85527800	-1.41595400
H	-5.21989000	4.68057300	0.16788600
C	-2.20522700	-0.58647000	-0.60403900
C	-0.85255000	-0.89231600	-0.31440800
C	0.03915300	0.09547400	0.07013200
C	-0.46446300	1.42555500	0.15669300
C	-1.79703900	1.66488700	-0.11083000
C	-3.17470400	-1.53453700	-1.08989400
C	-2.90900100	-2.88733300	-1.42387700
C	-3.92227300	-3.72644200	-1.85676900
C	-5.23232100	-3.17313400	-1.96101900
C	-5.42983800	-1.83926700	-1.66462100
H	-0.50950600	-1.92534500	-0.39587200
H	0.19020400	2.25523600	0.43172100
H	-2.19733800	2.67733000	-0.04657800
H	-1.88994200	-3.26940700	-1.34127500

H	-6.07577700	-3.79000100	-2.27829500
H	-6.41337500	-1.37414400	-1.76261000
N	-2.67878000	0.70624200	-0.47133900
N	-4.44404300	-1.02209100	-1.23617000
C	1.48007800	-0.19579000	0.38774600
H	1.72097600	0.09427000	1.42487200
H	1.72000200	-1.26210300	0.26533200
H	2.15178000	0.38656200	-0.26590500
C	-3.67659100	-5.16537400	-2.22023400
H	-4.31313100	-5.83586200	-1.61799400
H	-3.93272000	-5.35359100	-3.27696500
H	-2.62705600	-5.45514600	-2.06506800

UB3LYP-D3/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF)
HF= -2240.5636168
UM06/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF)
HF= -2239.8498736

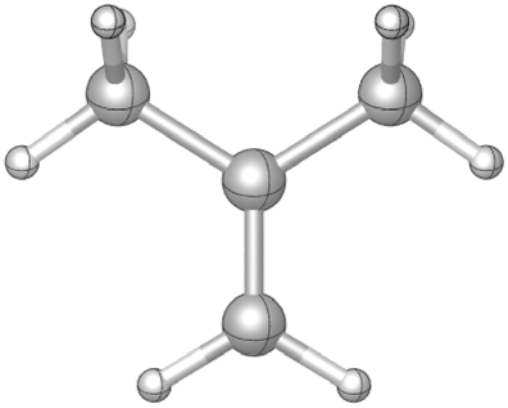


UB3LYP-D3/def2-SVP-CPCM(THF)
Zero-point correction= 0.218542 (Hartree/Particle)
Thermal correction to Energy= 0.233345
Thermal correction to Enthalpy= 0.234289
Thermal correction to Gibbs Free Energy= 0.174716
Sum of electronic and zero-point Energies= -2082.200898
Sum of electronic and thermal Energies= -2082.186094
Sum of electronic and thermal Enthalpies= -2082.185150
Sum of electronic and thermal Free Energies= -2082.244723

Ni	-4.14128400	1.35473100	-1.69261700
H	-5.44683100	2.14366100	-2.15615700
C	-1.98417500	-0.28633800	-0.86820800
C	-0.70498300	-0.64872200	-0.42793000
C	0.27134100	0.32654400	-0.20166200
C	-0.09836300	1.66595300	-0.43842900
C	-1.38204500	1.95976800	-0.87425400
C	-3.07986300	-1.24022000	-1.13348300
C	-2.98621500	-2.63051500	-0.98125800
C	-4.08889600	-3.44510900	-1.26067400
C	-5.26798000	-2.80868900	-1.69242600
C	-5.29004200	-1.42466400	-1.82069600
H	-0.46479800	-1.69941600	-0.25909600
H	0.61651500	2.47707900	-0.28247700
H	-1.69463300	2.98938000	-1.06507000
H	-2.05320000	-3.08385600	-0.64411100
H	-6.16263600	-3.39015800	-1.92588200
H	-6.18629700	-0.89328500	-2.15166600
N	-2.31931600	1.01465600	-1.08971900
N	-4.22769500	-0.65399600	-1.54992000
C	1.65392700	-0.02271100	0.27689900
H	1.84919000	0.42643700	1.26505500
H	1.79507800	-1.10967900	0.36065200
H	2.41867300	0.37455100	-0.41046400
C	-4.02947500	-4.94106600	-1.11192900
H	-3.05325800	-5.27716600	-0.73493400
H	-4.81014400	-5.29435300	-0.41873800
H	-4.21487300	-5.43465100	-2.08017100

UB3LYP-D3/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF)

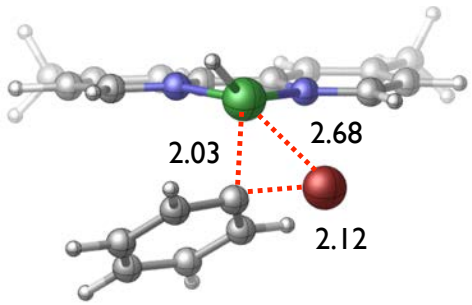
HF= -2083.2746658
UM06/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF)
HF= -2082.7071176



UB3LYP-D3/def2-SVP-CPCM(THF)
Zero-point correction= 0.107040 (Hartree/Particle)
Thermal correction to Energy= 0.112322
Thermal correction to Enthalpy= 0.113267
Thermal correction to Gibbs Free Energy= 0.079765
Sum of electronic and zero-point Energies= -157.012996
Sum of electronic and thermal Energies= -157.007713
Sum of electronic and thermal Enthalpies= -157.006769
Sum of electronic and thermal Free Energies= -157.040270

C	-5.45780700	2.07262200	0.23723400
C	-5.52946100	0.85899400	1.12932400
H	-6.18072200	0.07439500	0.71608900
H	-4.52384500	0.42950900	1.28546300
H	-5.90716300	1.13242700	2.13066000
C	-6.12859400	2.15207900	-0.92172300
H	-6.76266200	1.33174500	-1.27263500
H	-6.06610800	3.04018900	-1.55848800
C	-4.57879200	3.19055500	0.73860400
H	-3.54036500	2.83933200	0.87450700
H	-4.56607400	4.05129000	0.05348300
H	-4.91872000	3.53998000	1.72977100

UB3LYP-D3/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF)
HF= -157.3001298
UM06/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF)
HF= -157.1516226

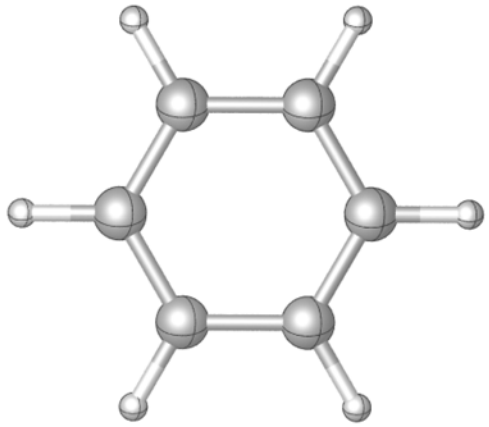


UB3LYP-D3/def2-SVP-CPCM(THF)
Zero-point correction= 0.309716 (Hartree/Particle)
Thermal correction to Energy= 0.331219
Thermal correction to Enthalpy= 0.332163
Thermal correction to Gibbs Free Energy= 0.255765
Sum of electronic and zero-point Energies= -4887.483265
Sum of electronic and thermal Energies= -4887.461762
Sum of electronic and thermal Enthalpies= -4887.460818
Sum of electronic and thermal Free Energies= -4887.537216

Ni	-0.79917400	-0.18317200	0.37337300
C	-1.59750800	0.64027300	-1.29816000
C	-0.96341900	3.22629700	-2.16800300
C	-2.36114100	1.73785700	-0.84662200
C	-0.61544700	0.82411200	-2.29669300
C	-0.27976900	2.11796100	-2.69156100
C	-2.01349800	3.02495500	-1.26137200
H	-3.17246700	1.57386600	-0.13808600
H	-0.08267700	-0.03906500	-2.69625000
H	0.52534700	2.26263500	-3.41731900
H	-2.56944300	3.88025800	-0.86738400
N	0.73831700	1.17004400	0.61386500
C	2.88889900	2.96658200	0.63201800
C	0.57718400	2.41769300	1.06391300
C	1.94612800	0.78038200	0.15858700
C	3.03910900	1.65625900	0.16120700
C	1.61503200	3.34445000	1.08820000
N	0.80701100	-1.25157900	-0.39748800
C	3.15053000	-2.56636100	-1.22288500
C	0.76597600	-2.51433900	-0.84472100
C	1.99870400	-0.61427200	-0.34700400
C	3.17962600	-1.24773700	-0.75376000
C	1.89886900	-3.20297600	-1.26433900
H	-0.42788700	2.66934600	1.41062100
H	4.00894200	1.32914000	-0.21439100
H	1.43146900	4.35481000	1.45993100
H	-0.22342900	-2.97575700	-0.87505900

H	4.13164700	-0.71891900	-0.70211900
H	1.80530400	-4.23033100	-1.62269200
Br	-2.58780400	-1.23666900	-1.32829200
H	-0.69604400	4.23708700	-2.48470300
C	4.40185400	-3.28332100	-1.64903900
H	4.66136500	-4.06629700	-0.91677400
H	4.25605200	-3.78560800	-2.61812300
H	5.25751200	-2.59854300	-1.73256300
C	4.04019800	3.93441300	0.65931400
H	3.75413400	4.89726400	0.20758700
H	4.33939300	4.14378400	1.69999600
H	4.91734100	3.54304800	0.12497400
H	-1.77995400	0.05875200	1.64063100

UB3LYP-D3/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF)
HF= -4889.1966238
UM06/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF)
HF= -4888.3092754

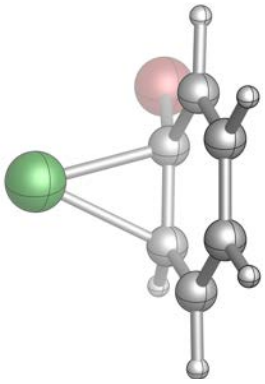


UB3LYP-D3/def2-SVP-CPCM(THF)
Zero-point correction= 0.100501 (Hartree/Particle)
Thermal correction to Energy= 0.104869
Thermal correction to Enthalpy= 0.105813
Thermal correction to Gibbs Free Energy= 0.073041
Sum of electronic and zero-point Energies= -231.991414
Sum of electronic and thermal Energies= -231.987046
Sum of electronic and thermal Enthalpies= -231.986102
Sum of electronic and thermal Free Energies= -232.018875

C	-1.78619400	0.38638600	-1.50220400
C	-1.08232300	3.09483000	-1.40580500
C	-2.51675000	1.27142400	-0.70025300
C	-0.70376700	0.85565300	-2.25604600
C	-0.35185200	2.20986100	-2.20777100
C	-2.16479500	2.62562500	-0.65210600
H	-3.36188700	0.90503200	-0.11142400
H	-0.13344100	0.16460300	-2.88246100
H	0.49324200	2.57637100	-2.79661600
H	-2.73519400	3.31669300	-0.02575100
H	-0.80755600	4.15235000	-1.36828900
H	-2.06099000	-0.67106600	-1.53988700

UB3LYP-D3/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF)
HF= -232.3465283
UM06/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF)
HF= -232.1429457

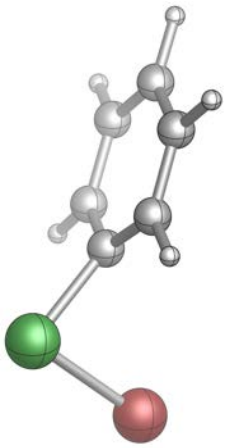
Figure S14



UB3LYP-D3/def2-SVP-CPCM(THF)
Zero-point correction= 0.090677 (Hartree/Particle)
Thermal correction to Energy= 0.098399
Thermal correction to Enthalpy= 0.099343
Thermal correction to Gibbs Free Energy= 0.055641
Sum of electronic and zero-point Energies= -4313.276593
Sum of electronic and thermal Energies= -4313.268871
Sum of electronic and thermal Enthalpies= -4313.267927
Sum of electronic and thermal Free Energies= -4313.311630

C	-3.04310700	0.16108800	1.66008100
C	-2.34670500	-0.85049300	0.93821400
C	-2.07481300	-0.67622800	-0.45526600
C	-2.52185500	0.51012300	-1.09572800
C	-3.19602600	1.48917000	-0.38006500
C	-3.44095600	1.31673200	1.00062000
Br	-2.20662100	-2.61196300	1.72318600
H	-1.71985100	-1.51667200	-1.05788600
H	-3.26327800	0.01302200	2.71784300
H	-3.96559900	2.09429900	1.56028000
H	-3.54390700	2.39323100	-0.88348800
H	-2.34869300	0.62453200	-2.16777600
Ni	-0.45364000	-0.16362000	0.82203800

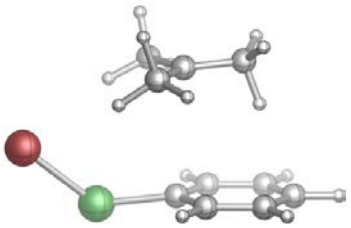
UB3LYP-D3/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF)
HF= -4314.14952807



UB3LYP-D3/def2-SVP-CPCM(THF)
Zero-point correction= 0.090158 (Hartree/Particle)
Thermal correction to Energy= 0.098267
Thermal correction to Enthalpy= 0.099211
Thermal correction to Gibbs Free Energy= 0.054044
Sum of electronic and zero-point Energies= -4313.273303
Sum of electronic and thermal Energies= -4313.265194
Sum of electronic and thermal Enthalpies= -4313.264250
Sum of electronic and thermal Free Energies= -4313.309417

C	-2.63732100	0.92656200	1.28790500
C	-1.85059900	-0.10489600	0.78343200
C	-1.92216100	-0.59087000	-0.51925500
C	-2.75164300	0.10387300	-1.41014300
C	-3.51157500	1.19149400	-0.96224800
C	-3.45850300	1.60214200	0.37557400
Br	-1.50891500	-2.09449000	2.65210700
H	-1.34389100	-1.45894000	-0.84267800
H	-2.60359000	1.21394500	2.34051600
H	-4.06526100	2.44163400	0.72291300
H	-4.17022700	1.71302600	-1.66029900
H	-2.80843700	-0.22077900	-2.45173900
Ni	-0.21539600	-0.46360600	1.69357600

UB3LYP-D3/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF)
HF= -4314.14216150

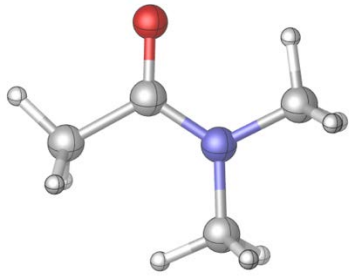


UB3LYP-D3/def2-SVP-CPCM(THF)
Zero-point correction= 0.208392 (Hartree/Particle)
Thermal correction to Energy= 0.223964
Thermal correction to Enthalpy= 0.224908
Thermal correction to Gibbs Free Energy= 0.162774
Sum of electronic and zero-point Energies= -4470.909091
Sum of electronic and thermal Energies= -4470.893518
Sum of electronic and thermal Enthalpies= -4470.892574
Sum of electronic and thermal Free Energies= -4470.954708

Ni	-5.69003100	0.64818100	0.19683600
C	-5.31262800	2.49967100	0.66139700
C	-6.23448800	3.52426700	0.36697900
C	-4.17964800	2.83013800	1.43170000
C	-6.03777200	4.83176200	0.82555600
H	-7.12224700	3.30081900	-0.23322700
C	-3.97330700	4.13463800	1.89512600
H	-3.44227800	2.05887000	1.67670000
C	-4.90263100	5.13978700	1.58920300
H	-6.76310200	5.61325100	0.58422500
H	-3.08705600	4.37265000	2.48928000
H	-4.74153100	6.16071500	1.94406100
Br	-5.68614100	-0.46437700	-1.89372500
C	-3.77679300	3.39391200	-1.98984200
C	-2.89096800	2.24435300	-1.77541200
H	-3.42256200	1.28372100	-1.75682300
H	-2.23827200	2.24155400	-2.67717100
H	-2.22444500	2.38095000	-0.91340100
C	-3.36068800	4.72070500	-1.55843600
H	-3.85202000	4.85510400	-0.56365600
H	-2.28012400	4.80823100	-1.38558500
H	-3.76455200	5.52248000	-2.19272700
C	-5.01632300	3.22690400	-2.75395700
H	-5.49823400	2.25608700	-2.56766100
H	-5.70555800	4.07386700	-2.65002300
H	-4.67682000	3.20337300	-3.81377000

UB3LYP-D3/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF)
HF= -4472.07517251

DMA

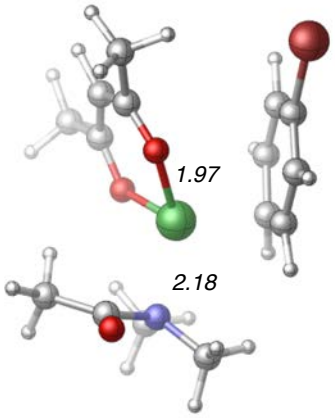


UB3LYP-D3/def2-SVP-CPCM(THF)
$<S^2>$ = 0.0000
Zero-point correction= 0.129574 (Hartree/Particle)
Thermal correction to Energy= 0.137214
Thermal correction to Enthalpy= 0.138159
Thermal correction to Gibbs Free Energy= 0.097818
Sum of electronic and zero-point Energies= -287.506478
Sum of electronic and thermal Energies= -287.498838
Sum of electronic and thermal Enthalpies= -287.497894
Sum of electronic and thermal Free Energies= -287.538234

C	-2.77549400	1.10576800	0.17344400
O	-3.37576400	0.04098600	0.30285000
N	-1.42066200	1.15712500	-0.02483700
C	-3.53169900	2.42604000	0.23195600
H	-3.17999200	3.06144900	1.05983000
H	-3.42570500	3.00001200	-0.70177600
H	-4.59143000	2.19194000	0.38873300
C	-0.64344600	2.37040000	-0.20318800
H	-1.25639800	3.26981200	-0.09049600
H	0.17034500	2.41803800	0.54165400
H	-0.18014800	2.39406000	-1.20606400
C	-0.65581000	-0.07661500	-0.10272300
H	-1.32981400	-0.92785900	0.04169300
H	-0.16180500	-0.16647800	-1.08632700
H	0.12810200	-0.09653400	0.67449200

UB3LYP-D3/def2-TZVPP-CPCM(THF)// UB3LYP-D3/def2-SVP-CPCM(THF)
HF= -287.968183
UM06/def2-TZVPP-CPCM(THF)// UB3LYP-D3/def2-SVP-CPCM(THF)
HF= -287.7556375

^{2}A-DMA-N



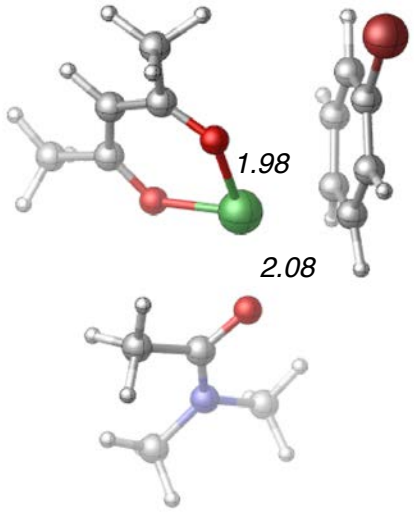
UB3LYP-D3/def2-SVP-CPCM(THF)
Zero-point correction= 0.334610 (Hartree/Particle)
Thermal correction to Energy= 0.359997
Thermal correction to Enthalpy= 0.360941
Thermal correction to Gibbs Free Energy= 0.276130
Sum of electronic and zero-point Energies= -4945.881912
Sum of electronic and thermal Energies= -4945.856525
Sum of electronic and thermal Enthalpies= -4945.855581
Sum of electronic and thermal Free Energies= -4945.940391

C	-2.38385200	1.54700000	-1.19046200
O	-2.56104700	1.50095400	-2.39614100
N	-1.37287000	0.74453500	-0.58367600
C	-3.17663100	2.47036200	-0.29399500
H	-3.55728500	1.94507700	0.59047500
H	-2.53641800	3.30063700	0.04600600
H	-4.00683300	2.87792300	-0.88264400
C	-0.33484600	0.28781600	-1.52187900
H	0.34963800	1.11482100	-1.77797300
H	0.24348600	-0.51919100	-1.05542400
H	-0.80658500	-0.07658600	-2.43881000
C	-0.81492300	1.17330700	0.71106500
H	-0.21818800	2.09533400	0.60455600
H	-1.61496000	1.31223300	1.44292300
H	-0.16279700	0.37309800	1.08604200
Ni	-2.85937700	-0.81031400	-0.20266100
C	-1.59741300	-2.49138000	0.12393600
C	-1.82822800	-2.75913400	-1.24900300
C	-2.83693300	-3.65734500	-1.64005400
C	-3.60617300	-4.28244600	-0.66447200
C	-3.38749600	-4.04805600	0.70562100
C	-2.38182400	-3.17159900	1.09077500
H	-0.68264900	-1.98414900	0.44480200
H	-1.16989500	-2.34103900	-2.01103100

H	-4.00662500	-4.54478200	1.45386400
H	-2.19922200	-2.99115700	2.15173500
H	-3.01374000	-3.85569400	-2.69803300
Br	-5.00080200	-5.48418200	-1.18944900
C	-5.66791900	-1.42806900	0.14358400
O	-4.68295600	-1.40061200	-0.65387600
C	-5.64863800	-0.98083500	1.48607200
H	-6.56505600	-1.09680800	2.06563100
C	-4.56163700	-0.34030500	2.11684600
O	-3.43375200	-0.09849100	1.58088900
C	-6.94534600	-2.01407900	-0.41916700
H	-6.76202500	-3.06891200	-0.68247200
H	-7.79456700	-1.95707900	0.27521100
H	-7.20169600	-1.49108000	-1.35446600
C	-4.71613900	0.13944400	3.54551000
H	-5.67601600	-0.14327700	3.99848000
H	-3.89140200	-0.26777100	4.15242000
H	-4.61752500	1.23764400	3.56964300

UB3LYP-D3/def2-TZVPP-CPCM(THF)// UB3LYP-D3/def2-SVP-CPCM(THF)
HF= -4947.7109019
UM06/def2-TZVPP-CPCM(THF)// UB3LYP-D3/def2-SVP-CPCM(THF)
HF= -4946.8406731

^{2}A-DMA-O



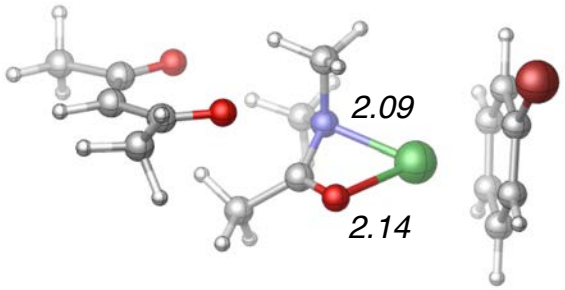
UB3LYP-D3/def2-SVP-CPCM(THF)
Zero-point correction= 0.333954 (Hartree/Particle)
Thermal correction to Energy= 0.359909
Thermal correction to Enthalpy= 0.360854
Thermal correction to Gibbs Free Energy= 0.272367
Sum of electronic and zero-point Energies= -4945.890866
Sum of electronic and thermal Energies= -4945.864911
Sum of electronic and thermal Enthalpies= -4945.863966
Sum of electronic and thermal Free Energies= -4945.952453

C	-0.86706700	1.17746200	-0.95642900
O	-1.02443200	-0.05873500	-1.01941100
N	0.37547300	1.70557900	-0.88856000
C	-2.05802200	2.11220400	-0.97006500
H	-2.12290700	2.68122800	-0.03129400
H	-1.99841800	2.82320400	-1.80761900
H	-2.96704100	1.50923000	-1.06437000
C	1.54849100	0.84014400	-0.89418900
H	2.19553900	1.08629000	-1.75258200
H	2.13121500	0.98605900	0.03045300
H	1.23403000	-0.20563700	-0.96489100
C	0.66981200	3.13028300	-0.83989000
H	1.19171200	3.44869700	-1.75861100
H	-0.23689200	3.73163700	-0.72865300
H	1.32934300	3.34351900	0.01719400
Ni	-2.70280800	-1.11931500	-0.39915300
C	-1.58501700	-2.90884700	-0.31627200
C	-2.03253700	-2.81770200	-1.66571600
C	-3.15090700	-3.57289500	-2.09104400
C	-3.81874500	-4.37156000	-1.17714900
C	-3.38044100	-4.49446100	0.15961000

C	-2.26391100	-3.78563400	0.57266500
H	-0.60565900	-2.51218800	-0.03522000
H	-1.42548700	-2.29945900	-2.41173600
H	-3.91793600	-5.14219300	0.85425500
H	-1.90366000	-3.89625500	1.59837400
H	-3.49011500	-3.51044800	-3.12624800
Br	-5.38985200	-5.32520000	-1.72296400
C	-5.45629800	-1.19052300	0.55674200
O	-4.63582000	-1.55383600	-0.33846700
C	-5.15679300	-0.35561800	1.65824300
H	-5.96562100	-0.13106600	2.35471000
C	-3.90139900	0.24895600	1.89761700
O	-2.86127100	0.09400400	1.18780900
C	-6.86784600	-1.71878700	0.39092700
H	-6.83210900	-2.81883500	0.33026100
H	-7.54664700	-1.41808400	1.20076700
H	-7.27395600	-1.36419700	-0.57092500
C	-3.74925500	1.18362100	3.08258300
H	-4.64679800	1.23904000	3.71390000
H	-2.89252300	0.85729700	3.69413900
H	-3.50941300	2.19501100	2.71330100

UB3LYP-D3/def2-TZVPP-CPCM(THF)// UB3LYP-D3/def2-SVP-CPCM(THF)
HF= -4947.7206989
UM06/def2-TZVPP-CPCM(THF)// UB3LYP-D3/def2-SVP-CPCM(THF)
HF= -4946.8519092

^{2}A-DMA'-conf1



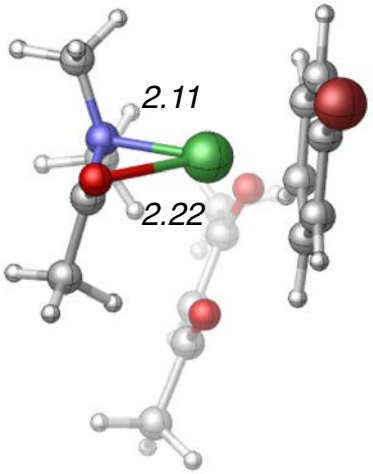
UB3LYP-D3/def2-SVP-CPCM(THF)
Zero-point correction= 0.333515 (Hartree/Particle)
Thermal correction to Energy= 0.359366
Thermal correction to Enthalpy= 0.360310
Thermal correction to Gibbs Free Energy= 0.272439
Sum of electronic and zero-point Energies= -4945.808783
Sum of electronic and thermal Energies= -4945.782931
Sum of electronic and thermal Enthalpies= -4945.781987
Sum of electronic and thermal Free Energies= -4945.869858

C	-1.76896800	-1.05834000	-1.69978000
O	-2.82325200	-1.09231900	-1.06125600
N	-0.58437700	-0.92091500	-0.90100900
C	-1.66946700	-1.35361400	-3.15555400
H	-0.93675900	-0.68494500	-3.62107200
H	-1.34230900	-2.39886300	-3.28715000
H	-2.65950300	-1.23344400	-3.60939200
C	0.66491700	-1.47728000	-1.45110200
H	1.03663800	-0.85964200	-2.28180700
H	1.40664000	-1.48964300	-0.64016800
H	0.49895100	-2.51356400	-1.77291100
C	-0.37715200	0.44648200	-0.33981100
H	0.04488100	1.08654600	-1.12503300
H	-1.34179300	0.85730100	-0.02381000
H	0.29271400	0.35645500	0.52685200
Ni	-1.69568400	-1.88151400	0.58388000
C	-1.09472400	-3.69294800	1.63628900
C	-2.50423200	-3.59613200	1.66638100
C	-3.12291600	-2.47049000	2.25486800
C	-2.33578900	-1.46444700	2.85918700
C	-0.93345900	-1.54421600	2.82530700
C	-0.32220300	-2.64999500	2.19317900
H	-0.60804800	-4.55054200	1.17173200
H	-3.12287000	-4.37377000	1.21740000
H	-0.32313000	-0.75156700	3.25781700
H	0.76606200	-2.68901400	2.12960900
H	-4.20838700	-2.37567100	2.23749800
Br	-3.18322100	0.01458400	3.69556100

C	-2.17004800	1.92339200	-3.58430000
O	-2.10679600	1.43491100	-2.43352100
C	-1.12117800	1.99559600	-4.54397800
H	-1.36831500	2.44927000	-5.50674100
C	0.22430400	1.56901900	-4.36536700
O	0.71147400	1.04080100	-3.33817400
C	-3.53208000	2.49251800	-4.00121100
H	-3.85742000	3.22898500	-3.24757500
H	-3.54184800	2.96506900	-4.99459900
H	-4.27716100	1.67856400	-3.98559300
C	1.18034500	1.76458300	-5.54801300
H	0.72798600	2.26269900	-6.41825500
H	2.05205800	2.34956500	-5.20985000
H	1.56650400	0.77976400	-5.86168700

UB3LYP-D3/def2-TZVPP-CPCM(THF)// UB3LYP-D3/def2-SVP-CPCM(THF)
HF= -4947.6428298
UM06/def2-TZVPP-CPCM(THF)// UB3LYP-D3/def2-SVP-CPCM(THF)
HF= -4946.781502

^{2}A-DMA'-conf2



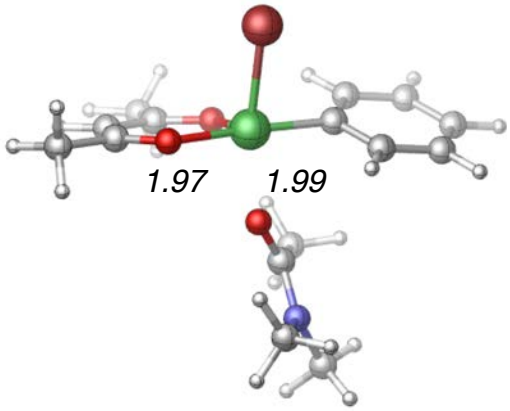
UB3LYP-D3/def2-SVP-CPCM(THF)
Zero-point correction= 0.333505 (Hartree/Particle)
Thermal correction to Energy= 0.359314
Thermal correction to Enthalpy= 0.360258
Thermal correction to Gibbs Free Energy= 0.274476
Sum of electronic and zero-point Energies= -4945.816723
Sum of electronic and thermal Energies= -4945.790914
Sum of electronic and thermal Enthalpies= -4945.789970
Sum of electronic and thermal Free Energies= -4945.875752

C	-1.88767300	-0.84033800	-1.04841300
O	-2.60783000	-0.12550100	-0.32523300
N	-0.51147500	-0.89937600	-0.73734300
C	-2.41367300	-1.63218500	-2.20696500
H	-1.85094300	-1.39745200	-3.12329500
H	-2.29278700	-2.71307000	-2.00725900
H	-3.47479500	-1.38929500	-2.33665700
C	0.36458600	-1.82564000	-1.47047100
H	0.60359700	-1.43086600	-2.47193300
H	1.29135100	-1.94890000	-0.89699700
H	-0.10477800	-2.81395900	-1.52797000
C	0.14916000	0.33936700	-0.28466600
H	0.59081300	0.86485400	-1.14804000
H	-0.58281200	0.98695400	0.20944900
H	0.94454500	0.08248800	0.42718100
Ni	-1.57854600	-1.64404200	0.92855200
C	-0.79633600	-3.62215300	1.45757300
C	-2.20485100	-3.71757600	1.42065400
C	-2.99164900	-2.89024200	2.24863300
C	-2.36196500	-1.98314200	3.13235800
C	-0.95844600	-1.88392400	3.19573600
C	-0.18778600	-2.70092100	2.33966500

H	-0.18540400	-4.18833100	0.74267700
H	-2.66798900	-4.38845500	0.69781200
H	-0.48285100	-1.17070700	3.86834800
H	0.89873400	-2.59778600	2.33882400
H	-4.07943500	-2.92305100	2.19034500
Br	-3.43403700	-0.86500700	4.23749400
C	-0.95743000	-5.24687700	-2.30010800
O	-1.46421300	-4.53735600	-1.39076400
C	0.40181000	-5.63448900	-2.40272300
H	0.67614500	-6.22996200	-3.27663100
C	1.44981000	-5.33198600	-1.48222200
O	1.35003400	-4.70111100	-0.40715000
C	-1.90361400	-5.68993500	-3.41763500
H	-2.24358200	-4.79740500	-3.97143400
H	-1.45719000	-6.39744000	-4.13178100
H	-2.80241400	-6.14381400	-2.96898600
C	2.85423500	-5.82774200	-1.84744000
H	2.90314100	-6.40103600	-2.78479600
H	3.52921700	-4.95856300	-1.92525300
H	3.23930700	-6.45079100	-1.02296600

UB3LYP-D3/def2-TZVPP-CPCM(THF)// UB3LYP-D3/def2-SVP-CPCM(THF)
HF= -4947.6480744
UM06/def2-TZVPP-CPCM(THF)// UB3LYP-D3/def2-SVP-CPCM(THF)
HF= -4946.7844496

^{2}C-DMA-O



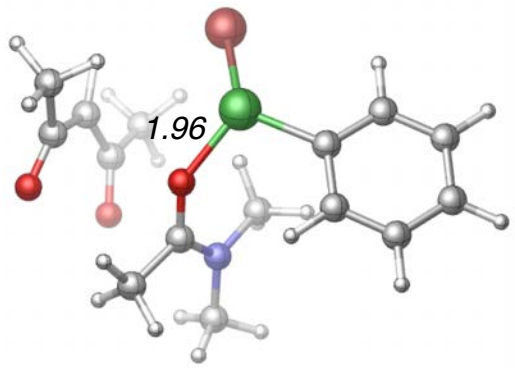
UB3LYP-D3/def2-SVP-CPCM(THF)
Zero-point correction= 0.335220 (Hartree/Particle)
Thermal correction to Energy= 0.360904
Thermal correction to Enthalpy= 0.361848
Thermal correction to Gibbs Free Energy= 0.275250
Sum of electronic and zero-point Energies= -4945.908362
Sum of electronic and thermal Energies= -4945.882678
Sum of electronic and thermal Enthalpies= -4945.881734
Sum of electronic and thermal Free Energies= -4945.968331

C	-2.72312300	0.16404400	-0.21128400
O	-1.94642200	-0.57518600	-0.86605100
N	-2.21526200	1.05771300	0.65247600
C	-4.21765800	0.07104800	-0.37844300
H	-4.65738900	-0.43891400	0.49349000
H	-4.68111300	1.06314300	-0.47105600
H	-4.42823600	-0.52882300	-1.26950100
C	-3.05005100	1.95397900	1.44806100
H	-2.48680000	2.25413600	2.34170300
H	-3.31813700	2.86365200	0.88478000
H	-3.96799200	1.45619400	1.78328200
C	-0.77110100	1.22317500	0.79533900
H	-0.49927800	2.27675700	0.62342000
H	-0.45500500	0.94083600	1.81257700
H	-0.25444200	0.59111300	0.06665600
Ni	-2.13583600	-2.30617300	-1.82492900
C	-3.38599700	-3.35898200	1.99830200
C	-2.61469400	-3.00223900	0.88261600
C	-3.20029800	-3.02036800	-0.38301800
C	-4.52367500	-3.41253300	-0.56565600
C	-5.28795800	-3.76754100	0.55458700
C	-4.72306500	-3.73915900	1.83541000
H	-2.93628800	-3.33712600	2.99500900
H	-1.57211100	-2.69925400	1.01066300

H	-4.95718000	-3.41711400	-1.56654900
H	-6.33158600	-4.06686500	0.42185700
H	-5.32322900	-4.01714000	2.70561000
Br	-1.57001500	-4.55993400	-2.32136400
C	-3.62262900	-1.35164500	-4.12517800
O	-3.69114100	-1.86408700	-2.95889500
C	-2.44511800	-0.99835600	-4.80590200
H	-2.54811400	-0.57952300	-5.80649000
C	-1.13753900	-1.12968700	-4.28123200
O	-0.85029900	-1.59082900	-3.13839600
C	-4.96290800	-1.11180700	-4.78276300
H	-5.53193500	-0.38740400	-4.17682500
H	-4.87724100	-0.73298200	-5.80965800
H	-5.53811100	-2.05118400	-4.78337100
C	0.04290300	-0.70039700	-5.12368000
H	-0.25102200	-0.25180500	-6.08169000
H	0.65229600	0.01769300	-4.55237700
H	0.67916200	-1.57992700	-5.31529200

UB3LYP-D3/def2-TZVPP-CPCM(THF)// UB3LYP-D3/def2-SVP-CPCM(THF)
HF= -4947.7369949
UM06/def2-TZVPP-CPCM(THF)// UB3LYP-D3/def2-SVP-CPCM(THF)
HF= -4946.8553074

^{2}C-DMA'-conf1



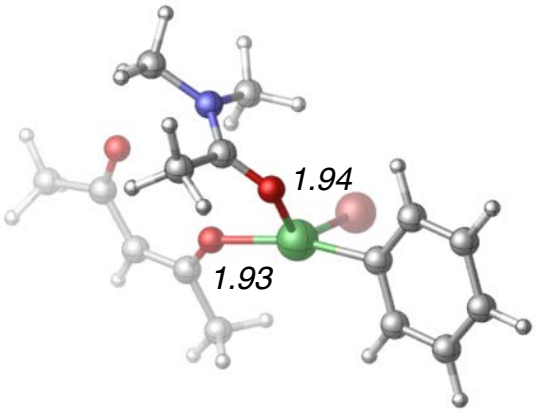
UB3LYP-D3/def2-SVP-CPCM(THF)
Zero-point correction= 0.332583 (Hartree/Particle)
Thermal correction to Energy= 0.359318
Thermal correction to Enthalpy= 0.360262
Thermal correction to Gibbs Free Energy= 0.270529
Sum of electronic and zero-point Energies= -4945.848754
Sum of electronic and thermal Energies= -4945.822019
Sum of electronic and thermal Enthalpies= -4945.821075
Sum of electronic and thermal Free Energies= -4945.910808

C	-0.46249000	-1.46454300	-4.21905300
O	-1.34334000	-0.66262100	-3.80734000
N	0.52565700	-1.90817000	-3.43606900
C	-0.52213100	-1.90221900	-5.65882300
H	0.39506000	-1.59029400	-6.17737700
H	-0.63077100	-2.99403300	-5.74388900
H	-1.37721000	-1.40913600	-6.13144800
C	1.58082300	-2.79211400	-3.92336500
H	2.43412700	-2.19163500	-4.27828900
H	1.91214400	-3.43893300	-3.09925300
H	1.22907500	-3.43654500	-4.73540200
C	0.73339300	-1.37632900	-2.09107200
H	1.81332300	-1.30158400	-1.90572000
H	0.29755800	-0.37667300	-1.99651800
H	0.27365300	-2.02967400	-1.33424600
Ni	-2.33094100	-0.14263900	-2.20039400
C	-2.74566800	-2.84195600	1.08050100
C	-2.61783000	-1.68172200	0.30469400
C	-2.54896800	-1.74000000	-1.10003100
C	-2.61071300	-3.01274100	-1.70061100
C	-2.73837300	-4.17978900	-0.93515800
C	-2.80601000	-4.09614500	0.46069300
H	-2.79457000	-2.76899800	2.17145900
H	-2.56040800	-0.70921100	0.80529100
H	-2.55297800	-3.10178500	-2.79133300

H	-2.78259600	-5.15644200	-1.42725500
H	-2.90224800	-5.00408200	1.06279200
Br	-1.43760100	1.85644400	-1.22776000
C	-0.69949200	1.75083400	-5.43385200
O	-0.35133500	1.07006000	-6.39037900
C	0.21237100	2.09348100	-4.33103900
H	-0.07679100	2.92195000	-3.68052400
C	1.45703600	1.39228200	-4.00544900
O	1.83329600	0.39214200	-4.61319600
C	-2.09775600	2.32091600	-5.32193000
H	-2.73897300	1.88686700	-6.10004300
H	-2.51633400	2.12603700	-4.32275000
H	-2.06112400	3.41653800	-5.44755000
C	2.23643700	1.94952500	-2.83293300
H	1.59769100	1.94290200	-1.93415400
H	3.13808400	1.34726900	-2.66201300
H	2.51748700	2.99881500	-3.02071500

UB3LYP-D3/def2-TZVPP-CPCM(THF)// UB3LYP-D3/def2-SVP-CPCM(THF)
HF= -4947.6653381
UM06/def2-TZVPP-CPCM(THF)// UB3LYP-D3/def2-SVP-CPCM(THF)
HF= -4946.7828069

^{2}C-DMA'-conf2



UB3LYP-D3/def2-SVP-CPCM(THF)
Zero-point correction= 0.334582 (Hartree/Particle)
Thermal correction to Energy= 0.360359
Thermal correction to Enthalpy= 0.361303
Thermal correction to Gibbs Free Energy= 0.275123
Sum of electronic and zero-point Energies= -4945.869422
Sum of electronic and thermal Energies= -4945.843645
Sum of electronic and thermal Enthalpies= -4945.842701
Sum of electronic and thermal Free Energies= -4945.928881

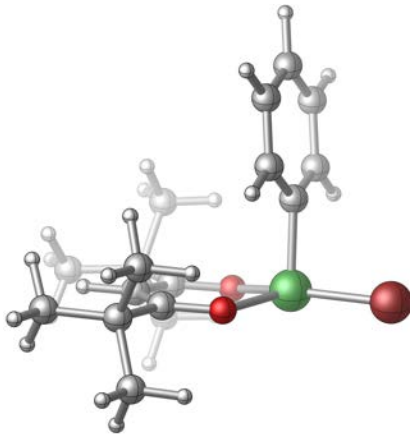
C	-2.01216100	0.86910700	-0.04072900
O	-2.27815700	-0.35815900	-0.22735100
N	-1.12610100	1.26725300	0.86415700
C	-2.77296000	1.87403300	-0.86856500
H	-3.23419700	2.66188900	-0.25677200
H	-2.08983800	2.35148400	-1.58917400
H	-3.55218800	1.33887400	-1.42306500
C	-0.72519000	2.65795000	1.06780000
H	-0.90266600	2.94235000	2.11693000
H	0.34350700	2.74853500	0.83116300
H	-1.28654200	3.33786700	0.42091000
C	-0.35376100	0.28037700	1.61671900
H	-0.02560500	0.73412200	2.56082000
H	-0.97005500	-0.59962400	1.83459000
H	0.51945900	-0.01674600	1.02005000
Ni	-1.14441600	-1.85866500	-0.70746700
C	-4.75390500	-3.68551400	0.41638200
C	-3.58731600	-2.91548200	0.50658100
C	-2.60890600	-3.08051400	-0.46876600
C	-2.72666600	-4.01280000	-1.49678300
C	-3.90637800	-4.76990100	-1.58229500
C	-4.91387700	-4.60767500	-0.62664800
H	-5.54179800	-3.55949200	1.16398500
H	-3.45768800	-2.18225800	1.30413600

H	-1.92404700	-4.16192300	-2.22475700
H	-4.02272900	-5.49525800	-2.39200600
H	-5.82484300	-5.20822200	-0.68808800
Br	0.08631200	-3.32753100	0.60460900
C	1.27103400	-0.89155200	-2.07248900
O	0.19192900	-0.64673100	-1.40498000
C	2.37996900	-0.05640200	-2.07907800
H	3.20646300	-0.33282200	-2.73794600
C	2.55225900	1.14703500	-1.29164100
O	1.74485000	1.58272700	-0.46372800
C	1.28738000	-2.16325800	-2.89682200
H	0.39033100	-2.19207500	-3.53830900
H	2.18589500	-2.27002900	-3.51926300
H	1.21862300	-3.02708800	-2.21395700
C	3.86097600	1.90096200	-1.52779500
H	3.93606300	2.22819800	-2.57835100
H	3.90766400	2.77801800	-0.86770600
H	4.72821700	1.24831600	-1.33297200

UB3LYP-D3/def2-TZVPP-CPCM(THF)// UB3LYP-D3/def2-SVP-CPCM(THF)
HF= -4947.6993646
UM06/def2-TZVPP-CPCM(THF)// UB3LYP-D3/def2-SVP-CPCM(THF)
HF= -4946.8143409

Figure S15

^{2}B^{TMHD}



UB3LYP-D3/def2-SVP-CPCM(THF)

Zero-point correction= 0.372835 (Hartree/Particle)

Thermal correction to Energy= 0.396936

Thermal correction to Enthalpy= 0.397880

Thermal correction to Gibbs Free Energy= 0.316227

Sum of electronic and zero-point Energies= -4893.938481

Sum of electronic and thermal Energies= -4893.914380

Sum of electronic and thermal Enthalpies= -4893.913436

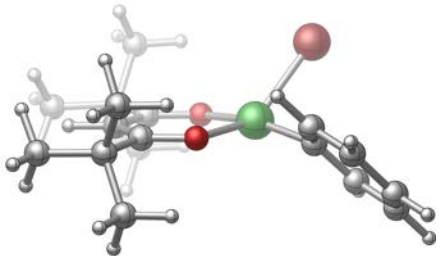
Sum of electronic and thermal Free Energies= -4893.995089

C	-2.56869900	1.06653100	1.31644600
C	-1.72660600	0.13435400	0.72201700
C	-1.72732600	-0.12971300	-0.64220700
C	-2.61211200	0.59908600	-1.45179000
C	-3.46751600	1.55172000	-0.88821000
C	-3.44801300	1.78355000	0.49177300
Br	-1.75701700	-2.55072000	2.20848200
H	-1.05887500	-0.87635900	-1.06983800
H	-2.54326000	1.24830600	2.39274000
H	-4.11359100	2.52760500	0.93735000
H	-4.15375800	2.11420600	-1.52591300
H	-2.62720700	0.41151600	-2.52880500
Ni	-0.42983800	-0.68760000	1.84004300
O	0.93295200	-1.16607200	0.54263200
O	0.39100300	0.96684900	2.23863900
C	1.28316400	1.56067900	1.53832600
C	1.79673800	-0.37119200	0.04939100
C	2.65607100	-0.99141700	-1.06922800
C	1.52176100	3.02424000	1.95026700
C	1.97810800	0.96352900	0.47281000
H	2.71755000	1.56234200	-0.04319500
C	1.69380800	-1.49935100	-2.16566200

H	0.98004100	-2.22654400	-1.75315500
H	1.12391500	-0.66664400	-2.60842600
H	2.26532700	-1.98824600	-2.97009600
C	3.66344500	-0.01191800	-1.68855700
H	4.38344600	0.36223100	-0.94467900
H	4.23705700	-0.52670700	-2.47498400
H	3.16265400	0.85147200	-2.15325400
C	3.41496200	-2.18645700	-0.45034800
H	3.99998400	-2.70370900	-1.22715900
H	4.11160300	-1.84858400	0.33394300
H	2.71297700	-2.90450200	-0.00295700
C	2.69077000	3.68788200	1.20795500
H	2.81275200	4.72079600	1.56925000
H	3.63951800	3.15753900	1.38389700
H	2.51530400	3.73733500	0.12249100
C	1.79255100	3.06090600	3.46923300
H	1.90301400	4.10371300	3.80558200
H	0.96580200	2.59911200	4.02657100
H	2.72094900	2.52151300	3.71750400
C	0.21249400	3.78414400	1.63441400
H	-0.00553100	3.76202100	0.55459400
H	-0.63914600	3.33245900	2.16268100
H	0.30437000	4.83669000	1.94595400

UB3LYP-D3/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF)
HF= -4895.7394255

^{2}C^{TMHD}



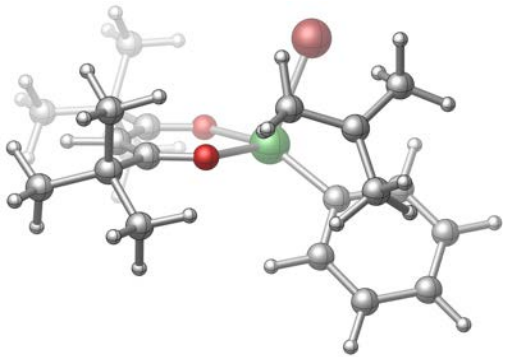
UB3LYP-D3/def2-SVP-CPCM(THF)
Zero-point correction= 0.372626 (Hartree/Particle)
Thermal correction to Energy= 0.396808
Thermal correction to Enthalpy= 0.397752
Thermal correction to Gibbs Free Energy= 0.315737
Sum of electronic and zero-point Energies= -4893.929733
Sum of electronic and thermal Energies= -4893.905551
Sum of electronic and thermal Enthalpies= -4893.904607
Sum of electronic and thermal Free Energies= -4893.986622

C	-3.03615900	-1.47922900	-1.00536000
O	-3.58360700	-0.31983100	-1.08381500
C	-3.72718600	-2.69444500	-0.92015000
H	-3.14584600	-3.60673300	-0.88326300
C	-5.13538500	-2.79891800	-0.83990500
O	-5.91740500	-1.79941500	-0.86169000
C	-5.84418000	-4.16080100	-0.71787200
C	-1.49617300	-1.41323600	-1.00946800
Ni	-5.43455200	0.05667100	-1.16028600
C	-5.07611800	1.92976300	-1.04472300
C	-4.02526300	2.51299000	-1.74720500
C	-5.81228300	2.63386400	-0.09387100
C	-3.67941300	3.84006300	-1.46191200
H	-3.47149700	1.93696700	-2.49080200
C	-5.44910000	3.95961700	0.19256000
H	-6.66031600	2.17381100	0.42047400
C	-4.38776800	4.56061800	-0.49129000
H	-2.85118600	4.30956500	-1.99978500
H	-6.00953300	4.52070500	0.94532200
H	-4.11536900	5.59643300	-0.27374000
Br	-7.01082900	0.53755800	-2.78894400
C	-0.82487900	-2.79026300	-0.90392000
H	0.26880700	-2.66309600	-0.90844200
H	-1.09603800	-3.30833600	0.02879000
H	-1.08623300	-3.44054200	-1.75290200
C	-1.06736500	-0.53931500	0.19008600
H	-1.52928500	0.45628300	0.13242800
H	-1.36436100	-1.00500600	1.14367200

H	0.02751600	-0.42002100	0.19436000
C	-1.06446000	-0.73322900	-2.32785900
H	-1.37069900	-1.33269600	-3.20032400
H	-1.51391800	0.26561900	-2.41892200
H	0.03150500	-0.62708200	-2.35371200
C	-4.88062500	-5.35397100	-0.64152600
H	-4.25497900	-5.43533600	-1.54363900
H	-4.21904700	-5.29123900	0.23639500
H	-5.45993100	-6.28646500	-0.55518600
C	-6.74880700	-4.30624300	-1.96245300
H	-7.43935700	-3.45456000	-2.04257700
H	-6.14709900	-4.34976800	-2.88470800
H	-7.33724200	-5.23482400	-1.89380000
C	-6.71490500	-4.12101300	0.55675900
H	-7.28836300	-5.05672800	0.64971000
H	-6.09018400	-4.01201200	1.45819700
H	-7.42044400	-3.27901100	0.52120300

UB3LYP-D3/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF)
HF= -4895.73076529

^{3}C-complex^{TMHD}



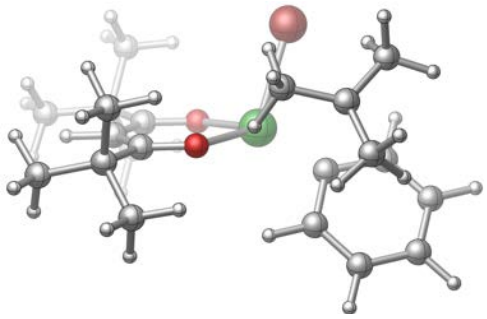
UB3LYP-D3/def2-SVP-CPCM(THF)
Zero-point correction= 0.489906 (Hartree/Particle)
Thermal correction to Energy= 0.521374
Thermal correction to Enthalpy= 0.522318
Thermal correction to Gibbs Free Energy= 0.425218
Sum of electronic and zero-point Energies= -5051.534392
Sum of electronic and thermal Energies= -5051.502925
Sum of electronic and thermal Enthalpies= -5051.501980
Sum of electronic and thermal Free Energies= -5051.599081

C	-4.19805300	-1.47087900	2.19745700
O	-4.50713200	-0.26041500	2.40633100
C	-3.64201300	-1.95701600	0.98997300
H	-3.38548300	-3.00792600	0.94331000
C	-3.40732200	-1.18306300	-0.16154400
O	-3.67565300	0.06084000	-0.26625000
C	-2.82101300	-1.83063900	-1.43715800
C	-4.49347400	-2.42012600	3.38050200
Ni	-4.38692600	1.27767400	1.14689900
C	-3.53261500	2.98911100	0.63333600
C	-4.09190300	4.26960500	0.82963200
C	-2.20030100	2.95478800	0.16314500
C	-3.37483200	5.44670800	0.57720100
H	-5.12660000	4.34462800	1.18194500
C	-1.46416700	4.11968700	-0.08781100
H	-1.72921700	1.98262600	-0.02135600
C	-2.05271000	5.37490200	0.11651100
H	-3.84425200	6.42272600	0.73669100
H	-0.43408700	4.05370600	-0.45251500
H	-1.48788900	6.28958100	-0.08493700
Br	-6.83112500	1.61530300	0.78921500
C	-4.86396000	3.06426000	-2.38815600
C	-3.64646000	3.80785300	-2.72703000
H	-2.77298600	3.16917100	-2.90126600
H	-3.89618800	4.33714800	-3.67169600

H	-3.43193200	4.59688000	-1.98973500
C	-6.02730300	3.75295600	-1.85560300
H	-6.27492900	3.23522900	-0.88809900
H	-5.88983200	4.82841100	-1.70092200
H	-6.91126200	3.52976500	-2.47876300
C	-4.92032100	1.62609300	-2.60312500
H	-4.39980600	1.18120800	-1.71248700
H	-5.93601900	1.21352600	-2.61584200
H	-4.31876400	1.30951200	-3.46806300
C	-3.99765900	-2.04299800	-2.41666900
H	-4.50980500	-1.09613700	-2.63543100
H	-3.62975600	-2.46321500	-3.36682800
H	-4.73811400	-2.74187400	-1.99634900
C	-1.79247300	-0.86164300	-2.05512900
H	-0.94894400	-0.69247700	-1.36629000
H	-1.39075900	-1.28343000	-2.98995400
H	-2.24412200	0.11364500	-2.27809000
C	-2.13552100	-3.18274700	-1.17725000
H	-1.33979400	-3.09453500	-0.42124800
H	-2.84676500	-3.95210300	-0.84154600
H	-1.67782500	-3.54796000	-2.11010200
C	-4.03481600	-3.86790200	3.15263100
H	-4.54509200	-4.33078300	2.29399500
H	-2.94829100	-3.93038100	2.98467900
H	-4.26982000	-4.47309900	4.04257900
C	-3.78742500	-1.85256500	4.62981700
H	-4.10196500	-0.81629000	4.81677700
H	-4.03378000	-2.46071900	5.51490000
H	-2.69233900	-1.86283400	4.50307800
C	-6.02375400	-2.39487900	3.59346500
H	-6.29684300	-3.00026000	4.47277700
H	-6.37558700	-1.36501800	3.74989800
H	-6.55016300	-2.80707100	2.71709800

UB3LYP-D3/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF)
HF= -5053.62941616

^{3}C-TS^{TMHD}



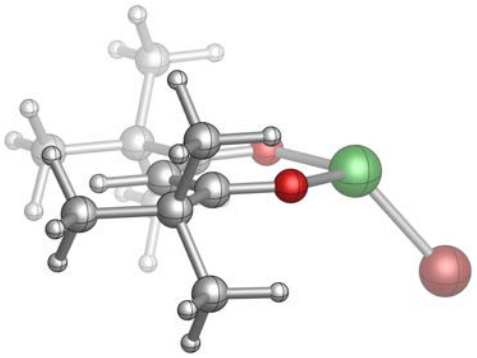
UB3LYP-D3/def2-SVP-CPCM(THF)
Zero-point correction= 0.490206 (Hartree/Particle)
Thermal correction to Energy= 0.521083
Thermal correction to Enthalpy= 0.522027
Thermal correction to Gibbs Free Energy= 0.426260
Sum of electronic and zero-point Energies= -5051.532776
Sum of electronic and thermal Energies= -5051.501899
Sum of electronic and thermal Enthalpies= -5051.500955
Sum of electronic and thermal Free Energies= -5051.596722

C	-4.14753400	-1.48132700	2.30746700
O	-4.44355000	-0.25668700	2.44671400
C	-3.54744000	-2.03086700	1.15083200
H	-3.31137500	-3.08747600	1.15977900
C	-3.22455700	-1.29905500	-0.00872700
O	-3.47446100	-0.06153200	-0.17935400
C	-2.54038500	-1.98320100	-1.21504200
C	-4.51150100	-2.36708500	3.51972900
Ni	-4.34960200	1.19437100	1.09370400
C	-3.58220100	2.93087200	0.48779900
C	-4.14597100	4.19912300	0.75030900
C	-2.24245000	2.92270400	0.02939800
C	-3.42897200	5.38828400	0.57152100
H	-5.18348000	4.25104300	1.09742400
C	-1.50639600	4.09787000	-0.14584200
H	-1.77131500	1.96058700	-0.20018500
C	-2.10333200	5.34043800	0.11802800
H	-3.90014900	6.35387200	0.77915200
H	-0.47168900	4.05531300	-0.49971000
H	-1.53881400	6.26508900	-0.03090500
Br	-6.81827500	1.41346700	0.81869300
C	-4.80157500	3.10131700	-2.19963000
C	-3.66950100	3.87909300	-2.71678800
H	-2.79502500	3.26976500	-2.96958300
H	-4.04306200	4.39922900	-3.62213900
H	-3.39483700	4.68633700	-2.01619500

C	-6.03327600	3.78608800	-1.79967500
H	-6.44540600	3.30572100	-0.89038200
H	-5.92497300	4.87084800	-1.68731900
H	-6.77949600	3.55714800	-2.58873600
C	-4.81055300	1.64007500	-2.33682300
H	-3.89070000	1.19522500	-1.92766300
H	-5.68174500	1.16981800	-1.86640100
H	-4.80286000	1.43280500	-3.42681200
C	-1.36682000	-1.09243100	-1.67365800
H	-0.60786900	-1.00101100	-0.87959800
H	-0.88241900	-1.53201300	-2.56002000
H	-1.71247300	-0.08167900	-1.93039000
C	-3.59341200	-2.07608500	-2.34200800
H	-4.44565900	-2.70332800	-2.03499400
H	-3.97871700	-1.08155200	-2.60630200
H	-3.14588500	-2.52411300	-3.24397500
C	-2.00793200	-3.39155900	-0.90638300
H	-2.81605800	-4.09348400	-0.65093200
H	-1.49371400	-3.79320600	-1.79391100
H	-1.28532900	-3.37895800	-0.07559900
C	-6.04880200	-2.30525100	3.66341200
H	-6.37116500	-2.86187300	4.55816400
H	-6.38771800	-1.26317100	3.75271400
H	-6.54428300	-2.75089000	2.78539500
C	-4.07225900	-3.83210800	3.38081800
H	-4.55138400	-4.32532800	2.52106400
H	-2.98057600	-3.92334400	3.26785400
H	-4.36123100	-4.39066500	4.28530800
C	-3.84905200	-1.75312600	4.77088600
H	-4.14529300	-2.31349400	5.67213300
H	-2.74995400	-1.78908800	4.69275900
H	-4.15064900	-0.70358900	4.89435000

UB3LYP-D3/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF)
HF= -5053.62798843

^3P_A^{TMHD}



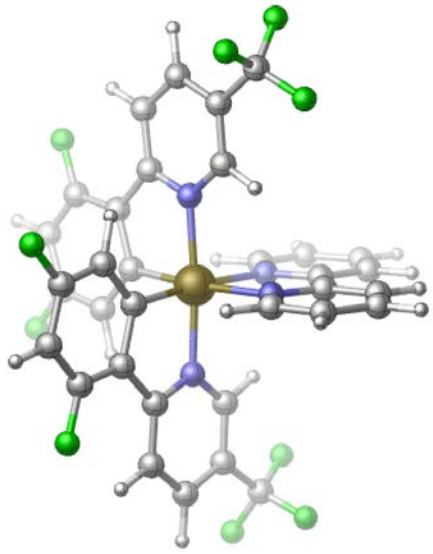
UB3LYP-D3/def2-SVP-CPCM(THF)
Zero-point correction= 0.282662 (Hartree/Particle)
Thermal correction to Energy= 0.301298
Thermal correction to Enthalpy= 0.302242
Thermal correction to Gibbs Free Energy= 0.233217
Sum of electronic and zero-point Energies= -4662.566267
Sum of electronic and thermal Energies= -4662.547631
Sum of electronic and thermal Enthalpies= -4662.546686
Sum of electronic and thermal Free Energies= -4662.615712

C	-4.16700400	-0.40222700	2.65529700
O	-5.13971600	0.35433000	2.31766400
C	-3.23345300	-0.95046200	1.75314300
H	-2.45486600	-1.58098000	2.16264600
C	-3.21113900	-0.71121000	0.36412700
O	-4.06759300	0.00109200	-0.26275100
C	-2.11244400	-1.30436300	-0.53872000
C	-4.08893700	-0.67638000	4.16906700
Ni	-5.62926000	0.77793600	0.52055600
Br	-7.73773800	0.11643200	-0.24995500
C	-2.90452500	-1.56399200	4.57828100
H	-1.93833400	-1.10485800	4.31781100
H	-2.91897000	-1.71112000	5.66947900
H	-2.95499600	-2.55864500	4.10923100
C	-3.97676100	0.68838700	4.88340500
H	-4.81907900	1.34057700	4.61305300
H	-3.98111300	0.54324000	5.97520400
H	-3.03991500	1.20067100	4.61027400
C	-5.41118300	-1.36744300	4.57247800
H	-6.27548000	-0.74839600	4.29302600
H	-5.51205200	-2.34592400	4.07557900
H	-5.43309500	-1.53298600	5.66122100
C	-1.08285500	-2.15697000	0.21714600
H	-0.54178200	-1.57110500	0.97611600
H	-1.55059600	-3.02123300	0.71340400

H	-0.33824900	-2.54663100	-0.49437100
C	-1.39251800	-0.12376400	-1.22725300
H	-0.63530700	-0.50315200	-1.93149900
H	-2.10740000	0.49898900	-1.78337600
H	-0.88157600	0.51258700	-0.48657700
C	-2.81648900	-2.17637200	-1.60240600
H	-3.33119000	-3.03092200	-1.13404800
H	-3.56097400	-1.58898700	-2.15814200
H	-2.07612800	-2.57259800	-2.31519100

UB3LYP-D3/def2-TZVPP-CPCM(THF)// UB3LYP-D3/def2-SVP-CPCM(THF)
HF= -4664.03136026

Figure S17
[Ir(II)]



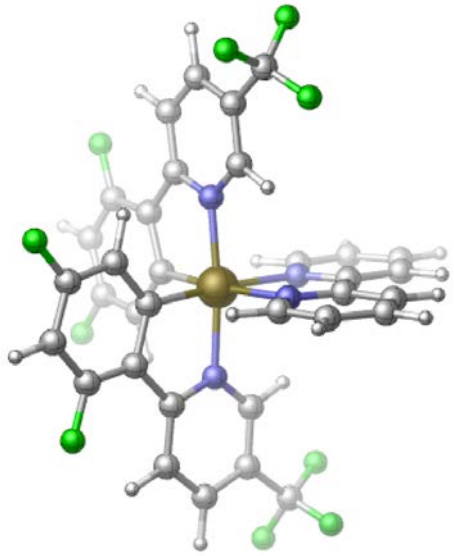
UB3LYP-D3/def2-SVP-CPCM(THF)
Zero-point correction= 0.456088 (Hartree/Particle)
Thermal correction to Energy= 0.496055
Thermal correction to Enthalpy= 0.496999
Thermal correction to Gibbs Free Energy= 0.378449
Sum of electronic and zero-point Energies= -2626.184144
Sum of electronic and thermal Energies= -2626.144177
Sum of electronic and thermal Enthalpies= -2626.143232
Sum of electronic and thermal Free Energies= -2626.261783

Ir	-0.38361500	0.77402400	0.05316900
C	2.34735200	1.55708000	1.07420000
C	2.41755700	1.29983400	-1.28265800
C	3.73792100	1.88540800	1.05493200
C	1.54618300	1.50257900	2.25738700
C	3.76397300	1.61776800	-1.34905400
H	1.85216300	1.05616000	-2.18579600
C	4.43596300	1.91595000	-0.13134000
H	4.24922400	2.11309300	1.99056100
C	2.02866400	1.78209300	3.57294900
H	4.27848300	1.63319400	-2.31040600
H	5.49928800	2.16794500	-0.13425200
C	-0.59876000	1.08108500	3.17806200
C	1.18832500	1.70340600	4.66064600
H	3.07308700	2.06117100	3.71419800
C	-0.17324600	1.33815200	4.47076900
H	-1.63515300	0.80142300	2.97206200
H	1.56779800	1.92063400	5.66211800
H	-0.87109400	1.26044100	5.30511000
C	-1.20298700	-1.96383800	0.73819500

C	1.11681300	-1.82859300	0.34511200
C	-1.07689600	-3.34293800	0.99669600
C	-2.43196900	-1.17336500	0.77340100
C	1.28877300	-3.18376500	0.59613000
H	1.95705500	-1.18870400	0.07846900
C	0.16627400	-3.95482400	0.92500200
H	-1.95872600	-3.92382500	1.24996100
C	-2.28624200	0.21283100	0.45110000
C	-3.71127200	-1.66010700	1.10138600
H	0.26512200	-5.02467200	1.11845200
C	-3.42294200	1.03566800	0.46870100
C	-4.83725100	-0.84913300	1.12405700
C	-4.66164900	0.49780900	0.80247100
H	-3.36520800	2.09860200	0.22890800
H	-5.81457800	-1.25438600	1.38393400
C	-0.76136600	0.59493300	-1.92704200
C	-1.08185900	1.82964800	-2.57472800
C	-0.70798800	-0.57879600	-2.69448400
C	-1.32492000	1.82253700	-3.96108600
C	-1.12033100	3.00700200	-1.70896600
C	-0.95672700	-0.52336500	-4.06206400
H	-0.47155300	-1.54613700	-2.24825800
C	-1.26781200	0.66511300	-4.72473000
C	-1.42632300	4.32796300	-2.09075400
H	-1.45934100	0.69105800	-5.79690900
C	-0.81789200	3.72327200	0.51586400
C	-1.42840100	5.34401800	-1.14574900
H	-1.66027100	4.54557000	-3.12862000
C	-1.11862300	5.03850900	0.18583900
H	-1.66255400	6.36897900	-1.43944600
N	1.71837900	1.25851900	-0.13231300
N	0.20508800	1.16057400	2.10042000
N	-0.08694600	-1.23930600	0.40954300
N	-0.82238600	2.74098200	-0.39775800
C	2.66020500	-3.80107100	0.55323200
F	3.14500300	-4.01512800	1.79241600
F	3.54522900	-3.02117500	-0.09014500
F	2.63996800	-4.99550400	-0.06605700
F	-3.88932800	-2.95793500	1.41527800
F	-5.73932900	1.29702900	0.81882300
F	-1.62428200	2.96511100	-4.60875900
F	-0.89844900	-1.65281300	-4.78414100
H	-0.56136900	3.43599300	1.53475600
C	-1.15339100	6.10205200	1.24945300
F	-0.61759400	7.25480300	0.80869300
F	-0.48167500	5.73342700	2.35350300

F -2.41670600 6.38074700 1.62781400
UB3LYP-D3/def2-TZVPP-CPCM(THF)// UB3LYP-D3/def2-SVP-CPCM(THF)
HF= -2629.5151152
UM06/def2-TZVPP-CPCM(THF)// UB3LYP-D3/def2-SVP-CPCM(THF)
HF= -2627.9322792

[Ir(III)]$^+$



UB3LYP-D3/def2-SVP-CPCM(THF)
Zero-point correction= 0.459873 (Hartree/Particle)
Thermal correction to Energy= 0.499499
Thermal correction to Enthalpy= 0.500443
Thermal correction to Gibbs Free Energy= 0.383450
Sum of electronic and zero-point Energies= -2626.063035
Sum of electronic and thermal Energies= -2626.023409
Sum of electronic and thermal Enthalpies= -2626.022465
Sum of electronic and thermal Free Energies= -2626.139458

Ir	-0.36720300	0.77952700	0.06402700
C	2.38652400	1.58502300	1.06698800
C	2.42805500	1.35755700	-1.25950400
C	3.73997300	1.94563400	1.07249400
C	1.56470700	1.49006000	2.29981200
C	3.77401700	1.71107200	-1.32161800
H	1.86155100	1.11139000	-2.15945200
C	4.43993800	2.00930000	-0.13187700
H	4.24890400	2.17751000	2.00668500
C	2.07363700	1.73195000	3.58207600
H	4.28084200	1.74808300	-2.28671300
H	5.49488900	2.28997700	-0.13730600
C	-0.54779900	1.03770800	3.19369300
C	1.23267100	1.61942200	4.68865100
H	3.11804600	2.00575800	3.72187300
C	-0.10296800	1.26420200	4.49413000
H	-1.58236600	0.75935700	2.98495900
H	1.62051500	1.80683600	5.69171500
H	-0.79616300	1.16232700	5.33004100
C	-1.21972100	-1.95400300	0.73314100

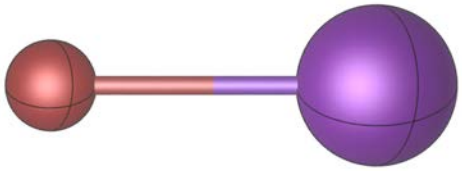
C	1.10163800	-1.85646100	0.34063800
C	-1.11821500	-3.33733900	0.97548300
C	-2.43541000	-1.14432500	0.77199500
C	1.25013700	-3.21667800	0.57522400
H	1.95744300	-1.23755900	0.07567900
C	0.11416200	-3.97017800	0.89631400
H	-2.01018300	-3.90644400	1.21964200
C	-2.27236700	0.23887500	0.45318600
C	-3.72190900	-1.61132400	1.10260600
H	0.19325500	-5.04396300	1.07620300
C	-3.39069500	1.08218300	0.47576200
C	-4.83382600	-0.78149000	1.12989900
C	-4.63836000	0.56239400	0.81197100
H	-3.32047300	2.14392000	0.23766600
H	-5.81688700	-1.17171500	1.39127000
C	-0.74495800	0.58128800	-1.90904100
C	-1.07074200	1.80607900	-2.56857000
C	-0.67417000	-0.60085500	-2.65716800
C	-1.30553300	1.78075600	-3.95663300
C	-1.12303600	2.99278100	-1.71722400
C	-0.91559400	-0.56296500	-4.02840200
H	-0.43349300	-1.56155800	-2.20088300
C	-1.23351300	0.61441100	-4.70518000
C	-1.45072100	4.30320700	-2.11465900
H	-1.41910400	0.62615600	-5.77867700
C	-0.83773400	3.74010900	0.49917100
C	-1.47314600	5.32942900	-1.18093400
H	-1.68875200	4.50473300	-3.15477800
C	-1.16335400	5.04493300	0.15494100
H	-1.72632500	6.34619300	-1.48708800
N	1.75547400	1.29387500	-0.09938000
N	0.26119100	1.15194300	2.12847300
N	-0.09061500	-1.24482100	0.41597400
N	-0.81828700	2.74747400	-0.40373300
C	2.61267600	-3.85661200	0.52181200
F	3.10234800	-4.07120500	1.75753400
F	3.50139300	-3.08854900	-0.13119600
F	2.56742400	-5.04948500	-0.09414100
F	-3.91702700	-2.90403800	1.41404900
F	-5.69845700	1.37943900	0.83251100
F	-1.60903600	2.91184300	-4.61605200
F	-0.84204900	-1.69891000	-4.73266500
H	-0.58538500	3.47760800	1.52538800
C	-1.22539400	6.11997400	1.20806100
F	-0.68430200	7.26779300	0.76615200
F	-0.57444400	5.76211400	2.32835200

F -2.49680900 6.39308100 1.55489100
UB3LYP-D3/def2-TZVPP-CPCM(THF)// UB3LYP-D3/def2-SVP-CPCM(THF)
HF= -2629.3946502
UM06/def2-TZVPP-CPCM(THF)// UB3LYP-D3/def2-SVP-CPCM(THF)
HF= -2627.8122578

K^+

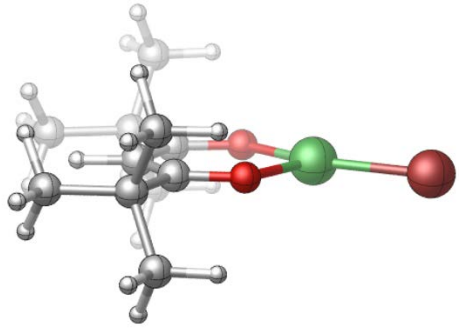
UB3LYP-D3/def2-SVP-CPCM(THF)
Zero-point correction= 0.000000 (Hartree/Particle)
Thermal correction to Energy= 0.001416
Thermal correction to Enthalpy= 0.002360
Thermal correction to Gibbs Free Energy= -0.015176
Sum of electronic and zero-point Energies= -599.792231
Sum of electronic and thermal Energies= -599.790815
Sum of electronic and thermal Enthalpies= -599.789871
Sum of electronic and thermal Free Energies= -599.807407
K 0.67977500 1.81953700 -2.01383600
UB3LYP-D3/def2-TZVPP-CPCM(THF)// UB3LYP-D3/def2-SVP-CPCM(THF)
HF= -599.8697705
UM06/def2-TZVPP-CPCM(THF)// UB3LYP-D3/def2-SVP-CPCM(THF)
HF= -599.8424387

KBr



UB3LYP-D3/def2-SVP-CPCM(THF)
Zero-point correction= 0.000291 (Hartree/Particle)
Thermal correction to Energy= 0.003334
Thermal correction to Enthalpy= 0.004279
Thermal correction to Gibbs Free Energy= -0.024774
Sum of electronic and zero-point Energies= -3173.856696
Sum of electronic and thermal Energies= -3173.853653
Sum of electronic and thermal Enthalpies= -3173.852709
Sum of electronic and thermal Free Energies= -3173.881762
K -0.27573900 1.80647700 -1.00469500
Br -3.38333800 1.80647700 -1.00469500
UB3LYP-D3/def2-TZVPP-CPCM(THF)// UB3LYP-D3/def2-SVP-CPCM(THF)
HF= -3174.256792
UM06/def2-TZVPP-CPCM(THF)// UB3LYP-D3/def2-SVP-CPCM(THF)
HF= -3174.1001508

^1P_A-TMHD



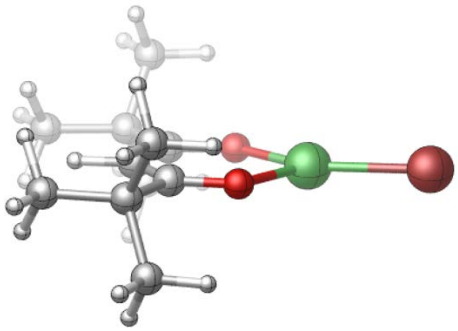
UB3LYP-D3/def2-SVP-CPCM(THF)
Zero-point correction= 0.282899 (Hartree/Particle)
Thermal correction to Energy= 0.301442
Thermal correction to Enthalpy= 0.302386
Thermal correction to Gibbs Free Energy= 0.234658
Sum of electronic and zero-point Energies= -4662.552097
Sum of electronic and thermal Energies= -4662.533554
Sum of electronic and thermal Enthalpies= -4662.532610
Sum of electronic and thermal Free Energies= -4662.600337

C	-2.67689100	1.50064700	-0.05133500
O	-1.42106200	1.53065300	-0.28586800
C	-3.43835400	0.32407000	0.07753400
H	-4.49775900	0.42432000	0.27535300
C	-2.90671800	-0.97398200	-0.03591800
O	-1.67346600	-1.22093200	-0.26675900
C	-3.30475800	2.90087100	0.08111300
C	-3.78209700	-2.23131300	0.10708500
Ni	-0.31332000	0.03984100	-0.51201000
Br	1.82020300	0.91198800	-0.90887100
C	-3.67744000	-3.01696800	-1.21927400
H	-2.63039000	-3.26130100	-1.44801600
H	-4.24888200	-3.95565800	-1.14550000
H	-4.08809500	-2.43169500	-2.05782800
C	-5.25691000	-1.91964900	0.40030800
H	-5.81737900	-2.86280300	0.49247700
H	-5.37928900	-1.36675700	1.34431100
H	-5.72151600	-1.33529900	-0.40862600
C	-3.19667000	-3.07570700	1.26065900
H	-3.25819300	-2.53293700	2.21771400
H	-3.76359900	-4.01435100	1.36297400
H	-2.14248000	-3.32164900	1.07013400
C	-3.04457300	3.64761900	-1.24638900
H	-3.42761500	4.67791500	-1.17842900
H	-1.96868200	3.68623800	-1.46782300
H	-3.55352200	3.14797900	-2.08647800

C	-4.81319500	2.87253300	0.36555800
H	-5.37475200	2.38061600	-0.44351400
H	-5.04277600	2.35931100	1.31202700
H	-5.18707500	3.90483500	0.44886800
C	-2.57677900	3.62410700	1.23623200
H	-2.95320300	4.65492400	1.32904500
H	-2.74929600	3.10915900	2.19514100
H	-1.49362900	3.66017400	1.05302600

UB3LYP-D3/def2-TZVPP-CPCM(THF)// UB3LYP-D3/def2-SVP-CPCM(THF)
HF= -4664.0202018
UM06/def2-TZVPP-CPCM(THF)// UB3LYP-D3/def2-SVP-CPCM(THF)
HF= -4663.333533

^3P_A-TMHD



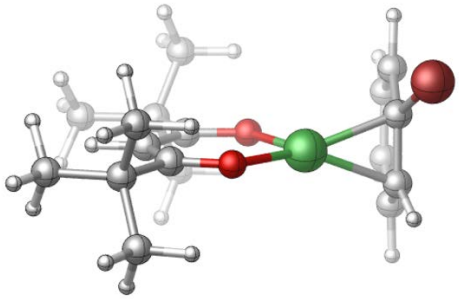
UB3LYP-D3/def2-SVP-CPCM(THF)
Zero-point correction= 0.282628 (Hartree/Particle)
Thermal correction to Energy= 0.301243
Thermal correction to Enthalpy= 0.302187
Thermal correction to Gibbs Free Energy= 0.233454
Sum of electronic and zero-point Energies= -4662.565357
Sum of electronic and thermal Energies= -4662.546741
Sum of electronic and thermal Enthalpies= -4662.545797
Sum of electronic and thermal Free Energies= -4662.614530

C	-2.71245200	1.52103100	-0.04857400
O	-1.45837800	1.56881700	-0.27941600
C	-3.45883500	0.33159800	0.07913400
H	-4.52137600	0.42417300	0.26347600
C	-2.92327900	-0.96773600	-0.01162300
O	-1.68892300	-1.22719900	-0.21770400
C	-3.37150100	2.90790100	0.08917000
C	-3.80975600	-2.22005900	0.12992000
Ni	-0.28827500	0.05093900	-0.50691000
Br	1.92911300	0.60440700	-1.08862900
C	-3.68687100	-3.01752700	-1.18789800
H	-2.63661800	-3.26429600	-1.39857800
H	-4.26046700	-3.95521300	-1.11606200
H	-4.08376300	-2.43856900	-2.03759700
C	-5.28877600	-1.90374100	0.39590100
H	-5.85325700	-2.84488000	0.48603200
H	-5.42618500	-1.34293600	1.33320700
H	-5.73872800	-1.32467400	-0.42510700
C	-3.24759500	-3.05863700	1.29887700
H	-3.32562900	-2.50982300	2.25143700
H	-3.81724600	-3.99619600	1.39731400
H	-2.19040400	-3.30667500	1.12888900
C	-3.09963700	3.68145600	-1.21992800
H	-3.49950700	4.70484300	-1.14282400
H	-2.02075400	3.73993500	-1.42127400
H	-3.58547300	3.18839400	-2.07755400

C	-4.88485300	2.85280500	0.34352000
H	-5.42231700	2.35841700	-0.48042200
H	-5.12521900	2.32757400	1.28069900
H	-5.27822900	3.87785000	0.42845200
C	-2.68038400	3.62616200	1.26988500
H	-3.07617000	4.64901400	1.37174600
H	-2.86289300	3.09311000	2.21711100
H	-1.59448700	3.68392200	1.10943900

UB3LYP-D3/def2-TZVPP-CPCM(THF)// UB3LYP-D3/def2-SVP-CPCM(THF)
HF= -4664.0306008
UM06/def2-TZVPP-CPCM(THF)// UB3LYP-D3/def2-SVP-CPCM(THF)
HF= -4663.3442077

^{2}A-TMHD



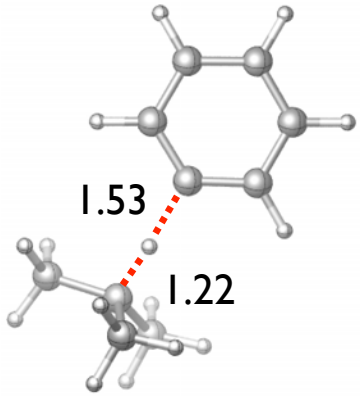
UB3LYP-D3/def2-SVP-CPCM(THF)
Zero-point correction= 0.371812 (Hartree/Particle)
Thermal correction to Energy= 0.396012
Thermal correction to Enthalpy= 0.396956
Thermal correction to Gibbs Free Energy= 0.314402
Sum of electronic and zero-point Energies= -4893.918513
Sum of electronic and thermal Energies= -4893.894313
Sum of electronic and thermal Enthalpies= -4893.893369
Sum of electronic and thermal Free Energies= -4893.975922

C	-2.35056300	1.49763400	-0.08085100
O	-1.10960500	1.45110100	-0.33763200
C	-3.19367000	0.36601100	0.03381700
H	-4.23921800	0.54154200	0.25423300
C	-2.77418500	-0.97096700	-0.12013600
O	-1.57666200	-1.32919700	-0.37629300
C	-2.90157200	2.93116400	0.09863400
C	-3.76813200	-2.14650600	0.00901700
Ni	-0.07491500	-0.16653800	-0.64206800
C	1.55418400	2.72254700	-1.71182500
C	1.45782900	1.54447300	-2.43036700
C	1.62478300	0.28492900	-1.78974300
C	1.91005300	0.27106800	-0.39159800
C	2.04367800	1.49041300	0.32913700
C	1.84316700	2.69133100	-0.32679000
H	1.41396600	3.68253200	-2.21343400
H	1.26792300	1.56399800	-3.50600800
H	2.28974700	1.46223700	1.39153000
H	1.91409000	3.62603100	0.23439000
H	1.76342200	-0.61570400	-2.39502800
Br	2.65175100	-1.34156700	0.40594200
C	-2.09139300	3.59678000	1.23197500
H	-1.01591800	3.56642800	1.00633500
H	-2.39813000	4.64815900	1.35425500
H	-2.25721700	3.07951100	2.19139100
C	-4.39753200	2.99040200	0.43959900
H	-5.01698000	2.54991700	-0.35695600

H	-4.62378400	2.46802800	1.38216500
H	-4.70817700	4.04070800	0.55863100
C	-2.64839900	3.68495300	-1.22544000
H	-3.21915200	3.23119400	-2.05236800
H	-2.96191300	4.73731100	-1.13208300
H	-1.58124000	3.65678700	-1.48825900
C	-3.24958800	-3.07040100	1.13205500
H	-3.88771200	-3.96486700	1.21565800
H	-2.21897900	-3.39134100	0.92429600
H	-3.25977900	-2.55155500	2.10463900
C	-5.20695800	-1.71727400	0.33082900
H	-5.26878700	-1.17815200	1.28885400
H	-5.62897000	-1.07314100	-0.45610100
H	-5.84886200	-2.60918200	0.40975400
C	-3.75272900	-2.90842500	-1.33445600
H	-2.73172900	-3.22922200	-1.58600900
H	-4.39793100	-3.79982300	-1.27598900
H	-4.12491600	-2.27066600	-2.15299400

UB3LYP-D3/def2-TZVPP-CPCM(THF)// UB3LYP-D3/def2-SVP-CPCM(THF)
HF= -4895.7207494
UM06/def2-TZVPP-CPCM(THF)// UB3LYP-D3/def2-SVP-CPCM(THF)
HF= -4894.8531818

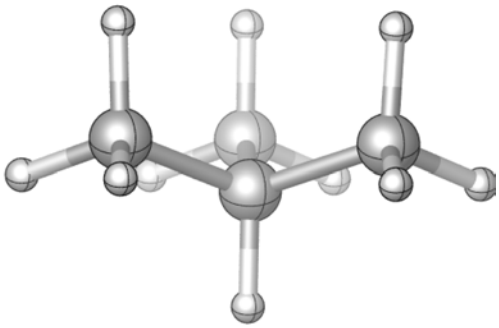
Figure S18



UB3LYP-D3/def2-SVP-CPCM(THF)
Zero-point correction= 0.213786 (Hartree/Particle)
Thermal correction to Energy= 0.225178
Thermal correction to Enthalpy= 0.226122
Thermal correction to Gibbs Free Energy= 0.173602
Sum of electronic and zero-point Energies= -389.540592
Sum of electronic and thermal Energies= -389.529200
Sum of electronic and thermal Enthalpies= -389.528256
Sum of electronic and thermal Free Energies= -389.580776

C	-1.32452900	-5.70999100	-0.64601400
C	-0.12003600	-5.86266600	-1.56424400
H	0.68500100	-6.43887600	-1.07969700
H	-0.40152200	-6.39634600	-2.49114200
H	0.29018200	-4.88221700	-1.85654500
C	-2.41255400	-4.81606700	-1.22439400
H	-2.85986500	-5.27816400	-2.12420100
H	-3.22412400	-4.64874100	-0.49758000
H	-2.01124200	-3.83307100	-1.52055000
C	-1.85409300	-7.03864200	-0.12381800
H	-1.05791200	-7.62793500	0.35995400
H	-2.66327700	-6.88962700	0.60966700
H	-2.26260400	-7.64800700	-0.95155300
H	-0.91115000	-5.12004400	0.34065500
C	-0.40944900	-4.39769200	1.59793900
C	-0.09322600	-3.04791900	1.51310700
C	-0.29669600	-5.12910100	2.77318600
C	0.36202000	-2.39719300	2.67184400
H	-0.19342200	-2.49804600	0.57204800
C	0.15955400	-4.46946500	3.92654200
H	-0.55527800	-6.19197700	2.80758700
C	0.48683500	-3.10845500	3.87230300
H	0.61887800	-1.33435500	2.63568700
H	0.25853600	-5.01968900	4.86691500

H 0.84136300 -2.59837600 4.77177200
UB3LYP-D3/def2-TZVPP-CPCM(THF)// UB3LYP-D3/def2-SVP-CPCM(THF)
HF= -390.1859701
UM06/def2-TZVPP-CPCM(THF)// UB3LYP-D3/def2-SVP-CPCM(THF)
HF= -389.8284779

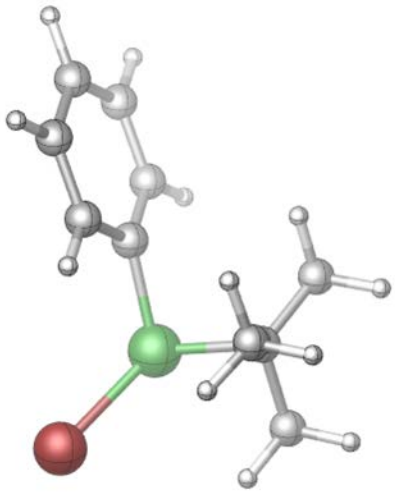


UB3LYP-D3/def2-SVP-CPCM(THF)
Zero-point correction= 0.130747 (Hartree/Particle)
Thermal correction to Energy= 0.136352
Thermal correction to Enthalpy= 0.137297
Thermal correction to Gibbs Free Energy= 0.103241
Sum of electronic and zero-point Energies= -158.220710
Sum of electronic and thermal Energies= -158.215105
Sum of electronic and thermal Enthalpies= -158.214161
Sum of electronic and thermal Free Energies= -158.248216

C	-1.35880900	-5.74058300	-0.69920900
C	-0.82369700	-4.98911000	-1.92428400
H	0.27857000	-4.96727300	-1.93406700
H	-1.15671900	-5.47685400	-2.85723600
H	-1.18260900	-3.94683300	-1.94599900
C	-2.89193400	-5.72268600	-0.66606700
H	-3.30687200	-6.23708900	-1.55062800
H	-3.28129200	-6.23329100	0.23015200
H	-3.28288100	-4.69183400	-0.66506000
C	-0.82205700	-7.17657400	-0.65350800
H	0.28028500	-7.19472100	-0.64411100
H	-1.17672700	-7.71082400	0.24334200
H	-1.15825600	-7.74716700	-1.53709700
H	-0.99537000	-5.21550400	0.20414900

UB3LYP-D3/def2-TZVPP-CPCM(THF)// UB3LYP-D3/def2-SVP-CPCM(THF)
HF= -158.5324782
UM06/def2-TZVPP-CPCM(THF)// UB3LYP-D3/def2-SVP-CPCM(THF)
HF= -158.3793557

Figure S19

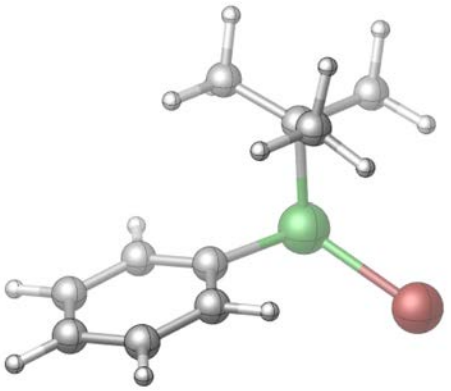


UB3LYP-D3/def2-SVP-CPCM(THF)
Zero-point correction= 0.211223 (Hartree/Particle)
Thermal correction to Energy= 0.225662
Thermal correction to Enthalpy= 0.226607
Thermal correction to Gibbs Free Energy= 0.167821
Sum of electronic and zero-point Energies= -4471.112669
Sum of electronic and thermal Energies= -4471.098230
Sum of electronic and thermal Enthalpies= -4471.097286
Sum of electronic and thermal Free Energies= -4471.156071

C	2.85880600	0.74317800	0.23337800
C	3.89346800	-0.36358800	0.23547100
C	2.89142500	1.59192300	-1.03876300
H	3.79736600	-1.00840200	-0.65008500
H	3.80865900	-0.98854000	1.13475300
H	2.83855000	0.98998300	-1.95855600
H	2.09760800	2.35745600	-1.06205300
Br	1.03762700	-1.52014500	-2.04620800
Ni	1.11076700	-0.01515500	-0.20188300
C	0.91749900	-0.80812000	1.49745800
C	0.23763100	-0.12580100	2.51524500
C	1.28575200	-2.14699300	1.68565300
C	-0.07912200	-0.78179600	3.71312800
H	-0.04145600	0.92453500	2.38833100
C	0.97451500	-2.79953400	2.88509200
H	1.80903300	-2.68372300	0.89031400
H	-0.61299000	-0.24450900	4.50216000
H	1.26392600	-3.84500600	3.02485900
C	0.29169800	-2.11808000	3.90012700
H	0.05055000	-2.62804200	4.83649700
H	4.90621400	0.08337100	0.22516700
H	3.85381700	2.13871200	-1.06186100

C	2.86935900	1.59626600	1.48856300
H	2.00503800	2.27775800	1.52880400
H	2.86822500	0.98299600	2.39880000
H	3.78220400	2.22164500	1.49347700

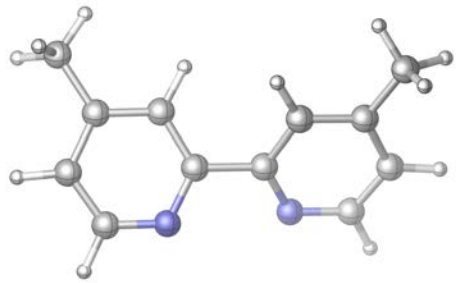
UB3LYP-D3/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF)
HF= -4472.2797924
UM06/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF)
HF= -4471.7023257



UB3LYP-D3/def2-SVP-CPCM(THF)
Zero-point correction= 0.211070 (Hartree/Particle)
Thermal correction to Energy= 0.225625
Thermal correction to Enthalpy= 0.226569
Thermal correction to Gibbs Free Energy= 0.166740
Sum of electronic and zero-point Energies= -4471.112594
Sum of electronic and thermal Energies= -4471.098040
Sum of electronic and thermal Enthalpies= -4471.097096
Sum of electronic and thermal Free Energies= -4471.156924

Ni	-0.69015100	-0.10048000	0.06690000
C	-1.96369900	1.24956000	-0.26283500
C	-3.75785000	3.24547600	-1.08695500
C	-3.28369100	0.91615600	-0.59356900
C	-1.54374900	2.58408400	-0.34634400
C	-2.43860100	3.58003200	-0.76273900
C	-4.17889400	1.91239800	-1.00231600
H	-3.61298600	-0.12420000	-0.53461900
H	-0.52004100	2.86087800	-0.07631200
H	-2.10321300	4.61904300	-0.82766500
H	-5.20867000	1.64572900	-1.25680800
Br	-1.01456200	-2.11044000	-1.14130800
C	-1.03216700	-0.11144300	1.98866700
H	-4.45861200	4.02270400	-1.40299600
C	0.07143200	-1.13149100	2.27540100
H	0.11860800	-1.28593800	3.37058600
H	-0.12193100	-2.10897700	1.81056400
H	1.07300700	-0.78180000	1.97154100
C	-2.41490100	-0.64855700	2.29100800
H	-3.19423400	0.09351200	2.07311600
H	-2.62479500	-1.55971000	1.71081700
H	-2.47953600	-0.90882600	3.36492000
C	-0.73489600	1.24114900	2.61122300
H	0.21051300	1.66488300	2.23478800
H	-1.53801100	1.96418300	2.41945300
H	-0.62753400	1.12405900	3.70638000

UB3LYP-D3/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF)
HF= -4472.279756
UM06/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF)
HF= -4471.7027401



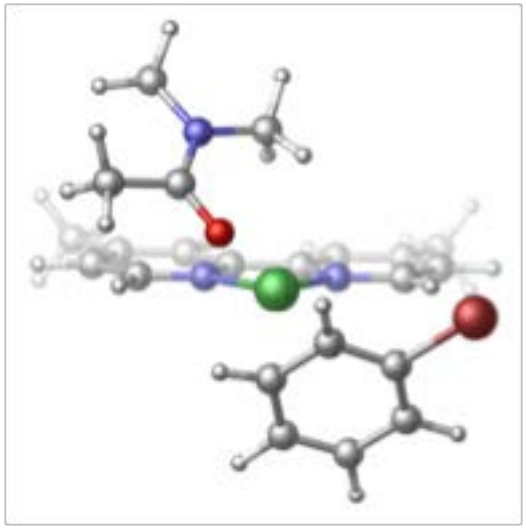
UB3LYP-D3/def2-SVP-CPCM(THF)
Zero-point correction= 0.212040 (Hartree/Particle)
Thermal correction to Energy= 0.224472
Thermal correction to Enthalpy= 0.225417
Thermal correction to Gibbs Free Energy= 0.170903
Sum of electronic and zero-point Energies= -573.414733
Sum of electronic and thermal Energies= -573.402300
Sum of electronic and thermal Enthalpies= -573.401356
Sum of electronic and thermal Free Energies= -573.455869

C	-2.31575100	-1.15742200	-0.05825600
C	-0.91697700	-1.27194600	0.02278700
C	-0.22447200	-0.70695500	1.10164900
C	-0.99218900	-0.04466300	2.07014800
C	-2.37809600	0.02559400	1.90563400
C	-3.07072300	-1.75985500	-1.20231200
C	-2.63843200	-2.95842800	-1.79813600
C	-3.35500200	-3.51359600	-2.86541400
C	-4.49796800	-2.81983100	-3.28994600
C	-4.85559900	-1.63801000	-2.63699400
H	-0.36149000	-1.78401300	-0.76571600
H	-0.51932900	0.41415800	2.94221800
H	-2.98834200	0.54166500	2.65702300
H	-1.75618600	-3.47459000	-1.41410900
H	-5.10737900	-3.19713900	-4.11514400
H	-5.74810300	-1.08816000	-2.96001800
N	-3.03302700	-0.50956800	0.87394100
N	-4.17073800	-1.11301100	-1.61872400
C	-2.91853600	-4.78894400	-3.53673600
H	-2.16322000	-5.32437400	-2.94346500
H	-3.77370400	-5.46175800	-3.70579800
H	-2.47910300	-4.57147800	-4.52509600
C	1.27668300	-0.77649400	1.19822700
H	1.60731200	-0.85611700	2.24488300
H	1.68075800	-1.63018200	0.63440200
H	1.72933200	0.14008200	0.78228300

UB3LYP-D3/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF)

HF= -574.2558479
UM06/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF)
HF= -573.7901558

^{1}F-DMA-O



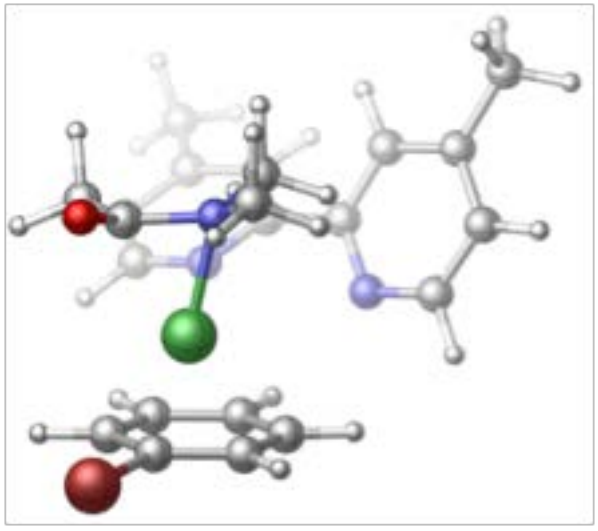
UB3LYP-D3/def2-SVP-CPCM(THF)
Zero-point correction= 0.435353 (Hartree/Particle)
Thermal correction to Energy= 0.465364
Thermal correction to Enthalpy= 0.466308
Thermal correction to Gibbs Free Energy= 0.371774
Sum of electronic and zero-point Energies= -5174.442026
Sum of electronic and thermal Energies= -5174.412014
Sum of electronic and thermal Enthalpies= -5174.411070
Sum of electronic and thermal Free Energies= -5174.505604

C	-1.99573800	1.70563600	1.27592200
O	-1.57857800	0.71672600	0.64048900
N	-2.89472400	2.56501500	0.75010400
C	-1.47410900	1.95364900	2.67628200
H	-1.11216300	2.98325600	2.81198000
H	-2.26334600	1.76787100	3.42184500
H	-0.65298600	1.24992700	2.85587800
C	-3.33995100	2.40820300	-0.63035700
H	-4.25568400	1.79961900	-0.69048700
H	-3.54156900	3.40275500	-1.05441600
H	-2.55717000	1.92011100	-1.22281600
C	-3.58663900	3.59887300	1.50728500
H	-4.67135200	3.39904700	1.50070200
H	-3.25493700	3.63050100	2.54901400
H	-3.41506200	4.58905900	1.05431700
Ni	-2.83422400	-0.70330200	-0.47307400
C	-2.12470800	-3.48520000	-0.24809200
C	-1.46424900	-2.23640700	-0.06587200
C	-0.92329800	-1.56582200	-1.20744300
C	-1.06246300	-2.17899900	-2.47563400
C	-1.73841200	-3.37384900	-2.65124100

C	-2.27633700	-4.02521900	-1.51351100
H	-2.51370100	-4.01365500	0.62537200
H	-1.14288900	-1.93603900	0.93594900
H	-1.85101900	-3.80954600	-3.64483900
H	-2.80536800	-4.97206300	-1.64706800
H	-0.24789300	-0.71828200	-1.08343100
Br	-0.30699000	-1.28484100	-3.99442100
C	-5.58488100	-0.71657100	-1.26670300
C	-6.73781400	-0.77640800	-2.10429200
C	-6.62620500	-0.92475200	-3.47360800
C	-5.31084700	-1.01892300	-4.02328900
C	-4.22414500	-0.96917600	-3.16702200
C	-5.62452000	-0.53277000	0.15671400
C	-6.81183900	-0.35572400	0.92827500
C	-6.75854700	-0.17742000	2.29830500
C	-5.47215700	-0.17843900	2.92135100
C	-4.35230300	-0.35121800	2.12428400
H	-7.72971900	-0.70607800	-1.65381300
H	-5.15633400	-1.12736700	-5.09888200
H	-3.20818600	-1.04370200	-3.56061600
H	-7.78206500	-0.35573300	0.42787800
H	-5.36804800	-0.05364900	4.00110500
H	-3.34962000	-0.36151400	2.56330400
N	-4.32004800	-0.82323300	-1.83343800
N	-4.39581800	-0.51921400	0.79480000
C	-7.99766800	0.01327800	3.13136200
H	-8.91250800	-0.01112300	2.52081600
H	-8.07819400	-0.77190300	3.90309800
H	-7.96779700	0.97738100	3.66821900
C	-7.82822500	-0.98815700	-4.37703000
H	-7.85017400	-1.93823500	-4.93878200
H	-8.77061600	-0.89980000	-3.81620200
H	-7.79867700	-0.18096600	-5.12951400

UB3LYP-D3/def2-TZVPP-CPCM(THF)// UB3LYP-D3/def2-SVP-CPCM(THF)
HF= -5176.5999679
UM06/def2-TZVPP-CPCM(THF)// UB3LYP-D3/def2-SVP-CPCM(THF)
HF= -5175.5019016

^{1}F-DMA'



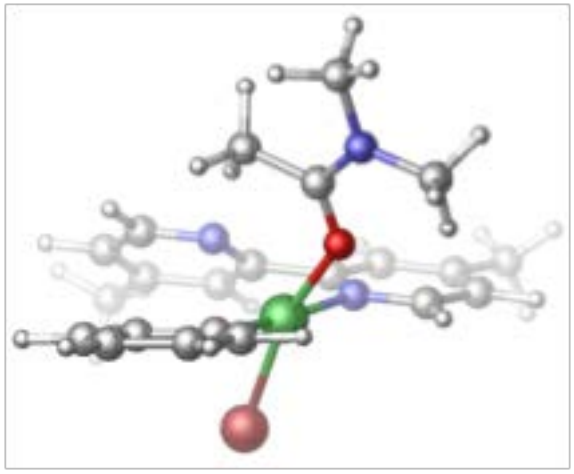
UB3LYP-D3/def2-SVP-CPCM(THF)
Zero-point correction= 0.434398 (Hartree/Particle)
Thermal correction to Energy= 0.465055
Thermal correction to Enthalpy= 0.465999
Thermal correction to Gibbs Free Energy= 0.367305
Sum of electronic and zero-point Energies= -5174.382824
Sum of electronic and thermal Energies= -5174.352168
Sum of electronic and thermal Enthalpies= -5174.351223
Sum of electronic and thermal Free Energies= -5174.449917

C	-1.97016600	-0.98194000	-1.08653400
O	-2.20401200	0.23211900	-0.94905100
N	-0.60758500	-1.45789200	-1.14294800
C	-3.05520500	-1.90925000	-1.62444700
H	-3.12003200	-1.79774700	-2.72214000
H	-2.91213600	-2.96911300	-1.38454000
H	-4.00633000	-1.56981000	-1.19390600
C	-0.25349500	-2.60168900	-1.99171600
H	-0.17849100	-2.30293900	-3.05367600
H	0.71643900	-3.00280500	-1.66692700
H	-0.99124600	-3.40058900	-1.88880200
C	0.42535300	-0.41680500	-1.13844900
H	0.58143400	-0.01349500	-2.15619400
H	0.11223800	0.39839900	-0.47949900
H	1.36587800	-0.85076800	-0.77147100
Ni	-1.23286100	-1.97005100	0.65837000
C	-1.08992900	-3.90407700	1.69927000
C	-2.39999500	-3.36935600	1.70329300
C	-2.63609200	-2.04654400	2.16848500
C	-1.53656200	-1.26833800	2.61729100
C	-0.22206000	-1.78959600	2.61961200

C	-0.01065000	-3.10841500	2.14799900
H	-0.90472400	-4.88789900	1.26762300
H	-3.23163500	-3.96770100	1.32849900
H	0.61175300	-1.18009900	2.96852300
H	1.00757500	-3.49857800	2.10094800
H	-3.64243600	-1.62574500	2.16820100
Br	-1.85461700	0.49234200	3.32735600
C	-0.09040200	-5.98907000	-1.79741600
C	0.72717800	-5.82898000	-2.92735000
C	2.08116800	-5.50137600	-2.77491200
C	2.55601200	-5.36665300	-1.46251900
C	1.67347400	-5.56036500	-0.39654700
C	-1.55072400	-6.27313800	-1.95183000
C	-2.01040200	-7.17779800	-2.92166800
C	-3.38412000	-7.41845300	-3.06355400
C	-4.24220200	-6.71770300	-2.20384900
C	-3.69645700	-5.83388600	-1.26960100
H	0.29925600	-5.92628100	-3.92752400
H	3.60125500	-5.11375200	-1.26868300
H	2.03505800	-5.46701800	0.63429100
H	-1.29511900	-7.71102700	-3.55197400
H	-5.32455600	-6.85832800	-2.25656300
H	-4.35677400	-5.27266200	-0.59793000
N	0.38261000	-5.86107300	-0.54841000
N	-2.38753300	-5.61150600	-1.13621600
C	-3.91142400	-8.36728900	-4.10664000
H	-3.18760700	-9.16524600	-4.32932600
H	-4.85947500	-8.82725000	-3.79075500
H	-4.10602100	-7.82680900	-5.04905000
C	2.96833300	-5.25888600	-3.96637600
H	4.01884800	-5.49575400	-3.74191900
H	2.64880300	-5.85264100	-4.83564100
H	2.92585600	-4.19588000	-4.26012500

UB3LYP-D3/def2-TZVPP-CPCM(THF)// UB3LYP-D3/def2-SVP-CPCM(THF)
HF= -5176.5457794
UM06/def2-TZVPP-CPCM(THF)// UB3LYP-D3/def2-SVP-CPCM(THF)
HF= -5175.463106

^{1}G-DMA-O



UB3LYP-D3/def2-SVP-CPCM(THF)
Zero-point correction= 0.437417 (Hartree/Particle)
Thermal correction to Energy= 0.467940
Thermal correction to Enthalpy= 0.468884
Thermal correction to Gibbs Free Energy= 0.371580
Sum of electronic and zero-point Energies= -5174.486401
Sum of electronic and thermal Energies= -5174.455878
Sum of electronic and thermal Enthalpies= -5174.454934
Sum of electronic and thermal Free Energies= -5174.552238

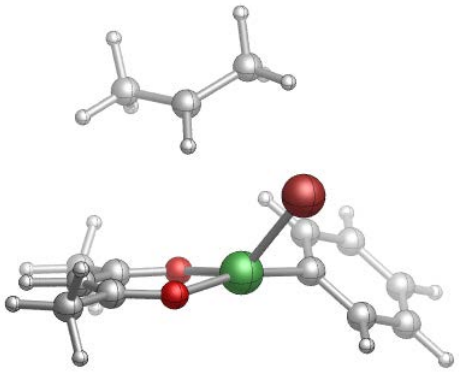
C	-2.51811700	0.31763100	0.07638600
O	-1.75704900	-0.42918400	-0.58355500
N	-2.03794100	0.99075400	1.13756200
C	-3.96681200	0.45866400	-0.30611300
H	-4.55773600	-0.27525200	0.26498400
H	-4.36819500	1.46308700	-0.12181600
H	-4.04949800	0.20330700	-1.37052500
C	-2.87060900	1.84720400	1.97767100
H	-2.39333500	1.94038300	2.96236100
H	-2.97962400	2.85839700	1.55033500
H	-3.86665800	1.41301600	2.13146500
C	-0.62541000	0.90751900	1.49514000
H	-0.19668200	1.92010700	1.56276800
H	-0.50684800	0.41033900	2.47185100
H	-0.08655700	0.33533700	0.73370900
Ni	-2.17675500	-1.82835800	-1.86714500
C	-3.43413900	-3.49580300	1.78010300
C	-2.67291600	-2.89108000	0.76966300
C	-3.15204600	-2.77163900	-0.54921900
C	-4.43301900	-3.29451900	-0.81448900
C	-5.20936200	-3.88521500	0.19066900
C	-4.71214100	-3.99090300	1.49636400
H	-3.02949300	-3.57586900	2.79444400

H	-1.68660800	-2.48703600	1.01852400
H	-4.82632300	-3.24467200	-1.83340900
H	-6.20606200	-4.27154400	-0.04668700
H	-5.31338900	-4.45711600	2.28225500
Br	-2.08778200	-3.71370700	-3.31942000
C	-3.16586000	-0.65969400	-4.64107200
C	-3.62524100	-0.99946500	-5.91967800
C	-4.96027400	-1.38708400	-6.10195100
C	-5.77973200	-1.40094300	-4.96412000
C	-5.23882800	-1.03497200	-3.72942700
C	-1.74267500	-0.29293700	-4.39998500
C	-0.99936100	0.43769100	-5.33616700
C	0.33428100	0.77675600	-5.07833500
C	0.86918600	0.36373200	-3.84796800
C	0.07257000	-0.35560600	-2.96397400
H	-2.93801600	-0.99718100	-6.76814700
H	-6.82987100	-1.69394000	-5.03522200
H	-5.86283400	-1.03861300	-2.82874600
H	-1.47541400	0.76390200	-6.26241400
H	1.90000700	0.60148200	-3.57663900
H	0.45598600	-0.68479900	-1.99576300
N	-3.96721800	-0.67229400	-3.56429500
N	-1.19861900	-0.68518600	-3.23111300
C	1.16437100	1.54228400	-6.07178600
H	0.54561600	1.98976200	-6.86246500
H	1.73798500	2.34099500	-5.57658600
H	1.89556400	0.87062000	-6.55264800
C	-5.47169300	-1.81243900	-7.45188100
H	-6.55881200	-1.66825800	-7.53590100
H	-4.97664600	-1.25818600	-8.26334200
H	-5.26605300	-2.88448100	-7.61430200

UB3LYP-D3/def2-TZVPP-CPCM(THF)// UB3LYP-D3/def2-SVP-CPCM(THF)
HF= -5176.6518013
UM06/def2-TZVPP-CPCM(THF)// UB3LYP-D3/def2-SVP-CPCM(THF)
HF= -5175.5492669

Figure S21 and S22

^{3}C-complex$^{i\text{-Pr}}$



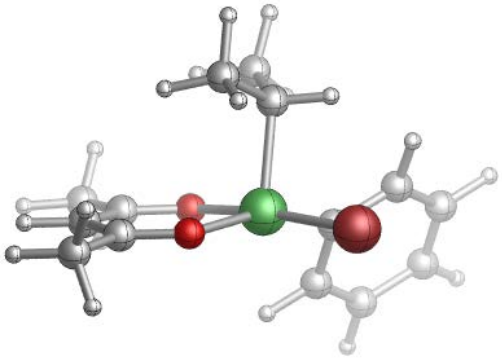
Zero-point correction= 0.291952 (Hartree/Particle)
Thermal correction to Energy= 0.315481
Thermal correction to Enthalpy= 0.316425
Thermal correction to Gibbs Free Energy= 0.234171
Sum of electronic and zero-point Energies= -4776.684870
Sum of electronic and thermal Energies= -4776.661341
Sum of electronic and thermal Enthalpies= -4776.660397
Sum of electronic and thermal Free Energies= -4776.742651

C	-4.50490500	-1.15068000	1.54684500
O	-4.87134800	-0.04408900	2.04910500
C	-3.52432800	-1.28040200	0.53511000
H	-3.27605100	-2.28174100	0.18558500
C	-2.79989200	-0.20410400	0.00948400
O	-2.98438600	1.03574600	0.29380900
C	-1.68382100	-0.44485200	-0.97467800
H	-1.88701900	0.12811000	-1.89226200
H	-0.74477400	-0.05402500	-0.55100500
H	-1.55837700	-1.50630900	-1.22338800
C	-5.16894900	-2.38075500	2.11256900
H	-4.95881100	-2.43565700	3.19298800
H	-6.26034900	-2.27831400	2.00323800
H	-4.83623000	-3.30840100	1.62959100
Ni	-4.33051200	1.72717800	1.44177200
C	-3.61921600	3.49090400	1.22127800
C	-3.45176700	4.23913100	2.38450900
C	-3.14520800	3.92205000	-0.01420600
C	-2.74296700	5.44886400	2.30885700
H	-3.86611500	3.90357200	3.33881300
C	-2.45130700	5.13718300	-0.07901100
H	-3.29581300	3.30994900	-0.90467200
C	-2.24808800	5.89722800	1.08026200
H	-2.59269300	6.04195100	3.21502900
H	-2.06601400	5.48690100	-1.04074500
H	-1.70799400	6.84565900	1.02331300

Br	-6.44771500	2.65360700	1.23309800
C	-5.11552700	1.62544300	-2.28403600
C	-4.42971800	0.77253600	-3.29549900
H	-4.25594200	-0.25077100	-2.92809100
H	-5.00850200	0.70566000	-4.23717200
H	-3.44069100	1.18927200	-3.58548700
C	-5.60698200	2.98852600	-2.63087500
H	-6.09475100	3.47343300	-1.77207700
H	-4.78208400	3.65352000	-2.96502400
H	-6.32623700	2.96524500	-3.47394800
H	-5.13465700	1.30791000	-1.23963800

UB3LYP-D3/def2-TZVPP-CPCM(DMA)// UB3LYP-D3/def2-SVP-CPCM(THF)
HF=-4817.61341725
UM06/def2-TZVPP-CPCM(DMA)// UB3LYP-D3/def2-SVP-CPCM(THF)
HF= -4816.80636293

^{1}C'*i*-Pr



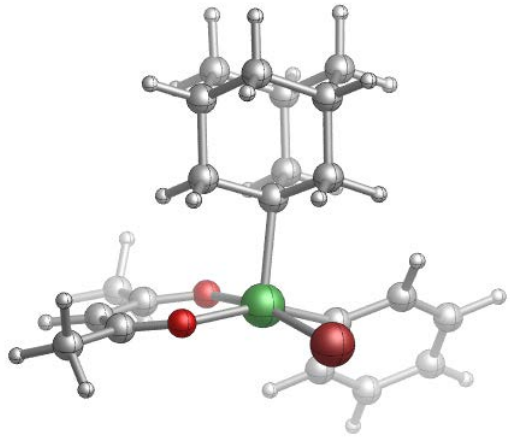
Zero-point correction= 0.297520 (Hartree/Particle)
Thermal correction to Energy= 0.318715
Thermal correction to Enthalpy= 0.319659
Thermal correction to Gibbs Free Energy= 0.246597
Sum of electronic and zero-point Energies= -4776.718715
Sum of electronic and thermal Energies= -4776.697520
Sum of electronic and thermal Enthalpies= -4776.696576
Sum of electronic and thermal Free Energies= -4776.769638

C	-4.26273100	-0.32975800	0.88325900
O	-5.48402200	0.00752800	0.68169600
C	-3.38034400	-0.82945700	-0.07996300
H	-2.36837900	-1.08522300	0.23092600
C	-3.76492900	-1.08155300	-1.41643700
O	-4.90428300	-0.79971000	-1.89114600
C	-2.79089900	-1.72159500	-2.37446300
H	-3.24196500	-2.63947000	-2.78393400
H	-2.62784600	-1.03858900	-3.22370400
H	-1.82661000	-1.96303700	-1.90881300
C	-3.81451800	-0.15170900	2.31204900
H	-2.78277800	-0.48724800	2.47756500
H	-3.90213400	0.91250200	2.58507400
H	-4.49525900	-0.70914500	2.97462600
Ni	-6.41932000	0.06169200	-0.95042200
C	-8.05687900	0.29108000	0.01760800
C	-9.04317800	1.26600900	-0.15218700
C	-8.23551000	-0.72293200	0.96570000
C	-10.19712900	1.24092600	0.64018600
H	-8.93270500	2.04653300	-0.90690000
C	-9.40114700	-0.75480000	1.74569400
H	-7.47139600	-1.48860900	1.11625400
C	-10.38063200	0.22978700	1.59065800
H	-10.95983800	2.01277900	0.50390800
H	-9.53226000	-1.55152300	2.48338700
H	-11.28413500	0.20987500	2.20541700
Br	-7.66733300	-0.10032400	-2.93012200

C	-6.09728600	2.06783100	-1.09823400
C	-4.86421300	2.12587800	-1.95693100
H	-3.98270700	1.71952500	-1.43941700
H	-4.99714800	1.61084700	-2.91533100
H	-4.66010000	3.19576300	-2.15927600
H	-7.00456200	2.34137600	-1.64664100
C	-5.98780400	2.75420900	0.23531300
H	-6.84282300	2.54899700	0.88981400
H	-5.06152300	2.49389800	0.76277600
H	-5.97146100	3.84284700	0.03369600

UB3LYP-D3/def2-TZVPP-CPCM(DMA)// UB3LYP-D3/def2-SVP-CPCM(THF)
HF= -4778.31828595
UM06/def2-TZVPP-CPCM(DMA)// UB3LYP-D3/def2-SVP-CPCM(THF)
HF= -4777.53911766

^{1}C'^{Ad}



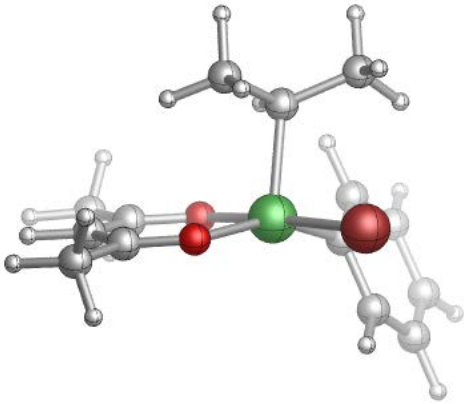
Zero-point correction= 0.437415 (Hartree/Particle)
Thermal correction to Energy= 0.461985
Thermal correction to Enthalpy= 0.462930
Thermal correction to Gibbs Free Energy= 0.382855
Sum of electronic and zero-point Energies= -5047.993260
Sum of electronic and thermal Energies= -5047.968689
Sum of electronic and thermal Enthalpies= -5047.967745
Sum of electronic and thermal Free Energies= -5048.047820

C	-4.43468200	-0.23717600	0.96563600
O	-5.63063900	0.17719300	0.76541200
C	-3.53913800	-0.66722700	-0.01969400
H	-2.54843700	-0.99537800	0.29203500
C	-3.86018300	-0.69469700	-1.39633600
O	-4.97313600	-0.33049400	-1.87551300
C	-2.82915900	-1.15406300	-2.39894800
H	-3.28876100	-1.88280400	-3.08401900
H	-2.52215300	-0.28777900	-3.00863400
H	-1.93913200	-1.59320500	-1.92938900
C	-4.01701000	-0.21032800	2.41514700
H	-4.75884300	-0.75938900	3.01585500
H	-3.01925100	-0.63829200	2.57712800
H	-4.02588200	0.83402600	2.76813400
Ni	-6.58537800	0.27486400	-0.87403600
C	-8.23065100	0.18830000	0.11302300
C	-9.38838100	0.95737400	-0.03924200
C	-8.23130200	-0.87031500	1.03189300
C	-10.51933900	0.70313800	0.74559700
H	-9.42878500	1.75477900	-0.78071100
C	-9.37136000	-1.13661200	1.80513200
H	-7.34523200	-1.49331100	1.16546000
C	-10.51541800	-0.34591600	1.67233500
H	-11.41160100	1.32293000	0.61937100
H	-9.35412900	-1.96526100	2.51897100

H	-11.40032900	-0.54739500	2.28160600
Br	-7.82631400	-0.08224600	-2.83680800
C	-4.86888900	2.49814000	-1.18010100
H	-4.66416300	2.08205600	-2.17429500
H	-4.24168300	1.97428200	-0.44909800
C	-6.34184500	2.39288000	-0.84527500
C	-4.50641700	4.01939000	-1.16399200
H	-3.43319900	4.10577900	-1.40007500
C	-5.34808000	4.75003500	-2.22143000
H	-5.13013300	4.34938300	-3.22530000
H	-5.08808900	5.82190700	-2.23530800
C	-7.18702000	3.04934700	-1.91445700
H	-8.25940200	2.91950200	-1.72799600
H	-6.96178200	2.63617100	-2.90423200
C	-6.83901300	4.57486400	-1.89206200
H	-7.46108900	5.06625700	-2.65779700
C	-7.14221400	5.15760600	-0.50287900
H	-6.91855300	6.23784100	-0.49205000
H	-8.21399500	5.04675800	-0.26777500
C	-6.65936500	2.91466300	0.54025900
H	-6.08277400	2.37795100	1.30202100
H	-7.72461700	2.79909500	0.77294500
C	-4.79585900	4.59391900	0.23195600
H	-4.18630300	4.07566800	0.99119800
H	-4.51625400	5.66051200	0.26485800
C	-6.29075800	4.43118800	0.55111100
H	-6.51108900	4.82321400	1.55745700

UB3LYP-D3/def2-TZVPP-CPCM(DMA)// UB3LYP-D3/def2-SVP-CPCM(THF)
HF= -5050.01092587
UM06/def2-TZVPP-CPCM(DMA)// UB3LYP-D3/def2-SVP-CPCM(THF)
HF= -5049.00795149

^{1}C''-complex$^{i\text{-Pr}}$



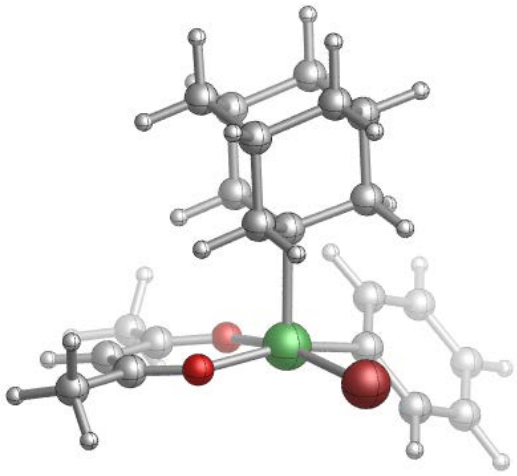
Zero-point correction= 0.297586 (Hartree/Particle)
Thermal correction to Energy= 0.318784
Thermal correction to Enthalpy= 0.319728
Thermal correction to Gibbs Free Energy= 0.246639
Sum of electronic and zero-point Energies= -4776.714077
Sum of electronic and thermal Energies= -4776.692879
Sum of electronic and thermal Enthalpies= -4776.691935
Sum of electronic and thermal Free Energies= -4776.765024

C	-4.71394900	-0.83682200	1.41221400
O	-4.96334000	0.31835300	1.91336500
C	-3.79101400	-1.11077400	0.39737800
H	-3.69214900	-2.14071900	0.05733900
C	-3.01247000	-0.11220400	-0.23128300
O	-3.01644500	1.10855800	0.10530200
C	-2.09747300	-0.47872000	-1.37378800
H	-2.11986300	-1.54930700	-1.61525800
H	-2.38705800	0.10316800	-2.26352600
H	-1.06870200	-0.17986100	-1.11674100
C	-5.53236100	-1.94915000	2.01885800
H	-5.31999400	-2.00026600	3.09889300
H	-6.60215600	-1.70916400	1.91294500
H	-5.32724400	-2.92455600	1.55948600
Ni	-4.09501000	1.95354900	1.54168100
C	-3.04178000	1.74801500	3.28615000
C	-2.78031600	3.00241500	4.07332000
H	-2.44997000	2.68019700	5.08024400
H	-1.98767900	3.61381600	3.62531200
H	-3.67732100	3.61969300	4.20166700
C	-1.81892600	1.00651300	2.82222100
H	-1.22553000	0.76413800	3.72576300
H	-2.05787700	0.05950600	2.32267400
H	-1.19275500	1.62443600	2.16442000
C	-5.60201600	2.80182900	2.36851200

C	-6.08675100	2.53451400	3.65025400
C	-6.37717500	3.55231700	1.47551300
C	-7.33172500	3.03849900	4.05039900
H	-5.51981400	1.92294500	4.35362900
C	-7.62931900	4.04192000	1.87471000
H	-6.01458000	3.77186700	0.46955100
C	-8.10706200	3.79351300	3.16459400
H	-7.69723100	2.82679200	5.05920700
H	-8.22491700	4.62800800	1.16911600
H	-9.07898300	4.18346400	3.47749200
Br	-3.10094400	4.00210200	0.96810200
H	-3.77534000	1.09081800	3.76577800

UB3LYP-D3/def2-TZVPP-CPCM(DMA)// UB3LYP-D3/def2-SVP-CPCM(THF)
HF= -4778.31370771
UM06/def2-TZVPP-CPCM(DMA)// UB3LYP-D3/def2-SVP-CPCM(THF)
HF= -4777.53485701

^{1}C''-complex^{Ad}



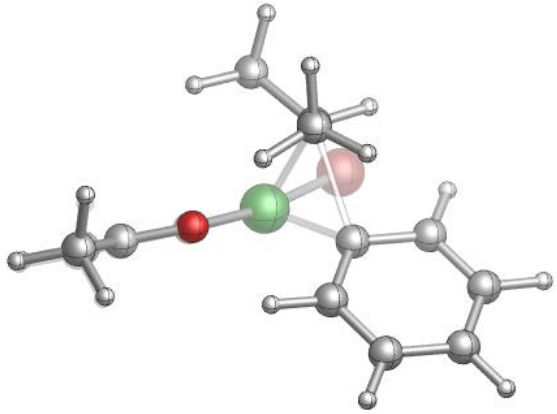
Zero-point correction= 0.437465 (Hartree/Particle)
Thermal correction to Energy= 0.462034
Thermal correction to Enthalpy= 0.462978
Thermal correction to Gibbs Free Energy= 0.382950
Sum of electronic and zero-point Energies= -5047.990295
Sum of electronic and thermal Energies= -5047.965725
Sum of electronic and thermal Enthalpies= -5047.964781
Sum of electronic and thermal Free Energies= -5048.044810

C	-5.00425600	-0.26788700	0.89142900
O	-6.20763300	-0.09658300	0.49061000
C	-3.92294100	-0.63981800	0.08489000
H	-2.94211000	-0.74516000	0.54650700
C	-4.05834100	-0.91786900	-1.29336000
O	-5.14597900	-0.82709000	-1.93726700
C	-2.85361600	-1.33961400	-2.09877100
H	-3.09933600	-2.24865600	-2.66908500
H	-2.62663900	-0.55028500	-2.83475200
H	-1.96501300	-1.51818300	-1.47930700
C	-4.80793300	-0.01038900	2.36445900
H	-3.78175400	-0.21092500	2.69861400
H	-5.06313200	1.04066800	2.57685000
H	-5.51238900	-0.63330200	2.93768500
Ni	-6.90807900	-0.25022800	-1.26341200
C	-8.63211600	-0.13074400	-0.38893200
C	-8.86934400	0.84796400	0.58480500
C	-9.56877900	-1.16303200	-0.53966600
C	-10.03786500	0.83357700	1.35447300
H	-8.13073900	1.62753500	0.77055200
C	-10.73242100	-1.19106000	0.24524300
H	-9.40861800	-1.95228000	-1.27397800
C	-10.97907400	-0.18855300	1.18566700
H	-10.20362900	1.61892600	2.09767500

H	-11.44968000	-2.00568000	0.10819400
H	-11.89158500	-0.20537700	1.78748400
Br	-7.87407100	-0.91544200	-3.32141600
C	-6.95241000	4.63241400	-1.45962800
H	-6.77787700	5.68900000	-1.72357900
H	-7.57063200	4.62556600	-0.54643000
C	-5.60910400	3.93191200	-1.19863500
H	-5.07774200	4.41776800	-0.36418300
C	-7.68932700	3.91934400	-2.60538300
H	-8.66405700	4.39922800	-2.79056300
C	-6.83291200	3.93696800	-3.87980400
H	-6.65234000	4.97726200	-4.19944100
H	-7.36516400	3.43248800	-4.70306600
C	-4.74589100	3.95079400	-2.46905000
H	-3.77825900	3.45721400	-2.27934300
H	-4.52747500	4.99215200	-2.75978100
C	-5.49624600	3.23318400	-3.60106100
H	-4.87864000	3.20487900	-4.51356400
C	-5.77110800	1.75099000	-3.18032800
H	-6.28957300	1.22636700	-3.98975300
H	-4.81947800	1.24232800	-2.99613300
C	-5.87600300	2.44612500	-0.78263100
H	-6.45320600	2.42802400	0.14897700
H	-4.91587500	1.94283500	-0.60564500
C	-7.96891600	2.43660100	-2.18948600
H	-8.60512100	2.43346300	-1.29925300
H	-8.49574500	1.90864900	-2.99410700
C	-6.62208300	1.80550400	-1.92723900

UB3LYP-D3/def2-TZVPP-CPCM(DMA)// UB3LYP-D3/def2-SVP-CPCM(THF)
HF= -5050.01092587
UM06/def2-TZVPP-CPCM(DMA)// UB3LYP-D3/def2-SVP-CPCM(THF)
HF= -5049.00795149

^{1}C'-TS$^{i\text{-Pr}}$



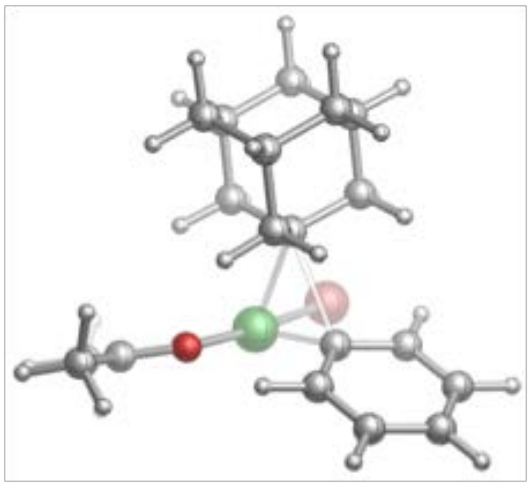
Zero-point correction= 0.297700 (Hartree/Particle)
Thermal correction to Energy= 0.318234
Thermal correction to Enthalpy= 0.319178
Thermal correction to Gibbs Free Energy= 0.247594
Sum of electronic and zero-point Energies= -4776.703604
Sum of electronic and thermal Energies= -4776.683070
Sum of electronic and thermal Enthalpies= -4776.682126
Sum of electronic and thermal Free Energies= -4776.753710

C	-3.98117100	-0.38342000	0.70411400
O	-5.08969800	0.21721900	0.49156100
C	-3.32399300	-1.20475000	-0.21926400
H	-2.38337900	-1.67194700	0.06838000
C	-3.85483700	-1.46525500	-1.49621700
O	-4.93772100	-0.97201700	-1.94555200
C	-3.13566300	-2.39152600	-2.44479200
H	-3.80094700	-3.23338200	-2.69534700
H	-2.93190400	-1.85372300	-3.38431600
H	-2.19593600	-2.77930000	-2.03101300
C	-3.39798000	-0.14585800	2.07400300
H	-2.44765700	-0.67334000	2.22592400
H	-3.24443600	0.93573600	2.21689000
H	-4.12400600	-0.47172600	2.83614500
Ni	-6.13948800	0.26022100	-1.10166300
C	-7.81306000	0.66666600	-0.10279400
C	-9.05265800	1.00209600	-0.67045700
C	-7.79056700	0.05730400	1.16296900
C	-10.24405400	0.69568300	-0.00790000
H	-9.09530700	1.49703500	-1.63995100
C	-8.98807100	-0.25809500	1.81696400
H	-6.84295300	-0.16692600	1.64708500
C	-10.21906500	0.05747300	1.23709300
H	-11.19717400	0.96200700	-0.47238400
H	-8.94779400	-0.74867400	2.79324000
H	-11.15168100	-0.18170300	1.75423300

Br	-7.17326300	0.42517600	-3.27868800
C	-6.51392300	2.34400900	-0.60210600
C	-5.16174000	2.60170600	-1.26675000
H	-4.31501000	2.28670100	-0.64282500
H	-5.06437200	2.17265500	-2.27356000
H	-5.09625500	3.69978600	-1.38743300
H	-7.31815200	2.70006500	-1.25050200
C	-6.56569800	2.90752400	0.80142100
H	-7.58235300	2.93153300	1.21220100
H	-5.91979500	2.32549000	1.47258200
H	-6.17602500	3.94075700	0.77039600

UB3LYP-D3/def2-TZVPP-CPCM(DMA)// UB3LYP-D3/def2-SVP-CPCM(THF)
HF= -4778.30356914
UM06/def2-TZVPP-CPCM(DMA)// UB3LYP-D3/def2-SVP-CPCM(THF)
HF= -4777.52976312

^{1}C'-TS^{Ad}



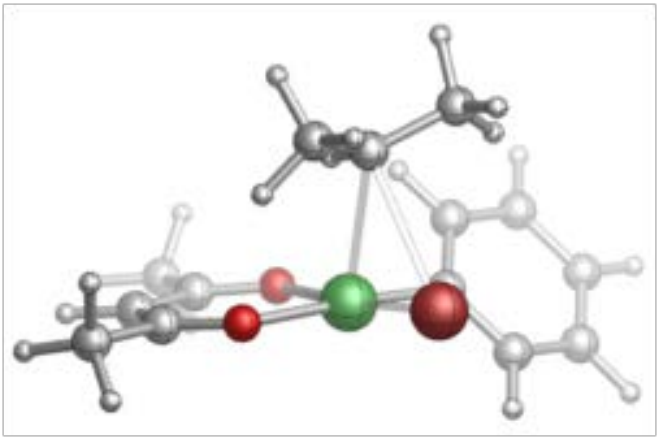
Zero-point correction= 0.437403 (Hartree/Particle)
Thermal correction to Energy= 0.461446
Thermal correction to Enthalpy= 0.462390
Thermal correction to Gibbs Free Energy= 0.382978
Sum of electronic and zero-point Energies= -5047.979137
Sum of electronic and thermal Energies= -5047.955094
Sum of electronic and thermal Enthalpies= -5047.954150
Sum of electronic and thermal Free Energies= -5048.033562

C	-4.15139200	-0.32333600	0.86761600
O	-5.33202900	0.08503200	0.60028300
C	-3.28524600	-0.92518300	-0.05312300
H	-2.29807700	-1.24196500	0.28039100
C	-3.67414100	-1.18129800	-1.38283800
O	-4.79198000	-0.84913700	-1.88498500
C	-2.74210200	-1.91202600	-2.31851000
H	-3.20762500	-2.86806000	-2.60894000
H	-2.62121000	-1.32162500	-3.24013500
H	-1.75870800	-2.10984600	-1.87251700
C	-3.72030600	-0.10058300	2.29585600
H	-4.45272300	-0.56802400	2.97288600
H	-2.71979700	-0.50074500	2.50485600
H	-3.73066700	0.98136300	2.50662900
Ni	-6.24602900	0.14729400	-1.08859200
C	-7.98762200	0.57629700	-0.17833400
C	-9.20253900	0.66459100	-0.87981900
C	-8.03340200	0.19172400	1.17451300
C	-10.41614200	0.34639100	-0.26192300
H	-9.20741400	0.97120500	-1.92361800
C	-9.24668200	-0.12980900	1.79215800
H	-7.11224400	0.13968000	1.75013500
C	-10.44603100	-0.05293300	1.07805200
H	-11.34361400	0.41580200	-0.83693300

H	-9.24851800	-0.43760300	2.84154300
H	-11.39547300	-0.29623200	1.56217100
Br	-7.11843200	0.19947500	-3.36062400
C	-5.28375200	2.52892500	-1.24878000
H	-5.30605900	2.19079400	-2.29364600
H	-4.52331400	1.95547200	-0.70399300
C	-6.66621600	2.43410400	-0.59177100
C	-4.85052900	4.03020500	-1.22245600
H	-3.85529700	4.08862300	-1.69206100
C	-5.86741000	4.86152700	-2.01666000
H	-5.89981800	4.52240400	-3.06533100
H	-5.56363200	5.92190700	-2.02670500
C	-7.69195500	3.21864500	-1.38395500
H	-8.68517300	3.14425400	-0.92525600
H	-7.75299900	2.84885700	-2.41591000
C	-7.25041000	4.71496200	-1.36622500
H	-8.00136400	5.28767600	-1.93433800
C	-7.19782800	5.20698000	0.09103600
H	-6.91456200	6.27252200	0.11987200
H	-8.19384400	5.12403000	0.55743900
C	-6.61585500	2.87362600	0.85785500
H	-5.90737800	2.25638300	1.42358300
H	-7.60348100	2.79088600	1.32881700
C	-4.78425100	4.50871200	0.23563300
H	-4.04311600	3.91510700	0.79703700
H	-4.45395100	5.56043200	0.27309400
C	-6.17330500	4.36820400	0.87545500
H	-6.14156600	4.69343500	1.92815500

UB3LYP-D3/def2-TZVPP-CPCM(DMA)// UB3LYP-D3/def2-SVP-CPCM(THF)
HF= -5049.99792520
UM06/def2-TZVPP-CPCM(DMA)// UB3LYP-D3/def2-SVP-CPCM(THF)
HF= -5048.99950709

^{1}C''-TS$^{i\text{-Pr}}$



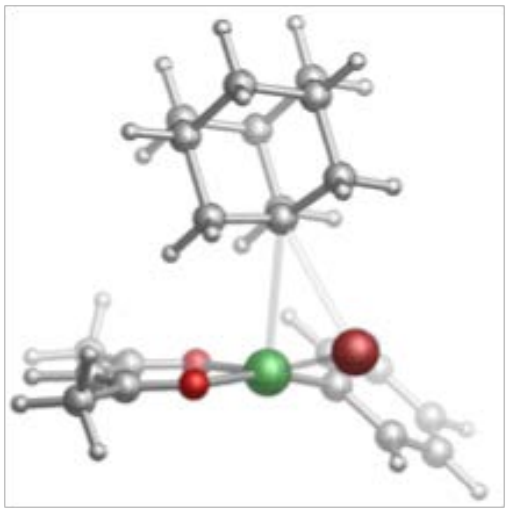
Zero-point correction= 0.295724 (Hartree/Particle)
Thermal correction to Energy= 0.316798
Thermal correction to Enthalpy= 0.317742
Thermal correction to Gibbs Free Energy= 0.244376
Sum of electronic and zero-point Energies= -4776.696349
Sum of electronic and thermal Energies= -4776.675275
Sum of electronic and thermal Enthalpies= -4776.674331
Sum of electronic and thermal Free Energies= -4776.747697

C	-5.04608300	-1.01406600	1.21106900
O	-5.32751400	0.16285200	1.62034400
C	-3.95817400	-1.36070000	0.39392100
H	-3.83217900	-2.40749900	0.11902000
C	-3.01109300	-0.42613100	-0.07225700
O	-3.04483700	0.82052700	0.17074100
C	-1.83955400	-0.89548300	-0.90294300
H	-1.92024200	-1.94887900	-1.20229400
H	-1.75036900	-0.26041400	-1.79788800
H	-0.91319000	-0.76089700	-0.31938400
C	-6.00259300	-2.08229600	1.68641000
H	-6.03083400	-2.07627200	2.78789300
H	-7.01889000	-1.83443700	1.33978700
H	-5.73264600	-3.08619400	1.33347400
Ni	-4.41067800	1.79213500	1.23167700
C	-2.57075800	2.20308600	3.02216800
C	-2.82417200	3.25030200	4.03568000
H	-2.53735600	2.79351300	5.00681500
H	-2.21473800	4.14976000	3.88032600
H	-3.88908900	3.50542500	4.10354200
C	-1.20542500	1.90133300	2.53608000
H	-0.75543000	1.23275600	3.29992000
H	-1.23654200	1.34670300	1.58995900
H	-0.58140300	2.79910800	2.43890900
C	-5.79914400	2.69344700	2.16757700

C	-6.17978900	2.25492700	3.44617500
C	-6.52459700	3.74546800	1.58528700
C	-7.23572400	2.86391200	4.13724900
H	-5.65589900	1.41241200	3.90724800
C	-7.59492600	4.34545600	2.26323800
H	-6.24598500	4.11342900	0.59465800
C	-7.94995400	3.91227500	3.54554300
H	-7.50686200	2.51117100	5.13705900
H	-8.14794900	5.16173000	1.78842100
H	-8.77793000	4.38672600	4.07943700
Br	-3.19307500	3.77569500	0.91731000
H	-3.24161700	1.33852300	3.07332400

UB3LYP-D3/def2-TZVPP-CPCM(DMA)// UB3LYP-D3/def2-SVP-CPCM(THF)
HF= -4778.29784834
UM06/def2-TZVPP-CPCM(DMA)// UB3LYP-D3/def2-SVP-CPCM(THF)
HF= -4777.52344646

^{1}C''-TS^{Ad}



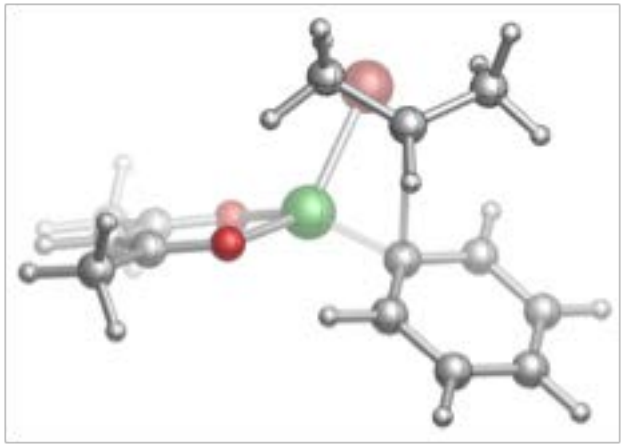
Zero-point correction= 0.435959 (Hartree/Particle)
Thermal correction to Energy= 0.460362
Thermal correction to Enthalpy= 0.461306
Thermal correction to Gibbs Free Energy= 0.380306
Sum of electronic and zero-point Energies= -5047.974046
Sum of electronic and thermal Energies= -5047.949643
Sum of electronic and thermal Enthalpies= -5047.948699
Sum of electronic and thermal Free Energies= -5048.029699

C	-4.70640500	-0.24338900	0.58006500
O	-5.97458200	-0.12831900	0.47699400
C	-3.85228100	-0.76873500	-0.40277800
H	-2.78784300	-0.83737700	-0.18002100
C	-4.31201900	-1.22967700	-1.65667100
O	-5.51710500	-1.16812900	-2.04300200
C	-3.33209400	-1.81335900	-2.64797000
H	-3.68092300	-2.81241100	-2.95423400
H	-3.32458100	-1.18588500	-3.55440000
H	-2.31077800	-1.88798900	-2.25150300
C	-4.13796000	0.25448500	1.88799800
H	-3.05636400	0.08748700	1.97593300
H	-4.34547400	1.33343400	1.97952500
H	-4.65733200	-0.24303300	2.72225700
Ni	-7.06881100	-0.54722400	-1.01368500
C	-8.60538600	-0.38655400	0.10336900
C	-8.68547700	0.51094000	1.18279500
C	-9.66517000	-1.30313800	-0.04643800
C	-9.78274500	0.52056400	2.05456800
H	-7.86177200	1.20203100	1.36953200
C	-10.75773200	-1.31420800	0.83143800
H	-9.64558000	-2.01968100	-0.87083800
C	-10.82770600	-0.39436100	1.88335900

H	-9.81496200	1.24065900	2.87856800
H	-11.56155900	-2.04311400	0.68677900
H	-11.68402100	-0.39280000	2.56374300
Br	-8.31327900	-0.51928400	-3.01682200
C	-7.41274300	4.85063700	-2.19040200
H	-7.04767900	5.88730600	-2.27380500
H	-8.47811100	4.90440700	-1.91455800
C	-6.61749100	4.10709200	-1.10810600
H	-6.75092400	4.58013100	-0.12309100
C	-7.24506500	4.12846500	-3.53562100
H	-7.83647000	4.62051700	-4.32301200
C	-5.76139800	4.05320100	-3.93024100
H	-5.35591700	5.07032300	-4.05623700
H	-5.64836100	3.53864300	-4.89788200
C	-5.12920000	4.03202000	-1.48564400
H	-4.56189000	3.50136600	-0.70414600
H	-4.71189100	5.04971300	-1.55445600
C	-4.97413900	3.31588400	-2.83695500
H	-3.91267100	3.21821500	-3.11167500
C	-5.53837000	1.83511100	-2.68920300
H	-5.43283400	1.29008600	-3.63465600
H	-4.98455500	1.32238000	-1.89644300
C	-7.17747600	2.62440500	-0.97500200
H	-8.23936600	2.64724600	-0.70277200
H	-6.60664700	2.09380900	-0.20610700
C	-7.80033700	2.65138900	-3.39786300
H	-8.86019700	2.67321400	-3.11572600
H	-7.68131800	2.12275100	-4.35041500
C	-6.94726400	2.08232300	-2.32846000

UB3LYP-D3/def2-TZVPP-CPCM(DMA)// UB3LYP-D3/def2-SVP-CPCM(THF)
HF= -5050.00227554
UM06/def2-TZVPP-CPCM(DMA)// UB3LYP-D3/def2-SVP-CPCM(THF)
HF= -5049.00355154

^{3}C-TS$^{i\text{-Pr}}$



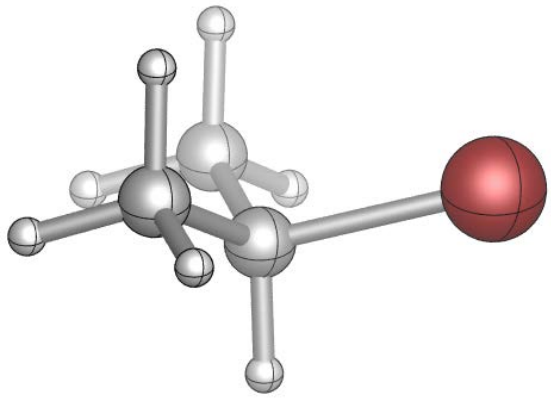
Zero-point correction= 0.291168 (Hartree/Particle)
Thermal correction to Energy= 0.314140
Thermal correction to Enthalpy= 0.315084
Thermal correction to Gibbs Free Energy= 0.234321
Sum of electronic and zero-point Energies= -4776.683307
Sum of electronic and thermal Energies= -4776.660335
Sum of electronic and thermal Enthalpies= -4776.659391
Sum of electronic and thermal Free Energies= -4776.740155

C	-2.36118600	-0.64377600	0.45185900
O	-3.12407300	0.38453200	0.41725900
C	-2.78580900	-1.98098800	0.41828900
H	-2.02349700	-2.75834000	0.45386000
C	-4.14152700	-2.37888300	0.40968500
O	-5.12445300	-1.57532400	0.35697800
C	-4.49654500	-3.84327300	0.48017400
H	-5.11652200	-4.01802700	1.37437500
H	-5.11524600	-4.10273900	-0.39380100
H	-3.61609400	-4.49770600	0.51421700
C	-0.89165200	-0.31740600	0.54991400
H	-0.71761600	0.28210100	1.45786000
H	-0.25571800	-1.21146100	0.57453900
H	-0.61047800	0.31243000	-0.30920600
Ni	-5.02932200	0.35599300	0.15613900
C	-5.28126300	2.24073700	0.47824200
C	-6.58594000	2.74199900	0.42739100
C	-4.21984700	3.01190600	0.95673400
C	-6.84311500	4.01928800	0.94287500
H	-7.39661700	2.14897500	0.00031200
C	-4.49017800	4.29328700	1.45962300
H	-3.20813100	2.61056000	0.95600400
C	-5.79496800	4.79583100	1.45187400
H	-7.86489500	4.40854200	0.93342600
H	-3.66792500	4.90225700	1.84538300

H	-5.99591200	5.79966300	1.83490400
Br	-5.82173700	0.50856100	-2.05487700
C	-2.99932200	3.69583100	-1.82226500
C	-2.43639500	2.38994100	-2.26258900
H	-2.47089500	2.27999300	-3.36550800
H	-1.39395400	2.25214000	-1.93660100
H	-3.03033300	1.54850300	-1.85893200
C	-4.31868200	4.17966700	-2.31192400
H	-4.23469800	4.66402400	-3.30939100
H	-5.02961500	3.34405400	-2.42737500
H	-4.76335300	4.92062300	-1.62850200
H	-2.40445600	4.34732800	-1.17510300

UB3LYP-D3/def2-TZVPP-CPCM(DMA)// UB3LYP-D3/def2-SVP-CPCM(THF)
HF= -4778.28000251
UM06/def2-TZVPP-CPCM(DMA)// UB3LYP-D3/def2-SVP-CPCM(THF)
HF= -4777.49651484

***i*Pr-Br**

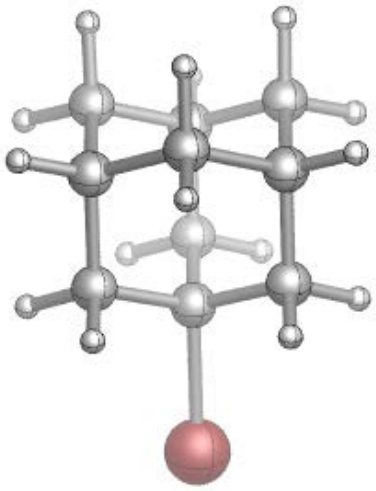


Zero-point correction= 0.093570 (Hartree/Particle)
Thermal correction to Energy= 0.098960
Thermal correction to Enthalpy= 0.099905
Thermal correction to Gibbs Free Energy= 0.064321
Sum of electronic and zero-point Energies= -2692.245354
Sum of electronic and thermal Energies= -2692.239964
Sum of electronic and thermal Enthalpies= -2692.239020
Sum of electronic and thermal Free Energies= -2692.274603

C	-1.76973700	2.94632600	2.80829800
C	-1.50495700	2.87037900	1.31519000
H	-0.41627400	2.79919900	1.14944300
H	-1.97839200	1.97918900	0.87478400
H	-1.87574800	3.76236000	0.79039500
Br	-3.74989200	3.16938400	3.11257100
C	-1.28411200	1.73632900	3.58641000
H	-0.19151300	1.64615500	3.46014100
H	-1.50019600	1.82967400	4.66027400
H	-1.75050200	0.81207500	3.21146000
H	-1.35916500	3.87336400	3.23130400

UB3LYP-D3/def2-TZVPP-CPCM(DMA)// UB3LYP-D3/def2-SVP-CPCM(THF)
HF= -2692.78972539
UM06/def2-TZVPP-CPCM(DMA)// UB3LYP-D3/def2-SVP-CPCM(THF)
HF= -2692.55656411

Ad-Br



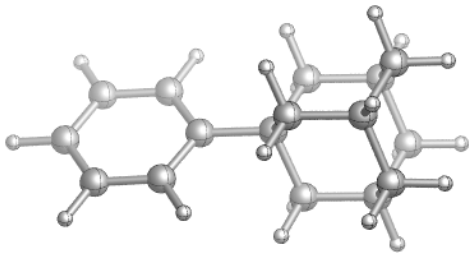
Zero-point correction= 0.233256 (Hartree/Particle)
Thermal correction to Energy= 0.241651
Thermal correction to Enthalpy= 0.242595
Thermal correction to Gibbs Free Energy= 0.199568
Sum of electronic and zero-point Energies= -2963.523396
Sum of electronic and thermal Energies= -2963.515001
Sum of electronic and thermal Enthalpies= -2963.514057
Sum of electronic and thermal Free Energies= -2963.557084

C	-1.88329500	1.37104900	-0.00315300
H	-0.78191400	1.37449800	0.00737900
H	-2.22085500	2.41940600	0.00779100
C	-2.41569700	0.63798100	1.23278300
C	-2.40864800	0.64841100	-1.26606800
H	-2.02694600	1.17358800	-2.15702900
C	-1.91092000	-0.81021500	-1.26434300
H	-0.80809900	-0.83507000	-1.28427500
H	-2.26341100	-1.32960300	-2.17139100
C	-1.91038800	-0.80883400	1.25596600
H	-2.26836300	-1.31683900	2.16532200
H	-0.80930600	-0.82190600	1.27737400
C	-2.43463400	-1.53167700	-0.00756200
H	-2.07298600	-2.57298400	0.00601100
C	-3.97509900	-1.51171600	-0.00439200
H	-4.36116700	-2.04310000	-0.89055900
H	-4.35988500	-2.04142200	0.88367200
C	-3.94751600	0.67076200	1.25572500
H	-4.30007200	1.71402200	1.27552400
H	-4.32001500	0.17411300	2.16540400
C	-3.94917600	0.67029900	-1.26386000
H	-4.31347900	1.71155400	-1.28172800
H	-4.33425000	0.17570100	-2.17139400

C	-4.47192100	-0.05272800	-0.00743600
H	-5.57405200	-0.03143000	0.00639700
Br	-1.72961200	1.58334000	2.88316800

UB3LYP-D3/def2-TZVPP-CPCM(DMA)// UB3LYP-D3/def2-SVP-CPCM(THF)
HF= -2692.78972539
UM06/def2-TZVPP-CPCM(DMA)// UB3LYP-D3/def2-SVP-CPCM(THF)
HF= -2692.55656411

Ad-Ph



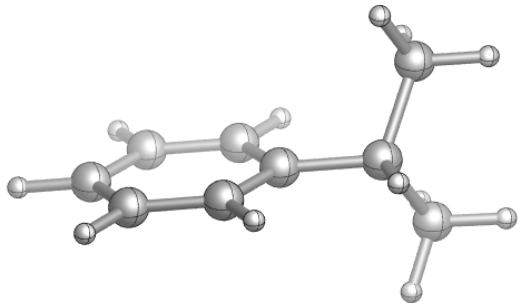
Zero-point correction= 0.324546 (Hartree/Particle)
Thermal correction to Energy= 0.335948
Thermal correction to Enthalpy= 0.336892
Thermal correction to Gibbs Free Energy= 0.287610
Sum of electronic and zero-point Energies= -621.049416
Sum of electronic and thermal Energies= -621.038014
Sum of electronic and thermal Enthalpies= -621.037070
Sum of electronic and thermal Free Energies= -621.086353

C	-9.05162300	0.85471200	0.04815300
C	-8.76142400	0.74758300	1.42334000
C	-10.16553900	0.14499500	-0.43192500
C	-9.54413700	-0.03042700	2.27881000
H	-7.90510000	1.28308600	1.83989900
C	-10.95474300	-0.63687700	0.42163000
H	-10.43668600	0.19213500	-1.48658400
C	-10.64968800	-0.73005800	1.78097200
H	-9.28914200	-0.09075600	3.34040300
H	-11.81463900	-1.17621500	0.01482700
H	-11.26506400	-1.34040000	2.44703400
C	-7.75260900	4.04495400	-2.68996900
H	-7.11367000	4.69035700	-3.31727000
H	-8.78114200	4.43953100	-2.76026000
C	-7.27177300	4.08183800	-1.22799900
H	-7.30785900	5.11786900	-0.85006300
C	-7.70650700	2.59392500	-3.20303400
H	-8.06397000	2.55806500	-4.24614000
C	-6.26146400	2.06767800	-3.13250800
H	-5.60116700	2.68458200	-3.76635600
H	-6.21435600	1.03603700	-3.52239900
C	-5.82724500	3.55160200	-1.14811100
H	-5.46724600	3.58930600	-0.10516500
H	-5.15543600	4.19174800	-1.74563400
C	-5.77961700	2.10281000	-1.67094500
H	-4.74640800	1.72033500	-1.61021100
C	-6.69528200	1.21605600	-0.80637400
H	-6.66147600	0.17105500	-1.15967100
H	-6.32977800	1.21373200	0.23318200

C	-8.18905000	3.19860600	-0.36157700
H	-9.22626000	3.57420400	-0.39577800
H	-7.86515600	3.25088600	0.69044200
C	-8.62079800	1.71159200	-2.33219600
H	-9.65923600	2.07586400	-2.40624800
H	-8.61137500	0.67811800	-2.71792900
C	-8.16600400	1.72198700	-0.85193500

UB3LYP-D3/def2-TZVPP-CPCM(DMA)// UB3LYP-D3/def2-SVP-CPCM(THF)
HF= -622.03871909
UM06/def2-TZVPP-CPCM(DMA)// UB3LYP-D3/def2-SVP-CPCM(THF)
HF= -621.50649605

***i*Pr-Ph**



Zero-point correction= 0.184466 (Hartree/Particle)
Thermal correction to Energy= 0.193027
Thermal correction to Enthalpy= 0.193971
Thermal correction to Gibbs Free Energy= 0.150892
Sum of electronic and zero-point Energies= -349.775767
Sum of electronic and thermal Energies= -349.767205
Sum of electronic and thermal Enthalpies= -349.766261
Sum of electronic and thermal Free Energies= -349.809340

C	-7.85943500	1.84940600	0.01558800
C	-9.01702800	1.45077700	-0.67127300
C	-7.00753200	0.84660600	0.51272700
C	-9.31823500	0.09662500	-0.85914900
H	-9.69435700	2.21412100	-1.06585100
C	-7.30281600	-0.50701700	0.32813500
H	-6.09905000	1.12607500	1.05317600
C	-8.46112100	-0.88852700	-0.35980900
H	-10.22624400	-0.18796500	-1.39771100
H	-6.62558100	-1.26896300	0.72361700
H	-8.69289700	-1.94693800	-0.50445000
C	-7.53947100	3.32441200	0.21624600
C	-6.22164800	3.71973500	-0.47099300
H	-5.36471200	3.18920800	-0.02409600
H	-6.24387100	3.47828000	-1.54546900
H	-6.03644800	4.80119500	-0.36592400
H	-8.34966000	3.89909500	-0.26480700
C	-7.52492300	3.70544400	1.70627000
H	-8.48052200	3.45256900	2.19213900
H	-6.72234500	3.17529600	2.24515400
H	-7.35204200	4.78702500	1.82998700

UB3LYP-D3/def2-TZVPP-CPCM(DMA)// UB3LYP-D3/def2-SVP-CPCM(THF)
HF= -350.34501770
UM06/def2-TZVPP-CPCM(DMA)// UB3LYP-D3/def2-SVP-CPCM(THF)
HF= -350.03343472

F. References

1. (a) Lee, C.; Yang, W.; Parr, R. G., Development of the Colle-Salvetti Correlation-Energy Formula into a Functional of the Electron Density. *Phys. Rev. B* **1988,** *37*, 785–789. (b) Becke, A. D., Density-Functional Thermochemistry. III. The Role of Exact Exchange. *J. Chem. Phys.* **1993,** *98*, 5648–5652.

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