

# Supporting Information

## Nickel-Catalyzed Ethylene Copolymerization with Vinylalkoxysilanes: A Computational Study

Zhihui Song <sup>1,\*</sup>, Rong Gao <sup>1</sup>, Changjiang Wu <sup>2</sup>, Qingqiang Gou <sup>1</sup>, Gang Zheng <sup>1</sup>, Junjie Liu <sup>3</sup>,  
Shifang Yang <sup>3</sup>, and Huasheng Feng <sup>4</sup>,

<sup>1</sup> Department of Polyethylene, SINOPEC (Beijing) Research Institute of Chemical Industry Co., Ltd., Beijing 100013, China; songzhz.bjhy@sinopec.com (Z.S.); gaor.bjhy@sinopec.com (R.G.); gouqq.bjhy@sinopec.com (Q.G.); zhenggang.bjhy@sinopec.com (G.Z.)

<sup>2</sup> SINOPEC (Beijing) Research Institute of Chemical Industry Co., Ltd., Beijing 100013, China; [wuchangjiang.bjhy@sinopec.com](mailto:wuchangjiang.bjhy@sinopec.com) (C.W.)

<sup>3</sup> Department of Ethylene, SINOPEC (Beijing) Research Institute of Chemical Industry Co., Ltd., Beijing 100013, China; liujj.bjhy@sinopec.com (J.L.); yangshf.bjhy@sinopec.com (S.Y.)

<sup>4</sup> Department of Catalytic Science, SINOPEC (Beijing) Research Institute of Chemical Industry Co., Ltd., Beijing 100013, China; fenghs.bjhy@sinopec.com (H.F.)

\* Correspondence: songzhz.bjhy@sinopec.com (Z.S.)

## 1. Computational Details

All density functional theory (DFT) calculations were performed with the Gaussian 16 program. Geometry optimizations employed the spin-unrestricted dispersion-corrected method (UB3LYP-D3), with the 6-31G(d) basis set for nonmetal atoms (C, N, H, Si, O) and the LANL2DZ basis set along with the associated pseudopotential for metal atoms (Ni), denoted as BSI. 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 (Hcorrection) and free energy (Gcorrection) at the temperature of 298K. Single-point energies based on BSI geometries were refined using a higher-level method denoted as BSII. For BSII, the 6-311G(d,p) basis set was applied to nonmetal atoms (C, N, H, Si, O), and the SDD basis set with its associated pseudopotential was used for metal atoms (Ni). To explore the effect of toluene solvent on the catalytic system, single point energies were performed in implicit toluene solvent through the SMD model, labeled as UB3LYP-D3/BSII(SMD)//B3LYP-D3/BSI. Energy profiles were constructed at the UB3LYP-D3/BSII(SMD)//B3LYP-D3/BSI level, including Gibbs free energy corrections taken from frequency calculations in the gas phase. All optimized geometrical figures were generated with CYLview, with distances presented in Å, and energies reported in kcal/mol.

## 2. Energetics with Different Methods from Optimizations

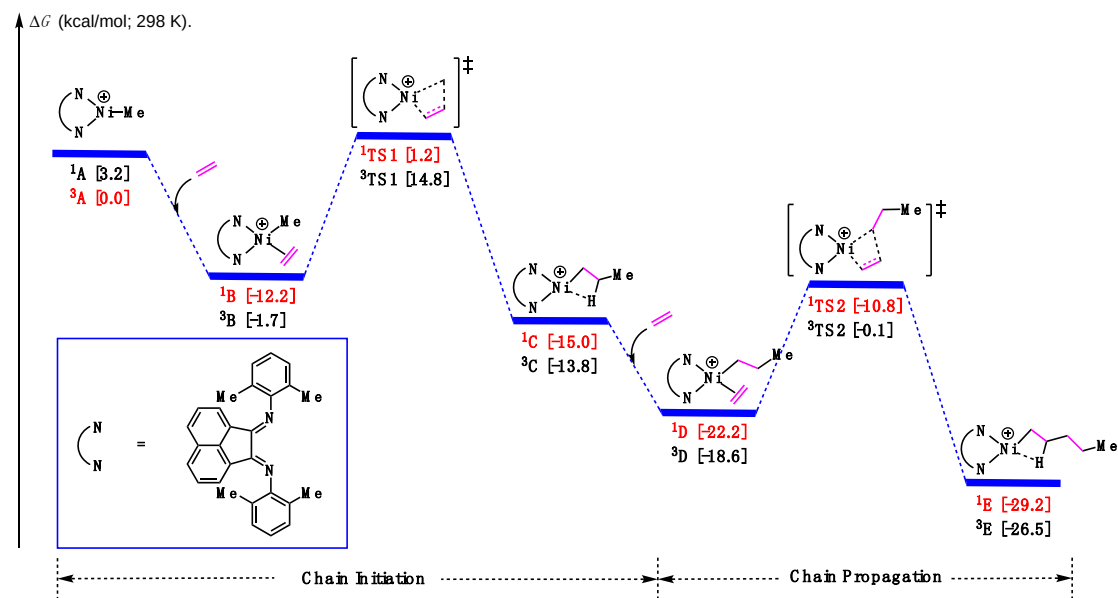
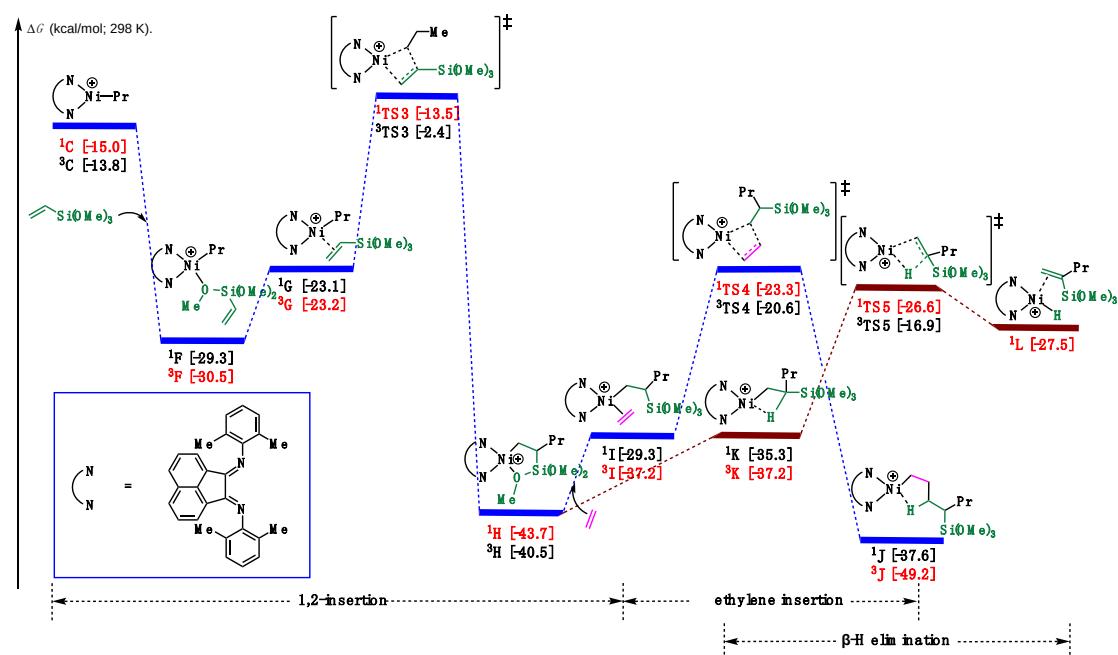
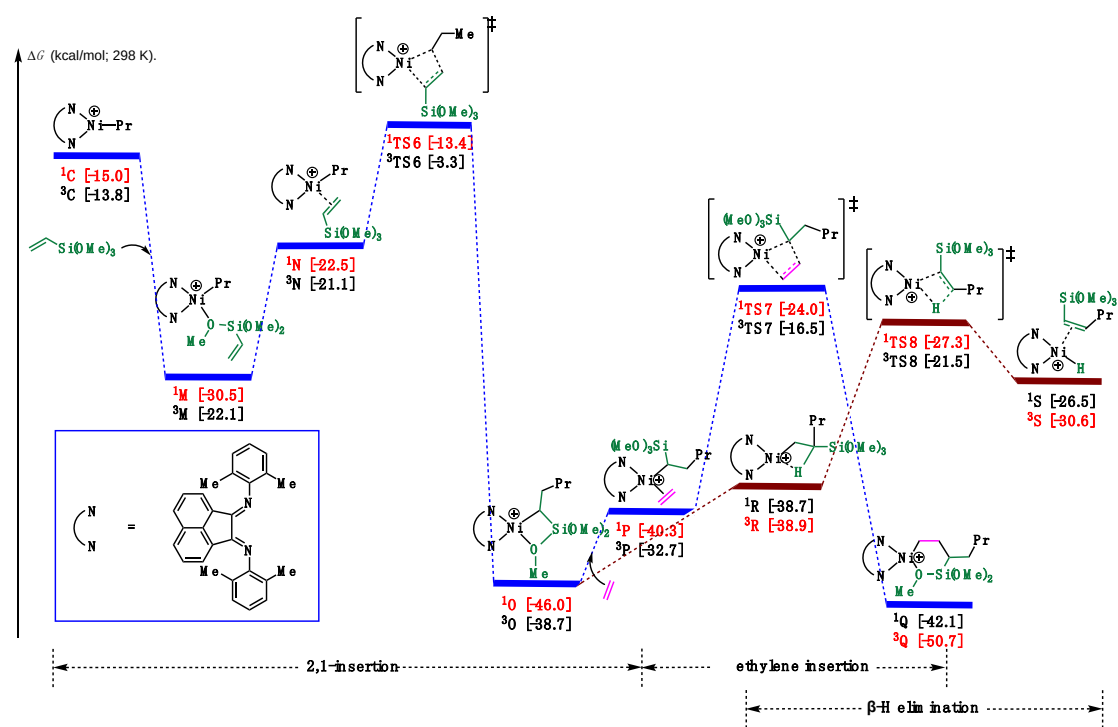


**Figure S1.** Calculated relative Gibbs free energies of optimization for the insertion of ethylene. Free energies (kcal/mol) were computed at the B3LYP-D3/BSI level of theory with the 6-31G(d) basis set for nonmetal atoms (C, N, H, Si, O) and the LANL2DZ basis set along with the associated pseudopotential for metal atoms (Ni), denoted as BSI.



(a)



(b)

**Figure S2.** Calculated relative Gibbs free energies of optimization for the (a) 1,2-insertion of vinyltrimethoxysilane (b) 2,1-insertion of vinyltrimethoxysilane, ethylene reinsertion, and  $\beta$ -H elimination. Free energies (kcal/mol) were computed at the B3LYP-D3/BSI level of theory with the 6-31G(d) basis set for nonmetal atoms (C, N, H, Si, O) and the LANL2DZ basis set along with the associated pseudopotential for metal atoms (Ni), denoted as BSI.

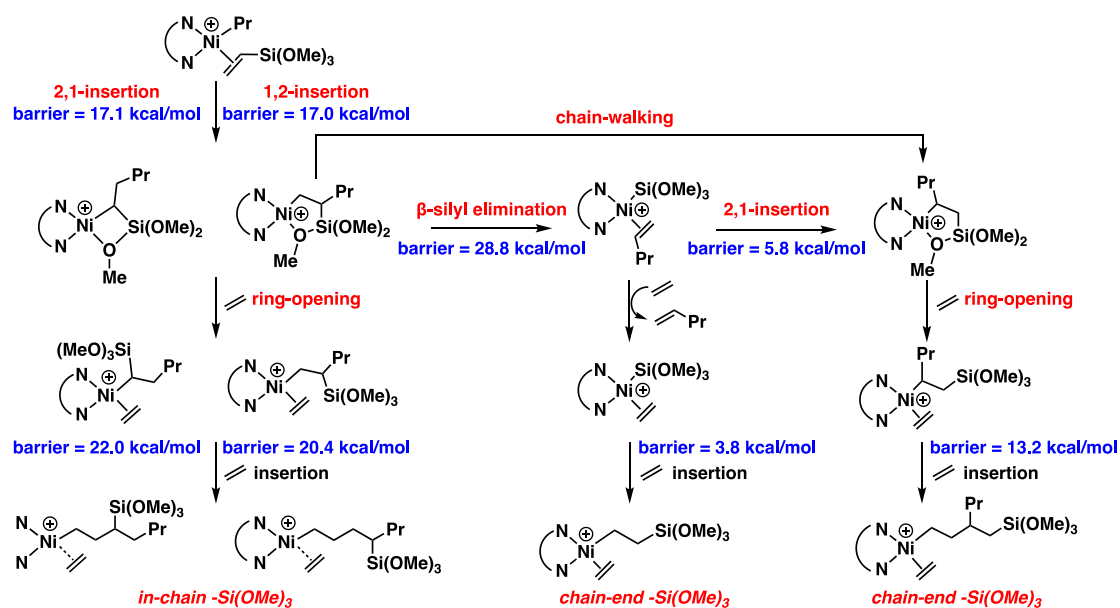


**Figure S3.** Calculated relative Gibbs free energies of optimization for the silane enchainment. Free energies (kcal/mol) were computed at the B3LYP-D3/BSI level of theory with the 6-31G(d) basis set for nonmetal atoms (C, N, H, Si, O) and the LANL2DZ basis set along with the associated pseudopotential for metal atoms (Ni), denoted as BSI.

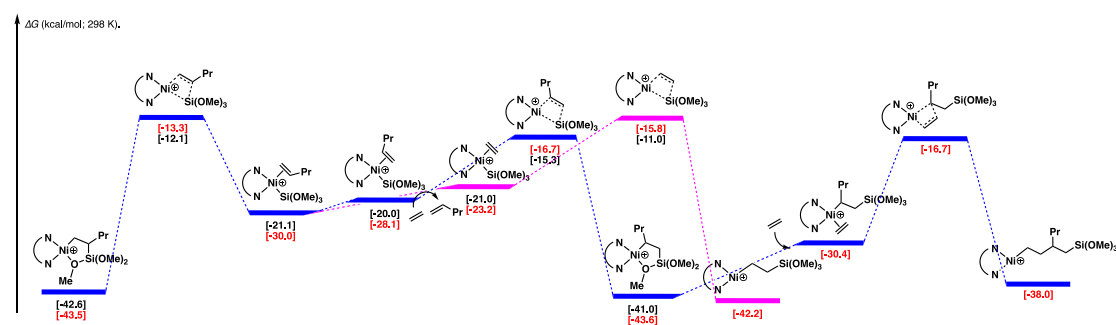
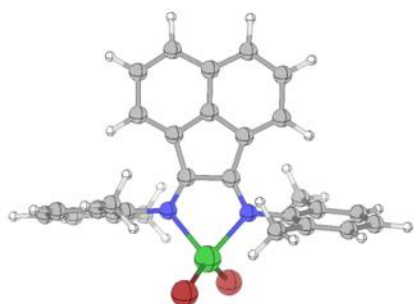


**Figure S4.** Calculated relative Gibbs free energies for the silane enchainment. Free energies (kcal/mol) were computed at the UB3LYP-D3/BSII(SMD)//B3LYP-D3/BSI level of theory with the 6-311G(d,p) basis set for nonmetal atoms (C, N, H, Si, O) and the SDD basis set along with the associated pseudopotential for metal atoms (Ni), denoted as BSII.

### 3. Coordinates and Energies of Optimized Structures in Computations



B3LYP-D3/BSI

Zero-point correction= 0.447859 (Hartree/Particle)

Thermal correction to Energy= 0.479246

Thermal correction to Enthalpy= 0.480191

Thermal correction to Gibbs Free Energy= 0.379854

Sum of electronic and zero-point Energies= -6502.838089

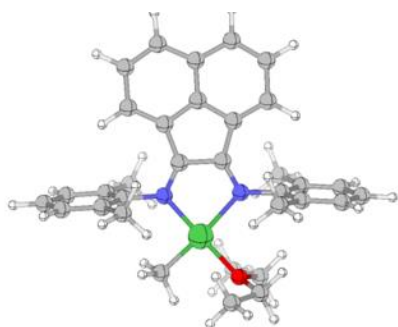
Sum of electronic and thermal Energies= -6502.806702

Sum of electronic and thermal Enthalpies= -6502.805758

Sum of electronic and thermal Free Energies= -6502.906095

|    |             |            |             |
|----|-------------|------------|-------------|
| Ni | -2.01261000 | 3.85067700 | -1.36050700 |
| Br | -1.90191100 | 4.01876200 | -3.72352600 |
| Br | -2.17416700 | 5.53661000 | 0.29933300  |
| N  | -0.61013900 | 2.41992600 | -0.77975400 |
| N  | -3.33649900 | 2.33065200 | -0.82542400 |
| C  | 0.82149800  | 2.50834300 | -0.79344800 |
| C  | 1.51508000  | 2.06055800 | -1.93285000 |
| C  | 1.47191000  | 3.03056800 | 0.33891300  |
| C  | 2.90957100  | 2.17715600 | -1.92556100 |
| C  | 2.86756900  | 3.12435800 | 0.29598100  |
| C  | 3.58267000  | 2.70961800 | -0.82658300 |
| H  | 3.46727400  | 1.84419800 | -2.79693400 |
| H  | 3.39208800  | 3.52808800 | 1.15798400  |
| H  | 4.66548500  | 2.79712900 | -0.84351100 |
| C  | -4.77079300 | 2.33986400 | -0.84837600 |
| C  | -5.42520700 | 1.95017500 | -2.03074700 |
| C  | -5.46249100 | 2.72779000 | 0.31392900  |
| C  | -6.82423700 | 1.98473500 | -2.03589200 |
| C  | -6.86056300 | 2.74637600 | 0.25592400  |
| C  | -7.53860100 | 2.38571000 | -0.90788100 |
| H  | -7.35198600 | 1.69132600 | -2.93952700 |
| H  | -7.41712900 | 3.04903600 | 1.13899400  |
| H  | -8.62442500 | 2.41276000 | -0.93400700 |
| C  | 0.69211200  | 3.42765400 | 1.56648000  |
| H  | -0.08646600 | 4.16025900 | 1.32914400  |
| H  | 0.18872200  | 2.55877600 | 2.01189700  |

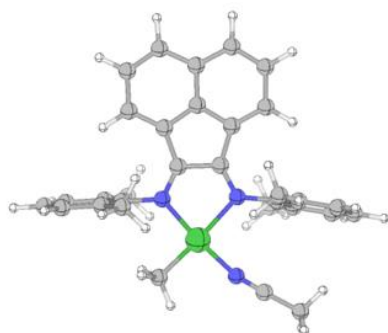
|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 1.35330200  | 3.85522900  | 2.32567000  |
| C | 0.78334100  | 1.44442700  | -3.09855400 |
| H | 0.28343500  | 0.51187300  | -2.80366800 |
| H | 0.01132500  | 2.11771200  | -3.48560200 |
| H | 1.47728700  | 1.20714100  | -3.91001500 |
| C | -4.72355100 | 3.07205000  | 1.58261000  |
| H | -4.17660400 | 2.20198300  | 1.97040000  |
| H | -3.98998900 | 3.86736000  | 1.41383800  |
| H | -5.41994700 | 3.39990400  | 2.35970800  |
| C | -4.64413000 | 1.46984300  | -3.22732900 |
| H | -3.91015700 | 2.21409200  | -3.55377800 |
| H | -4.08687900 | 0.55282900  | -2.99238500 |
| H | -5.31241800 | 1.24872100  | -4.06450600 |
| C | -2.69814500 | 1.29663500  | -0.41153700 |
| C | -1.19276500 | 1.34336200  | -0.39303900 |
| C | -3.10092100 | -0.02553800 | 0.08328500  |
| C | -4.31202700 | -0.65797900 | 0.29544800  |
| C | -1.89171900 | -0.71615600 | 0.37128300  |
| C | -4.29560400 | -1.98559400 | 0.79864900  |
| H | -5.25277900 | -0.16112500 | 0.08750300  |
| C | -1.85700800 | -2.03177400 | 0.87153700  |
| C | -0.72085400 | 0.04628500  | 0.10694900  |
| C | -3.11696200 | -2.65862100 | 1.08078500  |
| H | -5.24411600 | -2.48660800 | 0.96725900  |
| C | -0.56604700 | -2.58044100 | 1.10937200  |
| C | 0.52163300  | -0.51077700 | 0.34716100  |
| H | -3.15102800 | -3.67448800 | 1.46566600  |
| C | 0.57520600  | -1.83649900 | 0.85278100  |
| H | -0.47848000 | -3.59253300 | 1.49574300  |
| H | 1.43476100  | 0.04145400  | 0.15646500  |
| H | 1.54859600  | -2.27861700 | 1.04294000  |



B3LYP-D3/BSI

|    |             |             |             |
|----|-------------|-------------|-------------|
| Ni | -1.82272000 | 0.74040100  | 2.09963800  |
| N  | -0.37957600 | -0.76269500 | 1.81385500  |
| N  | -3.04957100 | -0.72238100 | 1.84579300  |
| C  | 1.05213100  | -0.71560800 | 1.80442300  |
| C  | 1.71084100  | -0.45693500 | 0.58953400  |
| C  | 1.74494600  | -0.91370700 | 3.01174300  |
| C  | 3.10668000  | -0.35574500 | 0.61324400  |
| C  | 3.14014200  | -0.80363500 | 2.98814400  |
| C  | 3.81759700  | -0.51955100 | 1.80222300  |
| H  | 3.63663400  | -0.15175400 | -0.31325200 |
| H  | 3.69628800  | -0.94808300 | 3.91046800  |
| H  | 4.89995000  | -0.43319800 | 1.80328900  |
| C  | -4.48540300 | -0.67093600 | 1.86773800  |
| C  | -5.16298500 | -0.41967100 | 0.66516700  |
| C  | -5.14191300 | -0.85956700 | 3.09326900  |
| C  | -6.56080700 | -0.37985400 | 0.70871900  |
| C  | -6.54012800 | -0.81120800 | 3.08997900  |
| C  | -7.24503000 | -0.57766200 | 1.90860400  |
| H  | -7.11289300 | -0.18669200 | -0.20694400 |
| H  | -7.07613400 | -0.95307200 | 4.02438600  |
| H  | -8.33014100 | -0.54051700 | 1.92475600  |
| C  | 1.00290000  | -1.28199400 | 4.27407800  |
| H  | 0.12268800  | -0.64963900 | 4.42814300  |
| H  | 0.64316500  | -2.31826000 | 4.22890900  |
| H  | 1.64837100  | -1.19362400 | 5.15209100  |
| C  | 0.93218600  | -0.34530600 | -0.69922100 |
| H  | 0.57855000  | -1.33076500 | -1.02968400 |
| H  | 0.04464300  | 0.28523900  | -0.58484200 |
| H  | 1.54984300  | 0.07029400  | -1.49995900 |
| C  | -4.35180200 | -1.11681100 | 4.35264300  |
| H  | -3.85853900 | -2.09712700 | 4.32333600  |
| H  | -3.56264300 | -0.36547700 | 4.48220600  |
| H  | -4.99701800 | -1.09430300 | 5.23469300  |
| C  | -4.39503500 | -0.21656000 | -0.61758700 |
| H  | -3.60530400 | 0.53428200  | -0.48863100 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -3.90494700 | -1.14354300 | -0.94270400 |
| H | -5.05487700 | 0.11258600  | -1.42449800 |
| C | -2.47643600 | -1.86199300 | 1.63746600  |
| C | -0.97778600 | -1.88536000 | 1.61890600  |
| C | -3.25883700 | 1.99530400  | 2.33996700  |
| H | -3.86589200 | 1.67633000  | 3.19422500  |
| H | -2.83504300 | 2.98564200  | 2.51816200  |
| H | -3.87864100 | 1.99762000  | 1.43673000  |
| C | -2.94797600 | -3.22338700 | 1.39789600  |
| C | -4.18749200 | -3.83303900 | 1.30042100  |
| C | -1.76845300 | -4.00932200 | 1.24511800  |
| C | -4.23019000 | -5.22875600 | 1.05020400  |
| H | -5.10691800 | -3.26947600 | 1.41059000  |
| C | -1.79438900 | -5.39390100 | 0.99647200  |
| C | -0.56100000 | -3.26477000 | 1.36666300  |
| C | -3.08189600 | -5.99272900 | 0.90167600  |
| H | -5.19941500 | -5.71136900 | 0.97307000  |
| C | -0.53004800 | -6.03454900 | 0.86849000  |
| C | 0.65494100  | -3.91310800 | 1.23755600  |
| H | -3.16260700 | -7.05931800 | 0.71090100  |
| C | 0.64668400  | -5.30950600 | 0.98668900  |
| H | -0.48977800 | -7.10314000 | 0.67611500  |
| H | 1.59423100  | -3.37814700 | 1.32404300  |
| H | 1.59699600  | -5.82403300 | 0.88446900  |
| O | -0.52689100 | 2.21504400  | 2.36418300  |
| C | 0.20816300  | 2.28390700  | 3.61156500  |
| H | 1.00516600  | 1.53315700  | 3.59360300  |
| H | 0.66844200  | 3.27720500  | 3.66245000  |
| C | -0.74747300 | 2.08484300  | 4.77356700  |
| H | -1.24540300 | 1.11026700  | 4.72247600  |
| H | -0.19078100 | 2.13389400  | 5.71510200  |
| H | -1.51909900 | 2.85922300  | 4.77726600  |
| C | 0.18805800  | 2.73765300  | 1.21654700  |
| H | 0.98094700  | 2.03324100  | 0.94399100  |
| H | 0.65329000  | 3.68045600  | 1.52602800  |
| C | -0.78726400 | 2.97884500  | 0.07918800  |
| H | -1.55226700 | 3.70290800  | 0.37170400  |
| H | -0.24475600 | 3.36694800  | -0.78906200 |
| H | -1.29261800 | 2.05412200  | -0.22022100 |

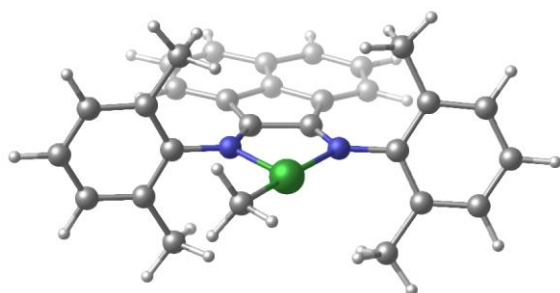


B3LYP-D3/BSI

|    |             |             |             |
|----|-------------|-------------|-------------|
| Ni | -1.84908000 | 0.71488900  | 2.13264100  |
| N  | -0.43498100 | -0.77378000 | 1.83993500  |
| N  | -3.09566500 | -0.73661100 | 1.85287000  |
| C  | 0.98293300  | -0.62714100 | 1.86134600  |
| C  | 1.68178400  | -0.47178800 | 0.65053400  |
| C  | 1.60800100  | -0.51312500 | 3.11645000  |
| C  | 3.05801000  | -0.22449700 | 0.72284200  |
| C  | 2.98604500  | -0.27224900 | 3.14065400  |
| C  | 3.70876200  | -0.12965100 | 1.95425500  |
| H  | 3.62047900  | -0.10247200 | -0.19889700 |
| H  | 3.49277800  | -0.19745300 | 4.09917600  |
| H  | 4.77840900  | 0.05545100  | 1.98914000  |
| C  | -4.53055900 | -0.68176600 | 1.89190700  |
| C  | -5.22613000 | -0.42433400 | 0.70040900  |
| C  | -5.16891200 | -0.86506600 | 3.12814000  |
| C  | -6.62268900 | -0.37226300 | 0.76790200  |
| C  | -6.56654200 | -0.80523800 | 3.14800900  |
| C  | -7.28875500 | -0.56452700 | 1.97883600  |
| H  | -7.18817500 | -0.17338800 | -0.13831900 |
| H  | -7.08802400 | -0.94406800 | 4.09103800  |
| H  | -8.37309700 | -0.51774900 | 2.01286000  |
| C  | 0.79792800  | -0.65559700 | 4.38090800  |
| H  | -0.05764800 | 0.03223800  | 4.37841200  |
| H  | 0.38760400  | -1.66792000 | 4.48200000  |
| H  | 1.40492800  | -0.45000400 | 5.26674100  |
| C  | 0.95977700  | -0.54918600 | -0.67306500 |
| H  | 0.60158500  | -1.56578200 | -0.87738100 |
| H  | 0.08193200  | 0.10875500  | -0.68463700 |
| H  | 1.61685700  | -0.25742000 | -1.49651600 |
| C  | -4.36037200 | -1.13177700 | 4.37372700  |
| H  | -3.86906000 | -2.11249000 | 4.33018000  |
| H  | -3.56737100 | -0.38342100 | 4.49766400  |
| H  | -4.99234100 | -1.11443200 | 5.26544400  |
| C  | -4.48080200 | -0.22876900 | -0.59702900 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -3.68057100 | 0.51350900  | -0.48617700 |
| H | -4.00866900 | -1.16137800 | -0.93242300 |
| H | -5.15351800 | 0.10745200  | -1.39028400 |
| C | -2.52130700 | -1.86470600 | 1.58820200  |
| C | -1.01943400 | -1.88687200 | 1.57025300  |
| C | -3.25522900 | 2.01505800  | 2.36600300  |
| H | -3.86439600 | 1.67904700  | 3.21250600  |
| H | -2.85950800 | 3.01563300  | 2.55265500  |
| H | -3.85945100 | 2.00674500  | 1.45211200  |
| C | -2.98875300 | -3.21654800 | 1.29327800  |
| C | -4.22643700 | -3.82601900 | 1.17610500  |
| C | -1.80731000 | -3.99251400 | 1.10689600  |
| C | -4.26549300 | -5.21115400 | 0.87170600  |
| H | -5.14688300 | -3.26939700 | 1.31095200  |
| C | -1.82919200 | -5.36674200 | 0.80610300  |
| C | -0.60118300 | -3.25111200 | 1.25672900  |
| C | -3.11527300 | -5.96523800 | 0.69070300  |
| H | -5.23339400 | -5.69355700 | 0.77841000  |
| C | -0.56291000 | -5.99816600 | 0.65310000  |
| C | 0.61623000  | -3.88963300 | 1.10270700  |
| H | -3.19341100 | -7.02385200 | 0.45886300  |
| C | 0.61239200  | -5.27530400 | 0.79874000  |
| H | -0.51969600 | -7.05834700 | 0.41931700  |
| H | 1.55307900  | -3.35298300 | 1.20803700  |
| H | 1.56384500  | -5.78324700 | 0.67637100  |
| N | -0.50747500 | 2.00800800  | 2.32497200  |
| C | 0.48159700  | 2.60422600  | 2.38817100  |
| C | 1.75582600  | 3.30354400  | 2.46174800  |
| H | 2.56333800  | 2.56683200  | 2.38281100  |
| H | 1.83733800  | 4.02507100  | 1.64275600  |
| H | 1.83938900  | 3.83457900  | 3.41522700  |

<sup>1</sup>A



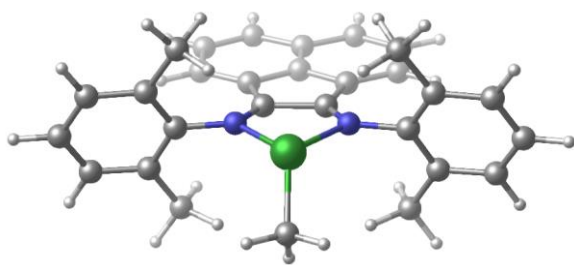
|    |             |             |             |
|----|-------------|-------------|-------------|
| Ni | -1.99154500 | 3.72921100  | -1.07778200 |
| N  | -0.56250000 | 2.35204400  | -0.62505400 |
| N  | -3.23625400 | 2.30486900  | -0.71881700 |
| C  | 0.85110600  | 2.53337900  | -0.67161800 |
| C  | 1.62098600  | 1.89586900  | -1.66673000 |
| C  | 1.41056200  | 3.44088100  | 0.25142800  |
| C  | 2.99662900  | 2.15582700  | -1.68062400 |
| C  | 2.78945700  | 3.65535800  | 0.20456200  |
| C  | 3.58003700  | 3.01501300  | -0.75076600 |
| H  | 3.61179700  | 1.68471300  | -2.44230600 |
| H  | 3.24457100  | 4.33387000  | 0.92054600  |
| H  | 4.64954500  | 3.19961000  | -0.78081200 |
| C  | -4.66338500 | 2.38992900  | -0.78057000 |
| C  | -5.30242400 | 2.06219200  | -1.98758300 |
| C  | -5.35167000 | 2.83793300  | 0.35880400  |
| C  | -6.69681300 | 2.16372000  | -2.02349200 |
| C  | -6.74494100 | 2.92364800  | 0.27555000  |
| C  | -7.41290400 | 2.58580500  | -0.90228900 |
| H  | -7.22116200 | 1.91644000  | -2.94226700 |
| H  | -7.30637100 | 3.26445100  | 1.14091800  |
| H  | -8.49498400 | 2.66183200  | -0.95014300 |
| C  | 0.54165400  | 4.12543700  | 1.27944100  |
| H  | -0.25291800 | 4.72419000  | 0.80806600  |
| H  | 0.04294800  | 3.40385800  | 1.93734800  |
| H  | 1.12938700  | 4.80329800  | 1.90371300  |
| C  | 0.99923100  | 0.99558000  | -2.70896600 |
| H  | 0.81312500  | -0.01317000 | -2.32070800 |
| H  | 0.03932100  | 1.38747500  | -3.06406100 |
| H  | 1.66082100  | 0.89632500  | -3.57350200 |
| C  | -4.59707500 | 3.20259200  | 1.61257200  |
| H  | -4.10761900 | 2.32702300  | 2.05801500  |
| H  | -3.80772700 | 3.93497300  | 1.39706900  |
| H  | -5.26420500 | 3.63122200  | 2.36462800  |
| C  | -4.49848100 | 1.62107900  | -3.18519900 |
| H  | -3.70699300 | 2.34591600  | -3.41617900 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -4.00804000 | 0.65509600  | -3.00904000 |
| H | -5.13305500 | 1.51633200  | -4.06876300 |
| C | -2.63501500 | 1.21130000  | -0.38611000 |
| C | -1.12752900 | 1.22859100  | -0.33716800 |
| C | -3.22774900 | 5.08040700  | -1.56563800 |
| H | -2.58648000 | 5.94815100  | -1.80223700 |
| H | -3.81074400 | 4.79128100  | -2.44681200 |
| H | -3.90635600 | 5.32503100  | -0.74144600 |
| C | -3.08032200 | -0.11975000 | 0.00034200  |
| C | -4.31188700 | -0.73572400 | 0.14697100  |
| C | -1.88881700 | -0.84882300 | 0.28181300  |
| C | -4.33537500 | -2.08608900 | 0.57794600  |
| H | -5.23665100 | -0.20809300 | -0.05859800 |
| C | -1.89670300 | -2.18557200 | 0.72009200  |
| C | -0.69319600 | -0.09795400 | 0.09316700  |
| C | -3.17546600 | -2.79492600 | 0.85871500  |
| H | -5.29608700 | -2.57751800 | 0.69402200  |
| C | -0.62577000 | -2.77122800 | 0.97903300  |
| C | 0.52872700  | -0.69279900 | 0.35683800  |
| H | -3.24119500 | -3.82740600 | 1.19057800  |
| C | 0.53944700  | -2.03882200 | 0.80357000  |
| H | -0.57101900 | -3.80166900 | 1.31886300  |
| H | 1.46017300  | -0.15301300 | 0.22486000  |
| H | 1.49553900  | -2.50876000 | 1.01112700  |

UB3LYP-D3/BSII(SMD)//B3LYP-D3/BSI

HF=-1402.0598939

<sup>3</sup>A



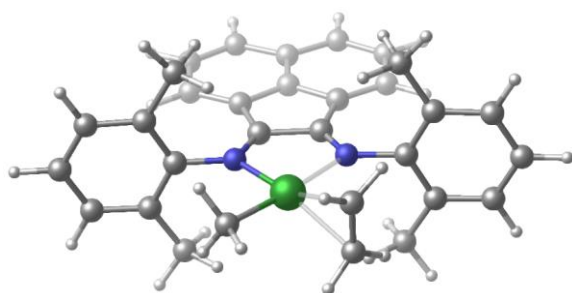
|                                              |                             |            |             |
|----------------------------------------------|-----------------------------|------------|-------------|
| Zero-point correction=                       | 0.481207 (Hartree/Particle) |            |             |
| Thermal correction to Energy=                | 0.511218                    |            |             |
| Thermal correction to Enthalpy=              | 0.512162                    |            |             |
| Thermal correction to Gibbs Free Energy=     | 0.418196                    |            |             |
| Sum of electronic and zero-point Energies=   | -1399.569944                |            |             |
| Sum of electronic and thermal Energies=      | -1399.539933                |            |             |
| Sum of electronic and thermal Enthalpies=    | -1399.538989                |            |             |
| Sum of electronic and thermal Free Energies= | -1399.632955                |            |             |
| Ni                                           | -2.04250100                 | 3.74505500 | -1.05138700 |
| N                                            | -0.65106000                 | 2.38756900 | -0.46541700 |
| N                                            | -3.36423000                 | 2.31108600 | -0.48647000 |
| C                                            | 0.76180900                  | 2.55960900 | -0.55443200 |
| C                                            | 1.48803300                  | 1.91890800 | -1.57786100 |
| C                                            | 1.35749900                  | 3.45805900 | 0.35151800  |
| C                                            | 2.86475700                  | 2.16294900 | -1.63653900 |
| C                                            | 2.73650100                  | 3.66063100 | 0.25870300  |
| C                                            | 3.48740600                  | 3.01416000 | -0.72360400 |
| H                                            | 3.44966500                  | 1.68713400 | -2.41877800 |
| H                                            | 3.22154200                  | 4.33487900 | 0.95888800  |
| H                                            | 4.55727300                  | 3.18737500 | -0.78868400 |
| C                                            | -4.78298400                 | 2.40316100 | -0.59717800 |
| C                                            | -5.45661700                 | 1.72059700 | -1.62952300 |
| C                                            | -5.44182600                 | 3.26846200 | 0.29730400  |
| C                                            | -6.84390200                 | 1.88652600 | -1.70913800 |
| C                                            | -6.82849400                 | 3.39273600 | 0.18363600  |
| C                                            | -7.52705600                 | 2.70295600 | -0.80781200 |
| H                                            | -7.38936500                 | 1.37704000 | -2.49863900 |
| H                                            | -7.36114600                 | 4.03991100 | 0.87470700  |
| H                                            | -8.60390600                 | 2.81539500 | -0.88910500 |
| C                                            | 0.52145800                  | 4.15606500 | 1.39610900  |
| H                                            | -0.28041400                 | 4.75309400 | 0.93415100  |
| H                                            | 0.03532400                  | 3.44432400 | 2.07412800  |
| H                                            | 1.12797200                  | 4.83732800 | 1.99823400  |
| C                                            | 0.80979600                  | 1.03271600 | -2.59565900 |
| H                                            | 0.54552900                  | 0.05434700 | -2.17590400 |
| H                                            | -0.11465500                 | 1.48856900 | -2.96881500 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 1.46677400  | 0.85610700  | -3.45114500 |
| C | -4.66215400 | 4.01496700  | 1.35193400  |
| H | -4.14452200 | 3.33353500  | 2.03770800  |
| H | -3.89040100 | 4.65751000  | 0.89978400  |
| H | -5.31546900 | 4.66032500  | 1.94458400  |
| C | -4.71473900 | 0.87198600  | -2.63486600 |
| H | -3.80901200 | 1.37585400  | -2.99179700 |
| H | -4.40702300 | -0.09140400 | -2.21010100 |
| H | -5.34634700 | 0.66158500  | -3.50174600 |
| C | -2.73847700 | 1.24140000  | -0.12852300 |
| C | -1.22100300 | 1.28407600  | -0.11718300 |
| C | -2.04108900 | 4.30983000  | -2.92084300 |
| H | -2.95719100 | 4.88548900  | -3.10577000 |
| H | -1.15611600 | 4.93740800  | -3.08776400 |
| H | -2.00919200 | 3.43460200  | -3.57722100 |
| C | -3.13908800 | -0.08184700 | 0.33832200  |
| C | -4.35149900 | -0.71020000 | 0.56868600  |
| C | -1.92796300 | -0.77421600 | 0.62143700  |
| C | -4.33634100 | -2.03172300 | 1.08174400  |
| H | -5.29362100 | -0.21448300 | 0.36233500  |
| C | -1.89485200 | -2.08439700 | 1.13382400  |
| C | -0.75360900 | -0.01498000 | 0.35541700  |
| C | -3.15522400 | -2.70605500 | 1.35692300  |
| H | -5.28387600 | -2.52903400 | 1.26296100  |
| C | -0.60490700 | -2.63470000 | 1.37462600  |
| C | 0.48872100  | -0.57456500 | 0.60291100  |
| H | -3.18950900 | -3.71901800 | 1.74818700  |
| C | 0.54037500  | -1.89523900 | 1.11580600  |
| H | -0.51949400 | -3.64437300 | 1.76657500  |
| H | 1.40437500  | -0.02666900 | 0.40982700  |
| H | 1.51161900  | -2.33890100 | 1.31029300  |

UB3LYP-D3/BSII(SMD)//B3LYP-D3/BSI

HF= -1402.0736328

**<sup>1</sup>B**



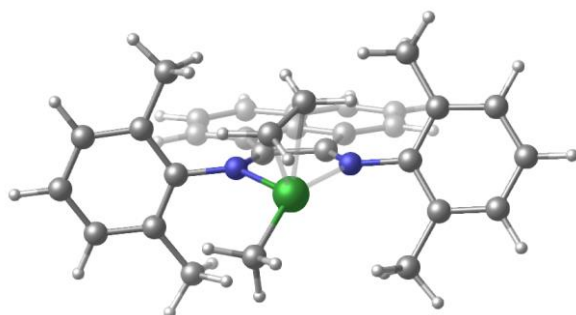
|                                              |                             |             |             |
|----------------------------------------------|-----------------------------|-------------|-------------|
| Zero-point correction=                       | 0.539821 (Hartree/Particle) |             |             |
| Thermal correction to Energy=                | 0.572074                    |             |             |
| Thermal correction to Enthalpy=              | 0.573018                    |             |             |
| Thermal correction to Gibbs Free Energy=     | 0.476017                    |             |             |
| Sum of electronic and zero-point Energies=   | -1478.147931                |             |             |
| Sum of electronic and thermal Energies=      | -1478.115678                |             |             |
| Sum of electronic and thermal Enthalpies=    | -1478.114734                |             |             |
| Sum of electronic and thermal Free Energies= | -1478.211736                |             |             |
| Ni                                           | -1.77400900                 | 0.76217400  | 2.11016100  |
| N                                            | -0.37826100                 | -0.79052100 | 1.81772700  |
| N                                            | -3.06311000                 | -0.72128800 | 1.82977800  |
| C                                            | 1.05091400                  | -0.73359500 | 1.82846300  |
| C                                            | 1.72181900                  | -0.45320100 | 0.62496700  |
| C                                            | 1.72203900                  | -0.90940200 | 3.05150800  |
| C                                            | 3.11596000                  | -0.33985500 | 0.67156200  |
| C                                            | 3.11617800                  | -0.78703300 | 3.04895300  |
| C                                            | 3.80870100                  | -0.50240400 | 1.87166500  |
| H                                            | 3.65892400                  | -0.12275900 | -0.24424900 |
| H                                            | 3.65931500                  | -0.91750600 | 3.98095400  |
| H                                            | 4.89004900                  | -0.40647900 | 1.88962000  |
| C                                            | -4.49602000                 | -0.64728600 | 1.84268600  |
| C                                            | -5.16195700                 | -0.36971900 | 0.63835200  |
| C                                            | -5.16385500                 | -0.82861700 | 3.06416700  |
| C                                            | -6.55849200                 | -0.29542900 | 0.67603400  |
| C                                            | -6.56036200                 | -0.74535400 | 3.05410600  |
| C                                            | -7.25318000                 | -0.48476500 | 1.87126500  |
| H                                            | -7.10127700                 | -0.08219600 | -0.24068700 |
| H                                            | -7.10459300                 | -0.88158600 | 3.98454000  |
| H                                            | -8.33703600                 | -0.42029500 | 1.88260200  |
| C                                            | 0.95501700                  | -1.25956900 | 4.30483300  |
| H                                            | 0.08278400                  | -0.60896600 | 4.44471100  |
| H                                            | 0.57426800                  | -2.28822800 | 4.26012900  |
| H                                            | 1.58938700                  | -1.17890500 | 5.19142000  |
| C                                            | 0.95471000                  | -0.32471300 | -0.66998700 |
| H                                            | 0.57894200                  | -1.30043100 | -1.00453400 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 0.07918000  | 0.32762900  | -0.56272800 |
| H | 1.58750900  | 0.07741200  | -1.46550400 |
| C | -4.38809000 | -1.11951800 | 4.32521400  |
| H | -3.92160100 | -2.11255400 | 4.28838500  |
| H | -3.57878400 | -0.39252100 | 4.46990100  |
| H | -5.03768200 | -1.08898000 | 5.20372600  |
| C | -4.38437600 | -0.18003900 | -0.64075000 |
| H | -3.57469200 | 0.54893900  | -0.50868300 |
| H | -3.91814800 | -1.11810500 | -0.96900000 |
| H | -5.03271400 | 0.17002800  | -1.44809500 |
| C | -2.49472300 | -1.86101300 | 1.61456900  |
| C | -0.99039000 | -1.90146600 | 1.60769600  |
| C | -3.19809000 | 2.03534200  | 2.35099400  |
| H | -3.80243000 | 1.68196000  | 3.19428000  |
| H | -2.84519000 | 3.05252700  | 2.54290800  |
| H | -3.80350500 | 2.01378100  | 1.43767800  |
| C | -0.25787500 | 2.42483100  | 1.72692900  |
| H | 0.46477600  | 1.93996000  | 1.07672600  |
| H | -0.86886300 | 3.20934800  | 1.29077500  |
| C | -0.25577200 | 2.17350300  | 3.06610200  |
| H | -0.86502500 | 2.74614500  | 3.75883900  |
| H | 0.46869200  | 1.48644500  | 3.49404600  |
| C | -2.97461400 | -3.21587500 | 1.35804000  |
| C | -4.21959200 | -3.81198300 | 1.24437100  |
| C | -1.80149000 | -4.01189300 | 1.20840800  |
| C | -4.27389600 | -5.20452200 | 0.98106600  |
| H | -5.13397400 | -3.23966300 | 1.35184700  |
| C | -1.83869700 | -5.39380000 | 0.94715100  |
| C | -0.58749400 | -3.28149800 | 1.34717700  |
| C | -3.13138100 | -5.97837000 | 0.83567200  |
| H | -5.24687200 | -5.67710900 | 0.89096500  |
| C | -0.57933500 | -6.04558700 | 0.82478900  |
| C | 0.62350500  | -3.93977600 | 1.22345500  |
| H | -3.22122700 | -7.04230300 | 0.63448500  |
| C | 0.60377500  | -5.33360900 | 0.96007300  |
| H | -0.54776200 | -7.11273100 | 0.62315000  |
| H | 1.56657300  | -3.41358900 | 1.32337100  |
| H | 1.54961200  | -5.85694600 | 0.86176700  |

UB3LYP-D3/BSII(SMD)//B3LYP-D3/BSI

HF=-1480.7208426

**<sup>3</sup>B**



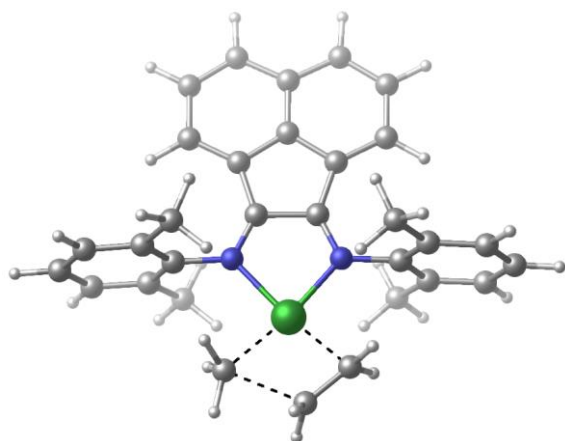
|                                              |                             |            |             |
|----------------------------------------------|-----------------------------|------------|-------------|
| Zero-point correction=                       | 0.536399 (Hartree/Particle) |            |             |
| Thermal correction to Energy=                | 0.569746                    |            |             |
| Thermal correction to Enthalpy=              | 0.570690                    |            |             |
| Thermal correction to Gibbs Free Energy=     | 0.470136                    |            |             |
| Sum of electronic and zero-point Energies=   | -1478.128599                |            |             |
| Sum of electronic and thermal Energies=      | -1478.095252                |            |             |
| Sum of electronic and thermal Enthalpies=    | -1478.094307                |            |             |
| Sum of electronic and thermal Free Energies= | -1478.194861                |            |             |
| Ni                                           | -2.11695100                 | 3.70291400 | -1.68136100 |
| N                                            | -0.71978500                 | 2.43449000 | -0.81424000 |
| N                                            | -3.43264900                 | 2.26951200 | -0.84272800 |
| C                                            | 0.70607700                  | 2.55599800 | -0.90493100 |
| C                                            | 1.33713500                  | 2.08284100 | -2.06941500 |
| C                                            | 1.41443300                  | 3.15300800 | 0.15195200  |
| C                                            | 2.72423200                  | 2.23489900 | -2.16439700 |
| C                                            | 2.80160900                  | 3.27750500 | 0.01413400  |
| C                                            | 3.45304900                  | 2.82889900 | -1.13438900 |
| H                                            | 3.23345100                  | 1.87926400 | -3.05582600 |
| H                                            | 3.37242100                  | 3.73148000 | 0.81952900  |
| H                                            | 4.52937300                  | 2.93934100 | -1.22501900 |
| C                                            | -4.85560400                 | 2.35304300 | -0.84938600 |
| C                                            | -5.48873600                 | 2.41223400 | -2.11016300 |
| C                                            | -5.57761300                 | 2.47242200 | 0.35779000  |
| C                                            | -6.87771200                 | 2.54546900 | -2.14336600 |
| C                                            | -6.96785400                 | 2.62472500 | 0.26829900  |
| C                                            | -7.61611400                 | 2.65248700 | -0.96369500 |
| H                                            | -7.38375000                 | 2.56916400 | -3.10438600 |
| H                                            | -7.54290400                 | 2.72758800 | 1.18463700  |
| H                                            | -8.69490600                 | 2.76714800 | -1.00701000 |
| C                                            | 0.71041000                  | 3.62566200 | 1.40158000  |
| H                                            | 0.06123400                  | 2.84921600 | 1.82347200  |
| H                                            | 1.43224400                  | 3.90979400 | 2.17172200  |
| H                                            | 0.08277000                  | 4.50263200 | 1.20380400  |
| C                                            | 0.54177900                  | 1.39722400 | -3.15318500 |
| H                                            | 0.16871000                  | 0.42150800 | -2.81462500 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -0.32870700 | 1.99256700  | -3.44798400 |
| H | 1.15414600  | 1.22767700  | -4.04248900 |
| C | -4.91536500 | 2.45028400  | 1.71640300  |
| H | -4.83351300 | 1.42872500  | 2.10744300  |
| H | -3.90324900 | 2.86401200  | 1.69487100  |
| H | -5.50018200 | 3.02891200  | 2.43700500  |
| C | -4.68661600 | 2.30039600  | -3.38548000 |
| H | -4.02182200 | 3.16559900  | -3.52748500 |
| H | -4.05331700 | 1.40566700  | -3.39381100 |
| H | -5.34305200 | 2.25678800  | -4.25852300 |
| C | -2.77914700 | 1.27984100  | -0.33489100 |
| C | -1.26656300 | 1.37084500  | -0.33653700 |
| C | -1.28833700 | 4.63884800  | -3.22110000 |
| H | -1.85977600 | 5.52757000  | -3.51454900 |
| H | -0.25393600 | 4.92626200  | -3.00722200 |
| H | -1.29659900 | 3.92906200  | -4.06075200 |
| C | -2.63603300 | 5.01388900  | 0.27110800  |
| H | -2.17865000 | 4.39006800  | 1.03266600  |
| H | -3.72256700 | 5.02974900  | 0.23799400  |
| C | -1.88947400 | 5.78636300  | -0.55049100 |
| H | -2.34763500 | 6.47046300  | -1.25778000 |
| H | -0.80601200 | 5.82155500  | -0.48012200 |
| C | -3.13204000 | -0.02346400 | 0.22745100  |
| C | -4.31701700 | -0.70559900 | 0.44791700  |
| C | -1.89666600 | -0.65979400 | 0.53719100  |
| C | -4.25145000 | -2.01473200 | 0.98863000  |
| H | -5.27807200 | -0.25915400 | 0.21778600  |
| C | -1.81275600 | -1.95620400 | 1.07862300  |
| C | -0.75145300 | 0.12655000  | 0.22999900  |
| C | -3.04694400 | -2.62728800 | 1.30274700  |
| H | -5.17895200 | -2.55084000 | 1.16322200  |
| C | -0.50218100 | -2.45054800 | 1.33029600  |
| C | 0.51246800  | -0.38033700 | 0.48041800  |
| H | -3.04245100 | -3.63050600 | 1.71979900  |
| C | 0.61405400  | -1.67999700 | 1.03922300  |
| H | -0.37830500 | -3.44429500 | 1.75173400  |
| H | 1.40642900  | 0.19070400  | 0.25657100  |
| H | 1.60175100  | -2.08303400 | 1.23952500  |

UB3LYP-D3/BSII(SMD)//B3LYP-D3/BSI

HF=-1480.7114892

<sup>1</sup>TS1

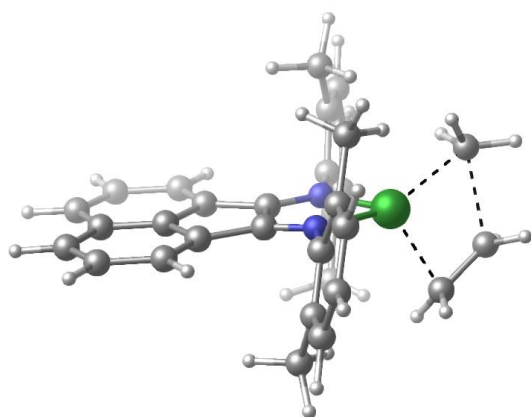


|                                              |                             |             |             |
|----------------------------------------------|-----------------------------|-------------|-------------|
| Zero-point correction=                       | 0.538963 (Hartree/Particle) |             |             |
| Thermal correction to Energy=                | 0.570527                    |             |             |
| Thermal correction to Enthalpy=              | 0.571471                    |             |             |
| Thermal correction to Gibbs Free Energy=     | 0.476147                    |             |             |
| Sum of electronic and zero-point Energies=   | -1478.127425                |             |             |
| Sum of electronic and thermal Energies=      | -1478.095861                |             |             |
| Sum of electronic and thermal Enthalpies=    | -1478.094917                |             |             |
| Sum of electronic and thermal Free Energies= | -1478.190241                |             |             |
| Ni                                           | -1.64563100                 | 0.76571900  | 2.03727700  |
| N                                            | -0.39841600                 | -0.74435100 | 1.77297500  |
| N                                            | -3.05387500                 | -0.71141300 | 1.79513300  |
| C                                            | 1.03746600                  | -0.70901700 | 1.76994100  |
| C                                            | 1.69922400                  | -0.46829200 | 0.55520200  |
| C                                            | 1.71483800                  | -0.88695100 | 2.98688200  |
| C                                            | 3.09765500                  | -0.42200000 | 0.57861000  |
| C                                            | 3.11296900                  | -0.83249100 | 2.96283800  |
| C                                            | 3.80024200                  | -0.60499100 | 1.77009000  |
| H                                            | 3.63567800                  | -0.23779300 | -0.34723000 |
| H                                            | 3.66288900                  | -0.96729000 | 3.89019700  |
| H                                            | 4.88524600                  | -0.56321100 | 1.77031000  |
| C                                            | -4.48290500                 | -0.62452900 | 1.81927300  |
| C                                            | -5.16045300                 | -0.35765500 | 0.61739700  |
| C                                            | -5.14392800                 | -0.76638700 | 3.05127100  |
| C                                            | -6.55395600                 | -0.24394100 | 0.67067100  |
| C                                            | -6.53774800                 | -0.64482200 | 3.05649700  |
| C                                            | -7.23843300                 | -0.38686100 | 1.87794200  |
| H                                            | -7.10276800                 | -0.03940800 | -0.24450800 |
| H                                            | -7.07397100                 | -0.75185600 | 3.99542600  |
| H                                            | -8.31986000                 | -0.29201500 | 1.90122700  |
| C                                            | 0.94718000                  | -1.14775200 | 4.25995500  |
| H                                            | 0.14276000                  | -0.41421200 | 4.39975000  |
| H                                            | 0.47227900                  | -2.13725800 | 4.24422500  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 1.60426200  | -1.10758900 | 5.13255600  |
| C | 0.91522500  | -0.28997900 | -0.72214300 |
| H | 0.43889400  | -1.22887300 | -1.03276200 |
| H | 0.11025900  | 0.44587400  | -0.59842800 |
| H | 1.56140300  | 0.04170400  | -1.53900000 |
| C | -4.36653000 | -1.07360600 | 4.30859700  |
| H | -3.95544700 | -2.09117800 | 4.28297100  |
| H | -3.51480100 | -0.39329900 | 4.43471200  |
| H | -5.00201700 | -0.99369300 | 5.19436500  |
| C | -4.40074800 | -0.23620800 | -0.68173300 |
| H | -3.54575300 | 0.44530800  | -0.58906100 |
| H | -3.99680000 | -1.20676800 | -0.99793800 |
| H | -5.04654800 | 0.13221300  | -1.48300400 |
| C | -2.49371300 | -1.85357700 | 1.59793200  |
| C | -0.99585200 | -1.87221600 | 1.58500500  |
| C | -3.16884200 | 2.13057500  | 2.27458500  |
| H | -3.60691300 | 1.56234100  | 3.09978100  |
| H | -3.37286000 | 3.18171500  | 2.45282400  |
| H | -3.61227100 | 1.86473200  | 1.31094700  |
| C | -0.14641900 | 2.00969100  | 2.24371900  |
| H | 0.41169800  | 1.67336100  | 3.11613200  |
| H | 0.40565000  | 1.98312100  | 1.30555600  |
| C | -1.19997700 | 2.92686900  | 2.40415400  |
| H | -1.42412900 | 3.61211600  | 1.59300600  |
| H | -1.41821400 | 3.30355900  | 3.39827400  |
| C | -2.95641900 | -3.22074100 | 1.36921600  |
| C | -4.19289500 | -3.83489200 | 1.27337800  |
| C | -1.77292300 | -4.00087900 | 1.22890200  |
| C | -4.22932900 | -5.23327800 | 1.03647800  |
| H | -5.11398900 | -3.27170500 | 1.37507600  |
| C | -1.79168000 | -5.38772800 | 0.99369100  |
| C | -0.56830800 | -3.24829900 | 1.34841500  |
| C | -3.07650500 | -5.99289800 | 0.89978600  |
| H | -5.19579500 | -5.72147900 | 0.96025300  |
| C | -0.52370700 | -6.02340900 | 0.87707100  |
| C | 0.65130000  | -3.89301500 | 1.23052000  |
| H | -3.15163900 | -7.06162200 | 0.71901700  |
| C | 0.64929300  | -5.29150600 | 0.99314700  |
| H | -0.47722700 | -7.09357800 | 0.69517200  |
| H | 1.58803500  | -3.35370000 | 1.31555300  |
| H | 1.60224800  | -5.80273900 | 0.89977300  |

UB3LYP-D3/BSII(SMD)//B3LYP-D3/BSI

HF=-1480.6979817

**<sup>3</sup>TS1**

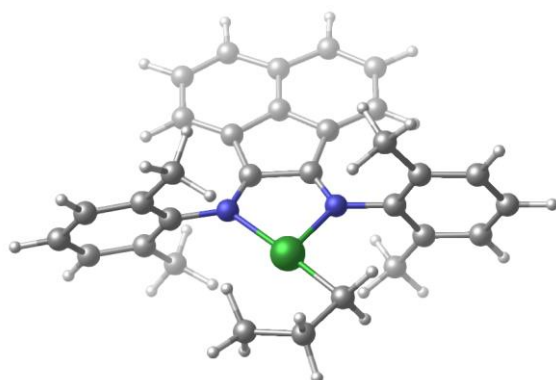
|                                              |                             |            |             |
|----------------------------------------------|-----------------------------|------------|-------------|
| Zero-point correction=                       | 0.536642 (Hartree/Particle) |            |             |
| Thermal correction to Energy=                | 0.568970                    |            |             |
| Thermal correction to Enthalpy=              | 0.569914                    |            |             |
| Thermal correction to Gibbs Free Energy=     | 0.471278                    |            |             |
| Sum of electronic and zero-point Energies=   | -1478.103349                |            |             |
| Sum of electronic and thermal Energies=      | -1478.071021                |            |             |
| Sum of electronic and thermal Enthalpies=    | -1478.070077                |            |             |
| Sum of electronic and thermal Free Energies= | -1478.168713                |            |             |
| Ni                                           | -2.19486800                 | 3.75188200 | -1.34254500 |
| N                                            | -0.74025000                 | 2.40559200 | -0.73565400 |
| N                                            | -3.43116800                 | 2.21684200 | -0.83469100 |
| C                                            | 0.68074700                  | 2.54238200 | -0.84515600 |
| C                                            | 1.28389400                  | 2.18742900 | -2.06536000 |
| C                                            | 1.40917800                  | 3.05853500 | 0.23967000  |
| C                                            | 2.66645000                  | 2.36767000 | -2.18365400 |
| C                                            | 2.78984700                  | 3.21699800 | 0.07688800  |
| C                                            | 3.41523500                  | 2.87826000 | -1.12342200 |
| H                                            | 3.15567000                  | 2.10146700 | -3.11660600 |
| H                                            | 3.37621900                  | 3.61137100 | 0.90228600  |
| H                                            | 4.48707400                  | 3.01317600 | -1.23254800 |
| C                                            | -4.85551500                 | 2.29690100 | -0.85016300 |
| C                                            | -5.49124700                 | 2.24942800 | -2.10570700 |
| C                                            | -5.56337000                 | 2.51331600 | 0.34897000  |
| C                                            | -6.88300800                 | 2.36842500 | -2.13964300 |
| C                                            | -6.95484100                 | 2.63864400 | 0.26229600  |
| C                                            | -7.61205500                 | 2.55761400 | -0.96512600 |
| H                                            | -7.39607900                 | 2.31600900 | -3.09588300 |
| H                                            | -7.52467500                 | 2.81114000 | 1.17127900  |
| H                                            | -8.69256500                 | 2.65580000 | -1.00800600 |
| C                                            | 0.71950500                  | 3.39732300 | 1.53828600  |
| H                                            | 0.29891300                  | 2.50206000 | 2.01374100  |
| H                                            | 1.41478800                  | 3.85597100 | 2.24607100  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -0.11246600 | 4.09215300  | 1.37851700  |
| C | 0.46127700  | 1.59885900  | -3.18673300 |
| H | 0.09901400  | 0.59511600  | -2.92949600 |
| H | -0.42339000 | 2.20978300  | -3.40309700 |
| H | 1.04907200  | 1.51554900  | -4.10453400 |
| C | -4.85313900 | 2.63160200  | 1.67698700  |
| H | -4.54060600 | 1.65221900  | 2.05970000  |
| H | -3.95152000 | 3.24948000  | 1.59523500  |
| H | -5.50817700 | 3.08338900  | 2.42661300  |
| C | -4.68204300 | 2.04783900  | -3.36367400 |
| H | -3.90744100 | 2.82117200  | -3.47021900 |
| H | -4.16108800 | 1.08277200  | -3.36107600 |
| H | -5.31659400 | 2.08816800  | -4.25276000 |
| C | -2.78477000 | 1.22516000  | -0.31738600 |
| C | -1.27904400 | 1.31295900  | -0.31352500 |
| C | -1.16844500 | 5.00343200  | -2.86199700 |
| H | -1.04899400 | 5.99849100  | -3.28119000 |
| H | -0.19369400 | 4.53624800  | -2.70464800 |
| H | -1.81418800 | 4.42471100  | -3.54136200 |
| C | -2.50223200 | 5.32889500  | -0.02691000 |
| H | -1.95906300 | 5.09833600  | 0.88508500  |
| H | -3.58382400 | 5.41478500  | 0.07176800  |
| C | -1.84515000 | 6.01158800  | -1.09275800 |
| H | -2.44779900 | 6.67305000  | -1.70651900 |
| H | -0.82099800 | 6.33731300  | -0.93934400 |
| C | -3.14815500 | -0.07414400 | 0.24428200  |
| C | -4.33839700 | -0.73533600 | 0.49436800  |
| C | -1.91528400 | -0.73055700 | 0.52280000  |
| C | -4.27972300 | -2.04880500 | 1.02684700  |
| H | -5.29714700 | -0.26889500 | 0.29581000  |
| C | -1.83843100 | -2.03214800 | 1.05114700  |
| C | -0.76635700 | 0.04780000  | 0.20723300  |
| C | -3.07787000 | -2.68488400 | 1.30167900  |
| H | -5.21106500 | -2.56961500 | 1.22584900  |
| C | -0.52950000 | -2.54625900 | 1.27081800  |
| C | 0.49504600  | -0.47680500 | 0.42934900  |
| H | -3.07941200 | -3.69120700 | 1.71123000  |
| C | 0.59062900  | -1.78615300 | 0.96718200  |
| H | -0.40996400 | -3.54575100 | 1.67976200  |
| H | 1.39178400  | 0.08832500  | 0.20015600  |
| H | 1.57672800  | -2.20400100 | 1.14388500  |

UB3LYP-D3/BSII(SMD)//B3LYP-D3/BSI

HF=-1480.6797945

<sup>13</sup>C



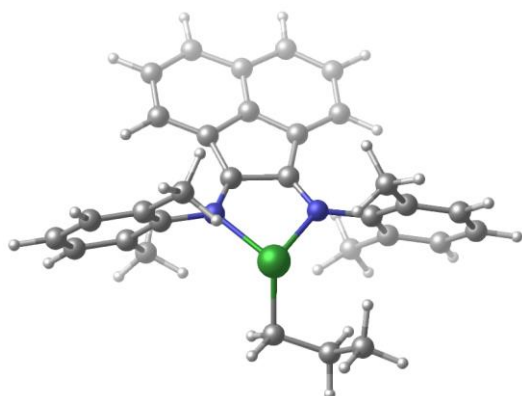
|                                              |                             |             |             |
|----------------------------------------------|-----------------------------|-------------|-------------|
| Zero-point correction=                       | 0.540394 (Hartree/Particle) |             |             |
| Thermal correction to Energy=                | 0.572271                    |             |             |
| Thermal correction to Enthalpy=              | 0.573216                    |             |             |
| Thermal correction to Gibbs Free Energy=     | 0.476808                    |             |             |
| Sum of electronic and zero-point Energies=   | -1478.152552                |             |             |
| Sum of electronic and thermal Energies=      | -1478.120675                |             |             |
| Sum of electronic and thermal Enthalpies=    | -1478.119731                |             |             |
| Sum of electronic and thermal Free Energies= | -1478.216138                |             |             |
| Ni                                           | -1.67855900                 | 0.61094000  | 1.90354700  |
| N                                            | -0.44454200                 | -0.81924900 | 1.70832400  |
| N                                            | -3.10710100                 | -0.83835000 | 1.70197500  |
| C                                            | 0.98512700                  | -0.71782800 | 1.69784000  |
| C                                            | 1.61861100                  | -0.42229700 | 0.48005500  |
| C                                            | 1.68109300                  | -0.87813500 | 2.90683000  |
| C                                            | 3.01320300                  | -0.31476300 | 0.48819600  |
| C                                            | 3.07462600                  | -0.76079900 | 2.86679700  |
| C                                            | 3.73636000                  | -0.48651900 | 1.66910900  |
| H                                            | 3.53158200                  | -0.08976700 | -0.43971900 |
| H                                            | 3.64129200                  | -0.87966600 | 3.78614600  |
| H                                            | 4.81841800                  | -0.39671000 | 1.65812300  |
| C                                            | -4.52410700                 | -0.67718900 | 1.73589700  |
| C                                            | -5.13161900                 | -0.07710400 | 0.61655200  |
| C                                            | -5.24358900                 | -1.02036100 | 2.89655100  |
| C                                            | -6.51173000                 | 0.14069700  | 0.66180500  |
| C                                            | -6.62149700                 | -0.77545400 | 2.89707000  |
| C                                            | -7.25344000                 | -0.20725100 | 1.79084700  |
| H                                            | -7.00514300                 | 0.58792000  | -0.19671000 |
| H                                            | -7.19995000                 | -1.02578800 | 3.78216900  |
| H                                            | -8.32367400                 | -0.02546100 | 1.81330700  |
| C                                            | 0.93928300                  | -1.17140600 | 4.18755200  |
| H                                            | 0.11995500                  | -0.45779300 | 4.34186700  |
| H                                            | 0.49226200                  | -2.17377900 | 4.17295600  |
| H                                            | 1.60769900                  | -1.11792800 | 5.05065800  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 0.80528200  | -0.24007100 | -0.77680600 |
| H | 0.32452800  | -1.17760100 | -1.08419500 |
| H | 0.00137500  | 0.49168400  | -0.62137700 |
| H | 1.42925200  | 0.10381900  | -1.60567300 |
| C | -4.55225400 | -1.60764400 | 4.10453200  |
| H | -4.25607600 | -2.65061100 | 3.93694800  |
| H | -3.64116300 | -1.05109500 | 4.35571900  |
| H | -5.21105400 | -1.58840100 | 4.97657600  |
| C | -4.31258300 | 0.27162600  | -0.60282700 |
| H | -3.43205400 | 0.87509400  | -0.34239400 |
| H | -3.93281100 | -0.62911500 | -1.10124800 |
| H | -4.90524000 | 0.83348800  | -1.32945100 |
| C | -2.53048900 | -1.98582900 | 1.60867500  |
| C | -1.02619300 | -1.96952600 | 1.60076900  |
| C | -2.78668700 | 2.59140300  | 2.55695300  |
| H | -2.84570700 | 2.20065900  | 3.57978600  |
| H | -3.55605400 | 3.36309800  | 2.45396600  |
| H | -3.16873600 | 1.81891900  | 1.84379700  |
| C | -0.39409400 | 1.98262700  | 2.16680900  |
| H | 0.11228100  | 1.78365200  | 3.11905700  |
| H | 0.33814100  | 2.00556600  | 1.35482300  |
| C | -1.37823800 | 3.14288200  | 2.20375900  |
| H | -1.43115400 | 3.63201600  | 1.22585900  |
| H | -1.10713100 | 3.90860300  | 2.94052900  |
| C | -2.95316800 | -3.37641500 | 1.45993100  |
| C | -4.17204700 | -4.02691500 | 1.38592700  |
| C | -1.74969300 | -4.13124100 | 1.36205100  |
| C | -4.17184600 | -5.43508400 | 1.21336500  |
| H | -5.10775500 | -3.48322500 | 1.45990600  |
| C | -1.73104900 | -5.52751500 | 1.19164600  |
| C | -0.56459000 | -3.34280200 | 1.44402100  |
| C | -2.99899500 | -6.17018000 | 1.11961900  |
| H | -5.12503800 | -5.95096300 | 1.15470300  |
| C | -0.44625800 | -6.13418100 | 1.10888600  |
| C | 0.67225000  | -3.95956600 | 1.35862400  |
| H | -3.04521700 | -7.24785900 | 0.98979100  |
| C | 0.70745300  | -5.36723900 | 1.19093200  |
| H | -0.37121200 | -7.21030200 | 0.97914000  |
| H | 1.59367700  | -3.39102400 | 1.41765900  |
| H | 1.67348500  | -5.85754400 | 1.12391600  |

UB3LYP-D3/BSII(SMD)//B3LYP-D3/BSI

HF=-1480.7262117

<sup>3</sup>C



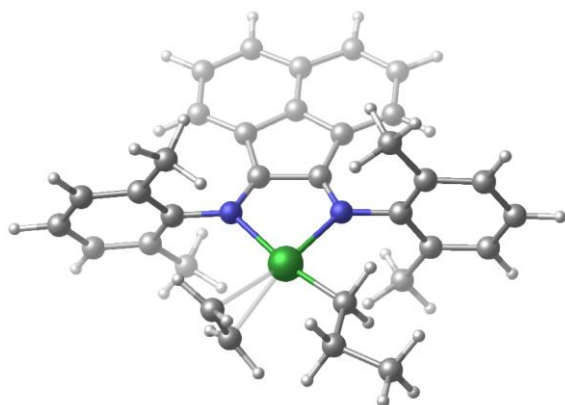
|                                              |                             |            |             |
|----------------------------------------------|-----------------------------|------------|-------------|
| Zero-point correction=                       | 0.539284 (Hartree/Particle) |            |             |
| Thermal correction to Energy=                | 0.571615                    |            |             |
| Thermal correction to Enthalpy=              | 0.572560                    |            |             |
| Thermal correction to Gibbs Free Energy=     | 0.473946                    |            |             |
| Sum of electronic and zero-point Energies=   | -1478.148816                |            |             |
| Sum of electronic and thermal Energies=      | -1478.116485                |            |             |
| Sum of electronic and thermal Enthalpies=    | -1478.115541                |            |             |
| Sum of electronic and thermal Free Energies= | -1478.214155                |            |             |
| Ni                                           | -2.30827100                 | 3.48010000 | -1.61908900 |
| N                                            | -0.84764600                 | 2.21650700 | -0.99659700 |
| N                                            | -3.55392400                 | 2.04146100 | -0.89946000 |
| C                                            | 0.55011000                  | 2.48592700 | -1.06325500 |
| C                                            | 1.15915300                  | 2.42111000 | -2.33100700 |
| C                                            | 1.24032400                  | 2.90771700 | 0.09054500  |
| C                                            | 2.51507300                  | 2.74511000 | -2.42156100 |
| C                                            | 2.59406100                  | 3.23237200 | -0.05370900 |
| C                                            | 3.22973300                  | 3.14561600 | -1.29219200 |
| H                                            | 3.01022300                  | 2.68731900 | -3.38677700 |
| H                                            | 3.14957100                  | 3.56790900 | 0.81767300  |
| H                                            | 4.28095100                  | 3.40286100 | -1.37962700 |
| C                                            | -4.97820400                 | 2.10752200 | -0.87967100 |
| C                                            | -5.64410100                 | 1.97699400 | -2.11353400 |
| C                                            | -5.65660300                 | 2.38995000 | 0.32252500  |
| C                                            | -7.03797300                 | 2.06930800 | -2.11691900 |
| C                                            | -7.05176100                 | 2.48492600 | 0.26558300  |
| C                                            | -7.73921300                 | 2.31538400 | -0.93608300 |
| H                                            | -7.57448600                 | 1.95282500 | -3.05437500 |
| H                                            | -7.60067600                 | 2.70758200 | 1.17643900  |
| H                                            | -8.82208200                 | 2.39232800 | -0.95528100 |
| C                                            | 0.54653100                  | 3.03611600 | 1.42621900  |
| H                                            | 0.37974500                  | 2.05820500 | 1.89420500  |
| H                                            | 1.14731000                  | 3.63305500 | 2.11726200  |
| H                                            | -0.43220800                 | 3.51932000 | 1.32557400  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 0.36308800  | 1.98974300  | -3.53802100 |
| H | -0.00804800 | 0.96295500  | -3.43430800 |
| H | -0.51911400 | 2.63015700  | -3.68721700 |
| H | 0.96542800  | 2.04207900  | -4.44854400 |
| C | -4.91411400 | 2.61704900  | 1.61821700  |
| H | -4.56433400 | 1.67598400  | 2.06015200  |
| H | -4.03401000 | 3.25331900  | 1.46890200  |
| H | -5.56097600 | 3.10407200  | 2.35251900  |
| C | -4.86243200 | 1.72500600  | -3.37950600 |
| H | -4.12695200 | 2.52409200  | -3.56127100 |
| H | -4.30070200 | 0.78426200  | -3.33292900 |
| H | -5.52179700 | 1.68340900  | -4.25022400 |
| C | -2.87269800 | 1.09954000  | -0.34012500 |
| C | -1.35987600 | 1.20111600  | -0.38892700 |
| C | -0.45274500 | 5.93820200  | -2.39018600 |
| H | 0.51351700  | 6.44755800  | -2.46432300 |
| H | -0.30502300 | 4.92293500  | -2.79032500 |
| H | -1.16349700 | 6.45759700  | -3.04373300 |
| C | -2.34285700 | 5.27355200  | -0.80014500 |
| H | -2.67462400 | 5.17374500  | 0.23932600  |
| H | -3.11235400 | 5.81295100  | -1.37569400 |
| C | -0.95946300 | 5.89747300  | -0.94212200 |
| H | -0.98465000 | 6.92415300  | -0.54321800 |
| H | -0.23893800 | 5.34905000  | -0.32237000 |
| C | -3.20116200 | -0.14386700 | 0.35215500  |
| C | -4.37669800 | -0.79858400 | 0.67874800  |
| C | -1.95330000 | -0.74220300 | 0.68533000  |
| C | -4.28795500 | -2.05025500 | 1.33920600  |
| H | -5.34564800 | -0.37249000 | 0.44308700  |
| C | -1.84676700 | -1.98403100 | 1.33871900  |
| C | -0.82226500 | 0.02223700  | 0.28291200  |
| C | -3.07106600 | -2.63168500 | 1.66491300  |
| H | -5.20691800 | -2.56671100 | 1.59775200  |
| C | -0.52696400 | -2.45104000 | 1.59337700  |
| C | 0.45050600  | -0.45817300 | 0.54031800  |
| H | -3.04904900 | -3.59179300 | 2.17293200  |
| C | 0.57619100  | -1.70581700 | 1.20209300  |
| H | -0.38508700 | -3.40232800 | 2.09866800  |
| H | 1.33459300  | 0.09873600  | 0.24982300  |
| H | 1.57158400  | -2.08664900 | 1.40755100  |

UB3LYP-D3/BSII(SMD)//B3LYP-D3/BSI

HF=-1480.7310112

**<sup>1</sup>D**



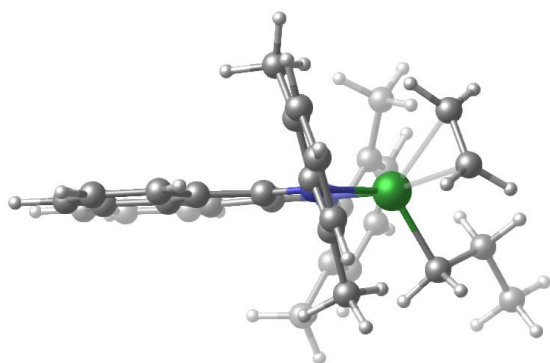
|                                              |                             |            |             |
|----------------------------------------------|-----------------------------|------------|-------------|
| Zero-point correction=                       | 0.597459 (Hartree/Particle) |            |             |
| Thermal correction to Energy=                | 0.632457                    |            |             |
| Thermal correction to Enthalpy=              | 0.633401                    |            |             |
| Thermal correction to Gibbs Free Energy=     | 0.530500                    |            |             |
| Sum of electronic and zero-point Energies=   | -1556.719924                |            |             |
| Sum of electronic and thermal Energies=      | -1556.684926                |            |             |
| Sum of electronic and thermal Enthalpies=    | -1556.683982                |            |             |
| Sum of electronic and thermal Free Energies= | -1556.786883                |            |             |
| Ni                                           | -2.21378700                 | 3.49860000 | -1.65330400 |
| N                                            | -0.83010900                 | 2.21088400 | -0.96711900 |
| N                                            | -3.50706100                 | 2.11084700 | -0.64586300 |
| C                                            | 0.59332000                  | 2.29053900 | -1.12644000 |
| C                                            | 1.18301300                  | 1.64330000 | -2.22450700 |
| C                                            | 1.32919200                  | 3.03887900 | -0.19375600 |
| C                                            | 2.57107100                  | 1.74590600 | -2.36607700 |
| C                                            | 2.71424200                  | 3.11459000 | -0.37529300 |
| C                                            | 3.33180100                  | 2.47217000 | -1.44912600 |
| H                                            | 3.05445800                  | 1.25484700 | -3.20612000 |
| H                                            | 3.30945700                  | 3.68622600 | 0.33145500  |
| H                                            | 4.40780200                  | 2.54421000 | -1.57601000 |
| C                                            | -4.93104300                 | 2.12916800 | -0.52810200 |
| C                                            | -5.68461800                 | 1.65751200 | -1.61896500 |
| C                                            | -5.52444700                 | 2.66514900 | 0.62925500  |
| C                                            | -7.07840600                 | 1.73384800 | -1.53026400 |
| C                                            | -6.92260100                 | 2.72544100 | 0.67007700  |
| C                                            | -7.69452900                 | 2.26591600 | -0.39707700 |
| H                                            | -7.68155800                 | 1.37216000 | -2.35852100 |
| H                                            | -7.40645500                 | 3.13901200 | 1.55076900  |
| H                                            | -8.77751300                 | 2.32448800 | -0.34637300 |
| C                                            | 0.63818300                  | 3.70840400 | 0.96876700  |
| H                                            | 0.26291100                  | 2.96970700 | 1.68900300  |
| H                                            | 1.32030300                  | 4.37591800 | 1.50165900  |
| H                                            | -0.22699300                 | 4.29430400 | 0.63406600  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 0.33503400  | 0.85870200  | -3.19498500 |
| H | -0.51004000 | 1.45747300  | -3.55864500 |
| H | 0.92154900  | 0.53423100  | -4.05837000 |
| H | -0.08947400 | -0.03655600 | -2.72261800 |
| C | -4.68342000 | 3.12015300  | 1.79927900  |
| H | -4.28369200 | 2.26189000  | 2.35476500  |
| H | -3.82091700 | 3.71706700  | 1.48036100  |
| H | -5.27401400 | 3.71921700  | 2.49739600  |
| C | -4.99079100 | 1.05631900  | -2.81778400 |
| H | -4.17421600 | 1.69748000  | -3.17486000 |
| H | -4.53982600 | 0.08689400  | -2.56948700 |
| H | -5.69067800 | 0.89757900  | -3.64244200 |
| C | -2.81350900 | 1.18341200  | -0.08860900 |
| C | -1.31993500 | 1.24610200  | -0.26217300 |
| C | -0.83433700 | 4.56255000  | -2.51836300 |
| H | -0.27994000 | 4.96702300  | -1.65848900 |
| H | -0.21218600 | 3.78646700  | -2.98002900 |
| C | -3.98343500 | 4.64023600  | -2.52480600 |
| H | -4.77360900 | 3.89626800  | -2.53697400 |
| H | -3.63068000 | 5.00299000  | -3.48271500 |
| C | -3.60634400 | 5.22425000  | -1.35131000 |
| H | -2.94090800 | 6.08129500  | -1.32230500 |
| H | -4.09344300 | 4.94814300  | -0.41972700 |
| C | -1.13656400 | 5.64879800  | -3.54099900 |
| H | -1.66371700 | 5.22040500  | -4.40356600 |
| H | -1.78615900 | 6.42872300  | -3.12416700 |
| C | 0.16403000  | 6.30896900  | -4.03590700 |
| H | -0.05003600 | 7.08126600  | -4.78318400 |
| H | 0.70465800  | 6.77898100  | -3.20626500 |
| H | 0.83033400  | 5.56884300  | -4.49364100 |
| C | -3.11313000 | 0.00028300  | 0.71828500  |
| C | -4.26997200 | -0.59058400 | 1.19565400  |
| C | -1.85255700 | -0.59195000 | 1.00999800  |
| C | -4.14945300 | -1.77604500 | 1.96556300  |
| H | -5.24743000 | -0.16664400 | 0.99373600  |
| C | -1.71495700 | -1.76620500 | 1.77326900  |
| C | -0.74365100 | 0.11093000  | 0.45582000  |
| C | -2.92039500 | -2.35197300 | 2.25164400  |
| H | -5.05331900 | -2.24431700 | 2.34234800  |
| C | -0.38619300 | -2.23226100 | 1.97760800  |
| C | 0.53863700  | -0.36687400 | 0.67070200  |
| H | -2.87374400 | -3.25978800 | 2.84674900  |
| C | 0.69437700  | -1.54769200 | 1.44067800  |
| H | -0.21977600 | -3.13403200 | 2.56040100  |

|   |            |             |            |
|---|------------|-------------|------------|
| H | 1.40786600 | 0.13884200  | 0.26638600 |
| H | 1.69738400 | -1.92551900 | 1.61220900 |

UB3LYP-D3/BSII(SMD)/B3LYP-D3/BSI  
HF=-1559.3733182

**<sup>3</sup>D**



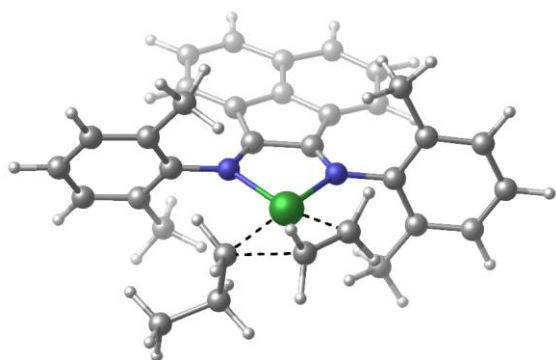
|                                              |                             |            |             |
|----------------------------------------------|-----------------------------|------------|-------------|
| Zero-point correction=                       | 0.594305 (Hartree/Particle) |            |             |
| Thermal correction to Energy=                | 0.630127                    |            |             |
| Thermal correction to Enthalpy=              | 0.631071                    |            |             |
| Thermal correction to Gibbs Free Energy=     | 0.525639                    |            |             |
| Sum of electronic and zero-point Energies=   | -1556.712470                |            |             |
| Sum of electronic and thermal Energies=      | -1556.676649                |            |             |
| Sum of electronic and thermal Enthalpies=    | -1556.675705                |            |             |
| Sum of electronic and thermal Free Energies= | -1556.781137                |            |             |
| Ni                                           | -1.83851000                 | 3.70519300 | -1.32615500 |
| N                                            | -0.46545000                 | 2.28703800 | -0.75438800 |
| N                                            | -3.16900400                 | 2.19392000 | -0.85136600 |
| C                                            | 0.94160300                  | 2.49095900 | -0.62521300 |
| C                                            | 1.70605000                  | 2.57063500 | -1.80531700 |
| C                                            | 1.50028000                  | 2.69671800 | 0.65212500  |
| C                                            | 3.07070400                  | 2.84919700 | -1.68310100 |
| C                                            | 2.86933900                  | 2.98200700 | 0.72184700  |
| C                                            | 3.65017700                  | 3.05635900 | -0.43086700 |
| H                                            | 3.68093100                  | 2.90392000 | -2.58038400 |
| H                                            | 3.32258500                  | 3.15034600 | 1.69500900  |
| H                                            | 4.70990700                  | 3.27993400 | -0.35383700 |
| C                                            | -4.57023200                 | 2.24757000 | -1.08734600 |
| C                                            | -5.15531600                 | 1.52991900 | -2.15252700 |
| C                                            | -5.31384700                 | 3.14734400 | -0.29332400 |
| C                                            | -6.52607000                 | 1.71438300 | -2.37891600 |
| C                                            | -6.67923900                 | 3.28157900 | -0.54723000 |
| C                                            | -7.28504100                 | 2.56980400 | -1.58418800 |
| H                                            | -6.99688800                 | 1.17958300 | -3.19945500 |
| H                                            | -7.26956200                 | 3.95533600 | 0.06744600  |
| H                                            | -8.34605600                 | 2.69270200 | -1.77931900 |
| C                                            | 0.66774300                  | 2.59875400 | 1.90973400  |
| H                                            | 1.17434700                  | 3.08087500 | 2.75012400  |
| H                                            | -0.31697200                 | 3.06548600 | 1.79199800  |
| H                                            | 0.48898200                  | 1.55262900 | 2.18832300  |
| C                                            | 1.06261500                  | 2.32438300 | -3.14749500 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 0.72998300  | 1.28301000  | -3.24355700 |
| H | 0.17254300  | 2.94902300  | -3.28395000 |
| H | 1.76025400  | 2.53037300  | -3.96356900 |
| C | -4.63762200 | 3.93160500  | 0.80390800  |
| H | -4.15833400 | 3.27642200  | 1.54047600  |
| H | -3.84666400 | 4.57923500  | 0.39741300  |
| H | -5.35133100 | 4.57150500  | 1.32937500  |
| C | -4.36882200 | 0.60188400  | -3.04896900 |
| H | -3.32404000 | 0.90816700  | -3.15298700 |
| H | -4.36615000 | -0.42398300 | -2.66056700 |
| H | -4.81134300 | 0.57162300  | -4.04872000 |
| C | -2.54496000 | 1.11610000  | -0.50738800 |
| C | -1.04091000 | 1.18302400  | -0.41367800 |
| C | -2.42439900 | 3.97265000  | -3.24670300 |
| H | -1.60514300 | 4.34648800  | -3.86841100 |
| H | -2.75783800 | 2.99555300  | -3.60765400 |
| C | -0.90225500 | 5.55334800  | -0.20406300 |
| H | -0.37747700 | 5.02963500  | 0.59035200  |
| H | -1.77360000 | 6.13965000  | 0.07977500  |
| C | -0.42070800 | 5.57037400  | -1.47028900 |
| H | -0.88127600 | 6.17659900  | -2.24394900 |
| H | 0.50608100  | 5.06307500  | -1.72675100 |
| C | -3.56870700 | 4.96816000  | -3.09467700 |
| H | -4.24294100 | 4.67224000  | -2.27744900 |
| H | -3.17646700 | 5.96057200  | -2.83381500 |
| C | -4.41899100 | 5.07700800  | -4.37796700 |
| H | -5.22041100 | 5.81403800  | -4.25282300 |
| H | -3.80222900 | 5.37901100  | -5.23126000 |
| H | -4.87758900 | 4.11010200  | -4.61259400 |
| C | -0.57044100 | -0.12190600 | 0.04750700  |
| C | 0.67026600  | -0.67385000 | 0.31627500  |
| C | -1.73913900 | -0.91579700 | 0.21514200  |
| C | 0.72570100  | -2.02103800 | 0.75645400  |
| H | 1.58257100  | -0.09871700 | 0.20239300  |
| C | -1.70391400 | -2.24845600 | 0.66621100  |
| C | -2.94607300 | -0.23302300 | -0.10602700 |
| C | -0.41534500 | -2.79000200 | 0.93274600  |
| H | 1.69640800  | -2.45884300 | 0.96694900  |
| C | -2.96068400 | -2.90032500 | 0.80771100  |
| C | -4.15411800 | -0.89081300 | 0.04853100  |
| H | -0.32818100 | -3.81599900 | 1.27947800  |
| C | -4.13905500 | -2.23156300 | 0.51181900  |
| H | -2.99380000 | -3.93004200 | 1.15263400  |
| H | -5.09627800 | -0.40460500 | -0.17931700 |

|   |             |             |            |
|---|-------------|-------------|------------|
| H | -5.08568300 | -2.74891800 | 0.63241500 |
|---|-------------|-------------|------------|

UB3LYP-D3/BSII(SMD)//B3LYP-D3/BSI  
HF=-1559.3694633

# <sup>1</sup>TS2



|                                              |                             |
|----------------------------------------------|-----------------------------|
| Zero-point correction=                       | 0.597130 (Hartree/Particle) |
| Thermal correction to Energy=                | 0.631214                    |
| Thermal correction to Enthalpy=              | 0.632158                    |
| Thermal correction to Gibbs Free Energy=     | 0.531954                    |
| Sum of electronic and zero-point Energies=   | -1556.703600                |
| Sum of electronic and thermal Energies=      | -1556.669515                |
| Sum of electronic and thermal Enthalpies=    | -1556.668571                |
| Sum of electronic and thermal Free Energies= | -1556.768775                |

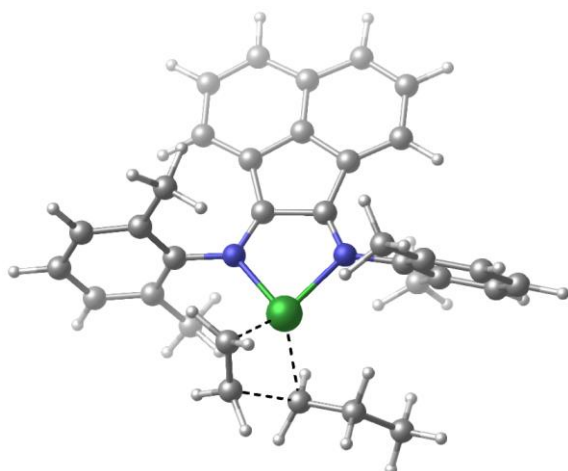
|    |             |            |             |
|----|-------------|------------|-------------|
| Ni | -2.37273300 | 3.80563000 | -1.19304200 |
| N  | -0.84118700 | 2.42774800 | -0.78523300 |
| N  | -3.48907800 | 2.33101300 | -0.50759600 |
| C  | 0.57329600  | 2.57379000 | -0.93380500 |
| C  | 1.24750500  | 1.92128800 | -1.98368500 |
| C  | 1.23087800  | 3.43956100 | -0.03701500 |
| C  | 2.62038300  | 2.16234800 | -2.11861400 |
| C  | 2.60321400  | 3.64391200 | -0.20939600 |
| C  | 3.29440300  | 3.01437100 | -1.24419600 |
| H  | 3.16223100  | 1.67452300 | -2.92440100 |
| H  | 3.12998900  | 4.30221800 | 0.47580400  |
| H  | 4.35862500  | 3.18869100 | -1.37068600 |
| C  | -4.92117700 | 2.31683600 | -0.40556900 |
| C  | -5.66211500 | 2.02838200 | -1.56324800 |
| C  | -5.52018900 | 2.62793800 | 0.82586800  |
| C  | -7.05718400 | 2.03513000 | -1.45930400 |
| C  | -6.91879600 | 2.62519500 | 0.88253200  |
| C  | -7.68227600 | 2.32792700 | -0.24670000 |
| H  | -7.65407000 | 1.81157000 | -2.33927200 |
| H  | -7.40910400 | 2.86317200 | 1.82254300  |
| H  | -8.76624400 | 2.33231700 | -0.18355800 |
| C  | 0.47069500  | 4.08440500 | 1.09659200  |
| H  | 0.11878000  | 3.33423600 | 1.81595300  |
| H  | 1.09777100  | 4.79931300 | 1.63567600  |
| H  | -0.42198600 | 4.61280800 | 0.73614700  |
| C  | 0.54179300  | 0.96704000 | -2.91818500 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -0.47068500 | 1.30055000  | -3.16388300 |
| H | 1.09810400  | 0.85686900  | -3.85291000 |
| H | 0.45073600  | -0.02980900 | -2.46816800 |
| C | -4.67691700 | 2.93281200  | 2.04037600  |
| H | -4.16663700 | 2.03324200  | 2.40803300  |
| H | -3.89668800 | 3.67007300  | 1.81383500  |
| H | -5.29025000 | 3.32342500  | 2.85653100  |
| C | -4.95688400 | 1.71215900  | -2.85926100 |
| H | -4.22088800 | 2.48806900  | -3.10977700 |
| H | -4.40517300 | 0.76555700  | -2.79532500 |
| H | -5.66660100 | 1.63086200  | -3.68667400 |
| C | -2.82382500 | 1.28173900  | -0.15956400 |
| C | -1.33162400 | 1.34590600  | -0.28713000 |
| C | -1.05259800 | 5.04878600  | -2.23865800 |
| H | -0.86630300 | 6.11220900  | -2.37513500 |
| H | -0.25720800 | 4.70555800  | -1.57480100 |
| C | -3.90650200 | 5.01483900  | -1.21113800 |
| H | -4.23287100 | 5.04897900  | -0.17256900 |
| H | -4.65036100 | 4.64086100  | -1.91258000 |
| C | -2.91560000 | 5.90823700  | -1.66123300 |
| H | -2.97068300 | 6.26186500  | -2.68521700 |
| H | -2.47953900 | 6.61202500  | -0.95785700 |
| C | -1.07461800 | 4.34203700  | -3.58992700 |
| H | -1.25082600 | 3.26591600  | -3.47271900 |
| H | -1.90919000 | 4.72481600  | -4.19137000 |
| C | 0.24876300  | 4.54933100  | -4.34818000 |
| H | 0.22053000  | 4.04391000  | -5.31974500 |
| H | 0.43526600  | 5.61440700  | -4.52643200 |
| H | 1.09199200  | 4.14699300  | -3.77731900 |
| C | -3.17095700 | -0.02923500 | 0.38432100  |
| C | -4.35027900 | -0.68018100 | 0.70456900  |
| C | -1.92654700 | -0.68691200 | 0.60525900  |
| C | -4.26858600 | -1.98874700 | 1.24587700  |
| H | -5.31603200 | -0.21185600 | 0.55218700  |
| C | -1.82844800 | -1.98088700 | 1.14993100  |
| C | -0.79176300 | 0.08754700  | 0.23076900  |
| C | -3.05650100 | -2.62581300 | 1.46752100  |
| H | -5.19030200 | -2.50417000 | 1.49691800  |
| C | -0.51271600 | -2.49399300 | 1.32323700  |
| C | 0.47618900  | -0.43670700 | 0.41260500  |
| H | -3.04070900 | -3.62713900 | 1.88895400  |
| C | 0.59367800  | -1.73735800 | 0.96658600  |
| H | -0.37714300 | -3.48811300 | 1.74013800  |
| H | 1.36448300  | 0.12235500  | 0.14044800  |

|   |            |             |            |
|---|------------|-------------|------------|
| H | 1.58654800 | -2.15141100 | 1.11163000 |
|---|------------|-------------|------------|

UB3LYP-D3/BSII(SMD)//B3LYP-D3/BSI  
HF=-1559.3549407

### <sup>3</sup>TS2



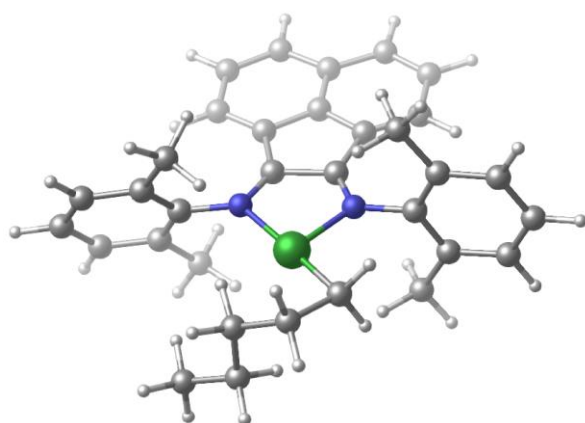
|                                              |                             |            |             |
|----------------------------------------------|-----------------------------|------------|-------------|
| Zero-point correction=                       | 0.594768 (Hartree/Particle) |            |             |
| Thermal correction to Energy=                | 0.629524                    |            |             |
| Thermal correction to Enthalpy=              | 0.630468                    |            |             |
| Thermal correction to Gibbs Free Energy=     | 0.526913                    |            |             |
| Sum of electronic and zero-point Energies=   | -1556.683727                |            |             |
| Sum of electronic and thermal Energies=      | -1556.648971                |            |             |
| Sum of electronic and thermal Enthalpies=    | -1556.648027                |            |             |
| Sum of electronic and thermal Free Energies= | -1556.751582                |            |             |
| Ni                                           | -1.86219000                 | 3.71932300 | -1.27154300 |
| N                                            | -0.45387200                 | 2.24682600 | -0.78801600 |
| N                                            | -3.15625200                 | 2.19457300 | -0.86034700 |
| C                                            | 0.94896000                  | 2.45526100 | -0.63595600 |
| C                                            | 1.73679600                  | 2.51741200 | -1.80027100 |
| C                                            | 1.48071100                  | 2.68598400 | 0.64878500  |
| C                                            | 3.10150300                  | 2.78191100 | -1.65466200 |
| C                                            | 2.85038200                  | 2.96025400 | 0.74261300  |
| C                                            | 3.65713400                  | 3.00209600 | -0.39395400 |
| H                                            | 3.73062500                  | 2.81749800 | -2.53984800 |
| H                                            | 3.28302300                  | 3.14818600 | 1.72150300  |
| H                                            | 4.71761300                  | 3.21468900 | -0.29816000 |
| C                                            | -4.56757700                 | 2.26995300 | -1.05995000 |
| C                                            | -5.14778100                 | 1.65473800 | -2.18729300 |
| C                                            | -5.31032400                 | 3.07081700 | -0.17128000 |
| C                                            | -6.52134300                 | 1.83369800 | -2.38714400 |
| C                                            | -6.68093300                 | 3.21154800 | -0.40738900 |
| C                                            | -7.28494300                 | 2.59729900 | -1.50470200 |
| H                                            | -6.99107800                 | 1.37439600 | -3.25265600 |
| H                                            | -7.27599200                 | 3.81181700 | 0.27525600  |
| H                                            | -8.34939400                 | 2.72279700 | -1.67844900 |
| C                                            | 0.60817400                  | 2.65070300 | 1.88191000  |
| H                                            | 1.12232400                  | 3.10391300 | 2.73358400  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -0.33347800 | 3.19021600  | 1.72571300  |
| H | 0.34747100  | 1.62258900  | 2.16224100  |
| C | 1.11612600  | 2.27483900  | -3.15383500 |
| H | 0.69863900  | 1.26331800  | -3.23110900 |
| H | 0.29093100  | 2.97250200  | -3.33896100 |
| H | 1.85153300  | 2.39728600  | -3.95340200 |
| C | -4.63665400 | 3.73266800  | 1.00569500  |
| H | -4.21377100 | 2.99339200  | 1.69677800  |
| H | -3.80113800 | 4.36936700  | 0.68268800  |
| H | -5.34058500 | 4.35504200  | 1.56433500  |
| C | -4.31951000 | 0.85243400  | -3.16332600 |
| H | -3.38256800 | 1.36456900  | -3.41317200 |
| H | -4.04924700 | -0.12981800 | -2.75710600 |
| H | -4.87032500 | 0.68458300  | -4.09264000 |
| C | -2.54591500 | 1.11037200  | -0.51152000 |
| C | -1.03996500 | 1.16016900  | -0.41571800 |
| C | -2.00747200 | 4.64505100  | -3.31727000 |
| H | -1.44286800 | 5.17836400  | -4.07956900 |
| H | -1.91649300 | 3.56757700  | -3.52201900 |
| C | -0.95413400 | 5.41209800  | -0.47034700 |
| H | -0.13679400 | 4.99013800  | 0.10861900  |
| H | -1.67118000 | 6.01949700  | 0.07828700  |
| C | -0.77839600 | 5.63729200  | -1.86797300 |
| H | -1.23239100 | 6.52905100  | -2.28824600 |
| H | 0.17580000  | 5.36176500  | -2.31010600 |
| C | -3.44331600 | 5.12368800  | -3.15784900 |
| H | -3.89927900 | 4.75506400  | -2.22223600 |
| H | -3.45549800 | 6.21737900  | -3.08077100 |
| C | -4.33702100 | 4.66287400  | -4.32186300 |
| H | -5.36078400 | 5.02818800  | -4.18870900 |
| H | -3.95907300 | 5.03841200  | -5.27879800 |
| H | -4.37528400 | 3.56966500  | -4.37333300 |
| C | -0.59236700 | -0.13866100 | 0.08779000  |
| C | 0.63652100  | -0.69949900 | 0.38741500  |
| C | -1.77205800 | -0.91848600 | 0.24510800  |
| C | 0.66932000  | -2.04169500 | 0.84668500  |
| H | 1.55652400  | -0.13478400 | 0.28309800  |
| C | -1.75918200 | -2.24792400 | 0.70603800  |
| C | -2.96719200 | -0.22745800 | -0.10371900 |
| C | -0.48176600 | -2.79873800 | 1.00643400  |
| H | 1.63123700  | -2.48557100 | 1.08329800  |
| C | -3.02520700 | -2.88731700 | 0.82054400  |
| C | -4.18504800 | -0.87447400 | 0.01929500  |
| H | -0.41157800 | -3.82180000 | 1.36539500  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -4.19128400 | -2.21294700 | 0.48811900  |
| H | -3.07571900 | -3.91410700 | 1.17219000  |
| H | -5.11610700 | -0.38151900 | -0.23826900 |
| H | -5.14385500 | -2.72417900 | 0.58568100  |

UB3LYP-D3/BSII(SMD)//B3LYP-D3/BSI  
HF=-1559.3383153

<sup>1</sup>E



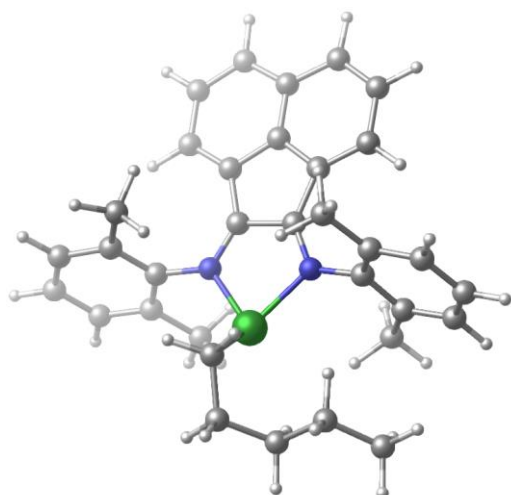
|                                              |                             |            |             |
|----------------------------------------------|-----------------------------|------------|-------------|
| Zero-point correction=                       | 0.598334 (Hartree/Particle) |            |             |
| Thermal correction to Energy=                | 0.632599                    |            |             |
| Thermal correction to Enthalpy=              | 0.633543                    |            |             |
| Thermal correction to Gibbs Free Energy=     | 0.532267                    |            |             |
| Sum of electronic and zero-point Energies=   | -1556.731923                |            |             |
| Sum of electronic and thermal Energies=      | -1556.697659                |            |             |
| Sum of electronic and thermal Enthalpies=    | -1556.696714                |            |             |
| Sum of electronic and thermal Free Energies= | -1556.797990                |            |             |
| Ni                                           | -2.27722700                 | 3.63243800 | -1.08386600 |
| N                                            | -0.75906800                 | 2.31783800 | -0.65720100 |
| N                                            | -3.41634900                 | 2.24402900 | -0.47321300 |
| C                                            | 0.64014200                  | 2.50134600 | -0.85837700 |
| C                                            | 1.29405900                  | 1.83726600 | -1.91553300 |
| C                                            | 1.29220500                  | 3.44153300 | -0.03731700 |
| C                                            | 2.65115600                  | 2.11759000 | -2.11240700 |
| C                                            | 2.64989600                  | 3.68032200 | -0.26791700 |
| C                                            | 3.32719100                  | 3.02328600 | -1.29527700 |
| H                                            | 3.17624300                  | 1.62651200 | -2.92706900 |
| H                                            | 3.17711200                  | 4.38907700 | 0.36467000  |
| H                                            | 4.37999900                  | 3.22586900 | -1.46693300 |
| C                                            | -4.84783700                 | 2.27932600 | -0.40608700 |
| C                                            | -5.57874200                 | 1.85881200 | -1.52832800 |
| C                                            | -5.44938800                 | 2.76783500 | 0.76451400  |
| C                                            | -6.97417700                 | 1.90989400 | -1.44326000 |
| C                                            | -6.84727900                 | 2.80093700 | 0.80438900  |
| C                                            | -7.60408700                 | 2.37152400 | -0.28671200 |
| H                                            | -7.56772900                 | 1.58975100 | -2.29511400 |
| H                                            | -7.34206100                 | 3.17252900 | 1.69743600  |
| H                                            | -8.68833300                 | 2.40649000 | -0.23938400 |
| C                                            | 0.54690000                  | 4.12833800 | 1.08135700  |
| H                                            | 0.22407200                  | 3.41261500 | 1.84749600  |
| H                                            | 1.17131300                  | 4.88303900 | 1.56662900  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -0.36319200 | 4.62522100  | 0.71780600  |
| C | 0.55400400  | 0.89341200  | -2.83424600 |
| H | -0.40815300 | 1.31454900  | -3.14932200 |
| H | 1.14190400  | 0.68943800  | -3.73290400 |
| H | 0.34409800  | -0.06831000 | -2.35090800 |
| C | -4.59986500 | 3.23049900  | 1.92175300  |
| H | -4.05737500 | 2.39471900  | 2.38210600  |
| H | -3.84469000 | 3.95477600  | 1.58892200  |
| H | -5.21014300 | 3.70060400  | 2.69710900  |
| C | -4.86694600 | 1.36722300  | -2.76427200 |
| H | -4.10020800 | 2.08302200  | -3.08767300 |
| H | -4.35532000 | 0.41349000  | -2.58103800 |
| H | -5.56741900 | 1.21667000  | -3.58968300 |
| C | -2.76874100 | 1.18550900  | -0.10903100 |
| C | -1.26922100 | 1.22046100  | -0.21539900 |
| C | -1.35870700 | 5.56078000  | -2.26419700 |
| H | -0.61655600 | 6.35822000  | -2.13346500 |
| H | -0.89672500 | 4.77033500  | -1.60733800 |
| C | -3.65204900 | 4.87374400  | -1.50101000 |
| H | -4.35582500 | 4.98657000  | -0.67204700 |
| H | -4.17898500 | 4.50609600  | -2.38910600 |
| C | -2.73763500 | 6.06198200  | -1.74569600 |
| H | -3.14359900 | 6.77279400  | -2.47860100 |
| H | -2.58459500 | 6.61364800  | -0.81185800 |
| C | -1.35193000 | 5.07067400  | -3.71810700 |
| H | -2.07684600 | 4.25414500  | -3.83872800 |
| H | -1.70876900 | 5.89267300  | -4.35236100 |
| C | 0.03294900  | 4.61012400  | -4.18073200 |
| H | 0.00753700  | 4.26073300  | -5.21791000 |
| H | 0.75956600  | 5.42874000  | -4.12052700 |
| H | 0.40778400  | 3.79171200  | -3.55593900 |
| C | -3.15081200 | -0.11589700 | 0.42392900  |
| C | -4.34862000 | -0.73381500 | 0.74145900  |
| C | -1.92417500 | -0.81089100 | 0.63470700  |
| C | -4.30294200 | -2.04870700 | 1.27061600  |
| H | -5.29980200 | -0.23457000 | 0.59414700  |
| C | -1.86238700 | -2.11272100 | 1.16444900  |
| C | -0.76808100 | -0.06493400 | 0.26760400  |
| C | -3.10857600 | -2.72356700 | 1.47990300  |
| H | -5.23798700 | -2.53974000 | 1.52101800  |
| C | -0.56114000 | -2.66613000 | 1.32565500  |
| C | 0.48472200  | -0.62771700 | 0.43613500  |
| H | -3.12140100 | -3.72959600 | 1.89008400  |
| C | 0.56601300  | -1.93850700 | 0.97252800  |

|   |             |             |            |
|---|-------------|-------------|------------|
| H | -0.45300100 | -3.66876700 | 1.72988900 |
| H | 1.38667400  | -0.08988200 | 0.16458500 |
| H | 1.54651500  | -2.38424500 | 1.10706000 |

UB3LYP-D3/BSII(SMD)//B3LYP-D3/BSI  
HF=-1559.3858533

<sup>3</sup>E



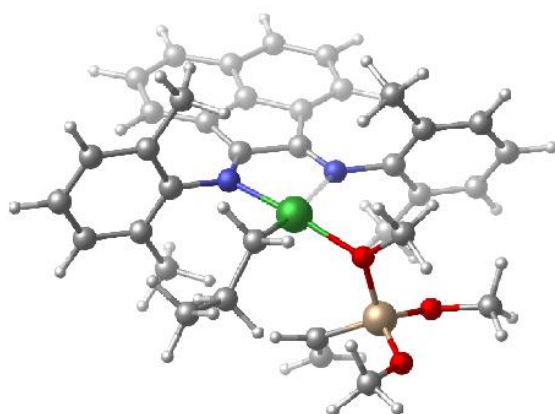
|                                              |                             |            |             |
|----------------------------------------------|-----------------------------|------------|-------------|
| Zero-point correction=                       | 0.596923 (Hartree/Particle) |            |             |
| Thermal correction to Energy=                | 0.631765                    |            |             |
| Thermal correction to Enthalpy=              | 0.632709                    |            |             |
| Thermal correction to Gibbs Free Energy=     | 0.527924                    |            |             |
| Sum of electronic and zero-point Energies=   | -1556.724707                |            |             |
| Sum of electronic and thermal Energies=      | -1556.689865                |            |             |
| Sum of electronic and thermal Enthalpies=    | -1556.688921                |            |             |
| Sum of electronic and thermal Free Energies= | -1556.793706                |            |             |
| Ni                                           | -1.46058100                 | 3.28349300 | -1.76721300 |
| N                                            | -0.19946100                 | 1.94805500 | -0.90164300 |
| N                                            | -2.89269800                 | 1.94992400 | -1.21983900 |
| C                                            | 1.20899600                  | 2.11840100 | -0.76804500 |
| C                                            | 1.98266700                  | 2.00238600 | -1.93910300 |
| C                                            | 1.76285000                  | 2.49104500 | 0.47302900  |
| C                                            | 3.36139500                  | 2.20038000 | -1.83417100 |
| C                                            | 3.14723400                  | 2.69039700 | 0.52454300  |
| C                                            | 3.94250800                  | 2.53575400 | -0.61073600 |
| H                                            | 3.98079200                  | 2.09645600 | -2.72062300 |
| H                                            | 3.60091100                  | 2.98349900 | 1.46732300  |
| H                                            | 5.01469500                  | 2.69420500 | -0.54576900 |
| C                                            | -4.29583800                 | 2.10630200 | -1.42220300 |
| C                                            | -4.77836900                 | 1.94662100 | -2.73452900 |
| C                                            | -5.11925600                 | 2.51528900 | -0.35515000 |
| C                                            | -6.14321400                 | 2.14369800 | -2.95735600 |
| C                                            | -6.47665300                 | 2.71510600 | -0.63119800 |
| C                                            | -6.98891500                 | 2.52114800 | -1.91410200 |
| H                                            | -6.54027900                 | 2.01230700 | -3.95981300 |
| H                                            | -7.13423900                 | 3.03720400 | 0.17147700  |
| H                                            | -8.04593200                 | 2.68059500 | -2.10434700 |
| C                                            | 0.90037300                  | 2.70738700 | 1.69416300  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 1.44823200  | 3.26468900  | 2.45845200  |
| H | -0.00596100 | 3.27304300  | 1.44830200  |
| H | 0.58073700  | 1.75935600  | 2.14378900  |
| C | 1.32846000  | 1.65669500  | -3.25438300 |
| H | 0.82781500  | 0.68167900  | -3.21896800 |
| H | 0.55959600  | 2.39708600  | -3.52538100 |
| H | 2.05998200  | 1.63324600  | -4.06616600 |
| C | -4.55822200 | 2.76420500  | 1.02477400  |
| H | -4.32409700 | 1.82772000  | 1.54574600  |
| H | -3.63301600 | 3.35070800  | 0.97966000  |
| H | -5.27576700 | 3.31263800  | 1.64047400  |
| C | -3.83614700 | 1.57431700  | -3.85196400 |
| H | -3.03234900 | 2.31877000  | -3.95471100 |
| H | -3.35175300 | 0.60656100  | -3.67532100 |
| H | -4.35949300 | 1.52239800  | -4.81011000 |
| C | -2.37150200 | 0.98884200  | -0.53574900 |
| C | -0.86546300 | 0.98784400  | -0.35604400 |
| C | -2.49133500 | 5.75454400  | -3.29095900 |
| H | -2.41835800 | 6.52857100  | -4.06615600 |
| H | -2.15917700 | 4.81974100  | -3.78753700 |
| C | -1.51910700 | 5.10585800  | -0.98154300 |
| H | -0.65015700 | 5.21630600  | -0.32315400 |
| H | -2.43664600 | 5.13780200  | -0.38317400 |
| C | -1.52025200 | 6.09948200  | -2.14371100 |
| H | -1.78352000 | 7.09812800  | -1.75723000 |
| H | -0.50565300 | 6.18879500  | -2.55219100 |
| C | -3.95581400 | 5.59539000  | -2.86331500 |
| H | -4.04543400 | 4.77384200  | -2.14004800 |
| H | -4.27310000 | 6.50504900  | -2.33502000 |
| C | -4.89165400 | 5.32823800  | -4.04539900 |
| H | -5.92491400 | 5.19322300  | -3.71043700 |
| H | -4.87026300 | 6.15778900  | -4.76164300 |
| H | -4.59678500 | 4.41781700  | -4.58218800 |
| C | -0.52100700 | -0.20382700 | 0.41465500  |
| C | 0.66044800  | -0.76545300 | 0.86815700  |
| C | -1.75265300 | -0.87235100 | 0.66363600  |
| C | 0.59394800  | -1.99542200 | 1.57067600  |
| H | 1.61711300  | -0.28358300 | 0.69879100  |
| C | -1.83680200 | -2.09406900 | 1.35700400  |
| C | -2.89000500 | -0.20088200 | 0.13318700  |
| C | -0.60734200 | -2.64532800 | 1.81452200  |
| H | 1.51751400  | -2.43894800 | 1.92899400  |
| C | -3.14126800 | -2.63974700 | 1.51628200  |
| C | -4.14707500 | -0.75681600 | 0.29998500  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -0.61291500 | -3.58560600 | 2.35879100  |
| C | -4.25065600 | -1.98538200 | 1.00027500  |
| H | -3.26614300 | -3.57954200 | 2.04694500  |
| H | -5.03593100 | -0.27204200 | -0.08848600 |
| H | -5.23393200 | -2.42486300 | 1.13480800  |

UB3LYP-D3/BSII(SMD)//B3LYP-D3/BSI  
HF=-1559.3874592

<sup>1</sup>F



|                                              |                             |            |             |
|----------------------------------------------|-----------------------------|------------|-------------|
| Zero-point correction=                       | 0.717826 (Hartree/Particle) |            |             |
| Thermal correction to Energy=                | 0.763587                    |            |             |
| Thermal correction to Enthalpy=              | 0.764531                    |            |             |
| Thermal correction to Gibbs Free Energy=     | 0.638806                    |            |             |
| Sum of electronic and zero-point Energies=   | -2191.049821                |            |             |
| Sum of electronic and thermal Energies=      | -2191.004060                |            |             |
| Sum of electronic and thermal Enthalpies=    | -2191.003116                |            |             |
| Sum of electronic and thermal Free Energies= | -2191.128841                |            |             |
| Ni                                           | -2.56900100                 | 3.78533000 | -1.52736300 |
| N                                            | -0.99011000                 | 2.39770800 | -1.51135200 |
| N                                            | -3.45046800                 | 2.42062000 | -0.47629900 |
| C                                            | 0.24385500                  | 2.42901600 | -2.23244300 |
| C                                            | 0.17810600                  | 2.21266300 | -3.62215000 |
| C                                            | 1.45135100                  | 2.70118700 | -1.56777800 |
| C                                            | 1.36727800                  | 2.28613700 | -4.35460700 |
| C                                            | 2.61678800                  | 2.76141700 | -2.34146900 |
| C                                            | 2.58011600                  | 2.56063700 | -3.72082900 |
| H                                            | 1.33944100                  | 2.11549800 | -5.42752600 |
| H                                            | 3.56154300                  | 2.97642200 | -1.84936900 |
| H                                            | 3.49584300                  | 2.61572700 | -4.30205200 |
| C                                            | -4.76697500                 | 2.47811900 | 0.09283600  |
| C                                            | -5.84761200                 | 2.01648800 | -0.67629600 |
| C                                            | -4.91899100                 | 3.00545100 | 1.38560300  |
| C                                            | -7.12671500                 | 2.11145500 | -0.11752600 |
| C                                            | -6.21678200                 | 3.08299500 | 1.90303600  |
| C                                            | -7.31222300                 | 2.64407100 | 1.15864700  |
| H                                            | -7.98126300                 | 1.76401700 | -0.69160300 |
| H                                            | -6.36497100                 | 3.49328200 | 2.89823600  |
| H                                            | -8.31267600                 | 2.71630500 | 1.57462800  |
| C                                            | 1.49425100                  | 2.89303100 | -0.07302200 |
| H                                            | 1.45294600                  | 1.92882700 | 0.45048700  |
| H                                            | 2.41649100                  | 3.39720300 | 0.22711800  |

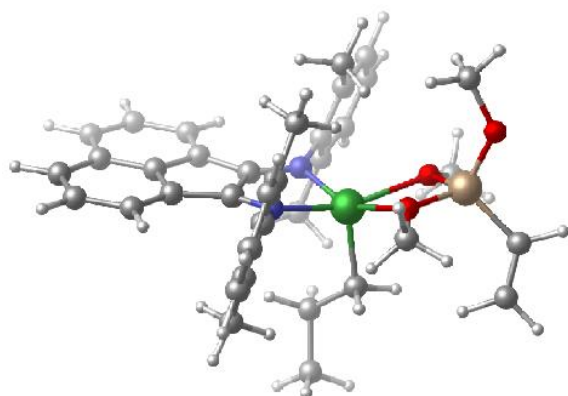
|    |             |            |             |
|----|-------------|------------|-------------|
| H  | 0.65205700  | 3.49445300 | 0.27679100  |
| C  | -1.13375900 | 1.85383300 | -4.27874000 |
| H  | -1.94393900 | 2.52224800 | -3.96224000 |
| H  | -1.05626900 | 1.89680700 | -5.36872000 |
| H  | -1.44574200 | 0.83742800 | -4.00557200 |
| C  | -3.71624500 | 3.43180300 | 2.19297500  |
| H  | -3.00039400 | 3.99500000 | 1.58479200  |
| H  | -4.01344600 | 4.05187900 | 3.04315500  |
| H  | -3.17899500 | 2.55990000 | 2.58929200  |
| C  | -5.61290900 | 1.40398000 | -2.03530000 |
| H  | -4.96132100 | 2.03464900 | -2.65192800 |
| H  | -5.11912000 | 0.42729700 | -1.94678200 |
| H  | -6.55520100 | 1.25430400 | -2.56887800 |
| C  | -2.70306000 | 1.39789500 | -0.21451700 |
| C  | -1.33369900 | 1.36498500 | -0.82696400 |
| C  | -1.05747300 | 5.93325700 | 0.41303700  |
| H  | -2.12118000 | 5.91500600 | 0.63819700  |
| C  | -0.18498000 | 5.80558900 | 1.42397400  |
| H  | 0.88955700  | 5.82613800 | 1.25885000  |
| C  | -4.15538400 | 4.85391300 | -1.79264800 |
| H  | -4.98537000 | 4.15139800 | -1.92030200 |
| H  | -3.98652100 | 5.36583400 | -2.75066400 |
| C  | -4.48142800 | 5.86257600 | -0.69891000 |
| H  | -4.48094300 | 5.37041800 | 0.28046500  |
| C  | -5.85407200 | 6.52313900 | -0.91079500 |
| H  | -6.64966800 | 5.76951300 | -0.88656600 |
| H  | -6.06374800 | 7.26288800 | -0.12939100 |
| H  | -5.90198000 | 7.03142700 | -1.88129300 |
| H  | -3.70961800 | 6.64045100 | -0.66448000 |
| H  | -0.51013900 | 5.67565300 | 2.45499400  |
| Si | -0.49894000 | 6.22571000 | -1.31961600 |
| O  | -0.68713400 | 7.73915300 | -1.93009500 |
| O  | 1.07986300  | 5.83585600 | -1.43048600 |
| O  | -1.46558400 | 5.21623900 | -2.31681300 |
| C  | -1.92243400 | 8.44510600 | -2.05026000 |
| H  | -1.72770600 | 9.36417100 | -2.60798200 |
| H  | -2.67222000 | 7.85194500 | -2.59021200 |
| H  | -2.32060500 | 8.70832500 | -1.06318800 |
| C  | 1.98167200  | 6.19793100 | -2.48087700 |
| H  | 2.99419500  | 6.18093400 | -2.07010400 |
| H  | 1.92063600  | 5.46555100 | -3.29294500 |
| H  | 1.76496200  | 7.20116100 | -2.86205500 |
| C  | -1.35614600 | 5.33408300 | -3.75699700 |
| H  | -0.56442000 | 4.67275400 | -4.11407400 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -2.31372500 | 5.04326000  | -4.19068800 |
| H | -1.13318100 | 6.36993800  | -4.02329200 |
| C | -3.71863700 | -1.68951700 | 1.83440100  |
| C | -2.55631500 | -2.41793000 | 1.62815800  |
| C | -1.49426900 | -1.88391300 | 0.84615000  |
| C | -1.69736600 | -0.59638300 | 0.31546500  |
| C | -2.89233400 | 0.15208400  | 0.52492600  |
| C | -3.91108200 | -0.39530900 | 1.28661600  |
| H | -0.04121600 | -3.49938200 | 0.91960000  |
| H | -4.51356400 | -2.12143100 | 2.43430200  |
| H | -2.45313600 | -3.40741100 | 2.06504300  |
| C | -0.25240700 | -2.50533300 | 0.53518900  |
| C | -0.73402000 | 0.07203000  | -0.49138900 |
| H | -4.83531500 | 0.14152800  | 1.46752400  |
| C | 0.46399300  | -0.55674600 | -0.78011100 |
| C | 0.68548400  | -1.85547300 | -0.25306400 |
| H | 1.22101000  | -0.07806500 | -1.39145200 |
| H | 1.62389800  | -2.35306600 | -0.47700800 |

UB3LYP-D3/BSII(SMD)//B3LYP-D3/BSI

HF=-2193.9537367

<sup>3</sup>F



|    |             |            |             |
|----|-------------|------------|-------------|
| Ni | -3.02073300 | 3.92698600 | -1.21070400 |
| N  | -1.19879500 | 2.93349400 | -1.02377300 |
| N  | -3.74016300 | 2.03526300 | -0.79346000 |
| C  | 0.07395400  | 3.41939200 | -1.45754600 |
| C  | 0.26868700  | 3.44365700 | -2.85593300 |
| C  | 1.04571400  | 3.90755600 | -0.56541000 |
| C  | 1.46320900  | 3.97141800 | -3.35123200 |
| C  | 2.22642700  | 4.43242300 | -1.11041700 |
| C  | 2.43725700  | 4.47111100 | -2.48624500 |
| H  | 1.63088000  | 3.98421400 | -4.42493000 |
| H  | 2.98856800  | 4.81340200 | -0.43571400 |
| H  | 3.36097900  | 4.88064000 | -2.88389800 |
| C  | -5.09795300 | 1.61029300 | -0.91524300 |
| C  | -5.54585800 | 1.34574700 | -2.22508200 |
| C  | -5.95576000 | 1.53721900 | 0.19762800  |
| C  | -6.88236300 | 0.97871000 | -2.40515200 |
| C  | -7.28948100 | 1.17521000 | -0.03342100 |
| C  | -7.75268500 | 0.89607200 | -1.31859000 |
| H  | -7.24034400 | 0.75872700 | -3.40743500 |
| H  | -7.96934900 | 1.11311000 | 0.81198500  |
| H  | -8.79011500 | 0.61464200 | -1.47241300 |
| C  | 0.84803400  | 3.91299500 | 0.93143300  |
| H  | 1.81288400  | 3.88225100 | 1.44654500  |
| H  | 0.33663700  | 4.82753100 | 1.25500200  |
| H  | 0.25299700  | 3.06657800 | 1.28155000  |
| C  | -0.78564300 | 2.89232900 | -3.78447700 |
| H  | -0.98729100 | 1.83263000 | -3.58722500 |
| H  | -1.73492400 | 3.42608800 | -3.65972400 |
| H  | -0.47641600 | 2.98678200 | -4.82937600 |
| C  | -5.47383800 | 1.85687500 | 1.59142400  |
| H  | -5.20060800 | 2.91225900 | 1.68180100  |
| H  | -6.25355700 | 1.64729100 | 2.32868500  |

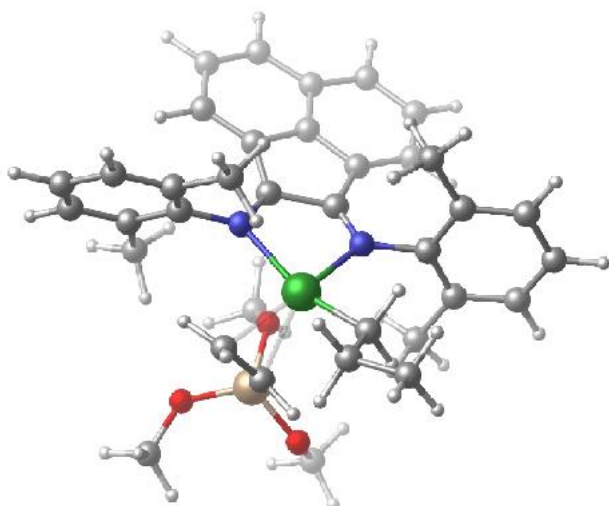
|    |             |             |             |
|----|-------------|-------------|-------------|
| H  | -4.58914400 | 1.27207400  | 1.86540000  |
| C  | -4.59673800 | 1.46436300  | -3.39257500 |
| H  | -4.17955000 | 2.47779200  | -3.45050700 |
| H  | -3.74749900 | 0.77682700  | -3.29957200 |
| H  | -5.10461000 | 1.24672800  | -4.33642200 |
| C  | -2.79436300 | 1.26429800  | -0.37381000 |
| C  | -1.37416000 | 1.75819100  | -0.51985900 |
| C  | -4.48006200 | 7.73372600  | -2.39316000 |
| H  | -4.49938500 | 8.58288100  | -3.07551400 |
| C  | -4.91076400 | 7.89976900  | -1.13339000 |
| H  | -5.26927500 | 8.86062800  | -0.76910700 |
| C  | -3.39081800 | 4.86390000  | 0.54532000  |
| H  | -4.49089600 | 4.86008800  | 0.60250000  |
| H  | -3.05751800 | 5.90165500  | 0.40351000  |
| C  | -2.76062800 | 4.24163500  | 1.78027800  |
| H  | -2.88770500 | 3.15003700  | 1.76445600  |
| C  | -3.32668600 | 4.79016900  | 3.10139400  |
| H  | -4.40455100 | 4.60085000  | 3.17844200  |
| H  | -2.84124500 | 4.32746100  | 3.96938100  |
| H  | -3.17851400 | 5.87446000  | 3.16799000  |
| H  | -1.68117200 | 4.41329900  | 1.75838600  |
| H  | -4.92233900 | 7.08607000  | -0.41098600 |
| Si | -3.88790400 | 6.11127700  | -3.02372600 |
| O  | -3.94730200 | 6.14493100  | -4.65391100 |
| O  | -4.68284300 | 4.79266400  | -2.35267000 |
| O  | -2.39059400 | 5.61152600  | -2.44133800 |
| C  | -3.55168100 | 5.09428100  | -5.53966200 |
| H  | -3.83773200 | 5.38961500  | -6.55128300 |
| H  | -2.46683300 | 4.94420700  | -5.50151600 |
| H  | -4.05425200 | 4.15278100  | -5.28622500 |
| C  | -6.10863000 | 4.65990800  | -2.18711700 |
| H  | -6.58483600 | 5.64431600  | -2.17413200 |
| H  | -6.51457500 | 4.05420300  | -3.00016400 |
| H  | -6.28278800 | 4.15106600  | -1.23814900 |
| C  | -1.25264900 | 6.46438000  | -2.20215700 |
| H  | -0.78292300 | 6.13056100  | -1.27616700 |
| H  | -0.54314100 | 6.35894200  | -3.02559500 |
| H  | -1.56754000 | 7.50704400  | -2.09838200 |
| C  | -3.20219700 | -2.35332200 | 0.86343800  |
| C  | -1.85269200 | -2.64728300 | 0.98465000  |
| C  | -0.86783100 | -1.67072600 | 0.66660800  |
| C  | -1.34550800 | -0.41590500 | 0.24506400  |
| C  | -2.72989300 | -0.11230400 | 0.12125100  |
| C  | -3.66557300 | -1.08522200 | 0.42672300  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 0.97040000  | -2.76999300 | 1.04055900  |
| H | -3.93425200 | -3.11670500 | 1.10803200  |
| H | -1.54034900 | -3.63210300 | 1.32100700  |
| C | 0.54585100  | -1.82353600 | 0.71718400  |
| C | -0.48970800 | 0.65826600  | -0.12753700 |
| H | -4.72936900 | -0.89618600 | 0.33728700  |
| C | 0.88161800  | 0.47721200  | -0.07771200 |
| C | 1.38155500  | -0.77885600 | 0.35282600  |
| H | 1.56799700  | 1.26708300  | -0.36033100 |
| H | 2.45684300  | -0.92179800 | 0.39557300  |

UB3LYP-D3/BSII(SMD)//B3LYP-D3/BSI

HF=-2193.954199

<sup>1</sup>G



|                                              |                             |
|----------------------------------------------|-----------------------------|
| Zero-point correction=                       | 0.717295 (Hartree/Particle) |
| Thermal correction to Energy=                | 0.763221                    |
| Thermal correction to Enthalpy=              | 0.764165                    |
| Thermal correction to Gibbs Free Energy=     | 0.637773                    |
| Sum of electronic and zero-point Energies=   | -2191.039540                |
| Sum of electronic and thermal Energies=      | -2190.993614                |
| Sum of electronic and thermal Enthalpies=    | -2190.992670                |
| Sum of electronic and thermal Free Energies= | -2191.119062                |

|    |             |            |             |
|----|-------------|------------|-------------|
| Ni | -2.21148300 | 4.10696100 | -0.76323500 |
| N  | -0.82969900 | 2.51776600 | -1.00559900 |
| N  | -3.43497300 | 2.61171100 | -0.30575700 |
| C  | 0.59305800  | 2.60369300 | -1.10359800 |
| C  | 1.29154800  | 2.28536700 | -2.28530500 |
| C  | 1.24778800  | 3.11655200 | 0.03681400  |
| C  | 2.68381800  | 2.44918200 | -2.27641600 |
| C  | 2.63674800  | 3.25632200 | -0.00273700 |
| C  | 3.35473900  | 2.92183300 | -1.15070100 |
| H  | 3.24310900  | 2.20683700 | -3.17598700 |
| H  | 3.15604300  | 3.63206300 | 0.87461800  |
| H  | 4.43424500  | 3.03725300 | -1.17029600 |
| C  | -4.76616400 | 2.67135900 | 0.22740100  |
| C  | -5.85716900 | 2.92446600 | -0.61970700 |
| C  | -4.90761100 | 2.50155900 | 1.61732700  |
| C  | -7.12874200 | 2.97707700 | -0.03619500 |
| C  | -6.19640300 | 2.57088400 | 2.15586900  |
| C  | -7.30096700 | 2.80195900 | 1.33669700  |
| H  | -7.99081000 | 3.16228600 | -0.67127800 |
| H  | -6.32952700 | 2.44239100 | 3.22653100  |
| H  | -8.29605700 | 2.85079500 | 1.76865600  |
| C  | 0.45744100  | 3.49191000 | 1.26695700  |

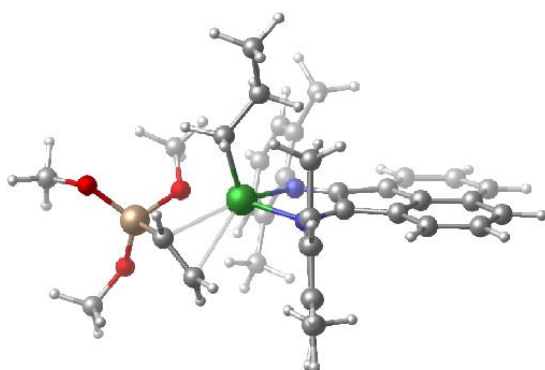
|    |             |            |             |
|----|-------------|------------|-------------|
| H  | -0.10965700 | 2.64235600 | 1.66553500  |
| H  | 1.11311600  | 3.86407200 | 2.05883400  |
| H  | -0.27526200 | 4.28172500 | 1.04157700  |
| C  | 0.59210500  | 1.83891700 | -3.54699800 |
| H  | -0.14313600 | 1.05205500 | -3.36351600 |
| H  | 0.06479500  | 2.67143200 | -4.02405500 |
| H  | 1.31892700  | 1.45264100 | -4.26738200 |
| C  | -3.70162900 | 2.23707300 | 2.48654700  |
| H  | -2.90113700 | 2.96239400 | 2.29334800  |
| H  | -3.96312000 | 2.28968500 | 3.54662200  |
| H  | -3.28106100 | 1.24112800 | 2.29583700  |
| C  | -5.66686000 | 3.13290100 | -2.10035700 |
| H  | -5.17803200 | 4.09122600 | -2.30986800 |
| H  | -5.02972900 | 2.36231700 | -2.54346500 |
| H  | -6.63021000 | 3.12989200 | -2.61843500 |
| C  | -2.92889400 | 1.46401700 | -0.60910600 |
| C  | -1.46121900 | 1.39906200 | -0.94707400 |
| C  | -2.08664300 | 5.38172400 | -2.44767800 |
| H  | -2.78301000 | 6.20273600 | -2.28486000 |
| C  | -0.87470500 | 5.43661900 | -1.78817600 |
| H  | -0.04213400 | 4.79619300 | -2.06493700 |
| C  | -3.39674700 | 5.38978800 | 0.07614800  |
| H  | -3.68333900 | 4.82000000 | 0.96791500  |
| H  | -4.28797000 | 5.52316300 | -0.54780400 |
| C  | -2.75031400 | 6.70615500 | 0.47650000  |
| H  | -1.79790800 | 6.51553000 | 0.99104400  |
| C  | -3.67125600 | 7.51017000 | 1.41391900  |
| H  | -3.88970400 | 6.94721100 | 2.32862500  |
| H  | -3.20173600 | 8.45734200 | 1.70197400  |
| H  | -4.62460400 | 7.73724100 | 0.92356800  |
| H  | -2.51916900 | 7.31881600 | -0.40331100 |
| H  | -0.62712100 | 6.26382600 | -1.12808500 |
| Si | -2.52866000 | 4.32181300 | -3.92933800 |
| O  | -3.93198500 | 5.01598800 | -4.43704300 |
| O  | -1.35975100 | 4.32080100 | -5.09390900 |
| O  | -2.69421900 | 2.73903400 | -3.49855000 |
| C  | -4.77247300 | 4.49280000 | -5.46649300 |
| H  | -5.46163800 | 5.28350000 | -5.77295400 |
| H  | -4.19304800 | 4.17218200 | -6.34145100 |
| H  | -5.35466000 | 3.64304000 | -5.08897700 |
| C  | -0.90043200 | 5.49367400 | -5.77192800 |
| H  | -0.38753400 | 6.17055200 | -5.07702200 |
| H  | -0.19451000 | 5.17720200 | -6.54341000 |
| H  | -1.73114200 | 6.02985400 | -6.24567000 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -2.76393900 | 1.63963800  | -4.40636400 |
| H | -2.00834200 | 1.72267900  | -5.19406100 |
| H | -2.58502800 | 0.72361800  | -3.83497700 |
| H | -3.75906200 | 1.57687200  | -4.86325400 |
| C | -4.76833900 | -1.89975900 | -0.35911500 |
| C | -3.66774400 | -2.71226400 | -0.58715900 |
| C | -2.38352000 | -2.14579400 | -0.82021700 |
| C | -2.31171000 | -0.73977100 | -0.81812800 |
| C | -3.43925100 | 0.09426100  | -0.57341000 |
| C | -4.67514100 | -0.48447500 | -0.33960700 |
| H | -1.15923300 | -3.92626700 | -1.06046100 |
| H | -5.73626000 | -2.35795000 | -0.18144700 |
| H | -3.78237000 | -3.79276600 | -0.58425200 |
| C | -1.16228800 | -2.83983800 | -1.04580800 |
| C | -1.10123200 | -0.02069300 | -1.02971100 |
| H | -5.55500300 | 0.11756000  | -0.14402800 |
| C | 0.07296600  | -0.72419100 | -1.23630800 |
| C | 0.01987200  | -2.14181500 | -1.24003800 |
| H | 1.01716600  | -0.21529300 | -1.39238500 |
| H | 0.94001400  | -2.69419600 | -1.40311400 |

UB3LYP-D3/BSII(SMD)//B3LYP-D3/BSI

HF=-2193.9416353

<sup>3</sup>G



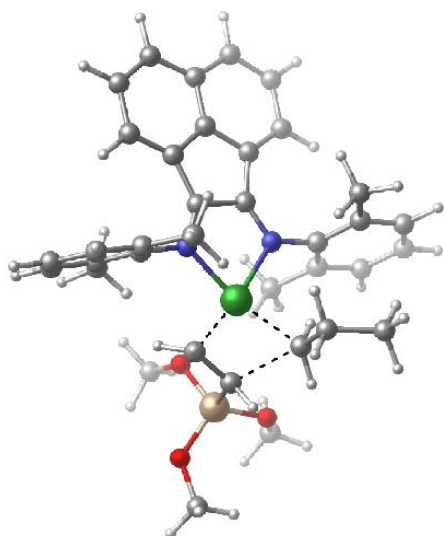
|                                              |                             |            |             |
|----------------------------------------------|-----------------------------|------------|-------------|
| Zero-point correction=                       | 0.715377 (Hartree/Particle) |            |             |
| Thermal correction to Energy=                | 0.762054                    |            |             |
| Thermal correction to Enthalpy=              | 0.762998                    |            |             |
| Thermal correction to Gibbs Free Energy=     | 0.632934                    |            |             |
| Sum of electronic and zero-point Energies=   | -2191.047720                |            |             |
| Sum of electronic and thermal Energies=      | -2191.001043                |            |             |
| Sum of electronic and thermal Enthalpies=    | -2191.000099                |            |             |
| Sum of electronic and thermal Free Energies= | -2191.130163                |            |             |
| Ni                                           | -3.02073300                 | 3.92698600 | -1.21070400 |
| N                                            | -1.19879500                 | 2.93349400 | -1.02377300 |
| N                                            | -3.74016300                 | 2.03526300 | -0.79346000 |
| C                                            | 0.07395400                  | 3.41939200 | -1.45754600 |
| C                                            | 0.26868700                  | 3.44365700 | -2.85593300 |
| C                                            | 1.04571400                  | 3.90755600 | -0.56541000 |
| C                                            | 1.46320900                  | 3.97141800 | -3.35123200 |
| C                                            | 2.22642700                  | 4.43242300 | -1.11041700 |
| C                                            | 2.43725700                  | 4.47111100 | -2.48624500 |
| H                                            | 1.63088000                  | 3.98421400 | -4.42493000 |
| H                                            | 2.98856800                  | 4.81340200 | -0.43571400 |
| H                                            | 3.36097900                  | 4.88064000 | -2.88389800 |
| C                                            | -5.09795300                 | 1.61029300 | -0.91524300 |
| C                                            | -5.54585800                 | 1.34574700 | -2.22508200 |
| C                                            | -5.95576000                 | 1.53721900 | 0.19762800  |
| C                                            | -6.88236300                 | 0.97871000 | -2.40515200 |
| C                                            | -7.28948100                 | 1.17521000 | -0.03342100 |
| C                                            | -7.75268500                 | 0.89607200 | -1.31859000 |
| H                                            | -7.24034400                 | 0.75872700 | -3.40743500 |
| H                                            | -7.96934900                 | 1.11311000 | 0.81198500  |
| H                                            | -8.79011500                 | 0.61464200 | -1.47241300 |
| C                                            | 0.84803400                  | 3.91299500 | 0.93143300  |
| H                                            | 1.81288400                  | 3.88225100 | 1.44654500  |
| H                                            | 0.33663700                  | 4.82753100 | 1.25500200  |
| H                                            | 0.25299700                  | 3.06657800 | 1.28155000  |

|    |             |            |             |
|----|-------------|------------|-------------|
| C  | -0.78564300 | 2.89232900 | -3.78447700 |
| H  | -0.98729100 | 1.83263000 | -3.58722500 |
| H  | -1.73492400 | 3.42608800 | -3.65972400 |
| H  | -0.47641600 | 2.98678200 | -4.82937600 |
| C  | -5.47383800 | 1.85687500 | 1.59142400  |
| H  | -5.20060800 | 2.91225900 | 1.68180100  |
| H  | -6.25355700 | 1.64729100 | 2.32868500  |
| H  | -4.58914400 | 1.27207400 | 1.86540000  |
| C  | -4.59673800 | 1.46436300 | -3.39257500 |
| H  | -4.17955000 | 2.47779200 | -3.45050700 |
| H  | -3.74749900 | 0.77682700 | -3.29957200 |
| H  | -5.10461000 | 1.24672800 | -4.33642200 |
| C  | -2.79436300 | 1.26429800 | -0.37381000 |
| C  | -1.37416000 | 1.75819100 | -0.51985900 |
| C  | -4.48006200 | 7.73372600 | -2.39316000 |
| H  | -4.49938500 | 8.58288100 | -3.07551400 |
| C  | -4.91076400 | 7.89976900 | -1.13339000 |
| H  | -5.26927500 | 8.86062800 | -0.76910700 |
| C  | -3.39081800 | 4.86390000 | 0.54532000  |
| H  | -4.49089600 | 4.86008800 | 0.60250000  |
| H  | -3.05751800 | 5.90165500 | 0.40351000  |
| C  | -2.76062800 | 4.24163500 | 1.78027800  |
| H  | -2.88770500 | 3.15003700 | 1.76445600  |
| C  | -3.32668600 | 4.79016900 | 3.10139400  |
| H  | -4.40455100 | 4.60085000 | 3.17844200  |
| H  | -2.84124500 | 4.32746100 | 3.96938100  |
| H  | -3.17851400 | 5.87446000 | 3.16799000  |
| H  | -1.68117200 | 4.41329900 | 1.75838600  |
| H  | -4.92233900 | 7.08607000 | -0.41098600 |
| Si | -3.88790400 | 6.11127700 | -3.02372600 |
| O  | -3.94730200 | 6.14493100 | -4.65391100 |
| O  | -4.68284300 | 4.79266400 | -2.35267000 |
| O  | -2.39059400 | 5.61152600 | -2.44133800 |
| C  | -3.55168100 | 5.09428100 | -5.53966200 |
| H  | -3.83773200 | 5.38961500 | -6.55128300 |
| H  | -2.46683300 | 4.94420700 | -5.50151600 |
| H  | -4.05425200 | 4.15278100 | -5.28622500 |
| C  | -6.10863000 | 4.65990800 | -2.18711700 |
| H  | -6.58483600 | 5.64431600 | -2.17413200 |
| H  | -6.51457500 | 4.05420300 | -3.00016400 |
| H  | -6.28278800 | 4.15106600 | -1.23814900 |
| C  | -1.25264900 | 6.46438000 | -2.20215700 |
| H  | -0.78292300 | 6.13056100 | -1.27616700 |
| H  | -0.54314100 | 6.35894200 | -3.02559500 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -1.56754000 | 7.50704400  | -2.09838200 |
| C | -3.20219700 | -2.35332200 | 0.86343800  |
| C | -1.85269200 | -2.64728300 | 0.98465000  |
| C | -0.86783100 | -1.67072600 | 0.66660800  |
| C | -1.34550800 | -0.41590500 | 0.24506400  |
| C | -2.72989300 | -0.11230400 | 0.12125100  |
| C | -3.66557300 | -1.08522200 | 0.42672300  |
| H | 0.97040000  | -2.76999300 | 1.04055900  |
| H | -3.93425200 | -3.11670500 | 1.10803200  |
| H | -1.54034900 | -3.63210300 | 1.32100700  |
| C | 0.54585100  | -1.82353600 | 0.71718400  |
| C | -0.48970800 | 0.65826600  | -0.12753700 |
| H | -4.72936900 | -0.89618600 | 0.33728700  |
| C | 0.88161800  | 0.47721200  | -0.07771200 |
| C | 1.38155500  | -0.77885600 | 0.35282600  |
| H | 1.56799700  | 1.26708300  | -0.36033100 |
| H | 2.45684300  | -0.92179800 | 0.39557300  |

UB3LYP-D3/BSII(SMD)/B3LYP-D3/BSI

HF=-2193.940966

**<sup>1</sup>TS3**

|                                              |                             |            |             |
|----------------------------------------------|-----------------------------|------------|-------------|
| Zero-point correction=                       | 0.716940 (Hartree/Particle) |            |             |
| Thermal correction to Energy=                | 0.762483                    |            |             |
| Thermal correction to Enthalpy=              | 0.763428                    |            |             |
| Thermal correction to Gibbs Free Energy=     | 0.635902                    |            |             |
| Sum of electronic and zero-point Energies=   | -2191.022626                |            |             |
| Sum of electronic and thermal Energies=      | -2190.977083                |            |             |
| Sum of electronic and thermal Enthalpies=    | -2190.976139                |            |             |
| Sum of electronic and thermal Free Energies= | -2191.103664                |            |             |
| Ni                                           | -1.96498600                 | 3.74190700 | -1.19265900 |
| N                                            | -0.74573700                 | 2.22940000 | -0.93392400 |
| N                                            | -3.35647000                 | 2.36782800 | -0.42084300 |
| C                                            | 0.65947800                  | 2.21165200 | -1.22279600 |
| C                                            | 1.08963600                  | 1.70906700 | -2.46187800 |
| C                                            | 1.53859900                  | 2.74422400 | -0.26707100 |
| C                                            | 2.46493500                  | 1.72386600 | -2.72068200 |
| C                                            | 2.90492000                  | 2.73597900 | -0.56754100 |
| C                                            | 3.36657400                  | 2.22635100 | -1.78156800 |
| H                                            | 2.82682100                  | 1.34257100 | -3.67168800 |
| H                                            | 3.60819700                  | 3.13719000 | 0.15715000  |
| H                                            | 4.43009200                  | 2.23035800 | -2.00085800 |
| C                                            | -4.75485400                 | 2.52556600 | -0.16384300 |
| C                                            | -5.62746000                 | 2.54684400 | -1.26823200 |
| C                                            | -5.20230400                 | 2.72278900 | 1.15659500  |
| C                                            | -6.98719900                 | 2.76520000 | -1.02225100 |
| C                                            | -6.57069300                 | 2.94250700 | 1.35154700  |
| C                                            | -7.45762300                 | 2.96460000 | 0.27486500  |
| H                                            | -7.67911100                 | 2.77801000 | -1.85994600 |
| H                                            | -6.93956600                 | 3.10051200 | 2.36138500  |
| H                                            | -8.51520600                 | 3.13977100 | 0.44798400  |
| C                                            | 1.00557700                  | 3.29121600 | 1.03400400  |

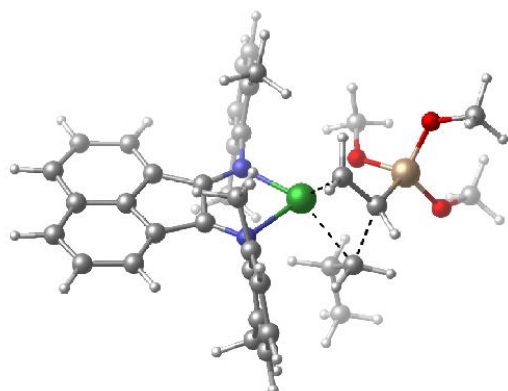
|    |             |            |             |
|----|-------------|------------|-------------|
| H  | 0.57308800  | 2.49746000 | 1.65669500  |
| H  | 1.79526000  | 3.77817300 | 1.61229000  |
| H  | 0.20574900  | 4.02184600 | 0.85428700  |
| C  | 0.09161500  | 1.18021300 | -3.46396300 |
| H  | -0.36109600 | 0.24107200 | -3.11995500 |
| H  | -0.72523900 | 1.89444400 | -3.62284300 |
| H  | 0.57280100  | 0.98325000 | -4.42595200 |
| C  | -4.24858200 | 2.67915800 | 2.32688700  |
| H  | -3.33689300 | 3.25233000 | 2.13032400  |
| H  | -4.71760300 | 3.08624200 | 3.22647900  |
| H  | -3.93989700 | 1.64997800 | 2.55013900  |
| C  | -5.10179000 | 2.30514400 | -2.66100000 |
| H  | -4.27729900 | 2.98056500 | -2.91176300 |
| H  | -4.71000900 | 1.28519600 | -2.76573100 |
| H  | -5.89323300 | 2.43705900 | -3.40440900 |
| C  | -2.78066700 | 1.23943200 | -0.19243500 |
| C  | -1.30955100 | 1.16647800 | -0.46906900 |
| C  | -1.76733200 | 5.57553900 | -2.41876300 |
| H  | -1.76103900 | 6.59778100 | -2.04935600 |
| C  | -0.61177100 | 4.80463800 | -2.09528700 |
| H  | -0.20412600 | 4.11985900 | -2.83557200 |
| C  | -3.32223200 | 5.34372400 | -1.00638900 |
| H  | -4.10865300 | 4.59031300 | -1.05473300 |
| H  | -3.71817200 | 6.18574000 | -1.56440000 |
| C  | -2.92567500 | 5.75696800 | 0.40613100  |
| H  | -2.49572900 | 4.91804300 | 0.97003700  |
| C  | -4.14133800 | 6.30209900 | 1.17726700  |
| H  | -4.92585300 | 5.54217200 | 1.25549600  |
| H  | -3.85409500 | 6.60596900 | 2.18987100  |
| H  | -4.56599000 | 7.17466300 | 0.66824700  |
| H  | -2.14063300 | 6.52250200 | 0.35712800  |
| H  | 0.12700400  | 5.20686500 | -1.40037200 |
| Si | -2.57731700 | 5.28115300 | -4.08403400 |
| O  | -4.15479100 | 5.73328000 | -3.92097800 |
| O  | -1.85578300 | 6.08592500 | -5.32489300 |
| O  | -2.37284000 | 3.67399200 | -4.39385900 |
| C  | -5.14378900 | 5.57474200 | -4.93849000 |
| H  | -6.00341100 | 6.19584100 | -4.67392000 |
| H  | -4.77106800 | 5.88858400 | -5.92172600 |
| H  | -5.46873000 | 4.52832100 | -4.99719600 |
| C  | -1.94741000 | 7.49295100 | -5.55494100 |
| H  | -1.25640100 | 8.03661600 | -4.89903800 |
| H  | -1.66639600 | 7.68246800 | -6.59394400 |
| H  | -2.96622000 | 7.86398500 | -5.38754000 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -2.50472900 | 3.07191500  | -5.68462500 |
| H | -2.06161900 | 3.70223900  | -6.46244900 |
| H | -1.98309700 | 2.11134100  | -5.66167200 |
| H | -3.56130300 | 2.89312000  | -5.91885200 |
| C | -4.41073600 | -1.99559500 | 1.09585700  |
| C | -3.25883600 | -2.76777000 | 1.11979400  |
| C | -2.00871000 | -2.21820000 | 0.71992100  |
| C | -2.02251800 | -0.87232600 | 0.30886500  |
| C | -3.20346800 | -0.07727900 | 0.28925600  |
| C | -4.40554700 | -0.63808300 | 0.68315500  |
| H | -0.67602300 | -3.91382000 | 0.99449100  |
| H | -5.35160300 | -2.43995300 | 1.40522000  |
| H | -3.30767300 | -3.80286100 | 1.44654000  |
| C | -0.74628400 | -2.87412600 | 0.68678700  |
| C | -0.85615300 | -0.18068300 | -0.12825100 |
| H | -5.32507600 | -0.06336200 | 0.68322000  |
| C | 0.35854300  | -0.84409400 | -0.15097500 |
| C | 0.39039400  | -2.19985700 | 0.26590500  |
| H | 1.26707000  | -0.35173400 | -0.47884400 |
| H | 1.34075800  | -2.72422200 | 0.25093400  |

UB3LYP-D3/BSII(SMD)//B3LYP-D3/BSI

HF=-2193.9225937

### <sup>3</sup>TS3



|                                              |                             |            |             |
|----------------------------------------------|-----------------------------|------------|-------------|
| Zero-point correction=                       | 0.715245 (Hartree/Particle) |            |             |
| Thermal correction to Energy=                | 0.762111                    |            |             |
| Thermal correction to Enthalpy=              | 0.763055                    |            |             |
| Thermal correction to Gibbs Free Energy=     | 0.631819                    |            |             |
| Sum of electronic and zero-point Energies=   | -2191.035778                |            |             |
| Sum of electronic and thermal Energies=      | -2190.988913                |            |             |
| Sum of electronic and thermal Enthalpies=    | -2190.987968                |            |             |
| Sum of electronic and thermal Free Energies= | -2191.119205                |            |             |
| Ni                                           | -2.73328600                 | 4.03558600 | -0.90395900 |
| N                                            | -1.08604900                 | 2.79406600 | -0.86909300 |
| N                                            | -3.66549800                 | 2.21464700 | -0.25586000 |
| C                                            | 0.25717700                  | 3.15060400 | -1.20977400 |
| C                                            | 0.59172600                  | 3.23745200 | -2.57148000 |
| C                                            | 1.17199100                  | 3.45274700 | -0.18524900 |
| C                                            | 1.89412900                  | 3.62745800 | -2.90088100 |
| C                                            | 2.46201300                  | 3.84505800 | -0.56131300 |
| C                                            | 2.82383900                  | 3.93097000 | -1.90662500 |
| H                                            | 2.17552600                  | 3.69707000 | -3.94816200 |
| H                                            | 3.18625900                  | 4.08621700 | 0.21211500  |
| H                                            | 3.82951900                  | 4.23708100 | -2.17877600 |
| C                                            | -5.06414000                 | 1.93973400 | -0.12460700 |
| C                                            | -5.76528700                 | 1.47103400 | -1.25587200 |
| C                                            | -5.70185700                 | 2.17306000 | 1.10667900  |
| C                                            | -7.14990100                 | 1.30851500 | -1.14210100 |
| C                                            | -7.08865900                 | 1.99046900 | 1.17247000  |
| C                                            | -7.81225100                 | 1.57687200 | 0.05616400  |
| H                                            | -7.71078600                 | 0.95869900 | -2.00476800 |
| H                                            | -7.59827300                 | 2.16816300 | 2.11596100  |
| H                                            | -8.88865500                 | 1.44964000 | 0.12204300  |
| C                                            | 0.76739400                  | 3.36319700 | 1.26635900  |
| H                                            | 0.51531700                  | 2.33470300 | 1.55279300  |
| H                                            | 1.57583700                  | 3.70169200 | 1.91979900  |
| H                                            | -0.11571900                 | 3.97975000 | 1.46992600  |

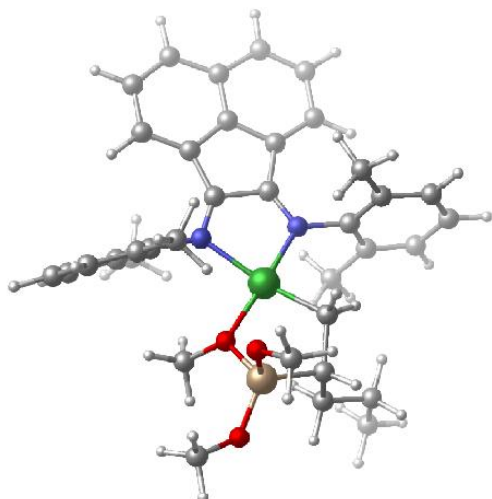
|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -0.43660400 | 2.92214700  | -3.62856900 |
| H  | -0.75751800 | 1.87406500  | -3.57894400 |
| H  | -1.33577600 | 3.53391600  | -3.48964100 |
| H  | -0.04288900 | 3.10716600  | -4.63152000 |
| C  | -4.91537500 | 2.50541200  | 2.35309100  |
| H  | -3.97026500 | 3.00221300  | 2.12713400  |
| H  | -5.49149800 | 3.14674900  | 3.02715500  |
| H  | -4.67045500 | 1.58853600  | 2.90561300  |
| C  | -5.04674000 | 1.07716700  | -2.52654900 |
| H  | -4.21707000 | 1.74961400  | -2.76180900 |
| H  | -4.62527600 | 0.06765300  | -2.43131800 |
| H  | -5.73388800 | 1.06635200  | -3.37739000 |
| C  | -2.80717500 | 1.25555700  | -0.22145400 |
| C  | -1.37144900 | 1.58162200  | -0.52942700 |
| C  | -4.21048700 | 5.65295000  | -1.59410000 |
| H  | -5.23099200 | 5.89426000  | -1.31280000 |
| C  | -4.03252000 | 4.51064000  | -2.45067900 |
| H  | -4.86314900 | 3.82162100  | -2.56952700 |
| C  | -3.99635800 | 5.46112700  | 0.54467100  |
| H  | -4.75894900 | 4.71094600  | 0.75315900  |
| H  | -4.42203700 | 6.46054500  | 0.58466700  |
| C  | -2.76069300 | 5.38792200  | 1.43681300  |
| H  | -2.35736900 | 4.36621200  | 1.49692800  |
| C  | -3.10019500 | 5.85526200  | 2.86797100  |
| H  | -3.88625700 | 5.23546500  | 3.31160200  |
| H  | -2.21478700 | 5.79691200  | 3.51150000  |
| H  | -3.44974900 | 6.89313200  | 2.85967800  |
| H  | -1.96368500 | 6.01967300  | 1.03137400  |
| H  | -3.35979100 | 4.57729200  | -3.30544800 |
| Si | -2.91094100 | 6.96088700  | -1.81532700 |
| O  | -3.17630800 | 8.19037500  | -0.76140400 |
| O  | -2.63502600 | 7.50866300  | -3.34039500 |
| O  | -1.57098000 | 6.01695300  | -1.45368100 |
| C  | -2.41944600 | 9.40094400  | -0.67847100 |
| H  | -3.05874800 | 10.16921300 | -0.23652000 |
| H  | -1.54359200 | 9.25519600  | -0.03501900 |
| H  | -2.08621300 | 9.73980300  | -1.66683200 |
| C  | -3.54114000 | 8.33184200  | -4.08140000 |
| H  | -4.42576300 | 7.75825300  | -4.38352200 |
| H  | -3.86120700 | 9.20443900  | -3.49872400 |
| H  | -3.02049800 | 8.67671200  | -4.97776300 |
| C  | -0.22995500 | 6.39952600  | -1.81554700 |
| H  | -0.09361400 | 7.47942200  | -1.69490700 |
| H  | 0.46136500  | 5.87302900  | -1.15856600 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -0.02892700 | 6.12479500  | -2.85354100 |
| C | -3.56680900 | -2.43284500 | 0.55622400  |
| C | -2.26890100 | -2.90531900 | 0.43330500  |
| C | -1.20459500 | -2.02073700 | 0.10197400  |
| C | -1.55153300 | -0.66971200 | -0.08403700 |
| C | -2.88276000 | -0.18484100 | 0.03852700  |
| C | -3.89891600 | -1.06689900 | 0.36028200  |
| H | 0.49586100  | -3.37519100 | 0.06439900  |
| H | -4.36110800 | -3.12844900 | 0.80867500  |
| H | -2.05907800 | -3.95999500 | 0.58879300  |
| C | 0.17002600  | -2.34701000 | -0.06714200 |
| C | -0.60503500 | 0.33909500  | -0.42132200 |
| H | -4.92652300 | -0.73503600 | 0.45899000  |
| C | 0.72546600  | -0.00852700 | -0.58296400 |
| C | 1.09305700  | -1.36649200 | -0.39908200 |
| H | 1.47718500  | 0.72872500  | -0.84082100 |
| H | 2.13557600  | -1.64236500 | -0.52368000 |

UB3LYP-D3/BSII(SMD)/B3LYP-D3/BSI

HF=-2193.9066338

<sup>1</sup>H



|                                              |                             |            |             |
|----------------------------------------------|-----------------------------|------------|-------------|
| Zero-point correction=                       | 0.720138 (Hartree/Particle) |            |             |
| Thermal correction to Energy=                | 0.765036                    |            |             |
| Thermal correction to Enthalpy=              | 0.765981                    |            |             |
| Thermal correction to Gibbs Free Energy=     | 0.639909                    |            |             |
| Sum of electronic and zero-point Energies=   | -2191.071589                |            |             |
| Sum of electronic and thermal Energies=      | -2191.026691                |            |             |
| Sum of electronic and thermal Enthalpies=    | -2191.025747                |            |             |
| Sum of electronic and thermal Free Energies= | -2191.151819                |            |             |
| Ni                                           | -2.60989400                 | 3.37570100 | -1.30732400 |
| N                                            | -1.11156600                 | 2.20213200 | -0.94181900 |
| N                                            | -3.68820000                 | 1.87483600 | -0.33705900 |
| C                                            | 0.27047900                  | 2.44647600 | -1.24116800 |
| C                                            | 0.83460200                  | 1.86195900 | -2.38625100 |
| C                                            | 0.98206800                  | 3.31552000 | -0.39670300 |
| C                                            | 2.17911900                  | 2.14137000 | -2.65654600 |
| C                                            | 2.32283600                  | 3.56592800 | -0.70600000 |
| C                                            | 2.91987600                  | 2.97957000 | -1.82265900 |
| H                                            | 2.64272100                  | 1.70213200 | -3.53563800 |
| H                                            | 2.89687500                  | 4.23209100 | -0.06789900 |
| H                                            | 3.96117700                  | 3.18651600 | -2.05075400 |
| C                                            | -5.09632600                 | 1.80159300 | -0.11288200 |
| C                                            | -5.93044500                 | 1.68803400 | -1.24093300 |
| C                                            | -5.60260600                 | 1.95243100 | 1.19211900  |
| C                                            | -7.31282200                 | 1.70597100 | -1.03029400 |
| C                                            | -6.99303500                 | 1.97487900 | 1.35055500  |
| C                                            | -7.84354200                 | 1.85145400 | 0.25215500  |
| H                                            | -7.97691200                 | 1.60662500 | -1.88463100 |
| H                                            | -7.40788500                 | 2.09858300 | 2.34728800  |
| H                                            | -8.91987000                 | 1.87094500 | 0.39510300  |
| C                                            | 0.29682500                  | 3.96155300 | 0.78079800  |
| H                                            | -0.02709300                 | 3.21832900 | 1.52014600  |

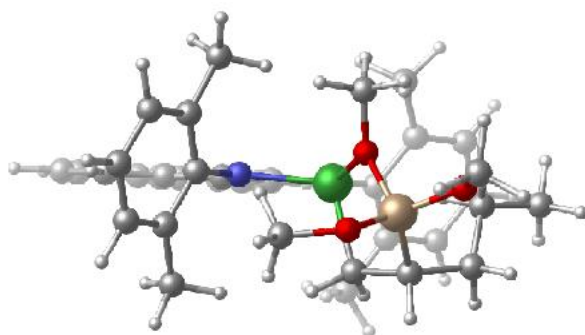
|    |             |            |             |
|----|-------------|------------|-------------|
| H  | 0.95820600  | 4.67272700 | 1.28245600  |
| H  | -0.60359900 | 4.49942000 | 0.45411300  |
| C  | 0.01217900  | 0.96951400 | -3.28353300 |
| H  | -0.22125000 | 0.01435000 | -2.79591400 |
| H  | -0.94323300 | 1.44168000 | -3.54209200 |
| H  | 0.54675700  | 0.74673900 | -4.21064300 |
| C  | -4.68240100 | 2.11599900 | 2.37911400  |
| H  | -3.88404700 | 2.84078800 | 2.17688100  |
| H  | -5.23665300 | 2.45884500 | 3.25687700  |
| H  | -4.19259200 | 1.17138100 | 2.64553500  |
| C  | -5.34373100 | 1.54848400 | -2.62431700 |
| H  | -4.81820500 | 2.46285700 | -2.92391000 |
| H  | -4.62303400 | 0.72357100 | -2.67534800 |
| H  | -6.12764900 | 1.35667100 | -3.36228400 |
| C  | -2.89952700 | 0.90446500 | -0.03142300 |
| C  | -1.44366700 | 1.11060900 | -0.33179900 |
| C  | -2.11866400 | 5.93629800 | -2.68474800 |
| H  | -1.70786600 | 6.39061000 | -3.59989900 |
| C  | -1.56266000 | 4.51412000 | -2.50709300 |
| H  | -1.59154900 | 3.93553800 | -3.44334100 |
| C  | -1.78847900 | 6.84666700 | -1.47743500 |
| H  | -2.13729000 | 6.34832900 | -0.55898400 |
| H  | -2.34999700 | 7.78686900 | -1.55158100 |
| C  | -0.29505600 | 7.17450300 | -1.32846800 |
| H  | 0.29335200  | 6.24969600 | -1.27887400 |
| C  | -0.00783600 | 8.02050700 | -0.08398900 |
| H  | -0.30189200 | 7.48760800 | 0.82953500  |
| H  | 1.05763300  | 8.26140800 | -0.00213700 |
| H  | -0.56327300 | 8.96559600 | -0.10876300 |
| H  | 0.04407000  | 7.70622700 | -2.22805800 |
| H  | -0.53172400 | 4.52636400 | -2.15189000 |
| Si | -3.94594000 | 5.64723200 | -2.81578400 |
| O  | -4.86217500 | 6.98534000 | -2.58969100 |
| O  | -4.44702000 | 4.72466000 | -4.08393300 |
| O  | -4.15926300 | 4.58409500 | -1.48660600 |
| C  | -6.26242000 | 7.11080400 | -2.86072700 |
| H  | -6.46159900 | 8.15022500 | -3.13176600 |
| H  | -6.57314400 | 6.45591100 | -3.68257300 |
| H  | -6.84124200 | 6.85880700 | -1.96432600 |
| C  | -4.15578000 | 5.01086600 | -5.45489800 |
| H  | -3.07478000 | 5.10194300 | -5.62095200 |
| H  | -4.53478800 | 4.18007900 | -6.05462000 |
| H  | -4.64742800 | 5.93519900 | -5.78139300 |
| C  | -4.98440600 | 4.93403900 | -0.34928200 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -5.98177500 | 4.50981200  | -0.48262200 |
| H | -4.52564300 | 4.51069200  | 0.54339300  |
| H | -5.03688100 | 6.02095500  | -0.25474800 |
| C | -3.82737100 | -2.47443700 | 1.54818400  |
| C | -2.53787800 | -2.97616600 | 1.64383100  |
| C | -1.42629000 | -2.21114900 | 1.19212600  |
| C | -1.71861500 | -0.94371600 | 0.65464300  |
| C | -3.04100800 | -0.42514400 | 0.56358600  |
| C | -4.10318100 | -1.19072100 | 1.01067000  |
| H | 0.23119000  | -3.54935900 | 1.62577700  |
| H | -4.65766900 | -3.07960600 | 1.89847000  |
| H | -2.37089100 | -3.96284100 | 2.06701400  |
| C | -0.05297800 | -2.58229700 | 1.22005900  |
| C | -0.71845700 | -0.06359000 | 0.14799800  |
| H | -5.12331200 | -0.82642200 | 0.95873800  |
| C | 0.60988700  | -0.45248400 | 0.18710800  |
| C | 0.92190300  | -1.72327900 | 0.73445500  |
| H | 1.39915000  | 0.18749000  | -0.19045400 |
| H | 1.96228100  | -2.03109200 | 0.76874500  |

UB3LYP-D3/BSII(SMD)//B3LYP-D3/BSI

HF=-2193.9768404

<sup>3</sup>H



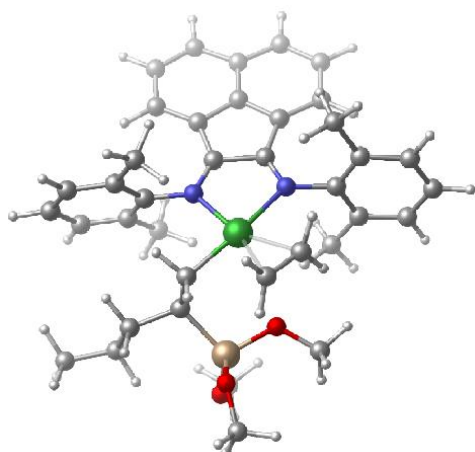
|                                              |                             |            |             |
|----------------------------------------------|-----------------------------|------------|-------------|
| Zero-point correction=                       | 0.718050 (Hartree/Particle) |            |             |
| Thermal correction to Energy=                | 0.763517                    |            |             |
| Thermal correction to Enthalpy=              | 0.764461                    |            |             |
| Thermal correction to Gibbs Free Energy=     | 0.636712                    |            |             |
| Sum of electronic and zero-point Energies=   | -2191.065410                |            |             |
| Sum of electronic and thermal Energies=      | -2191.019943                |            |             |
| Sum of electronic and thermal Enthalpies=    | -2191.018999                |            |             |
| Sum of electronic and thermal Free Energies= | -2191.146748                |            |             |
| Ni                                           | -2.63037700                 | 3.72982400 | 0.33954500  |
| N                                            | -0.99106000                 | 2.68242200 | -0.33172400 |
| N                                            | -3.49684400                 | 1.86317700 | 0.23787000  |
| C                                            | 0.29937700                  | 3.23676800 | -0.58517800 |
| C                                            | 0.65376900                  | 3.62522400 | -1.89064800 |
| C                                            | 1.14344700                  | 3.45066100 | 0.52055400  |
| C                                            | 1.88447500                  | 4.27016500 | -2.06267800 |
| C                                            | 2.36298800                  | 4.09890100 | 0.30027000  |
| C                                            | 2.72952400                  | 4.51442700 | -0.97998700 |
| H                                            | 2.17686200                  | 4.58691000 | -3.06020300 |
| H                                            | 3.03053500                  | 4.27089700 | 1.14040500  |
| H                                            | 3.67599800                  | 5.02349300 | -1.13520500 |
| C                                            | -4.86007200                 | 1.58584500 | 0.54057500  |
| C                                            | -5.79787700                 | 1.36085200 | -0.48731800 |
| C                                            | -5.23677800                 | 1.66659000 | 1.89723000  |
| C                                            | -7.13400800                 | 1.17028500 | -0.11144600 |
| C                                            | -6.57711900                 | 1.45211800 | 2.22270600  |
| C                                            | -7.52207700                 | 1.20266100 | 1.22645600  |
| H                                            | -7.87722700                 | 1.00194300 | -0.88618600 |
| H                                            | -6.88272500                 | 1.49234100 | 3.26450200  |
| H                                            | -8.56353500                 | 1.04973000 | 1.49278300  |
| C                                            | 0.76669000                  | 2.92074400 | 1.88256200  |
| H                                            | 0.96030600                  | 1.84191900 | 1.94665300  |
| H                                            | 1.34296800                  | 3.40770100 | 2.67436000  |
| H                                            | -0.29903500                 | 3.05886500 | 2.09148300  |
| C                                            | -0.24894900                 | 3.34200200 | -3.06714500 |

|    |             |            |             |
|----|-------------|------------|-------------|
| H  | -0.19914600 | 2.28433800 | -3.35643500 |
| H  | -1.29596900 | 3.56135300 | -2.83823700 |
| H  | 0.04435600  | 3.93550800 | -3.93731800 |
| C  | -4.20875600 | 1.98018900 | 2.95662600  |
| H  | -3.76198100 | 2.97203800 | 2.78918200  |
| H  | -4.65921800 | 1.98741100 | 3.95273800  |
| H  | -3.38596300 | 1.25587500 | 2.95888500  |
| C  | -5.40593900 | 1.34239000 | -1.94610300 |
| H  | -4.61569400 | 2.06713900 | -2.16481600 |
| H  | -5.03538500 | 0.35649000 | -2.25302100 |
| H  | -6.26657100 | 1.57973800 | -2.57757800 |
| C  | -2.69331100 | 0.99780400 | -0.28566600 |
| C  | -1.29291500 | 1.45771200 | -0.59975900 |
| C  | -3.90231700 | 6.17210000 | -0.68770100 |
| H  | -3.96904600 | 6.87457400 | -1.53604700 |
| C  | -3.41024500 | 4.80948000 | -1.20690900 |
| H  | -4.22431700 | 4.22164200 | -1.64838700 |
| C  | -5.30808500 | 6.10282700 | -0.04151800 |
| H  | -6.00358400 | 5.70272200 | -0.79402600 |
| H  | -5.65077700 | 7.11764700 | 0.19475300  |
| C  | -5.40899000 | 5.24161000 | 1.22425600  |
| H  | -5.02220300 | 4.23446100 | 1.00752600  |
| C  | -6.84425500 | 5.09956900 | 1.73659300  |
| H  | -7.48216900 | 4.62303800 | 0.98334800  |
| H  | -6.88405600 | 4.48356000 | 2.64116100  |
| H  | -7.27371600 | 6.07978500 | 1.97409100  |
| H  | -4.77432000 | 5.66487500 | 2.01339600  |
| H  | -2.60655400 | 4.91827200 | -1.94248800 |
| Si | -2.60868800 | 6.87949400 | 0.46438700  |
| O  | -3.21229700 | 7.94079100 | 1.54796200  |
| O  | -1.28188800 | 7.56121500 | -0.22523000 |
| O  | -2.09475200 | 5.47533400 | 1.31743900  |
| C  | -2.64658500 | 9.17229100 | 2.00812700  |
| H  | -3.41947100 | 9.94414100 | 1.95903000  |
| H  | -2.32642000 | 9.05647600 | 3.04965800  |
| H  | -1.79063700 | 9.47449800 | 1.39709700  |
| C  | -0.25127300 | 6.86164800 | -0.92289100 |
| H  | 0.16966700  | 6.05631600 | -0.31144600 |
| H  | -0.62751100 | 6.43251600 | -1.85928700 |
| H  | 0.53885300  | 7.57836700 | -1.15914600 |
| C  | -1.34514100 | 5.60047100 | 2.54071800  |
| H  | -1.66618800 | 6.49621200 | 3.07893100  |
| H  | -1.54933000 | 4.72229600 | 3.15726900  |
| H  | -0.27535200 | 5.65608900 | 2.31943700  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -3.42592600 | -2.71631700 | -0.96132900 |
| C | -2.17244500 | -3.05309800 | -1.44978100 |
| C | -1.14599500 | -2.07234100 | -1.54555300 |
| C | -1.48501400 | -0.77167600 | -1.12881400 |
| C | -2.77355200 | -0.42148300 | -0.63533900 |
| C | -3.74971100 | -1.39864800 | -0.54652100 |
| H | 0.50193800  | -3.24183200 | -2.34749600 |
| H | -4.19098600 | -3.48345500 | -0.89386400 |
| H | -1.96801300 | -4.07405700 | -1.76008600 |
| C | 0.18671300  | -2.25890000 | -2.00837400 |
| C | -0.56404400 | 0.31253200  | -1.14308900 |
| H | -4.74273100 | -1.17403300 | -0.17289400 |
| C | 0.72741600  | 0.10180400  | -1.59330600 |
| C | 1.08369100  | -1.20105200 | -2.02737900 |
| H | 1.45632400  | 0.90452500  | -1.61794000 |
| H | 2.09483200  | -1.37121300 | -2.38374000 |

UB3LYP-D3/BSII(SMD)//B3LYP-D3/BSI

HF=-2193.9751616



|                                              |                             |             |             |
|----------------------------------------------|-----------------------------|-------------|-------------|
| Zero-point correction=                       | 0.776001 (Hartree/Particle) |             |             |
| Thermal correction to Energy=                | 0.824220                    |             |             |
| Thermal correction to Enthalpy=              | 0.825164                    |             |             |
| Thermal correction to Gibbs Free Energy=     | 0.693177                    |             |             |
| Sum of electronic and zero-point Energies=   | -2269.605266                |             |             |
| Sum of electronic and thermal Energies=      | -2269.557047                |             |             |
| Sum of electronic and thermal Enthalpies=    | -2269.556102                |             |             |
| Sum of electronic and thermal Free Energies= | -2269.688090                |             |             |
| Ni                                           | -0.02345600                 | 1.05827700  | -0.07128200 |
| N                                            | 1.29537300                  | -0.49120100 | -0.15705400 |
| N                                            | -1.38614100                 | -0.54778200 | -0.21229900 |
| C                                            | 2.73001500                  | -0.45517800 | -0.17540200 |
| C                                            | 3.41026200                  | -0.67962100 | -1.38672100 |
| C                                            | 3.40085200                  | -0.17090400 | 1.02881800  |
| C                                            | 4.80583700                  | -0.56888700 | -1.37351700 |
| C                                            | 4.79570900                  | -0.07907400 | 0.99388400  |
| C                                            | 5.49430600                  | -0.26568900 | -0.19928800 |
| H                                            | 5.35419400                  | -0.72351300 | -2.29871300 |
| H                                            | 5.33397100                  | 0.14277300  | 1.91110700  |
| H                                            | 6.57664200                  | -0.17944500 | -0.21311400 |
| C                                            | -2.81380300                 | -0.54864000 | -0.35693700 |
| C                                            | -3.33751100                 | -0.36718600 | -1.64867700 |
| C                                            | -3.62627900                 | -0.70378000 | 0.77872800  |
| C                                            | -4.72930200                 | -0.32129200 | -1.78373500 |
| C                                            | -5.01333900                 | -0.64891600 | 0.59533100  |
| C                                            | -5.56239300                 | -0.45482200 | -0.67212000 |
| H                                            | -5.15950400                 | -0.18508000 | -2.77237900 |
| H                                            | -5.66431800                 | -0.76096300 | 1.45814200  |
| H                                            | -6.64049700                 | -0.41142600 | -0.79426500 |
| C                                            | 2.62565400                  | -0.01623200 | 2.31429900  |
| H                                            | 2.18249300                  | -0.97165600 | 2.62378100  |

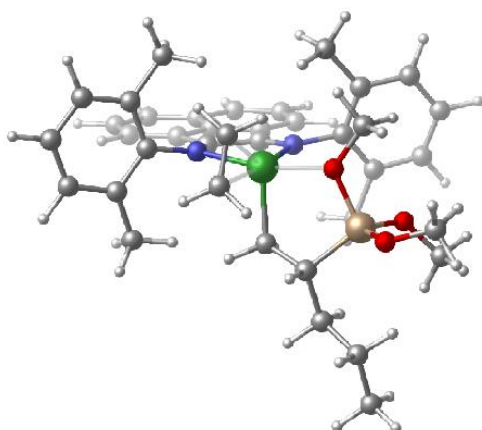
|    |             |             |             |
|----|-------------|-------------|-------------|
| H  | 3.27054600  | 0.33302200  | 3.12488300  |
| H  | 1.79644000  | 0.69325700  | 2.19949200  |
| C  | 2.68888700  | -1.09292700 | -2.64901300 |
| H  | 2.53255400  | -2.17934200 | -2.66625000 |
| H  | 1.70371800  | -0.62610900 | -2.74189300 |
| H  | 3.27412400  | -0.83014700 | -3.53457400 |
| C  | -3.02081200 | -0.96833700 | 2.13720500  |
| H  | -2.18230200 | -0.29556900 | 2.35399500  |
| H  | -3.76538600 | -0.85268100 | 2.92924100  |
| H  | -2.62569800 | -1.99075000 | 2.19857600  |
| C  | -2.41259600 | -0.27814700 | -2.83835600 |
| H  | -1.62697800 | 0.47021300  | -2.68577100 |
| H  | -1.91362900 | -1.23996900 | -3.01740000 |
| H  | -2.96544400 | -0.02071100 | -3.74632400 |
| C  | -0.77262500 | -1.67921700 | -0.21634800 |
| C  | 0.72158000  | -1.64798800 | -0.14730400 |
| C  | 1.85913800  | 2.39300200  | -1.73136900 |
| H  | 1.80776500  | 1.38348600  | -2.15644200 |
| C  | 1.48057900  | 2.33571100  | -0.24311900 |
| H  | 2.26249000  | 1.84327800  | 0.33817200  |
| C  | 3.33639200  | 2.86518700  | -1.85996900 |
| H  | 3.41512800  | 3.91695000  | -1.55323100 |
| H  | 1.37300100  | 3.34107000  | 0.16323500  |
| Si | 0.64888900  | 3.45144800  | -2.69180800 |
| O  | 1.01064800  | 3.75643100  | -4.27461500 |
| O  | -0.81448600 | 2.64449200  | -2.61994300 |
| O  | 0.53990900  | 4.91240900  | -1.93731900 |
| C  | 0.92454200  | 2.78520700  | -5.31403200 |
| H  | 1.81731400  | 2.14726300  | -5.32246100 |
| H  | 0.03511900  | 2.15151700  | -5.20103100 |
| H  | 0.86328600  | 3.31430800  | -6.26887000 |
| C  | -2.01666500 | 3.27788900  | -3.06091000 |
| H  | -1.94542700 | 3.58764200  | -4.11091000 |
| H  | -2.83622200 | 2.55977200  | -2.96332500 |
| H  | -2.24418800 | 4.15861700  | -2.44682200 |
| C  | 0.28853400  | 6.17947100  | -2.54993700 |
| H  | 0.73391100  | 6.23304200  | -3.54826200 |
| H  | -0.79099800 | 6.35783900  | -2.62980400 |
| H  | 0.72797000  | 6.95351700  | -1.91495100 |
| C  | -2.38188100 | -5.16607300 | -0.42331100 |
| C  | -1.20776800 | -5.89916000 | -0.34017800 |
| C  | 0.05013700  | -5.24339600 | -0.23009700 |
| C  | 0.02085400  | -3.83616000 | -0.21315600 |
| C  | -1.18463600 | -3.08313100 | -0.28959600 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -2.39426200 | -3.74754900 | -0.39770700 |
| H | 1.41587600  | -6.93235400 | -0.14012400 |
| H | -3.32824700 | -5.69092100 | -0.50858400 |
| H | -1.24452900 | -6.98490100 | -0.35897600 |
| C | 1.33377200  | -5.84895700 | -0.13401800 |
| C | 1.19402500  | -3.03385300 | -0.11927400 |
| H | -3.33338100 | -3.21002800 | -0.46116900 |
| C | 2.42988600  | -3.65169800 | -0.02653500 |
| C | 2.47623500  | -5.06935100 | -0.03214100 |
| H | 3.34692800  | -3.07867500 | 0.04702400  |
| H | 3.44370200  | -5.55594400 | 0.04258900  |
| H | 3.93240000  | 2.28844600  | -1.13981500 |
| C | -1.87521600 | 2.19783500  | 0.41280200  |
| H | -2.27355000 | 1.59003800  | 1.21762300  |
| H | -2.39941700 | 2.15372400  | -0.53595600 |
| C | -0.91565200 | 3.12580300  | 0.64652400  |
| H | -0.64788400 | 3.86024500  | -0.10354100 |
| H | -0.48494900 | 3.25445400  | 1.63559000  |
| C | 3.95531600  | 2.67963300  | -3.25308900 |
| H | 3.76367200  | 1.65114800  | -3.59336800 |
| H | 3.46499700  | 3.34457900  | -3.97254200 |
| C | 5.46511900  | 2.93856500  | -3.24856200 |
| H | 5.89626400  | 2.80924000  | -4.24744800 |
| H | 5.68890500  | 3.95991500  | -2.91838100 |
| H | 5.97778700  | 2.24911300  | -2.56633400 |

UB3LYP-D3/BSII(SMD)//B3LYP-D3/BSI

HF=-2193.9751616

<sup>3</sup>I



|                                              |                             |            |             |
|----------------------------------------------|-----------------------------|------------|-------------|
| Zero-point correction=                       | 0.772437 (Hartree/Particle) |            |             |
| Thermal correction to Energy=                | 0.820781                    |            |             |
| Thermal correction to Enthalpy=              | 0.821725                    |            |             |
| Thermal correction to Gibbs Free Energy=     | 0.688853                    |            |             |
| Sum of electronic and zero-point Energies=   | -2269.617155                |            |             |
| Sum of electronic and thermal Energies=      | -2269.568811                |            |             |
| Sum of electronic and thermal Enthalpies=    | -2269.567867                |            |             |
| Sum of electronic and thermal Free Energies= | -2269.700739                |            |             |
| Ni                                           | -2.69353500                 | 3.87487300 | -0.04985700 |
| N                                            | -1.03511900                 | 2.58894400 | -0.33832800 |
| N                                            | -3.69269500                 | 2.05726100 | -0.47275400 |
| C                                            | 0.34265200                  | 2.95223000 | -0.47200300 |
| C                                            | 0.74836500                  | 3.40157600 | -1.74193900 |
| C                                            | 1.22737800                  | 2.88112100 | 0.61666400  |
| C                                            | 2.07798100                  | 3.80340000 | -1.90648900 |
| C                                            | 2.55047100                  | 3.28371200 | 0.40393100  |
| C                                            | 2.97528100                  | 3.74807000 | -0.84061500 |
| H                                            | 2.40973200                  | 4.15022600 | -2.88162000 |
| H                                            | 3.25360800                  | 3.23186500 | 1.23109300  |
| H                                            | 4.00612100                  | 4.05931800 | -0.98133800 |
| C                                            | -5.08810700                 | 1.86689700 | -0.72700900 |
| C                                            | -5.50981500                 | 1.98898700 | -2.06808700 |
| C                                            | -5.98866300                 | 1.61600400 | 0.32139300  |
| C                                            | -6.87817800                 | 1.90312900 | -2.33671400 |
| C                                            | -7.35226600                 | 1.54125400 | 0.00304500  |
| C                                            | -7.79783400                 | 1.69308500 | -1.30770100 |
| H                                            | -7.22259000                 | 1.99627800 | -3.36318800 |
| H                                            | -8.06648800                 | 1.35416900 | 0.80086200  |
| H                                            | -8.85900300                 | 1.63717100 | -1.53095800 |
| C                                            | 0.77042200                  | 2.39852400 | 1.96978300  |
| H                                            | 0.25896400                  | 1.43133000 | 1.91282700  |
| H                                            | 1.61918600                  | 2.28762700 | 2.65044900  |

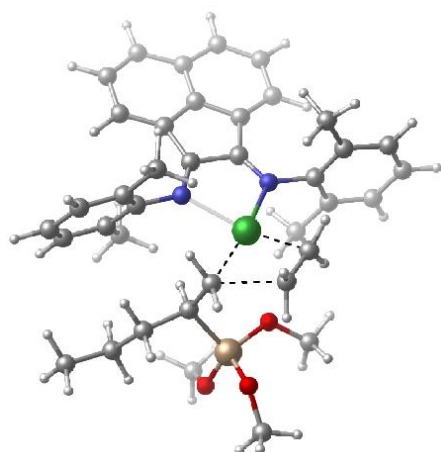
|    |             |             |             |
|----|-------------|-------------|-------------|
| H  | 0.07400100  | 3.11439100  | 2.41514200  |
| C  | -0.22288500 | 3.39539100  | -2.89775600 |
| H  | -1.19537100 | 3.81418300  | -2.61049900 |
| H  | 0.16441800  | 3.96712100  | -3.74573400 |
| H  | -0.41833000 | 2.37243100  | -3.24504600 |
| C  | -5.52201200 | 1.35146300  | 1.73351900  |
| H  | -4.51536000 | 1.72923500  | 1.91555900  |
| H  | -6.19767400 | 1.80611500  | 2.46532700  |
| H  | -5.50746900 | 0.27213800  | 1.93443600  |
| C  | -4.49792000 | 2.13629600  | -3.18119900 |
| H  | -3.96352500 | 1.19189600  | -3.34885100 |
| H  | -4.98253900 | 2.41468100  | -4.12103400 |
| H  | -3.73362600 | 2.88724100  | -2.94872500 |
| C  | -2.87789100 | 1.06108600  | -0.47666800 |
| C  | -1.40088200 | 1.35567100  | -0.40987200 |
| C  | -2.33328400 | 5.16931000  | 2.67410100  |
| H  | -3.19666300 | 5.85126300  | 2.70333000  |
| C  | -2.77540400 | 3.85652400  | 2.01295100  |
| H  | -2.11977700 | 3.02105400  | 2.28170600  |
| C  | -1.86976800 | 4.95440000  | 4.13907500  |
| H  | -2.65049700 | 4.38457300  | 4.66240000  |
| H  | -3.80061000 | 3.60268800  | 2.29609100  |
| Si | -1.09245400 | 6.08784600  | 1.62171000  |
| O  | -1.27517500 | 7.70774100  | 1.83127400  |
| O  | -1.51047300 | 5.66541600  | 0.03022200  |
| O  | 0.49154700  | 5.64628700  | 1.71586100  |
| C  | -0.33357400 | 8.74121600  | 1.54713100  |
| H  | 0.61227500  | 8.34397300  | 1.15886300  |
| H  | -0.76237500 | 9.42508700  | 0.80698200  |
| H  | -0.13202900 | 9.30053700  | 2.46654400  |
| C  | -0.86246200 | 6.32055900  | -1.07467200 |
| H  | -0.94480000 | 7.40681700  | -0.96596900 |
| H  | 0.18721400  | 6.02158900  | -1.12831100 |
| H  | -1.37328700 | 6.01777300  | -1.99071600 |
| C  | 1.41606500  | 5.87626900  | 2.77300500  |
| H  | 1.43915700  | 6.93120000  | 3.07229800  |
| H  | 1.17107100  | 5.26695200  | 3.65082200  |
| H  | 2.40694300  | 5.59016600  | 2.41028800  |
| C  | -3.85087200 | -2.62978400 | -0.92599300 |
| C  | -2.56320800 | -3.14361400 | -0.96044800 |
| C  | -1.43605800 | -2.28414500 | -0.83585200 |
| C  | -1.71153100 | -0.91387400 | -0.67055300 |
| C  | -3.03180300 | -0.38616100 | -0.63632100 |
| C  | -4.10997400 | -1.24378600 | -0.76706000 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 0.20996400  | -3.69670200 | -0.98792900 |
| H | -4.69341200 | -3.30701000 | -1.02591400 |
| H | -2.40952700 | -4.21184500 | -1.08645400 |
| C | -0.06187600 | -2.65180500 | -0.86585200 |
| C | -0.69674600 | 0.07611500  | -0.54392400 |
| H | -5.13044400 | -0.87758800 | -0.75186500 |
| C | 0.63185400  | -0.31045900 | -0.58330900 |
| C | 0.92832200  | -1.68891700 | -0.74408700 |
| H | 1.43523000  | 0.41155000  | -0.49339500 |
| H | 1.96960000  | -1.99459700 | -0.77279900 |
| H | -0.97918300 | 4.30919300  | 4.14845100  |
| C | -4.34956200 | 5.26150300  | -1.22029700 |
| H | -3.70479900 | 6.04477700  | -1.60721500 |
| H | -4.76603800 | 4.55682300  | -1.93124800 |
| C | -4.70209300 | 5.22430300  | 0.08068500  |
| H | -5.40142800 | 4.48113100  | 0.45289700  |
| H | -4.36038400 | 5.97987700  | 0.77969800  |
| C | -1.58214500 | 6.24156100  | 4.92593700  |
| H | -0.80238900 | 6.82892400  | 4.42202700  |
| H | -2.47919300 | 6.87481200  | 4.91895400  |
| C | -1.15169200 | 5.95771400  | 6.36830000  |
| H | -0.95960400 | 6.88564300  | 6.91748100  |
| H | -1.92709500 | 5.40262400  | 6.90945000  |
| H | -0.23426400 | 5.35615600  | 6.39594400  |

UB3LYP-D3/BSII(SMD)//B3LYP-D3/BSI

HF=-2272.6038475

# <sup>1</sup>TS4



Zero-point correction= 0.776360 (Hartree/Particle)

Thermal correction to Energy= 0.823771

Thermal correction to Enthalpy= 0.824715

Thermal correction to Gibbs Free Energy= 0.694544

Sum of electronic and zero-point Energies= -2269.596820

Sum of electronic and thermal Energies= -2269.549408

Sum of electronic and thermal Enthalpies= -2269.548464

Sum of electronic and thermal Free Energies= -2269.678636

|    |             |             |             |
|----|-------------|-------------|-------------|
| Ni | -0.20003900 | 1.02335800  | -0.05634500 |
| N  | 1.34016700  | -0.57338100 | -0.20245300 |
| N  | -1.36043400 | -0.58367700 | -0.19502300 |
| C  | 2.76172400  | -0.46944300 | -0.19519900 |
| C  | 3.48361200  | -0.63777300 | -1.39394300 |
| C  | 3.38727800  | -0.12540100 | 1.01878700  |
| C  | 4.86682400  | -0.43371000 | -1.35155300 |
| C  | 4.77300100  | 0.06792400  | 1.01053600  |
| C  | 5.50868100  | -0.07858200 | -0.16467500 |
| H  | 5.44355700  | -0.54736400 | -2.26524000 |
| H  | 5.27500800  | 0.33129500  | 1.93746500  |
| H  | 6.58255700  | 0.08188900  | -0.15690400 |
| C  | -2.79479500 | -0.55504200 | -0.24738500 |
| C  | -3.40557500 | -0.37410900 | -1.49907600 |
| C  | -3.52131200 | -0.67172500 | 0.94785500  |
| C  | -4.80287000 | -0.31229400 | -1.53334400 |
| C  | -4.91708900 | -0.60339700 | 0.86555500  |
| C  | -5.55427000 | -0.42492300 | -0.36254100 |
| H  | -5.30220100 | -0.17610300 | -2.48894900 |
| H  | -5.50459000 | -0.69018100 | 1.77554600  |
| H  | -6.63794900 | -0.37169300 | -0.40729900 |
| C  | 2.58790700  | -0.04708000 | 2.29802000  |
| H  | 2.30501400  | -1.05023000 | 2.64311000  |

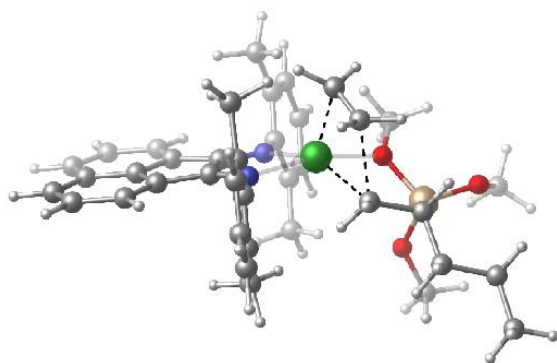
|    |             |             |             |
|----|-------------|-------------|-------------|
| H  | 3.16450500  | 0.42953900  | 3.09543800  |
| H  | 1.65267100  | 0.51044200  | 2.16503800  |
| C  | 2.80108600  | -1.05017200 | -2.67738200 |
| H  | 2.54227500  | -2.11625900 | -2.66453900 |
| H  | 1.86957000  | -0.49852800 | -2.84550300 |
| H  | 3.45512200  | -0.87985100 | -3.53681100 |
| C  | -2.81048100 | -0.89578300 | 2.26048600  |
| H  | -1.98125800 | -0.19033000 | 2.39502100  |
| H  | -3.49659100 | -0.78659400 | 3.10455200  |
| H  | -2.37801900 | -1.90367900 | 2.30970600  |
| C  | -2.56507200 | -0.27998700 | -2.74907900 |
| H  | -1.77921500 | 0.47773800  | -2.64718700 |
| H  | -2.06707700 | -1.23509400 | -2.96233900 |
| H  | -3.18054900 | -0.02848000 | -3.61751500 |
| C  | -0.75088000 | -1.71793700 | -0.27883700 |
| C  | 0.75236800  | -1.71536700 | -0.25418500 |
| C  | 1.73156600  | 2.48065600  | -1.59927100 |
| H  | 1.67857800  | 1.43832900  | -1.93703800 |
| C  | 1.28269600  | 2.56816300  | -0.13341800 |
| H  | 1.86144900  | 1.91892000  | 0.53195100  |
| C  | 3.22730900  | 2.91156100  | -1.65325700 |
| H  | 3.30584000  | 3.97600700  | -1.39295100 |
| H  | 1.43828900  | 3.57958800  | 0.23322900  |
| Si | 0.61823800  | 3.46829200  | -2.74453100 |
| O  | 1.11980400  | 3.60847100  | -4.31046800 |
| O  | -0.85377000 | 2.68793200  | -2.71019800 |
| O  | 0.50847400  | 4.99409800  | -2.13563300 |
| C  | 1.07978000  | 2.54894000  | -5.26333200 |
| H  | 1.96161600  | 1.90427400  | -5.15871500 |
| H  | 0.17479600  | 1.93836900  | -5.14907600 |
| H  | 1.08553100  | 2.99098000  | -6.26323800 |
| C  | -2.03776700 | 3.30143400  | -3.22178000 |
| H  | -1.95020800 | 3.50779400  | -4.29579200 |
| H  | -2.87189800 | 2.61194400  | -3.06372900 |
| H  | -2.25256200 | 4.24015700  | -2.69567200 |
| C  | 0.31251900  | 6.20226500  | -2.87642700 |
| H  | 0.82933600  | 6.16336500  | -3.84039100 |
| H  | -0.75660600 | 6.37589100  | -3.04924000 |
| H  | 0.71319000  | 7.02830900  | -2.28298900 |
| C  | -2.43425000 | -5.16410900 | -0.53182500 |
| C  | -1.27276500 | -5.92188100 | -0.52014500 |
| C  | 0.00165000  | -5.29420800 | -0.43895900 |
| C  | 0.00102300  | -3.88798000 | -0.37642100 |
| C  | -1.19133300 | -3.10922100 | -0.38226300 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -2.41763900 | -3.74715400 | -0.46097100 |
| H | 1.33666000  | -7.00988900 | -0.45620500 |
| H | -3.39360500 | -5.66815500 | -0.59485000 |
| H | -1.33261100 | -7.00551600 | -0.57241400 |
| C | 1.27618300  | -5.92598200 | -0.41116500 |
| C | 1.19157400  | -3.11343100 | -0.29611800 |
| H | -3.34746400 | -3.19002500 | -0.46838200 |
| C | 2.41757100  | -3.75429000 | -0.26974000 |
| C | 2.43707300  | -5.17187800 | -0.32640700 |
| H | 3.34604600  | -3.19722200 | -0.21014700 |
| H | 3.39672500  | -5.67882800 | -0.30476600 |
| H | 3.76380500  | 2.35933100  | -0.86980200 |
| C | -1.70634600 | 2.23089500  | 0.33092900  |
| H | -2.17119800 | 1.82088900  | 1.22661500  |
| H | -2.33009000 | 2.22876900  | -0.56014800 |
| C | -0.70638000 | 3.21739600  | 0.46652200  |
| H | -0.61553600 | 3.99763400  | -0.27943600 |
| H | -0.37182000 | 3.48570600  | 1.46441400  |
| C | 3.93416800  | 2.65628900  | -2.99263300 |
| H | 3.76392400  | 1.61340300  | -3.29345300 |
| H | 3.49463100  | 3.28536900  | -3.77363100 |
| C | 5.44027200  | 2.91940700  | -2.89989300 |
| H | 5.93608900  | 2.73779100  | -3.85986700 |
| H | 5.64175100  | 3.95814300  | -2.61228800 |
| H | 5.90530600  | 2.26948200  | -2.14911700 |

UB3LYP-D3/BSII(SMD)//B3LYP-D3/BSI

HF=-2272.5778781

### <sup>3</sup>TS4



|                                              |                             |
|----------------------------------------------|-----------------------------|
| Zero-point correction=                       | 0.773501 (Hartree/Particle) |
| Thermal correction to Energy=                | 0.821523                    |
| Thermal correction to Enthalpy=              | 0.822467                    |
| Thermal correction to Gibbs Free Energy=     | 0.688719                    |
| Sum of electronic and zero-point Energies=   | -2269.589533                |
| Sum of electronic and thermal Energies=      | -2269.541511                |
| Sum of electronic and thermal Enthalpies=    | -2269.540567                |
| Sum of electronic and thermal Free Energies= | -2269.674315                |

|    |             |            |             |
|----|-------------|------------|-------------|
| Ni | -2.20751600 | 3.78078900 | -0.18183600 |
| N  | -0.72737200 | 2.42535100 | -0.76910300 |
| N  | -3.36387000 | 1.96160300 | -0.28916100 |
| C  | 0.64680600  | 2.73278600 | -1.01503400 |
| C  | 1.04331900  | 3.10552700 | -2.31095700 |
| C  | 1.53180200  | 2.71891500 | 0.07615800  |
| C  | 2.37987300  | 3.47365900 | -2.50071300 |
| C  | 2.86068400  | 3.08736300 | -0.16212200 |
| C  | 3.28346400  | 3.46534100 | -1.43725600 |
| H  | 2.71019000  | 3.77068000 | -3.49248900 |
| H  | 3.56681300  | 3.07717500 | 0.66390700  |
| H  | 4.31756500  | 3.75277700 | -1.60281700 |
| C  | -4.71542900 | 1.76573500 | 0.13625600  |
| C  | -5.77824100 | 1.98165100 | -0.75826200 |
| C  | -4.92755900 | 1.40299200 | 1.48182900  |
| C  | -7.08244400 | 1.85550500 | -0.26187000 |
| C  | -6.24651900 | 1.29878300 | 1.93295000  |
| C  | -7.31959700 | 1.53046400 | 1.07199900  |
| H  | -7.91849000 | 2.01050700 | -0.93891800 |
| H  | -6.42995900 | 1.02353500 | 2.96813300  |
| H  | -8.33843100 | 1.44333900 | 1.43736300  |
| C  | 1.04613200  | 2.32044300 | 1.44737800  |
| H  | 0.61766900  | 1.31069300 | 1.44363200  |
| H  | 1.86595300  | 2.33419300 | 2.17119600  |
| H  | 0.27214000  | 3.00969900 | 1.80442400  |
| C  | 0.04708900  | 3.11553700 | -3.44531200 |

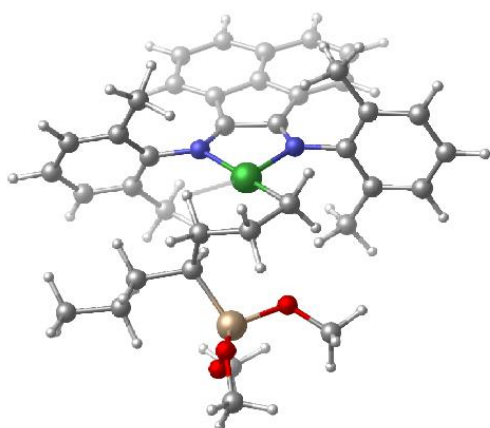
|    |             |             |             |
|----|-------------|-------------|-------------|
| H  | -0.85719000 | 3.67328300  | -3.17311900 |
| H  | 0.47668200  | 3.56860000  | -4.34277000 |
| H  | -0.27311700 | 2.09851500  | -3.70556100 |
| C  | -3.76468500 | 1.08050100  | 2.39095000  |
| H  | -2.97248200 | 1.83582900  | 2.33710900  |
| H  | -4.09065600 | 1.00216200  | 3.43159100  |
| H  | -3.30336300 | 0.12346600  | 2.11381400  |
| C  | -5.54642800 | 2.31624800  | -2.21402800 |
| H  | -6.37574300 | 1.95224000  | -2.82780400 |
| H  | -5.47845000 | 3.39866300  | -2.37527000 |
| H  | -4.62390600 | 1.87097500  | -2.59802000 |
| C  | -2.64401900 | 0.97942600  | -0.70301300 |
| C  | -1.19100200 | 1.24586400  | -1.00539100 |
| C  | -3.02400200 | 5.99540200  | 2.14233500  |
| H  | -3.42322000 | 6.91096200  | 1.67998000  |
| C  | -3.60494800 | 4.78142300  | 1.42646700  |
| H  | -3.18769500 | 3.83518700  | 1.80475000  |
| C  | -3.46113900 | 6.00339400  | 3.63320800  |
| H  | -4.55444300 | 5.89547100  | 3.67186000  |
| H  | -4.68819400 | 4.70240400  | 1.51270000  |
| Si | -1.16470300 | 6.07448900  | 1.92576800  |
| O  | -0.63977200 | 7.62500700  | 2.00465600  |
| O  | -0.87742800 | 5.43269600  | 0.38973000  |
| O  | -0.30556900 | 5.07188700  | 2.91937500  |
| C  | 0.69362600  | 8.08289400  | 2.23490000  |
| H  | 1.39204800  | 7.25505900  | 2.40795800  |
| H  | 1.03182300  | 8.65618500  | 1.36581600  |
| H  | 0.69451100  | 8.73754300  | 3.11194200  |
| C  | 0.19788000  | 5.90888000  | -0.44381900 |
| H  | 0.20886500  | 7.00247400  | -0.44585600 |
| H  | 1.15612500  | 5.51625700  | -0.09333900 |
| H  | 0.01635500  | 5.54390800  | -1.45424500 |
| C  | 0.00068700  | 5.25984800  | 4.30043800  |
| H  | 0.35061900  | 6.27903600  | 4.50320800  |
| H  | -0.87379900 | 5.05679700  | 4.92842000  |
| H  | 0.79567800  | 4.55682400  | 4.56320400  |
| C  | -3.84140400 | -2.63403800 | -1.22964300 |
| C  | -2.63502800 | -3.15095400 | -1.67815200 |
| C  | -1.48604500 | -2.31884500 | -1.79076300 |
| C  | -1.65584600 | -0.97015300 | -1.42700700 |
| C  | -2.89233100 | -0.43990100 | -0.96562200 |
| C  | -3.99390200 | -1.27099400 | -0.86511200 |
| H  | 0.00447300  | -3.72275800 | -2.52269700 |
| H  | -4.70212900 | -3.29110900 | -1.15286700 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -2.56264500 | -4.20132300 | -1.94670800 |
| C | -0.18482500 | -2.69430400 | -2.22763700 |
| C | -0.60596400 | -0.01037500 | -1.47946800 |
| H | -4.95210800 | -0.90072900 | -0.51785200 |
| C | 0.65064300  | -0.40462600 | -1.90524900 |
| C | 0.83946000  | -1.76071500 | -2.27860000 |
| H | 1.47645700  | 0.29583100  | -1.95792100 |
| H | 1.82314000  | -2.07322900 | -2.61507800 |
| H | -3.05736200 | 5.11314200  | 4.13614500  |
| C | -3.04089800 | 4.90204500  | -1.73492300 |
| H | -2.28075800 | 5.60583600  | -2.06479700 |
| H | -3.35942000 | 4.16694200  | -2.46798600 |
| C | -3.91718200 | 5.27348300  | -0.67904200 |
| H | -4.89352100 | 4.80177900  | -0.65108700 |
| H | -3.89484400 | 6.30216500  | -0.33640000 |
| C | -3.06440600 | 7.26681800  | 4.41225200  |
| H | -1.97529800 | 7.40424600  | 4.38700100  |
| H | -3.48485900 | 8.14589400  | 3.90624600  |
| C | -3.53896100 | 7.22251500  | 5.86781800  |
| H | -3.25844900 | 8.13425800  | 6.40573400  |
| H | -4.62928600 | 7.12208700  | 5.92493200  |
| H | -3.09962500 | 6.37022400  | 6.40150600  |

UB3LYP-D3/BSII(SMD)/B3LYP-D3/BSI

HF=-2272.5761181

1J



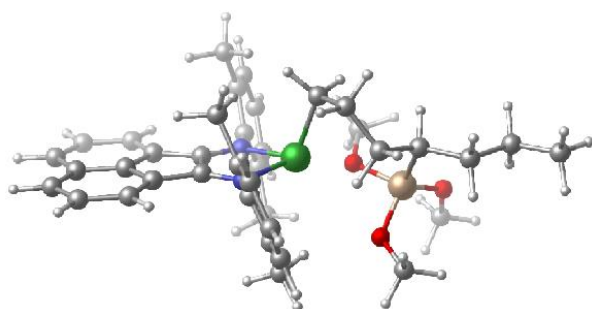
|                                              |                             |             |             |
|----------------------------------------------|-----------------------------|-------------|-------------|
| Zero-point correction=                       | 0.776524 (Hartree/Particle) |             |             |
| Thermal correction to Energy=                | 0.824233                    |             |             |
| Thermal correction to Enthalpy=              | 0.825178                    |             |             |
| Thermal correction to Gibbs Free Energy=     | 0.693459                    |             |             |
| Sum of electronic and zero-point Energies=   | -2269.618371                |             |             |
| Sum of electronic and thermal Energies=      | -2269.570661                |             |             |
| Sum of electronic and thermal Enthalpies=    | -2269.569717                |             |             |
| Sum of electronic and thermal Free Energies= | -2269.701436                |             |             |
| Ni                                           | -0.05949800                 | 0.78615000  | 0.04744800  |
| N                                            | 1.39640400                  | -0.68211500 | -0.07844600 |
| N                                            | -1.26989700                 | -0.65912400 | -0.13958700 |
| C                                            | 2.81456600                  | -0.53876400 | -0.09713600 |
| C                                            | 3.51869000                  | -0.71831800 | -1.30438900 |
| C                                            | 3.44721500                  | -0.13371300 | 1.09355300  |
| C                                            | 4.89965100                  | -0.49607300 | -1.28622600 |
| C                                            | 4.82931400                  | 0.07647800  | 1.06077400  |
| C                                            | 5.55267800                  | -0.10367700 | -0.11786200 |
| H                                            | 5.46377900                  | -0.61683700 | -2.20669100 |
| H                                            | 5.33943200                  | 0.37993400  | 1.97080400  |
| H                                            | 6.62459600                  | 0.06905600  | -0.12877400 |
| C                                            | -2.69835100                 | -0.56282100 | -0.21618100 |
| C                                            | -3.27956200                 | -0.34446300 | -1.47601600 |
| C                                            | -3.44315700                 | -0.65151400 | 0.96972900  |
| C                                            | -4.67346900                 | -0.23872100 | -1.52960900 |
| C                                            | -4.83405900                 | -0.53799600 | 0.86704700  |
| C                                            | -5.44536700                 | -0.33719000 | -0.37093600 |
| H                                            | -5.15384500                 | -0.07463300 | -2.49040700 |
| H                                            | -5.43767300                 | -0.60350400 | 1.76810000  |
| H                                            | -6.52606500                 | -0.25023200 | -0.43225000 |
| C                                            | 2.66118800                  | -0.00156400 | 2.37582300  |
| H                                            | 2.34132500                  | -0.98407900 | 2.74617100  |
| H                                            | 3.25949600                  | 0.47279400  | 3.15826700  |

|    |             |             |             |
|----|-------------|-------------|-------------|
| H  | 1.74678900  | 0.58944000  | 2.23935300  |
| C  | 2.81425400  | -1.11988500 | -2.57924900 |
| H  | 2.52193400  | -2.17676400 | -2.56640700 |
| H  | 1.90118000  | -0.53438900 | -2.73789700 |
| H  | 3.46558700  | -0.96917200 | -3.44412800 |
| C  | -2.75094800 | -0.87020500 | 2.29215200  |
| H  | -1.93529600 | -0.14963400 | 2.43314100  |
| H  | -3.45047700 | -0.76723800 | 3.12572700  |
| H  | -2.30526700 | -1.87174100 | 2.35050800  |
| C  | -2.41671000 | -0.22787100 | -2.70844800 |
| H  | -1.69400500 | 0.59230500  | -2.61065400 |
| H  | -1.84518000 | -1.14763800 | -2.88684500 |
| H  | -3.02764300 | -0.04055200 | -3.59596100 |
| C  | -0.68616400 | -1.80941100 | -0.22497300 |
| C  | 0.81541000  | -1.82681500 | -0.18470900 |
| C  | 1.51872400  | 2.65998000  | -1.54035700 |
| H  | 1.33642400  | 1.61620600  | -1.84867800 |
| C  | 1.06500300  | 2.85924900  | -0.05857900 |
| H  | 1.40983100  | 1.98105900  | 0.55001900  |
| C  | 3.05040500  | 2.89637700  | -1.59409800 |
| H  | 3.24857500  | 3.94876100  | -1.34419600 |
| H  | 1.70129000  | 3.63914400  | 0.37246300  |
| Si | 0.51315300  | 3.67054900  | -2.76851500 |
| O  | 1.09709800  | 3.71927500  | -4.31361700 |
| O  | -0.96827700 | 2.91542400  | -2.79159200 |
| O  | 0.44918400  | 5.22342700  | -2.23734100 |
| C  | 0.97938000  | 2.65821500  | -5.25640500 |
| H  | 1.82663800  | 1.96693100  | -5.16206800 |
| H  | 0.04567500  | 2.09797800  | -5.11988200 |
| H  | 0.99107500  | 3.09046000  | -6.26090900 |
| C  | -2.13940000 | 3.50723000  | -3.34985900 |
| H  | -2.01195900 | 3.72083300  | -4.41888100 |
| H  | -2.96451600 | 2.79898300  | -3.22860200 |
| H  | -2.39634600 | 4.43816200  | -2.82911300 |
| C  | 0.26549500  | 6.39356100  | -3.03860500 |
| H  | 0.77587100  | 6.29901000  | -4.00244800 |
| H  | -0.80238400 | 6.57379000  | -3.21305200 |
| H  | 0.68100100  | 7.24324100  | -2.49046800 |
| C  | -2.42069900 | -5.21576800 | -0.56679000 |
| C  | -1.26920800 | -5.98966100 | -0.57686100 |
| C  | 0.01493400  | -5.38372000 | -0.47946300 |
| C  | 0.03481100  | -3.98055200 | -0.37778500 |
| C  | -1.14819300 | -3.18589800 | -0.36260100 |
| C  | -2.38424600 | -3.80190200 | -0.45818600 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 1.32623500  | -7.11667300 | -0.54681700 |
| H | -3.38667100 | -5.70506700 | -0.64248900 |
| H | -1.34497900 | -7.07042500 | -0.65900200 |
| C | 1.28086300  | -6.03376600 | -0.47124100 |
| C | 1.23718500  | -3.22494300 | -0.27663200 |
| H | -3.30459700 | -3.22871800 | -0.44965200 |
| C | 2.45408600  | -3.88333000 | -0.27155600 |
| C | 2.45285900  | -5.29880100 | -0.36798600 |
| H | 3.39007300  | -3.33987900 | -0.20065300 |
| H | 3.40500500  | -5.82002600 | -0.36314700 |
| H | 3.51403600  | 2.29987000  | -0.79427200 |
| C | -1.37880400 | 2.12662700  | 0.19127500  |
| H | -2.00470200 | 1.93803400  | 1.06913000  |
| H | -1.97118800 | 2.11907600  | -0.72409600 |
| C | -0.40340400 | 3.27842900  | 0.31855800  |
| H | -0.67794300 | 4.14153300  | -0.29489900 |
| H | -0.36027000 | 3.61741000  | 1.35913000  |
| C | 3.74987200  | 2.55719900  | -2.91612400 |
| H | 3.52674600  | 1.51599000  | -3.18537600 |
| H | 3.34979300  | 3.18302400  | -3.71948700 |
| C | 5.26680500  | 2.75214700  | -2.82656100 |
| H | 5.75781400  | 2.49204900  | -3.77090100 |
| H | 5.51418500  | 3.79619700  | -2.60038800 |
| H | 5.69908300  | 2.12868500  | -2.03588000 |

UB3LYP-D3/BSII(SMD)//B3LYP-D3/BSI

HF=-2272.6022786



|                                              |                             |            |             |
|----------------------------------------------|-----------------------------|------------|-------------|
| Zero-point correction=                       | 0.776464 (Hartree/Particle) |            |             |
| Thermal correction to Energy=                | 0.824088                    |            |             |
| Thermal correction to Enthalpy=              | 0.825032                    |            |             |
| Thermal correction to Gibbs Free Energy=     | 0.693014                    |            |             |
| Sum of electronic and zero-point Energies=   | -2269.636393                |            |             |
| Sum of electronic and thermal Energies=      | -2269.588769                |            |             |
| Sum of electronic and thermal Enthalpies=    | -2269.587824                |            |             |
| Sum of electronic and thermal Free Energies= | -2269.719843                |            |             |
| Ni                                           | -1.82427600                 | 3.36357200 | 0.29515300  |
| N                                            | -0.49653900                 | 2.30641300 | -0.84290900 |
| N                                            | -2.89752400                 | 1.61550400 | 0.17904500  |
| C                                            | 0.78727400                  | 2.75047400 | -1.28095500 |
| C                                            | 0.93444300                  | 3.29914500 | -2.56708500 |
| C                                            | 1.84102300                  | 2.69872600 | -0.35118900 |
| C                                            | 2.19971300                  | 3.78028500 | -2.92365200 |
| C                                            | 3.08983000                  | 3.18154300 | -0.75552400 |
| C                                            | 3.27060600                  | 3.71762100 | -2.03127300 |
| H                                            | 2.34049900                  | 4.21152800 | -3.91106500 |
| H                                            | 3.92349400                  | 3.14033400 | -0.05959000 |
| H                                            | 4.24513000                  | 4.09373400 | -2.32805800 |
| C                                            | -4.18456800                 | 1.41300500 | 0.75405400  |
| C                                            | -5.34775200                 | 1.48623100 | -0.03821800 |
| C                                            | -4.23325300                 | 1.24294400 | 2.15223600  |
| C                                            | -6.58140200                 | 1.36953700 | 0.61447700  |
| C                                            | -5.48726800                 | 1.11904500 | 2.75491200  |
| C                                            | -6.65533300                 | 1.18476100 | 1.99417400  |
| H                                            | -7.49347400                 | 1.43310400 | 0.02715400  |
| H                                            | -5.54557900                 | 0.96877200 | 3.82956300  |
| H                                            | -7.62368000                 | 1.09634900 | 2.47762700  |
| C                                            | 1.60403100                  | 2.15458000 | 1.03673600  |
| H                                            | 1.27674300                  | 1.10803300 | 1.01217400  |
| H                                            | 2.51410800                  | 2.20713900 | 1.64067300  |
| H                                            | 0.81818800                  | 2.72527800 | 1.54911400  |
| C                                            | -0.23861300                 | 3.37384000 | -3.51464000 |
| H                                            | -1.11194600                 | 3.82469000 | -3.02906300 |

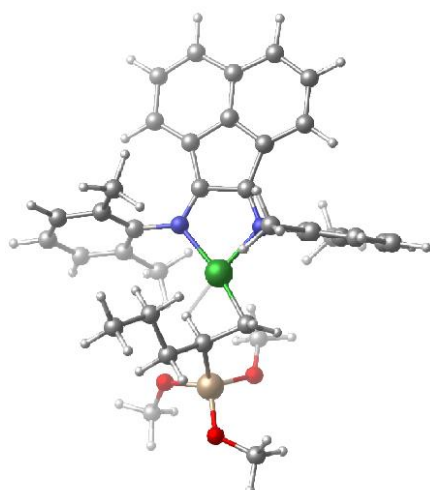
|    |             |             |             |
|----|-------------|-------------|-------------|
| H  | 0.00876800  | 3.96882600  | -4.39772500 |
| H  | -0.54085600 | 2.37668600  | -3.85895400 |
| C  | -2.95619200 | 1.15794400  | 2.95145400  |
| H  | -2.33480300 | 2.05292100  | 2.82143200  |
| H  | -3.16974600 | 1.04993300  | 4.01861000  |
| H  | -2.34745300 | 0.29929400  | 2.64253500  |
| C  | -5.28604500 | 1.70106700  | -1.53208200 |
| H  | -6.23557900 | 2.09510700  | -1.90451200 |
| H  | -4.49529500 | 2.40539600  | -1.80704500 |
| H  | -5.08626200 | 0.76382500  | -2.06606500 |
| C  | -2.33875400 | 0.78640100  | -0.63736700 |
| C  | -0.98826600 | 1.16502800  | -1.18909300 |
| C  | -3.05698500 | 6.35040400  | 1.93958700  |
| H  | -2.82849800 | 6.95066200  | 1.04556500  |
| C  | -4.02742000 | 5.19697700  | 1.51086800  |
| H  | -3.73126100 | 4.23078000  | 1.95243400  |
| C  | -3.72882800 | 7.30326800  | 2.96451400  |
| H  | -4.74629800 | 7.51005400  | 2.60186700  |
| H  | -5.01529100 | 5.39903400  | 1.94344800  |
| Si | -1.43507400 | 5.60403700  | 2.50953200  |
| O  | -0.42080600 | 6.72171100  | 3.14915800  |
| O  | -0.64912100 | 4.85132700  | 1.19483700  |
| O  | -1.63188800 | 4.27387200  | 3.47307900  |
| C  | 0.85332300  | 6.42043900  | 3.73045300  |
| H  | 0.80667400  | 5.51696700  | 4.34909400  |
| H  | 1.60719000  | 6.28033900  | 2.94642100  |
| H  | 1.14317900  | 7.26914700  | 4.35389100  |
| C  | 0.25202700  | 5.61822700  | 0.35792000  |
| H  | 0.19074400  | 6.68288100  | 0.59826200  |
| H  | 1.26897900  | 5.25807500  | 0.52235600  |
| H  | -0.02221700 | 5.45641700  | -0.68505400 |
| C  | -2.45651400 | 4.25425700  | 4.64231300  |
| H  | -2.24354300 | 5.10605000  | 5.29913600  |
| H  | -3.51896500 | 4.26705300  | 4.37083100  |
| H  | -2.24108600 | 3.33028200  | 5.18391300  |
| C  | -3.65854400 | -2.67728300 | -1.65685700 |
| C  | -2.57944400 | -3.04705400 | -2.44558200 |
| C  | -1.47576200 | -2.16622000 | -2.62119500 |
| C  | -1.55714000 | -0.92511300 | -1.96303700 |
| C  | -2.66707500 | -0.54085000 | -1.15932300 |
| C  | -3.72278600 | -1.42119800 | -1.00001300 |
| H  | -0.18135100 | -3.33949000 | -3.91528400 |
| H  | -4.48651600 | -3.36873900 | -1.53538000 |
| H  | -2.57202100 | -4.01803700 | -2.93303500 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -0.29603000 | -2.39981900 | -3.38195300 |
| C | -0.52800700 | 0.05581000  | -2.02397000 |
| H | -4.58391700 | -1.16711400 | -0.39165500 |
| C | 0.61074100  | -0.19974900 | -2.76778900 |
| C | 0.70558300  | -1.44247300 | -3.44573000 |
| H | 1.41559500  | 0.52358300  | -2.83779300 |
| H | 1.59605500  | -1.64699100 | -4.03191200 |
| H | -3.86169000 | 6.79198800  | 3.92950300  |
| C | -2.93089300 | 4.66832400  | -0.78714000 |
| H | -2.27924300 | 5.54147400  | -0.91791700 |
| H | -3.15565500 | 4.25619100  | -1.77656800 |
| C | -4.20342600 | 5.00842600  | -0.00996900 |
| H | -4.94154100 | 4.21149500  | -0.15354500 |
| H | -4.65670300 | 5.92654900  | -0.41910900 |
| C | -3.01740800 | 8.64477300  | 3.18677100  |
| H | -2.00912800 | 8.47728500  | 3.57955200  |
| H | -2.89070100 | 9.14269600  | 2.21463300  |
| C | -3.79920000 | 9.56035600  | 4.13488600  |
| H | -3.28470900 | 10.51680800 | 4.27637900  |
| H | -4.80202000 | 9.77433100  | 3.74558100  |
| H | -3.91868600 | 9.09721900  | 5.12230300  |

UB3LYP-D3/BSII(SMD)//B3LYP-D3/BSI

HF=-2272.6282077

<sup>1</sup>K



|                                              |                             |            |             |
|----------------------------------------------|-----------------------------|------------|-------------|
| Zero-point correction=                       | 0.717518 (Hartree/Particle) |            |             |
| Thermal correction to Energy=                | 0.763262                    |            |             |
| Thermal correction to Enthalpy=              | 0.764206                    |            |             |
| Thermal correction to Gibbs Free Energy=     | 0.635033                    |            |             |
| Sum of electronic and zero-point Energies=   | -2191.055971                |            |             |
| Sum of electronic and thermal Energies=      | -2191.010227                |            |             |
| Sum of electronic and thermal Enthalpies=    | -2191.009282                |            |             |
| Sum of electronic and thermal Free Energies= | -2191.138456                |            |             |
| Ni                                           | -1.83117800                 | 3.68651200 | -1.20016900 |
| N                                            | -0.64057500                 | 2.21295600 | -0.94264000 |
| N                                            | -3.26806800                 | 2.42575800 | -0.63261400 |
| C                                            | 0.77806100                  | 2.20995400 | -1.14763600 |
| C                                            | 1.25370600                  | 1.99734600 | -2.45188600 |
| C                                            | 1.62676200                  | 2.45957000 | -0.05676000 |
| C                                            | 2.63828500                  | 2.02154100 | -2.64871000 |
| C                                            | 3.00437100                  | 2.47743700 | -0.30154800 |
| C                                            | 3.50817900                  | 2.25774200 | -1.58403700 |
| H                                            | 3.03290300                  | 1.85498300 | -3.64731000 |
| H                                            | 3.68432200                  | 2.67044900 | 0.52376100  |
| H                                            | 4.58036900                  | 2.27690300 | -1.75473100 |
| C                                            | -4.67873000                 | 2.64692400 | -0.68201500 |
| C                                            | -5.43051000                 | 2.05527100 | -1.72013600 |
| C                                            | -5.25000900                 | 3.53403100 | 0.24920300  |
| C                                            | -6.79798100                 | 2.34530400 | -1.77647500 |
| C                                            | -6.62448800                 | 3.77561100 | 0.16185500  |
| C                                            | -7.39578900                 | 3.18731400 | -0.83931300 |
| H                                            | -7.39568900                 | 1.90788200 | -2.57151300 |
| H                                            | -7.08916900                 | 4.43887400 | 0.88643400  |
| H                                            | -8.46038300                 | 3.39338200 | -0.89655100 |
| C                                            | 1.06100900                  | 2.69608400 | 1.32217400  |

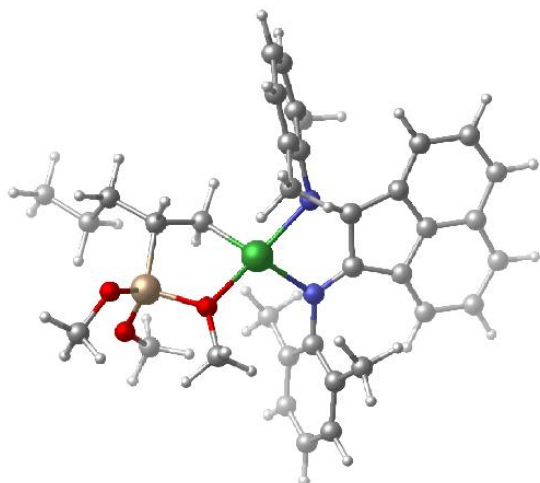
|    |             |            |             |
|----|-------------|------------|-------------|
| H  | 0.59713500  | 1.78832800 | 1.72913400  |
| H  | 1.84262100  | 3.01065500 | 2.01871800  |
| H  | 0.28605800  | 3.47133600 | 1.30316300  |
| C  | 0.28932000  | 1.73216600 | -3.58083300 |
| H  | -0.21696800 | 0.76597900 | -3.45682500 |
| H  | -0.49632600 | 2.49706900 | -3.61511200 |
| H  | 0.80275200  | 1.71939600 | -4.54584100 |
| C  | -4.41238300 | 4.22760700 | 1.29651300  |
| H  | -4.00270800 | 5.16481700 | 0.89786800  |
| H  | -5.01900200 | 4.48807200 | 2.16929900  |
| H  | -3.57463000 | 3.61183500 | 1.63697600  |
| C  | -4.78948000 | 1.16957100 | -2.76392200 |
| H  | -3.83776500 | 1.58504800 | -3.11467300 |
| H  | -4.58318300 | 0.16400700 | -2.37754000 |
| H  | -5.44766200 | 1.05953200 | -3.62989100 |
| C  | -2.75224500 | 1.27543400 | -0.35525400 |
| C  | -1.25919800 | 1.16678600 | -0.50423400 |
| C  | -2.03563700 | 5.75870900 | -1.84029500 |
| H  | -2.78577900 | 5.10985300 | -1.20042200 |
| C  | -0.71669300 | 5.06040500 | -1.87090600 |
| H  | -0.28733200 | 4.85103900 | -2.85304000 |
| C  | -2.75912000 | 5.95630500 | -3.19229800 |
| H  | -2.09757000 | 6.53877900 | -3.84502300 |
| H  | -3.65728400 | 6.56510800 | -3.03266400 |
| C  | -3.16696000 | 4.64632000 | -3.88098200 |
| H  | -2.27885700 | 4.01643900 | -4.03083600 |
| C  | -3.87058600 | 4.87166600 | -5.22181400 |
| H  | -3.21701700 | 5.39778900 | -5.92722300 |
| H  | -4.16358900 | 3.92109900 | -5.68056000 |
| H  | -4.77632000 | 5.47526700 | -5.09156100 |
| H  | -3.83362000 | 4.09034800 | -3.20531900 |
| H  | 0.03789400  | 5.35921300 | -1.14012500 |
| Si | -2.05787300 | 7.29511500 | -0.72756500 |
| O  | -3.62748400 | 7.40741100 | -0.25625900 |
| O  | -1.00933200 | 7.08011700 | 0.52972100  |
| O  | -1.60688200 | 8.63806000 | -1.53960200 |
| C  | -4.18870900 | 8.54459200 | 0.41154000  |
| H  | -3.76643000 | 8.65440700 | 1.41790200  |
| H  | -4.00364700 | 9.46125600 | -0.15796700 |
| H  | -5.26614600 | 8.38193700 | 0.49276900  |
| C  | -1.19340600 | 6.12055300 | 1.56307900  |
| H  | -0.28512500 | 6.09729100 | 2.17135200  |
| H  | -2.04453200 | 6.38298800 | 2.20356200  |
| H  | -1.36545300 | 5.11382100 | 1.15319900  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -0.25968900 | 9.04956200  | -1.78596600 |
| H | 0.32811300  | 9.04875300  | -0.86186000 |
| H | 0.21965400  | 8.38832000  | -2.51942100 |
| H | -0.29272000 | 10.06261500 | -2.19375000 |
| C | -4.55152000 | -1.89826400 | 0.84636100  |
| C | -3.42384600 | -2.69783000 | 0.96417500  |
| C | -2.13440000 | -2.18551300 | 0.64761900  |
| C | -2.08435000 | -0.84603300 | 0.22011800  |
| C | -3.24221200 | -0.02546100 | 0.09459300  |
| C | -4.48340600 | -0.55090400 | 0.40787100  |
| H | -0.86813600 | -3.90934300 | 1.03663700  |
| H | -5.52283100 | -2.31477400 | 1.09403800  |
| H | -3.52270200 | -3.72634800 | 1.30008700  |
| C | -0.88938600 | -2.87217900 | 0.71355700  |
| C | -0.86942900 | -0.18715800 | -0.12787700 |
| H | -5.38664300 | 0.04277500  | 0.31731500  |
| C | 0.32697600  | -0.87926400 | -0.05506600 |
| C | 0.29283700  | -2.23189000 | 0.37082000  |
| H | 1.26945400  | -0.40781100 | -0.31115300 |
| H | 1.22742600  | -2.78070800 | 0.43067200  |

UB3LYP-D3/BSII(SMD)//B3LYP-D3/BSI

HF=-2193.9621976

<sup>3</sup>K



|                                              |                             |
|----------------------------------------------|-----------------------------|
| Zero-point correction=                       | 0.717863 (Hartree/Particle) |
| Thermal correction to Energy=                | 0.763611                    |
| Thermal correction to Enthalpy=              | 0.764555                    |
| Thermal correction to Gibbs Free Energy=     | 0.635009                    |
| Sum of electronic and zero-point Energies=   | -2191.058637                |
| Sum of electronic and thermal Energies=      | -2191.012889                |
| Sum of electronic and thermal Enthalpies=    | -2191.011945                |
| Sum of electronic and thermal Free Energies= | -2191.141491                |

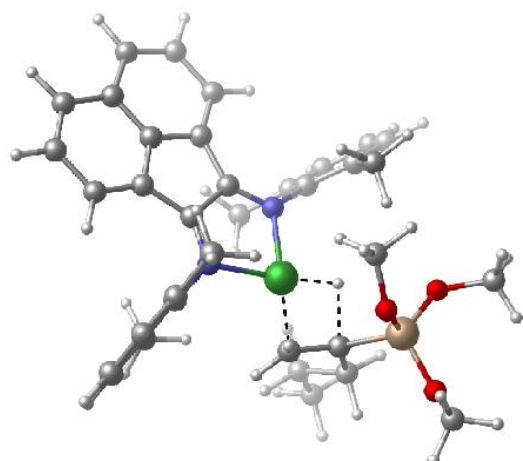
|    |             |            |             |
|----|-------------|------------|-------------|
| Ni | -2.37603700 | 3.63105900 | -0.92606100 |
| N  | -0.85932600 | 2.42641900 | -0.27610000 |
| N  | -3.48282000 | 1.92965000 | -0.69049400 |
| C  | 0.50612500  | 2.81321900 | -0.16377200 |
| C  | 1.44736500  | 2.40395900 | -1.13116900 |
| C  | 0.83364400  | 3.70712100 | 0.87458300  |
| C  | 2.75956200  | 2.87163000 | -0.99224900 |
| C  | 2.15879600  | 4.13571800 | 0.97902200  |
| C  | 3.11874500  | 3.71687800 | 0.05685000  |
| H  | 3.50235000  | 2.57679700 | -1.72847700 |
| H  | 2.43664200  | 4.80811100 | 1.78594900  |
| H  | 4.14353800  | 4.06471100 | 0.14543700  |
| C  | -4.89218300 | 1.81109700 | -0.88564100 |
| C  | -5.39453700 | 1.29319500 | -2.09223600 |
| C  | -5.72532400 | 2.30062700 | 0.13603100  |
| C  | -6.78474100 | 1.26381400 | -2.25014800 |
| C  | -7.10852800 | 2.25230100 | -0.06703800 |
| C  | -7.63656400 | 1.73782900 | -1.25160600 |
| H  | -7.19932600 | 0.87067900 | -3.17437000 |
| H  | -7.77184600 | 2.61579100 | 0.71324200  |
| H  | -8.71228300 | 1.70655400 | -1.39712200 |
| C  | -0.22637400 | 4.16839600 | 1.84473800  |
| H  | -1.05017600 | 4.67805300 | 1.32147800  |

|    |             |             |             |
|----|-------------|-------------|-------------|
| H  | -0.67373500 | 3.32990100  | 2.39162500  |
| H  | 0.18446500  | 4.87072200  | 2.57477200  |
| C  | 1.05578800  | 1.54034400  | -2.30686100 |
| H  | 0.08551000  | 1.84195600  | -2.71619300 |
| H  | 1.79841500  | 1.62027000  | -3.10518900 |
| H  | 0.97933900  | 0.48159300  | -2.03152200 |
| C  | -5.12702400 | 2.82706400  | 1.41772700  |
| H  | -5.88932300 | 3.28842500  | 2.05140700  |
| H  | -4.64973800 | 2.02519900  | 1.99505100  |
| H  | -4.34875700 | 3.57550800  | 1.21854900  |
| C  | -4.46573500 | 0.80633400  | -3.17578400 |
| H  | -3.87360200 | -0.05574500 | -2.84567900 |
| H  | -5.02848200 | 0.50466200  | -4.06297300 |
| H  | -3.77426100 | 1.60083800  | -3.47157200 |
| C  | -2.73365500 | 0.93499500  | -0.35901900 |
| C  | -1.26400800 | 1.20575200  | -0.14674600 |
| C  | -0.64831900 | 4.84381200  | -2.97114600 |
| H  | 0.08114800  | 4.40667900  | -2.27538200 |
| H  | -0.79463100 | 5.87881100  | -2.62959200 |
| C  | -1.96663000 | 4.06616400  | -2.91780800 |
| C  | 0.00821800  | 4.85901800  | -4.36949000 |
| H  | 0.23343000  | 3.82185100  | -4.65941800 |
| H  | 0.97602600  | 5.37422300  | -4.29215200 |
| C  | -0.83297900 | 5.51817200  | -5.46803200 |
| H  | -1.78283500 | 4.97919700  | -5.57906700 |
| C  | -0.10863400 | 5.55767700  | -6.81721700 |
| H  | 0.14137100  | 4.54591900  | -7.15960200 |
| H  | -0.72768600 | 6.02790100  | -7.58887500 |
| H  | 0.82772200  | 6.12450800  | -6.74718400 |
| H  | -1.09696600 | 6.53963800  | -5.16109800 |
| H  | -1.92463700 | 3.13589900  | -3.49266500 |
| Si | -3.56492400 | 4.95940600  | -3.01694200 |
| O  | -4.73708600 | 4.01290900  | -3.65258200 |
| O  | -3.73455600 | 6.47113500  | -3.63655600 |
| O  | -3.76793800 | 5.12823300  | -1.30671700 |
| C  | -6.08497600 | 4.38791800  | -3.94428600 |
| H  | -6.73027100 | 4.13207900  | -3.09631800 |
| H  | -6.16580900 | 5.45739500  | -4.16596300 |
| H  | -6.41191800 | 3.81837200  | -4.81842700 |
| C  | -3.15812800 | 7.67219100  | -3.12888200 |
| H  | -3.83749900 | 8.49857700  | -3.35619900 |
| H  | -3.00739500 | 7.62363400  | -2.04258800 |
| H  | -2.19458400 | 7.86418300  | -3.61317100 |
| C  | -4.95363600 | 5.65447500  | -0.68571600 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -5.74408900 | 4.89832000  | -0.68545300 |
| H | -4.70904200 | 5.93131300  | 0.34213300  |
| H | -5.28906000 | 6.54349000  | -1.22870800 |
| C | -3.89351500 | -2.67627000 | 0.24061600  |
| C | -2.65621300 | -3.19663000 | 0.59023700  |
| C | -1.49972100 | -2.36752500 | 0.61266200  |
| C | -1.69213300 | -1.01967100 | 0.25711100  |
| C | -2.96206600 | -0.48441800 | -0.09578200 |
| C | -4.07084700 | -1.31227400 | -0.10688700 |
| H | 0.03550800  | -3.77416800 | 1.23897200  |
| H | -4.75938400 | -3.33085900 | 0.23225100  |
| H | -2.56528700 | -4.24737500 | 0.85137300  |
| C | -0.17228500 | -2.74528800 | 0.95846800  |
| C | -0.63919600 | -0.06148600 | 0.23281000  |
| H | -5.05306800 | -0.93852800 | -0.37420600 |
| C | 0.64124300  | -0.45729900 | 0.57995600  |
| C | 0.85381000  | -1.81217400 | 0.94225100  |
| H | 1.47042600  | 0.24155500  | 0.57465500  |
| H | 1.85741200  | -2.12482800 | 1.21308500  |

UB3LYP-D3/BSII(SMD)//B3LYP-D3/BSI

HF=-2193.9704071

**<sup>1</sup>TS5**

Zero-point correction= 0.713911 (Hartree/Particle)

Thermal correction to Energy= 0.758537

Thermal correction to Enthalpy= 0.759482

Thermal correction to Gibbs Free Energy= 0.633534

Sum of electronic and zero-point Energies= -2191.044158

Sum of electronic and thermal Energies= -2190.999532

Sum of electronic and thermal Enthalpies= -2190.998588

Sum of electronic and thermal Free Energies= -2191.124536

|    |             |            |             |
|----|-------------|------------|-------------|
| Ni | -1.94445500 | 3.71394400 | -1.25300500 |
| N  | -0.69662800 | 2.22560900 | -0.97743200 |
| N  | -3.31061300 | 2.47012500 | -0.61257500 |
| C  | 0.70306000  | 2.17318600 | -1.28032500 |
| C  | 1.07434700  | 1.83738000 | -2.59301100 |
| C  | 1.63639200  | 2.50368500 | -0.28512800 |
| C  | 2.43985500  | 1.81999700 | -2.89639400 |
| C  | 2.99139000  | 2.47370500 | -0.63394900 |
| C  | 3.39216900  | 2.13304800 | -1.92622500 |
| H  | 2.75410200  | 1.55996800 | -3.90353400 |
| H  | 3.73510600  | 2.72560200 | 0.11712800  |
| H  | 4.44806500  | 2.11783400 | -2.17900700 |
| C  | -4.73381200 | 2.64458100 | -0.63430300 |
| C  | -5.47209200 | 2.01889400 | -1.65783900 |
| C  | -5.32949600 | 3.47754100 | 0.32765300  |
| C  | -6.85619100 | 2.22237000 | -1.67495200 |
| C  | -6.71808200 | 3.63686700 | 0.27880100  |
| C  | -7.47854500 | 3.01435200 | -0.71036000 |
| H  | -7.44719200 | 1.75612000 | -2.45858700 |
| H  | -7.20247700 | 4.26233100 | 1.02370700  |
| H  | -8.55497500 | 3.15508700 | -0.73658800 |
| C  | 1.17896700  | 2.87243500 | 1.10468000  |
| H  | 0.70410500  | 2.02283300 | 1.61204600  |

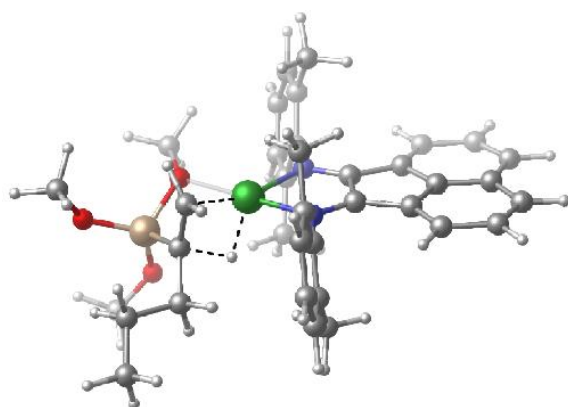
|    |             |            |             |
|----|-------------|------------|-------------|
| H  | 2.01949200  | 3.20161200 | 1.72124800  |
| H  | 0.43960100  | 3.68101500 | 1.07434600  |
| C  | 0.02247600  | 1.48929000 | -3.61784700 |
| H  | -0.47059500 | 0.53832300 | -3.37720100 |
| H  | -0.76608000 | 2.25132600 | -3.65496400 |
| H  | 0.45873300  | 1.39552100 | -4.61585800 |
| C  | -4.49377100 | 4.19548200 | 1.35587800  |
| H  | -3.95792100 | 5.02822500 | 0.88483500  |
| H  | -5.12090300 | 4.60800600 | 2.15157000  |
| H  | -3.74812600 | 3.53816100 | 1.81674000  |
| C  | -4.79853500 | 1.17654900 | -2.71655000 |
| H  | -3.89876300 | 1.66681500 | -3.10701700 |
| H  | -4.49101600 | 0.19869000 | -2.32499800 |
| H  | -5.47609300 | 0.99595400 | -3.55524200 |
| C  | -2.78537100 | 1.34117100 | -0.26815500 |
| C  | -1.30123500 | 1.21067600 | -0.45932900 |
| C  | -1.75942700 | 5.78440700 | -2.08127800 |
| H  | -2.95857400 | 4.85371600 | -1.35251700 |
| C  | -0.60228700 | 4.97007300 | -1.99795300 |
| H  | -0.18446400 | 4.50510200 | -2.89002800 |
| C  | -2.49370800 | 5.99075600 | -3.40462800 |
| H  | -1.94924100 | 6.78494900 | -3.93564700 |
| H  | -3.49268400 | 6.39147800 | -3.19608000 |
| C  | -2.62404800 | 4.75653500 | -4.30585500 |
| H  | -1.63041000 | 4.38542600 | -4.58662500 |
| C  | -3.43849900 | 5.04330100 | -5.57049900 |
| H  | -2.96725500 | 5.82807400 | -6.17353400 |
| H  | -3.52615600 | 4.14852400 | -6.19595300 |
| H  | -4.45130300 | 5.37881900 | -5.31826700 |
| H  | -3.10596000 | 3.95355800 | -3.72651300 |
| H  | 0.11657600  | 5.14360600 | -1.19716700 |
| Si | -1.94603200 | 7.15020700 | -0.78933200 |
| O  | -3.54036100 | 7.14759000 | -0.37962100 |
| O  | -0.95586300 | 6.84528400 | 0.49556800  |
| O  | -1.49046200 | 8.56420600 | -1.46482800 |
| C  | -4.20242400 | 8.23328600 | 0.27529300  |
| H  | -3.94015600 | 8.26367800 | 1.34038000  |
| H  | -3.93977800 | 9.19163100 | -0.18667300 |
| H  | -5.27925900 | 8.07356700 | 0.17991300  |
| C  | -1.27784800 | 5.99146800 | 1.58669600  |
| H  | -0.41371900 | 5.95854300 | 2.25585800  |
| H  | -2.14601800 | 6.36304100 | 2.14459100  |
| H  | -1.49881200 | 4.97068200 | 1.24374700  |
| C  | -0.48069100 | 9.48205700 | -1.03616900 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 0.02465300  | 9.13033000  | -0.13119600 |
| H | 0.25317100  | 9.59844700  | -1.83954400 |
| H | -0.94798400 | 10.45172900 | -0.83777800 |
| C | -4.57823600 | -1.75104700 | 1.13663100  |
| C | -3.45555300 | -2.55764300 | 1.25474100  |
| C | -2.17171500 | -2.07532800 | 0.87455700  |
| C | -2.12163900 | -0.75664000 | 0.38687400  |
| C | -3.27498300 | 0.07132000  | 0.26191800  |
| C | -4.51130200 | -0.42530300 | 0.63640200  |
| H | -0.91131100 | -3.79534900 | 1.29777200  |
| H | -5.54527200 | -2.14505700 | 1.43306200  |
| H | -3.55420300 | -3.56894800 | 1.63948200  |
| C | -0.93253900 | -2.77346500 | 0.92917300  |
| C | -0.91293900 | -0.12990000 | -0.03360800 |
| H | -5.41094000 | 0.17366400  | 0.54770500  |
| C | 0.27752600  | -0.83288600 | 0.02813400  |
| C | 0.24390100  | -2.16411200 | 0.51712300  |
| H | 1.21487300  | -0.38593900 | -0.28457100 |
| H | 1.17389700  | -2.72144800 | 0.56934700  |

UB3LYP-D3/BSII(SMD)//B3LYP-D3/BSI

HF=-2193.9466587

<sup>3</sup>TS5



|                                              |                             |            |             |
|----------------------------------------------|-----------------------------|------------|-------------|
| Zero-point correction=                       | 0.711745 (Hartree/Particle) |            |             |
| Thermal correction to Energy=                | 0.757811                    |            |             |
| Thermal correction to Enthalpy=              | 0.758755                    |            |             |
| Thermal correction to Gibbs Free Energy=     | 0.627739                    |            |             |
| Sum of electronic and zero-point Energies=   | -2191.025155                |            |             |
| Sum of electronic and thermal Energies=      | -2190.979090                |            |             |
| Sum of electronic and thermal Enthalpies=    | -2190.978146                |            |             |
| Sum of electronic and thermal Free Energies= | -2191.109161                |            |             |
| Ni                                           | -2.60740800                 | 3.44319000 | -1.58428600 |
| N                                            | -1.03195300                 | 2.08806900 | -1.27138000 |
| N                                            | -3.62585700                 | 1.99837300 | -0.52396000 |
| C                                            | 0.29664100                  | 2.22457800 | -1.77085300 |
| C                                            | 0.52022300                  | 1.89017100 | -3.11892900 |
| C                                            | 1.29752500                  | 2.76305300 | -0.94291500 |
| C                                            | 1.80198600                  | 2.10674600 | -3.63598600 |
| C                                            | 2.56371100                  | 2.96257700 | -1.50559300 |
| C                                            | 2.81590800                  | 2.64060700 | -2.83967500 |
| H                                            | 2.00275100                  | 1.85154300 | -4.67294000 |
| H                                            | 3.35327600                  | 3.38447000 | -0.88964500 |
| H                                            | 3.80357800                  | 2.80680800 | -3.25929200 |
| C                                            | -5.02935300                 | 1.99765200 | -0.26022500 |
| C                                            | -5.87792800                 | 1.46267800 | -1.24428400 |
| C                                            | -5.50625900                 | 2.60067600 | 0.91488600  |
| C                                            | -7.25524500                 | 1.50893300 | -1.00515300 |
| C                                            | -6.89259300                 | 2.63385700 | 1.10659900  |
| C                                            | -7.76065900                 | 2.08756400 | 0.15989000  |
| H                                            | -7.93472600                 | 1.09557100 | -1.74579700 |
| H                                            | -7.29007900                 | 3.09400500 | 2.00719400  |
| H                                            | -8.83313800                 | 2.12011300 | 0.32709400  |
| C                                            | 0.99479200                  | 3.14191200 | 0.48644300  |
| H                                            | 0.10048300                  | 3.77448300 | 0.54261300  |
| H                                            | 0.80523200                  | 2.25704700 | 1.10715100  |

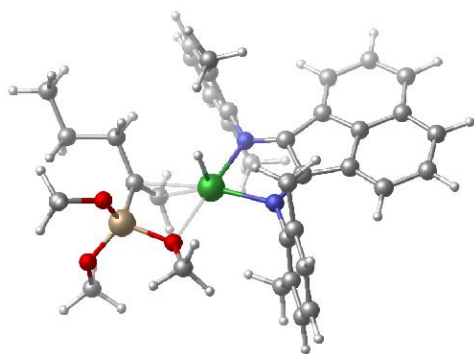
|    |             |            |             |
|----|-------------|------------|-------------|
| H  | 1.83096400  | 3.68722400 | 0.93202100  |
| C  | -0.58478600 | 1.28445200 | -3.95081200 |
| H  | -1.49232200 | 1.90051700 | -3.94347700 |
| H  | -0.27041300 | 1.16158500 | -4.99080800 |
| H  | -0.86968500 | 0.29567500 | -3.56864900 |
| C  | -4.54186500 | 3.18796000 | 1.91631800  |
| H  | -5.07219700 | 3.73312300 | 2.70158500  |
| H  | -3.94104900 | 2.40621700 | 2.39886300  |
| H  | -3.83811300 | 3.87572900 | 1.43031400  |
| C  | -5.30222900 | 0.89537700 | -2.51933400 |
| H  | -4.65104300 | 0.03441300 | -2.32410600 |
| H  | -6.09588400 | 0.56494300 | -3.19531400 |
| H  | -4.69220000 | 1.64255100 | -3.04495300 |
| C  | -2.85147100 | 1.05818400 | -0.10831200 |
| C  | -1.39834700 | 1.11092300 | -0.52140800 |
| C  | -1.56089100 | 5.53385700 | -2.21123100 |
| H  | -1.95550800 | 4.71735300 | -0.74837300 |
| H  | -2.32563800 | 6.25262800 | -1.91703400 |
| C  | -1.82416100 | 4.72793600 | -3.34165300 |
| C  | -0.14506100 | 5.90668800 | -1.83192200 |
| H  | 0.49557500  | 5.02397700 | -1.91451400 |
| H  | -0.10743500 | 6.24201200 | -0.78926900 |
| C  | 0.40304900  | 7.01590300 | -2.75230000 |
| H  | 0.34573200  | 6.67593300 | -3.79415800 |
| C  | 1.84963700  | 7.37482500 | -2.39831900 |
| H  | 2.50112400  | 6.49709400 | -2.48895800 |
| H  | 2.23770200  | 8.15354500 | -3.06311900 |
| H  | 1.92557700  | 7.74399900 | -1.36860900 |
| H  | -0.23472100 | 7.90744600 | -2.67718000 |
| H  | -0.97127400 | 4.22223300 | -3.79022700 |
| Si | -3.50919000 | 4.61848200 | -4.06489400 |
| O  | -3.63259400 | 3.27471400 | -4.99172200 |
| O  | -4.15183300 | 5.87878300 | -4.89669800 |
| O  | -4.34350200 | 4.43066200 | -2.59678200 |
| C  | -4.57676600 | 3.03342400 | -6.03958100 |
| H  | -5.50385500 | 2.62006100 | -5.62405900 |
| H  | -4.80467600 | 3.95196600 | -6.58939500 |
| H  | -4.13791200 | 2.30174000 | -6.72251800 |
| C  | -4.04112800 | 7.24980500 | -4.51099800 |
| H  | -4.45276900 | 7.85803300 | -5.31958100 |
| H  | -4.60859200 | 7.44981700 | -3.59274200 |
| H  | -2.99281400 | 7.53220300 | -4.35235600 |
| C  | -5.76083500 | 4.57169200 | -2.40676400 |
| H  | -6.29661100 | 3.75371500 | -2.89722500 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -5.96152500 | 4.53194100  | -1.33531600 |
| H | -6.09789200 | 5.52882900  | -2.81666500 |
| C | -3.89548300 | -1.96805500 | 2.01055300  |
| C | -2.65056600 | -2.57865800 | 2.06059100  |
| C | -1.52694400 | -1.99306200 | 1.41263400  |
| C | -1.76038600 | -0.78069200 | 0.73770900  |
| C | -3.03769900 | -0.15440300 | 0.68507000  |
| C | -4.11394500 | -0.74701800 | 1.32224900  |
| H | 0.04381800  | -3.42474000 | 1.87193800  |
| H | -4.73489500 | -2.43776200 | 2.51362100  |
| H | -2.52896600 | -3.51464700 | 2.59887200  |
| C | -0.19517100 | -2.49294300 | 1.36680800  |
| C | -0.74370300 | -0.07198100 | 0.03840400  |
| H | -5.10073900 | -0.29765500 | 1.30196500  |
| C | 0.54209400  | -0.58132300 | 0.00853600  |
| C | 0.79610500  | -1.80284200 | 0.68490900  |
| H | 1.34178100  | -0.06702800 | -0.51319700 |
| H | 1.80348900  | -2.20674900 | 0.66552400  |

UB3LYP-D3/BSII(SMD)//B3LYP-D3/BSI

HF=-2193.9286758

<sup>3</sup>L



|                                              |                             |
|----------------------------------------------|-----------------------------|
| Zero-point correction=                       | 0.713345 (Hartree/Particle) |
| Thermal correction to Energy=                | 0.759783                    |
| Thermal correction to Enthalpy=              | 0.760727                    |
| Thermal correction to Gibbs Free Energy=     | 0.628756                    |
| Sum of electronic and zero-point Energies=   | -2191.041455                |
| Sum of electronic and thermal Energies=      | -2190.995017                |
| Sum of electronic and thermal Enthalpies=    | -2190.994073                |
| Sum of electronic and thermal Free Energies= | -2191.126043                |

|    |             |            |             |
|----|-------------|------------|-------------|
| Ni | -2.61367300 | 3.47787200 | -1.55188900 |
| N  | -1.06262700 | 2.11680300 | -1.28332200 |
| N  | -3.67194600 | 1.95248700 | -0.62030900 |
| C  | 0.28581100  | 2.29380700 | -1.71348700 |
| C  | 0.59253600  | 1.94854500 | -3.04185500 |
| C  | 1.22209400  | 2.87798800 | -0.84236300 |
| C  | 1.88779400  | 2.21314300 | -3.49973500 |
| C  | 2.50596600  | 3.12009300 | -1.34368500 |
| C  | 2.83756600  | 2.79719000 | -2.66009100 |
| H  | 2.15112500  | 1.95336500 | -4.52154500 |
| H  | 3.24652900  | 3.57983200 | -0.69491900 |
| H  | 3.83741600  | 3.00035900 | -3.03203900 |
| C  | -5.07560100 | 1.93519400 | -0.36192200 |
| C  | -5.91652400 | 1.43377600 | -1.37052700 |
| C  | -5.56453300 | 2.47974200 | 0.83816300  |
| C  | -7.29620500 | 1.46715600 | -1.14245000 |
| C  | -6.95296100 | 2.50166500 | 1.01730800  |
| C  | -7.81278000 | 1.99858300 | 0.04018400  |
| H  | -7.96777200 | 1.07597300 | -1.90216800 |
| H  | -7.35883300 | 2.91939100 | 1.93469300  |
| H  | -8.88670600 | 2.02289400 | 0.19959400  |
| C  | 0.83677100  | 3.25085600 | 0.56842600  |
| H  | -0.10954200 | 3.80480600 | 0.58508500  |
| H  | 0.69860500  | 2.35947600 | 1.19391100  |
| H  | 1.61069600  | 3.86600000 | 1.03548900  |
| C  | -0.43688500 | 1.26760400 | -3.91218600 |

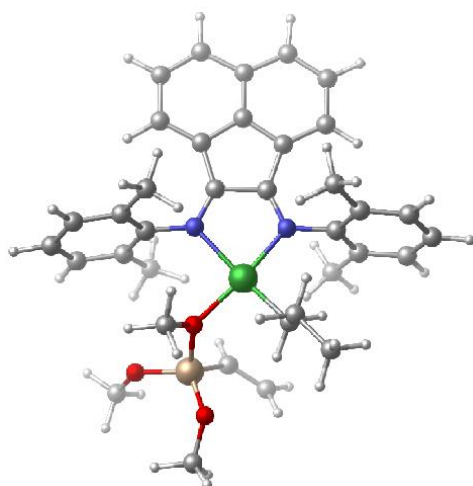
|    |             |            |             |
|----|-------------|------------|-------------|
| H  | -1.41499600 | 1.76031900 | -3.85817800 |
| H  | -0.12040400 | 1.24955300 | -4.95885200 |
| H  | -0.59284500 | 0.22849200 | -3.59403400 |
| C  | -4.61618700 | 3.01598200 | 1.88262300  |
| H  | -5.15878000 | 3.54609400 | 2.66996000  |
| H  | -4.04899200 | 2.20448300 | 2.35723700  |
| H  | -3.88408500 | 3.69987400 | 1.43692300  |
| C  | -5.32894300 | 0.88933100 | -2.64957700 |
| H  | -4.69955300 | 0.01032800 | -2.46240600 |
| H  | -6.11628300 | 0.59050400 | -3.34749200 |
| H  | -4.69443900 | 1.63416700 | -3.14548400 |
| C  | -2.88499700 | 1.04140400 | -0.16902400 |
| C  | -1.42525100 | 1.13439100 | -0.53681500 |
| C  | -1.35735600 | 5.47117300 | -2.69817800 |
| H  | -2.34598000 | 4.39411800 | -0.29306900 |
| H  | -2.05429200 | 6.12214400 | -2.16757300 |
| C  | -1.83112600 | 4.62029600 | -3.64789200 |
| C  | 0.08483400  | 5.66595100 | -2.34805800 |
| H  | 0.69923200  | 4.89926900 | -2.83066700 |
| H  | 0.19949700  | 5.54142300 | -1.26352500 |
| C  | 0.59295700  | 7.06887200 | -2.74183600 |
| H  | 0.47649800  | 7.20231100 | -3.82533800 |
| C  | 2.05957400  | 7.26397000 | -2.34481400 |
| H  | 2.69739100  | 6.50949500 | -2.82041900 |
| H  | 2.42271500  | 8.25219600 | -2.64515400 |
| H  | 2.18771300  | 7.17310600 | -1.25946700 |
| H  | -0.03032000 | 7.83524400 | -2.26134700 |
| H  | -1.10414600 | 4.01745800 | -4.18905000 |
| Si | -3.62703500 | 4.56884000 | -4.10066000 |
| O  | -3.91025800 | 3.24490700 | -5.01278700 |
| O  | -4.29168000 | 5.87542300 | -4.82854400 |
| O  | -4.25626400 | 4.40570200 | -2.53899600 |
| C  | -5.05077800 | 3.00640500 | -5.84639100 |
| H  | -5.89178200 | 2.64509500 | -5.24267800 |
| H  | -5.34770900 | 3.91549600 | -6.37860700 |
| H  | -4.77621000 | 2.23559600 | -6.57006500 |
| C  | -4.05741000 | 7.24077100 | -4.47451000 |
| H  | -4.52502200 | 7.86605200 | -5.23799600 |
| H  | -4.50108800 | 7.47773400 | -3.49929500 |
| H  | -2.98336500 | 7.46041000 | -4.44160000 |
| C  | -5.58657000 | 4.74064300 | -2.09665100 |
| H  | -6.28982200 | 3.95886100 | -2.39249500 |
| H  | -5.56032900 | 4.80591400 | -1.00883900 |
| H  | -5.88891100 | 5.69968900 | -2.52601000 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -3.89257200 | -1.97764500 | 1.98224500  |
| C | -2.63095100 | -2.54564300 | 2.08104300  |
| C | -1.50863400 | -1.93478300 | 1.45450700  |
| C | -1.76165800 | -0.74400900 | 0.74861800  |
| C | -3.05590900 | -0.16139200 | 0.64615800  |
| C | -4.12992500 | -0.77711800 | 1.26385800  |
| H | 0.09443100  | -3.30221300 | 1.99081400  |
| H | -4.73109500 | -2.46468300 | 2.47015100  |
| H | -2.49451000 | -3.46616300 | 2.64194600  |
| C | -0.16005700 | -2.38910900 | 1.45973600  |
| C | -0.74808700 | -0.01371300 | 0.06695300  |
| H | -5.12971600 | -0.36079300 | 1.20799100  |
| C | 0.55470500  | -0.47906700 | 0.08748400  |
| C | 0.82842300  | -1.67801400 | 0.79542300  |
| H | 1.35316500  | 0.05249500  | -0.41844300 |
| H | 1.84913800  | -2.04695400 | 0.81569700  |

UB3LYP-D3/BSII(SMD)//B3LYP-D3/BSI

HF=-2193.9469254

<sup>1</sup>M



Zero-point correction= 0.716551 (Hartree/Particle)  
Thermal correction to Energy= 0.763195  
Thermal correction to Enthalpy= 0.764139  
Thermal correction to Gibbs Free Energy= 0.633092  
Sum of electronic and zero-point Energies= -2191.047403  
Sum of electronic and thermal Energies= -2191.000760  
Sum of electronic and thermal Enthalpies= -2190.999815  
Sum of electronic and thermal Free Energies= -2191.130862

|    |             |            |             |
|----|-------------|------------|-------------|
| Ni | -1.91424100 | 3.50186500 | -1.52730600 |
| N  | -0.53733500 | 1.93120400 | -1.55102700 |
| N  | -3.03443000 | 2.18063500 | -0.64668200 |
| C  | 0.81797000  | 1.97271000 | -1.99308600 |
| C  | 1.07022500  | 1.93907600 | -3.37456100 |
| C  | 1.84227800  | 2.15904500 | -1.04395800 |
| C  | 2.39056500  | 2.10069900 | -3.80463000 |
| C  | 3.14807000  | 2.31628600 | -1.51987500 |
| C  | 3.42345900  | 2.29118500 | -2.88797900 |
| H  | 2.60510500  | 2.07794300 | -4.86977100 |
| H  | 3.95415300  | 2.46847700 | -0.80712100 |
| H  | 4.44306400  | 2.42274300 | -3.23766700 |
| C  | -4.37513300 | 2.35910900 | -0.16857200 |
| C  | -5.41197100 | 2.38989500 | -1.11830900 |
| C  | -4.59953300 | 2.52853200 | 1.20875300  |
| C  | -6.71442000 | 2.59329300 | -0.65368700 |
| C  | -5.91972300 | 2.74015600 | 1.62504700  |
| C  | -6.96837900 | 2.77142600 | 0.70676000  |
| H  | -7.53298100 | 2.61594000 | -1.36784100 |
| H  | -6.12110100 | 2.88146700 | 2.68350000  |
| H  | -7.98477900 | 2.93745400 | 1.05113500  |
| C  | 1.53684600  | 2.20205300 | 0.43505700  |
| H  | 2.40206300  | 2.55424500 | 1.00296200  |

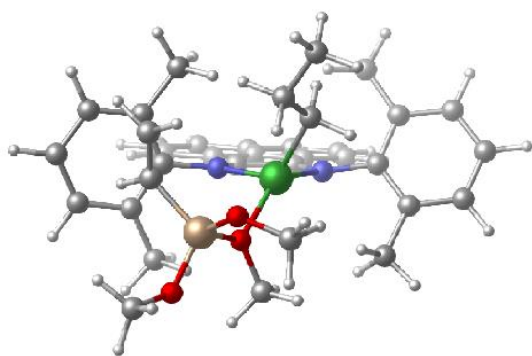
|    |             |            |             |
|----|-------------|------------|-------------|
| H  | 0.69077300  | 2.86499100 | 0.65623200  |
| H  | 1.26893500  | 1.20993800 | 0.81959300  |
| C  | -0.05050600 | 1.67877200 | -4.34765100 |
| H  | -0.24281900 | 0.60238900 | -4.44839500 |
| H  | -0.98332700 | 2.13514700 | -4.00410700 |
| H  | 0.18824100  | 2.06962900 | -5.34044700 |
| C  | -3.47602600 | 2.44036300 | 2.21510800  |
| H  | -3.24358800 | 1.39410400 | 2.45303600  |
| H  | -2.55431800 | 2.89933000 | 1.84387500  |
| H  | -3.75114000 | 2.93729800 | 3.14942300  |
| C  | -5.10759800 | 2.19344100 | -2.58215700 |
| H  | -4.36299300 | 2.92059400 | -2.93011400 |
| H  | -4.69163100 | 1.19609700 | -2.77410600 |
| H  | -6.01003500 | 2.30385900 | -3.18976900 |
| C  | -2.46379100 | 1.02647500 | -0.51018600 |
| C  | -1.04773400 | 0.89436200 | -0.98909200 |
| C  | -3.64631000 | 5.06287800 | -4.89592400 |
| H  | -4.51702900 | 4.60079600 | -5.35782200 |
| H  | -3.79265700 | 6.06519300 | -4.49913700 |
| C  | -2.46397900 | 4.43501100 | -4.80609400 |
| H  | -2.37708700 | 3.43304700 | -5.22527500 |
| C  | -3.11452500 | 4.98415700 | -1.23811400 |
| H  | -4.15155300 | 4.63679200 | -1.27074400 |
| H  | -2.95849500 | 5.70897300 | -2.04370000 |
| C  | -2.77350700 | 5.59922000 | 0.11383900  |
| H  | -2.90506000 | 4.85609600 | 0.90854300  |
| C  | -3.65174700 | 6.82326500 | 0.42958800  |
| H  | -4.71039500 | 6.53960800 | 0.45693600  |
| H  | -3.39128600 | 7.26050600 | 1.40059700  |
| H  | -3.53056300 | 7.59828100 | -0.33624100 |
| H  | -1.71650000 | 5.90005600 | 0.13533300  |
| Si | -0.99003200 | 5.27324400 | -4.07105600 |
| O  | -1.28033800 | 6.86567300 | -3.79180600 |
| O  | 0.39151900  | 4.99643300 | -4.91129100 |
| O  | -0.66267200 | 4.65044900 | -2.52668300 |
| C  | 0.43506300  | 5.24284200 | -1.77841700 |
| H  | 0.52962600  | 4.69285400 | -0.84350700 |
| H  | 1.35493800  | 5.13851000 | -2.35781200 |
| H  | 0.21124000  | 6.29291800 | -1.57863300 |
| C  | 0.54734800  | 4.90973100 | -6.32560800 |
| H  | -0.36524000 | 4.54882600 | -6.81705300 |
| H  | 0.80999000  | 5.88912300 | -6.74088700 |
| H  | 1.36147800  | 4.20959700 | -6.53375100 |
| C  | -1.16534000 | 7.90411800 | -4.76754100 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -1.38314000 | 8.85215300  | -4.27039200 |
| H | -0.15049100 | 7.94520100  | -5.18105500 |
| H | -1.88283100 | 7.76085900  | -5.58550500 |
| C | -2.87194000 | -0.27197400 | 0.02601300  |
| C | -4.03314600 | -0.79158100 | 0.57274300  |
| C | -1.73081200 | -1.11527900 | -0.11161500 |
| C | -4.03672800 | -2.15105500 | 0.97798900  |
| H | -4.92279000 | -0.18445400 | 0.69556400  |
| C | -1.71676500 | -2.46481200 | 0.28751000  |
| C | -0.60704000 | -0.46960800 | -0.69842000 |
| C | -2.92368400 | -2.96844100 | 0.84782800  |
| H | -4.94596500 | -2.56072700 | 1.40677900  |
| C | -0.49824700 | -3.17064800 | 0.08094000  |
| C | 0.56468400  | -1.17886200 | -0.88948700 |
| H | -2.97083100 | -4.00361800 | 1.17456200  |
| C | 0.59804900  | -2.53953100 | -0.48796900 |
| H | -0.43004100 | -4.21497800 | 0.37294500  |
| H | 1.43998000  | -0.71454200 | -1.33097200 |
| H | 1.51511500  | -3.10183600 | -0.63358800 |

UB3LYP-D3/BSII(SMD)//B3LYP-D3/BSI

HF=-2193.9513608

<sup>3</sup>M



|                                              |                             |
|----------------------------------------------|-----------------------------|
| Zero-point correction=                       | 0.714605 (Hartree/Particle) |
| Thermal correction to Energy=                | 0.761644                    |
| Thermal correction to Enthalpy=              | 0.762588                    |
| Thermal correction to Gibbs Free Energy=     | 0.630962                    |
| Sum of electronic and zero-point Energies=   | -2191.033796                |
| Sum of electronic and thermal Energies=      | -2190.986757                |
| Sum of electronic and thermal Enthalpies=    | -2190.985813                |
| Sum of electronic and thermal Free Energies= | -2191.117440                |

|    |             |            |             |
|----|-------------|------------|-------------|
| Ni | -2.59626700 | 3.49258000 | -1.55671900 |
| N  | -1.09041500 | 2.23152500 | -0.96654600 |
| N  | -3.78095000 | 2.04484200 | -0.59521300 |
| C  | 0.31913100  | 2.41792600 | -1.13242700 |
| C  | 0.96710500  | 1.84906000 | -2.24169800 |
| C  | 0.98952800  | 3.20942900 | -0.18499900 |
| C  | 2.33947300  | 2.08535200 | -2.38319200 |
| C  | 2.36115400  | 3.41742100 | -0.36451700 |
| C  | 3.03376700  | 2.86130000 | -1.45318700 |
| H  | 2.86342800  | 1.65778400 | -3.23367100 |
| H  | 2.90182000  | 4.02418300 | 0.35678700  |
| H  | 4.09800900  | 3.03578900 | -1.58025900 |
| C  | -5.15173800 | 2.19662200 | -0.25213000 |
| C  | -6.08105700 | 2.26382200 | -1.31151700 |
| C  | -5.54170200 | 2.39550100 | 1.09157200  |
| C  | -7.42936100 | 2.44637400 | -1.00429300 |
| C  | -6.90452000 | 2.59572600 | 1.34700900  |
| C  | -7.84377900 | 2.60518500 | 0.31895200  |
| H  | -8.15810900 | 2.47374000 | -1.80969100 |
| H  | -7.22522300 | 2.75744400 | 2.37266900  |
| H  | -8.89505600 | 2.75601900 | 0.54501000  |
| C  | 0.23897500  | 3.79687700 | 0.98359900  |
| H  | -0.66709900 | 4.31375600 | 0.64897400  |
| H  | -0.08005300 | 3.01470500 | 1.68502300  |
| H  | 0.86067100  | 4.50672300 | 1.53564100  |
| C  | 0.20071800  | 1.01303400 | -3.23616500 |

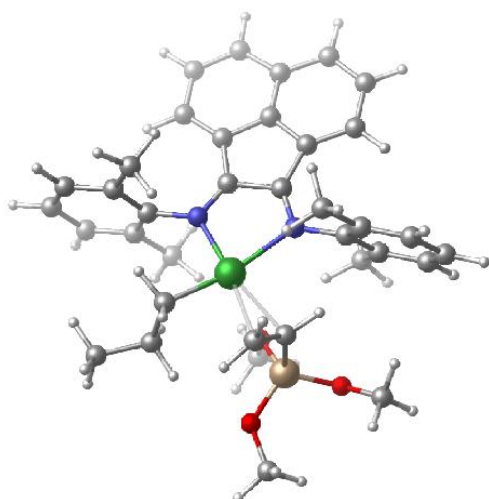
|    |             |            |             |
|----|-------------|------------|-------------|
| H  | -0.19242800 | 0.09792400 | -2.77562400 |
| H  | -0.65261400 | 1.57123800 | -3.63349100 |
| H  | 0.83625000  | 0.71855400 | -4.07539600 |
| C  | -4.55770600 | 2.43776000 | 2.23771900  |
| H  | -4.93271200 | 3.08744700 | 3.03358200  |
| H  | -4.39820300 | 1.44382100 | 2.67303000  |
| H  | -3.57952800 | 2.81822900 | 1.92853700  |
| C  | -5.61450700 | 2.14858500 | -2.74005000 |
| H  | -5.02500600 | 1.24091600 | -2.91330200 |
| H  | -6.45916900 | 2.14446500 | -3.43438000 |
| H  | -4.97565600 | 3.00342200 | -3.00309600 |
| C  | -3.04045500 | 1.09265700 | -0.13368300 |
| C  | -1.55186400 | 1.18715500 | -0.36651700 |
| C  | 0.69450400  | 6.50840700 | -2.07636000 |
| H  | 0.01252000  | 7.35366000 | -2.11831900 |
| H  | 1.54702500  | 6.60860700 | -1.40633100 |
| C  | 0.49946300  | 5.40103900 | -2.80592900 |
| C  | -3.24078400 | 5.02753800 | -0.45175100 |
| H  | -3.29311200 | 4.68219500 | 0.58797800  |
| H  | -4.27784900 | 5.10669200 | -0.82502500 |
| C  | -2.48853100 | 6.34096500 | -0.58388200 |
| H  | -1.45067600 | 6.21066200 | -0.25219400 |
| C  | -3.13633600 | 7.47768500 | 0.22807000  |
| H  | -3.17290200 | 7.22546800 | 1.29460300  |
| H  | -2.57409900 | 8.41314800 | 0.11946700  |
| H  | -4.16480300 | 7.65997100 | -0.10579600 |
| H  | -2.42937300 | 6.63894700 | -1.63642300 |
| H  | 1.22367500  | 4.59255200 | -2.72982900 |
| Si | -0.88121500 | 5.21832100 | -4.00312400 |
| O  | -0.39523100 | 4.73663700 | -5.50035900 |
| O  | -1.74301100 | 6.61728400 | -4.01342500 |
| O  | -1.91302800 | 3.93551700 | -3.54844300 |
| C  | 0.48178700  | 5.50638000 | -6.33067300 |
| H  | 0.69959500  | 4.91325800 | -7.22195600 |
| H  | 0.00796900  | 6.44725100 | -6.63339700 |
| H  | 1.42196700  | 5.72957900 | -5.81178400 |
| C  | -3.08973900 | 6.74366700 | -4.46492500 |
| H  | -3.77080100 | 6.17927300 | -3.81392300 |
| H  | -3.36078400 | 7.80114100 | -4.42263600 |
| H  | -3.20268800 | 6.39243100 | -5.49854000 |
| C  | -2.62693300 | 3.17407000 | -4.55559100 |
| H  | -1.97615300 | 2.98235600 | -5.40945600 |
| H  | -2.93157300 | 2.22827700 | -4.10217500 |
| H  | -3.51586100 | 3.72338100 | -4.88118200 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -4.24350000 | -2.04682800 | 1.73474800  |
| C | -2.99703700 | -2.62489900 | 1.92328500  |
| C | -1.82182700 | -1.97956700 | 1.44772600  |
| C | -2.00715800 | -0.74811400 | 0.79164600  |
| C | -3.28321900 | -0.14624200 | 0.61015200  |
| C | -4.40938000 | -0.79920500 | 1.08040500  |
| H | -0.27700000 | -3.38142800 | 2.05924100  |
| H | -5.12603900 | -2.55968700 | 2.10420300  |
| H | -2.91359200 | -3.57835500 | 2.43747300  |
| C | -0.47954200 | -2.43851700 | 1.55873400  |
| C | -0.93477100 | 0.00910300  | 0.24363400  |
| H | -5.39962600 | -0.37233400 | 0.96485400  |
| C | 0.36162600  | -0.46145700 | 0.36594400  |
| C | 0.56774800  | -1.69541800 | 1.03478100  |
| H | 1.20477600  | 0.08738000  | -0.03770400 |
| H | 1.58238900  | -2.06828900 | 1.13392500  |

UB3LYP-D3/BSII(SMD)//B3LYP-D3/BSI

HF=-2193.9431886

<sup>1</sup>N



|                                              |                             |            |             |
|----------------------------------------------|-----------------------------|------------|-------------|
| Zero-point correction=                       | 0.717932 (Hartree/Particle) |            |             |
| Thermal correction to Energy=                | 0.764148                    |            |             |
| Thermal correction to Enthalpy=              | 0.765093                    |            |             |
| Thermal correction to Gibbs Free Energy=     | 0.635948                    |            |             |
| Sum of electronic and zero-point Energies=   | -2191.036132                |            |             |
| Sum of electronic and thermal Energies=      | -2190.989915                |            |             |
| Sum of electronic and thermal Enthalpies=    | -2190.988971                |            |             |
| Sum of electronic and thermal Free Energies= | -2191.118115                |            |             |
| Ni                                           | -1.86638900                 | 3.61766800 | -1.47361800 |
| N                                            | -0.50744600                 | 1.95088600 | -1.52083400 |
| N                                            | -3.00285600                 | 2.24569000 | -0.57062400 |
| C                                            | 0.81160300                  | 1.84788100 | -2.06644300 |
| C                                            | 0.93653800                  | 1.79801400 | -3.46705500 |
| C                                            | 1.92507800                  | 1.89239300 | -1.20602900 |
| C                                            | 2.22545100                  | 1.76791300 | -4.00870200 |
| C                                            | 3.19533700                  | 1.86546300 | -1.79542100 |
| C                                            | 3.34826900                  | 1.80059800 | -3.18089900 |
| H                                            | 2.34529900                  | 1.72086800 | -5.08764400 |
| H                                            | 4.07163400                  | 1.90075900 | -1.15369900 |
| H                                            | 4.34306600                  | 1.78229500 | -3.61595500 |
| C                                            | -4.30239600                 | 2.42502600 | 0.01393000  |
| C                                            | -5.43608600                 | 2.19965500 | -0.78530300 |
| C                                            | -4.38100700                 | 2.83581400 | 1.35420800  |
| C                                            | -6.69064800                 | 2.40778800 | -0.20306300 |
| C                                            | -5.65692100                 | 3.03716900 | 1.89257700  |
| C                                            | -6.80191500                 | 2.82734500 | 1.12328300  |
| H                                            | -7.58404300                 | 2.24427600 | -0.79931500 |
| H                                            | -5.74824400                 | 3.36118800 | 2.92572100  |
| H                                            | -7.78330300                 | 2.99255800 | 1.55776700  |
| C                                            | 1.75532500                  | 1.96064100 | 0.29271900  |

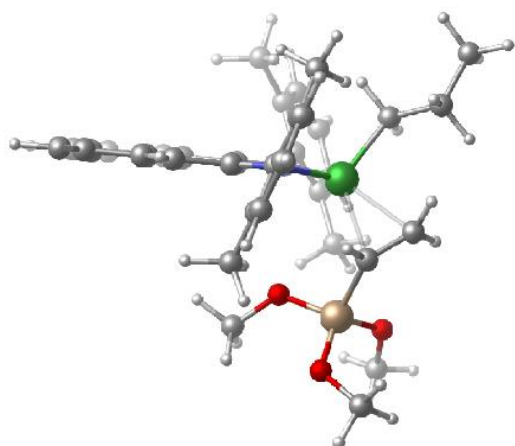
|    |             |            |             |
|----|-------------|------------|-------------|
| H  | 2.68659800  | 2.27059400 | 0.77379000  |
| H  | 0.97370000  | 2.67007900 | 0.58034700  |
| H  | 1.47709300  | 0.98043300 | 0.70142100  |
| C  | -0.29649900 | 1.75833100 | -4.33657700 |
| H  | -0.82084200 | 0.79878600 | -4.24090000 |
| H  | -1.01587100 | 2.53447000 | -4.04484600 |
| H  | -0.04361100 | 1.89810900 | -5.39100000 |
| C  | -3.13228200 | 2.99985200 | 2.18637000  |
| H  | -2.75978800 | 2.02344100 | 2.52545900  |
| H  | -2.32588800 | 3.47295100 | 1.61797700  |
| H  | -3.33290600 | 3.60307100 | 3.07639000  |
| C  | -5.28178800 | 1.73465300 | -2.21214100 |
| H  | -4.58538900 | 2.37740400 | -2.76557200 |
| H  | -4.87794700 | 0.71487600 | -2.25663900 |
| H  | -6.24205600 | 1.73760000 | -2.73433800 |
| C  | -2.43659500 | 1.09432700 | -0.42979500 |
| C  | -1.05767900 | 0.91780100 | -0.98934800 |
| C  | -0.91631500 | 5.37024800 | -2.71648100 |
| H  | -0.97336000 | 4.98948600 | -3.73518600 |
| H  | -1.49825500 | 6.25996300 | -2.50799600 |
| C  | -0.03672500 | 4.86874400 | -1.80405200 |
| H  | 0.63420400  | 4.09291700 | -2.16395300 |
| C  | -3.36124400 | 4.88758700 | -1.48538300 |
| H  | -4.24390400 | 4.25047600 | -1.42182500 |
| H  | -3.40950300 | 5.41507400 | -2.44466300 |
| C  | -3.30608800 | 5.84840700 | -0.30549200 |
| H  | -3.07311600 | 5.30001600 | 0.61300600  |
| C  | -4.64625800 | 6.58219600 | -0.11873600 |
| H  | -5.45236800 | 5.86883400 | 0.08910200  |
| H  | -4.59147700 | 7.28714300 | 0.71888400  |
| H  | -4.91826400 | 7.14675100 | -1.01845900 |
| H  | -2.49926400 | 6.57831600 | -0.43269600 |
| Si | 0.43107300  | 5.63109700 | -0.15546100 |
| O  | -0.10044900 | 7.18319900 | -0.05098400 |
| O  | 2.06300900  | 5.51556200 | 0.02412800  |
| O  | -0.28159400 | 4.74434400 | 1.03491400  |
| C  | -0.04029800 | 5.02771900 | 2.42106200  |
| H  | -0.60917200 | 4.30507700 | 3.01070300  |
| H  | 1.02468300  | 4.92553600 | 2.65705100  |
| H  | -0.37645100 | 6.03950600 | 2.67288600  |
| C  | 3.05416700  | 5.64389200 | -0.99349700 |
| H  | 3.04423400  | 4.77142900 | -1.65850200 |
| H  | 2.91505200  | 6.55384800 | -1.59134900 |
| H  | 4.02980400  | 5.69938700 | -0.50375900 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 0.64054600  | 8.34751400  | -0.41790800 |
| H | 0.11326200  | 9.21789200  | -0.01987800 |
| H | 1.65348900  | 8.32281800  | 0.00023500  |
| H | 0.70388600  | 8.44420900  | -1.50986100 |
| C | -2.84267600 | -0.17952600 | 0.16445300  |
| C | -3.96680500 | -0.64219600 | 0.82798400  |
| C | -1.75904900 | -1.07253300 | -0.07690500 |
| C | -3.99124800 | -1.99828900 | 1.24348300  |
| H | -4.81260300 | 0.00418600  | 1.03119700  |
| C | -1.76986900 | -2.42158800 | 0.32452600  |
| C | -0.66662500 | -0.47636400 | -0.76701700 |
| C | -2.93691300 | -2.86725200 | 1.00542100  |
| H | -4.87029500 | -2.36392300 | 1.76494400  |
| C | -0.61399200 | -3.18528100 | 0.00053400  |
| C | 0.44459800  | -1.24328200 | -1.07034900 |
| H | -2.99958200 | -3.89921900 | 1.33961700  |
| C | 0.44925800  | -2.60593800 | -0.67563500 |
| H | -0.56790900 | -4.23246900 | 0.28653700  |
| H | 1.29643400  | -0.82426500 | -1.59396100 |
| H | 1.31861300  | -3.21140800 | -0.91220600 |

UB3LYP-D3/BSII(SMD)//B3LYP-D3/BSI

HF=-2193.9374693

<sup>3</sup>N



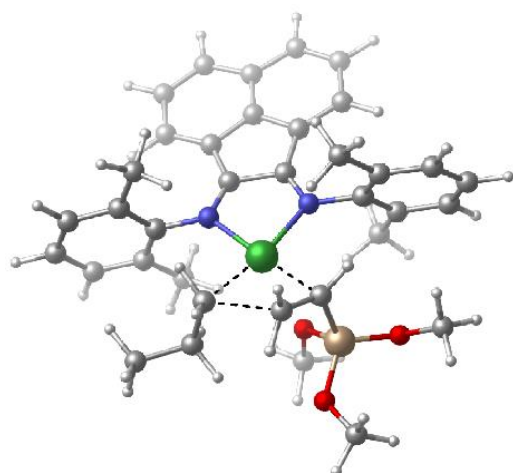
|                                              |                             |            |             |
|----------------------------------------------|-----------------------------|------------|-------------|
| Zero-point correction=                       | 0.714941 (Hartree/Particle) |            |             |
| Thermal correction to Energy=                | 0.761966                    |            |             |
| Thermal correction to Enthalpy=              | 0.762910                    |            |             |
| Thermal correction to Gibbs Free Energy=     | 0.630600                    |            |             |
| Sum of electronic and zero-point Energies=   | -2191.031407                |            |             |
| Sum of electronic and thermal Energies=      | -2190.984382                |            |             |
| Sum of electronic and thermal Enthalpies=    | -2190.983438                |            |             |
| Sum of electronic and thermal Free Energies= | -2191.115749                |            |             |
| Ni                                           | -2.23360100                 | 3.86584200 | -1.10794900 |
| N                                            | -0.80684900                 | 2.44679800 | -0.54807700 |
| N                                            | -3.53641400                 | 2.37807600 | -0.50083900 |
| C                                            | 0.61560800                  | 2.59642700 | -0.55667700 |
| C                                            | 1.40577000                  | 2.03300400 | -1.58015300 |
| C                                            | 1.17444900                  | 3.39321700 | 0.46539700  |
| C                                            | 2.78262400                  | 2.29735300 | -1.55814500 |
| C                                            | 2.55277000                  | 3.61500200 | 0.45041300  |
| C                                            | 3.35507900                  | 3.07721700 | -0.55726500 |
| H                                            | 3.40607600                  | 1.88019500 | -2.34478700 |
| H                                            | 2.99924400                  | 4.21488500 | 1.23864300  |
| H                                            | 4.42411700                  | 3.26781200 | -0.56083600 |
| C                                            | -4.91727500                 | 2.54828000 | -0.20332700 |
| C                                            | -5.77710100                 | 2.94198700 | -1.24961200 |
| C                                            | -5.36817200                 | 2.45027000 | 1.13326700  |
| C                                            | -7.12595600                 | 3.14975900 | -0.95540100 |
| C                                            | -6.72623300                 | 2.68601800 | 1.37874600  |
| C                                            | -7.60365700                 | 3.01577400 | 0.34831900  |
| H                                            | -7.80431600                 | 3.42927900 | -1.75680000 |
| H                                            | -7.09205800                 | 2.62097900 | 2.39991600  |
| H                                            | -8.65377800                 | 3.18921100 | 0.56351200  |
| C                                            | 0.30360100                  | 3.94053300 | 1.56812600  |
| H                                            | -0.54375600                 | 4.50164000 | 1.16439700  |
| H                                            | -0.11834000                 | 3.13168200 | 2.17865300  |

|    |             |            |             |
|----|-------------|------------|-------------|
| H  | 0.87253800  | 4.59926600 | 2.22960500  |
| C  | 0.83287100  | 1.15971900 | -2.67159200 |
| H  | -0.23978200 | 1.30319800 | -2.79896600 |
| H  | 1.31495500  | 1.36924100 | -3.63175000 |
| H  | 0.99678700  | 0.09773900 | -2.44844700 |
| C  | -4.44373000 | 2.14671300 | 2.28985500  |
| H  | -4.85209700 | 2.55636200 | 3.21788500  |
| H  | -4.31302000 | 1.06787200 | 2.43668300  |
| H  | -3.44846600 | 2.57872900 | 2.14297200  |
| C  | -5.24689100 | 3.13377600 | -2.64547200 |
| H  | -4.68863300 | 2.26378600 | -3.00077800 |
| H  | -6.05857700 | 3.34425700 | -3.34740800 |
| H  | -4.54954000 | 3.98210100 | -2.69538500 |
| C  | -2.89444500 | 1.28733300 | -0.25280700 |
| C  | -1.38330700 | 1.31931300 | -0.30092600 |
| C  | -1.38577700 | 5.44572600 | -2.68476100 |
| H  | -2.32684700 | 5.88370900 | -3.01398300 |
| H  | -0.76693000 | 6.06152200 | -2.03638300 |
| C  | -0.95734200 | 4.24689900 | -3.15816900 |
| C  | -2.91585200 | 5.23611400 | 0.21329400  |
| H  | -2.88394800 | 4.71181300 | 1.17637700  |
| H  | -3.96801300 | 5.29380800 | -0.10861900 |
| C  | -2.25964800 | 6.60460300 | 0.27586900  |
| H  | -1.17257900 | 6.50511200 | 0.40755300  |
| C  | -2.81891000 | 7.46791200 | 1.42249700  |
| H  | -2.64480600 | 6.98692700 | 2.39225700  |
| H  | -2.34265900 | 8.45517300 | 1.44202700  |
| H  | -3.89946700 | 7.61287200 | 1.30990300  |
| H  | -2.40827400 | 7.13428200 | -0.67377600 |
| H  | 0.02721200  | 3.91141200 | -2.83300100 |
| Si | -1.84392500 | 3.20040100 | -4.42808100 |
| O  | -0.84797200 | 2.69797900 | -5.63559900 |
| O  | -3.07707200 | 4.15258300 | -4.95588800 |
| O  | -2.35241000 | 1.82959500 | -3.66203800 |
| C  | -0.26014800 | 3.56173900 | -6.61359800 |
| H  | 0.20292800  | 2.93278400 | -7.37750200 |
| H  | -1.01394600 | 4.20216600 | -7.08687500 |
| H  | 0.51122500  | 4.19578700 | -6.15966700 |
| C  | -4.05875900 | 3.75223300 | -5.91466000 |
| H  | -4.68471200 | 2.94345200 | -5.51872400 |
| H  | -4.69185500 | 4.61714500 | -6.12641300 |
| H  | -3.59066100 | 3.41846500 | -6.84862100 |
| C  | -2.51795800 | 0.53388800 | -4.24364100 |
| H  | -1.76158200 | 0.34416700 | -5.01136200 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -2.41635300 | -0.20602200 | -3.44401600 |
| H | -3.51666100 | 0.44062800  | -4.68654900 |
| C | -4.48166200 | -2.10339600 | 0.61826600  |
| C | -3.30005800 | -2.80781100 | 0.79485000  |
| C | -2.04225400 | -2.16399300 | 0.63036200  |
| C | -2.07854400 | -0.80173400 | 0.27551300  |
| C | -3.28910500 | -0.07423200 | 0.11391600  |
| C | -4.49847300 | -0.72526900 | 0.28324800  |
| H | -0.66301900 | -3.78665800 | 1.06809200  |
| H | -5.42890400 | -2.61696300 | 0.75025000  |
| H | -3.33113400 | -3.85972600 | 1.06506600  |
| C | -0.75143100 | -2.73952900 | 0.79193300  |
| C | -0.90913900 | -0.02017400 | 0.05996900  |
| H | -5.44173200 | -0.20083800 | 0.17720400  |
| C | 0.33308900  | -0.60581600 | 0.23522700  |
| C | 0.38953300  | -1.97402800 | 0.60590100  |
| H | 1.24955100  | -0.04446400 | 0.09535600  |
| H | 1.36343400  | -2.43364300 | 0.74272100  |

UB3LYP-D3/BSII(SMD)//B3LYP-D3/BSI

HF=-2193.9383111

**<sup>1</sup>TS6**

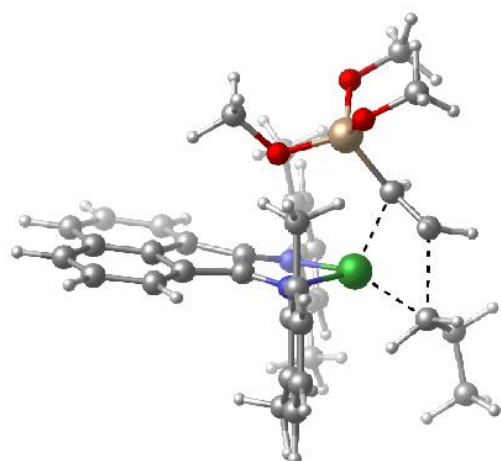
|                                              |                             |            |             |
|----------------------------------------------|-----------------------------|------------|-------------|
| Zero-point correction=                       | 0.718177 (Hartree/Particle) |            |             |
| Thermal correction to Energy=                | 0.763248                    |            |             |
| Thermal correction to Enthalpy=              | 0.764192                    |            |             |
| Thermal correction to Gibbs Free Energy=     | 0.639196                    |            |             |
| Sum of electronic and zero-point Energies=   | -2191.024481                |            |             |
| Sum of electronic and thermal Energies=      | -2190.979410                |            |             |
| Sum of electronic and thermal Enthalpies=    | -2190.978466                |            |             |
| Sum of electronic and thermal Free Energies= | -2191.103462                |            |             |
| Ni                                           | -1.72648500                 | 3.65649600 | -1.40382400 |
| N                                            | -0.47908900                 | 2.06739000 | -1.37391400 |
| N                                            | -3.00231800                 | 2.28370200 | -0.53428000 |
| C                                            | 0.85837900                  | 1.97969400 | -1.88968300 |
| C                                            | 1.01480100                  | 1.93586600 | -3.28837800 |
| C                                            | 1.95075500                  | 1.96091700 | -1.00387800 |
| C                                            | 2.31471600                  | 1.87127000 | -3.80050600 |
| C                                            | 3.23218600                  | 1.89148700 | -1.56511200 |
| C                                            | 3.41762300                  | 1.84819900 | -2.94618100 |
| H                                            | 2.45776000                  | 1.83099600 | -4.87686400 |
| H                                            | 4.09267500                  | 1.87737400 | -0.90165500 |
| H                                            | 4.42139700                  | 1.79834200 | -3.35770400 |
| C                                            | -4.31756100                 | 2.47238800 | -0.00057300 |
| C                                            | -5.42090600                 | 2.34136000 | -0.86163700 |
| C                                            | -4.44909100                 | 2.80637200 | 1.35976400  |
| C                                            | -6.69390600                 | 2.57184000 | -0.32691300 |
| C                                            | -5.74028900                 | 3.02779100 | 1.84912000  |
| C                                            | -6.85404800                 | 2.91512700 | 1.01528300  |
| H                                            | -7.56317300                 | 2.47652500 | -0.97174700 |
| H                                            | -5.86985500                 | 3.29372900 | 2.89467700  |
| H                                            | -7.84811900                 | 3.09644400 | 1.41285300  |
| C                                            | 1.76128600                  | 1.97017100 | 0.49348200  |
| H                                            | 2.67373400                  | 2.30631500 | 0.99255700  |

|    |             |            |             |
|----|-------------|------------|-------------|
| H  | 0.94782900  | 2.63477000 | 0.79243400  |
| H  | 1.52834100  | 0.96278400 | 0.86290100  |
| C  | -0.19303600 | 1.91408400 | -4.19357600 |
| H  | -0.76293800 | 0.98408300 | -4.07201600 |
| H  | -0.88591800 | 2.73394800 | -3.96344300 |
| H  | 0.09901200  | 1.99370100 | -5.24409900 |
| C  | -3.23956700 | 2.87738900 | 2.26240100  |
| H  | -2.91986500 | 1.87168200 | 2.56654600  |
| H  | -2.38518100 | 3.34713100 | 1.76417400  |
| H  | -3.46492800 | 3.44043900 | 3.17250300  |
| C  | -5.23036200 | 1.90031500 | -2.29341800 |
| H  | -4.43085800 | 2.46112100 | -2.79259800 |
| H  | -4.94754100 | 0.84055900 | -2.34184300 |
| H  | -6.15017800 | 2.02672800 | -2.87055800 |
| C  | -2.42858700 | 1.14177200 | -0.37586100 |
| C  | -1.02854100 | 1.00663700 | -0.88712400 |
| C  | -1.40757200 | 5.58873800 | -2.47960900 |
| H  | -1.67946800 | 5.45795000 | -3.52572700 |
| H  | -1.63879700 | 6.56802000 | -2.07639800 |
| C  | -0.29562900 | 4.88844400 | -1.95537100 |
| H  | 0.29985800  | 4.30728900 | -2.65651400 |
| C  | -3.26430800 | 5.09962300 | -1.55352600 |
| H  | -3.91520100 | 4.23106000 | -1.65676400 |
| H  | -3.58381400 | 5.77814200 | -2.34401200 |
| C  | -3.36200500 | 5.76261900 | -0.18536900 |
| H  | -3.03133900 | 5.07555100 | 0.59749300  |
| C  | -4.80050700 | 6.21895700 | 0.10591700  |
| H  | -5.49212000 | 5.37035000 | 0.09383700  |
| H  | -4.86310800 | 6.69145000 | 1.09254300  |
| H  | -5.14109600 | 6.94798000 | -0.63893600 |
| H  | -2.67906500 | 6.61938800 | -0.13549400 |
| Si | 0.49060700  | 5.49704200 | -0.37200200 |
| O  | 0.12563400  | 7.09220700 | -0.14212000 |
| O  | 2.10933800  | 5.20161800 | -0.34494900 |
| O  | -0.21776400 | 4.69654200 | 0.88922600  |
| C  | 0.02430800  | 5.06757200 | 2.25296600  |
| H  | -0.69212500 | 4.52745100 | 2.87713100  |
| H  | 1.04118400  | 4.78827800 | 2.55152600  |
| H  | -0.11538300 | 6.14435500 | 2.39418200  |
| C  | 3.02099400  | 5.33810400 | -1.43237500 |
| H  | 2.69228200  | 4.76215000 | -2.30564900 |
| H  | 3.14830500  | 6.38980700 | -1.71752000 |
| H  | 3.98748300  | 4.94464800 | -1.10864000 |
| C  | 0.84057500  | 8.18271300 | -0.71859500 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 0.36308500  | 9.10928400  | -0.38952500 |
| H | 1.88648000  | 8.18912900  | -0.38891500 |
| H | 0.81286500  | 8.14732900  | -1.81704600 |
| C | -2.82876500 | -0.15237200 | 0.17684400  |
| C | -3.96709900 | -0.64907300 | 0.78766800  |
| C | -1.72334900 | -1.01952000 | -0.05386700 |
| C | -3.98401500 | -2.01663100 | 1.16501900  |
| H | -4.82842300 | -0.01912100 | 0.97930200  |
| C | -1.72690800 | -2.37980500 | 0.30760300  |
| C | -0.61920400 | -0.38594600 | -0.69365400 |
| C | -2.90830100 | -2.86188200 | 0.93748500  |
| H | -4.87342100 | -2.41059600 | 1.64679100  |
| C | -0.55101100 | -3.11787600 | -0.00299000 |
| C | 0.51052400  | -1.13077500 | -0.98616100 |
| H | -2.96505900 | -3.90384900 | 1.24021600  |
| C | 0.52243700  | -2.50409200 | -0.63087800 |
| H | -0.49777100 | -4.17221900 | 0.25403400  |
| H | 1.37227900  | -0.68741700 | -1.47164500 |
| H | 1.40707300  | -3.09024600 | -0.85936900 |

UB3LYP-D3/BSII(SMD)//B3LYP-D3/BSI

HF=-2193.9240474

**<sup>3</sup>TS6**

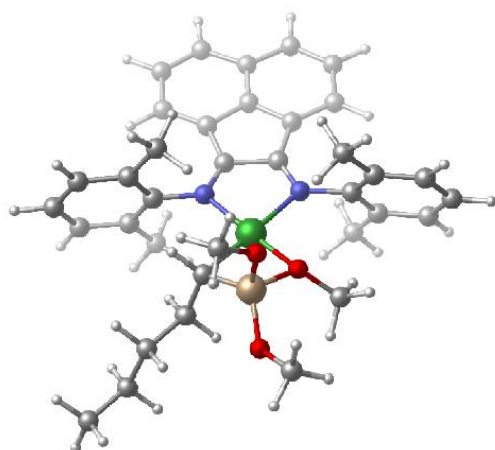
|                                              |                             |            |             |
|----------------------------------------------|-----------------------------|------------|-------------|
| Zero-point correction=                       | 0.714441 (Hartree/Particle) |            |             |
| Thermal correction to Energy=                | 0.760599                    |            |             |
| Thermal correction to Enthalpy=              | 0.761543                    |            |             |
| Thermal correction to Gibbs Free Energy=     | 0.631182                    |            |             |
| Sum of electronic and zero-point Energies=   | -2191.004193                |            |             |
| Sum of electronic and thermal Energies=      | -2190.958035                |            |             |
| Sum of electronic and thermal Enthalpies=    | -2190.957091                |            |             |
| Sum of electronic and thermal Free Energies= | -2191.087452                |            |             |
| Ni                                           | -2.11413100                 | 3.87478800 | -1.00875700 |
| N                                            | -0.78464000                 | 2.43605100 | -0.49253900 |
| N                                            | -3.48645300                 | 2.42888300 | -0.51027600 |
| C                                            | 0.62368500                  | 2.63167600 | -0.35558200 |
| C                                            | 1.53812400                  | 2.24228900 | -1.35281800 |
| C                                            | 1.03279500                  | 3.30483000 | 0.81669300  |
| C                                            | 2.89279600                  | 2.52930000 | -1.13306100 |
| C                                            | 2.39348200                  | 3.56633800 | 0.98879800  |
| C                                            | 3.32122100                  | 3.18238400 | 0.01992100  |
| H                                            | 3.61695300                  | 2.23505000 | -1.88823400 |
| H                                            | 2.72647300                  | 4.06828100 | 1.89310700  |
| H                                            | 4.37681700                  | 3.39157600 | 0.16528400  |
| C                                            | -4.86752100                 | 2.59720100 | -0.16358700 |
| C                                            | -5.88556900                 | 2.42219100 | -1.11522400 |
| C                                            | -5.13658900                 | 2.97934700 | 1.16661400  |
| C                                            | -7.20429400                 | 2.65622100 | -0.70452200 |
| C                                            | -6.46762100                 | 3.21086100 | 1.52670800  |
| C                                            | -7.49666400                 | 3.05535600 | 0.59847800  |
| H                                            | -8.00813300                 | 2.51981900 | -1.42303400 |
| H                                            | -6.69539200                 | 3.50487800 | 2.54772500  |
| H                                            | -8.52600700                 | 3.23631700 | 0.89326800  |
| C                                            | 0.02433500                  | 3.68467900 | 1.87446200  |
| H                                            | -0.77439000                 | 4.31863000 | 1.46720700  |

|    |             |            |             |
|----|-------------|------------|-------------|
| H  | -0.46818000 | 2.80089400 | 2.29806100  |
| H  | 0.49960300  | 4.23231500 | 2.69267200  |
| C  | 1.11111300  | 1.58857500 | -2.64460000 |
| H  | 0.21040700  | 0.98243600 | -2.54460700 |
| H  | 0.89141000  | 2.33749000 | -3.41304400 |
| H  | 1.91129000  | 0.95157400 | -3.03424800 |
| C  | -4.02540800 | 3.07565700 | 2.18614000  |
| H  | -4.38688200 | 3.51276400 | 3.12072600  |
| H  | -3.61495600 | 2.08411900 | 2.41828900  |
| H  | -3.18435600 | 3.68216400 | 1.83008600  |
| C  | -5.57516800 | 1.98938500 | -2.52387300 |
| H  | -4.83185000 | 1.18755800 | -2.55271900 |
| H  | -6.47874100 | 1.64012700 | -3.03179900 |
| H  | -5.15754000 | 2.80629900 | -3.11968700 |
| C  | -2.88440700 | 1.29878400 | -0.38233900 |
| C  | -1.37281200 | 1.29110500 | -0.42147800 |
| C  | -2.75188000 | 5.17409800 | -2.67073900 |
| H  | -3.80412400 | 4.97715100 | -2.86557600 |
| H  | -2.47097100 | 6.21734400 | -2.78342300 |
| C  | -1.79836400 | 4.17004600 | -3.04190100 |
| C  | -2.97399900 | 5.78475200 | -0.59278100 |
| H  | -3.36000900 | 5.15371400 | 0.22608200  |
| H  | -3.81381700 | 6.38443600 | -0.93877300 |
| C  | -1.75428400 | 6.61027000 | -0.19925300 |
| H  | -0.84725700 | 5.98630400 | -0.12744700 |
| C  | -1.95354700 | 7.32895900 | 1.14528800  |
| H  | -2.11217000 | 6.60677200 | 1.95517800  |
| H  | -1.07688200 | 7.93498500 | 1.39872700  |
| H  | -2.82668400 | 7.98941500 | 1.10887500  |
| H  | -1.54103100 | 7.34371100 | -0.98661700 |
| H  | -0.75911000 | 4.51509600 | -3.07829100 |
| Si | -2.15261500 | 2.69509600 | -4.10567500 |
| O  | -0.89558600 | 2.48092500 | -5.15613500 |
| O  | -3.60569900 | 2.87764500 | -4.87472200 |
| O  | -2.25789400 | 1.29855500 | -3.23050200 |
| C  | -0.39092800 | 3.43977700 | -6.07926300 |
| H  | 0.65261500  | 3.19124000 | -6.29318500 |
| H  | -0.95673500 | 3.41099100 | -7.01782300 |
| H  | -0.43021800 | 4.46109000 | -5.67505600 |
| C  | -3.88282200 | 3.83585900 | -5.89099000 |
| H  | -4.96869200 | 3.93695400 | -5.97459800 |
| H  | -3.45874800 | 4.82173800 | -5.65298500 |
| H  | -3.48645900 | 3.50469500 | -6.85800900 |
| C  | -2.42387700 | 0.02041600 | -3.85346900 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -1.59289500 | -0.19151000 | -4.53511800 |
| H | -2.43920200 | -0.73238000 | -3.05979200 |
| H | -3.36867300 | -0.02356800 | -4.40706600 |
| C | -4.57347700 | -2.08013600 | 0.29941200  |
| C | -3.41466000 | -2.83904700 | 0.37304500  |
| C | -2.13743200 | -2.23280500 | 0.21029400  |
| C | -2.13231900 | -0.84668900 | -0.03302200 |
| C | -3.32055300 | -0.06792000 | -0.10583600 |
| C | -4.54939700 | -0.68181500 | 0.06124400  |
| H | -0.80827400 | -3.93664600 | 0.45370500  |
| H | -5.53433200 | -2.56819000 | 0.42954200  |
| H | -3.47869900 | -3.90761100 | 0.55941800  |
| C | -0.86499900 | -2.86708200 | 0.27106400  |
| C | -0.93932600 | -0.09040100 | -0.21263300 |
| H | -5.47433800 | -0.11801800 | 0.01349300  |
| C | 0.28380800  | -0.73315500 | -0.13971900 |
| C | 0.29814400  | -2.13116600 | 0.10319700  |
| H | 1.21502100  | -0.19308200 | -0.26569100 |
| H | 1.25676700  | -2.63768400 | 0.15713600  |

UB3LYP-D3/BSII(SMD)//B3LYP-D3/BSI

HF=-2193.9117833



|                                              |                             |            |             |
|----------------------------------------------|-----------------------------|------------|-------------|
| Zero-point correction=                       | 0.719722 (Hartree/Particle) |            |             |
| Thermal correction to Energy=                | 0.765485                    |            |             |
| Thermal correction to Enthalpy=              | 0.766429                    |            |             |
| Thermal correction to Gibbs Free Energy=     | 0.635687                    |            |             |
| Sum of electronic and zero-point Energies=   | -2191.071529                |            |             |
| Sum of electronic and thermal Energies=      | -2191.025766                |            |             |
| Sum of electronic and thermal Enthalpies=    | -2191.024822                |            |             |
| Sum of electronic and thermal Free Energies= | -2191.155564                |            |             |
| Ni                                           | -2.04870100                 | 3.79241000 | -1.26824700 |
| N                                            | -1.04629700                 | 2.14441700 | -1.25364900 |
| N                                            | -3.42232500                 | 2.70935800 | -0.22040100 |
| C                                            | 0.25157200                  | 1.91718200 | -1.81847000 |
| C                                            | 0.35323700                  | 1.28116600 | -3.06743600 |
| C                                            | 1.37035200                  | 2.37555700 | -1.10082600 |
| C                                            | 1.63512400                  | 1.12243800 | -3.60723000 |
| C                                            | 2.63049900                  | 2.18963800 | -1.67785400 |
| C                                            | 2.76361300                  | 1.57329700 | -2.92269200 |
| H                                            | 1.74311300                  | 0.64235800 | -4.57596100 |
| H                                            | 3.51233500                  | 2.53258400 | -1.14363300 |
| H                                            | 3.74911600                  | 1.44359200 | -3.35984000 |
| C                                            | -4.66805600                 | 3.15711200 | 0.31396700  |
| C                                            | -5.86766100                 | 2.78566900 | -0.32244500 |
| C                                            | -4.63009800                 | 4.03652400 | 1.41179500  |
| C                                            | -7.06079100                 | 3.31096500 | 0.18744000  |
| C                                            | -5.84908500                 | 4.52691200 | 1.89062300  |
| C                                            | -7.05494700                 | 4.17091900 | 1.28579800  |
| H                                            | -8.00024400                 | 3.04482300 | -0.28938400 |
| H                                            | -5.84773300                 | 5.19764500 | 2.74549700  |
| H                                            | -7.99086600                 | 4.56794400 | 1.66742500  |
| C                                            | 1.19989800                  | 3.01388400 | 0.25614300  |
| H                                            | 2.14813100                  | 3.41370900 | 0.62545400  |
| H                                            | 0.46587400                  | 3.82934800 | 0.22777100  |

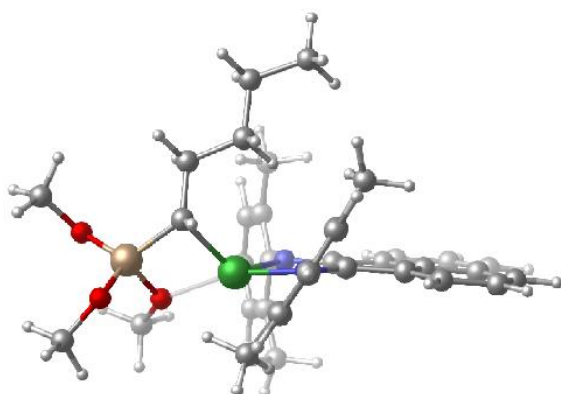
|    |             |             |             |
|----|-------------|-------------|-------------|
| H  | 0.83324600  | 2.28772200  | 0.99305400  |
| C  | -0.87206900 | 0.76303700  | -3.78307600 |
| H  | -1.24703100 | -0.15463700 | -3.31141700 |
| H  | -1.69010800 | 1.49181600  | -3.76655800 |
| H  | -0.64513300 | 0.52975600  | -4.82669300 |
| C  | -3.31522000 | 4.42017500  | 2.04531800  |
| H  | -2.76299800 | 3.53801100  | 2.39213700  |
| H  | -2.67371500 | 4.94500200  | 1.32778000  |
| H  | -3.47228900 | 5.07699300  | 2.90520300  |
| C  | -5.86194200 | 1.87541300  | -1.52820700 |
| H  | -5.13226800 | 2.20743300  | -2.27721400 |
| H  | -5.59749900 | 0.84554400  | -1.25783300 |
| H  | -6.84677300 | 1.84994300  | -2.00194800 |
| C  | -2.99795400 | 1.50707200  | -0.04258400 |
| C  | -1.65580500 | 1.18798000  | -0.63204100 |
| C  | -0.83459100 | 4.60008900  | -3.76207900 |
| H  | -1.84452900 | 4.84294300  | -4.12110500 |
| H  | -0.68096300 | 3.53315000  | -3.96100800 |
| C  | -0.71584300 | 4.85683200  | -2.25941400 |
| H  | 0.29230600  | 4.62860000  | -1.90364000 |
| C  | 0.19813700  | 5.39036700  | -4.58713900 |
| H  | 1.20402900  | 5.16418200  | -4.20374100 |
| H  | 0.03491100  | 6.46567300  | -4.43479400 |
| C  | 0.13904100  | 5.06333700  | -6.08401300 |
| H  | 0.29900200  | 3.98421700  | -6.22274500 |
| C  | 1.17001400  | 5.84656500  | -6.90288600 |
| H  | 2.19037800  | 5.62805000  | -6.56460100 |
| H  | 1.10956900  | 5.59593800  | -7.96763400 |
| H  | 1.01212100  | 6.92737500  | -6.80407200 |
| H  | -0.87134200 | 5.27611600  | -6.46101200 |
| Si | -1.49707600 | 6.37139800  | -1.59144400 |
| O  | -1.87920900 | 7.53493100  | -2.67994300 |
| O  | -0.92541300 | 6.96816700  | -0.16920200 |
| O  | -2.93095200 | 5.53910200  | -1.13047900 |
| C  | -4.26939200 | 5.91945200  | -1.51320500 |
| H  | -4.89890800 | 5.03200900  | -1.47982300 |
| H  | -4.64442700 | 6.65257000  | -0.79399300 |
| H  | -4.26557600 | 6.34422500  | -2.52085900 |
| C  | 0.39793500  | 7.48047300  | 0.01061800  |
| H  | 1.15398200  | 6.74555200  | -0.29487500 |
| H  | 0.54782600  | 8.40426200  | -0.56132100 |
| H  | 0.52761600  | 7.69909400  | 1.07306600  |
| C  | -2.33661900 | 8.86088600  | -2.39347900 |
| H  | -3.43251500 | 8.88608100  | -2.39517100 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -1.97287400 | 9.21131800  | -1.42088400 |
| H | -1.96505500 | 9.52457000  | -3.17795100 |
| C | -3.46889600 | 0.31187600  | 0.65520700  |
| C | -4.59409900 | -0.01375900 | 1.39131500  |
| C | -2.44447100 | -0.66053000 | 0.47482900  |
| C | -4.68191200 | -1.31866200 | 1.94140800  |
| H | -5.39379100 | 0.70203700  | 1.54744100  |
| C | -2.51447900 | -1.95788500 | 1.01508500  |
| C | -1.33565900 | -0.19514000 | -0.29089900 |
| C | -3.68413100 | -2.26594700 | 1.76512300  |
| H | -5.56276200 | -1.57994200 | 2.51942600  |
| C | -1.40493400 | -2.80969000 | 0.75387400  |
| C | -0.26833800 | -1.04523200 | -0.52576800 |
| H | -3.79244400 | -3.25392500 | 2.20404000  |
| C | -0.32537600 | -2.35771700 | 0.00894400  |
| H | -1.40566700 | -3.82336900 | 1.14501200  |
| H | 0.59263800  | -0.72742600 | -1.10306400 |
| H | 0.50838800  | -3.02834600 | -0.17372300 |

UB3LYP-D3/BSII(SMD)//B3LYP-D3/BSI

HF=-2193.9771875

<sup>3</sup>O



|                                              |                             |             |             |
|----------------------------------------------|-----------------------------|-------------|-------------|
| Zero-point correction=                       | 0.718182 (Hartree/Particle) |             |             |
| Thermal correction to Energy=                | 0.764052                    |             |             |
| Thermal correction to Enthalpy=              | 0.764996                    |             |             |
| Thermal correction to Gibbs Free Energy=     | 0.634811                    |             |             |
| Sum of electronic and zero-point Energies=   | -2191.060442                |             |             |
| Sum of electronic and thermal Energies=      | -2191.014571                |             |             |
| Sum of electronic and thermal Enthalpies=    | -2191.013627                |             |             |
| Sum of electronic and thermal Free Energies= | -2191.143813                |             |             |
| Ni                                           | -1.97719300                 | 3.02668000  | -1.35027000 |
| N                                            | -0.57042800                 | 2.11543700  | -0.19746300 |
| N                                            | -3.24031100                 | 2.41943000  | 0.17859000  |
| C                                            | 0.79927800                  | 1.87762400  | -0.54222500 |
| C                                            | 1.08453200                  | 0.77630200  | -1.36992400 |
| C                                            | 1.79103800                  | 2.75864500  | -0.08383800 |
| C                                            | 2.41838800                  | 0.56417200  | -1.73481800 |
| C                                            | 3.11239200                  | 2.50395300  | -0.46901800 |
| C                                            | 3.42656800                  | 1.41836000  | -1.28671600 |
| H                                            | 2.66386400                  | -0.27930500 | -2.37448700 |
| H                                            | 3.89903400                  | 3.16912400  | -0.12362100 |
| H                                            | 4.45724900                  | 1.23969900  | -1.57794300 |
| C                                            | -4.59667700                 | 2.81053300  | 0.28608500  |
| C                                            | -5.40121000                 | 2.61283000  | -0.86316100 |
| C                                            | -5.09398900                 | 3.48121900  | 1.42989000  |
| C                                            | -6.73514300                 | 3.01353700  | -0.81805100 |
| C                                            | -6.43612500                 | 3.88503000  | 1.41167200  |
| C                                            | -7.25616000                 | 3.64241300  | 0.31439700  |
| H                                            | -7.36973800                 | 2.84005200  | -1.68262400 |
| H                                            | -6.83316500                 | 4.40967000  | 2.27671900  |
| H                                            | -8.29485500                 | 3.95841800  | 0.33123900  |
| C                                            | 1.42996400                  | 3.92740400  | 0.79766000  |
| H                                            | 0.72588200                  | 4.59542300  | 0.29160600  |
| H                                            | 0.94579600                  | 3.60124900  | 1.72651600  |
| H                                            | 2.31646000                  | 4.50767100  | 1.06664400  |

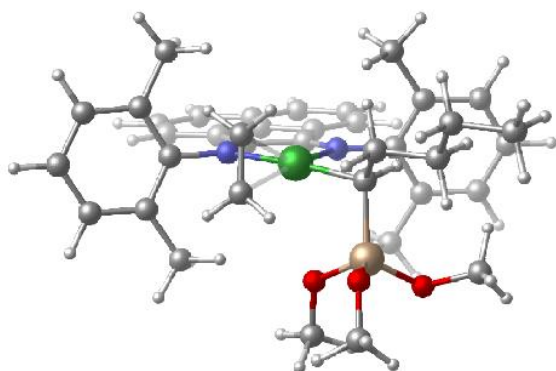
|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -0.02197600 | -0.13935400 | -1.83664600 |
| H  | -0.45242300 | -0.70818700 | -1.00276400 |
| H  | -0.84410800 | 0.42748700  | -2.29377300 |
| H  | 0.34591400  | -0.85713900 | -2.57457500 |
| C  | -4.25213900 | 3.83632800  | 2.63372000  |
| H  | -4.53066000 | 4.82758300  | 3.00405700  |
| H  | -4.40212500 | 3.12825300  | 3.45742000  |
| H  | -3.18363400 | 3.85642100  | 2.41415300  |
| C  | -4.83472200 | 1.99427200  | -2.12044100 |
| H  | -4.16978100 | 1.14913000  | -1.91318500 |
| H  | -5.63518900 | 1.63578700  | -2.77415300 |
| H  | -4.27143200 | 2.73933300  | -2.70455500 |
| C  | -2.59914800 | 1.69871700  | 1.03882100  |
| C  | -1.11512000 | 1.51656900  | 0.80797900  |
| C  | -1.60323900 | 5.99436600  | -0.76686700 |
| H  | -1.87421000 | 7.04000200  | -0.98926800 |
| H  | -0.52927900 | 5.91509900  | -0.98757300 |
| C  | -2.39867400 | 5.04519600  | -1.65700900 |
| C  | -1.83875800 | 5.74248400  | 0.72817400  |
| H  | -1.55435200 | 4.70473800  | 0.95416800  |
| H  | -2.91590600 | 5.81250300  | 0.93339300  |
| C  | -1.07294800 | 6.69276000  | 1.65354300  |
| H  | -0.00155700 | 6.65373200  | 1.41118800  |
| C  | -1.27465500 | 6.35823600  | 3.13500800  |
| H  | -0.93055300 | 5.33945100  | 3.35813100  |
| H  | -0.72071700 | 7.04563400  | 3.78307900  |
| H  | -2.33413200 | 6.41758500  | 3.41281300  |
| H  | -1.39154300 | 7.72572900  | 1.45884600  |
| H  | -3.47836200 | 5.13016400  | -1.48387700 |
| Si | -1.89711800 | 4.84205900  | -3.40839600 |
| O  | -0.66046700 | 5.73878300  | -4.02152600 |
| O  | -3.21685000 | 4.79626800  | -4.39372200 |
| O  | -1.21441000 | 3.27779900  | -3.29307500 |
| C  | -0.75944300 | 7.13279400  | -4.32877800 |
| H  | 0.14845900  | 7.42111000  | -4.86395500 |
| H  | -1.62840900 | 7.34311800  | -4.96419300 |
| H  | -0.83417400 | 7.72814200  | -3.41081400 |
| C  | -3.18107600 | 4.41508400  | -5.77089400 |
| H  | -2.98066200 | 3.34023600  | -5.87096100 |
| H  | -4.15968100 | 4.63293600  | -6.20537100 |
| H  | -2.41547100 | 4.97338100  | -6.32361500 |
| C  | -0.20914700 | 2.69774600  | -4.14699100 |
| H  | 0.55628700  | 2.24180900  | -3.51640000 |
| H  | -0.67043000 | 1.93548000  | -4.78235100 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 0.24562500  | 3.47639200  | -4.76361500 |
| C | -4.09300900 | -0.35777600 | 3.92682600  |
| C | -2.90889600 | -0.93351200 | 4.36108300  |
| C | -1.68053100 | -0.63794700 | 3.70696600  |
| C | -1.74705600 | 0.26519100  | 2.62955600  |
| C | -2.95653100 | 0.88182000  | 2.20067700  |
| C | -4.13876000 | 0.55705400  | 2.84350100  |
| H | -0.28296100 | -1.86069900 | 4.83629600  |
| H | -5.02030300 | -0.60861500 | 4.43235600  |
| H | -2.91651300 | -1.62309300 | 5.20058600  |
| C | -0.39394700 | -1.16571500 | 4.00845900  |
| C | -0.61435400 | 0.61733500  | 1.84408500  |
| H | -5.08601100 | 0.98472400  | 2.53432600  |
| C | 0.62469300  | 0.08155800  | 2.15345100  |
| C | 0.71397600  | -0.80820800 | 3.25392400  |
| H | 1.50801600  | 0.32488300  | 1.57392600  |
| H | 1.68285300  | -1.22847400 | 3.50473300  |

UB3LYP-D3/BSII(SMD)/B3LYP-D3/BSI

HF=-2193.9695596

**1p**



|                                              |                             |
|----------------------------------------------|-----------------------------|
| Zero-point correction=                       | 0.776535 (Hartree/Particle) |
| Thermal correction to Energy=                | 0.824987                    |
| Thermal correction to Enthalpy=              | 0.825932                    |
| Thermal correction to Gibbs Free Energy=     | 0.693109                    |
| Sum of electronic and zero-point Energies=   | -2269.622258                |
| Sum of electronic and thermal Energies=      | -2269.573805                |
| Sum of electronic and thermal Enthalpies=    | -2269.572861                |
| Sum of electronic and thermal Free Energies= | -2269.705683                |

|    |             |             |             |
|----|-------------|-------------|-------------|
| Ni | -0.40050300 | -0.83562000 | -0.50129600 |
| N  | 0.18159800  | 1.09531100  | -0.32017800 |
| N  | 1.68369300  | -1.13757800 | -0.34590700 |
| C  | -0.65456600 | 2.26014900  | -0.31077800 |
| C  | -1.15829700 | 2.71302700  | -1.54372500 |
| C  | -1.00069900 | 2.85040900  | 0.91721000  |
| C  | -2.01758300 | 3.81551700  | -1.53094200 |
| C  | -1.86844700 | 3.94844800  | 0.88005400  |
| C  | -2.37018200 | 4.43088800  | -0.32880400 |
| H  | -2.41614700 | 4.18676200  | -2.47101800 |
| H  | -2.15657200 | 4.42104900  | 1.81506300  |
| H  | -3.04411600 | 5.28244400  | -0.33394900 |
| C  | 2.41478000  | -2.36705800 | -0.34477200 |
| C  | 3.01823500  | -2.80820100 | -1.53639100 |
| C  | 2.45806600  | -3.10822700 | 0.84958000  |
| C  | 3.67381600  | -4.04467500 | -1.51085900 |
| C  | 3.12773000  | -4.33647900 | 0.82715200  |
| C  | 3.72777200  | -4.80465500 | -0.34214100 |
| H  | 4.14485200  | -4.41076000 | -2.41909000 |
| H  | 3.17739900  | -4.92709400 | 1.73792600  |
| H  | 4.23812900  | -5.76307700 | -0.34295500 |
| C  | -0.44922400 | 2.32647400  | 2.22010400  |
| H  | -1.04846500 | 2.67883100  | 3.06318000  |
| H  | -0.44953100 | 1.23390600  | 2.23732400  |
| H  | 0.58398200  | 2.66420700  | 2.37532600  |

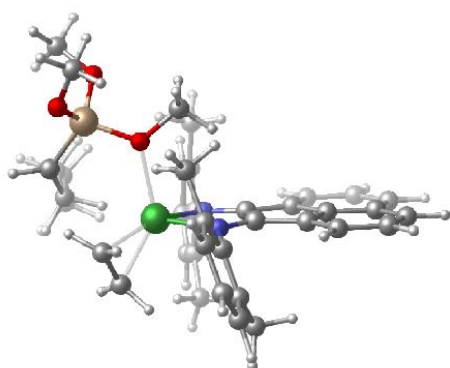
|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -0.78053000 | 2.00543200  | -2.82013200 |
| H  | -1.00318200 | 0.93239100  | -2.74787800 |
| H  | -1.32346900 | 2.41464900  | -3.67609100 |
| H  | 0.29360500  | 2.09218300  | -3.02674100 |
| C  | 1.83720400  | -2.55713200 | 2.11094900  |
| H  | 2.42579900  | -1.71544600 | 2.50035400  |
| H  | 0.82443500  | -2.17766100 | 1.93497500  |
| H  | 1.79369800  | -3.32038700 | 2.89300700  |
| C  | 2.98707900  | -1.95524500 | -2.78309300 |
| H  | 1.98272300  | -1.56521500 | -2.98780700 |
| H  | 3.64865700  | -1.08501400 | -2.68247800 |
| H  | 3.31801600  | -2.52372700 | -3.65622100 |
| C  | 2.29614300  | -0.01834300 | -0.18675600 |
| C  | 1.45875000  | 1.22974300  | -0.18934200 |
| C  | -3.23754100 | -0.94626600 | -1.50320400 |
| H  | -3.37893000 | -2.02602900 | -1.38134100 |
| H  | -2.78636300 | -0.78995800 | -2.49422300 |
| C  | -2.31037100 | -0.37317100 | -0.42620200 |
| H  | -2.29991900 | 0.71322700  | -0.54955300 |
| C  | -4.62524100 | -0.27662800 | -1.50863100 |
| H  | -5.12103600 | -0.46942200 | -0.54816300 |
| Si | -2.74943900 | -0.72012300 | 1.35690000  |
| O  | -3.79656700 | -2.00119800 | 1.34033300  |
| O  | -3.35502300 | 0.57344700  | 2.19379900  |
| O  | -1.34839700 | -1.09082200 | 2.18500700  |
| C  | -1.23066500 | -1.05175900 | 3.60953100  |
| H  | -0.16621800 | -1.08015700 | 3.86032000  |
| H  | -1.67292000 | -0.13663500 | 4.01648800  |
| H  | -1.71989100 | -1.92173900 | 4.06449500  |
| C  | -4.43268900 | 1.40023300  | 1.76246500  |
| H  | -4.17608900 | 1.92907100  | 0.83628900  |
| H  | -5.34893000 | 0.81900400  | 1.60121400  |
| H  | -4.62054700 | 2.13927600  | 2.54626000  |
| C  | -4.40476000 | -2.57372900 | 2.49779900  |
| H  | -3.69787400 | -3.22894400 | 3.02271000  |
| H  | -4.75743200 | -1.80102100 | 3.19226800  |
| H  | -5.26033700 | -3.17118100 | 2.17140600  |
| C  | 3.68999500  | 0.38473700  | 0.00180000  |
| C  | 4.89685800  | -0.28478400 | 0.10246600  |
| C  | 3.66863900  | 1.80555900  | 0.07782500  |
| C  | 6.07707900  | 0.48279100  | 0.27850300  |
| H  | 4.95091700  | -1.36638900 | 0.04783600  |
| C  | 4.83026500  | 2.58223400  | 0.24615000  |
| C  | 2.36453900  | 2.36824000  | -0.03441400 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 6.05687200  | 1.86790100  | 0.34747500  |
| H | 7.02670100  | -0.03684000 | 0.35919000  |
| C | 4.64407000  | 3.99186900  | 0.29452900  |
| C | 2.21444000  | 3.74372500  | 0.01587700  |
| H | 6.98522600  | 2.41673900  | 0.47960800  |
| C | 3.37568700  | 4.54150500  | 0.17982100  |
| H | 5.50586100  | 4.64105500  | 0.42265200  |
| H | 1.23950100  | 4.21069800  | -0.06381900 |
| H | 3.26157900  | 5.62028300  | 0.21881100  |
| H | -4.50146800 | 0.81364600  | -1.58807200 |
| C | -0.92477300 | -3.11197300 | -0.38746100 |
| H | -1.94548800 | -3.12871600 | -0.01871500 |
| H | -0.15299500 | -3.46551100 | 0.28894400  |
| C | -0.62760400 | -2.81036100 | -1.68024900 |
| H | 0.38180100  | -2.93770300 | -2.05809400 |
| H | -1.39959400 | -2.57745400 | -2.40488100 |
| C | -5.52429600 | -0.77362700 | -2.64729200 |
| H | -5.02886200 | -0.58325400 | -3.61004600 |
| H | -5.63590500 | -1.86397600 | -2.56820800 |
| C | -6.90609700 | -0.11208300 | -2.63838400 |
| H | -7.53109700 | -0.48062500 | -3.45895500 |
| H | -7.43395000 | -0.31562900 | -1.69864000 |
| H | -6.82320300 | 0.97674500  | -2.74383300 |

UB3LYP-D3/BSII(SMD)//B3LYP-D3/BSI

HF=-2272.6060627

**<sup>3</sup>P**



|                                              |                             |            |             |
|----------------------------------------------|-----------------------------|------------|-------------|
| Zero-point correction=                       | 0.772440 (Hartree/Particle) |            |             |
| Thermal correction to Energy=                | 0.821704                    |            |             |
| Thermal correction to Enthalpy=              | 0.822648                    |            |             |
| Thermal correction to Gibbs Free Energy=     | 0.686589                    |            |             |
| Sum of electronic and zero-point Energies=   | -2269.607721                |            |             |
| Sum of electronic and thermal Energies=      | -2269.558457                |            |             |
| Sum of electronic and thermal Enthalpies=    | -2269.557513                |            |             |
| Sum of electronic and thermal Free Energies= | -2269.693572                |            |             |
| Ni                                           | -1.52095000                 | 3.80846800 | -1.01059500 |
| N                                            | -0.41394200                 | 2.10425000 | -0.55620800 |
| N                                            | -3.11000700                 | 2.50246300 | -0.64255200 |
| C                                            | 0.96813300                  | 2.08742800 | -0.20941000 |
| C                                            | 1.92000700                  | 2.36562300 | -1.21129800 |
| C                                            | 1.33831000                  | 1.92643100 | 1.14500800  |
| C                                            | 3.26737900                  | 2.42440100 | -0.84631200 |
| C                                            | 2.69964500                  | 2.00868900 | 1.46172900  |
| C                                            | 3.65961400                  | 2.24449000 | 0.47991200  |
| H                                            | 4.01327300                  | 2.61991300 | -1.61182000 |
| H                                            | 3.00384600                  | 1.89435300 | 2.49871400  |
| H                                            | 4.70986600                  | 2.30242200 | 0.74939800  |
| C                                            | -4.50917400                 | 2.77907500 | -0.47232600 |
| C                                            | -5.40304900                 | 2.70561600 | -1.55457200 |
| C                                            | -4.93089500                 | 3.12264500 | 0.82668600  |
| C                                            | -6.75735000                 | 2.95307400 | -1.29804800 |
| C                                            | -6.29244000                 | 3.36893500 | 1.03328500  |
| C                                            | -7.20423000                 | 3.27609700 | -0.01746500 |
| H                                            | -7.46616700                 | 2.89054000 | -2.11917800 |
| H                                            | -6.63544500                 | 3.63042200 | 2.03062900  |
| H                                            | -8.25857900                 | 3.46721400 | 0.15753400  |
| C                                            | 0.32346400                  | 1.69759500 | 2.24231500  |
| H                                            | 0.03789800                  | 0.64117500 | 2.31554800  |
| H                                            | 0.73512600                  | 1.99338400 | 3.21124600  |
| C                                            | 1.49017700                  | 2.56786700 | -2.64164200 |

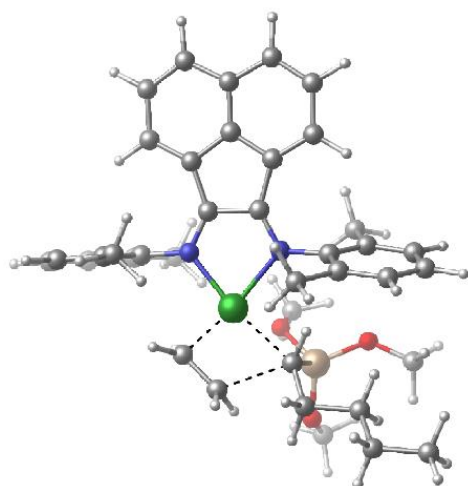
|    |             |             |             |
|----|-------------|-------------|-------------|
| H  | 1.04877900  | 1.65441100  | -3.05728000 |
| H  | 0.73131700  | 3.35505000  | -2.72024200 |
| H  | 2.34108400  | 2.84576400  | -3.27010100 |
| C  | -3.93798000 | 3.18392300  | 1.96180800  |
| H  | -3.05889200 | 3.77749800  | 1.68559400  |
| H  | -4.38885300 | 3.62125500  | 2.85663400  |
| H  | -3.57292500 | 2.18275200  | 2.22679100  |
| C  | -4.92947300 | 2.36294900  | -2.94407400 |
| H  | -4.29066100 | 1.47312500  | -2.94610900 |
| H  | -5.77729200 | 2.16807900  | -3.60669900 |
| H  | -4.34946800 | 3.18284200  | -3.37978600 |
| C  | -2.67690600 | 1.29931800  | -0.47736600 |
| C  | -1.18162300 | 1.07873700  | -0.40793500 |
| C  | -3.57627200 | 6.33079100  | -1.82967600 |
| H  | -3.42215300 | 7.06004200  | -1.02305100 |
| H  | -3.55029000 | 5.33369900  | -1.36080900 |
| C  | -2.51594000 | 6.48357900  | -2.87805900 |
| C  | -5.01059100 | 6.50914000  | -2.39467700 |
| H  | -5.06520400 | 7.44559900  | -2.96553400 |
| H  | -2.12573300 | 7.48950600  | -3.02947500 |
| Si | -1.99569100 | 5.18913700  | -4.06137900 |
| O  | -0.62759800 | 5.72711400  | -4.79313300 |
| O  | -3.14053900 | 4.70217200  | -5.14971300 |
| O  | -1.72701700 | 3.75593800  | -3.20211200 |
| C  | 0.09217800  | 5.03977300  | -5.81675600 |
| H  | 0.78943000  | 4.31897600  | -5.37141000 |
| H  | -0.58150300 | 4.51121900  | -6.50292600 |
| H  | 0.66513100  | 5.77859000  | -6.38275200 |
| C  | -3.77247700 | 5.57858300  | -6.08685100 |
| H  | -3.03510900 | 6.07518900  | -6.72917200 |
| H  | -4.43591400 | 4.97523700  | -6.71129600 |
| H  | -4.36740400 | 6.34085000  | -5.56912900 |
| C  | -1.66237200 | 2.48864400  | -3.88647800 |
| H  | -0.74488100 | 2.42606500  | -4.47829700 |
| H  | -1.65037200 | 1.70640600  | -3.12662100 |
| H  | -2.52802500 | 2.36262900  | -4.53806500 |
| C  | -4.85973800 | -1.80648900 | 0.14924200  |
| C  | -3.82542100 | -2.71100000 | 0.33431400  |
| C  | -2.46967500 | -2.28577500 | 0.25705300  |
| C  | -2.25907100 | -0.92044900 | -0.01434900 |
| C  | -3.31927900 | 0.00769100  | -0.21137700 |
| C  | -4.62864900 | -0.43336600 | -0.12599700 |
| H  | -1.40654900 | -4.14372400 | 0.63583700  |
| H  | -5.88554900 | -2.15552000 | 0.21568300  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -4.04792200 | -3.75402300 | 0.54216400  |
| C | -1.30346300 | -3.08257500 | 0.42625700  |
| C | -0.96522400 | -0.33799400 | -0.10603500 |
| H | -5.46542900 | 0.24145600  | -0.26510700 |
| C | 0.15209900  | -1.13620100 | 0.06634500  |
| C | -0.04057400 | -2.51663700 | 0.32894300  |
| H | 1.15420100  | -0.72453000 | 0.01310000  |
| H | 0.83324300  | -3.14661900 | 0.46319100  |
| H | -5.21067100 | 5.69454900  | -3.10418900 |
| C | -0.89309200 | 5.14203500  | 0.50957000  |
| H | -0.51455900 | 4.51519300  | 1.31308900  |
| H | -1.75320100 | 5.76458300  | 0.75063200  |
| C | -0.13888000 | 5.38225400  | -0.61990600 |
| H | -0.38524600 | 6.19589000  | -1.29762100 |
| H | 0.84433000  | 4.93309200  | -0.74094900 |
| H | -0.59713200 | 2.26803400  | 2.07794800  |
| C | -6.06558300 | 6.50986600  | -1.28268500 |
| H | -5.90599700 | 7.38584300  | -0.63892500 |
| H | -5.92089600 | 5.62666300  | -0.64951800 |
| C | -7.49604200 | 6.51868300  | -1.82703700 |
| H | -7.68546800 | 5.62804700  | -2.43834100 |
| H | -8.22916200 | 6.52590500  | -1.01296100 |
| H | -7.68064800 | 7.40055900  | -2.45204800 |

UB3LYP-D3/BSII(SMD)//B3LYP-D3/BSI

HF=-2272.5906992

<sup>1</sup>TS7



|                                              |                             |
|----------------------------------------------|-----------------------------|
| Zero-point correction=                       | 0.776152 (Hartree/Particle) |
| Thermal correction to Energy=                | 0.823917                    |
| Thermal correction to Enthalpy=              | 0.824862                    |
| Thermal correction to Gibbs Free Energy=     | 0.693306                    |
| Sum of electronic and zero-point Energies=   | -2269.596861                |
| Sum of electronic and thermal Energies=      | -2269.549095                |
| Sum of electronic and thermal Enthalpies=    | -2269.548151                |
| Sum of electronic and thermal Free Energies= | -2269.679706                |

|    |             |             |             |
|----|-------------|-------------|-------------|
| Ni | -0.10019400 | -1.06816900 | -0.61201400 |
| N  | 0.12423300  | 1.03606400  | -0.30897700 |
| N  | 1.87442100  | -0.98824200 | -0.41392500 |
| C  | -0.89393900 | 2.03540200  | -0.27301800 |
| C  | -1.47229500 | 2.41841100  | -1.49882000 |
| C  | -1.36759700 | 2.50291300  | 0.96726600  |
| C  | -2.53176400 | 3.33034500  | -1.46575900 |
| C  | -2.43472500 | 3.40804000  | 0.95009400  |
| C  | -3.01022400 | 3.82354800  | -0.25127000 |
| H  | -2.98670400 | 3.64719100  | -2.40020900 |
| H  | -2.82050600 | 3.78181900  | 1.89461100  |
| H  | -3.83857200 | 4.52580100  | -0.24058000 |
| C  | 2.78037000  | -2.09832700 | -0.49046100 |
| C  | 3.37987200  | -2.39417400 | -1.72510400 |
| C  | 2.99349900  | -2.86572900 | 0.66535400  |
| C  | 4.24516600  | -3.49278300 | -1.77694400 |
| C  | 3.86733800  | -3.95396900 | 0.56794200  |
| C  | 4.49209500  | -4.26413600 | -0.64064200 |
| H  | 4.72383800  | -3.74413400 | -2.71952400 |
| H  | 4.05283500  | -4.56310300 | 1.44847900  |
| H  | 5.16534600  | -5.11409000 | -0.69956200 |
| C  | -0.74708900 | 2.03781600  | 2.26129100  |
| H  | -1.40080400 | 2.26344300  | 3.10688600  |

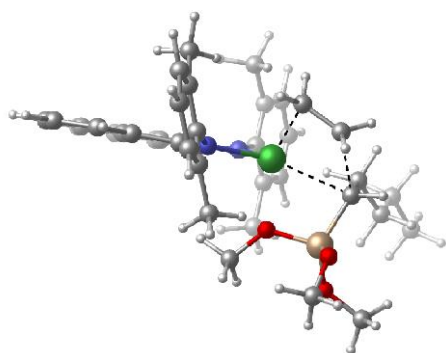
|    |             |             |             |
|----|-------------|-------------|-------------|
| H  | -0.57674600 | 0.95788400  | 2.24620200  |
| H  | 0.21935300  | 2.52734700  | 2.43753300  |
| C  | -0.95068200 | 1.84670800  | -2.79358000 |
| H  | -0.93544000 | 0.74845300  | -2.76085800 |
| H  | -1.56825200 | 2.15756800  | -3.64037100 |
| H  | 0.08012300  | 2.16713700  | -2.98914200 |
| C  | 2.29974400  | -2.50224800 | 1.95472000  |
| H  | 2.68754300  | -1.55984200 | 2.36396300  |
| H  | 1.22454900  | -2.35965500 | 1.79490800  |
| H  | 2.44212800  | -3.27831300 | 2.71174200  |
| C  | 3.09777200  | -1.54012200 | -2.93705200 |
| H  | 2.01871600  | -1.40088400 | -3.08215600 |
| H  | 3.53480100  | -0.53864900 | -2.83182100 |
| H  | 3.51200200  | -1.99122200 | -3.84254600 |
| C  | 2.34008800  | 0.18864900  | -0.16176400 |
| C  | 1.36076500  | 1.32505000  | -0.10524200 |
| C  | -3.49389900 | -1.05424800 | -1.60016600 |
| H  | -3.93390200 | -2.05688700 | -1.56490400 |
| H  | -3.09164700 | -0.91176300 | -2.61347100 |
| C  | -2.35628000 | -0.89504000 | -0.58495900 |
| H  | -2.00272900 | 0.12686200  | -0.71039500 |
| C  | -4.61193000 | -0.01836600 | -1.37647700 |
| H  | -5.14614100 | -0.25823000 | -0.44855600 |
| Si | -2.72251800 | -1.21716500 | 1.21769900  |
| O  | -3.79339600 | -2.47372600 | 1.22037200  |
| O  | -3.27825100 | 0.05655700  | 2.10977400  |
| O  | -1.26807200 | -1.57765200 | 1.93965000  |
| C  | -1.07126100 | -1.59242300 | 3.35699100  |
| H  | -0.00280400 | -1.46575400 | 3.55185000  |
| H  | -1.62229800 | -0.78038700 | 3.84212100  |
| H  | -1.39263300 | -2.55259500 | 3.77816300  |
| C  | -4.57283000 | 0.64744400  | 2.10614400  |
| H  | -4.63933000 | 1.40998900  | 1.32254100  |
| H  | -5.36234600 | -0.09803500 | 1.95103100  |
| H  | -4.72760000 | 1.12401700  | 3.07885900  |
| C  | -4.30235600 | -3.11370100 | 2.39084500  |
| H  | -3.55526700 | -3.79676500 | 2.81376900  |
| H  | -4.59190100 | -2.38414100 | 3.15788700  |
| H  | -5.18498500 | -3.69144800 | 2.10430000  |
| C  | 3.67285300  | 0.73697900  | 0.08506900  |
| C  | 4.95145300  | 0.21233200  | 0.16375600  |
| C  | 3.47954300  | 2.13676100  | 0.26605300  |
| C  | 6.02648200  | 1.10122300  | 0.42346800  |
| H  | 5.13865900  | -0.84725300 | 0.03110800  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 4.53513300  | 3.03213200  | 0.52002000  |
| C | 2.12056900  | 2.54708800  | 0.16300200  |
| C | 5.83786500  | 2.46444100  | 0.59618400  |
| H | 7.03099800  | 0.69460300  | 0.48667900  |
| C | 4.17760700  | 4.40123900  | 0.67020300  |
| C | 1.80146000  | 3.88471100  | 0.31359500  |
| H | 6.69098300  | 3.10845000  | 0.79117100  |
| C | 2.85372100  | 4.80209100  | 0.56701800  |
| H | 4.95202800  | 5.13725300  | 0.86796700  |
| H | 0.77662400  | 4.23263800  | 0.24462600  |
| H | 2.60877400  | 5.85297400  | 0.68543100  |
| H | -4.17226400 | 0.97934500  | -1.23930500 |
| C | -0.07741300 | -3.01256600 | -0.99119500 |
| H | 0.25440200  | -3.50550800 | -0.07885200 |
| H | 0.59912300  | -3.10570500 | -1.84010900 |
| C | -1.45339800 | -2.85243300 | -1.22943000 |
| H | -1.79176000 | -2.72677900 | -2.25132800 |
| H | -2.18221900 | -3.26790000 | -0.54310200 |
| C | -5.61955900 | 0.02874500  | -2.53213700 |
| H | -5.08909900 | 0.27367400  | -3.46319800 |
| H | -6.05458700 | -0.96928000 | -2.67885700 |
| C | -6.73456100 | 1.05093500  | -2.28982600 |
| H | -7.43907800 | 1.08123900  | -3.12780500 |
| H | -7.30316600 | 0.80749300  | -1.38396400 |
| H | -6.32174700 | 2.05957400  | -2.16171300 |

UB3LYP-D3/BSII(SMD)//B3LYP-D3/BSI

HF=-2272.5779061

<sup>3</sup>TS7



|                                              |                             |            |             |
|----------------------------------------------|-----------------------------|------------|-------------|
| Zero-point correction=                       | 0.773454 (Hartree/Particle) |            |             |
| Thermal correction to Energy=                | 0.821553                    |            |             |
| Thermal correction to Enthalpy=              | 0.822497                    |            |             |
| Thermal correction to Gibbs Free Energy=     | 0.689802                    |            |             |
| Sum of electronic and zero-point Energies=   | -2269.584138                |            |             |
| Sum of electronic and thermal Energies=      | -2269.536040                |            |             |
| Sum of electronic and thermal Enthalpies=    | -2269.535095                |            |             |
| Sum of electronic and thermal Free Energies= | -2269.667791                |            |             |
| Ni                                           | -1.63911800                 | 3.76536500 | -1.07092600 |
| N                                            | -0.44999100                 | 2.07487100 | -0.69342500 |
| N                                            | -3.15165000                 | 2.44265600 | -0.52698200 |
| C                                            | 0.95361500                  | 2.07656200 | -0.43590100 |
| C                                            | 1.84394600                  | 2.27983300 | -1.50751200 |
| C                                            | 1.40253300                  | 1.99552100 | 0.90210700  |
| C                                            | 3.21203100                  | 2.33504800 | -1.22892000 |
| C                                            | 2.78131700                  | 2.07297200 | 1.13126800  |
| C                                            | 3.68230200                  | 2.22833100 | 0.07965100  |
| H                                            | 3.91228700                  | 2.47045100 | -2.04859500 |
| H                                            | 3.14637700                  | 2.01944100 | 2.15334800  |
| H                                            | 4.74799700                  | 2.28258600 | 0.28070100  |
| C                                            | -4.53971200                 | 2.69768400 | -0.25649900 |
| C                                            | -5.47708000                 | 2.69030400 | -1.30340900 |
| C                                            | -4.90184300                 | 2.97036400 | 1.07608300  |
| C                                            | -6.81366300                 | 2.95668200 | -0.98359900 |
| C                                            | -6.24694300                 | 3.24313300 | 1.34589000  |
| C                                            | -7.19917200                 | 3.23452400 | 0.32737300  |
| H                                            | -7.55464200                 | 2.95211600 | -1.77834200 |
| H                                            | -6.54599900                 | 3.45893300 | 2.36796500  |
| H                                            | -8.23975800                 | 3.44619400 | 0.55411100  |
| C                                            | 0.44703300                  | 1.86172000 | 2.06588600  |
| H                                            | 0.11823400                  | 0.82465100 | 2.20466400  |
| H                                            | 0.92904700                  | 2.17981700 | 2.99430500  |
| C                                            | 1.32880300                  | 2.41062400 | -2.91722400 |
| H                                            | 0.81223300                  | 1.49923300 | -3.23979200 |

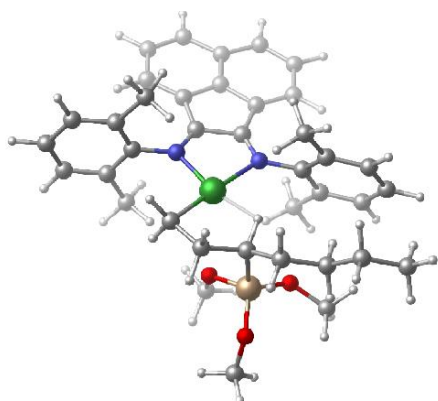
|    |             |             |             |
|----|-------------|-------------|-------------|
| H  | 0.61008800  | 3.23309100  | -3.00012300 |
| H  | 2.14828700  | 2.59882300  | -3.61655100 |
| C  | -3.87181600 | 2.93389400  | 2.17868800  |
| H  | -2.97963700 | 3.50840200  | 1.90944200  |
| H  | -4.27765500 | 3.33858800  | 3.10957000  |
| H  | -3.54086600 | 1.90611300  | 2.37843100  |
| C  | -5.05719600 | 2.41080200  | -2.72349400 |
| H  | -4.50435800 | 1.46783600  | -2.80305100 |
| H  | -5.92672500 | 2.34863400  | -3.38320800 |
| H  | -4.40148300 | 3.20057300  | -3.10277300 |
| C  | -2.68405800 | 1.24968800  | -0.37783800 |
| C  | -1.18880900 | 1.05057900  | -0.43212900 |
| C  | -3.78696400 | 5.98804300  | -1.66520700 |
| H  | -3.80980500 | 6.62131400  | -0.76678600 |
| H  | -4.05993900 | 4.98428200  | -1.31956400 |
| C  | -2.38114200 | 6.01111500  | -2.25589000 |
| C  | -4.88844000 | 6.46777000  | -2.63161200 |
| H  | -4.59494900 | 7.43274800  | -3.07007200 |
| H  | -2.01676900 | 7.03212500  | -2.38924500 |
| Si | -1.94057300 | 5.04127200  | -3.75789300 |
| O  | -0.46102300 | 5.56816300  | -4.25161900 |
| O  | -2.98821200 | 4.91054500  | -5.02616500 |
| O  | -1.87856300 | 3.45500300  | -3.18480200 |
| C  | 0.21499000  | 5.15811500  | -5.44132700 |
| H  | 0.89074000  | 4.32369400  | -5.21963000 |
| H  | -0.48724400 | 4.84915700  | -6.22526700 |
| H  | 0.80591900  | 6.00195300  | -5.80730500 |
| C  | -3.30955500 | 5.96319100  | -5.93978600 |
| H  | -2.41828000 | 6.53180600  | -6.23204100 |
| H  | -3.74758500 | 5.50910900  | -6.83209600 |
| H  | -4.03941300 | 6.64751200  | -5.49321900 |
| C  | -1.90728900 | 2.26810500  | -3.98791100 |
| H  | -1.01937300 | 2.21505900  | -4.62458200 |
| H  | -1.91397500 | 1.41301700  | -3.30882300 |
| H  | -2.80451000 | 2.25861900  | -4.61033600 |
| C  | -4.76577900 | -1.86165400 | 0.50288300  |
| C  | -3.70555800 | -2.74454200 | 0.64302400  |
| C  | -2.36588500 | -2.30405000 | 0.45307600  |
| C  | -2.19795500 | -0.94644800 | 0.12150900  |
| C  | -3.28459600 | -0.04027600 | -0.02587600 |
| C  | -4.57755600 | -0.49555400 | 0.16780400  |
| H  | -1.24651100 | -4.13199600 | 0.81749200  |
| H  | -5.77819800 | -2.22293900 | 0.65427500  |
| H  | -3.89565500 | -3.78261600 | 0.90162100  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -1.17712000 | -3.07778300 | 0.56384200  |
| C | -0.92493700 | -0.34896700 | -0.08788700 |
| H | -5.43244600 | 0.16341400  | 0.06796100  |
| C | 0.21510000  | -1.12469100 | 0.02812600  |
| C | 0.06515400  | -2.49725000 | 0.35392300  |
| H | 1.20352100  | -0.70192500 | -0.11517700 |
| H | 0.95714300  | -3.10912400 | 0.44561100  |
| H | -4.96890600 | 5.75742600  | -3.46510500 |
| C | -0.85657300 | 4.95708900  | 0.41121300  |
| H | 0.12293700  | 4.49639200  | 0.53384700  |
| H | -1.48320800 | 4.96414000  | 1.29997700  |
| C | -0.98176700 | 6.03367600  | -0.50464700 |
| H | -1.62374600 | 6.86298400  | -0.23207100 |
| H | -0.12761500 | 6.29442200  | -1.12334100 |
| H | -0.45107500 | 2.47254100  | 1.92448100  |
| C | -6.25369000 | 6.60831300  | -1.94623500 |
| H | -6.18392200 | 7.36911400  | -1.15651800 |
| H | -6.50191900 | 5.66446800  | -1.44340300 |
| C | -7.36953700 | 6.97982900  | -2.92738700 |
| H | -7.48356700 | 6.21161400  | -3.70266900 |
| H | -8.33279900 | 7.08439700  | -2.41619400 |
| H | -7.15511200 | 7.93003300  | -3.43150200 |

UB3LYP-D3/BSII(SMD)/B3LYP-D3/BSI

HF=-2272.5707502

<sup>1</sup>Q



|                                              |                             |             |             |
|----------------------------------------------|-----------------------------|-------------|-------------|
| Zero-point correction=                       | 0.777072 (Hartree/Particle) |             |             |
| Thermal correction to Energy=                | 0.824852                    |             |             |
| Thermal correction to Enthalpy=              | 0.825796                    |             |             |
| Thermal correction to Gibbs Free Energy=     | 0.693977                    |             |             |
| Sum of electronic and zero-point Energies=   | -2269.625432                |             |             |
| Sum of electronic and thermal Energies=      | -2269.577652                |             |             |
| Sum of electronic and thermal Enthalpies=    | -2269.576707                |             |             |
| Sum of electronic and thermal Free Energies= | -2269.708526                |             |             |
| Ni                                           | 0.00738700                  | -0.94620800 | 0.64859100  |
| N                                            | -0.15127400                 | 1.07318800  | 0.32294600  |
| N                                            | -1.87891500                 | -0.95394700 | 0.43159500  |
| C                                            | 0.89995600                  | 2.03659300  | 0.30217300  |
| C                                            | 1.48322900                  | 2.38032200  | 1.53675700  |
| C                                            | 1.39004100                  | 2.51640900  | -0.92668800 |
| C                                            | 2.55206400                  | 3.28105800  | 1.52657500  |
| C                                            | 2.47134100                  | 3.40386600  | -0.88705400 |
| C                                            | 3.04286900                  | 3.79256000  | 0.32477700  |
| H                                            | 3.00895500                  | 3.57148500  | 2.46846200  |
| H                                            | 2.87133600                  | 3.78566500  | -1.82246900 |
| H                                            | 3.87952600                  | 4.48483400  | 0.33247000  |
| C                                            | -2.74594200                 | -2.08983100 | 0.53850200  |
| C                                            | -3.25852100                 | -2.41744500 | 1.80339600  |
| C                                            | -3.00457200                 | -2.84696000 | -0.61445600 |
| C                                            | -4.09484800                 | -3.53543900 | 1.89002500  |
| C                                            | -3.84589300                 | -3.95644700 | -0.48092600 |
| C                                            | -4.39188900                 | -4.29539300 | 0.75796300  |
| H                                            | -4.50910300                 | -3.81222300 | 2.85561100  |
| H                                            | -4.06577400                 | -4.56130100 | -1.35639400 |
| H                                            | -5.04117100                 | -5.16158100 | 0.84366200  |
| C                                            | 0.79125700                  | 2.06334300  | -2.23532900 |
| H                                            | 1.43817200                  | 2.34054800  | -3.07152200 |
| H                                            | 0.67256000                  | 0.97580400  | -2.25059700 |
| H                                            | -0.19369000                 | 2.51378900  | -2.40976200 |

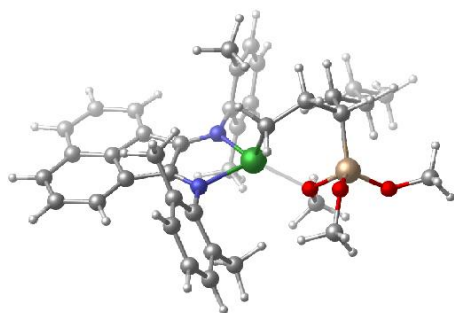
|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 0.94917000  | 1.79981800  | 2.82325000  |
| H  | 0.92028200  | 0.70209100  | 2.78433800  |
| H  | 1.56916200  | 2.09210000  | 3.67488100  |
| H  | -0.07788500 | 2.13042100  | 3.02128800  |
| C  | -2.38268100 | -2.45933800 | -1.93271700 |
| H  | -2.79957200 | -1.51710500 | -2.31231100 |
| H  | -1.30211600 | -2.31274500 | -1.82023900 |
| H  | -2.55366900 | -3.22896100 | -2.69019600 |
| C  | -2.90503900 | -1.57996600 | 3.00673600  |
| H  | -1.81709400 | -1.45532500 | 3.08836300  |
| H  | -3.33552600 | -0.57260300 | 2.93702400  |
| H  | -3.27144500 | -2.03790000 | 3.92916100  |
| C  | -2.35201700 | 0.21091900  | 0.12963800  |
| C  | -1.37885600 | 1.35583500  | 0.05796100  |
| C  | 3.62169100  | -1.12832700 | 1.66160700  |
| H  | 4.24949300  | -2.02795200 | 1.69502200  |
| H  | 3.25026300  | -0.97410500 | 2.68491200  |
| C  | 2.39573700  | -1.44115700 | 0.76339100  |
| H  | 1.77018000  | -0.52286800 | 0.93623100  |
| C  | 4.45962900  | 0.08427900  | 1.23534700  |
| H  | 5.11773900  | -0.20241800 | 0.40590000  |
| Si | 2.79075600  | -1.48755600 | -1.08317500 |
| O  | 4.02941400  | -2.55830200 | -1.23563500 |
| O  | 3.15455600  | -0.02310400 | -1.74528900 |
| O  | 1.38709600  | -1.94328100 | -1.84588500 |
| C  | 1.20078400  | -1.81564200 | -3.25833800 |
| H  | 0.12664300  | -1.81608300 | -3.46133800 |
| H  | 1.63462700  | -0.88212800 | -3.63356700 |
| H  | 1.65497800  | -2.66318200 | -3.78522700 |
| C  | 4.41420400  | 0.52661100  | -2.11107300 |
| H  | 4.63319600  | 1.38714300  | -1.47135200 |
| H  | 5.22412400  | -0.20567600 | -2.01566200 |
| H  | 4.35989100  | 0.86132900  | -3.15272800 |
| C  | 4.44535600  | -3.19983100 | -2.44065100 |
| H  | 3.69414200  | -3.92639200 | -2.77320500 |
| H  | 4.62320500  | -2.47516500 | -3.24620800 |
| H  | 5.37948200  | -3.72845400 | -2.23483100 |
| C  | -3.68221300 | 0.73591900  | -0.15713200 |
| C  | -4.95452100 | 0.19607700  | -0.23443000 |
| C  | -3.49685000 | 2.13101500  | -0.38303000 |
| C  | -6.03300400 | 1.06584800  | -0.53875100 |
| H  | -5.13186100 | -0.86075200 | -0.06842700 |
| C  | -4.55652100 | 3.00716600  | -0.68109100 |
| C  | -2.14310300 | 2.55791100  | -0.27184700 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -5.85286600 | 2.42436000  | -0.75577200 |
| H | -7.03330300 | 0.64903100  | -0.60151000 |
| C | -4.20877400 | 4.37415500  | -0.87101700 |
| C | -1.83360900 | 3.89274000  | -0.46124300 |
| H | -6.70886100 | 3.05326900  | -0.98449100 |
| C | -2.89023100 | 4.79101500  | -0.76102400 |
| H | -4.98657400 | 5.09597000  | -1.10446200 |
| H | -0.81249700 | 4.25117600  | -0.38747100 |
| H | -2.65332300 | 5.83978100  | -0.91024100 |
| H | 3.80437400  | 0.87749000  | 0.85469100  |
| C | 0.23114600  | -2.80638700 | 0.91904700  |
| H | 0.01113700  | -3.28888500 | -0.03714500 |
| H | -0.43011300 | -3.18033700 | 1.70606300  |
| C | 1.70488900  | -2.75775500 | 1.28576700  |
| H | 1.81025300  | -2.76847200 | 2.37667900  |
| H | 2.27344300  | -3.61465000 | 0.90177200  |
| C | 5.31434100  | 0.65360700  | 2.37335100  |
| H | 4.65093100  | 0.98476400  | 3.18556600  |
| H | 5.94441400  | -0.14067500 | 2.79641800  |
| C | 6.18996300  | 1.82340400  | 1.91398200  |
| H | 6.77606200  | 2.23694000  | 2.74166200  |
| H | 6.89225300  | 1.50674800  | 1.13318600  |
| H | 5.57383900  | 2.63050400  | 1.49848000  |

UB3LYP-D3/BSII(SMD)//B3LYP-D3/BSI

HF=-2272.6090285

<sup>3</sup>Q



|                                              |                             |            |             |
|----------------------------------------------|-----------------------------|------------|-------------|
| Zero-point correction=                       | 0.775629 (Hartree/Particle) |            |             |
| Thermal correction to Energy=                | 0.823757                    |            |             |
| Thermal correction to Enthalpy=              | 0.824701                    |            |             |
| Thermal correction to Gibbs Free Energy=     | 0.690983                    |            |             |
| Sum of electronic and zero-point Energies=   | -2269.637589                |            |             |
| Sum of electronic and thermal Energies=      | -2269.589462                |            |             |
| Sum of electronic and thermal Enthalpies=    | -2269.588518                |            |             |
| Sum of electronic and thermal Free Energies= | -2269.722235                |            |             |
| Ni                                           | -1.80472200                 | 3.28373300 | -1.42717500 |
| N                                            | -0.59637200                 | 1.71412000 | -0.90146800 |
| N                                            | -3.25042100                 | 2.10394600 | -0.58631800 |
| C                                            | 0.81615200                  | 1.72073600 | -1.06729700 |
| C                                            | 1.30323200                  | 1.66470500 | -2.39051800 |
| C                                            | 1.67193200                  | 1.89681900 | 0.04010800  |
| C                                            | 2.68407400                  | 1.72821700 | -2.58734200 |
| C                                            | 3.04804600                  | 1.97114300 | -0.21176300 |
| C                                            | 3.55420800                  | 1.87864800 | -1.50632900 |
| H                                            | 3.07841200                  | 1.66161500 | -3.59769200 |
| H                                            | 3.72626700                  | 2.11399900 | 0.62512300  |
| H                                            | 4.62533000                  | 1.93558400 | -1.67538400 |
| C                                            | -4.66099500                 | 2.34741400 | -0.54737200 |
| C                                            | -5.47278700                 | 1.77026500 | -1.54096600 |
| C                                            | -5.17212400                 | 3.19634000 | 0.44899200  |
| C                                            | -6.84189400                 | 2.05886000 | -1.51056700 |
| C                                            | -6.54731800                 | 3.45183100 | 0.44281200  |
| C                                            | -7.37784500                 | 2.88936700 | -0.52624100 |
| H                                            | -7.48933400                 | 1.62628600 | -2.26856400 |
| H                                            | -6.96561000                 | 4.10214200 | 1.20613000  |
| H                                            | -8.44205200                 | 3.10480800 | -0.51978200 |
| C                                            | 1.14913200                  | 2.03724000 | 1.45024400  |
| H                                            | 0.95161900                  | 1.06152600 | 1.91066700  |
| H                                            | 1.87907400                  | 2.55458600 | 2.07869500  |
| C                                            | 0.35058400                  | 1.53149300 | -3.55430000 |
| H                                            | -0.32416600                 | 0.67579300 | -3.43511400 |
| H                                            | -0.27428600                 | 2.42904800 | -3.65046600 |

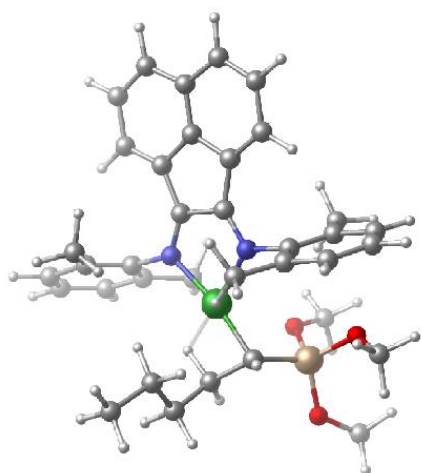
|    |             |             |             |
|----|-------------|-------------|-------------|
| H  | 0.89555600  | 1.40417900  | -4.49376200 |
| C  | -4.25568000 | 3.78402500  | 1.49170900  |
| H  | -3.40358300 | 4.28682600  | 1.02373900  |
| H  | -4.78416300 | 4.50627300  | 2.11959400  |
| H  | -3.84544500 | 3.00486600  | 2.14720400  |
| C  | -4.88474800 | 0.85022500  | -2.58406200 |
| H  | -4.59707700 | -0.11514600 | -2.14801000 |
| H  | -5.60400900 | 0.65174100  | -3.38319600 |
| H  | -3.98104900 | 1.27622500  | -3.03489000 |
| C  | -2.73928100 | 1.02327500  | -0.10012200 |
| C  | -1.25178000 | 0.81527600  | -0.24715100 |
| C  | -3.87938700 | 6.01202200  | -1.51756100 |
| H  | -4.30918700 | 6.32944600  | -0.55702600 |
| H  | -3.86365000 | 4.91294900  | -1.46778500 |
| C  | -2.43240700 | 6.55501600  | -1.60124000 |
| C  | -4.82934200 | 6.43848000  | -2.64377000 |
| H  | -4.93336300 | 7.53329500  | -2.63409600 |
| H  | -2.49047800 | 7.65258000  | -1.64671500 |
| Si | -1.56581000 | 5.94088000  | -3.14279700 |
| O  | 0.05288400  | 6.06990000  | -2.92469000 |
| O  | -2.07924700 | 6.52393600  | -4.59361900 |
| O  | -1.92830100 | 4.27132600  | -3.27947700 |
| C  | 1.05362000  | 5.47955300  | -3.75720400 |
| H  | 1.28497400  | 4.46857200  | -3.40092600 |
| H  | 0.73836900  | 5.43230400  | -4.80671600 |
| H  | 1.95484800  | 6.09372600  | -3.68735600 |
| C  | -2.18728400 | 7.91190500  | -4.92288900 |
| H  | -1.24042100 | 8.43799300  | -4.75276900 |
| H  | -2.44417000 | 7.98248600  | -5.98233600 |
| H  | -2.97976900 | 8.38898800  | -4.33388400 |
| C  | -2.85679800 | 3.71299800  | -4.23675300 |
| H  | -2.84430800 | 4.30075300  | -5.15532000 |
| H  | -2.53976100 | 2.68798400  | -4.44450500 |
| H  | -3.86475900 | 3.71003400  | -3.81003000 |
| C  | -4.66585400 | -1.76255400 | 1.71000900  |
| C  | -3.58008100 | -2.59155700 | 1.95110000  |
| C  | -2.27373000 | -2.21971900 | 1.52615100  |
| C  | -2.16197300 | -0.98068200 | 0.86860500  |
| C  | -3.27689700 | -0.13418700 | 0.61255000  |
| C  | -4.53701400 | -0.52190600 | 1.03402400  |
| H  | -1.09526400 | -3.92302100 | 2.18822700  |
| H  | -5.65127600 | -2.07124500 | 2.04467100  |
| H  | -3.72503500 | -3.53625900 | 2.46792000  |
| C  | -1.06894400 | -2.95967700 | 1.68650300  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -0.92681500 | -0.46311100 | 0.38617000  |
| H | -5.40943100 | 0.09653400  | 0.85425200  |
| C | 0.22780700  | -1.20806200 | 0.55059400  |
| C | 0.13362500  | -2.46256500 | 1.20657000  |
| H | 1.18738500  | -0.84921400 | 0.19427200  |
| H | 1.03819900  | -3.04804200 | 1.33816000  |
| H | -4.40332500 | 6.18632900  | -3.62404200 |
| C | -1.02838400 | 4.75258200  | -0.26225300 |
| H | -0.00013300 | 4.72443500  | -0.64874200 |
| H | -1.02484800 | 4.36608800  | 0.76192900  |
| C | -1.61478100 | 6.17275700  | -0.32907300 |
| H | -2.27101200 | 6.33801500  | 0.53556100  |
| H | -0.78863300 | 6.88950700  | -0.22750900 |
| H | 0.21561700  | 2.60704000  | 1.48041200  |
| C | -6.21142500 | 5.78613300  | -2.51913100 |
| H | -6.64472100 | 6.03571900  | -1.54112100 |
| H | -6.09399600 | 4.69328400  | -2.52016200 |
| C | -7.17270400 | 6.20271300  | -3.63558300 |
| H | -6.77258200 | 5.93507100  | -4.62171800 |
| H | -8.14694400 | 5.71350500  | -3.52658600 |
| H | -7.34073600 | 7.28632400  | -3.63029700 |

UB3LYP-D3/BSII(SMD)//B3LYP-D3/BSI

HF=-2272.6270402

<sup>1</sup>R



|    |             |            |             |
|----|-------------|------------|-------------|
| Ni | -1.52023200 | 3.44826000 | -1.36032800 |
| N  | -0.32165900 | 1.93387400 | -1.38575700 |
| N  | -2.86215200 | 2.17569700 | -0.65640800 |
| C  | 1.05593200  | 1.87123600 | -1.78589500 |
| C  | 1.34214100  | 1.79321600 | -3.15902200 |
| C  | 2.05391100  | 1.87607100 | -0.79710100 |
| C  | 2.68574900  | 1.69830000 | -3.53877500 |
| C  | 3.38208400  | 1.77381400 | -1.22381700 |
| C  | 3.69848000  | 1.68107300 | -2.57946500 |
| H  | 2.93294100  | 1.62843700 | -4.59460100 |
| H  | 4.17408400  | 1.77782600 | -0.47998900 |
| H  | 4.73658300  | 1.60473600 | -2.88935800 |
| C  | -4.21774800 | 2.47419000 | -0.31754900 |
| C  | -5.25869600 | 2.06569500 | -1.17236500 |
| C  | -4.43913500 | 3.25372300 | 0.83363000  |
| C  | -6.56213300 | 2.43983500 | -0.82528300 |
| C  | -5.75953200 | 3.59386200 | 1.14227600  |
| C  | -6.81414200 | 3.19101000 | 0.32246500  |
| H  | -7.38432100 | 2.14310100 | -1.47085100 |
| H  | -5.95835600 | 4.18214500 | 2.03391500  |
| H  | -7.83298200 | 3.47047100 | 0.57347300  |
| C  | 1.69729900  | 1.97539400 | 0.66481800  |
| H  | 2.58132400  | 2.21133900 | 1.26260400  |
| H  | 0.95212800  | 2.75845700 | 0.83118200  |
| H  | 1.28182700  | 1.03058200 | 1.03946600  |
| C  | 0.22593200  | 1.75346600 | -4.17229100 |
| H  | -0.52633700 | 2.52227800 | -3.96594500 |
| H  | 0.60601500  | 1.90010500 | -5.18702300 |
| H  | -0.29686500 | 0.78804500 | -4.14812400 |
| C  | -3.28465000 | 3.66993000 | 1.71323700  |
| H  | -2.79076800 | 2.79756000 | 2.16033200  |

|    |             |             |             |
|----|-------------|-------------|-------------|
| H  | -2.51009500 | 4.20982700  | 1.15305100  |
| H  | -3.62764900 | 4.31446000  | 2.52731700  |
| C  | -4.98194000 | 1.27291000  | -2.42822400 |
| H  | -4.14668600 | 1.69833200  | -2.99711800 |
| H  | -4.71989600 | 0.23177200  | -2.20211200 |
| H  | -5.86045500 | 1.25773400  | -3.07864800 |
| C  | -2.35449000 | 0.99536700  | -0.55821800 |
| C  | -0.91639300 | 0.86191700  | -0.97338800 |
| C  | -1.89895100 | 5.51270400  | -2.00512400 |
| H  | -2.00951800 | 6.34690600  | -1.30323900 |
| H  | -2.61198300 | 4.74449100  | -1.45257700 |
| C  | -0.51611600 | 4.93769000  | -2.01061700 |
| H  | -0.07130700 | 4.76592700  | -2.99324200 |
| C  | -2.60215400 | 5.80136800  | -3.33852000 |
| H  | -2.06262400 | 6.62069400  | -3.82997200 |
| H  | -3.61252400 | 6.17440300  | -3.12675700 |
| C  | -2.69467100 | 4.59479300  | -4.27862400 |
| H  | -1.68752600 | 4.28546500  | -4.58288500 |
| C  | -3.53941200 | 4.87832700  | -5.52394300 |
| H  | -3.12062300 | 5.71080900  | -6.10119400 |
| H  | -3.58296400 | 4.00382200  | -6.18180100 |
| H  | -4.56678400 | 5.14626100  | -5.25067200 |
| H  | -3.12322300 | 3.74487800  | -3.72385400 |
| Si | 0.59542900  | 5.55662400  | -0.66043400 |
| O  | 0.62533500  | 7.20169700  | -0.78424000 |
| O  | 2.12669300  | 4.94603200  | -0.64508600 |
| O  | -0.13747500 | 5.03020200  | 0.73376000  |
| C  | 0.33823200  | 5.30025900  | 2.05229700  |
| H  | 0.30114700  | 6.37402100  | 2.27318900  |
| H  | -0.31418000 | 4.77684500  | 2.75703700  |
| H  | 1.36573300  | 4.94063000  | 2.18189600  |
| C  | 3.04454100  | 5.13588000  | -1.72292500 |
| H  | 2.76700600  | 4.50972300  | -2.57901700 |
| H  | 3.08738200  | 6.18663400  | -2.03671600 |
| H  | 4.03504100  | 4.82867100  | -1.37937300 |
| C  | 1.49862900  | 8.07887200  | -0.07288200 |
| H  | 1.68227600  | 8.95858600  | -0.69618900 |
| H  | 1.03046900  | 8.40416700  | 0.86406200  |
| H  | 2.45901800  | 7.60041700  | 0.15667400  |
| C  | -2.81156700 | -0.31846000 | -0.11526500 |
| C  | -3.99761200 | -0.82610100 | 0.38478300  |
| C  | -1.69210900 | -1.18367700 | -0.27890600 |
| C  | -4.05008100 | -2.20391000 | 0.71807500  |
| H  | -4.87004500 | -0.19537300 | 0.51764100  |

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -1.72943800 | -2.55352700 | 0.04043600  |
| C  | -0.53133700 | -0.53554700 | -0.79388300 |
| C  | -2.96140000 | -3.04789500 | 0.55362700  |
| H  | -4.97743100 | -2.60782400 | 1.11192900  |
| C  | -0.53067300 | -3.28593300 | -0.18673400 |
| C  | 0.62103000  | -1.27362800 | -1.00396100 |
| H  | -3.04678500 | -4.09836100 | 0.81767000  |
| C  | 0.59747800  | -2.65747000 | -0.69337700 |
| H  | -0.50213300 | -4.34801300 | 0.04067500  |
| H  | 1.52438100  | -0.81559500 | -1.39049700 |
| H  | 1.49836000  | -3.24045000 | -0.85716000 |
| Ni | -2.37603700 | 3.63105900  | -0.92606100 |
| N  | -0.85932600 | 2.42641900  | -0.27610000 |
| N  | -3.48282000 | 1.92965000  | -0.69049400 |
| C  | 0.50612500  | 2.81321900  | -0.16377200 |
| C  | 1.44736500  | 2.40395900  | -1.13116900 |
| C  | 0.83364400  | 3.70712100  | 0.87458300  |
| C  | 2.75956200  | 2.87163000  | -0.99224900 |
| C  | 2.15879600  | 4.13571800  | 0.97902200  |
| C  | 3.11874500  | 3.71687800  | 0.05685000  |
| H  | 3.50235000  | 2.57679700  | -1.72847700 |
| H  | 2.43664200  | 4.80811100  | 1.78594900  |
| H  | 4.14353800  | 4.06471100  | 0.14543700  |
| C  | -4.89218300 | 1.81109700  | -0.88564100 |
| C  | -5.39453700 | 1.29319500  | -2.09223600 |
| C  | -5.72532400 | 2.30062700  | 0.13603100  |
| C  | -6.78474100 | 1.26381400  | -2.25014800 |
| C  | -7.10852800 | 2.25230100  | -0.06703800 |
| C  | -7.63656400 | 1.73782900  | -1.25160600 |
| H  | -7.19932600 | 0.87067900  | -3.17437000 |
| H  | -7.77184600 | 2.61579100  | 0.71324200  |
| H  | -8.71228300 | 1.70655400  | -1.39712200 |
| C  | -0.22637400 | 4.16839600  | 1.84473800  |
| H  | -1.05017600 | 4.67805300  | 1.32147800  |
| H  | -0.67373500 | 3.32990100  | 2.39162500  |
| H  | 0.18446500  | 4.87072200  | 2.57477200  |
| C  | 1.05578800  | 1.54034400  | -2.30686100 |
| H  | 0.08551000  | 1.84195600  | -2.71619300 |
| H  | 1.79841500  | 1.62027000  | -3.10518900 |
| H  | 0.97933900  | 0.48159300  | -2.03152200 |
| C  | -5.12702400 | 2.82706400  | 1.41772700  |
| H  | -5.88932300 | 3.28842500  | 2.05140700  |
| H  | -4.64973800 | 2.02519900  | 1.99505100  |
| H  | -4.34875700 | 3.57550800  | 1.21854900  |

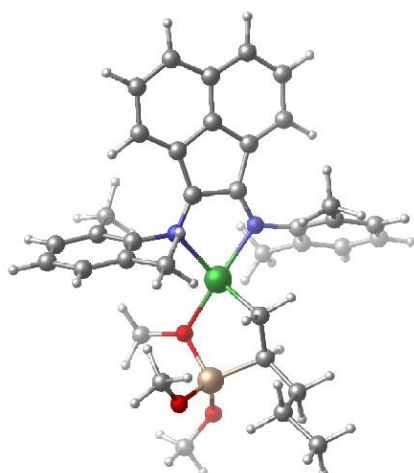
|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -4.46573500 | 0.80633400  | -3.17578400 |
| H  | -3.87360200 | -0.05574500 | -2.84567900 |
| H  | -5.02848200 | 0.50466200  | -4.06297300 |
| H  | -3.77426100 | 1.60083800  | -3.47157200 |
| C  | -2.73365500 | 0.93499500  | -0.35901900 |
| C  | -1.26400800 | 1.20575200  | -0.14674600 |
| C  | -0.64831900 | 4.84381200  | -2.97114600 |
| H  | 0.08114800  | 4.40667900  | -2.27538200 |
| H  | -0.79463100 | 5.87881100  | -2.62959200 |
| C  | -1.96663000 | 4.06616400  | -2.91780800 |
| C  | 0.00821800  | 4.85901800  | -4.36949000 |
| H  | 0.23343000  | 3.82185100  | -4.65941800 |
| H  | 0.97602600  | 5.37422300  | -4.29215200 |
| C  | -0.83297900 | 5.51817200  | -5.46803200 |
| H  | -1.78283500 | 4.97919700  | -5.57906700 |
| C  | -0.10863400 | 5.55767700  | -6.81721700 |
| H  | 0.14137100  | 4.54591900  | -7.15960200 |
| H  | -0.72768600 | 6.02790100  | -7.58887500 |
| H  | 0.82772200  | 6.12450800  | -6.74718400 |
| H  | -1.09696600 | 6.53963800  | -5.16109800 |
| H  | -1.92463700 | 3.13589900  | -3.49266500 |
| Si | -3.56492400 | 4.95940600  | -3.01694200 |
| O  | -4.73708600 | 4.01290900  | -3.65258200 |
| O  | -3.73455600 | 6.47113500  | -3.63655600 |
| O  | -3.76793800 | 5.12823300  | -1.30671700 |
| C  | -6.08497600 | 4.38791800  | -3.94428600 |
| H  | -6.73027100 | 4.13207900  | -3.09631800 |
| H  | -6.16580900 | 5.45739500  | -4.16596300 |
| H  | -6.41191800 | 3.81837200  | -4.81842700 |
| C  | -3.15812800 | 7.67219100  | -3.12888200 |
| H  | -3.83749900 | 8.49857700  | -3.35619900 |
| H  | -3.00739500 | 7.62363400  | -2.04258800 |
| H  | -2.19458400 | 7.86418300  | -3.61317100 |
| C  | -4.95363600 | 5.65447500  | -0.68571600 |
| H  | -5.74408900 | 4.89832000  | -0.68545300 |
| H  | -4.70904200 | 5.93131300  | 0.34213300  |
| H  | -5.28906000 | 6.54349000  | -1.22870800 |
| C  | -3.89351500 | -2.67627000 | 0.24061600  |
| C  | -2.65621300 | -3.19663000 | 0.59023700  |
| C  | -1.49972100 | -2.36752500 | 0.61266200  |
| C  | -1.69213300 | -1.01967100 | 0.25711100  |
| C  | -2.96206600 | -0.48441800 | -0.09578200 |
| C  | -4.07084700 | -1.31227400 | -0.10688700 |
| H  | 0.03550800  | -3.77416800 | 1.23897200  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -4.75938400 | -3.33085900 | 0.23225100  |
| H | -2.56528700 | -4.24737500 | 0.85137300  |
| C | -0.17228500 | -2.74528800 | 0.95846800  |
| C | -0.63919600 | -0.06148600 | 0.23281000  |
| H | -5.05306800 | -0.93852800 | -0.37420600 |
| C | 0.64124300  | -0.45729900 | 0.57995600  |
| C | 0.85381000  | -1.81217400 | 0.94225100  |
| H | 1.47042600  | 0.24155500  | 0.57465500  |
| H | 1.85741200  | -2.12482800 | 1.21308500  |

UB3LYP-D3/BSII(SMD)//B3LYP-D3/BSI

HF=-2193.9691734

<sup>3</sup>R



|                                              |                             |            |             |
|----------------------------------------------|-----------------------------|------------|-------------|
| Zero-point correction=                       | 0.718794 (Hartree/Particle) |            |             |
| Thermal correction to Energy=                | 0.764299                    |            |             |
| Thermal correction to Enthalpy=              | 0.765244                    |            |             |
| Thermal correction to Gibbs Free Energy=     | 0.637614                    |            |             |
| Sum of electronic and zero-point Energies=   | -2191.063000                |            |             |
| Sum of electronic and thermal Energies=      | -2191.017495                |            |             |
| Sum of electronic and thermal Enthalpies=    | -2191.016550                |            |             |
| Sum of electronic and thermal Free Energies= | -2191.144179                |            |             |
| Ni                                           | -2.37603700                 | 3.63105900 | -0.92606100 |
| N                                            | -0.85932600                 | 2.42641900 | -0.27610000 |
| N                                            | -3.48282000                 | 1.92965000 | -0.69049400 |
| C                                            | 0.50612500                  | 2.81321900 | -0.16377200 |
| C                                            | 1.44736500                  | 2.40395900 | -1.13116900 |
| C                                            | 0.83364400                  | 3.70712100 | 0.87458300  |
| C                                            | 2.75956200                  | 2.87163000 | -0.99224900 |
| C                                            | 2.15879600                  | 4.13571800 | 0.97902200  |
| C                                            | 3.11874500                  | 3.71687800 | 0.05685000  |
| H                                            | 3.50235000                  | 2.57679700 | -1.72847700 |
| H                                            | 2.43664200                  | 4.80811100 | 1.78594900  |
| H                                            | 4.14353800                  | 4.06471100 | 0.14543700  |
| C                                            | -4.89218300                 | 1.81109700 | -0.88564100 |
| C                                            | -5.39453700                 | 1.29319500 | -2.09223600 |
| C                                            | -5.72532400                 | 2.30062700 | 0.13603100  |
| C                                            | -6.78474100                 | 1.26381400 | -2.25014800 |
| C                                            | -7.10852800                 | 2.25230100 | -0.06703800 |
| C                                            | -7.63656400                 | 1.73782900 | -1.25160600 |
| H                                            | -7.19932600                 | 0.87067900 | -3.17437000 |
| H                                            | -7.77184600                 | 2.61579100 | 0.71324200  |
| H                                            | -8.71228300                 | 1.70655400 | -1.39712200 |
| C                                            | -0.22637400                 | 4.16839600 | 1.84473800  |
| H                                            | -1.05017600                 | 4.67805300 | 1.32147800  |

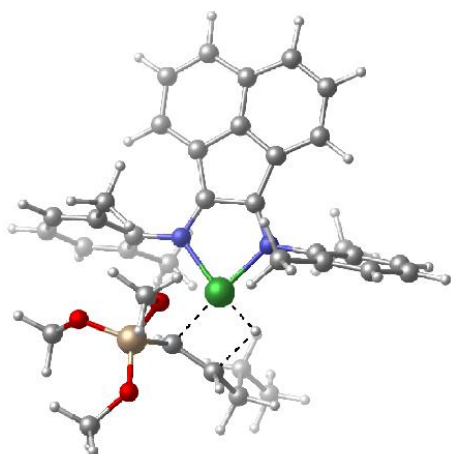
|    |             |             |             |
|----|-------------|-------------|-------------|
| H  | -0.67373500 | 3.32990100  | 2.39162500  |
| H  | 0.18446500  | 4.87072200  | 2.57477200  |
| C  | 1.05578800  | 1.54034400  | -2.30686100 |
| H  | 0.08551000  | 1.84195600  | -2.71619300 |
| H  | 1.79841500  | 1.62027000  | -3.10518900 |
| H  | 0.97933900  | 0.48159300  | -2.03152200 |
| C  | -5.12702400 | 2.82706400  | 1.41772700  |
| H  | -5.88932300 | 3.28842500  | 2.05140700  |
| H  | -4.64973800 | 2.02519900  | 1.99505100  |
| H  | -4.34875700 | 3.57550800  | 1.21854900  |
| C  | -4.46573500 | 0.80633400  | -3.17578400 |
| H  | -3.87360200 | -0.05574500 | -2.84567900 |
| H  | -5.02848200 | 0.50466200  | -4.06297300 |
| H  | -3.77426100 | 1.60083800  | -3.47157200 |
| C  | -2.73365500 | 0.93499500  | -0.35901900 |
| C  | -1.26400800 | 1.20575200  | -0.14674600 |
| C  | -0.64831900 | 4.84381200  | -2.97114600 |
| H  | 0.08114800  | 4.40667900  | -2.27538200 |
| H  | -0.79463100 | 5.87881100  | -2.62959200 |
| C  | -1.96663000 | 4.06616400  | -2.91780800 |
| C  | 0.00821800  | 4.85901800  | -4.36949000 |
| H  | 0.23343000  | 3.82185100  | -4.65941800 |
| H  | 0.97602600  | 5.37422300  | -4.29215200 |
| C  | -0.83297900 | 5.51817200  | -5.46803200 |
| H  | -1.78283500 | 4.97919700  | -5.57906700 |
| C  | -0.10863400 | 5.55767700  | -6.81721700 |
| H  | 0.14137100  | 4.54591900  | -7.15960200 |
| H  | -0.72768600 | 6.02790100  | -7.58887500 |
| H  | 0.82772200  | 6.12450800  | -6.74718400 |
| H  | -1.09696600 | 6.53963800  | -5.16109800 |
| H  | -1.92463700 | 3.13589900  | -3.49266500 |
| Si | -3.56492400 | 4.95940600  | -3.01694200 |
| O  | -4.73708600 | 4.01290900  | -3.65258200 |
| O  | -3.73455600 | 6.47113500  | -3.63655600 |
| O  | -3.76793800 | 5.12823300  | -1.30671700 |
| C  | -6.08497600 | 4.38791800  | -3.94428600 |
| H  | -6.73027100 | 4.13207900  | -3.09631800 |
| H  | -6.16580900 | 5.45739500  | -4.16596300 |
| H  | -6.41191800 | 3.81837200  | -4.81842700 |
| C  | -3.15812800 | 7.67219100  | -3.12888200 |
| H  | -3.83749900 | 8.49857700  | -3.35619900 |
| H  | -3.00739500 | 7.62363400  | -2.04258800 |
| H  | -2.19458400 | 7.86418300  | -3.61317100 |
| C  | -4.95363600 | 5.65447500  | -0.68571600 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -5.74408900 | 4.89832000  | -0.68545300 |
| H | -4.70904200 | 5.93131300  | 0.34213300  |
| H | -5.28906000 | 6.54349000  | -1.22870800 |
| C | -3.89351500 | -2.67627000 | 0.24061600  |
| C | -2.65621300 | -3.19663000 | 0.59023700  |
| C | -1.49972100 | -2.36752500 | 0.61266200  |
| C | -1.69213300 | -1.01967100 | 0.25711100  |
| C | -2.96206600 | -0.48441800 | -0.09578200 |
| C | -4.07084700 | -1.31227400 | -0.10688700 |
| H | 0.03550800  | -3.77416800 | 1.23897200  |
| H | -4.75938400 | -3.33085900 | 0.23225100  |
| H | -2.56528700 | -4.24737500 | 0.85137300  |
| C | -0.17228500 | -2.74528800 | 0.95846800  |
| C | -0.63919600 | -0.06148600 | 0.23281000  |
| H | -5.05306800 | -0.93852800 | -0.37420600 |
| C | 0.64124300  | -0.45729900 | 0.57995600  |
| C | 0.85381000  | -1.81217400 | 0.94225100  |
| H | 1.47042600  | 0.24155500  | 0.57465500  |
| H | 1.85741200  | -2.12482800 | 1.21308500  |

UB3LYP-D3/BSII(SMD)//B3LYP-D3/BSI

HF=-2193.9745854

**<sup>1</sup>TS8**



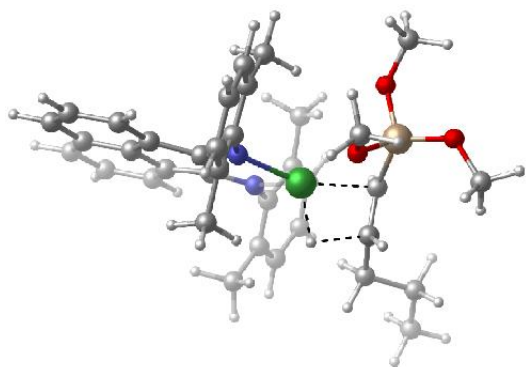
|    |             |            |             |
|----|-------------|------------|-------------|
| Ni | -1.63824500 | 3.51936400 | -1.30871100 |
| N  | -0.35211600 | 1.98675400 | -1.35381800 |
| N  | -2.89817500 | 2.21154000 | -0.62970400 |
| C  | 1.01592800  | 1.91476400 | -1.78652300 |
| C  | 1.26396300  | 1.85144000 | -3.16937400 |
| C  | 2.04683200  | 1.88652500 | -0.83025100 |
| C  | 2.59467100  | 1.76023800 | -3.59316700 |
| C  | 3.36097900  | 1.78938900 | -1.30173700 |
| C  | 3.63707700  | 1.72576300 | -2.66736300 |
| H  | 2.80742200  | 1.70229600 | -4.65726000 |
| H  | 4.17474000  | 1.76978100 | -0.58196500 |
| H  | 4.66505200  | 1.65305100 | -3.01015300 |
| C  | -4.26313300 | 2.45139500 | -0.26036200 |
| C  | -5.28830900 | 2.07309500 | -1.14314500 |
| C  | -4.50542400 | 3.10838600 | 0.95729800  |
| C  | -6.60507800 | 2.34790700 | -0.75686500 |
| C  | -5.83761500 | 3.35725800 | 1.30303200  |
| C  | -6.88022800 | 2.97811600 | 0.45711100  |
| H  | -7.41858000 | 2.06941700 | -1.42133800 |
| H  | -6.05428000 | 3.85665500 | 2.24345500  |
| H  | -7.90858400 | 3.18305900 | 0.73941300  |
| C  | 1.74921800  | 1.91954600 | 0.64814100  |
| H  | 2.64152200  | 2.20020000 | 1.21372900  |
| H  | 0.95817400  | 2.63726600 | 0.87668000  |
| H  | 1.42344800  | 0.93356800 | 1.00528300  |
| C  | 0.12100000  | 1.79527800 | -4.15216700 |
| H  | -0.67459700 | 2.49725900 | -3.88737400 |
| H  | 0.45930600  | 2.01751800 | -5.16822100 |
| H  | -0.33415900 | 0.79579200 | -4.16536400 |
| C  | -3.35649300 | 3.51155000 | 1.84820100  |
| H  | -2.82227800 | 2.63366600 | 2.23460300  |

|    |             |             |             |
|----|-------------|-------------|-------------|
| H  | -2.61682300 | 4.10902700  | 1.30001600  |
| H  | -3.70944300 | 4.09325200  | 2.70424200  |
| C  | -4.97168400 | 1.40948900  | -2.46199600 |
| H  | -4.20957100 | 1.97161800  | -3.01626500 |
| H  | -4.58315900 | 0.39273100  | -2.32167900 |
| H  | -5.86490800 | 1.33891800  | -3.08829500 |
| C  | -2.36622500 | 1.04356100  | -0.50438800 |
| C  | -0.93267800 | 0.91459000  | -0.92776500 |
| C  | -1.69294400 | 5.64007300  | -2.09465300 |
| H  | -1.96380000 | 6.36301100  | -1.32475700 |
| H  | -2.76817900 | 4.56370900  | -1.32280500 |
| C  | -0.43958900 | 4.99437800  | -1.94090100 |
| H  | 0.04525100  | 4.60678100  | -2.83823200 |
| C  | -2.42340000 | 5.85416500  | -3.40484600 |
| H  | -1.99545900 | 6.76727300  | -3.84675200 |
| H  | -3.47261900 | 6.08712900  | -3.18748000 |
| C  | -2.34858600 | 4.70630300  | -4.41409100 |
| H  | -1.30515700 | 4.53201600  | -4.70332500 |
| C  | -3.18932600 | 4.97193100  | -5.66599600 |
| H  | -2.85066000 | 5.87632100  | -6.18474000 |
| H  | -3.12142600 | 4.13706600  | -6.37126600 |
| H  | -4.24615200 | 5.11075100  | -5.40933800 |
| H  | -2.69401500 | 3.78640900  | -3.91823400 |
| Si | 0.58135900  | 5.48925400  | -0.45466100 |
| O  | 0.45483700  | 7.10997600  | -0.17944000 |
| O  | 2.15218000  | 5.01663600  | -0.57636000 |
| O  | -0.13786200 | 4.73887000  | 0.83115600  |
| C  | 0.13726500  | 5.07130300  | 2.19631400  |
| H  | 0.19018300  | 6.15667100  | 2.33181400  |
| H  | -0.67719200 | 4.67188600  | 2.80653200  |
| H  | 1.08181400  | 4.61675500  | 2.51691300  |
| C  | 2.95485300  | 5.12572100  | -1.75113200 |
| H  | 2.56674500  | 4.48501300  | -2.55108200 |
| H  | 3.01318400  | 6.16221100  | -2.10761300 |
| H  | 3.96162600  | 4.78589000  | -1.49981300 |
| C  | 1.44342300  | 8.10319700  | -0.44051700 |
| H  | 1.45132000  | 8.37750100  | -1.50365000 |
| H  | 1.19233700  | 8.99118500  | 0.14577700  |
| H  | 2.44376100  | 7.75926500  | -0.15222700 |
| C  | -2.81745500 | -0.26553600 | -0.04324400 |
| C  | -3.99956300 | -0.77181400 | 0.46804100  |
| C  | -1.69910500 | -1.13105200 | -0.21557300 |
| C  | -4.04852000 | -2.14899900 | 0.80442300  |
| H  | -4.87085300 | -0.14148300 | 0.60759600  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -1.73441200 | -2.50058400 | 0.10594100  |
| C | -0.54514600 | -0.48449500 | -0.74646000 |
| C | -2.96153600 | -2.99341400 | 0.63196300  |
| H | -4.97226000 | -2.55200100 | 1.20762200  |
| C | -0.53945800 | -3.23484300 | -0.13376300 |
| C | 0.60281700  | -1.22525500 | -0.97025000 |
| H | -3.04450200 | -4.04330900 | 0.89913000  |
| C | 0.58236800  | -2.60847000 | -0.65625600 |
| H | -0.50920200 | -4.29643400 | 0.09571300  |
| H | 1.50159600  | -0.77040000 | -1.37080200 |
| H | 1.48066500  | -3.19240800 | -0.83063100 |

UB3LYP-D3/BSII(SMD)//B3LYP-D3/BSI

HF=-2193.9505661

**<sup>3</sup>TS8**

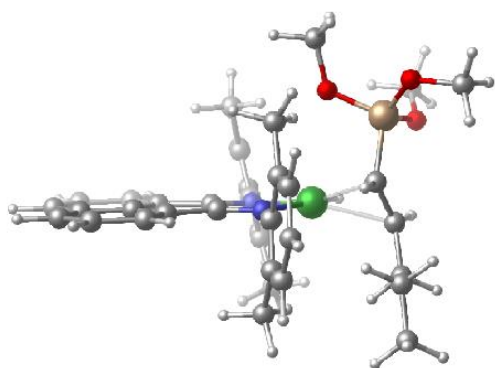
|                                              |                             |            |             |
|----------------------------------------------|-----------------------------|------------|-------------|
| Zero-point correction=                       | 0.715387 (Hartree/Particle) |            |             |
| Thermal correction to Energy=                | 0.761274                    |            |             |
| Thermal correction to Enthalpy=              | 0.762218                    |            |             |
| Thermal correction to Gibbs Free Energy=     | 0.631328                    |            |             |
| Sum of electronic and zero-point Energies=   | -2191.032363                |            |             |
| Sum of electronic and thermal Energies=      | -2190.986477                |            |             |
| Sum of electronic and thermal Enthalpies=    | -2190.985533                |            |             |
| Sum of electronic and thermal Free Energies= | -2191.116423                |            |             |
| Ni                                           | -2.60740800                 | 3.44319000 | -1.58428600 |
| N                                            | -1.03195300                 | 2.08806900 | -1.27138000 |
| N                                            | -3.62585700                 | 1.99837300 | -0.52396000 |
| C                                            | 0.29664100                  | 2.22457800 | -1.77085300 |
| C                                            | 0.52022300                  | 1.89017100 | -3.11892900 |
| C                                            | 1.29752500                  | 2.76305300 | -0.94291500 |
| C                                            | 1.80198600                  | 2.10674600 | -3.63598600 |
| C                                            | 2.56371100                  | 2.96257700 | -1.50559300 |
| C                                            | 2.81590800                  | 2.64060700 | -2.83967500 |
| H                                            | 2.00275100                  | 1.85154300 | -4.67294000 |
| H                                            | 3.35327600                  | 3.38447000 | -0.88964500 |
| H                                            | 3.80357800                  | 2.80680800 | -3.25929200 |
| C                                            | -5.02935300                 | 1.99765200 | -0.26022500 |
| C                                            | -5.87792800                 | 1.46267800 | -1.24428400 |
| C                                            | -5.50625900                 | 2.60067600 | 0.91488600  |
| C                                            | -7.25524500                 | 1.50893300 | -1.00515300 |
| C                                            | -6.89259300                 | 2.63385700 | 1.10659900  |
| C                                            | -7.76065900                 | 2.08756400 | 0.15989000  |
| H                                            | -7.93472600                 | 1.09557100 | -1.74579700 |
| H                                            | -7.29007900                 | 3.09400500 | 2.00719400  |
| H                                            | -8.83313800                 | 2.12011300 | 0.32709400  |
| C                                            | 0.99479200                  | 3.14191200 | 0.48644300  |
| H                                            | 0.10048300                  | 3.77448300 | 0.54261300  |
| H                                            | 0.80523200                  | 2.25704700 | 1.10715100  |
| H                                            | 1.83096400                  | 3.68722400 | 0.93202100  |
| C                                            | -0.58478600                 | 1.28445200 | -3.95081200 |

|    |             |            |             |
|----|-------------|------------|-------------|
| H  | -1.49232200 | 1.90051700 | -3.94347700 |
| H  | -0.27041300 | 1.16158500 | -4.99080800 |
| H  | -0.86968500 | 0.29567500 | -3.56864900 |
| C  | -4.54186500 | 3.18796000 | 1.91631800  |
| H  | -5.07219700 | 3.73312300 | 2.70158500  |
| H  | -3.94104900 | 2.40621700 | 2.39886300  |
| H  | -3.83811300 | 3.87572900 | 1.43031400  |
| C  | -5.30222900 | 0.89537700 | -2.51933400 |
| H  | -4.65104300 | 0.03441300 | -2.32410600 |
| H  | -6.09588400 | 0.56494300 | -3.19531400 |
| H  | -4.69220000 | 1.64255100 | -3.04495300 |
| C  | -2.85147100 | 1.05818400 | -0.10831200 |
| C  | -1.39834700 | 1.11092300 | -0.52140800 |
| C  | -1.56089100 | 5.53385700 | -2.21123100 |
| H  | -1.95550800 | 4.71735300 | -0.74837300 |
| H  | -2.32563800 | 6.25262800 | -1.91703400 |
| C  | -1.82416100 | 4.72793600 | -3.34165300 |
| C  | -0.14506100 | 5.90668800 | -1.83192200 |
| H  | 0.49557500  | 5.02397700 | -1.91451400 |
| H  | -0.10743500 | 6.24201200 | -0.78926900 |
| C  | 0.40304900  | 7.01590300 | -2.75230000 |
| H  | 0.34573200  | 6.67593300 | -3.79415800 |
| C  | 1.84963700  | 7.37482500 | -2.39831900 |
| H  | 2.50112400  | 6.49709400 | -2.48895800 |
| H  | 2.23770200  | 8.15354500 | -3.06311900 |
| H  | 1.92557700  | 7.74399900 | -1.36860900 |
| H  | -0.23472100 | 7.90744600 | -2.67718000 |
| H  | -0.97127400 | 4.22223300 | -3.79022700 |
| Si | -3.50919000 | 4.61848200 | -4.06489400 |
| O  | -3.63259400 | 3.27471400 | -4.99172200 |
| O  | -4.15183300 | 5.87878300 | -4.89669800 |
| O  | -4.34350200 | 4.43066200 | -2.59678200 |
| C  | -4.57676600 | 3.03342400 | -6.03958100 |
| H  | -5.50385500 | 2.62006100 | -5.62405900 |
| H  | -4.80467600 | 3.95196600 | -6.58939500 |
| H  | -4.13791200 | 2.30174000 | -6.72251800 |
| C  | -4.04112800 | 7.24980500 | -4.51099800 |
| H  | -4.45276900 | 7.85803300 | -5.31958100 |
| H  | -4.60859200 | 7.44981700 | -3.59274200 |
| H  | -2.99281400 | 7.53220300 | -4.35235600 |
| C  | -5.76083500 | 4.57169200 | -2.40676400 |
| H  | -6.29661100 | 3.75371500 | -2.89722500 |
| H  | -5.96152500 | 4.53194100 | -1.33531600 |
| H  | -6.09789200 | 5.52882900 | -2.81666500 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -3.89548300 | -1.96805500 | 2.01055300  |
| C | -2.65056600 | -2.57865800 | 2.06059100  |
| C | -1.52694400 | -1.99306200 | 1.41263400  |
| C | -1.76038600 | -0.78069200 | 0.73770900  |
| C | -3.03769900 | -0.15440300 | 0.68507000  |
| C | -4.11394500 | -0.74701800 | 1.32224900  |
| H | 0.04381800  | -3.42474000 | 1.87193800  |
| H | -4.73489500 | -2.43776200 | 2.51362100  |
| H | -2.52896600 | -3.51464700 | 2.59887200  |
| C | -0.19517100 | -2.49294300 | 1.36680800  |
| C | -0.74370300 | -0.07198100 | 0.03840400  |
| H | -5.10073900 | -0.29765500 | 1.30196500  |
| C | 0.54209400  | -0.58132300 | 0.00853600  |
| C | 0.79610500  | -1.80284200 | 0.68490900  |
| H | 1.34178100  | -0.06702800 | -0.51319700 |
| H | 1.80348900  | -2.20674900 | 0.66552400  |

UB3LYP-D3/BSII(SMD)//B3LYP-D3/BSI

HF=-2193.9390128



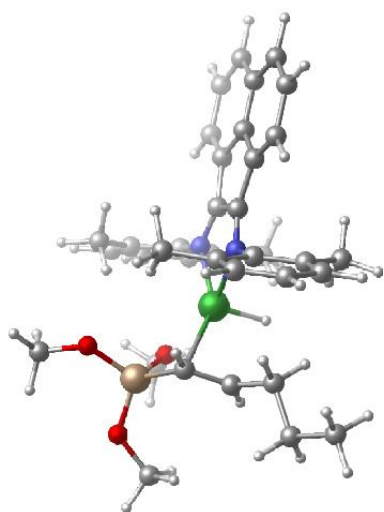
|    |             |             |             |
|----|-------------|-------------|-------------|
| Ni | -1.73997800 | 3.50841900  | -1.38395400 |
| N  | -0.59178200 | 1.81579800  | -1.64570800 |
| N  | -2.92268600 | 2.31463100  | -0.44450200 |
| C  | 0.59862600  | 1.57317800  | -2.40729100 |
| C  | 0.45686200  | 1.11398600  | -3.73008000 |
| C  | 1.85075600  | 1.82503500  | -1.82275800 |
| C  | 1.62107400  | 0.91382300  | -4.47849100 |
| C  | 2.98849100  | 1.61514700  | -2.61222600 |
| C  | 2.87833900  | 1.16486400  | -3.92714100 |
| H  | 1.53589900  | 0.56679900  | -5.50462000 |
| H  | 3.96845900  | 1.80470300  | -2.18273100 |
| H  | 3.77217100  | 1.01083400  | -4.52419700 |
| C  | -4.14607400 | 2.69086000  | 0.20284700  |
| C  | -5.28584200 | 2.85758500  | -0.59999500 |
| C  | -4.14442600 | 2.92452900  | 1.58864900  |
| C  | -6.47592700 | 3.22913000  | 0.03301200  |
| C  | -5.35710800 | 3.30134400  | 2.17666800  |
| C  | -6.51490300 | 3.44402100  | 1.41082700  |
| H  | -7.37522500 | 3.35497700  | -0.56365900 |
| H  | -5.38658900 | 3.49264700  | 3.24600900  |
| H  | -7.44605800 | 3.73605700  | 1.88721200  |
| C  | 1.95827000  | 2.24859300  | -0.37873300 |
| H  | 2.94460600  | 2.66939300  | -0.16445500 |
| H  | 1.19927800  | 2.98819900  | -0.11053200 |
| H  | 1.81219300  | 1.38922400  | 0.28988800  |
| C  | -0.91196800 | 0.85498900  | -4.31180400 |
| H  | -1.38245000 | -0.02571800 | -3.85605400 |
| H  | -1.58548900 | 1.70259400  | -4.13674600 |
| H  | -0.85357500 | 0.68153200  | -5.38933200 |
| C  | -2.87426800 | 2.80279500  | 2.39623800  |
| H  | -2.55956200 | 1.75640200  | 2.50209200  |
| H  | -2.05321700 | 3.34690700  | 1.91578600  |
| H  | -3.01587000 | 3.20568300  | 3.40299300  |
| C  | -5.20238300 | 2.64226000  | -2.08954900 |

|    |             |             |             |
|----|-------------|-------------|-------------|
| H  | -4.41895300 | 3.27850600  | -2.52463800 |
| H  | -4.94223900 | 1.60517400  | -2.33661300 |
| H  | -6.15136400 | 2.87827700  | -2.57827600 |
| C  | -2.45737400 | 1.11511400  | -0.33999800 |
| C  | -1.15927800 | 0.83089500  | -1.03879700 |
| C  | -1.23626800 | 5.26157000  | -2.80013900 |
| H  | -1.95098200 | 6.00779400  | -2.46096500 |
| H  | -2.70760400 | 4.56259600  | -1.11691200 |
| C  | -0.24808500 | 4.87847300  | -1.91724100 |
| H  | 0.57187300  | 4.27334300  | -2.30507000 |
| C  | -1.34877800 | 4.88145000  | -4.25643200 |
| H  | -1.72854600 | 5.75934300  | -4.79739000 |
| H  | -2.14528600 | 4.12686700  | -4.35295100 |
| C  | -0.06282300 | 4.37669600  | -4.92116200 |
| H  | 0.70247000  | 5.16129600  | -4.85483000 |
| C  | -0.28345100 | 3.98131800  | -6.38355100 |
| H  | -0.64224100 | 4.82875900  | -6.97921100 |
| H  | 0.64752100  | 3.62390000  | -6.83567200 |
| H  | -1.02642200 | 3.17840400  | -6.46609900 |
| H  | 0.32910100  | 3.51665500  | -4.37269600 |
| Si | 0.00114500  | 5.72683900  | -0.26617500 |
| O  | -1.12950100 | 6.91846600  | -0.20039200 |
| O  | 1.54460200  | 6.28344200  | -0.12910400 |
| O  | -0.18179000 | 4.61767200  | 0.94545800  |
| C  | 0.52426800  | 4.63402300  | 2.19056700  |
| H  | 0.40394100  | 3.65006400  | 2.65214900  |
| H  | 1.58792400  | 4.83905200  | 2.03666300  |
| H  | 0.10482900  | 5.39244400  | 2.86238100  |
| C  | 2.08167900  | 7.36411000  | -0.89532600 |
| H  | 3.08756800  | 7.57034900  | -0.52172700 |
| H  | 2.14771200  | 7.09709400  | -1.95821300 |
| H  | 1.46864000  | 8.26684200  | -0.79105900 |
| C  | -1.76599500 | 7.36172500  | 0.99917600  |
| H  | -2.16853500 | 6.51252800  | 1.56489800  |
| H  | -1.06686800 | 7.92022800  | 1.63385500  |
| H  | -2.58872800 | 8.02321900  | 0.71711000  |
| C  | -2.91313700 | -0.12637900 | 0.27815800  |
| C  | -4.00887400 | -0.50242100 | 1.03587000  |
| C  | -1.93022600 | -1.10058800 | -0.06263400 |
| C  | -4.10749900 | -1.85654400 | 1.44640200  |
| H  | -4.77374500 | 0.21256900  | 1.31751800  |
| C  | -2.01276600 | -2.44684400 | 0.33825200  |
| C  | -0.86049400 | -0.58854500 | -0.85121800 |
| C  | -3.14925700 | -2.80395000 | 1.11669500  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -4.96450000 | -2.15655200 | 2.04122400  |
| C | -0.95089100 | -3.29539600 | -0.08316600 |
| C | 0.15858300  | -1.43693500 | -1.24800200 |
| H | -3.26442700 | -3.83016000 | 1.45457400  |
| C | 0.09311100  | -2.79659300 | -0.84833600 |
| H | -0.96187000 | -4.34475900 | 0.19839500  |
| H | 0.98766600  | -1.08297800 | -1.85038000 |
| H | 0.88963100  | -3.46662400 | -1.15641000 |

UB3LYP-D3/BSII(SMD)//B3LYP-D3/BSI

HF=-2193.9475446



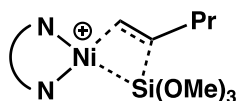
|                                              |             |            |                             |
|----------------------------------------------|-------------|------------|-----------------------------|
| Zero-point correction=                       |             |            | 0.713716 (Hartree/Particle) |
| Thermal correction to Energy=                |             |            | 0.760073                    |
| Thermal correction to Enthalpy=              |             |            | 0.761017                    |
| Thermal correction to Gibbs Free Energy=     |             |            | 0.630074                    |
| Sum of electronic and zero-point Energies=   |             |            | -2191.047376                |
| Sum of electronic and thermal Energies=      |             |            | -2191.001019                |
| Sum of electronic and thermal Enthalpies=    |             |            | -2191.000075                |
| Sum of electronic and thermal Free Energies= |             |            | -2191.131019                |
| Ni                                           | -2.61367300 | 3.47787200 | -1.55188900                 |
| N                                            | -1.06262700 | 2.11680300 | -1.28332200                 |
| N                                            | -3.67194600 | 1.95248700 | -0.62030900                 |
| C                                            | 0.28581100  | 2.29380700 | -1.71348700                 |
| C                                            | 0.59253600  | 1.94854500 | -3.04185500                 |
| C                                            | 1.22209400  | 2.87798800 | -0.84236300                 |
| C                                            | 1.88779400  | 2.21314300 | -3.49973500                 |
| C                                            | 2.50596600  | 3.12009300 | -1.34368500                 |
| C                                            | 2.83756600  | 2.79719000 | -2.66009100                 |
| H                                            | 2.15112500  | 1.95336500 | -4.52154500                 |
| H                                            | 3.24652900  | 3.57983200 | -0.69491900                 |
| H                                            | 3.83741600  | 3.00035900 | -3.03203900                 |
| C                                            | -5.07560100 | 1.93519400 | -0.36192200                 |
| C                                            | -5.91652400 | 1.43377600 | -1.37052700                 |
| C                                            | -5.56453300 | 2.47974200 | 0.83816300                  |
| C                                            | -7.29620500 | 1.46715600 | -1.14245000                 |
| C                                            | -6.95296100 | 2.50166500 | 1.01730800                  |
| C                                            | -7.81278000 | 1.99858300 | 0.04018400                  |
| H                                            | -7.96777200 | 1.07597300 | -1.90216800                 |
| H                                            | -7.35883300 | 2.91939100 | 1.93469300                  |
| H                                            | -8.88670600 | 2.02289400 | 0.19959400                  |
| C                                            | 0.83677100  | 3.25085600 | 0.56842600                  |

|    |             |            |             |
|----|-------------|------------|-------------|
| H  | -0.10954200 | 3.80480600 | 0.58508500  |
| H  | 0.69860500  | 2.35947600 | 1.19391100  |
| H  | 1.61069600  | 3.86600000 | 1.03548900  |
| C  | -0.43688500 | 1.26760400 | -3.91218600 |
| H  | -1.41499600 | 1.76031900 | -3.85817800 |
| H  | -0.12040400 | 1.24955300 | -4.95885200 |
| H  | -0.59284500 | 0.22849200 | -3.59403400 |
| C  | -4.61618700 | 3.01598200 | 1.88262300  |
| H  | -5.15878000 | 3.54609400 | 2.66996000  |
| H  | -4.04899200 | 2.20448300 | 2.35723700  |
| H  | -3.88408500 | 3.69987400 | 1.43692300  |
| C  | -5.32894300 | 0.88933100 | -2.64957700 |
| H  | -4.69955300 | 0.01032800 | -2.46240600 |
| H  | -6.11628300 | 0.59050400 | -3.34749200 |
| H  | -4.69443900 | 1.63416700 | -3.14548400 |
| C  | -2.88499700 | 1.04140400 | -0.16902400 |
| C  | -1.42525100 | 1.13439100 | -0.53681500 |
| C  | -1.35735600 | 5.47117300 | -2.69817800 |
| H  | -2.34598000 | 4.39411800 | -0.29306900 |
| H  | -2.05429200 | 6.12214400 | -2.16757300 |
| C  | -1.83112600 | 4.62029600 | -3.64789200 |
| C  | 0.08483400  | 5.66595100 | -2.34805800 |
| H  | 0.69923200  | 4.89926900 | -2.83066700 |
| H  | 0.19949700  | 5.54142300 | -1.26352500 |
| C  | 0.59295700  | 7.06887200 | -2.74183600 |
| H  | 0.47649800  | 7.20231100 | -3.82533800 |
| C  | 2.05957400  | 7.26397000 | -2.34481400 |
| H  | 2.69739100  | 6.50949500 | -2.82041900 |
| H  | 2.42271500  | 8.25219600 | -2.64515400 |
| H  | 2.18771300  | 7.17310600 | -1.25946700 |
| H  | -0.03032000 | 7.83524400 | -2.26134700 |
| H  | -1.10414600 | 4.01745800 | -4.18905000 |
| Si | -3.62703500 | 4.56884000 | -4.10066000 |
| O  | -3.91025800 | 3.24490700 | -5.01278700 |
| O  | -4.29168000 | 5.87542300 | -4.82854400 |
| O  | -4.25626400 | 4.40570200 | -2.53899600 |
| C  | -5.05077800 | 3.00640500 | -5.84639100 |
| H  | -5.89178200 | 2.64509500 | -5.24267800 |
| H  | -5.34770900 | 3.91549600 | -6.37860700 |
| H  | -4.77621000 | 2.23559600 | -6.57006500 |
| C  | -4.05741000 | 7.24077100 | -4.47451000 |
| H  | -4.52502200 | 7.86605200 | -5.23799600 |
| H  | -4.50108800 | 7.47773400 | -3.49929500 |
| H  | -2.98336500 | 7.46041000 | -4.44160000 |

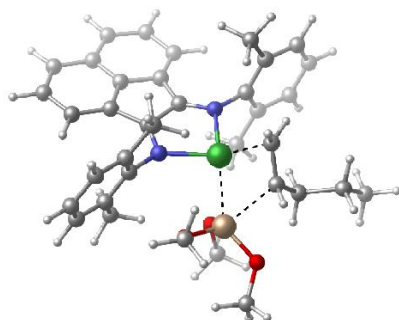
|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -5.58657000 | 4.74064300  | -2.09665100 |
| H | -6.28982200 | 3.95886100  | -2.39249500 |
| H | -5.56032900 | 4.80591400  | -1.00883900 |
| H | -5.88891100 | 5.69968900  | -2.52601000 |
| C | -3.89257200 | -1.97764500 | 1.98224500  |
| C | -2.63095100 | -2.54564300 | 2.08104300  |
| C | -1.50863400 | -1.93478300 | 1.45450700  |
| C | -1.76165800 | -0.74400900 | 0.74861800  |
| C | -3.05590900 | -0.16139200 | 0.64615800  |
| C | -4.12992500 | -0.77711800 | 1.26385800  |
| H | 0.09443100  | -3.30221300 | 1.99081400  |
| H | -4.73109500 | -2.46468300 | 2.47015100  |
| H | -2.49451000 | -3.46616300 | 2.64194600  |
| C | -0.16005700 | -2.38910900 | 1.45973600  |
| C | -0.74808700 | -0.01371300 | 0.06695300  |
| H | -5.12971600 | -0.36079300 | 1.20799100  |
| C | 0.55470500  | -0.47906700 | 0.08748400  |
| C | 0.82842300  | -1.67801400 | 0.79542300  |
| H | 1.35316500  | 0.05249500  | -0.41844300 |
| H | 1.84913800  | -2.04695400 | 0.81569700  |

UB3LYP-D3/BSII(SMD)//B3LYP-D3/BSI

HF=-2193.954489



Singlet



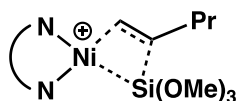
|                                              |                             |            |             |
|----------------------------------------------|-----------------------------|------------|-------------|
| Zero-point correction=                       | 0.718642 (Hartree/Particle) |            |             |
| Thermal correction to Energy=                | 0.763563                    |            |             |
| Thermal correction to Enthalpy=              | 0.764507                    |            |             |
| Thermal correction to Gibbs Free Energy=     | 0.639414                    |            |             |
| Sum of electronic and zero-point Energies=   | -2191.026725                |            |             |
| Sum of electronic and thermal Energies=      | -2190.981805                |            |             |
| Sum of electronic and thermal Enthalpies=    | -2190.980861                |            |             |
| Sum of electronic and thermal Free Energies= | -2191.105953                |            |             |
| Ni                                           | -2.58691800                 | 3.33231000 | -1.66972600 |
| N                                            | -1.09147600                 | 2.14584600 | -1.10668600 |
| N                                            | -3.74357600                 | 1.84310500 | -0.83404200 |
| C                                            | 0.29811000                  | 2.48606300 | -1.12626100 |
| C                                            | 1.07512000                  | 2.07801200 | -2.22301700 |
| C                                            | 0.81231400                  | 3.26454500 | -0.07282400 |
| C                                            | 2.42050900                  | 2.46194600 | -2.24457500 |
| C                                            | 2.16085200                  | 3.63124500 | -0.14214600 |
| C                                            | 2.96015300                  | 3.23323000 | -1.21501200 |
| H                                            | 3.04497300                  | 2.15349400 | -3.07853900 |
| H                                            | 2.58501700                  | 4.23500200 | 0.65563400  |
| H                                            | 4.00458700                  | 3.52830500 | -1.24999900 |
| C                                            | -5.14832700                 | 1.55746600 | -0.95169900 |
| C                                            | -5.60713000                 | 1.11063300 | -2.20100000 |
| C                                            | -6.00006900                 | 1.73247300 | 0.15031300  |
| C                                            | -6.96726400                 | 0.80698800 | -2.32964700 |
| C                                            | -7.35358200                 | 1.42613100 | -0.02546000 |
| C                                            | -7.83626100                 | 0.96010100 | -1.25011800 |
| H                                            | -7.34243700                 | 0.45341000 | -3.28631400 |
| H                                            | -8.03477100                 | 1.55760600 | 0.81099800  |
| H                                            | -8.89024100                 | 0.72408100 | -1.36343500 |
| C                                            | -0.06129000                 | 3.66903100 | 1.09234100  |
| H                                            | -0.27542900                 | 2.81013000 | 1.74193100  |
| H                                            | 0.43420400                  | 4.42839100 | 1.70377300  |

|    |             |             |             |
|----|-------------|-------------|-------------|
| H  | -1.02975400 | 4.06463700  | 0.76364900  |
| C  | 0.46448200  | 1.23177300  | -3.31219700 |
| H  | 0.21131400  | 0.23001800  | -2.94184700 |
| H  | -0.46750300 | 1.67519400  | -3.68356200 |
| H  | 1.15153400  | 1.11388000  | -4.15428700 |
| C  | -5.46453400 | 2.22627900  | 1.47014600  |
| H  | -4.81844200 | 3.09726900  | 1.32651200  |
| H  | -6.28116500 | 2.50090000  | 2.14366300  |
| H  | -4.86748100 | 1.45319500  | 1.97162500  |
| C  | -4.65217800 | 0.97074700  | -3.36174400 |
| H  | -4.11141400 | 1.91049500  | -3.54436100 |
| H  | -3.88941900 | 0.20496500  | -3.17267900 |
| H  | -5.18110200 | 0.69895100  | -4.27924600 |
| C  | -2.98313000 | 0.92331600  | -0.34075000 |
| C  | -1.50409000 | 1.15733000  | -0.38865500 |
| C  | -2.24918500 | 5.35646400  | -2.44137700 |
| H  | -2.97113500 | 5.88623900  | -3.06293900 |
| C  | -1.61222600 | 4.22961200  | -3.04977900 |
| H  | -2.01922800 | 3.82926500  | -3.98215500 |
| C  | -1.34746300 | 6.26103900  | -1.59903700 |
| H  | -0.67560300 | 5.66333500  | -0.97815800 |
| H  | -1.89984700 | 6.95648500  | -0.96764700 |
| H  | -0.53662000 | 4.11397700  | -2.93140000 |
| Si | -4.02752600 | 5.14737000  | -1.00092200 |
| O  | -4.27644000 | 6.75936200  | -1.29268300 |
| O  | -5.49252000 | 4.40923800  | -1.15639600 |
| O  | -3.44420300 | 4.90845300  | 0.52698100  |
| C  | -5.43503700 | 7.47806000  | -0.85551800 |
| H  | -5.70903300 | 8.19041500  | -1.63852300 |
| H  | -6.28287000 | 6.81099300  | -0.66384800 |
| H  | -5.20366400 | 8.03163700  | 0.06153000  |
| C  | -6.27059800 | 4.36763700  | -2.35223300 |
| H  | -5.70830100 | 3.90759600  | -3.17475200 |
| H  | -7.14677600 | 3.75070300  | -2.14678500 |
| H  | -6.58834200 | 5.37299000  | -2.65396500 |
| C  | -3.47924900 | 5.86782000  | 1.59027700  |
| H  | -2.71660700 | 5.58210800  | 2.31906000  |
| H  | -3.26381400 | 6.87708800  | 1.22325800  |
| H  | -4.46100200 | 5.86012600  | 2.07703300  |
| C  | -4.08241800 | -2.38925700 | 1.28335800  |
| C  | -2.82371500 | -2.80539900 | 1.68972300  |
| C  | -1.67534300 | -2.01241400 | 1.41300700  |
| C  | -1.90172500 | -0.80722300 | 0.72239600  |
| C  | -3.19516800 | -0.37390900 | 0.30990000  |

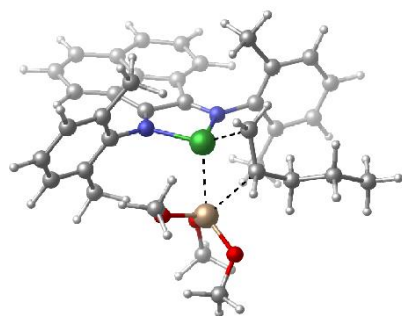
|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -4.29305300 | -1.16972700 | 0.58933300  |
| H | -0.09209300 | -3.21769300 | 2.28784500  |
| H | -4.94228500 | -3.01464100 | 1.50228100  |
| H | -2.70905400 | -3.74576400 | 2.22182100  |
| C | -0.32359300 | -2.30211800 | 1.75051800  |
| C | -0.85275600 | 0.08400800  | 0.35726400  |
| H | -5.29380200 | -0.88019500 | 0.29097600  |
| C | 0.45395100  | -0.22557900 | 0.69156600  |
| C | 0.69697300  | -1.43104700 | 1.39871900  |
| H | 1.27647600  | 0.42985100  | 0.42750100  |
| H | 1.71910500  | -1.67743600 | 1.66867500  |
| H | -0.73617300 | 6.85673300  | -2.28807800 |

UB3LYP-D3/BSII(SMD)//B3LYP-D3/BSI

HF=-2193.9296826



Triplet



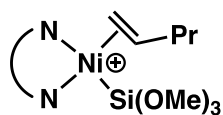
|                                              |                             |            |             |
|----------------------------------------------|-----------------------------|------------|-------------|
| Zero-point correction=                       | 0.716509 (Hartree/Particle) |            |             |
| Thermal correction to Energy=                | 0.762307                    |            |             |
| Thermal correction to Enthalpy=              | 0.763251                    |            |             |
| Thermal correction to Gibbs Free Energy=     | 0.634770                    |            |             |
| Sum of electronic and zero-point Energies=   | -2191.017098                |            |             |
| Sum of electronic and thermal Energies=      | -2190.971300                |            |             |
| Sum of electronic and thermal Enthalpies=    | -2190.970356                |            |             |
| Sum of electronic and thermal Free Energies= | -2191.098837                |            |             |
| Ni                                           | -2.86239700                 | 3.25282400 | -1.72829600 |
| N                                            | -1.23499200                 | 2.39228100 | -0.78954900 |
| N                                            | -3.81116000                 | 1.64752200 | -1.00479700 |
| C                                            | 0.14657700                  | 2.75012500 | -0.89667100 |
| C                                            | 0.86680900                  | 2.27618700 | -2.00938500 |
| C                                            | 0.71745700                  | 3.59704600 | 0.06874500  |
| C                                            | 2.19112000                  | 2.70349200 | -2.15673500 |
| C                                            | 2.04717900                  | 3.99184200 | -0.11623200 |
| C                                            | 2.77765100                  | 3.55796400 | -1.22295900 |
| H                                            | 2.76559400                  | 2.35626100 | -3.01129500 |
| H                                            | 2.50817700                  | 4.64949700 | 0.61569500  |
| H                                            | 3.80563100                  | 3.88191700 | -1.35516500 |
| C                                            | -5.20209900                 | 1.37755200 | -1.18520100 |
| C                                            | -5.62472500                 | 1.01961200 | -2.47984200 |
| C                                            | -6.10509200                 | 1.56471700 | -0.12089700 |
| C                                            | -6.99119200                 | 0.81488900 | -2.69221900 |
| C                                            | -7.46445400                 | 1.36102100 | -0.38618400 |
| C                                            | -7.90765000                 | 0.98555200 | -1.65449000 |
| H                                            | -7.33553000                 | 0.52164300 | -3.68020700 |
| H                                            | -8.18231600                 | 1.50704700 | 0.41639300  |
| H                                            | -8.96732600                 | 0.83083500 | -1.83496600 |
| C                                            | -0.08645900                 | 4.04374200 | 1.26362900  |
| H                                            | -0.24492800                 | 3.21323100 | 1.96452100  |
| H                                            | 0.42655100                  | 4.84354800 | 1.80509500  |

|    |             |            |             |
|----|-------------|------------|-------------|
| H  | -1.07830300 | 4.39519100 | 0.96584100  |
| C  | 0.24153600  | 1.30074700 | -2.97871800 |
| H  | 0.16449100  | 0.30121600 | -2.53052700 |
| H  | -0.77437900 | 1.59941400 | -3.26067600 |
| H  | 0.84142700  | 1.20998900 | -3.88835000 |
| C  | -5.63780200 | 1.99036900 | 1.24908200  |
| H  | -4.90497500 | 2.79953100 | 1.18623800  |
| H  | -6.48241100 | 2.33823100 | 1.85036600  |
| H  | -5.16916900 | 1.15902700 | 1.79062700  |
| C  | -4.62271900 | 0.84412300 | -3.59528400 |
| H  | -4.04165500 | 1.76142000 | -3.76316700 |
| H  | -3.89567600 | 0.05564900 | -3.36576900 |
| H  | -5.11975700 | 0.58366100 | -4.53361600 |
| C  | -3.03247700 | 0.88871200 | -0.30405400 |
| C  | -1.58685000 | 1.28734800 | -0.22336500 |
| C  | -2.38237700 | 5.26140200 | -2.50795700 |
| H  | -3.17756800 | 5.93909700 | -2.82584400 |
| C  | -2.14595000 | 4.17547700 | -3.41721600 |
| H  | -2.83123200 | 4.00547700 | -4.24644100 |
| C  | -1.17408800 | 5.95582700 | -1.88415600 |
| H  | -0.49678800 | 5.19688700 | -1.48504000 |
| H  | -1.47671500 | 6.59471400 | -1.04825500 |
| C  | -0.41775400 | 6.81294200 | -2.91483900 |
| H  | -0.14141800 | 6.18561900 | -3.77199200 |
| C  | 0.83853700  | 7.44299600 | -2.30510400 |
| H  | 1.52382100  | 6.66835800 | -1.93957300 |
| H  | 1.37494900  | 8.04906500 | -3.04267100 |
| H  | 0.58442100  | 8.09298000 | -1.45898700 |
| H  | -1.08556200 | 7.59503100 | -3.30015300 |
| H  | -1.13022700 | 3.81325200 | -3.55513200 |
| Si | -3.84954400 | 5.18032500 | -0.62655400 |
| O  | -3.94395100 | 6.82629100 | -0.72751100 |
| O  | -5.32125300 | 4.49805000 | -0.97230000 |
| O  | -3.42094100 | 4.72094100 | 0.89891500  |
| C  | -5.06225200 | 7.59380600 | -0.26212800 |
| H  | -4.92269500 | 7.87026400 | 0.78899300  |
| H  | -5.11694000 | 8.50427900 | -0.86397900 |
| H  | -6.00213900 | 7.03851300 | -0.36227500 |
| C  | -6.00684200 | 4.54085000 | -2.22598700 |
| H  | -5.35255000 | 4.22599200 | -3.05059800 |
| H  | -6.84207000 | 3.84080300 | -2.16401100 |
| H  | -6.38108000 | 5.54984400 | -2.43461400 |
| C  | -3.40187700 | 5.57454000 | 2.05137800  |
| H  | -2.72933900 | 5.12388600 | 2.78528900  |

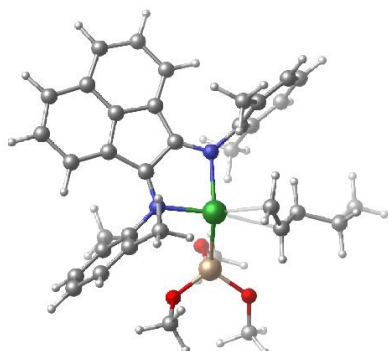
|   |             |             |            |
|---|-------------|-------------|------------|
| H | -3.03864300 | 6.57634800  | 1.79926100 |
| H | -4.40681000 | 5.64745900  | 2.48192000 |
| C | -3.95347400 | -2.45564700 | 1.35009600 |
| C | -2.67944100 | -2.78644600 | 1.78745100 |
| C | -1.57950600 | -1.91920800 | 1.53609500 |
| C | -1.86849800 | -0.73313300 | 0.83724600 |
| C | -3.17705100 | -0.38827800 | 0.39238600 |
| C | -4.22641900 | -1.25463000 | 0.64580600 |
| H | 0.06188100  | -3.01606500 | 2.44760800 |
| H | -4.77501900 | -3.13580700 | 1.55226100 |
| H | -2.51573900 | -3.71649300 | 2.32480700 |
| C | -0.21895800 | -2.11821300 | 1.90395500 |
| C | -0.87670100 | 0.22717400  | 0.49231900 |
| H | -5.23651500 | -1.02932100 | 0.32202200 |
| C | 0.43919100  | 0.00694500  | 0.85855400 |
| C | 0.74758300  | -1.18075800 | 1.57179600 |
| H | 1.22213900  | 0.71495900  | 0.61016900 |
| H | 1.77830000  | -1.35830200 | 1.86255500 |

UB3LYP-D3/BSII(SMD)//B3LYP-D3/BSI

HF=-2193.923159



Singlet



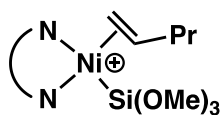
|                                              |                             |            |             |
|----------------------------------------------|-----------------------------|------------|-------------|
| Zero-point correction=                       | 0.718913 (Hartree/Particle) |            |             |
| Thermal correction to Energy=                | 0.765083                    |            |             |
| Thermal correction to Enthalpy=              | 0.766027                    |            |             |
| Thermal correction to Gibbs Free Energy=     | 0.636742                    |            |             |
| Sum of electronic and zero-point Energies=   | -2191.036594                |            |             |
| Sum of electronic and thermal Energies=      | -2190.990424                |            |             |
| Sum of electronic and thermal Enthalpies=    | -2190.989479                |            |             |
| Sum of electronic and thermal Free Energies= | -2191.118765                |            |             |
| Ni                                           | -2.59626900                 | 3.75197000 | -1.01764100 |
| N                                            | -0.91328600                 | 2.32528900 | -0.84344000 |
| N                                            | -3.59513400                 | 2.17611200 | -0.35014800 |
| C                                            | 0.46129600                  | 2.48073400 | -1.18453100 |
| C                                            | 0.76654900                  | 2.61420700 | -2.55497300 |
| C                                            | 1.44548300                  | 2.57662100 | -0.18097200 |
| C                                            | 2.09797600                  | 2.84038400 | -2.91280700 |
| C                                            | 2.76391400                  | 2.81664300 | -0.59014600 |
| C                                            | 3.09170200                  | 2.94605800 | -1.93852300 |
| H                                            | 2.35442500                  | 2.93547000 | -3.96437100 |
| H                                            | 3.53978400                  | 2.90271600 | 0.16599500  |
| H                                            | 4.12066500                  | 3.13228300 | -2.23087300 |
| C                                            | -4.99211300                 | 2.06845400 | -0.00756400 |
| C                                            | -5.85739900                 | 1.37221300 | -0.86585500 |
| C                                            | -5.41241000                 | 2.63360200 | 1.20733800  |
| C                                            | -7.18955200                 | 1.22768600 | -0.45861500 |
| C                                            | -6.74720400                 | 2.45094300 | 1.58023700  |
| C                                            | -7.62957700                 | 1.74821100 | 0.75823300  |
| H                                            | -7.88137300                 | 0.69264900 | -1.10350600 |
| H                                            | -7.09487500                 | 2.87010900 | 2.52047900  |
| H                                            | -8.66440100                 | 1.61770200 | 1.06084100  |
| C                                            | 1.12141800                  | 2.39777400 | 1.28463900  |
| H                                            | 1.14688500                  | 1.33750300 | 1.56621200  |

|    |             |             |             |
|----|-------------|-------------|-------------|
| H  | 1.85102800  | 2.92017000  | 1.90999600  |
| H  | 0.12547000  | 2.77175700  | 1.54045700  |
| C  | -0.32233300 | 2.47212100  | -3.59081800 |
| H  | -0.72323400 | 1.45067100  | -3.60960300 |
| H  | -1.17075900 | 3.13569600  | -3.37593600 |
| H  | 0.05092900  | 2.70588600  | -4.59151100 |
| C  | -4.44279900 | 3.40768200  | 2.06223300  |
| H  | -4.02255800 | 4.24018600  | 1.48435000  |
| H  | -4.93641100 | 3.81948200  | 2.94635400  |
| H  | -3.60659500 | 2.78277300  | 2.40013300  |
| C  | -5.35776200 | 0.74872100  | -2.14446500 |
| H  | -4.64368100 | 1.40341300  | -2.64845000 |
| H  | -4.85615000 | -0.20775800 | -1.94608000 |
| H  | -6.18571800 | 0.55263300  | -2.83107800 |
| C  | -2.84816600 | 1.15342000  | -0.07516800 |
| C  | -1.37887200 | 1.21050400  | -0.40784600 |
| C  | -1.70648700 | 5.76352200  | -0.49389300 |
| H  | -2.55280400 | 6.44438900  | -0.44623500 |
| C  | -1.26580500 | 5.35969800  | -1.72965000 |
| H  | -1.73634500 | 5.74704400  | -2.62730000 |
| H  | -0.31219700 | 4.84929000  | -1.83260000 |
| Si | -4.46355100 | 4.83779500  | -1.74266100 |
| O  | -3.99847100 | 6.26151600  | -2.47009800 |
| O  | -5.21901800 | 3.87705400  | -2.87225200 |
| O  | -5.55364100 | 5.15163700  | -0.55044500 |
| C  | -4.95557400 | 7.27358500  | -2.80659300 |
| H  | -4.40813100 | 8.12724800  | -3.21436700 |
| H  | -5.66396200 | 6.91313600  | -3.56345900 |
| H  | -5.51244600 | 7.59576800  | -1.91893400 |
| C  | -4.70711100 | 3.71672400  | -4.19389100 |
| H  | -4.49289000 | 4.68458200  | -4.66222900 |
| H  | -3.78515300 | 3.11747500  | -4.18989500 |
| H  | -5.46158000 | 3.19043300  | -4.78428200 |
| C  | -6.97531700 | 5.02174900  | -0.66623100 |
| H  | -7.39566300 | 5.09935100  | 0.33855600  |
| H  | -7.38573200 | 5.82470600  | -1.29041400 |
| H  | -7.24718500 | 4.05319200  | -1.09400100 |
| C  | -4.07513100 | -2.13471400 | 1.50647000  |
| C  | -2.87845600 | -2.82833600 | 1.40928500  |
| C  | -1.72538200 | -2.20619000 | 0.85624000  |
| C  | -1.87929100 | -0.87365700 | 0.42763500  |
| C  | -3.11356000 | -0.16508400 | 0.50654400  |
| C  | -4.21810400 | -0.79786100 | 1.05597700  |
| H  | -0.26112800 | -3.80570500 | 1.00080400  |

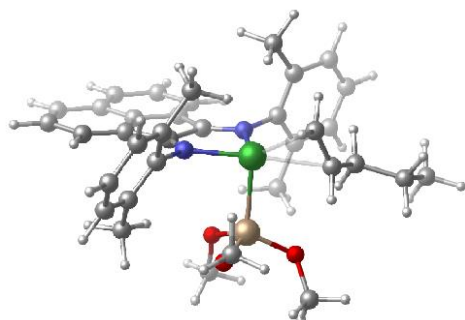
|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -4.93984200 | -2.62931600 | 1.93770900  |
| H | -2.81644800 | -3.85500600 | 1.75954000  |
| C | -0.43414000 | -2.77926300 | 0.68941700  |
| C | -0.81415900 | -0.11133400 | -0.12437000 |
| H | -5.17524800 | -0.29925100 | 1.14626600  |
| C | 0.43202800  | -0.69384000 | -0.27583800 |
| C | 0.60033100  | -2.04087400 | 0.13499100  |
| H | 1.26729000  | -0.14339200 | -0.69408100 |
| H | 1.57552900  | -2.50230900 | 0.01513900  |
| C | -0.97721900 | 5.50032500  | 0.79033900  |
| H | -0.61924600 | 6.45222600  | 1.20503700  |
| H | -1.64237000 | 5.05803800  | 1.54157300  |
| H | -0.11809900 | 4.84429200  | 0.63695500  |

UB3LYP-D3/BSII(SMD)//B3LYP-D3/BSI

HF=-2193.9394361



Triplet



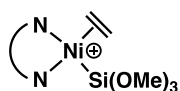
|                                              |                             |            |             |
|----------------------------------------------|-----------------------------|------------|-------------|
| Zero-point correction=                       | 0.717167 (Hartree/Particle) |            |             |
| Thermal correction to Energy=                | 0.764015                    |            |             |
| Thermal correction to Enthalpy=              | 0.764959                    |            |             |
| Thermal correction to Gibbs Free Energy=     | 0.633251                    |            |             |
| Sum of electronic and zero-point Energies=   | -2191.039948                |            |             |
| Sum of electronic and thermal Energies=      | -2190.993100                |            |             |
| Sum of electronic and thermal Enthalpies=    | -2190.992155                |            |             |
| Sum of electronic and thermal Free Energies= | -2191.123864                |            |             |
| Ni                                           | -2.89529800                 | 3.22147900 | -1.93293100 |
| N                                            | -1.30713600                 | 2.42292800 | -0.94962000 |
| N                                            | -3.85584700                 | 1.58341900 | -1.19149600 |
| C                                            | 0.05347900                  | 2.85399200 | -1.04008900 |
| C                                            | 0.77813300                  | 2.39399900 | -2.15791400 |
| C                                            | 0.59660600                  | 3.75732800 | -0.10999900 |
| C                                            | 2.07607700                  | 2.87706000 | -2.34538300 |
| C                                            | 1.90296300                  | 4.20932200 | -0.33776900 |
| C                                            | 2.63510100                  | 3.78519800 | -1.44545700 |
| H                                            | 2.65119100                  | 2.53337700 | -3.20091400 |
| H                                            | 2.34414300                  | 4.91036800 | 0.36558200  |
| H                                            | 3.64374400                  | 4.15522500 | -1.60330700 |
| C                                            | -5.21931100                 | 1.26690800 | -1.46497800 |
| C                                            | -5.50778100                 | 0.91470700 | -2.80516800 |
| C                                            | -6.23382100                 | 1.39030900 | -0.49313300 |
| C                                            | -6.83505500                 | 0.67947900 | -3.16075600 |
| C                                            | -7.55415300                 | 1.15609100 | -0.90791600 |
| C                                            | -7.85866000                 | 0.80690400 | -2.21899500 |
| H                                            | -7.06800500                 | 0.38985900 | -4.18172500 |
| H                                            | -8.35133300                 | 1.25669000 | -0.17581300 |
| H                                            | -8.88999400                 | 0.63114200 | -2.51011300 |
| C                                            | -0.19440900                 | 4.26140100 | 1.07170000  |
| H                                            | -0.82135200                 | 3.48379600 | 1.51376600  |
| H                                            | 0.47743900                  | 4.64780800 | 1.84381100  |

|    |             |             |             |
|----|-------------|-------------|-------------|
| H  | -0.86837300 | 5.07523800  | 0.77810900  |
| C  | 0.17050700  | 1.38163300  | -3.09910400 |
| H  | 0.10540400  | 0.39263900  | -2.62696600 |
| H  | -0.85295400 | 1.65512400  | -3.38266200 |
| H  | 0.76766100  | 1.27784700  | -4.00914500 |
| C  | -5.98596100 | 1.76246200  | 0.94928300  |
| H  | -4.98108100 | 2.13724600  | 1.13394200  |
| H  | -6.68494400 | 2.54597700  | 1.25716500  |
| H  | -6.15156400 | 0.89563500  | 1.60155300  |
| C  | -4.39462600 | 0.74086000  | -3.81094700 |
| H  | -3.80649900 | 1.65955400  | -3.93706600 |
| H  | -3.68772300 | -0.03685700 | -3.49771400 |
| H  | -4.79107100 | 0.46459900  | -4.79166300 |
| C  | -3.10208400 | 0.95257400  | -0.34935700 |
| C  | -1.67987000 | 1.42505100  | -0.21990600 |
| C  | -2.25115900 | 5.21779900  | -3.15991500 |
| H  | -3.09305900 | 5.86872400  | -2.92640200 |
| C  | -2.45621000 | 4.16396100  | -3.99584400 |
| H  | -3.42523100 | 4.00013400  | -4.46598100 |
| C  | -0.92374900 | 5.65197600  | -2.61518700 |
| H  | -0.14959300 | 4.92221000  | -2.87379100 |
| H  | -0.99554500 | 5.68856300  | -1.52349000 |
| C  | -0.52071500 | 7.05276900  | -3.11787800 |
| H  | -0.45198600 | 7.04385100  | -4.21324900 |
| C  | 0.81384900  | 7.49372800  | -2.50850100 |
| H  | 1.61224900  | 6.78444600  | -2.75646600 |
| H  | 1.10968800  | 8.48109600  | -2.87750800 |
| H  | 0.74559300  | 7.54650500  | -1.41522100 |
| H  | -1.30771600 | 7.77295000  | -2.85644100 |
| H  | -1.62631500 | 3.55564900  | -4.34945600 |
| Si | -3.74064200 | 4.57610700  | -0.17581300 |
| O  | -3.06387200 | 6.09800500  | -0.14575200 |
| O  | -5.40094700 | 4.70432600  | -0.28068100 |
| O  | -3.40136100 | 3.79898000  | 1.25414900  |
| C  | -3.72681000 | 7.30991700  | 0.22501600  |
| H  | -3.56172600 | 7.51907500  | 1.28873100  |
| H  | -3.30289600 | 8.12811500  | -0.36496100 |
| H  | -4.80540500 | 7.25198200  | 0.04080400  |
| C  | -6.10751800 | 4.76797100  | -1.51420700 |
| H  | -5.69047300 | 4.06909200  | -2.25594200 |
| H  | -7.14475500 | 4.47736500  | -1.32967000 |
| H  | -6.08984500 | 5.78263600  | -1.93322200 |
| C  | -3.45287900 | 4.44577400  | 2.52762200  |
| H  | -3.07342800 | 3.74422200  | 3.27580600  |

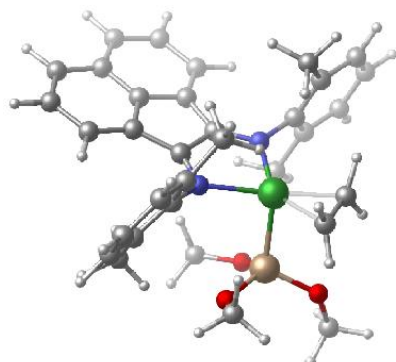
|   |             |             |            |
|---|-------------|-------------|------------|
| H | -2.82622400 | 5.34600300  | 2.53832300 |
| H | -4.48269300 | 4.71892000  | 2.78835600 |
| C | -4.00976400 | -2.19593000 | 1.66093500 |
| C | -2.77586300 | -2.37368900 | 2.26832300 |
| C | -1.70386400 | -1.47629700 | 2.00338900 |
| C | -1.98029800 | -0.41849000 | 1.11819400 |
| C | -3.25165400 | -0.22297000 | 0.50701900 |
| C | -4.27008200 | -1.12195400 | 0.77115700 |
| H | -0.11256100 | -2.32587200 | 3.21699800 |
| H | -4.80921100 | -2.89949100 | 1.87150900 |
| H | -2.62079800 | -3.20779900 | 2.94707800 |
| C | -0.38013300 | -1.53372100 | 2.52308000 |
| C | -1.00488500 | 0.54003800  | 0.72602700 |
| H | -5.24701000 | -1.02110000 | 0.31259400 |
| C | 0.27696000  | 0.45635700  | 1.23996900 |
| C | 0.56845600  | -0.59369000 | 2.14858800 |
| H | 1.04572000  | 1.16870300  | 0.96200100 |
| H | 1.57142200  | -0.66225300 | 2.55818500 |

UB3LYP-D3/BSII(SMD)//B3LYP-D3/BSI

HF=-2193.9501853



Singlet



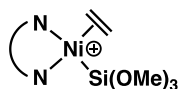
|                                              |                             |             |             |
|----------------------------------------------|-----------------------------|-------------|-------------|
| Zero-point correction=                       | 0.632777 (Hartree/Particle) |             |             |
| Thermal correction to Energy=                | 0.674359                    |             |             |
| Thermal correction to Enthalpy=              | 0.675303                    |             |             |
| Thermal correction to Gibbs Free Energy=     | 0.558346                    |             |             |
| Sum of electronic and zero-point Energies=   | -2073.170529                |             |             |
| Sum of electronic and thermal Energies=      | -2073.128948                |             |             |
| Sum of electronic and thermal Enthalpies=    | -2073.128004                |             |             |
| Sum of electronic and thermal Free Energies= | -2073.244961                |             |             |
| Ni                                           | -0.44993500                 | -1.37432100 | 0.75065500  |
| N                                            | 1.38401800                  | -0.51561000 | 0.34043400  |
| N                                            | -1.11333100                 | 0.53212300  | 0.30955700  |
| C                                            | 2.66345300                  | -1.12513100 | 0.53744500  |
| C                                            | 3.13350600                  | -1.18569300 | 1.86291500  |
| C                                            | 3.37616600                  | -1.67303500 | -0.54268300 |
| C                                            | 4.35548200                  | -1.82425000 | 2.09604900  |
| C                                            | 4.59389900                  | -2.30316200 | -0.25968300 |
| C                                            | 5.08098400                  | -2.38343200 | 1.04486300  |
| H                                            | 4.73902400                  | -1.87697500 | 3.11142500  |
| H                                            | 5.16190200                  | -2.73769900 | -1.07783000 |
| H                                            | 6.02603400                  | -2.88069800 | 1.24125400  |
| C                                            | -2.41728300                 | 1.05701800  | 0.61178400  |
| C                                            | -2.75979700                 | 1.10536800  | 1.97987200  |
| C                                            | -3.30647200                 | 1.48145500  | -0.39281500 |
| C                                            | -4.04051900                 | 1.54194700  | 2.32812100  |
| C                                            | -4.57924500                 | 1.91223300  | 0.00819700  |
| C                                            | -4.95364400                 | 1.93187900  | 1.34910100  |
| H                                            | -4.31564500                 | 1.58755400  | 3.37825500  |
| H                                            | -5.28237800                 | 2.23796100  | -0.75368900 |
| H                                            | -5.94714800                 | 2.26591600  | 1.63241200  |
| C                                            | 2.84940000                  | -1.57638100 | -1.95299800 |
| H                                            | 2.78324600                  | -0.53146200 | -2.28401300 |

|    |             |             |             |
|----|-------------|-------------|-------------|
| H  | 3.50695800  | -2.10206300 | -2.65065800 |
| H  | 1.84479900  | -2.00176100 | -2.03522100 |
| C  | 2.36478300  | -0.52115400 | 2.97978300  |
| H  | 2.41886700  | 0.57290400  | 2.90200600  |
| H  | 1.29876200  | -0.78001300 | 2.95358500  |
| H  | 2.76150500  | -0.80558500 | 3.95806100  |
| C  | -2.95014700 | 1.47369800  | -1.85897300 |
| H  | -3.02110000 | 0.45931100  | -2.26022900 |
| H  | -3.63602400 | 2.11335900  | -2.42166500 |
| H  | -1.93534500 | 1.83704100  | -2.04320000 |
| C  | -1.74505000 | 0.76589700  | 3.04577200  |
| H  | -1.35278100 | -0.25198500 | 2.93412200  |
| H  | -0.88122400 | 1.44112800  | 3.00356000  |
| H  | -2.18258100 | 0.84354300  | 4.04459000  |
| C  | -0.12970300 | 1.31135800  | 0.00964800  |
| C  | 1.26145500  | 0.70611500  | -0.03647400 |
| C  | -1.42887600 | -2.85270300 | 1.70945000  |
| H  | -1.84288900 | -2.37877600 | 2.59944300  |
| C  | -0.04608500 | -3.10608000 | 1.60089200  |
| Si | -1.38352000 | -2.24212200 | -1.09623800 |
| O  | -1.30923000 | -3.88100300 | -1.04334500 |
| O  | -2.89837300 | -1.63828500 | -1.29526900 |
| O  | -0.45066400 | -1.78218600 | -2.36673800 |
| C  | -1.18708700 | -4.72366600 | -2.20101700 |
| H  | -1.01610200 | -5.74108800 | -1.84263500 |
| H  | -2.10861700 | -4.70152400 | -2.79356400 |
| H  | -0.34599400 | -4.40855100 | -2.82603800 |
| C  | -3.99959700 | -1.81809900 | -0.39914500 |
| H  | -3.74527200 | -1.45890200 | 0.60385500  |
| H  | -4.83120100 | -1.22357200 | -0.78220200 |
| H  | -4.29496700 | -2.87218000 | -0.35372800 |
| C  | -0.38177600 | -0.58065300 | -3.11922500 |
| H  | -0.08273300 | 0.26537900  | -2.49011800 |
| H  | 0.37486800  | -0.72313600 | -3.89481000 |
| H  | -1.34356500 | -0.35417800 | -3.58826500 |
| C  | -0.30129100 | 5.11778600  | -0.51415100 |
| C  | 1.05076100  | 5.32081100  | -0.74835100 |
| C  | 1.96277500  | 4.22955300  | -0.72130400 |
| C  | 1.41092800  | 2.96154100  | -0.45799800 |
| C  | 0.02151100  | 2.74908200  | -0.22365000 |
| C  | -0.84018000 | 3.83380300  | -0.24766800 |
| H  | 3.84913100  | 5.22954500  | -1.12994000 |
| H  | -0.97533600 | 5.96836800  | -0.53471500 |
| H  | 1.42097400  | 6.32230200  | -0.94968800 |

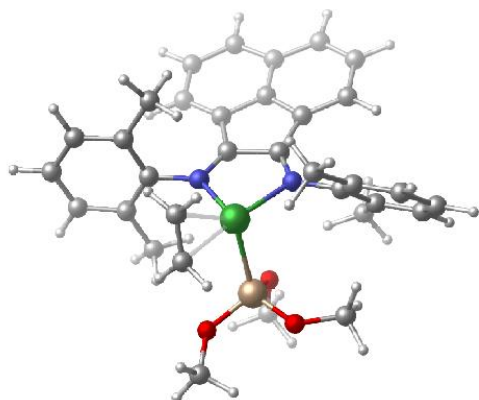
|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 3.37143900  | 4.27689200  | -0.91840500 |
| C | 2.19689900  | 1.77946900  | -0.37038300 |
| H | -1.90249300 | 3.71732200  | -0.06852900 |
| C | 3.56613600  | 1.85477800  | -0.55571900 |
| C | 4.13642400  | 3.12313400  | -0.83686300 |
| H | 4.19503500  | 0.97400000  | -0.48926900 |
| H | 5.20935100  | 3.18779000  | -0.98816300 |
| H | 0.31259300  | -3.85636600 | 0.90148900  |
| H | -2.13599700 | -3.47244300 | 1.16632200  |
| H | 0.63964500  | -2.85985800 | 2.41131600  |

UB3LYP-D3/BSII(SMD)//B3LYP-D3/BSI

HF=-2075.957666



Triplet



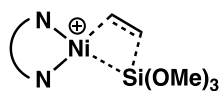
|                                              |                             |             |             |
|----------------------------------------------|-----------------------------|-------------|-------------|
| Zero-point correction=                       | 0.631719 (Hartree/Particle) |             |             |
| Thermal correction to Energy=                | 0.674155                    |             |             |
| Thermal correction to Enthalpy=              | 0.675099                    |             |             |
| Thermal correction to Gibbs Free Energy=     | 0.553646                    |             |             |
| Sum of electronic and zero-point Energies=   | -2073.165057                |             |             |
| Sum of electronic and thermal Energies=      | -2073.122622                |             |             |
| Sum of electronic and thermal Enthalpies=    | -2073.121678                |             |             |
| Sum of electronic and thermal Free Energies= | -2073.243131                |             |             |
| Ni                                           | 0.60573800                  | -1.12841500 | 0.92238700  |
| N                                            | 0.93646900                  | 0.86447600  | 0.59170700  |
| N                                            | -1.27474300                 | -0.66837300 | 0.31716000  |
| C                                            | 2.19276300                  | 1.52267700  | 0.69868600  |
| C                                            | 2.86144700                  | 1.40375900  | 1.93861100  |
| C                                            | 2.79622800                  | 2.16074600  | -0.40997400 |
| C                                            | 4.10979700                  | 2.00840100  | 2.08467400  |
| C                                            | 4.05721900                  | 2.74101600  | -0.21358300 |
| C                                            | 4.70490400                  | 2.68289600  | 1.01695300  |
| H                                            | 4.62240300                  | 1.94406200  | 3.04040800  |
| H                                            | 4.54053100                  | 3.23115400  | -1.05451800 |
| H                                            | 5.68008600                  | 3.14405800  | 1.14104600  |
| C                                            | -2.42947900                 | -1.51400400 | 0.35230100  |
| C                                            | -3.26273800                 | -1.44253300 | 1.48946100  |
| C                                            | -2.67237600                 | -2.40591700 | -0.70620500 |
| C                                            | -4.35715200                 | -2.31051000 | 1.55217600  |
| C                                            | -3.79098700                 | -3.24296600 | -0.60291300 |
| C                                            | -4.62244000                 | -3.20489000 | 0.51462100  |
| H                                            | -5.00939400                 | -2.27606400 | 2.42063900  |
| H                                            | -4.00671800                 | -3.93127900 | -1.41578900 |
| H                                            | -5.48008000                 | -3.86808300 | 0.57632900  |
| C                                            | 2.18494600                  | 2.17805600  | -1.79161300 |

|    |             |             |             |
|----|-------------|-------------|-------------|
| H  | 1.55452700  | 3.06050300  | -1.95025800 |
| H  | 2.97703100  | 2.20878300  | -2.54625900 |
| H  | 1.57834200  | 1.28910700  | -1.98074900 |
| C  | 2.25171300  | 0.61845500  | 3.07522900  |
| H  | 1.19640600  | 0.86212600  | 3.23566500  |
| H  | 2.31327300  | -0.46315400 | 2.87324900  |
| H  | 2.79011100  | 0.79453900  | 4.01052100  |
| C  | -1.77320900 | -2.46857100 | -1.91660900 |
| H  | -1.31033600 | -1.50418000 | -2.14150000 |
| H  | -0.95547700 | -3.18163400 | -1.76109700 |
| H  | -2.33609700 | -2.79677600 | -2.79595400 |
| C  | -3.00613800 | -0.43714300 | 2.58892500  |
| H  | -1.94385100 | -0.37976900 | 2.85408700  |
| H  | -3.31019400 | 0.57147600  | 2.28136500  |
| H  | -3.57074500 | -0.69133200 | 3.49007300  |
| C  | -1.37284300 | 0.58703300  | 0.03227800  |
| C  | -0.14814200 | 1.44661900  | 0.18219100  |
| C  | 0.72560700  | -3.25669800 | 1.73221100  |
| H  | 1.79814700  | -3.40802200 | 1.83932400  |
| C  | 0.00934100  | -2.57196800 | 2.66540900  |
| H  | -1.07486500 | -2.54243400 | 2.62197800  |
| Si | 1.77449000  | -1.96127000 | -0.97335200 |
| O  | 1.37908600  | -3.52411600 | -1.36394200 |
| O  | 3.41318800  | -1.98490100 | -0.70833400 |
| O  | 1.33439100  | -0.98422900 | -2.24031100 |
| C  | 2.19781800  | -4.68408900 | -1.20305400 |
| H  | 3.25742100  | -4.44926900 | -1.34025300 |
| H  | 2.05589800  | -5.11757400 | -0.20469700 |
| H  | 1.88459000  | -5.41870600 | -1.95004300 |
| C  | 4.31819500  | -0.88395600 | -0.77615700 |
| H  | 5.31807900  | -1.28776700 | -0.95765000 |
| H  | 4.05517700  | -0.19833400 | -1.58912100 |
| H  | 4.32480600  | -0.32745700 | 0.16712200  |
| C  | 1.45810200  | -1.38147000 | -3.61394800 |
| H  | 1.07388900  | -0.56309400 | -4.22839800 |
| H  | 2.50636400  | -1.56376300 | -3.87984600 |
| H  | 0.87625900  | -2.28797400 | -3.80990300 |
| C  | -4.59518800 | 2.37937200  | -1.04054700 |
| C  | -4.07424400 | 3.66443300  | -1.06404900 |
| C  | -2.70679900 | 3.89921100  | -0.74747300 |
| C  | -1.93471500 | 2.76470300  | -0.43553900 |
| C  | -2.47418700 | 1.45018000  | -0.39021000 |
| C  | -3.80928700 | 1.25005400  | -0.69455400 |
| H  | -2.58338400 | 6.06273900  | -0.92829700 |

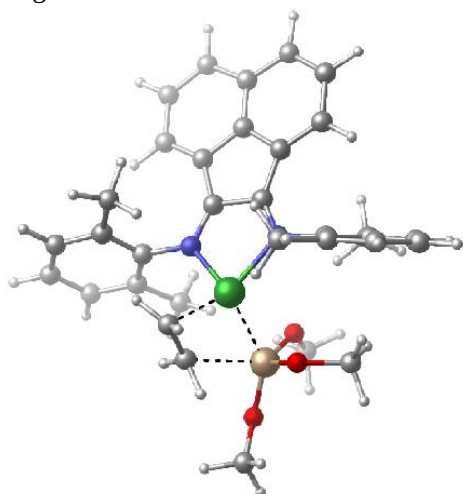
|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -5.64197900 | 2.22809700  | -1.28484100 |
| H | -4.71445600 | 4.50377900  | -1.32129600 |
| C | -2.03678500 | 5.15289000  | -0.69628000 |
| C | -0.55123500 | 2.82595500  | -0.10182700 |
| H | -4.25457400 | 0.26187800  | -0.66704600 |
| C | 0.06683000  | 4.06403800  | -0.04246600 |
| C | -0.69756200 | 5.22025000  | -0.34315100 |
| H | 1.11310500  | 4.16224500  | 0.22424700  |
| H | -0.20972100 | 6.18899000  | -0.29893000 |
| H | 0.23434900  | -3.81029100 | 0.93736600  |
| H | 0.48575000  | -2.11611900 | 3.53031300  |

UB3LYP-D3/BSII(SMD)//B3LYP-D3/BSI

HF=-2075.9564871



Singlet



|                                              |                             |
|----------------------------------------------|-----------------------------|
| Zero-point correction=                       | 0.632681 (Hartree/Particle) |
| Thermal correction to Energy=                | 0.673272                    |
| Thermal correction to Enthalpy=              | 0.674216                    |
| Thermal correction to Gibbs Free Energy=     | 0.559482                    |
| Sum of electronic and zero-point Energies=   | -2073.165636                |
| Sum of electronic and thermal Energies=      | -2073.125045                |
| Sum of electronic and thermal Enthalpies=    | -2073.124100                |
| Sum of electronic and thermal Free Energies= | -2073.238835                |

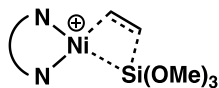
|    |             |             |             |
|----|-------------|-------------|-------------|
| Ni | -0.74681200 | -1.09767700 | 0.57988300  |
| N  | 1.17672100  | -1.00393000 | 0.24387400  |
| N  | -0.69259100 | 0.92693500  | 0.16742400  |
| C  | 2.12531500  | -2.06537900 | 0.42061000  |
| C  | 2.81351300  | -2.13210300 | 1.64444000  |
| C  | 2.29299400  | -3.01287800 | -0.60070700 |
| C  | 3.71656200  | -3.18555700 | 1.82283200  |
| C  | 3.21027400  | -4.04617300 | -0.37930000 |
| C  | 3.91880300  | -4.13309800 | 0.81931300  |
| H  | 4.26096400  | -3.26098200 | 2.76024700  |
| H  | 3.36287500  | -4.79031200 | -1.15626900 |
| H  | 4.62326200  | -4.94470500 | 0.97459700  |
| C  | -1.66229100 | 1.93027500  | 0.51887800  |
| C  | -1.84155600 | 2.16340800  | 1.89838000  |
| C  | -2.39618100 | 2.62592600  | -0.45598400 |
| C  | -2.81342000 | 3.08946300  | 2.29009800  |
| C  | -3.35143500 | 3.55151600  | -0.01440400 |
| C  | -3.57105500 | 3.77669000  | 1.34252400  |
| H  | -2.96352800 | 3.28030200  | 3.34922500  |
| H  | -3.92904600 | 4.09880700  | -0.75461800 |

|    |             |             |             |
|----|-------------|-------------|-------------|
| H  | -4.32082700 | 4.49453500  | 1.66117200  |
| C  | 1.50723900  | -2.90153800 | -1.88257300 |
| H  | 1.76106900  | -1.98375300 | -2.42889700 |
| H  | 1.70954600  | -3.74914200 | -2.54292400 |
| H  | 0.42993200  | -2.86489900 | -1.68440200 |
| C  | 2.58363700  | -1.09261800 | 2.71501300  |
| H  | 3.00013300  | -0.11879800 | 2.42578100  |
| H  | 1.51279200  | -0.93786900 | 2.89746700  |
| H  | 3.05329600  | -1.38765100 | 3.65697900  |
| C  | -2.19980900 | 2.38788000  | -1.93125100 |
| H  | -2.72797800 | 1.47879000  | -2.23279200 |
| H  | -2.59910300 | 3.22248900  | -2.51450100 |
| H  | -1.14470400 | 2.26972100  | -2.19687500 |
| C  | -0.96755400 | 1.48103800  | 2.92474500  |
| H  | -0.96812900 | 0.39080900  | 2.81104500  |
| H  | 0.07814800  | 1.80112200  | 2.83037300  |
| H  | -1.29735700 | 1.71648600  | 3.94006200  |
| C  | 0.52111700  | 1.26728700  | -0.10739300 |
| C  | 1.55530800  | 0.16731200  | -0.13879800 |
| C  | -2.23604600 | -2.00614100 | 1.57439000  |
| H  | -2.46795600 | -1.25243000 | 2.32940300  |
| C  | -0.95317300 | -2.68324200 | 1.62901200  |
| Si | -2.68195100 | -1.62395300 | -0.62831000 |
| O  | -3.49798400 | -3.05500600 | -0.61578800 |
| O  | -3.63320900 | -0.29584400 | -0.74641400 |
| O  | -1.72344900 | -1.75016500 | -1.96365900 |
| C  | -3.98013400 | -3.69992100 | -1.80522900 |
| H  | -4.38189700 | -4.66981300 | -1.50447900 |
| H  | -4.77824300 | -3.11013200 | -2.27041500 |
| H  | -3.16796600 | -3.84525000 | -2.52360900 |
| C  | -4.58978800 | 0.13924000  | 0.22700900  |
| H  | -4.08335300 | 0.47672900  | 1.13766600  |
| H  | -5.12912100 | 0.98506100  | -0.20239000 |
| H  | -5.29983600 | -0.66043700 | 0.46646200  |
| C  | -1.16082000 | -0.81085100 | -2.87005600 |
| H  | -0.50405900 | -0.10527100 | -2.35274900 |
| H  | -0.57370200 | -1.37475400 | -3.59879200 |
| H  | -1.94660700 | -0.25669000 | -3.39125100 |
| C  | 1.86242300  | 4.82541800  | -0.67044500 |
| C  | 3.18450600  | 4.47498100  | -0.90215500 |
| C  | 3.59249200  | 3.11250000  | -0.85767900 |
| C  | 2.58605000  | 2.17024400  | -0.57600200 |
| C  | 1.22669100  | 2.52784700  | -0.34076900 |
| C  | 0.86051300  | 3.86253600  | -0.38605800 |

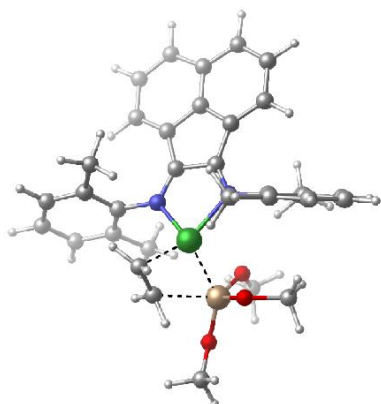
|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 5.71837200  | 3.27675700  | -1.28120500 |
| H | 1.57917700  | 5.87267100  | -0.70676300 |
| H | 3.91903200  | 5.24626700  | -1.11696400 |
| C | 4.90295200  | 2.59442000  | -1.05753300 |
| C | 2.83969800  | 0.77278500  | -0.47752500 |
| H | -0.16216300 | 4.17516500  | -0.20915100 |
| C | 4.12491800  | 0.29605000  | -0.66762000 |
| C | 5.14846800  | 1.23209100  | -0.96500800 |
| H | 4.35221600  | -0.76162100 | -0.59238600 |
| H | 6.15817300  | 0.86523900  | -1.12036200 |
| H | -0.85520800 | -3.64315400 | 1.12235600  |
| H | -3.10970300 | -2.62335400 | 1.36466300  |
| H | -0.30349800 | -2.56900400 | 2.49718100  |

UB3LYP-D3/BSII(SMD)//B3LYP-D3/BSI

HF=-2075.9505901



Triplet



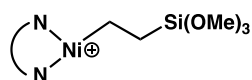
|                                              |                             |             |             |
|----------------------------------------------|-----------------------------|-------------|-------------|
| Zero-point correction=                       | 0.631491 (Hartree/Particle) |             |             |
| Thermal correction to Energy=                | 0.672696                    |             |             |
| Thermal correction to Enthalpy=              | 0.673640                    |             |             |
| Thermal correction to Gibbs Free Energy=     | 0.556584                    |             |             |
| Sum of electronic and zero-point Energies=   | -2073.153249                |             |             |
| Sum of electronic and thermal Energies=      | -2073.112044                |             |             |
| Sum of electronic and thermal Enthalpies=    | -2073.111100                |             |             |
| Sum of electronic and thermal Free Energies= | -2073.228155                |             |             |
| Ni                                           | 1.00797300                  | -0.63615500 | 0.81287100  |
| N                                            | 0.33395500                  | 1.21612100  | 0.47379100  |
| N                                            | -0.89560200                 | -1.16504300 | 0.23841800  |
| C                                            | 1.11941700                  | 2.40526900  | 0.55179000  |
| C                                            | 1.62968600                  | 2.76165000  | 1.81673900  |
| C                                            | 1.43957000                  | 3.12846100  | -0.61654400 |
| C                                            | 2.44156500                  | 3.89560200  | 1.90486400  |
| C                                            | 2.26486100                  | 4.25156800  | -0.47700600 |
| C                                            | 2.75766000                  | 4.63966600  | 0.76736700  |
| H                                            | 2.82831600                  | 4.19498500  | 2.87505900  |
| H                                            | 2.52858100                  | 4.82054600  | -1.36453500 |
| H                                            | 3.39430200                  | 5.51545500  | 0.85067800  |
| C                                            | -1.46730100                 | -2.47125900 | 0.29671000  |
| C                                            | -2.20194300                 | -2.84316200 | 1.44244600  |
| C                                            | -1.20499100                 | -3.37157100 | -0.75190800 |
| C                                            | -2.67026600                 | -4.15945900 | 1.51564100  |
| C                                            | -1.69853600                 | -4.67570800 | -0.63496600 |
| C                                            | -2.42209800                 | -5.07090700 | 0.48907200  |
| H                                            | -3.23280700                 | -4.46995700 | 2.39197600  |
| H                                            | -1.51239500                 | -5.38368200 | -1.43823200 |
| H                                            | -2.79139500                 | -6.08906600 | 0.56707000  |
| C                                            | 0.95426500                  | 2.70442900  | -1.98273900 |

|    |             |             |             |
|----|-------------|-------------|-------------|
| H  | -0.08088400 | 3.01873300  | -2.16186900 |
| H  | 1.57130000  | 3.15960200  | -2.76313200 |
| H  | 0.99972900  | 1.61795500  | -2.09933300 |
| C  | 1.29494600  | 1.94593400  | 3.04165900  |
| H  | 0.21250000  | 1.84810000  | 3.18334400  |
| H  | 1.69686500  | 0.92658900  | 2.96220900  |
| H  | 1.71727400  | 2.39907300  | 3.94256200  |
| C  | -0.47593000 | -2.92263700 | -1.99442800 |
| H  | 0.29622200  | -2.18354900 | -1.76777600 |
| H  | -0.01495600 | -3.77013400 | -2.51044100 |
| H  | -1.16799900 | -2.44316000 | -2.69995700 |
| C  | -2.48845900 | -1.85423100 | 2.54877300  |
| H  | -1.60220600 | -1.26358600 | 2.80838600  |
| H  | -3.27015400 | -1.14318900 | 2.25330300  |
| H  | -2.83297400 | -2.36780200 | 3.45036200  |
| C  | -1.60126900 | -0.10871700 | 0.00940000  |
| C  | -0.91182500 | 1.22107900  | 0.11226400  |
| C  | 2.00809300  | -2.51062500 | 1.12384700  |
| H  | 3.09048100  | -2.55889000 | 1.22899000  |
| C  | 1.30776700  | -2.08749800 | 2.29037700  |
| H  | 0.32458600  | -2.48815900 | 2.51190100  |
| Si | 2.73146500  | -1.16683000 | -0.71543500 |
| O  | 3.67495400  | -2.37331200 | -1.30957000 |
| O  | 3.52892800  | -0.07260900 | 0.24681500  |
| O  | 2.07605800  | -0.45479100 | -2.04914300 |
| C  | 4.78984400  | -3.02017200 | -0.69445700 |
| H  | 5.28127400  | -2.36932600 | 0.03883800  |
| H  | 4.46518000  | -3.94431200 | -0.20343200 |
| H  | 5.50647600  | -3.27192900 | -1.48062200 |
| C  | 4.20836700  | 1.10921700  | -0.22280600 |
| H  | 5.27303200  | 0.88533800  | -0.34330100 |
| H  | 3.78993600  | 1.45014500  | -1.17363900 |
| H  | 4.07589600  | 1.89091400  | 0.52654300  |
| C  | 2.26735900  | -0.81299700 | -3.42545800 |
| H  | 1.46026900  | -1.47803900 | -3.74951700 |
| H  | 2.22871200  | 0.10970800  | -4.01077300 |
| H  | 3.22763300  | -1.31197000 | -3.57884700 |
| C  | -5.33754300 | -0.01829600 | -0.88209800 |
| C  | -5.46013900 | 1.36076100  | -0.96165400 |
| C  | -4.33699600 | 2.20331200  | -0.72818900 |
| C  | -3.12400800 | 1.55675500  | -0.42830400 |
| C  | -3.00022300 | 0.14296000  | -0.33627900 |
| C  | -4.10859300 | -0.65274400 | -0.56362200 |
| H  | -5.21102800 | 4.17836600  | -0.98182200 |

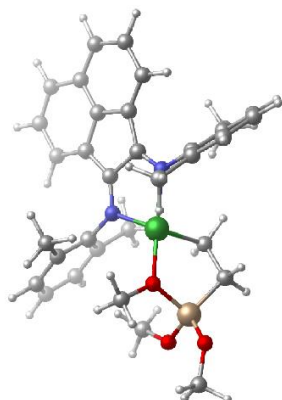
|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -6.21012700 | -0.63825200 | -1.06290000 |
| H | -6.42189100 | 1.80616700  | -1.20074400 |
| C | -4.30341700 | 3.62547500  | -0.75585100 |
| C | -1.90819100 | 2.25378600  | -0.17199500 |
| H | -4.05233400 | -1.73383300 | -0.49643000 |
| C | -1.90920800 | 3.63819700  | -0.19942800 |
| C | -3.12476600 | 4.30776800  | -0.49351600 |
| H | -1.00728800 | 4.20866600  | -0.00744500 |
| H | -3.12565700 | 5.39309300  | -0.51622800 |
| H | 1.57419400  | -3.31401900 | 0.53141900  |
| H | 1.85343400  | -1.63592400 | 3.11554000  |

UB3LYP-D3/BSII(SMD)//B3LYP-D3/BSI

HF=-2075.940064



Triplet



|                                              |                             |
|----------------------------------------------|-----------------------------|
| Zero-point correction=                       | 0.631789 (Hartree/Particle) |
| Thermal correction to Energy=                | 0.673374                    |
| Thermal correction to Enthalpy=              | 0.674318                    |
| Thermal correction to Gibbs Free Energy=     | 0.553785                    |
| Sum of electronic and zero-point Energies=   | -2073.195402                |
| Sum of electronic and thermal Energies=      | -2073.153817                |
| Sum of electronic and thermal Enthalpies=    | -2073.152873                |
| Sum of electronic and thermal Free Energies= | -2073.273406                |

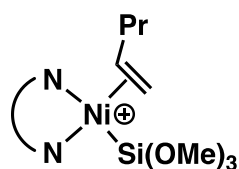
|    |             |             |             |
|----|-------------|-------------|-------------|
| Ni | 0.88549000  | 0.61374100  | 0.07564700  |
| N  | -0.10218900 | -1.17959300 | 0.12559500  |
| N  | -1.02659600 | 1.34848500  | 0.16679400  |
| C  | 0.51906700  | -2.46493200 | 0.11218800  |
| C  | 0.68198600  | -3.14736500 | -1.10727200 |
| C  | 1.03056100  | -2.95625700 | 1.32723900  |
| C  | 1.40570800  | -4.34529600 | -1.08715700 |
| C  | 1.74739800  | -4.15720500 | 1.29863700  |
| C  | 1.94199800  | -4.84424600 | 0.10037100  |
| H  | 1.55124400  | -4.88757400 | -2.01750000 |
| H  | 2.14933500  | -4.55599900 | 2.22619900  |
| H  | 2.50693400  | -5.77150100 | 0.09224900  |
| C  | -1.33823000 | 2.73317900  | 0.09738900  |
| C  | -1.92563500 | 3.28976900  | -1.05877000 |
| C  | -0.92358200 | 3.53053900  | 1.18601200  |
| C  | -2.14357100 | 4.67360200  | -1.06929200 |
| C  | -1.17817600 | 4.90147900  | 1.13385800  |
| C  | -1.78929900 | 5.47199600  | 0.01591300  |
| H  | -2.58837400 | 5.12672800  | -1.95120300 |
| H  | -0.88839600 | 5.52722400  | 1.97343200  |
| H  | -1.97263600 | 6.54178400  | -0.01521300 |
| C  | 0.74723800  | -2.23562800 | 2.62283800  |
| H  | -0.27999600 | -2.42779200 | 2.95919600  |

|    |             |             |             |
|----|-------------|-------------|-------------|
| H  | 1.42273500  | -2.56361200 | 3.41794400  |
| H  | 0.84081200  | -1.15001500 | 2.51313000  |
| C  | 0.08526300  | -2.61117100 | -2.38586000 |
| H  | -1.00650200 | -2.72443000 | -2.39034800 |
| H  | 0.29567800  | -1.54467400 | -2.51335600 |
| H  | 0.47642700  | -3.14563400 | -3.25565400 |
| C  | -0.23638900 | 2.90545800  | 2.37691900  |
| H  | 0.73455900  | 2.46968400  | 2.09426400  |
| H  | -0.04217000 | 3.65003100  | 3.15357100  |
| H  | -0.83242600 | 2.09882600  | 2.81912900  |
| C  | -2.28130100 | 2.45966600  | -2.27035100 |
| H  | -1.58314700 | 1.62952500  | -2.41671300 |
| H  | -3.28612600 | 2.02776400  | -2.18860500 |
| H  | -2.26366600 | 3.07697400  | -3.17287900 |
| C  | -1.90303600 | 0.40054300  | 0.11447000  |
| C  | -1.38062900 | -1.01390100 | 0.10019000  |
| C  | 2.87253400  | 1.76696000  | -1.70245600 |
| H  | 3.38292400  | 1.83477600  | -2.67549800 |
| C  | 1.50802300  | 1.06964400  | -1.81004300 |
| H  | 0.74449900  | 1.70704000  | -2.26798200 |
| Si | 3.96559400  | 0.90330200  | -0.46925800 |
| O  | 4.62565800  | -0.53896400 | -0.89692500 |
| O  | 2.82234000  | 0.59774900  | 0.78510300  |
| O  | 5.15164700  | 1.84327100  | 0.13489500  |
| C  | 3.90358100  | -1.74778600 | -1.13404400 |
| H  | 3.29418800  | -2.02687900 | -0.26716700 |
| H  | 3.24851800  | -1.65450600 | -2.00830700 |
| H  | 4.63095300  | -2.54032200 | -1.32483400 |
| C  | 3.27041400  | 0.17361200  | 2.08737400  |
| H  | 4.21934000  | 0.66154700  | 2.32532700  |
| H  | 2.51975900  | 0.47650700  | 2.82062300  |
| H  | 3.38949500  | -0.91373500 | 2.10629700  |
| C  | 6.50806800  | 1.49750700  | 0.43546400  |
| H  | 7.16260700  | 2.24058800  | -0.02798600 |
| H  | 6.65344400  | 1.52351700  | 1.52095300  |
| H  | 6.76192600  | 0.50226000  | 0.05802400  |
| C  | -5.72997500 | 0.76603000  | 0.20077600  |
| C  | -6.03305100 | -0.58702900 | 0.17332500  |
| C  | -4.99555300 | -1.55965500 | 0.12427600  |
| C  | -3.67816200 | -1.06577500 | 0.09857300  |
| C  | -3.36461000 | 0.32291300  | 0.11360800  |
| C  | -4.39486300 | 1.24529600  | 0.17048200  |
| H  | -6.13292000 | -3.41235800 | 0.11823000  |
| H  | -6.53898100 | 1.48853400  | 0.24374800  |

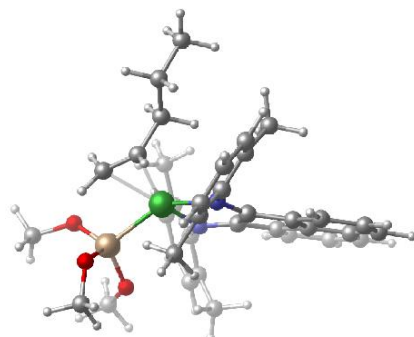
|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -7.07000500 | -0.91066900 | 0.19286300  |
| C | -5.13814500 | -2.97554600 | 0.10567300  |
| C | -2.53383200 | -1.91071800 | 0.07553900  |
| H | -4.19825700 | 2.31178200  | 0.18902500  |
| C | -2.70091100 | -3.28434100 | 0.06257200  |
| C | -4.02259800 | -3.79963400 | 0.07455900  |
| H | -1.85072900 | -3.95763000 | 0.04453200  |
| H | -4.16060200 | -4.87625200 | 0.06213700  |
| H | 2.74916100  | 2.79922700  | -1.34791800 |
| H | 1.57094900  | 0.12934500  | -2.36749900 |

UB3LYP-D3/BSII(SMD)//B3LYP-D3/BSI

HF=-2075.9869062



Singlet



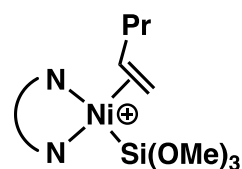
|                                              |                             |            |             |
|----------------------------------------------|-----------------------------|------------|-------------|
| Zero-point correction=                       | 0.719843 (Hartree/Particle) |            |             |
| Thermal correction to Energy=                | 0.765347                    |            |             |
| Thermal correction to Enthalpy=              | 0.766291                    |            |             |
| Thermal correction to Gibbs Free Energy=     | 0.640701                    |            |             |
| Sum of electronic and zero-point Energies=   | -2191.036710                |            |             |
| Sum of electronic and thermal Energies=      | -2190.991207                |            |             |
| Sum of electronic and thermal Enthalpies=    | -2190.990262                |            |             |
| Sum of electronic and thermal Free Energies= | -2191.115852                |            |             |
| Ni                                           | -2.63171900                 | 3.44826700 | -1.56175900 |
| N                                            | -1.02601500                 | 2.24813100 | -0.88589000 |
| N                                            | -3.71114500                 | 1.92924300 | -0.93911300 |
| C                                            | 0.36051600                  | 2.57661700 | -0.82819900 |
| C                                            | 1.31238700                  | 1.88733900 | -1.60796700 |
| C                                            | 0.71035800                  | 3.69693800 | -0.04018900 |
| C                                            | 2.63717000                  | 2.34726300 | -1.57074000 |
| C                                            | 2.04587700                  | 4.10185500 | -0.02429700 |
| C                                            | 3.00656800                  | 3.43696000 | -0.78850900 |
| H                                            | 3.38369200                  | 1.83409900 | -2.17153400 |
| H                                            | 2.33299300                  | 4.95037700 | 0.59055100  |
| H                                            | 4.03940700                  | 3.77166800 | -0.77507400 |
| C                                            | -5.13291500                 | 1.74029100 | -1.05882700 |
| C                                            | -5.69720500                 | 1.79173900 | -2.34595000 |
| C                                            | -5.90770500                 | 1.52172600 | 0.09756500  |
| C                                            | -7.07473300                 | 1.57882500 | -2.46643400 |
| C                                            | -7.28026000                 | 1.31329300 | -0.07592100 |
| C                                            | -7.86253400                 | 1.33376600 | -1.34304300 |
| H                                            | -7.52709500                 | 1.60358100 | -3.45391400 |
| H                                            | -7.89932400                 | 1.14641100 | 0.80156200  |
| H                                            | -8.93027300                 | 1.16925100 | -1.45327800 |
| C                                            | -0.33487300                 | 4.42251700 | 0.77247300  |

|    |             |             |             |
|----|-------------|-------------|-------------|
| H  | -0.88911800 | 3.73823400  | 1.42550500  |
| H  | 0.12602400  | 5.19015600  | 1.40044100  |
| H  | -1.07917100 | 4.91636700  | 0.13365700  |
| C  | 0.98622100  | 0.68663400  | -2.46745200 |
| H  | 1.30659200  | -0.24204900 | -1.97986000 |
| H  | -0.08083500 | 0.58404100  | -2.67619800 |
| H  | 1.51056100  | 0.74982600  | -3.42587800 |
| C  | -5.30415700 | 1.54307800  | 1.48129800  |
| H  | -4.63074400 | 2.39787800  | 1.59162800  |
| H  | -6.08933800 | 1.62664500  | 2.23810400  |
| H  | -4.73967300 | 0.62942200  | 1.69972200  |
| C  | -4.84552100 | 2.06865800  | -3.56019100 |
| H  | -4.48763900 | 3.10612500  | -3.54544300 |
| H  | -3.96217300 | 1.42106500  | -3.60086400 |
| H  | -5.41567300 | 1.92397900  | -4.48185300 |
| C  | -2.97669400 | 0.91542300  | -0.59940000 |
| C  | -1.49613100 | 1.13260400  | -0.44866300 |
| C  | -2.34873100 | 5.19691600  | -2.88548300 |
| H  | -3.12930000 | 5.14859600  | -3.63838000 |
| C  | -1.28130800 | 4.32926500  | -2.91699900 |
| Si | -4.15548700 | 5.02914400  | -0.92798000 |
| O  | -5.13345900 | 5.59078400  | -2.14005300 |
| O  | -5.08822400 | 4.43850700  | 0.31025500  |
| O  | -3.24124100 | 6.25939600  | -0.27548800 |
| C  | -5.78093900 | 6.86610900  | -2.14270600 |
| H  | -5.15652600 | 7.63152400  | -1.66634100 |
| H  | -5.96091900 | 7.15142100  | -3.18279200 |
| H  | -6.74371900 | 6.81127000  | -1.62076900 |
| C  | -6.49866400 | 4.64831500  | 0.40519600  |
| H  | -7.00669000 | 4.36430200  | -0.52200800 |
| H  | -6.87294400 | 4.02126400  | 1.21747600  |
| H  | -6.72222900 | 5.69724600  | 0.63803100  |
| C  | -3.30970100 | 6.75743600  | 1.06188900  |
| H  | -2.30699300 | 6.72506200  | 1.50080700  |
| H  | -3.65145900 | 7.79786500  | 1.03708800  |
| H  | -3.99157700 | 6.16528100  | 1.67977100  |
| C  | -4.20407700 | -2.66392300 | 0.11642200  |
| C  | -3.00561100 | -3.15998100 | 0.60685700  |
| C  | -1.85106900 | -2.33180500 | 0.66509100  |
| C  | -2.00470000 | -1.01149200 | 0.19977100  |
| C  | -3.24332500 | -0.48925500 | -0.27313700 |
| C  | -4.34828200 | -1.32353000 | -0.32274500 |
| H  | -0.38546100 | -3.69330700 | 1.51501300  |
| H  | -5.06989200 | -3.31734100 | 0.07474100  |

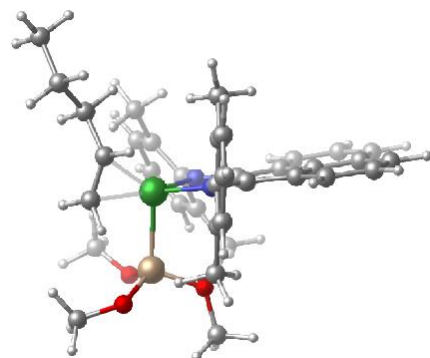
|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -2.94356600 | -4.18965300 | 0.94809300  |
| C | -0.55797300 | -2.68880000 | 1.13862200  |
| C | -0.93346900 | -0.07735800 | 0.15481400  |
| H | -5.30963500 | -0.97154500 | -0.67703200 |
| C | 0.31364400  | -0.45151300 | 0.62257100  |
| C | 0.47870700  | -1.76798400 | 1.12400400  |
| H | 1.15245300  | 0.23540700  | 0.60766300  |
| H | 1.45446400  | -2.06289500 | 1.49720200  |
| C | -1.10861000 | 3.27773100  | -3.98560000 |
| H | -1.99646100 | 3.25898100  | -4.62955100 |
| H | -1.02493200 | 2.28171600  | -3.53597300 |
| H | -0.40321800 | 4.55468700  | -2.31319500 |
| H | -2.28642500 | 6.11674700  | -2.31417100 |
| C | 0.15816000  | 3.53333200  | -4.82753600 |
| H | 1.03081000  | 3.51923200  | -4.16120700 |
| H | 0.10792400  | 4.54073600  | -5.25978400 |
| C | 0.32824200  | 2.49425500  | -5.93944400 |
| H | -0.51862000 | 2.51662800  | -6.63540400 |
| H | 1.23973900  | 2.68113000  | -6.51653200 |
| H | 0.39318000  | 1.47995400  | -5.52685300 |

UB3LYP-D3/BSII(SMD)//B3LYP-D3/BSI

HF=-2193.9416719



Triplet



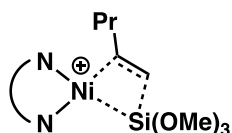
|                                              |                             |            |             |
|----------------------------------------------|-----------------------------|------------|-------------|
| Zero-point correction=                       | 0.717644 (Hartree/Particle) |            |             |
| Thermal correction to Energy=                | 0.764062                    |            |             |
| Thermal correction to Enthalpy=              | 0.765007                    |            |             |
| Thermal correction to Gibbs Free Energy=     | 0.635110                    |            |             |
| Sum of electronic and zero-point Energies=   | -2191.038324                |            |             |
| Sum of electronic and thermal Energies=      | -2190.991906                |            |             |
| Sum of electronic and thermal Enthalpies=    | -2190.990961                |            |             |
| Sum of electronic and thermal Free Energies= | -2191.120858                |            |             |
| Ni                                           | -2.93895600                 | 3.31196100 | -1.83739100 |
| N                                            | -1.33273000                 | 2.45520200 | -0.95216600 |
| N                                            | -3.91599200                 | 1.65486700 | -1.11855500 |
| C                                            | 0.04503300                  | 2.82103200 | -1.09260600 |
| C                                            | 0.79021700                  | 2.15568600 | -2.08927300 |
| C                                            | 0.59343400                  | 3.84489800 | -0.30137500 |
| C                                            | 2.12159200                  | 2.53780400 | -2.27846600 |
| C                                            | 1.93545800                  | 4.18284100 | -0.51997700 |
| C                                            | 2.69436400                  | 3.54220300 | -1.49769700 |
| H                                            | 2.71150700                  | 2.03875200 | -3.04256100 |
| H                                            | 2.38460700                  | 4.96220400 | 0.08967400  |
| H                                            | 3.73132500                  | 3.82505900 | -1.65226300 |
| C                                            | -5.31042800                 | 1.39350600 | -1.24946200 |
| C                                            | -5.78898000                 | 1.24009300 | -2.57130900 |
| C                                            | -6.18695200                 | 1.39530300 | -0.14182100 |
| C                                            | -7.15161300                 | 1.02686500 | -2.77137300 |
| C                                            | -7.55176100                 | 1.19423000 | -0.39881600 |
| C                                            | -8.03394900                 | 1.00119500 | -1.68937100 |
| H                                            | -7.52481200                 | 0.88503400 | -3.78184300 |
| H                                            | -8.24240500                 | 1.19995200 | 0.44036800  |
| H                                            | -9.09520500                 | 0.84247000 | -1.85611100 |
| C                                            | -0.22362700                 | 4.55679600 | 0.74690600  |

|    |             |             |             |
|----|-------------|-------------|-------------|
| H  | -0.87774900 | 3.87281300  | 1.29286500  |
| H  | 0.42785800  | 5.06603200  | 1.46310000  |
| H  | -0.87637100 | 5.31544400  | 0.29819800  |
| C  | 0.16665400  | 1.05813900  | -2.91916500 |
| H  | 0.02552300  | 0.14241200  | -2.33104300 |
| H  | -0.82274800 | 1.34915700  | -3.29221900 |
| H  | 0.79760900  | 0.80788600  | -3.77626800 |
| C  | -5.74912500 | 1.63234800  | 1.28354400  |
| H  | -4.77121300 | 2.10677300  | 1.35665900  |
| H  | -6.46960200 | 2.28580600  | 1.78501000  |
| H  | -5.71216800 | 0.69095800  | 1.84565000  |
| C  | -4.84091900 | 1.31866200  | -3.74149800 |
| H  | -4.45502400 | 2.34167100  | -3.86114200 |
| H  | -3.97216500 | 0.66265800  | -3.62005100 |
| H  | -5.34252100 | 1.05515500  | -4.67672500 |
| C  | -3.11312100 | 0.94496100  | -0.38663900 |
| C  | -1.67934500 | 1.38709200  | -0.31221200 |
| C  | -2.35023700 | 5.15664500  | -3.00791100 |
| H  | -3.30691700 | 5.55046000  | -3.35108700 |
| C  | -1.70086800 | 4.18962900  | -3.71632700 |
| H  | -0.69348200 | 3.91527000  | -3.40566900 |
| Si | -3.83091100 | 4.65039500  | -0.09592000 |
| O  | -3.23739100 | 6.20562900  | -0.02795200 |
| O  | -5.49055400 | 4.68398900  | -0.19741000 |
| O  | -3.38604200 | 3.92423800  | 1.32126900  |
| C  | -3.89888700 | 7.35045100  | -0.56188700 |
| H  | -4.97585800 | 7.32212200  | -0.36064500 |
| H  | -3.47049800 | 8.23736900  | -0.08727700 |
| H  | -3.74003700 | 7.42658900  | -1.64635900 |
| C  | -6.24647900 | 4.64676500  | -1.40207200 |
| H  | -5.67115300 | 4.21170400  | -2.23438300 |
| H  | -7.12748200 | 4.01996000  | -1.24264900 |
| H  | -6.56297900 | 5.65719700  | -1.68644000 |
| C  | -3.51199400 | 4.54629800  | 2.60694000  |
| H  | -3.20200400 | 5.59586800  | 2.56842200  |
| H  | -4.54852400 | 4.48468100  | 2.95841200  |
| H  | -2.86528400 | 4.00548300  | 3.30325200  |
| C  | -3.91472900 | -2.39965500 | 1.34050900  |
| C  | -2.64606300 | -2.64311800 | 1.84391100  |
| C  | -1.58681300 | -1.72418800 | 1.60405600  |
| C  | -1.91160000 | -0.57846100 | 0.85484200  |
| C  | -3.21984200 | -0.31089300 | 0.35878700  |
| C  | -4.22416600 | -1.23502100 | 0.59175500  |
| H  | 0.07262500  | -2.70068900 | 2.61324100  |

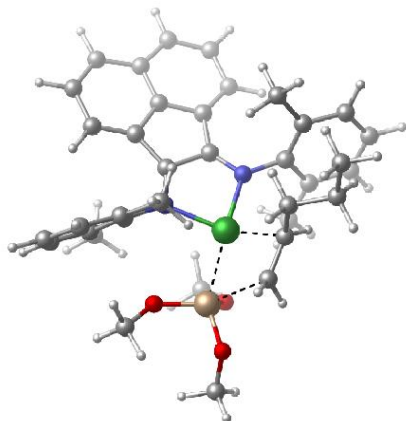
|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -4.70494200 | -3.12059700 | 1.52570000  |
| H | -2.45385400 | -3.54476200 | 2.41884200  |
| C | -0.23209700 | -1.83988300 | 2.02436500  |
| C | -0.95299100 | 0.40700300  | 0.49200800  |
| H | -5.22937600 | -1.08608400 | 0.21473000  |
| C | 0.35986300  | 0.26648100  | 0.90657400  |
| C | 0.69941300  | -0.86999000 | 1.68495300  |
| H | 1.11748500  | 0.99708300  | 0.64604400  |
| H | 1.72663700  | -0.98369800 | 2.01703800  |
| H | -1.85977000 | 5.70435800  | -2.20836400 |
| C | -2.19700500 | 3.55497600  | -4.98387900 |
| H | -2.21301900 | 2.46116600  | -4.87638100 |
| H | -3.22662900 | 3.87381800  | -5.19182800 |
| C | -1.28786400 | 3.90896400  | -6.18153800 |
| H | -0.25925300 | 3.59974700  | -5.95252000 |
| H | -1.26698300 | 4.99908300  | -6.30389000 |
| C | -1.75940700 | 3.24011400  | -7.47584200 |
| H | -1.10435700 | 3.50221800  | -8.31283100 |
| H | -1.75979100 | 2.14758100  | -7.37903100 |
| H | -2.77695200 | 3.55485100  | -7.73609200 |

UB3LYP-D3/BSII(SMD)//B3LYP-D3/BSI

HF= -2193.9490144



Singlet



|                                              |                             |
|----------------------------------------------|-----------------------------|
| Zero-point correction=                       | 0.719662 (Hartree/Particle) |
| Thermal correction to Energy=                | 0.764359                    |
| Thermal correction to Enthalpy=              | 0.765303                    |
| Thermal correction to Gibbs Free Energy=     | 0.641461                    |
| Sum of electronic and zero-point Energies=   | -2191.033427                |
| Sum of electronic and thermal Energies=      | -2190.988729                |
| Sum of electronic and thermal Enthalpies=    | -2190.987785                |
| Sum of electronic and thermal Free Energies= | -2191.111627                |

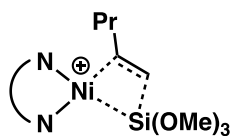
|    |             |            |             |
|----|-------------|------------|-------------|
| Ni | -2.65408600 | 3.49193300 | -1.61086600 |
| N  | -1.11573900 | 2.33286300 | -0.92506600 |
| N  | -3.78402000 | 1.95741400 | -0.87153100 |
| C  | 0.29088500  | 2.57659400 | -1.03991500 |
| C  | 1.07018500  | 1.78941800 | -1.91108600 |
| C  | 0.83009400  | 3.66766900 | -0.32864200 |
| C  | 2.41895900  | 2.13799400 | -2.06669200 |
| C  | 2.18352000  | 3.96486800 | -0.50690100 |
| C  | 2.97429100  | 3.21233500 | -1.37625800 |
| H  | 3.03596000  | 1.55051800 | -2.74157200 |
| H  | 2.61728300  | 4.79708600 | 0.04055300  |
| H  | 4.02172700  | 3.46341200 | -1.51353200 |
| C  | -5.17244600 | 1.65074800 | -1.09089200 |
| C  | -5.57198000 | 1.41521300 | -2.41784600 |
| C  | -6.07233300 | 1.58219100 | -0.01186000 |
| C  | -6.90676200 | 1.06280600 | -2.65151700 |
| C  | -7.39727200 | 1.23163800 | -0.29396100 |
| C  | -7.81421500 | 0.96334100 | -1.59823500 |
| H  | -7.22985000 | 0.86506300 | -3.66993800 |
| H  | -8.11027100 | 1.17670900 | 0.52426800  |

|    |             |             |             |
|----|-------------|-------------|-------------|
| H  | -8.84676800 | 0.68991500  | -1.79359200 |
| C  | -0.03445700 | 4.46633200  | 0.61355300  |
| H  | -0.42723200 | 3.83702800  | 1.42203900  |
| H  | 0.53201800  | 5.28263700  | 1.06987500  |
| H  | -0.90528000 | 4.89814300  | 0.10645500  |
| C  | 0.52840800  | 0.58121100  | -2.64146700 |
| H  | 0.72408000  | -0.33652400 | -2.07279100 |
| H  | -0.55140300 | 0.63143000  | -2.80494700 |
| H  | 1.01110400  | 0.47236900  | -3.61730300 |
| C  | -5.63752100 | 1.89449600  | 1.39769800  |
| H  | -5.12551500 | 2.85934800  | 1.42921800  |
| H  | -6.50096400 | 1.94323100  | 2.06686300  |
| H  | -4.95471600 | 1.13491800  | 1.79615700  |
| C  | -4.58466800 | 1.53172900  | -3.55297400 |
| H  | -4.16673800 | 2.54652900  | -3.60596100 |
| H  | -3.73497500 | 0.84948000  | -3.42940000 |
| H  | -5.05819500 | 1.31164000  | -4.51354600 |
| C  | -3.03222100 | 1.02807300  | -0.37613600 |
| C  | -1.55438500 | 1.29166500  | -0.30616200 |
| C  | -2.53817200 | 5.30369200  | -2.74526000 |
| H  | -3.25072900 | 5.38657100  | -3.56338000 |
| C  | -1.44878400 | 4.41263700  | -2.85925800 |
| Si | -4.13079000 | 5.25817100  | -1.02954800 |
| O  | -4.62413400 | 6.63600700  | -1.80188300 |
| O  | -5.49456700 | 4.48447600  | -0.51536700 |
| O  | -3.23226000 | 5.66755200  | 0.30019700  |
| C  | -5.22457900 | 7.72156100  | -1.08423100 |
| H  | -4.50904500 | 8.16045300  | -0.37993800 |
| H  | -5.51864500 | 8.47579400  | -1.81795500 |
| H  | -6.11549800 | 7.39944200  | -0.53053400 |
| C  | -6.78610500 | 4.57476800  | -1.12692800 |
| H  | -6.94024500 | 3.72690300  | -1.79900800 |
| H  | -7.53312600 | 4.53412100  | -0.32996000 |
| H  | -6.90074100 | 5.50684400  | -1.68829100 |
| C  | -3.36669500 | 5.10958400  | 1.60608100  |
| H  | -3.00790600 | 4.07285000  | 1.62423400  |
| H  | -2.75278200 | 5.70692700  | 2.28477100  |
| H  | -4.40846700 | 5.13378900  | 1.94234200  |
| C  | -4.13296800 | -2.46210900 | 0.83613200  |
| C  | -2.89903800 | -2.87526100 | 1.31394300  |
| C  | -1.76364000 | -2.02544400 | 1.20861900  |
| C  | -1.97606600 | -0.76980100 | 0.60733600  |
| C  | -3.24834400 | -0.33145500 | 0.13700900  |
| C  | -4.33183600 | -1.18837000 | 0.24488700  |

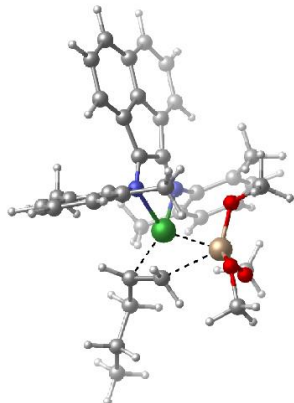
|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -0.21841900 | -3.25837700 | 2.11129100  |
| H | -4.98386500 | -3.13101100 | 0.91935200  |
| H | -2.79331800 | -3.85646500 | 1.76845900  |
| C | -0.43590200 | -2.30630500 | 1.63508900  |
| C | -0.93018800 | 0.16951800  | 0.39335000  |
| H | -5.31682500 | -0.90555800 | -0.10567000 |
| C | 0.35400000  | -0.13185700 | 0.81152800  |
| C | 0.57909600  | -1.38046300 | 1.44498900  |
| H | 1.17545500  | 0.55908200  | 0.65854800  |
| H | 1.58334100  | -1.61897800 | 1.78100700  |
| C | -1.25962700 | 3.50072500  | -4.04856200 |
| H | -2.16290300 | 3.50588600  | -4.67155100 |
| H | -1.11492000 | 2.46647800  | -3.71548600 |
| H | -0.53766300 | 4.66616400  | -2.31841300 |
| H | -2.34401800 | 6.24643500  | -2.23979300 |
| C | -0.03141000 | 3.90429000  | -4.88976700 |
| H | 0.85424600  | 3.89400000  | -4.24089800 |
| H | -0.15541500 | 4.93665200  | -5.24112800 |
| C | 0.18478000  | 2.96411600  | -6.07866500 |
| H | -0.68059000 | 2.96821800  | -6.75205700 |
| H | 1.06306400  | 3.26054100  | -6.66140500 |
| H | 0.33933300  | 1.93184100  | -5.74003400 |

UB3LYP-D3/BSII(SMD)/B3LYP-D3/BSI

HF=-2193.9372067



Triplet



|                                              |                             |
|----------------------------------------------|-----------------------------|
| Zero-point correction=                       | 0.717272 (Hartree/Particle) |
| Thermal correction to Energy=                | 0.762672                    |
| Thermal correction to Enthalpy=              | 0.763616                    |
| Thermal correction to Gibbs Free Energy=     | 0.635923                    |
| Sum of electronic and zero-point Energies=   | -2191.021177                |
| Sum of electronic and thermal Energies=      | -2190.975778                |
| Sum of electronic and thermal Enthalpies=    | -2190.974834                |
| Sum of electronic and thermal Free Energies= | -2191.102526                |

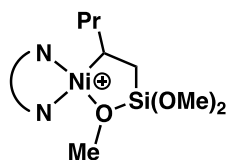
|    |             |             |             |
|----|-------------|-------------|-------------|
| Ni | -2.85123500 | 3.01985500  | -1.85361600 |
| N  | -1.28561300 | 2.31053800  | -0.76880700 |
| N  | -3.81912400 | 1.45805800  | -1.10370800 |
| C  | 0.08403000  | 2.70463100  | -0.87689700 |
| C  | 0.87611300  | 2.04659300  | -1.84313200 |
| C  | 0.58219700  | 3.75598800  | -0.08820800 |
| C  | 2.19479600  | 2.47775000  | -2.01243100 |
| C  | 1.91447700  | 4.14245200  | -0.28571300 |
| C  | 2.71372700  | 3.51849200  | -1.24094400 |
| H  | 2.82009400  | 1.98646100  | -2.75305800 |
| H  | 2.32379300  | 4.94333400  | 0.32457400  |
| H  | 3.74214400  | 3.83761300  | -1.38140600 |
| C  | -5.18612100 | 1.10728800  | -1.33525200 |
| C  | -5.52442000 | 0.64552200  | -2.62289900 |
| C  | -6.15452700 | 1.29501400  | -0.32750500 |
| C  | -6.86616200 | 0.36014200  | -2.89065500 |
| C  | -7.48644100 | 1.00139800  | -0.64667100 |
| C  | -7.84390700 | 0.53865900  | -1.91209800 |
| H  | -7.14225300 | -0.00873600 | -3.87468200 |
| H  | -8.25048800 | 1.14586900  | 0.11248900  |
| H  | -8.88348600 | 0.31895400  | -2.13613900 |

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -0.26940000 | 4.44985300  | 0.94818000  |
| H  | -1.06744800 | 3.80486600  | 1.32101900  |
| H  | 0.34433700  | 4.77145400  | 1.79550200  |
| H  | -0.74812700 | 5.34730400  | 0.53669400  |
| C  | 0.32098300  | 0.89671000  | -2.65168300 |
| H  | 0.22078700  | -0.00755300 | -2.03774900 |
| H  | -0.67609500 | 1.12358300  | -3.04803600 |
| H  | 0.97912200  | 0.65520100  | -3.49072700 |
| C  | -5.78943700 | 1.80694400  | 1.04535300  |
| H  | -5.03852400 | 2.59897500  | 0.98846800  |
| H  | -6.67335000 | 2.19933000  | 1.55653500  |
| H  | -5.37680100 | 1.00706800  | 1.67305900  |
| C  | -4.45510500 | 0.43049200  | -3.66528400 |
| H  | -3.88291400 | 1.34747100  | -3.84996900 |
| H  | -3.73054600 | -0.32839500 | -3.34535900 |
| H  | -4.88951300 | 0.10633500  | -4.61479900 |
| C  | -3.05873900 | 0.78105600  | -0.29508200 |
| C  | -1.64055100 | 1.23680100  | -0.14279600 |
| C  | -2.11198800 | 4.88945700  | -2.52464900 |
| H  | -2.71991700 | 5.71531000  | -2.90394300 |
| C  | -1.90254400 | 3.83937300  | -3.49908200 |
| H  | -0.91356900 | 3.38761100  | -3.53784800 |
| Si | -3.50706600 | 5.13829900  | -0.76976300 |
| O  | -2.83017700 | 6.58110000  | -0.37723900 |
| O  | -4.96234000 | 5.45596400  | -1.47462800 |
| O  | -3.56209800 | 4.29316100  | 0.64575900  |
| C  | -2.91095200 | 7.80361300  | -1.11191200 |
| H  | -3.88850300 | 7.91550600  | -1.59294800 |
| H  | -2.76147000 | 8.62531000  | -0.40717700 |
| H  | -2.12055100 | 7.84405500  | -1.87182500 |
| C  | -5.91036500 | 4.50686200  | -1.96238900 |
| H  | -5.44940900 | 3.79495200  | -2.66349200 |
| H  | -6.36009400 | 3.93843400  | -1.14302900 |
| H  | -6.68956200 | 5.05827900  | -2.49306300 |
| C  | -3.67360400 | 4.91291800  | 1.94115900  |
| H  | -2.83593600 | 5.59325500  | 2.11606300  |
| H  | -4.61468300 | 5.46623800  | 2.02872700  |
| H  | -3.65791800 | 4.10990500  | 2.68210600  |
| C  | -3.96900100 | -2.49620500 | 1.50157400  |
| C  | -2.72078200 | -2.74158500 | 2.05392300  |
| C  | -1.64117000 | -1.84262500 | 1.82747300  |
| C  | -1.92383400 | -0.71731100 | 1.03278700  |
| C  | -3.20757900 | -0.45581900 | 0.47173100  |
| C  | -4.23573800 | -1.35423300 | 0.70276600  |

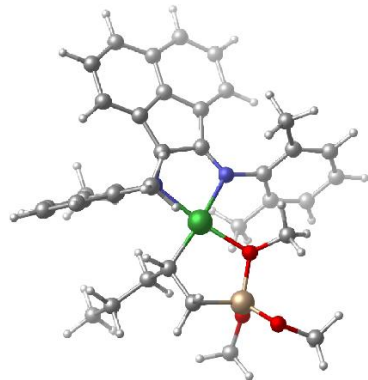
|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -0.03081900 | -2.80575800 | 2.92648200  |
| H | -4.77572800 | -3.19911400 | 1.68494300  |
| H | -2.56156800 | -3.62804300 | 2.66167800  |
| C | -0.30511200 | -1.95759600 | 2.30524200  |
| C | -0.94681900 | 0.25936100  | 0.69433400  |
| H | -5.22687100 | -1.19932300 | 0.29133400  |
| C | 0.34543600  | 0.12199600  | 1.16793000  |
| C | 0.64602800  | -1.00167400 | 1.98144000  |
| H | 1.11613800  | 0.84605500  | 0.92698800  |
| H | 1.65819400  | -1.11431800 | 2.35736300  |
| H | -1.22526500 | 5.21767100  | -1.98363000 |
| C | -2.74411100 | 3.76239800  | -4.74430800 |
| H | -2.70969300 | 2.74685700  | -5.15832200 |
| H | -3.79789500 | 3.97281700  | -4.50456000 |
| C | -2.28023000 | 4.75705900  | -5.83615000 |
| H | -1.22879300 | 4.55354400  | -6.07673900 |
| H | -2.31502500 | 5.77547300  | -5.42700900 |
| C | -3.13828900 | 4.66831600  | -7.10113800 |
| H | -2.79399300 | 5.37831100  | -7.86028700 |
| H | -3.09516000 | 3.66364600  | -7.53836800 |
| H | -4.18920900 | 4.89419300  | -6.88283000 |

UB3LYP-D3/BSII(SMD)//B3LYP-D3/BSI

HF=-2193.9294142



Singlet



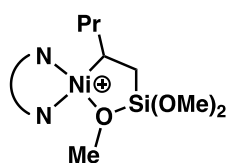
|                                              |                             |            |             |
|----------------------------------------------|-----------------------------|------------|-------------|
| Zero-point correction=                       | 0.720868 (Hartree/Particle) |            |             |
| Thermal correction to Energy=                | 0.765464                    |            |             |
| Thermal correction to Enthalpy=              | 0.766409                    |            |             |
| Thermal correction to Gibbs Free Energy=     | 0.642660                    |            |             |
| Sum of electronic and zero-point Energies=   | -2191.072122                |            |             |
| Sum of electronic and thermal Energies=      | -2191.027526                |            |             |
| Sum of electronic and thermal Enthalpies=    | -2191.026582                |            |             |
| Sum of electronic and thermal Free Energies= | -2191.150330                |            |             |
| Ni                                           | -2.61891100                 | 3.36274200 | -1.31607900 |
| N                                            | -1.09890100                 | 2.17157200 | -0.92729100 |
| N                                            | -3.69603400                 | 1.83569800 | -0.37117900 |
| C                                            | 0.28131800                  | 2.40628500 | -1.23622700 |
| C                                            | 0.91061500                  | 1.68120900 | -2.26521400 |
| C                                            | 0.94288600                  | 3.41990600 | -0.51343300 |
| C                                            | 2.23852600                  | 2.01177800 | -2.56889300 |
| C                                            | 2.27006800                  | 3.70226900 | -0.84396800 |
| C                                            | 2.91420500                  | 3.00922500 | -1.86997700 |
| H                                            | 2.74262700                  | 1.47222600 | -3.36635500 |
| H                                            | 2.79893800                  | 4.47555000 | -0.29381500 |
| H                                            | 3.94278600                  | 3.24766800 | -2.12354600 |
| C                                            | -5.10964600                 | 1.73537300 | -0.20023500 |
| C                                            | -5.89868000                 | 1.66535300 | -1.36470800 |
| C                                            | -5.67157500                 | 1.82092100 | 1.08869400  |
| C                                            | -7.28816800                 | 1.65178400 | -1.21010000 |
| C                                            | -7.06767300                 | 1.81608200 | 1.19053000  |
| C                                            | -7.87210900                 | 1.72906200 | 0.05491800  |
| H                                            | -7.91573700                 | 1.58310200 | -2.09451000 |
| H                                            | -7.52384100                 | 1.89000200 | 2.17411000  |
| H                                            | -8.95342000                 | 1.72551400 | 0.15509400  |

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 0.23000800  | 4.15782700  | 0.59200300  |
| H  | -0.08018600 | 3.47673700  | 1.39419400  |
| H  | 0.87146100  | 4.92686800  | 1.03033500  |
| H  | -0.68345400 | 4.64011700  | 0.21854800  |
| C  | 0.23676200  | 0.54949300  | -3.00675800 |
| H  | 0.48974300  | -0.41638200 | -2.55129000 |
| H  | -0.85298200 | 0.63096900  | -3.00514800 |
| H  | 0.56994700  | 0.51921000  | -4.04837600 |
| C  | -4.80980700 | 1.94917200  | 2.32327500  |
| H  | -3.98039600 | 2.65029200  | 2.17093500  |
| H  | -5.40009500 | 2.30270800  | 3.17301500  |
| H  | -4.36375700 | 0.98874100  | 2.60857400  |
| C  | -5.25977600 | 1.61015800  | -2.73118300 |
| H  | -4.79266900 | 2.56959900  | -2.98356400 |
| H  | -4.48121900 | 0.84073800  | -2.78559900 |
| H  | -6.00527300 | 1.39231400  | -3.50108400 |
| C  | -2.90404700 | 0.87448400  | -0.04404300 |
| C  | -1.44056900 | 1.09362800  | -0.29767700 |
| C  | -2.18169500 | 5.88277700  | -2.77501800 |
| H  | -1.84186300 | 6.33678700  | -3.71563500 |
| C  | -1.60104200 | 4.47120900  | -2.58211500 |
| H  | -0.58890000 | 4.53700100  | -2.17387300 |
| Si | -4.02287800 | 5.75514600  | -2.65356100 |
| O  | -4.75219400 | 7.15752000  | -2.22650200 |
| O  | -4.80384500 | 4.99336400  | -3.88928600 |
| O  | -4.13349900 | 4.63522700  | -1.36793800 |
| C  | -6.13510200 | 7.49064300  | -2.38631800 |
| H  | -6.20116700 | 8.54767800  | -2.65534200 |
| H  | -6.60884300 | 6.88680300  | -3.16852300 |
| H  | -6.66687600 | 7.32962500  | -1.44164100 |
| C  | -4.77141200 | 5.42909300  | -5.25149400 |
| H  | -3.74181400 | 5.47310300  | -5.62893600 |
| H  | -5.33228000 | 4.70358900  | -5.84514300 |
| H  | -5.23686700 | 6.41551400  | -5.36609300 |
| C  | -5.00528300 | 4.85762800  | -0.23432700 |
| H  | -5.98897900 | 4.42821400  | -0.43546900 |
| H  | -4.56128600 | 4.36561000  | 0.62928700  |
| H  | -5.08237200 | 5.93048500  | -0.04362800 |
| C  | -3.85284100 | -2.52425100 | 1.48495000  |
| C  | -2.56155500 | -3.00068900 | 1.65393100  |
| C  | -1.44216000 | -2.21579900 | 1.26000000  |
| C  | -1.72846800 | -0.95689800 | 0.69844600  |
| C  | -3.05262300 | -0.46064100 | 0.53975800  |
| C  | -4.12238200 | -1.24614600 | 0.93137400  |

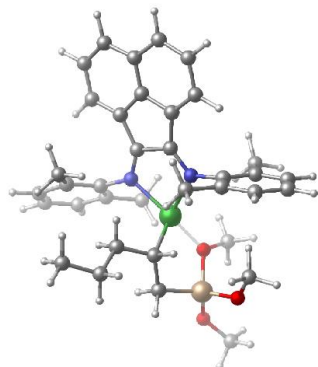
|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 0.21290500  | -3.51843500 | 1.79831100  |
| H | -4.68988900 | -3.14409500 | 1.79074900  |
| H | -2.39891300 | -3.98215200 | 2.09072100  |
| C | -0.06626300 | -2.55997600 | 1.36941000  |
| C | -0.72033200 | -0.06355900 | 0.23451900  |
| H | -5.14503500 | -0.90129700 | 0.82625100  |
| C | 0.61046000  | -0.42633900 | 0.35503000  |
| C | 0.91707600  | -1.68399100 | 0.93458600  |
| H | 1.40804800  | 0.22435200  | 0.01532400  |
| H | 1.96005600  | -1.96855100 | 1.03259200  |
| H | -1.85662700 | 6.54977800  | -1.96675700 |
| C | -1.59470400 | 3.63353700  | -3.86525700 |
| H | -2.57703900 | 3.68662100  | -4.35314200 |
| H | -1.43993800 | 2.57569900  | -3.62671300 |
| C | -0.49428400 | 4.04344900  | -4.86482600 |
| H | -0.60989000 | 5.10046700  | -5.13830400 |
| H | 0.47925600  | 3.95619200  | -4.36451400 |
| C | -0.50923300 | 3.18097900  | -6.13053400 |
| H | -0.36109500 | 2.12150900  | -5.88638800 |
| H | -1.46771000 | 3.26659900  | -6.65734900 |
| H | 0.28281600  | 3.47778100  | -6.82650700 |

UB3LYP-D3/BSII(SMD)//B3LYP-D3/BSI

HF=-2193.9771189



Triplet



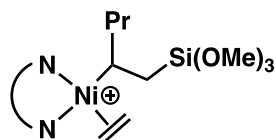
|                                              |                             |            |             |
|----------------------------------------------|-----------------------------|------------|-------------|
| Zero-point correction=                       | 0.717875 (Hartree/Particle) |            |             |
| Thermal correction to Energy=                | 0.763629                    |            |             |
| Thermal correction to Enthalpy=              | 0.764574                    |            |             |
| Thermal correction to Gibbs Free Energy=     | 0.635111                    |            |             |
| Sum of electronic and zero-point Energies=   | -2191.063223                |            |             |
| Sum of electronic and thermal Energies=      | -2191.017469                |            |             |
| Sum of electronic and thermal Enthalpies=    | -2191.016524                |            |             |
| Sum of electronic and thermal Free Energies= | -2191.145987                |            |             |
| Ni                                           | -2.51176300                 | 3.76445900 | 0.20107300  |
| N                                            | -0.93063600                 | 2.68726200 | -0.49367700 |
| N                                            | -3.46212900                 | 1.92937200 | 0.06374200  |
| C                                            | 0.35008400                  | 3.23475600 | -0.80548900 |
| C                                            | 0.64665300                  | 3.60658400 | -2.13043700 |
| C                                            | 1.23757400                  | 3.47126600 | 0.26043000  |
| C                                            | 1.86583800                  | 4.25367300 | -2.36349100 |
| C                                            | 2.44740000                  | 4.11336300 | -0.02182200 |
| C                                            | 2.75782300                  | 4.51123900 | -1.32205600 |
| H                                            | 2.11408900                  | 4.55769100 | -3.37677100 |
| H                                            | 3.14827600                  | 4.30106200 | 0.78713600  |
| H                                            | 3.69654600                  | 5.01776200 | -1.52534900 |
| C                                            | -4.84099300                 | 1.71077500 | 0.33276900  |
| C                                            | -5.73401500                 | 1.26130800 | -0.66669300 |
| C                                            | -5.29637000                 | 2.07531800 | 1.62190600  |
| C                                            | -7.08811900                 | 1.14402700 | -0.32189900 |
| C                                            | -6.64929300                 | 1.91873100 | 1.91957200  |
| C                                            | -7.54504900                 | 1.45378400 | 0.95485000  |
| H                                            | -7.79034500                 | 0.80837300 | -1.08058800 |
| H                                            | -7.00533800                 | 2.16951700 | 2.91498400  |
| H                                            | -8.59803000                 | 1.34638500 | 1.19714500  |
| C                                            | 0.90043300                  | 2.99424700 | 1.65115400  |

|    |             |             |             |
|----|-------------|-------------|-------------|
| H  | 1.01170100  | 1.90510200  | 1.73227200  |
| H  | 1.55434200  | 3.45200900  | 2.39872600  |
| H  | -0.13838700 | 3.22203900  | 1.91140000  |
| C  | -0.30553600 | 3.30129600  | -3.26148200 |
| H  | -0.32786300 | 2.22590900  | -3.48000700 |
| H  | -1.32976800 | 3.60036200  | -3.02140300 |
| H  | -0.00400100 | 3.81802700  | -4.17649300 |
| C  | -4.34114500 | 2.62203600  | 2.65727900  |
| H  | -4.06013800 | 3.65995600  | 2.42529000  |
| H  | -4.80276900 | 2.63132800  | 3.64865100  |
| H  | -3.41649300 | 2.03749700  | 2.71881300  |
| C  | -5.32103900 | 0.93483700  | -2.08339100 |
| H  | -4.35405500 | 1.36108700  | -2.35275000 |
| H  | -5.25539600 | -0.14871500 | -2.23958900 |
| H  | -6.06073100 | 1.32388500  | -2.78980900 |
| C  | -2.65009700 | 1.01974400  | -0.36964700 |
| C  | -1.24815900 | 1.45677800  | -0.71379800 |
| C  | -3.66917900 | 6.28075100  | -0.63971900 |
| H  | -3.82480300 | 7.09663700  | -1.36344800 |
| C  | -3.09072700 | 5.02490600  | -1.30494400 |
| H  | -2.14934100 | 5.25883400  | -1.82018500 |
| Si | -2.56753100 | 6.86369500  | 0.73941000  |
| O  | -3.30631400 | 7.81458700  | 1.83776600  |
| O  | -1.14821600 | 7.57620200  | 0.32323300  |
| O  | -2.21125100 | 5.35999600  | 1.49655300  |
| C  | -2.80105100 | 8.98318100  | 2.49286700  |
| H  | -3.58645900 | 9.74346100  | 2.48607500  |
| H  | -2.55118400 | 8.73866200  | 3.53135600  |
| H  | -1.91120900 | 9.37224400  | 1.98884800  |
| C  | -0.13132100 | 7.01444300  | -0.50872000 |
| H  | 0.13131400  | 5.99774800  | -0.19528700 |
| H  | -0.45192200 | 6.99175900  | -1.55701100 |
| H  | 0.75494100  | 7.64825400  | -0.42645600 |
| C  | -1.63535200 | 5.32985900  | 2.81751900  |
| H  | -2.15012000 | 6.05275300  | 3.45626700  |
| H  | -1.77456600 | 4.32560900  | 3.22332900  |
| H  | -0.56796300 | 5.56467500  | 2.76907600  |
| C  | -3.34353000 | -2.74924200 | -0.71914500 |
| C  | -2.10271700 | -3.10793100 | -1.22363000 |
| C  | -1.09464200 | -2.12487300 | -1.42780800 |
| C  | -1.43969300 | -0.80000700 | -1.10208200 |
| C  | -2.71989400 | -0.42488500 | -0.60439300 |
| C  | -3.67492800 | -1.40634900 | -0.40319200 |
| H  | 0.54514900  | -3.33367100 | -2.18671300 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -4.09334500 | -3.51837400 | -0.56212900 |
| H | -1.89293100 | -4.14754900 | -1.45943400 |
| C | 0.22744300  | -2.33148600 | -1.91242000 |
| C | -0.52898300 | 0.28681300  | -1.21293700 |
| H | -4.65810300 | -1.16703600 | -0.01346700 |
| C | 0.75342600  | 0.05704700  | -1.67915400 |
| C | 1.11160700  | -1.26949600 | -2.03235700 |
| H | 1.47359500  | 0.86244400  | -1.77459100 |
| H | 2.11477800  | -1.45555900 | -2.40302200 |
| H | -4.65690900 | 6.06181400  | -0.20838000 |
| C | -4.04026300 | 4.27202100  | -2.22108800 |
| H | -3.54369600 | 3.35665300  | -2.57151400 |
| H | -4.91920500 | 3.94074100  | -1.64906800 |
| C | -4.51629500 | 5.06421900  | -3.45500800 |
| H | -5.04793200 | 5.96625400  | -3.12667300 |
| H | -3.63887800 | 5.40855500  | -4.02032800 |
| C | -5.42774600 | 4.23022900  | -4.36110900 |
| H | -5.76266700 | 4.80441800  | -5.23161600 |
| H | -4.90794300 | 3.33676500  | -4.72949200 |
| H | -6.32050400 | 3.89574800  | -3.81781100 |

UB3LYP-D3/BSII(SMD)//B3LYP-D3/BSI

HF=-2193.9736642



Singlet

Zero-point correction= 0.775141 (Hartree/Particle)

Thermal correction to Energy= 0.823697

Thermal correction to Enthalpy= 0.824642

Thermal correction to Gibbs Free Energy= 0.691212

Sum of electronic and zero-point Energies= -2269.611669

Sum of electronic and thermal Energies= -2269.563113

Sum of electronic and thermal Enthalpies= -2269.562169

Sum of electronic and thermal Free Energies= -2269.695598

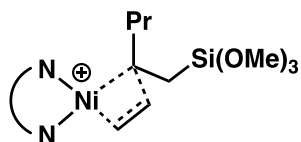
|    |             |             |             |
|----|-------------|-------------|-------------|
| Ni | 0.34492400  | 1.08379400  | -0.33801800 |
| N  | 1.55460300  | -0.52989900 | -0.13043100 |
| N  | -1.14903200 | -0.48338300 | -0.38147400 |
| C  | 2.97197900  | -0.51991700 | 0.09373500  |
| C  | 3.83361700  | -0.73137200 | -0.99581600 |
| C  | 3.43979900  | -0.26032100 | 1.39268500  |
| C  | 5.21093500  | -0.67426300 | -0.75449600 |
| C  | 4.82389400  | -0.20909400 | 1.58670800  |
| C  | 5.70447100  | -0.41250900 | 0.52366900  |
| H  | 5.89816100  | -0.83464100 | -1.58068100 |
| H  | 5.21034900  | -0.00712600 | 2.58198900  |
| H  | 6.77627700  | -0.36570400 | 0.69150200  |
| C  | -2.53233600 | -0.42907600 | -0.75146400 |
| C  | -2.83895800 | -0.53822500 | -2.12305000 |
| C  | -3.52308600 | -0.25314200 | 0.22926900  |
| C  | -4.18254800 | -0.45758700 | -2.49929700 |
| C  | -4.85622900 | -0.17848400 | -0.19720400 |
| C  | -5.18696500 | -0.27593200 | -1.54719900 |
| H  | -4.43983500 | -0.53744100 | -3.55201000 |
| H  | -5.63902300 | -0.05126800 | 0.54587600  |
| H  | -6.22594900 | -0.21694500 | -1.85744400 |
| C  | 2.47107100  | -0.07510600 | 2.53401100  |
| H  | 1.99088200  | -1.02472600 | 2.80542200  |
| H  | 2.97706000  | 0.30919100  | 3.42363500  |
| H  | 1.66979000  | 0.62021400  | 2.26176100  |
| C  | 3.27924600  | -1.03852400 | -2.36508200 |
| H  | 2.78569500  | -2.01878200 | -2.38350800 |
| H  | 2.53089800  | -0.29832500 | -2.66778200 |
| H  | 4.07195600  | -1.04976700 | -3.11763400 |
| C  | -3.18375500 | -0.16054700 | 1.69927100  |
| H  | -2.95608700 | 0.87175700  | 1.99170700  |

|    |             |             |             |
|----|-------------|-------------|-------------|
| H  | -4.02800100 | -0.48865700 | 2.31250900  |
| H  | -2.31833700 | -0.77655100 | 1.96275800  |
| C  | -1.74573500 | -0.73988500 | -3.14350600 |
| H  | -0.98850400 | 0.04487800  | -3.05381300 |
| H  | -1.24828800 | -1.70971900 | -3.01620400 |
| H  | -2.14998200 | -0.70400200 | -4.15857800 |
| C  | -0.57853400 | -1.62691600 | -0.23268100 |
| C  | 0.91127700  | -1.64380500 | -0.01974700 |
| C  | 1.30301000  | 2.38427100  | -2.47065200 |
| H  | 1.17599500  | 1.39273300  | -2.92948000 |
| C  | 1.74815100  | 2.25802000  | -1.00138700 |
| H  | 2.63441500  | 1.61803300  | -0.95111400 |
| Si | -0.19780900 | 3.39059400  | -2.96645000 |
| O  | 0.03549700  | 3.73137600  | -4.56189000 |
| O  | -1.53370000 | 2.46078500  | -2.66895500 |
| O  | -0.44883900 | 4.78347200  | -2.10283900 |
| C  | -0.95972300 | 4.28570600  | -5.42180000 |
| H  | -0.47486300 | 4.56913300  | -6.35953900 |
| H  | -1.74186800 | 3.54741000  | -5.63850500 |
| H  | -1.42445800 | 5.17848500  | -4.98287300 |
| C  | -2.87329200 | 2.95416700  | -2.60436900 |
| H  | -3.30744100 | 3.01591900  | -3.60942800 |
| H  | -3.46470200 | 2.24848300  | -2.01620500 |
| H  | -2.91030800 | 3.94431000  | -2.13662300 |
| C  | 0.23421000  | 6.01847500  | -2.31993500 |
| H  | 0.52072100  | 6.14137400  | -3.37095100 |
| H  | -0.43687600 | 6.83391300  | -2.03589900 |
| H  | 1.13523800  | 6.06844900  | -1.69711400 |
| C  | -2.31392900 | -5.05695800 | -0.23320000 |
| C  | -1.18902300 | -5.81736800 | 0.04959000  |
| C  | 0.08100000  | -5.19865000 | 0.21996000  |
| C  | 0.11466100  | -3.79806100 | 0.08552300  |
| C  | -1.03917200 | -3.01734600 | -0.20418400 |
| C  | -2.26214900 | -3.64509300 | -0.36419400 |
| H  | 1.35356200  | -6.91366100 | 0.62716300  |
| H  | -3.27026100 | -5.55474600 | -0.35981500 |
| H  | -1.27436300 | -6.89658300 | 0.14235000  |
| C  | 1.32047600  | -5.83385200 | 0.51094000  |
| C  | 1.30732300  | -3.03164700 | 0.22253600  |
| H  | -3.16209500 | -3.08339700 | -0.58732000 |
| C  | 2.49979100  | -3.67700200 | 0.50329300  |
| C  | 2.48211300  | -5.08826900 | 0.64683600  |
| H  | 3.42887100  | -3.12953500 | 0.61358600  |
| H  | 3.41431800  | -5.59789800 | 0.86965100  |

|   |             |            |             |
|---|-------------|------------|-------------|
| C | -1.21215100 | 2.65630200 | 0.34028400  |
| H | -2.12298200 | 2.13097500 | 0.07182500  |
| H | -1.00646000 | 3.57491200 | -0.19744700 |
| C | -0.45334500 | 2.27205400 | 1.40529000  |
| H | 0.37197000  | 2.87978800 | 1.75762100  |
| H | -0.74213700 | 1.43651600 | 2.03812200  |
| H | 2.14509000  | 2.83117300 | -3.02672100 |
| C | 2.06113600  | 3.57194400 | -0.30058700 |
| H | 2.60292200  | 4.21550300 | -1.01506500 |
| H | 1.14553500  | 4.12587000 | -0.06289900 |
| C | 2.93746900  | 3.41094900 | 0.94814600  |
| H | 3.89060100  | 2.94986300 | 0.65679900  |
| H | 2.46932300  | 2.69974900 | 1.64012100  |
| C | 3.19478500  | 4.73879900 | 1.66534500  |
| H | 3.83629700  | 4.60298900 | 2.54259800  |
| H | 3.68782600  | 5.45737600 | 0.99960900  |
| H | 2.25573600  | 5.19450900 | 2.00455900  |

UB3LYP-D3/BSII(SMD)/B3LYP-D3/BSI

HF=-2272.5949902



Singlet

Zero-point correction= 0.775273 (Hartree/Particle)

Thermal correction to Energy= 0.823061

Thermal correction to Enthalpy= 0.824005

Thermal correction to Gibbs Free Energy= 0.691488

Sum of electronic and zero-point Energies= -2269.590815

Sum of electronic and thermal Energies= -2269.543027

Sum of electronic and thermal Enthalpies= -2269.542083

Sum of electronic and thermal Free Energies= -2269.674600

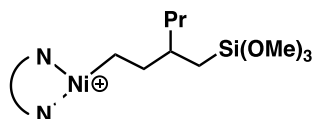
|    |             |             |             |
|----|-------------|-------------|-------------|
| Ni | -0.09790400 | 1.00545500  | -0.04153600 |
| N  | 1.40036700  | -0.59275500 | -0.10777100 |
| N  | -1.28755000 | -0.58925700 | -0.19175600 |
| C  | 2.81699800  | -0.48230700 | 0.00074300  |
| C  | 3.63576300  | -0.64345400 | -1.13372900 |
| C  | 3.33483000  | -0.10617300 | 1.25768100  |
| C  | 5.00851800  | -0.41560900 | -0.97773600 |
| C  | 4.71277600  | 0.10248300  | 1.36446300  |
| C  | 5.54522600  | -0.04570800 | 0.25494900  |
| H  | 5.66053700  | -0.52899200 | -1.83973100 |
| H  | 5.13197500  | 0.38367300  | 2.32665600  |
| H  | 6.61280100  | 0.12831900  | 0.35049500  |
| C  | -2.72160300 | -0.55356100 | -0.24231400 |
| C  | -3.34443600 | -0.38945800 | -1.49044100 |
| C  | -3.43719500 | -0.64663700 | 0.96200100  |
| C  | -4.74220300 | -0.32357600 | -1.51019600 |
| C  | -4.83328100 | -0.57455300 | 0.89379300  |
| C  | -5.48241900 | -0.41462500 | -0.33049700 |
| H  | -5.25079100 | -0.20094700 | -2.46277700 |
| H  | -5.41129900 | -0.64401000 | 1.81132500  |
| H  | -6.56635800 | -0.35891900 | -0.36546400 |
| C  | 2.41699100  | 0.02730500  | 2.44828500  |
| H  | 1.97555600  | -0.93973800 | 2.72017400  |
| H  | 2.95433400  | 0.41110400  | 3.31947400  |
| H  | 1.57979800  | 0.70558600  | 2.23671600  |
| C  | 3.07610000  | -1.07859500 | -2.46770600 |
| H  | 2.95605500  | -2.16885100 | -2.50768200 |
| H  | 2.09235500  | -0.64321800 | -2.66779900 |
| H  | 3.74543900  | -0.79050500 | -3.28293500 |
| C  | -2.71211700 | -0.84659100 | 2.27065200  |
| H  | -1.88446600 | -0.13525300 | 2.38374400  |

|    |             |             |             |
|----|-------------|-------------|-------------|
| H  | -3.38973300 | -0.72630100 | 3.12006400  |
| H  | -2.27414600 | -1.85146800 | 2.33197600  |
| C  | -2.52017300 | -0.30815000 | -2.75170600 |
| H  | -1.76896100 | 0.48806400  | -2.69138000 |
| H  | -1.98363800 | -1.24804300 | -2.93604600 |
| H  | -3.15471000 | -0.11493900 | -3.62137700 |
| C  | -0.68543700 | -1.72698600 | -0.27775800 |
| C  | 0.81523900  | -1.73349200 | -0.20399600 |
| C  | 1.63186100  | 2.38527700  | -1.81898300 |
| H  | 1.48806800  | 1.34077900  | -2.12166800 |
| C  | 1.51704700  | 2.53031400  | -0.30225600 |
| H  | 2.04698200  | 1.72452300  | 0.20390100  |
| Si | 0.53636600  | 3.39503200  | -2.94254400 |
| O  | 1.21372500  | 3.38303400  | -4.44351500 |
| O  | -0.96226200 | 2.67587000  | -2.96588000 |
| O  | 0.38327100  | 4.93630000  | -2.36258700 |
| C  | 0.49511000  | 3.37686200  | -5.67542100 |
| H  | 1.19106100  | 3.09865000  | -6.47111900 |
| H  | -0.32790500 | 2.65189200  | -5.65283300 |
| H  | 0.08888600  | 4.37196900  | -5.89968800 |
| C  | -2.18083400 | 3.37896400  | -3.19714400 |
| H  | -2.27884300 | 3.67060200  | -4.25070300 |
| H  | -3.00942800 | 2.71000000  | -2.94565000 |
| H  | -2.24590400 | 4.27728100  | -2.57136200 |
| C  | 0.32164800  | 6.12560500  | -3.15083800 |
| H  | 0.99793900  | 6.06659800  | -4.01119200 |
| H  | -0.70105300 | 6.30039900  | -3.50883100 |
| H  | 0.62102800  | 6.96650600  | -2.51971200 |
| C  | -2.37999600 | -5.16320800 | -0.58190700 |
| C  | -1.22349700 | -5.92727900 | -0.53686600 |
| C  | 0.05149800  | -5.30672700 | -0.41752000 |
| C  | 0.05689400  | -3.90057700 | -0.35566500 |
| C  | -1.13067400 | -3.11546800 | -0.39636800 |
| C  | -2.35771700 | -3.74631400 | -0.50963700 |
| H  | 1.37679900  | -7.02983800 | -0.39237300 |
| H  | -3.33984200 | -5.66204800 | -0.67282700 |
| H  | -1.28772600 | -7.01056600 | -0.59117800 |
| C  | 1.32092800  | -5.94562100 | -0.34868900 |
| C  | 1.24877300  | -3.13260300 | -0.23516200 |
| H  | -3.28365300 | -3.18358500 | -0.54288900 |
| C  | 2.46932800  | -3.78062200 | -0.16715600 |
| C  | 2.48266000  | -5.19819800 | -0.22463400 |
| H  | 3.39822700  | -3.22893500 | -0.07307600 |
| H  | 3.43811100  | -5.71069600 | -0.17116600 |

|   |             |            |             |
|---|-------------|------------|-------------|
| C | -1.61928900 | 2.22794500 | 0.24480100  |
| H | -2.09529200 | 1.86281700 | 1.15405200  |
| H | -2.23058900 | 2.17382400 | -0.65291000 |
| C | -0.59766400 | 3.18675800 | 0.32997000  |
| H | -0.46631000 | 3.90261300 | -0.47004700 |
| H | -0.25733200 | 3.50774800 | 1.30677100  |
| H | 2.66926800  | 2.62381900 | -2.10385000 |
| C | 2.07990600  | 3.82761300 | 0.27530100  |
| H | 3.02291200  | 4.00993200 | -0.26517700 |
| H | 1.45467100  | 4.69787600 | 0.04818700  |
| C | 2.40882800  | 3.75550700 | 1.77292600  |
| H | 3.12675900  | 2.93978000 | 1.93573400  |
| H | 1.51307300  | 3.48674300 | 2.34983000  |
| C | 2.98632000  | 5.06888000 | 2.30864700  |
| H | 3.23256100  | 4.99132600 | 3.37291200  |
| H | 3.90219100  | 5.34392000 | 1.77202600  |
| H | 2.27166900  | 5.89191600 | 2.18879900  |

UB3LYP-D3/BSII(SMD)//B3LYP-D3/BSI

HF=-2272.5734439



Singlet

Zero-point correction= 0.776026 (Hartree/Particle)

Thermal correction to Energy= 0.824269

Thermal correction to Enthalpy= 0.825213

Thermal correction to Gibbs Free Energy= 0.689601

Sum of electronic and zero-point Energies= -2269.620097

Sum of electronic and thermal Energies= -2269.571854

Sum of electronic and thermal Enthalpies= -2269.570910

Sum of electronic and thermal Free Energies= -2269.706522

|    |             |             |             |
|----|-------------|-------------|-------------|
| Ni | -0.09902200 | 0.69515900  | 0.16910300  |
| N  | 1.36668400  | -0.73601300 | 0.13244800  |
| N  | -1.28726700 | -0.76044800 | -0.04412500 |
| C  | 2.76416900  | -0.47566900 | 0.17074100  |
| C  | 3.52878500  | -0.53926000 | -1.01203000 |
| C  | 3.29410400  | 0.00085000  | 1.38743400  |
| C  | 4.86498400  | -0.12689200 | -0.93943100 |
| C  | 4.63474100  | 0.39283000  | 1.40990500  |
| C  | 5.41661300  | 0.33261700  | 0.25566600  |
| H  | 5.47280100  | -0.15727900 | -1.83961600 |
| H  | 5.06550300  | 0.75065800  | 2.34096700  |
| H  | 6.45441700  | 0.65055500  | 0.28621800  |
| C  | -2.71374400 | -0.67407800 | -0.15008800 |
| C  | -3.28346600 | -0.49190600 | -1.42141700 |
| C  | -3.46967100 | -0.72322300 | 1.03146600  |
| C  | -4.67779900 | -0.39435400 | -1.48887000 |
| C  | -4.85969600 | -0.61900600 | 0.91409300  |
| C  | -5.46032200 | -0.46148000 | -0.33524600 |
| H  | -5.14994000 | -0.25902100 | -2.45815600 |
| H  | -5.47073100 | -0.65748600 | 1.81170500  |
| H  | -6.54082300 | -0.38225900 | -0.40964900 |
| C  | 2.43731700  | 0.04481800  | 2.62934100  |
| H  | 2.14282000  | -0.96283100 | 2.94804600  |
| H  | 2.96881300  | 0.51973900  | 3.45829200  |
| H  | 1.50620500  | 0.60220400  | 2.46031900  |
| C  | 2.93030700  | -0.99254600 | -2.32272700 |
| H  | 2.78929800  | -2.07969800 | -2.35285000 |
| H  | 1.95039700  | -0.53476100 | -2.49782300 |
| H  | 3.58033000  | -0.72060400 | -3.15846200 |
| C  | -2.78421500 | -0.88262900 | 2.36550500  |
| H  | -1.98793800 | -0.13634800 | 2.48588800  |
| H  | -3.49251200 | -0.76948300 | 3.19032600  |

|    |             |             |             |
|----|-------------|-------------|-------------|
| H  | -2.31209000 | -1.86902500 | 2.46069700  |
| C  | -2.41742400 | -0.38730900 | -2.65322500 |
| H  | -1.77646200 | 0.50307500  | -2.61495900 |
| H  | -1.76313700 | -1.26037700 | -2.76550400 |
| H  | -3.03178600 | -0.31456900 | -3.55473000 |
| C  | -0.67708200 | -1.89635000 | -0.15514300 |
| C  | 0.82542700  | -1.88633000 | -0.06871100 |
| C  | 1.17832200  | 2.35831100  | -1.64352400 |
| H  | 0.69098200  | 1.39124000  | -1.84900000 |
| C  | 1.04857100  | 2.76478100  | -0.14925400 |
| H  | 1.35689500  | 1.88598600  | 0.48627300  |
| Si | 0.39664800  | 3.47810200  | -2.91820100 |
| O  | 1.20635200  | 3.25538000  | -4.33651300 |
| O  | -1.17760500 | 2.97478400  | -3.07476400 |
| O  | 0.43728800  | 5.05417900  | -2.42502600 |
| C  | 0.62176000  | 3.35718500  | -5.63401200 |
| H  | 1.28044500  | 2.84856000  | -6.34314600 |
| H  | -0.36748500 | 2.88391100  | -5.66331600 |
| H  | 0.52463500  | 4.40712000  | -5.93902800 |
| C  | -2.31068900 | 3.82438400  | -3.22902100 |
| H  | -2.48541400 | 4.05006100  | -4.28866200 |
| H  | -3.18645900 | 3.30023000  | -2.83393000 |
| H  | -2.18364300 | 4.76511800  | -2.68026000 |
| C  | 0.58390600  | 6.18394600  | -3.28540300 |
| H  | 1.36122700  | 6.01163300  | -4.03903600 |
| H  | -0.36173000 | 6.41586700  | -3.79264600 |
| H  | 0.86950100  | 7.04152600  | -2.67056000 |
| C  | -2.32241900 | -5.32052100 | -0.69500200 |
| C  | -1.15297800 | -6.06702800 | -0.71618100 |
| C  | 0.11437000  | -5.43806700 | -0.56050000 |
| C  | 0.09850500  | -4.04164900 | -0.39089200 |
| C  | -1.10306500 | -3.27496500 | -0.36507400 |
| C  | -2.32175900 | -3.91294300 | -0.51868200 |
| H  | 1.46837900  | -7.13489000 | -0.68281000 |
| H  | -3.27463000 | -5.82734200 | -0.81617000 |
| H  | -1.20177300 | -7.14387500 | -0.85246400 |
| C  | 1.39543000  | -6.05837200 | -0.55537500 |
| C  | 1.28062600  | -3.26594200 | -0.22521400 |
| H  | -3.25480200 | -3.36051000 | -0.50579300 |
| C  | 2.51252700  | -3.89454300 | -0.22392700 |
| C  | 2.54751200  | -5.30324000 | -0.38990700 |
| H  | 3.43249600  | -3.33224100 | -0.10211100 |
| H  | 3.51126400  | -5.80267600 | -0.38902100 |
| C  | -1.38374300 | 2.08866100  | 0.13315300  |

|   |             |            |             |
|---|-------------|------------|-------------|
| H | -2.09574200 | 1.97979900 | 0.95716200  |
| H | -1.89924900 | 2.05253400 | -0.82959600 |
| C | -0.38516000 | 3.23088000 | 0.27207600  |
| H | -0.64890500 | 4.10872400 | -0.33091600 |
| H | -0.34073400 | 3.55444500 | 1.31533500  |
| H | 2.23565400  | 2.20143500 | -1.88284200 |
| C | 2.12631300  | 3.80438700 | 0.23267900  |
| H | 3.07845700  | 3.48059800 | -0.20821600 |
| H | 1.85670400  | 4.75151700 | -0.25211300 |
| C | 2.33854500  | 4.00778700 | 1.73740400  |
| H | 2.53277500  | 3.03248500 | 2.20775200  |
| H | 1.42826600  | 4.40356500 | 2.20432000  |
| C | 3.50805400  | 4.95455800 | 2.02821400  |
| H | 3.64689900  | 5.09592700 | 3.10530600  |
| H | 4.44483000  | 4.55989000 | 1.61636600  |
| H | 3.33705100  | 5.94054600 | 1.58036000  |

UB3LYP-D3/BSII(SMD)//B3LYP-D3/BSI

HF=-2272.6053804