

## Supporting Information

### **Mechanistic insight into aryl-nickel-catalyzed benzylic dehydrogenation of electron-deficient heteroarenes by using DFT calculations**

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## I. Complete Gaussian 09 Reference

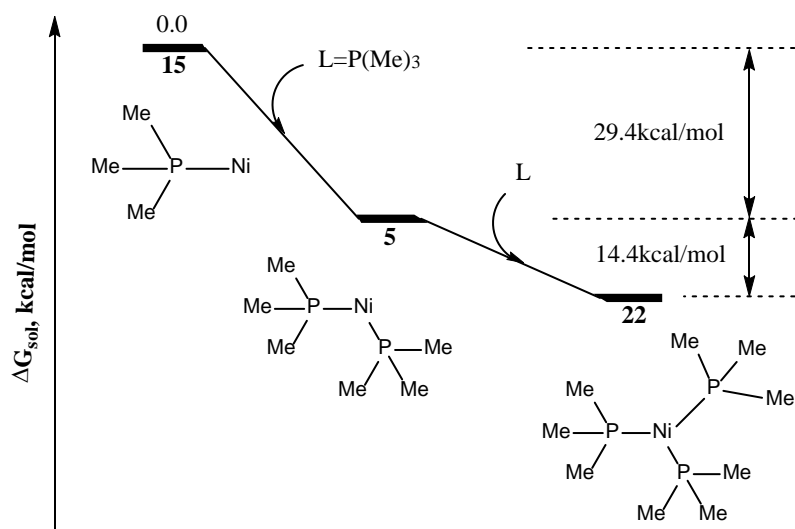
Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, J. A., Jr.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, J. M.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, Ö.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. Gaussian 09, revision D.01; Gaussian, Inc.: Wallingford, CT, 2010.

## II. Influence of dispersion correction and solvent on barrier in optimization

**Table S1.** Comparison of relative free energy barriers for selected key transition state optimized in gas phases without dispersion correction and in solvent phases with dispersion correction. The optimizations were performed using B3LYP/6-31G\*\*/Lan12dz method and single point energy corrections were added using M06/6-311++G\*\*/SDD method.

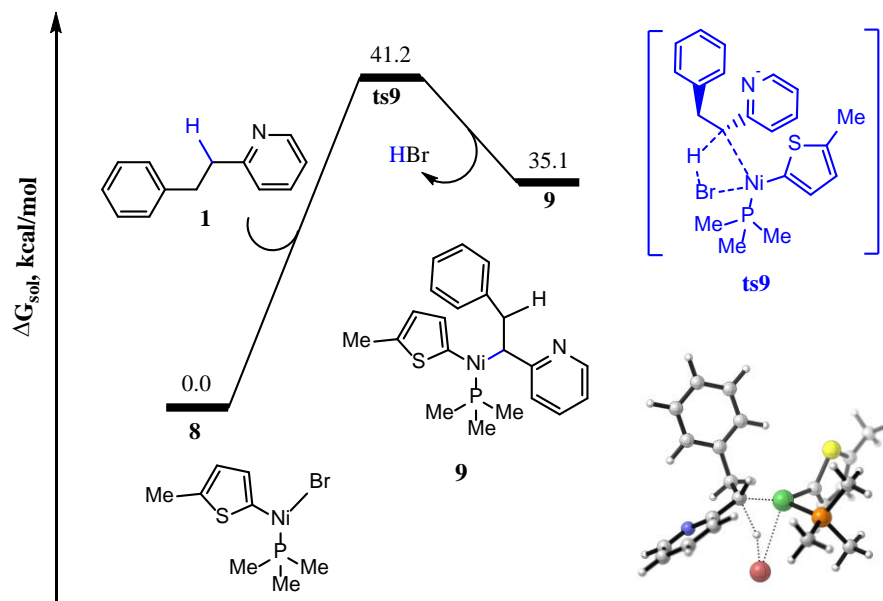
Selected transition state	Optimized in gas phase without dispersion correction ( <i>kcal/mol</i> )	Optimized in solvent phase with dispersion correction ( <i>kcal/mol</i> )
ts1	32.9	34.6
ts4	9.6	10.3
ts6	57.4	51.9
ts8	5.7	7.5

### III. The possible forms of nickel catalysts in this system



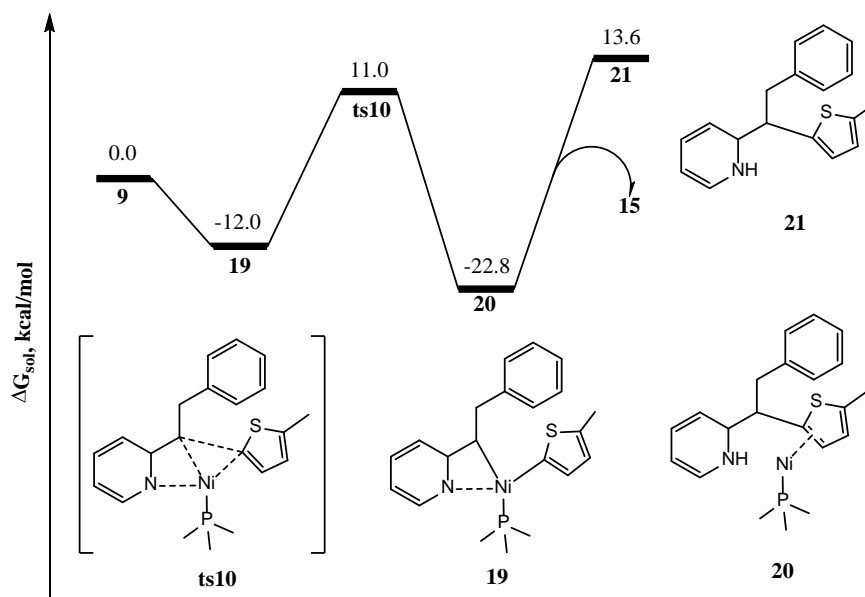
**Figure S1.** Comparison of the free energy of several possible nickel catalyst species

#### IV. Formation mechanism of species **9** without the participation of zinc salt



**Figure S2.** Reaction energy profile for the formation mechanism of species **9** without the participation of zinc salt

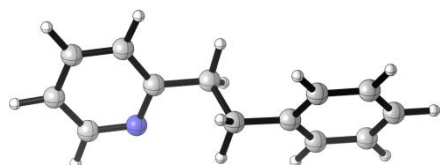
V. Possible competitive mechanism (reductive elimination) of  $\beta$ -hydride elimination



**Figure S3.** Reaction energy profile for possible competitive mechanism (reductive elimination) of  $\beta$ -hydride elimination

## VI. Cartesian Coordinates

1



B3LYP electronic energy: -557.9895753 a.u.  
B3LYP enthalpy: -557.750287 a.u.  
B3LYP free energy: -557.803090 a.u.  
M06 SCF energy in solution: -557.676868136 a.u.  
M06 enthalpy in solution: -557.437580136 a.u.  
M06 free energy in solution: -557.490383136 a.u.

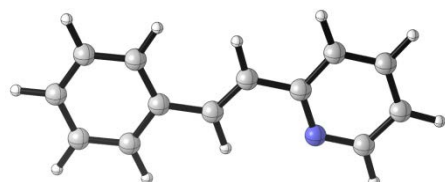
### Cartesian coordinates

ATOM	X	Y	Z
C	-0.44758500	-0.20371300	0.61088500
H	-0.18182100	0.54120400	1.36999800
C	-3.68503500	1.23765600	-0.31314000
C	-4.60633600	0.19327100	-0.22228600
C	-4.13748200	-1.05932700	0.16759800
C	-2.78050000	-1.21085900	0.44673300
C	-1.93006000	-0.10379500	0.33116300
N	-2.38192400	1.10568200	-0.04655500
H	-4.81507300	-1.90411500	0.25372300
H	-4.01185300	2.23203200	-0.61368400
H	-5.65397300	0.36166000	-0.44988600
H	-2.38069400	-2.17240500	0.75433600
C	0.41001800	0.05469300	-0.65175000
H	0.11283500	1.02430000	-1.06399800
H	0.16797800	-0.70161100	-1.40781500
C	1.89452300	0.03687600	-0.36154000
C	2.54797100	1.19083700	0.09332900
C	2.64496700	-1.13743200	-0.50589000
C	3.90935400	1.17214800	0.39646900
H	1.98243500	2.11300900	0.20492600
C	4.00735700	-1.16150300	-0.20436100
H	2.15645900	-2.04086900	-0.86390800
C	4.64432600	-0.00568000	0.24914200
H	4.39768200	2.07866700	0.74311700



H	4.57163400	-2.08174900	-0.32756000
H	5.70519300	-0.02099200	0.48157500
H	-0.20645100	-1.18793700	1.02695100

2



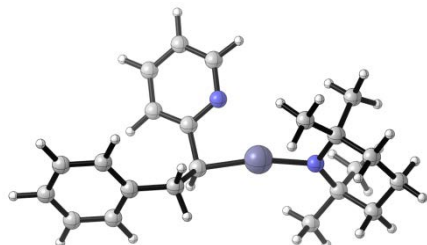
B3LYP electronic energy:	-556.7678206 a.u.
B3LYP enthalpy:	-556.552491 a.u.
B3LYP free energy:	-556.603288 a.u.
M06 SCF energy in solution:	-556.455757474 a.u.
M06 enthalpy in solution:	-556.240427474 a.u.
M06 free energy in solution:	-556.291224474 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	-0.51939900	-0.55929700	-0.00006100
C	-3.62921500	1.32923100	-0.00008500
C	-4.63803600	0.36129600	0.00002400
C	-4.25526500	-0.97870600	0.00010000
C	-2.89896400	-1.28900400	0.00006300
C	-1.95220200	-0.24856500	-0.00007000
N	-2.32664400	1.04943300	-0.00010200
H	-5.00001500	-1.76949000	0.00020200
H	-3.88890800	2.38705300	-0.00006200
H	-5.68271500	0.65441000	0.00006500
H	-2.56489000	-2.32235100	0.00017000
C	0.45187700	0.37472100	0.00003700
H	0.12709500	1.41308300	0.00001500
C	1.89897100	0.15522700	0.00003000
C	2.74983000	1.27637800	0.00007100
C	2.49386300	-1.12224600	-0.00005600
C	4.13554900	1.13285300	0.00006500
H	2.30954100	2.26997100	0.00012300
C	3.87697200	-1.26627600	-0.00005700
H	1.86881900	-2.00977200	-0.00013500
C	4.70621800	-0.14017800	0.00000800
H	4.76937600	2.01493200	0.00008100
H	4.31334500	-2.26108800	-0.00011500
H	5.78589400	-0.25681200	0.00002300

H -0.27222000 -1.61857800 -0.00006900

3



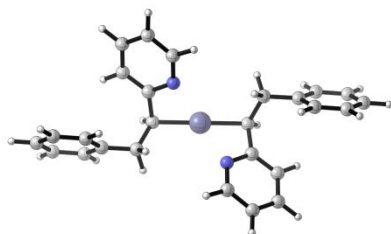
B3LYP electronic energy: -1031.5322184 a.u.  
B3LYP enthalpy: -1031.031644 a.u.  
B3LYP free energy: -1031.117881 a.u.  
M06 SCF energy in solution: -1192.62827997 a.u.  
M06 enthalpy in solution: -1192.12770497 a.u.  
M06 free energy in solution: -1192.21394297 a.u.

#### Cartesian coordinates

ATOM	X	Y	Z
C	-1.33086900	-0.42929400	-0.47806300
Zn	0.70230700	-0.15707400	-0.19217500
H	-1.61424300	-0.92804500	-1.41308300
C	-0.84042300	3.18892500	-0.19219800
C	-2.01337600	3.78604800	-0.64303100
C	-3.04898500	2.95475600	-1.07574800
C	-2.88056300	1.57321700	-1.03277900
C	-1.66932800	1.03751800	-0.56390200
N	-0.66881000	1.85905700	-0.15949900
H	-3.97897700	3.38100800	-1.44219300
H	0.00205900	3.78879900	0.14411100
H	-2.10707300	4.86678100	-0.66311700
H	-3.67145900	0.90579900	-1.35531900
C	-2.03327000	-1.17556800	0.69417700
H	-1.61669100	-2.18937800	0.74133800
H	-1.77770300	-0.69492600	1.64702200
C	-3.54449200	-1.27452700	0.58578400
C	-4.13843900	-2.14227400	-0.34436200
C	-4.38557900	-0.49460200	1.39073500
C	-5.52498700	-2.22421900	-0.46927800
H	-3.50414200	-2.76281700	-0.97383700
C	-5.77534200	-0.57340300	1.27142400
H	-3.94500300	0.17990700	2.12108300
C	-6.35030500	-1.43777000	0.33946300

H	-5.96311400	-2.90689500	-1.19249600
H	-6.40743400	0.03909600	1.90885900
H	-7.43062300	-1.50318500	0.24596900
N	2.60873600	-0.30379800	0.04192700
C	4.54079800	-1.85544000	-0.20814600
C	3.39676600	-1.08996400	-0.92310500
C	3.29032900	0.51790500	1.05772700
C	4.44496100	-0.27347200	1.72705400
C	5.36697400	-0.95474000	0.71323900
H	4.09089200	-2.65323500	0.39814800
H	5.18275900	-2.34258700	-0.95350600
H	5.01595700	0.39526400	2.38422900
H	4.00204800	-1.04872800	2.36679800
H	5.91591500	-0.20608500	0.12761900
H	6.12794200	-1.54758800	1.23570000
C	3.97674600	-0.24527100	-2.09160700
H	4.41991500	-0.88810600	-2.86244600
H	3.17939300	0.34499400	-2.55584700
H	4.75218500	0.44990900	-1.76434300
C	2.26024600	0.85519600	2.15527200
H	2.71762900	1.42821500	2.96932600
H	1.44058300	1.46779200	1.75631100
H	1.84003000	-0.06273000	2.58222100
C	2.46007200	-2.13654800	-1.55835900
H	1.65713500	-1.65433700	-2.13547900
H	3.00139800	-2.78386200	-2.25652000
H	2.00485600	-2.76817300	-0.78779800
C	3.82487600	1.87076600	0.51135700
H	3.02719600	2.39737000	-0.02311700
H	4.17657600	2.51523300	1.32676700
H	4.65845300	1.74247500	-0.18208400

4



B3LYP electronic energy: -1180.324118 a.u.  
 B3LYP enthalpy: -1179.866474 a.u.  
 B3LYP free energy: -1179.956816 a.u.  
 M06 SCF energy in solution: -1341.33893416 a.u.

M06 enthalpy in solution: -1340.88129016 a.u.

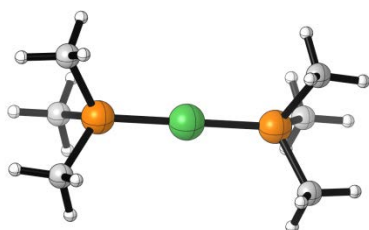
M06 free energy in solution: -1340.97163216 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	-2.08619100	0.03460500	-0.93243700
Zn	0.00000000	0.00007200	-0.72738000
H	-2.51981600	0.09662300	-1.93738300
C	-1.16741300	2.87445100	1.18348900
C	-2.24811200	3.75086300	1.16505800
C	-3.36581100	3.39915400	0.40419000
C	-3.36804600	2.19232400	-0.28941200
C	-2.24288100	1.35193300	-0.22534600
N	-1.15673000	1.71902900	0.50330500
H	-4.22818100	4.05897000	0.35772200
H	-0.26671100	3.10769900	1.74674600
H	-2.20909700	4.68288500	1.71918900
H	-4.22809000	1.88701800	-0.87492700
C	-2.76164100	-1.15236200	-0.18467000
H	-2.48989200	-2.07761500	-0.70771500
H	-2.34455700	-1.23759800	0.82668400
C	-4.27447300	-1.07100500	-0.08756000
C	-5.07877000	-1.35885000	-1.20165400
C	-4.90995500	-0.68282500	1.09990000
C	-6.46824100	-1.26051500	-1.13285600
H	-4.60638100	-1.66760700	-2.13186400
C	-6.30131700	-0.58264000	1.17541900
H	-4.30617000	-0.46082500	1.97675500
C	-7.08634500	-0.87057800	0.05852100
H	-7.07062900	-1.49462500	-2.00672900
H	-6.77090700	-0.28264500	2.10857100
H	-8.16876800	-0.79687100	0.11505700
C	2.08620400	-0.03446900	-0.93231600
H	2.51980400	-0.09646100	-1.93727700
C	1.16724100	-2.87452100	1.18325900
C	2.24795000	-3.75092200	1.16486100
C	3.36572500	-3.39913000	0.40414300
C	3.36801700	-2.19223600	-0.28934800
C	2.24283600	-1.35186200	-0.22532500
N	1.15661900	-1.71903400	0.50318700
H	4.22810900	-4.05892900	0.35770400
H	0.26647700	-3.10783200	1.74639200
H	2.20888800	-4.68299600	1.71890000
H	4.22811600	-1.88688000	-0.87475700

C	2.76173200	1.15243300	-0.18452000
H	2.49001400	2.07770900	-0.70753700
H	2.34467300	1.23765800	0.82684300
C	4.27455900	1.07100200	-0.08746300
C	5.07883100	1.35906100	-1.20152100
C	4.91006300	0.68251600	1.09988500
C	6.46829900	1.26063900	-1.13279700
H	4.60641700	1.66805200	-2.13164000
C	6.30142300	0.58224500	1.17533100
H	4.30630100	0.46034900	1.97671400
C	7.08642500	0.87040000	0.05847100
H	7.07066700	1.49491600	-2.00663800
H	6.77103100	0.28201700	2.10839900
H	8.16884600	0.79662600	0.11495200

5



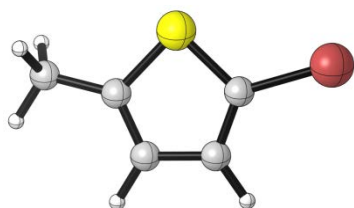
B3LYP electronic energy: -1091.5479367 a.u.  
 B3LYP enthalpy: -1091.302258 a.u.  
 B3LYP free energy: -1091.363370 a.u.  
 M06 SCF energy in solution: -1093.04565715 a.u.  
 M06 enthalpy in solution: -1092.79997815 a.u.  
 M06 free energy in solution: -1092.86109015 a.u.

Cartesian coordinates

ATOM	X	Y	Z
Ni	0.00014500	0.00012300	0.00061700
P	-2.14475000	-0.00010400	-0.00082100
C	-2.99751000	0.30692900	1.62283900
H	-4.08893300	0.28724700	1.52397100
H	-2.68976300	-0.45509400	2.34408400
H	-2.69148500	1.28117200	2.01376600
C	-3.00530500	1.25063600	-1.07464200
H	-2.70607500	1.10315700	-2.11604900
H	-4.09615600	1.17236300	-1.00077900
H	-2.69798300	2.25700700	-0.77715400
C	-3.00291500	-1.55769500	-0.54465400
H	-4.09407200	-1.45826300	-0.51134200

H	-2.69749400	-1.80333600	-1.56550100
H	-2.69925600	-2.38444000	0.10361700
P	2.14507100	0.00058000	-0.00022100
C	3.00034500	1.39195700	-0.88884100
H	4.09151400	1.30436800	-0.83570600
H	2.69257100	1.39604100	-1.93809400
H	2.69632600	2.34497700	-0.44721700
C	3.00523600	0.07179800	1.64713600
H	2.69935100	-0.78582700	2.25254400
H	4.09623500	0.06454800	1.54108600
H	2.70345700	0.97995200	2.17639700
C	2.99944600	-1.46455000	-0.76226900
H	4.09083000	-1.37651300	-0.71128200
H	2.68951600	-2.37526900	-0.24242200
H	2.69676700	-1.55711300	-1.80899000

6



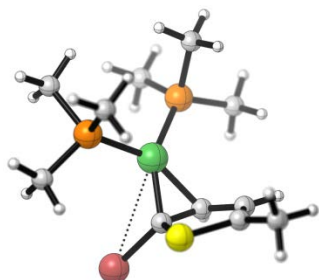
B3LYP electronic energy: -604.8751531 a.u.  
 B3LYP enthalpy: -604.782352 a.u.  
 B3LYP free energy: -604.823763 a.u.  
 M06 SCF energy in solution: -604.9532996 a.u.  
 M06 enthalpy in solution: -604.8604986 a.u.  
 M06 free energy in solution: -604.9019096 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	0.24751400	0.26473200	0.00019300
C	-0.35545200	1.48629600	-0.00015200
C	-1.78198200	1.36840900	0.00008200
C	-2.23960100	0.07859100	-0.00014400
S	-0.89446600	-1.04715100	-0.00005200
H	0.18363100	2.42521900	-0.00026500
H	-2.44891400	2.22421600	0.00022900
C	-3.65702400	-0.41087100	0.00005600
H	-3.88108700	-1.02069800	-0.88243100
H	-3.88208500	-1.01662900	0.88509400
H	-4.33859600	0.44437500	-0.00230100

Br 2.15422200 -0.08642900 0.00000900

7



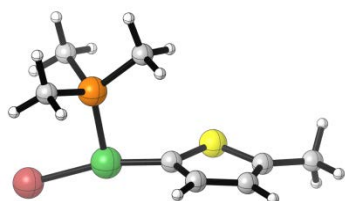
B3LYP electronic energy: -1696.4597147 a.u.  
B3LYP enthalpy: -1696.118948 a.u.  
B3LYP free energy: -1696.202034 a.u.  
M06 SCF energy in solution: -1698.05570577 a.u.  
M06 enthalpy in solution: -1697.71493877 a.u.  
M06 free energy in solution: -1697.79802477 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	1.42865900	-0.20791600	0.35439700
C	0.85369000	-1.42780400	0.84784200
C	1.16795200	-2.54678100	-0.03435400
C	1.96623700	-2.25301600	-1.08952100
S	2.43804400	-0.53888400	-1.09983400
H	0.68969200	-1.59047100	1.90970900
H	0.81139200	-3.55690300	0.15052700
Ni	-0.47342800	-0.06171400	0.17125700
Br	2.25874200	1.10226000	1.68920600
P	-2.47494000	-0.97876800	0.56544200
C	-2.50430700	-2.64941100	1.36887500
H	-3.52563600	-3.01345900	1.52427800
H	-1.96123100	-3.36014100	0.74020000
H	-1.99317300	-2.59688500	2.33418500
C	-3.60033700	-0.03188100	1.69727200
H	-3.80024400	0.95661100	1.27542200
H	-4.55098100	-0.55146900	1.85869400
H	-3.10412900	0.10965400	2.66163700
C	-3.59217200	-1.28881000	-0.88611300
H	-4.53923500	-1.74826800	-0.58283500
H	-3.80484000	-0.34769700	-1.40122800
H	-3.08736400	-1.95254100	-1.59404600
P	-0.78474600	1.82846600	-0.99419000
C	0.48058200	3.17283400	-0.86840300

H	0.27243900	3.98562900	-1.57258600
H	0.49667600	3.56766500	0.15019300
H	1.46951600	2.75742600	-1.07463200
C	-0.74257500	1.46108400	-2.81101400
H	-1.56331200	0.78611600	-3.07009700
H	-0.82394100	2.37196100	-3.41394700
H	0.19893400	0.95566700	-3.04285000
C	-2.34649900	2.82923900	-0.86386000
H	-2.35084900	3.66810000	-1.56814600
H	-3.21669100	2.19762800	-1.06639000
H	-2.44251300	3.22405200	0.15199600
C	2.43121700	-3.16094000	-2.18717600
H	2.10552600	-4.18609800	-1.98611300
H	2.02777700	-2.86596000	-3.16399800
H	3.52412200	-3.16461300	-2.27648500

8



B3LYP electronic energy:	-1235.372981 a.u.
B3LYP enthalpy:	-1235.153775 a.u.
B3LYP free energy:	-1235.219662 a.u.
M06 SCF energy in solution:	-1237.03262984 a.u.
M06 enthalpy in solution:	-1236.81342384 a.u.
M06 free energy in solution:	-1236.87931084 a.u.

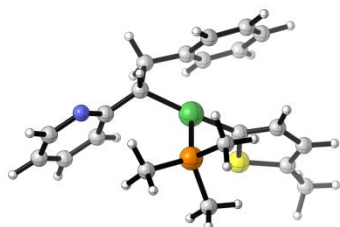
Cartesian coordinates

ATOM	X	Y	Z
Ni	-0.51316600	-0.56046100	0.13438200
Br	-2.69520700	-1.44484000	-0.06817900
P	-0.96803200	1.52634200	-0.03456300
C	0.38400000	2.76818600	0.02018900
H	-0.02937000	3.77739900	-0.07583100
H	0.92751400	2.67738000	0.96233500
H	1.08735300	2.57896200	-0.79325900
C	-1.84605300	1.88556500	-1.60896600
H	-2.72714700	1.24446400	-1.67189900
H	-2.13715300	2.94022500	-1.65478100
H	-1.18900900	1.65613400	-2.45167600
C	-2.12212200	2.05334500	1.29584200
H	-2.40887300	3.10165000	1.16199500



H	-3.00505900	1.41227000	1.26707700
H	-1.63701800	1.93429400	2.26787100
C	1.30570200	-0.29245900	0.36105800
C	2.04589500	-0.24043700	1.52349700
S	2.39542000	-0.36174800	-1.01576400
C	3.45859200	-0.31262300	1.31689400
H	1.59618400	-0.16566300	2.50893700
C	3.82477800	-0.37867700	-0.00331200
H	4.18417400	-0.32308800	2.12464300
C	5.20287600	-0.49770600	-0.58237200
H	5.94792400	-0.43872700	0.21638100
H	5.34580800	-1.45208000	-1.10263600
H	5.41731600	0.30075700	-1.30188400

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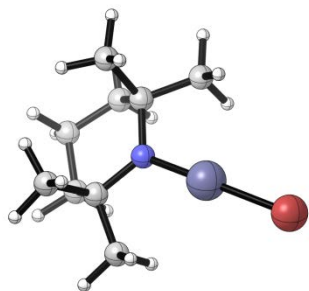


B3LYP electronic energy: -1779.5069362 a.u.  
 B3LYP enthalpy: -1779.062715 a.u.  
 B3LYP free energy: -1779.151485 a.u.  
 M06 SCF energy in solution: -1780.70373401 a.u.  
 M06 enthalpy in solution: -1780.25951301 a.u.  
 M06 free energy in solution: -1780.34828201 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	-1.69698300	-0.55976100	-0.08481700
C	-2.81033200	-0.73589500	-0.87751100
C	-3.96799900	-1.25636700	-0.20832400
C	-3.77021700	-1.50699900	1.12220400
S	-2.11847900	-1.08855900	1.54485100
H	-2.82014000	-0.47965400	-1.93383700
H	-4.91984200	-1.43582500	-0.70123900
C	-4.74728500	-2.03337500	2.13114500
H	-4.40077300	-2.96441700	2.59605500
H	-4.92945000	-1.31737800	2.94201300
H	-5.70797100	-2.23991400	1.64916100
Ni	0.07181600	0.20128700	-0.33281100
P	0.74125600	-1.69252400	-1.15983200
C	0.10545500	-1.83766600	-2.88692900

H	0.39471900	-2.79827700	-3.32569300
H	-0.98285800	-1.75642000	-2.87309400
H	0.51440000	-1.02858200	-3.49751900
C	2.53498000	-2.06426700	-1.36561800
H	2.99551200	-2.20710300	-0.38514200
H	2.66034300	-2.97838100	-1.95542400
H	3.04838100	-1.23152500	-1.84931600
C	0.13586700	-3.23958100	-0.36039200
H	0.51174300	-4.11407700	-0.90177800
H	0.48594800	-3.28016600	0.67410200
H	-0.95424000	-3.24235700	-0.35113400
C	5.19567000	0.04699900	0.24706100
C	5.24392800	-0.32103700	1.58998100
C	4.07454100	-0.17326100	2.34182900
C	2.93580800	0.32934800	1.72617300
C	2.97159900	0.68674800	0.35860200
N	4.10797400	0.53665600	-0.36092800
H	4.05271900	-0.45064300	3.39265800
H	6.08217000	-0.05323300	-0.37888700
H	6.15889900	-0.70685700	2.02794900
H	2.01326800	0.43952200	2.28886700
C	1.78450300	1.22689800	-0.34843100
H	2.08194000	1.46302700	-1.37441700
C	1.14983000	2.46240100	0.32946700
H	1.25011000	2.40245700	1.41759400
H	1.66187900	3.38880000	0.02593100
C	-0.33171300	2.55882900	-0.01747300
C	-1.31815400	2.65710800	0.98068200
C	-0.74192400	2.61405500	-1.36653600
C	-2.66084900	2.82214800	0.64891100
H	-1.02008700	2.60992900	2.02484200
C	-2.08729700	2.78280900	-1.69818100
H	0.00673400	2.57262100	-2.15273900
C	-3.04751200	2.88692800	-0.69144000
H	-3.40679300	2.89109400	1.43485400
H	-2.38327200	2.83784600	-2.74196000
H	-4.09465800	3.01531800	-0.94919400



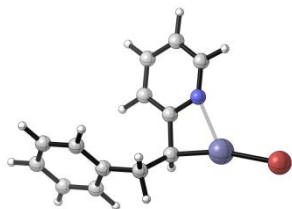
B3LYP electronic energy: -487.3888414 a.u.  
 B3LYP enthalpy: -487.113489 a.u.  
 B3LYP free energy: -487.172063 a.u.  
 M06 SCF energy in solution: -648.959480017 a.u.  
 M06 enthalpy in solution: -648.684127017 a.u.  
 M06 free energy in solution: -648.742701017 a.u.

Cartesian coordinates

ATOM	X	Y	Z
Zn	1.00439400	-0.00003000	0.03541800
N	-0.87855400	-0.00013000	0.05220300
C	-2.78168200	-1.25661800	-0.90967300
C	-1.59838900	-1.28618100	0.09189700
C	-1.59796700	1.28616900	0.09186800
C	-2.78118600	1.25699400	-0.90975800
C	-3.64603900	0.00036100	-0.76389600
H	-2.37027400	-1.28201600	-1.92740000
H	-3.38975600	-2.16135000	-0.78631200
H	-3.38892600	2.16197500	-0.78658500
H	-2.36967700	1.28209500	-1.92745600
H	-4.16105600	0.00050200	0.20493800
H	-4.43416300	0.00047500	-1.52586100
C	-2.09584000	-1.67327000	1.50862400
H	-2.48019700	-2.69982700	1.51923000
H	-1.27106300	-1.60935300	2.22602900
H	-2.89642500	-1.02280800	1.86485000
C	-0.60936300	2.37902900	-0.35488200
H	-1.08181000	3.36573800	-0.38161600
H	0.23312200	2.46168900	0.35062100
H	-0.21887800	2.16795000	-1.35751000
C	-0.61010500	-2.37925800	-0.35508200
H	0.23265100	-2.46186800	0.35008700
H	-1.08272800	-3.36589000	-0.38152700
H	-0.21998200	-2.16828100	-1.35785900
C	-2.09541100	1.67339800	1.50857600
H	-1.27064600	1.60922300	2.22596200
H	-2.47945700	2.70005900	1.51910800

H	-2.89617700	1.02313600	1.86471500
Br	3.38455400	-0.00009700	-0.07335500

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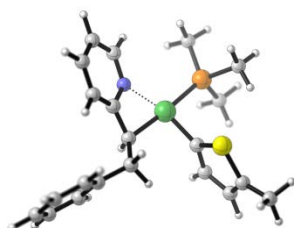
B3LYP electronic energy:	-636.1882813 a.u.
B3LYP enthalpy:	-635.955623 a.u.
B3LYP free energy:	-636.019300 a.u.
M06 SCF energy in solution:	-797.676846996 a.u.
M06 enthalpy in solution:	-797.444188996 a.u.
M06 free energy in solution:	-797.507865996 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	-0.30953800	-0.45349600	-0.49846200
Zn	1.73503200	-0.41102500	-0.16567000
H	-0.58879500	-0.72691000	-1.52282500
C	0.83725800	2.95131700	0.22622800
C	-0.25626400	3.78926100	0.04093000
C	-1.46871600	3.21543800	-0.35000800
C	-1.55215900	1.83748500	-0.53580800
C	-0.41272400	1.04560700	-0.32661400
N	0.75805100	1.62367700	0.04638600
H	-2.34253700	3.84027800	-0.51246000
H	1.80877400	3.33855000	0.52021800
H	-0.15815800	4.85894400	0.19126600
H	-2.48172500	1.37170700	-0.83989200
C	-1.15489100	-1.29869800	0.49016600
H	-0.86438400	-2.34807300	0.35817100
H	-0.89255000	-1.03758200	1.52257900
C	-2.66035600	-1.18271400	0.32215400
C	-3.29495900	-1.70500200	-0.81588100
C	-3.45217900	-0.54605200	1.28699300
C	-4.67398900	-1.58864800	-0.98683200
H	-2.70092800	-2.21225000	-1.57298000
C	-4.83456000	-0.42745000	1.12142100
H	-2.98060000	-0.14133700	2.17944300
C	-5.45015300	-0.94674000	-0.01763300
H	-5.14533700	-2.00461000	-1.87310600

H	-5.42869300	0.06834200	1.88427100
H	-6.52481100	-0.85815900	-0.14837200
Br	4.08690900	-0.89502100	0.13483300

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B3LYP electronic energy:	-1779.5359337 a.u.
B3LYP enthalpy:	-1779.091664 a.u.
B3LYP free energy:	-1779.181649 a.u.
M06 SCF energy in solution:	-1780.72176515 a.u.
M06 enthalpy in solution:	-1780.27749515 a.u.
M06 free energy in solution:	-1780.36748015 a.u.

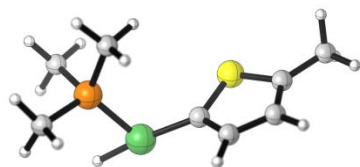
Cartesian coordinates

ATOM	X	Y	Z
C	1.29279600	1.28473500	0.27792500
C	1.43065400	2.21887100	1.28041700
C	1.66768000	3.56194000	0.82925700
C	1.71316700	3.69145600	-0.53078900
S	1.45701400	2.11575000	-1.26693900
H	1.35176600	1.96387200	2.33375700
H	1.79691700	4.40625500	1.50111000
C	1.93629400	4.92721500	-1.35046400
H	2.83138700	4.85190000	-1.98043000
H	1.09069300	5.14004900	-2.01598500
H	2.06597000	5.79201800	-0.69229700
Ni	0.90852200	-0.57161500	0.31887800
P	3.12634900	-1.09739600	0.36021800
C	4.01529800	-0.30763200	1.77203800
H	5.09354600	-0.48925300	1.71988500
H	3.81537800	0.76567100	1.75158300
H	3.63064300	-0.70921300	2.71414000
C	3.64648600	-2.86897000	0.53422600
H	3.31438900	-3.43811800	-0.33842000
H	4.73403500	-2.96138900	0.62008300
H	3.18393100	-3.30152500	1.42599000
C	4.11795200	-0.56052400	-1.10177000
H	5.18576400	-0.75039100	-0.95164900

H	3.77956000	-1.10235700	-1.98971900
H	3.95129800	0.50509100	-1.27294500
C	0.11930400	-3.59681400	-0.16557800
C	-0.79073600	-4.22670900	-1.00118700
C	-1.88853200	-3.48501400	-1.46891600
C	-2.06655500	-2.17288700	-1.06027300
C	-1.15368400	-1.62250900	-0.13543000
N	-0.05020700	-2.33281800	0.25829200
H	-2.60577900	-3.94562000	-2.14301500
H	1.01310600	-4.10640400	0.18283600
H	-0.64428900	-5.26166000	-1.29037000
H	-2.91036900	-1.58365100	-1.39945000
C	-1.07233200	-0.27924400	0.42558700
H	-1.06750200	-0.30557500	1.52023900
C	-1.88518000	0.86494400	-0.15498600
H	-1.47437100	1.79686700	0.25005300
H	-1.72885000	0.92071100	-1.23828600
C	-3.38104700	0.81384500	0.12905900
C	-4.31461600	0.86259500	-0.91521900
C	-3.86780700	0.74060800	1.44333100
C	-5.68843700	0.83170300	-0.66117100
H	-3.95907800	0.93342000	-1.94116300
C	-5.23740400	0.71103700	1.70323900
H	-3.16508700	0.70966600	2.27225700
C	-6.15557500	0.75405500	0.65061600
H	-6.39131100	0.87069100	-1.48925800
H	-5.59005800	0.65665400	2.72986300
H	-7.22266900	0.72996600	0.85282900
C	-5.37494600	1.96773400	-0.23889800
C	-5.62176600	0.65983600	0.12859100
C	-4.56517600	-0.28194300	0.06030100
N	-3.30536900	0.10785500	-0.24282000
H	-6.17891500	2.69467700	-0.22480700
H	-2.07839400	1.61696900	-0.93369600
O	-4.81382400	-1.55320200	0.28184400
H	-4.14668400	-2.10215700	-0.26979100
C	-3.81011600	3.74599600	-1.08347800
C	-7.00295100	0.20452900	0.52753200
F	-4.79767800	4.22786400	-1.87023800
F	-2.65162600	3.84233100	-1.77705500
F	-3.71309500	4.57651800	-0.02518900
F	-7.00628100	-0.37651700	1.74087700
F	-7.51151300	-0.68028400	-0.35123700
F	-7.85556600	1.25474200	0.57904100

C	-2.97163700	-3.93397800	-1.14708800
O	-3.08719900	-2.62619100	-1.27649000
O	-2.11408900	-4.49605700	-0.46798300
C	-4.01760800	-4.72213200	-1.92495600
H	-3.85977300	-5.79435400	-1.79466700
H	-5.02272200	-4.45526500	-1.57877700
H	-3.96579800	-4.46287800	-2.98787300
C	3.30367100	1.16862100	-1.79279800
C	4.24051700	1.93514700	-2.52519200
N	2.12985900	0.77624300	-2.28654900
C	3.87249800	2.27307300	-3.83213100
C	1.81411900	1.10400000	-3.54279700
C	2.65159800	1.85908200	-4.35924700
H	4.55794900	2.86230300	-4.43678600
H	0.84850100	0.75125700	-3.89982700
H	2.35908900	2.11346200	-5.37351700
C	5.55770600	2.40749600	-1.96636800
H	6.25966800	2.63501000	-2.77524100
H	5.41126400	3.31346100	-1.36873800
H	6.01638800	1.65884200	-1.31396700

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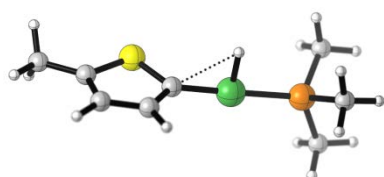
B3LYP electronic energy:	-1222.720508 a.u.
B3LYP enthalpy:	-1222.497287 a.u.
B3LYP free energy:	-1222.558866 a.u.
M06 SCF energy in solution:	-1224.18854699 a.u.
M06 enthalpy in solution:	-1223.96532599 a.u.
M06 free energy in solution:	-1224.02690499 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	-0.90189300	0.57309000	-0.04931200
C	-1.67133600	1.29182900	0.85137500
C	-3.02921800	0.86660200	0.97014800
C	-3.33909000	-0.21607400	0.18497900
S	-1.92195600	-0.70018500	-0.71766900
H	-1.27116900	2.12549500	1.42273500
H	-3.75917600	1.34617300	1.61618500
C	-4.65649800	-0.92170300	0.05699500

H	-4.98564500	-0.98826100	-0.98682800
H	-4.61615200	-1.94565100	0.44978600
H	-5.42626200	-0.38019800	0.61555200
Ni	0.82233300	0.93422600	-0.75856200
P	2.20155600	-0.30464800	0.21358900
C	3.06501000	-1.47436200	-0.91636400
H	3.76556800	-2.10533300	-0.36000400
H	2.32802900	-2.11104900	-1.41226100
H	3.60055800	-0.90766100	-1.67990600
C	3.56442600	0.58674600	1.07224900
H	3.14309700	1.26978700	1.81402400
H	4.23242200	-0.11996000	1.57512300
H	4.12392400	1.17336100	0.34163200
C	1.52448500	-1.40817800	1.52652300
H	2.31099700	-2.03242400	1.96408500
H	1.06153200	-0.79750900	2.30472800
H	0.74550800	-2.04035500	1.09511200
H	2.11407300	1.34023100	-1.42091600

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B3LYP electronic energy: -1222.7292014 a.u.  
 B3LYP enthalpy: -1222.506534 a.u.  
 B3LYP free energy: -1222.570024 a.u.  
 M06 SCF energy in solution: -1224.19193671 a.u.  
 M06 enthalpy in solution: -1223.96926971 a.u.  
 M06 free energy in solution: -1224.03275871 a.u.

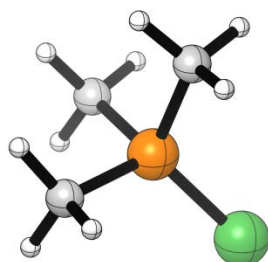
Cartesian coordinates

ATOM	X	Y	Z
C	-1.28824200	0.38536700	-0.11348500
C	-2.07074700	1.52488300	-0.04000300
C	-3.47138500	1.27883800	0.07386400
C	-3.80340800	-0.05357200	0.05441500
S	-2.35421200	-1.01725000	-0.10547500
H	-1.64903300	2.52493500	-0.06918500
H	-4.21641800	2.06404100	0.16560600
C	-5.16598200	-0.67037700	0.16528700
H	-5.39822300	-1.30981400	-0.69453600



H	-5.26493200	-1.28953500	1.06521100
H	-5.92846200	0.11284800	0.21486200
Ni	0.54170200	0.16924100	-0.00791000
P	2.76741800	-0.07314400	0.05718200
C	3.38948700	-1.59922100	-0.77816700
H	4.48346000	-1.64188200	-0.78039000
H	2.99707300	-2.48215400	-0.26640100
H	3.02383000	-1.61749100	-1.80791600
C	3.69845100	1.26574900	-0.81143100
H	3.49794100	2.22459500	-0.32575000
H	4.77703400	1.07811500	-0.80455500
H	3.34810500	1.33238000	-1.84447500
C	3.62181300	-0.14655400	1.69943500
H	4.70450600	-0.26552700	1.58779500
H	3.42125500	0.77153800	2.25894500
H	3.23024000	-0.98740700	2.27894500
H	0.50216100	0.20911200	-1.42627900

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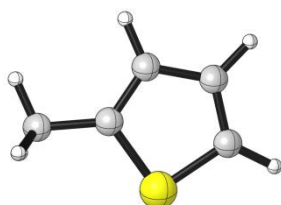
B3LYP electronic energy: -630.3819249 a.u.  
 B3LYP enthalpy: -630.257988 a.u.  
 B3LYP free energy: -630.300092 a.u.  
 M06 SCF energy in solution: -631.96261886 a.u.  
 M06 enthalpy in solution: -631.83868186 a.u.  
 M06 free energy in solution: -631.88078586 a.u.

Cartesian coordinates

ATOM	X	Y	Z
Ni	1.56724100	0.00007000	0.00000500
P	-0.47160200	-0.00000600	0.00028200
C	-1.31046900	-1.49529800	0.71364400
H	-2.40218200	-1.40478700	0.67355600
H	-1.00387700	-2.38432500	0.15650500
H	-0.99938700	-1.62536400	1.75338600
C	-1.31087700	1.36582800	0.93762700
H	-1.00033500	2.33092100	0.52911500

H	-2.40254200	1.28528300	0.87922300
H	-1.00418600	1.32938200	1.98614900
C	-1.31045100	0.12928400	-1.65157700
H	-2.40222600	0.12072200	-1.55317600
H	-1.00228000	1.05500100	-2.14442600
H	-1.00092000	-0.70760600	-2.28288200

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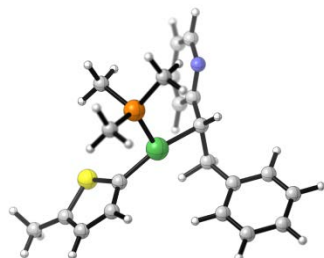


B3LYP electronic energy:	-592.3306807 a.u.
B3LYP enthalpy:	-592.229335 a.u.
B3LYP free energy:	-592.265819 a.u.
M06 SCF energy in solution:	-592.208780221 a.u.
M06 enthalpy in solution:	-592.107434221 a.u.
M06 free energy in solution:	-592.143919221 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	1.68238200	-0.22945700	0.00057800
C	1.38712300	1.10314300	-0.00010500
C	-0.02002900	1.35790400	-0.00018900
C	-0.78677000	0.22340800	-0.00043500
S	0.23778800	-1.19627200	-0.00013300
H	2.14185700	1.88147000	-0.00016100
H	-0.45211200	2.35304300	0.00047300
C	-2.28168800	0.10561700	0.00024400
H	-2.65156600	-0.43071200	-0.88091700
H	-2.65132800	-0.42433600	0.88537500
H	-2.73032400	1.10283500	-0.00324800
H	2.65276300	-0.70565200	0.00004400

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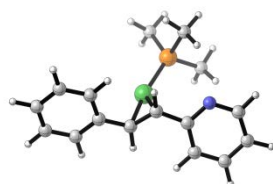
B3LYP electronic energy: -1779.51940713 a.u.  
 B3LYP enthalpy: -1779.075875 a.u.  
 B3LYP free energy: -1779.166170 a.u.  
 M06 SCF energy in solution: -1780.71133127 a.u.  
 M06 enthalpy in solution: -1780.26779927 a.u.  
 M06 free energy in solution: -1780.35809427 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	-1.96321000	-0.68513900	-0.08323200
C	-2.61910600	-1.81689300	0.35356700
C	-3.94788700	-1.99153700	-0.15674000
C	-4.35475300	-0.98992500	-0.99579800
S	-3.06085700	0.18498400	-1.15393900
H	-2.16355300	-2.52709200	1.03940900
H	-4.58289800	-2.83725800	0.09313100
C	-5.66434800	-0.84217500	-1.71194800
H	-6.18705600	0.08061800	-1.43199600
H	-5.53892100	-0.82403000	-2.80141400
H	-6.32082100	-1.68303800	-1.46762100
Ni	-0.16619800	-0.02637800	0.16160200
P	-0.55231400	1.13402500	1.94041800
C	-1.69641100	0.34549400	3.14851200
H	-1.91209000	1.02512700	3.97930300
H	-2.61806900	0.06516700	2.63630200
H	-1.23571800	-0.56488300	3.54152500
C	0.88312000	1.63310300	2.98153000
H	1.61720800	2.14586200	2.35312600
H	0.56649600	2.28482300	3.80259000
H	1.35045000	0.73649900	3.39880700
C	-1.37434900	2.73043200	1.52759700
H	-1.62762400	3.28963200	2.43426100
H	-0.70111500	3.33133100	0.91120500
H	-2.28323800	2.52625500	0.95639600
C	2.56155000	3.90176000	-0.33641300
C	2.10780300	4.33346000	-1.58315100
C	1.48814500	3.39090700	-2.40550400
C	1.36012300	2.08036100	-1.95962500
C	1.85970500	1.72255300	-0.68608200
N	2.44969400	2.64759400	0.11131200
H	1.10953700	3.67271100	-3.38431000
H	3.04687300	4.60365100	0.34106800
H	2.23410200	5.36580700	-1.89209700
H	0.87548700	1.33955300	-2.58705500

C	1.73216100	0.36470400	-0.13110000
H	2.39573200	0.18577000	0.71128600
C	1.53881700	-0.80840500	-1.06352700
H	0.41313900	-1.01828900	-1.22721700
H	1.84404100	-0.57329400	-2.09134900
C	2.14797700	-2.11634800	-0.60087600
C	3.54209700	-2.25515800	-0.54013400
C	1.34527200	-3.20434100	-0.23731800
C	4.11919000	-3.45417400	-0.12385000
H	4.17579500	-1.41726500	-0.81986700
C	1.92293400	-4.40579500	0.18143300
H	0.26324900	-3.10791600	-0.28322400
C	3.31053500	-4.53451600	0.23928200
H	5.20104800	-3.54606700	-0.08357200
H	1.28543900	-5.24012300	0.46049300
H	3.76043600	-5.46843900	0.56380400

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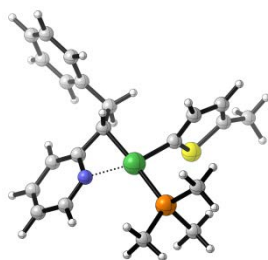
B3LYP electronic energy:	-1187.198136 a.u.
B3LYP enthalpy:	-1186.857773 a.u.
B3LYP free energy:	-1186.931863 a.u.
M06 SCF energy in solution:	-1188.48867114 a.u.
M06 enthalpy in solution:	-1188.14830814 a.u.
M06 free energy in solution:	-1188.22239814 a.u.

Cartesian coordinates

ATOM	X	Y	Z
Ni	-0.15586200	0.61117500	-0.49985100
P	1.20546900	2.28807800	-0.15101100
C	0.70223000	4.04511700	-0.47137300
H	1.48800900	4.75168100	-0.18300800
H	0.47894000	4.17748400	-1.53396200
H	-0.20561400	4.27164200	0.09458200
C	1.72846600	2.34673800	1.62232200
H	2.09078100	1.35399000	1.90419600
H	2.51040800	3.09483900	1.79308800
H	0.86300800	2.58380400	2.24744600
C	2.83940000	2.20357900	-1.02118700

H	3.50850600	3.01274400	-0.70882100
H	3.30892500	1.24241300	-0.79669600
H	2.68718600	2.26366400	-2.10249200
C	3.47203600	-1.84955900	1.10400300
C	3.85951000	-2.71517100	0.08110100
C	2.89347800	-3.07574400	-0.86104600
C	1.60898800	-2.55931100	-0.74651100
C	1.30694600	-1.67534600	0.30966300
N	2.24341600	-1.33898700	1.22914200
H	3.13667700	-3.76064500	-1.66905800
H	4.18863400	-1.55266300	1.86916900
H	4.87357300	-3.09853600	0.03378800
H	0.83897700	-2.84442700	-1.45483100
C	-0.02234900	-1.06898300	0.51164000
H	-0.19979600	-0.80281200	1.55251400
C	-1.10418500	-1.13999600	-0.39826900
H	-0.96018900	-1.66457500	-1.34319500
C	-2.51125800	-0.84721300	-0.08002900
C	-3.48417800	-0.97951000	-1.09365200
C	-2.95333900	-0.41246600	1.18848500
C	-4.82602700	-0.69021600	-0.85749100
H	-3.17284700	-1.32086000	-2.07847900
C	-4.29565900	-0.12579600	1.42319700
H	-2.24025700	-0.30876300	2.00023700
C	-5.24280900	-0.25935300	0.40388300
H	-5.54954700	-0.80641400	-1.66017200
H	-4.60595400	0.20122200	2.41225300
H	-6.28874800	-0.03557900	0.59201800

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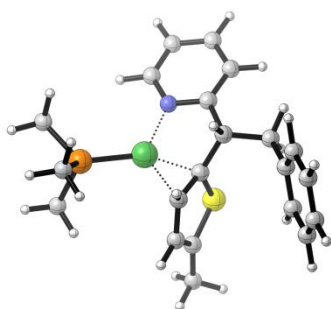
B3LYP electronic energy: -1779.5359338 a.u.  
 B3LYP enthalpy: -1779.091663 a.u.  
 B3LYP free energy: -1779.181634 a.u.  
 M06 SCF energy in solution: -1780.72177107 a.u.  
 M06 enthalpy in solution: -1780.27750007 a.u.  
 M06 free energy in solution: -1780.36747207 a.u.

## Cartesian coordinates

ATOM	X	Y	Z
C	-1.29328600	1.28457200	-0.27765500
C	-1.43261600	2.21849000	-1.28014900
C	-1.66955000	3.56156100	-0.82895400
C	-1.71355600	3.69128100	0.53111900
S	-1.45605100	2.11578200	1.26725600
H	-1.35476600	1.96335300	-2.33353500
H	-1.79980500	4.40572000	-1.50080600
C	-1.93626600	4.92709700	1.35082200
H	-2.83092500	4.85174900	1.98140200
H	-1.09023800	5.14008800	2.01574800
H	-2.06648300	5.79181900	0.69265500
Ni	-0.90847400	-0.57168400	-0.31872500
P	-3.12608500	-1.09783500	-0.36039100
C	-4.01439900	-0.31010800	-1.77376800
H	-5.09268100	-0.49158400	-1.72176000
H	-3.81449600	0.76322700	-1.75473500
H	-3.62941800	-0.71309400	-2.71513400
C	-3.64612400	-2.86966200	-0.53212700
H	-3.31405100	-3.43767800	0.34126600
H	-4.73366200	-2.96224000	-0.61795600
H	-3.18349000	-3.30333800	-1.42330800
C	-4.11848200	-0.55884800	1.10027000
H	-5.18616000	-0.74927600	0.94992500
H	-3.78037000	-1.09911300	1.98927700
H	-3.95219100	0.50708200	1.26979500
C	-0.11879100	-3.59656100	0.16553100
C	0.79109900	-4.22624600	1.00145000
C	1.88864400	-3.48432800	1.46944900
C	2.06656200	-2.17219800	1.06081000
C	1.15387700	-1.62201900	0.13563500
N	0.05064200	-2.33256400	-0.25839500
H	2.60576400	-3.94476900	2.14379800
H	-1.01241800	-4.10631000	-0.18310000
H	0.64475100	-5.26120500	1.29065700
H	2.91019100	-1.58281800	1.40018800
C	1.07243400	-0.27881100	-0.42537300
H	1.06742900	-0.30506300	-1.52002300
C	1.88519100	0.86552200	0.15504400
H	1.47434700	1.79735700	-0.25013400
H	1.72894100	0.92143900	1.23834700
C	3.38100500	0.81428600	-0.12919600

C	3.86744700	0.74203400	-1.44363400
C	4.31478600	0.86171000	0.91495100
C	5.23697700	0.71208700	-1.70385400
H	3.16448800	0.71216500	-2.27240400
C	5.68854000	0.83046700	0.66058300
H	3.95947400	0.93180500	1.94102800
C	6.15537100	0.75375700	-0.65137100
H	5.58940500	0.65847500	-2.73059600
H	6.39161000	0.86844000	1.48855100
H	7.22241400	0.72938000	-0.85381600

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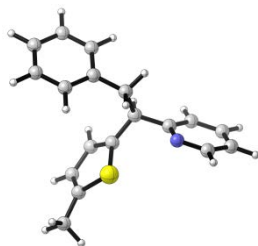
B3LYP electronic energy:	-1779.5470847 a.u.
B3LYP enthalpy:	-1779.102104 a.u.
B3LYP free energy:	-1779.190685 a.u.
M06 SCF energy in solution:	-1780.74120629 a.u.
M06 enthalpy in solution:	-1780.29622529 a.u.
M06 free energy in solution:	-1780.38480629 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	-0.47130500	-0.10839000	0.38564500
C	-0.30850000	-1.34592400	-0.31321200
C	-0.38860200	-2.49462300	0.57191900
C	-0.55279400	-2.20553200	1.88685700
S	-0.65094100	-0.45476700	2.15162700
H	-0.54926300	-1.44050600	-1.37009700
H	-0.31568200	-3.51753200	0.21158500
C	-0.59519200	-3.14530100	3.05310100
H	0.25910000	-3.00321400	3.72737100
H	-1.50408100	-3.01647200	3.65365500
H	-0.57163500	-4.18019500	2.69792000
Ni	1.38781100	-0.14944000	-0.16770800
P	3.16731200	-1.13560800	-0.95350600
C	2.97320500	-1.94564100	-2.61488800

H	3.87699200	-2.48451100	-2.92096900
H	2.13285600	-2.64389100	-2.57768700
H	2.74335100	-1.18421700	-3.36602300
C	4.77223400	-0.22854100	-1.23472200
H	5.12610200	0.19011300	-0.28734700
H	5.55353600	-0.87943300	-1.64345800
H	4.60574700	0.60083100	-1.92903000
C	3.78015200	-2.56399000	0.06428500
H	4.62250500	-3.08089900	-0.40930300
H	4.09401800	-2.20006700	1.04701100
H	2.96061500	-3.27089000	0.21762000
C	2.31934700	2.70173700	0.42743200
C	2.10732800	4.04762700	0.71472000
C	0.79714800	4.51962900	0.73394600
C	-0.24612200	3.63328100	0.46041400
C	0.03816400	2.29569400	0.18318400
N	1.32086000	1.83928400	0.17516600
H	0.58542100	5.56084800	0.95880600
H	3.32063500	2.28376800	0.39985800
H	2.94964400	4.69946500	0.92163100
H	-1.27166100	3.98282300	0.47280400
C	-0.98818000	1.21848400	-0.16583600
H	-0.94161400	1.10992000	-1.26027000
C	-2.45714100	1.58065600	0.18426800
H	-2.57100500	1.61192700	1.27321100
H	-2.67103800	2.58807800	-0.19084200
C	-3.46929600	0.63029400	-0.42175600
C	-3.93761800	-0.48665900	0.28286000
C	-3.95402900	0.85141300	-1.71889500
C	-4.86278200	-1.35794200	-0.29444700
H	-3.56744100	-0.67421300	1.28643900
C	-4.87725100	-0.01856200	-2.30028900
H	-3.60893900	1.71976600	-2.27680000
C	-5.33575500	-1.12810300	-1.58758800
H	-5.21483900	-2.21799400	0.26866100
H	-5.24297700	0.17396200	-3.30531900
H	-6.05777300	-1.80537800	-2.03517500





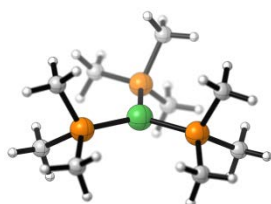
B3LYP electronic energy: -1149.11658054 a.u.  
 B3LYP enthalpy: -1148.796130 a.u.  
 B3LYP free energy: -1148.863089 a.u.  
 M06 SCF energy in solution: -1148.69947558 a.u.  
 M06 enthalpy in solution: -1148.37902558 a.u.  
 M06 free energy in solution: -1148.44598358 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	0.14737100	0.73481500	0.54306600
C	-0.55156100	1.32810000	1.55920800
C	-0.72103300	2.73720700	1.39736300
C	-0.15436000	3.22574600	0.25261900
S	0.61533800	1.93660900	-0.64885900
H	-0.94646700	0.76694700	2.39957200
H	-1.24542100	3.36651600	2.10899900
C	-0.12103500	4.64211400	-0.23880500
H	0.90337300	5.02088100	-0.33189500
H	-0.59806900	4.74851900	-1.21991600
H	-0.65387200	5.28938500	0.46355000
C	3.75408400	-0.84422200	-1.22391900
C	4.61002100	-1.43765100	-0.29602700
C	4.07738300	-1.82409700	0.93248700
C	2.72413400	-1.60167500	1.17843100
C	1.94256500	-0.99900200	0.18549800
N	2.45372500	-0.63024600	-0.99907900
H	4.70433900	-2.29000100	1.68739700
H	4.12933600	-0.52656400	-2.19507600
H	5.65799700	-1.58994600	-0.53283300
H	2.27676800	-1.88658300	2.12579200
C	0.45612700	-0.73625200	0.39397100
H	0.16707600	-1.19784700	1.34572200
C	-0.37284500	-1.43279700	-0.73295500
H	-0.12524700	-0.95298200	-1.68349700
H	-0.02395100	-2.46987400	-0.80360400
C	-1.86496200	-1.41804800	-0.49187500
C	-2.68268000	-0.42647600	-1.04969200
C	-2.46368700	-2.39687000	0.31391300

C	-4.05705300	-0.41226500	-0.80848800
H	-2.23653000	0.33849600	-1.67895400
C	-3.83677700	-2.38616500	0.55922900
H	-1.84669900	-3.18141100	0.74695700
C	-4.63910400	-1.39138900	-0.00230000
H	-4.67359300	0.36407700	-1.25288400
H	-4.28073800	-3.15759300	1.18239000
H	-5.70932100	-1.38249800	0.18323000

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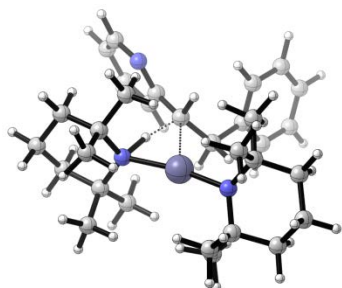
B3LYP electronic energy:	-1552.6863131 a.u.
B3LYP enthalpy:	-1552.318244 a.u.
B3LYP free energy:	-1552.397028 a.u.
M06 SCF energy in solution:	-1554.10675451 a.u.
M06 enthalpy in solution:	-1553.73868551 a.u.
M06 free energy in solution:	-1553.81746951 a.u.

Cartesian coordinates

ATOM	X	Y	Z
Ni	-0.01852500	-0.03348700	-0.08264100
P	1.71141500	-1.36558700	-0.02761600
C	3.25348400	-0.93458800	-0.98728300
H	4.05210700	-1.67351900	-0.85033300
H	3.01147400	-0.87111600	-2.05250500
H	3.61843100	0.04622400	-0.66889100
C	2.45089600	-1.59285500	1.66750300
H	1.69729200	-2.00882900	2.34224400
H	3.31972200	-2.26089400	1.64978800
H	2.75562100	-0.62057900	2.06443700
C	1.56373300	-3.15494900	-0.53896900
H	2.50380500	-3.70762300	-0.42075000
H	0.78734600	-3.63777100	0.06118900
H	1.25356600	-3.20569400	-1.58712900
P	-2.06967900	-0.78362800	-0.02418100
C	-2.92648200	-0.59709200	1.62006700
H	-3.95640100	-0.97165000	1.59430600
H	-2.36944300	-1.14568800	2.38517300
H	-2.93799500	0.45836400	1.90563400

C	-3.33398900	0.01521400	-1.13805200
H	-3.02633600	-0.10823300	-2.18079200
H	-4.33474100	-0.41449000	-1.01111300
H	-3.37444300	1.08705400	-0.92593200
C	-2.47677500	-2.57232900	-0.37163100
H	-3.54985500	-2.78515100	-0.29331100
H	-2.13700500	-2.83066900	-1.37900500
H	-1.93605100	-3.20784600	0.33580900
P	0.33754900	2.12058800	-0.01979400
C	-1.06529700	3.34989500	-0.13475800
H	-0.72337000	4.38994900	-0.06781200
H	-1.58960800	3.21112700	-1.08514700
H	-1.77892700	3.15936600	0.67257800
C	1.15326000	2.75741500	1.53074400
H	2.12363500	2.26884900	1.65684000
H	1.30056300	3.84348300	1.50445500
H	0.53609500	2.50538500	2.39804300
C	1.46437100	2.86771700	-1.30397300
H	1.59670400	3.94681500	-1.16217800
H	2.44086900	2.37826700	-1.25976600
H	1.04716600	2.69135500	-2.29991300

ts1



B3LYP electronic energy: -1440.6601618 a.u.  
 B3LYP enthalpy: -1439.880142 a.u.  
 B3LYP free energy: -1439.989280 a.u.  
 M06 SCF energy in solution: -1601.56480782 a.u.  
 M06 enthalpy in solution: -1600.78478882 a.u.  
 M06 free energy in solution: -1600.89392582 a.u.

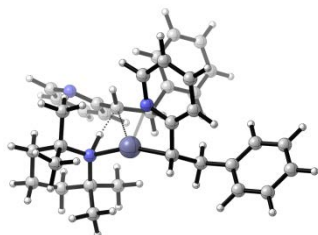
Cartesian coordinates

ATOM	X	Y	Z
C	1.37406000	0.55120600	-0.27003500
Zn	-1.13772800	-0.59321100	-0.01017900
H	0.99462100	0.78246100	-1.27188300
N	0.31396500	-2.01376100	0.16541800

C	1.94583500	-3.40302300	1.45086700
C	0.62414200	-2.59790300	1.51624300
C	0.38260600	-2.92847900	-1.03323700
C	1.70776200	-3.72757000	-1.01966200
C	1.97564200	-4.42739300	0.31447100
H	2.77173900	-2.69507600	1.30757400
H	2.10868900	-3.89087400	2.41988400
H	1.68887900	-4.45304600	-1.84211000
H	2.52670400	-3.02946800	-1.22680500
H	1.24201000	-5.22417700	0.49029200
H	2.95482100	-4.91924500	0.28573500
C	-0.51402200	-3.47885500	2.08082800
H	-0.33624800	-3.67492300	3.14376900
H	-1.48347900	-2.97700900	1.99379000
H	-0.59747400	-4.44669900	1.58603700
C	0.36670200	-2.05557300	-2.30250500
H	0.42294300	-2.69911700	-3.18639400
H	-0.57562600	-1.49460100	-2.39722900
H	1.20917600	-1.35970800	-2.32797300
C	0.83395100	-1.43065500	2.49955900
H	-0.06052200	-0.80231700	2.59239000
H	1.05206600	-1.82389800	3.49733200
H	1.66984100	-0.79873700	2.19505000
C	-0.83017600	-3.88345200	-1.12119400
H	-1.77184400	-3.32820500	-1.03340800
H	-0.83374300	-4.38458300	-2.09517200
H	-0.83000600	-4.66077900	-0.35717200
C	4.51125300	-0.66059900	-1.68819200
C	5.48665700	-0.46347900	-0.71201500
C	5.08028200	0.13492000	0.48310200
C	3.74997700	0.50092900	0.64680300
C	2.81789600	0.26169100	-0.39191800
N	3.22589800	-0.32141900	-1.54956800
H	5.79811900	0.32665500	1.27694200
H	4.77854300	-1.11586900	-2.64226300
H	6.51679700	-0.75648300	-0.88611200
H	3.43389400	0.99700600	1.55794400
C	0.97718600	1.64815200	0.72892400
H	-0.11896400	1.76653000	0.71163700
H	1.19865100	1.33805700	1.75881900
C	1.56633500	3.04627900	0.53524100
C	2.00218200	3.50950600	-0.71265200
C	1.63719200	3.92561900	1.62624100
C	2.48886600	4.80974900	-0.86569500

H	1.97557600	2.84252700	-1.56864600
C	2.12218200	5.22513000	1.47923700
H	1.30789800	3.58369000	2.60585000
C	2.55048600	5.67390500	0.22802300
H	2.82577200	5.14504300	-1.84312400
H	2.17018900	5.88538700	2.34135900
H	2.93255900	6.68397300	0.10898300
H	0.95008800	-0.91049000	-0.00396900
N	-2.75665500	0.44389700	-0.10103600
C	-4.05328100	2.29560200	-1.14541300
C	-3.15061900	1.05776600	-1.38910000
C	-3.76758900	0.22131400	0.95497300
C	-4.65285500	1.48200800	1.13575600
C	-5.20918800	2.01209900	-0.18594800
H	-3.43217800	3.09277200	-0.71660900
H	-4.42757700	2.66429600	-2.10856000
H	-5.46432400	1.25700300	1.83933600
H	-4.03914400	2.26834400	1.59469500
H	-5.91069900	1.29218900	-0.62618600
H	-5.78523100	2.92854400	-0.01005700
C	-3.85703200	0.07647200	-2.36369900
H	-3.99936100	0.53714200	-3.34855000
H	-3.24953400	-0.82575200	-2.49901800
H	-4.83927700	-0.23994500	-2.00717700
C	-3.01870500	-0.00502600	2.28147700
H	-3.71547300	-0.10960000	3.11985200
H	-2.43060900	-0.93395100	2.25549800
H	-2.34538700	0.83148900	2.49366700
C	-1.87239800	1.55199900	-2.08940800
H	-1.20612200	0.71852700	-2.35222100
H	-2.11137800	2.06136100	-3.02889400
H	-1.32015400	2.24839600	-1.45237400
C	-4.66428900	-1.02479900	0.72166500
H	-4.04144200	-1.91082900	0.55109500
H	-5.30042000	-1.22198400	1.59305800
H	-5.32020800	-0.91393500	-0.14343900

ts2



B3LYP electronic energy: -1589.4595395 a.u.  
 B3LYP enthalpy: -1588.722629 a.u.  
 B3LYP free energy: -1588.838222 a.u.  
 M06 SCF energy in solution: -1750.27989869 a.u.  
 M06 enthalpy in solution: -1749.54298769 a.u.  
 M06 free energy in solution: -1749.65858069 a.u.

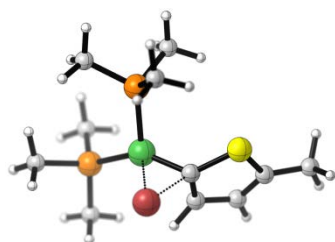
Cartesian coordinates

ATOM	X	Y	Z
C	-1.69976100	0.95513800	0.21763400
Zn	0.31340300	-1.34136700	0.13563200
H	-1.49079500	0.93917000	1.29179300
N	-1.65353200	-1.82746300	-0.16277200
C	-3.47521100	-2.44595900	-1.77324500
C	-1.95225500	-2.25608100	-1.57703800
C	-2.31290900	-2.58360700	0.96627000
C	-3.82057400	-2.78179300	0.67932800
C	-4.10891100	-3.34761600	-0.71224600
H	-3.95328600	-1.45962300	-1.72735400
H	-3.65527900	-2.84097500	-2.78080800
H	-4.24318200	-3.42858400	1.45807900
H	-4.31064800	-1.80582800	0.77204300
H	-3.73610000	-4.37564900	-0.80395500
H	-5.19188000	-3.40328200	-0.87272900
C	-1.18927800	-3.53594800	-1.99082200
H	-1.28876000	-3.69291500	-3.07049200
H	-0.11904400	-3.44298200	-1.76959500
H	-1.55290800	-4.43843900	-1.49864700
C	-2.18770300	-1.74058100	2.25044100
H	-2.63264800	-2.29204800	3.08556800
H	-1.13795300	-1.55552700	2.51103900
H	-2.70787600	-0.78495600	2.15072500
C	-1.48787900	-1.12946100	-2.52088300
H	-0.40839500	-0.94172700	-2.43760300
H	-1.67925800	-1.41815000	-3.55921500
H	-2.01741500	-0.19641900	-2.32279400
C	-1.62617900	-3.94177700	1.23747100
H	-0.54432700	-3.81449400	1.37399100

H	-2.02047900	-4.37680700	2.16221800
H	-1.77526600	-4.67566200	0.44488600
C	-5.29028200	1.20877500	0.74740500
C	-5.81363300	1.83204300	-0.38512700
C	-4.90268500	2.22402500	-1.37101000
C	-3.54832000	1.98217500	-1.18807600
C	-3.09308700	1.33229100	-0.00947400
N	-3.99368600	0.95769100	0.94527100
H	-5.24703100	2.72874300	-2.27091800
H	-5.95824100	0.89293500	1.55030900
H	-6.87949000	2.01058500	-0.48258100
H	-2.83389700	2.31557500	-1.93348200
C	-0.61763500	1.71436400	-0.54917600
H	0.36676500	1.28889800	-0.28284700
H	-0.70252200	1.54408000	-1.63168300
C	-0.48899600	3.22581300	-0.33771400
C	-0.96664100	3.86003300	0.81563700
C	0.16508100	4.01072500	-1.29931000
C	-0.79033400	5.23256100	1.00504700
H	-1.49407200	3.27405900	1.56186400
C	0.34430500	5.38198600	-1.11571400
H	0.53599300	3.53786600	-2.20729900
C	-0.13300800	5.99981400	0.04234300
H	-1.17429700	5.70425100	1.90601500
H	0.85071100	5.96872500	-1.87799900
H	0.00009400	7.06825100	0.18854000
H	-1.81489500	-0.60132200	-0.05071200
C	2.38828000	-1.30351600	-0.10161700
H	2.82484800	-2.30791300	-0.18424000
C	1.45052800	-0.08366400	3.22437600
C	2.63343100	0.18100100	3.90457200
C	3.84057700	-0.06157400	3.24479900
C	3.82786300	-0.54681600	1.93939700
C	2.59926200	-0.78147800	1.30237300
N	1.43706100	-0.55122600	1.96644100
H	4.78588100	0.12488800	3.74696200
H	0.48028200	0.07849100	3.68601000
H	2.60826200	0.56186200	4.91985300
H	4.75243200	-0.74212000	1.41012100
C	2.96511100	-0.42319200	-1.24076900
H	2.61715800	-0.85001800	-2.19047300
H	2.53539300	0.58410900	-1.18584200
C	4.47933300	-0.30411900	-1.29381700
C	5.27485400	-1.41118700	-1.62861000

C	5.12135400	0.90768600	-1.00552600
C	6.66542400	-1.31262800	-1.66649300
H	4.79726900	-2.35956400	-1.86543800
C	6.51421300	1.01249800	-1.04272900
H	4.52258800	1.77893000	-0.75074100
C	7.29157500	-0.09834500	-1.37139600
H	7.26164100	-2.18146700	-1.93213500
H	6.98964700	1.96317700	-0.81697900
H	8.37452100	-0.01965500	-1.40279100

ts3



B3LYP electronic energy:	-1696.44805186 a.u.
B3LYP enthalpy:	-1696.108171 a.u.
B3LYP free energy:	-1696.191760 a.u.
M06 SCF energy in solution:	-1698.03532154 a.u.
M06 enthalpy in solution:	-1697.69543454 a.u.
M06 free energy in solution:	-1697.77902454 a.u.

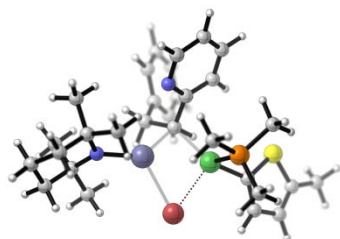
Cartesian coordinates

ATOM	X	Y	Z
C	1.34573700	-0.34869000	0.29974900
C	1.32870700	-1.69333900	-0.09398300
C	2.42774200	-2.01497400	-0.97040800
C	3.32074700	-1.00249100	-1.15339200
S	2.80553100	0.45507200	-0.28549600
H	0.73925400	-2.44855600	0.40889600
H	2.57793700	-3.00336600	-1.39518600
Ni	-0.44359800	-0.16974800	-0.10835900
Br	0.65111400	-0.09079100	2.49675800
P	-2.41770500	-1.23391800	-0.45097600
C	-2.39356000	-3.06705300	-0.17344400
H	-3.38103100	-3.51579600	-0.32681000
H	-1.67867100	-3.52916500	-0.85956400
H	-2.06362700	-3.27142600	0.84901000
C	-3.84161400	-0.73751600	0.62606500
H	-4.07325300	0.31916700	0.46877200
H	-4.73594000	-1.33508000	0.41970200



H	-3.55796900	-0.86711200	1.67419800
C	-3.17341100	-1.13980200	-2.14143000
H	-4.10654200	-1.70982700	-2.20469100
H	-3.37863600	-0.09630700	-2.39668600
H	-2.46547100	-1.53238000	-2.87677000
P	-0.65714800	2.04422600	-0.51157900
C	0.37372300	3.20573400	0.49389800
H	0.17930200	4.25006900	0.22734100
H	0.16356500	3.04816600	1.55424400
H	1.43142200	2.98754500	0.32792900
C	-0.18769200	2.52889900	-2.23865300
H	-0.83953700	2.01799400	-2.95322000
H	-0.26076400	3.61040400	-2.39782300
H	0.83970800	2.20526500	-2.42590800
C	-2.32793400	2.83994100	-0.35392700
H	-2.30320000	3.90091100	-0.62558100
H	-3.04738200	2.32927700	-1.00108200
H	-2.67415000	2.74853500	0.67957200
C	4.58478000	-1.00171300	-1.95731500
H	4.75281900	-1.99642300	-2.38116900
H	4.54722000	-0.28704800	-2.78871900
H	5.45763100	-0.74398600	-1.34562300

ts4



B3LYP electronic energy: -2266.8882194 a.u.  
 B3LYP enthalpy: -2266.167818 a.u.  
 B3LYP free energy: -2266.295478 a.u.  
 M06 SCF energy in solution: -2429.6707073 a.u.  
 M06 enthalpy in solution: -2428.9503063 a.u.  
 M06 free energy in solution: -2429.0779663 a.u.

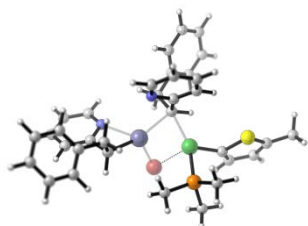
Cartesian coordinates

ATOM	X	Y	Z
Ni	1.36397800	-0.82612800	-0.09829700
Br	-0.28329300	-2.64248200	-1.33690500
P	1.84516700	-2.04452200	1.64878600
C	3.07873900	-1.40116300	2.85341700

H	3.16882300	-2.08368200	3.70456000
H	4.04869000	-1.29524300	2.36412900
H	2.75947500	-0.41868700	3.20922800
C	0.34061800	-2.31396400	2.67764100
H	-0.41307700	-2.83039700	2.07965800
H	0.58907900	-2.92500600	3.55196800
H	-0.06570700	-1.35582800	3.00808000
C	2.40864900	-3.74930000	1.26558300
H	2.46472400	-4.34500100	2.18195700
H	1.69444800	-4.19946400	0.57227500
H	3.38686600	-3.71172100	0.78407300
C	0.16165700	1.05891200	-0.04808800
Zn	-1.46877400	-0.48099800	-0.29643000
H	1.14460700	1.08014200	-0.57436400
C	-0.58541000	1.68310500	3.48025800
C	0.54898700	2.29263900	4.01373600
C	1.63465700	2.50512800	3.16079300
C	1.53901400	2.10879500	1.82976800
C	0.35908100	1.48867900	1.37420900
N	-0.68244800	1.27980900	2.20649800
H	2.53750000	2.98912800	3.52355800
H	-1.45920800	1.49865900	4.10307000
H	0.57684700	2.59165700	5.05643900
H	2.35539000	2.28676900	1.13749800
C	3.10522400	-1.13455900	-0.64415400
C	3.51589000	-2.00290600	-1.62804800
S	4.39832600	-0.00385700	-0.26800100
C	4.83695400	-1.73501600	-2.10897900
H	2.88049000	-2.79273200	-2.01290600
C	5.46170600	-0.68810300	-1.48299000
H	5.30797000	-2.30198300	-2.90625800
C	6.82411700	-0.12018800	-1.74718500
H	7.32952900	-0.71554100	-2.51312900
H	6.77455300	0.91411200	-2.10729500
H	7.45322300	-0.12380100	-0.84962900
C	-0.68398600	2.11377700	-0.85116600
H	-0.87889600	1.72602300	-1.85844600
H	-1.65631700	2.24499100	-0.36664800
C	0.00626100	3.45883600	-0.97970400
C	0.99216100	3.66325100	-1.95662500
C	-0.30860100	4.51886300	-0.11883000
C	1.64659200	4.89011200	-2.06913100
H	1.24158100	2.85565500	-2.64191700
C	0.34343400	5.74867800	-0.22873600

H	-1.07585900	4.37966600	0.63850500
C	1.32408000	5.93810800	-1.20351100
H	2.40143500	5.03079900	-2.83791100
H	0.08105600	6.55976400	0.44505800
H	1.82900000	6.89577200	-1.29287000
N	-3.41333700	-0.39985400	-0.33495700
C	-5.42709200	-1.44057300	0.71291300
C	-4.16524100	-0.56125200	0.92203700
C	-4.13025100	-0.09608600	-1.58698300
C	-5.38204900	-1.00085500	-1.74345200
C	-6.26216300	-1.00857100	-0.49285700
H	-5.09810400	-2.47601600	0.55108200
H	-6.03312900	-1.43589400	1.62877100
H	-5.95862300	-0.68264700	-2.62203200
H	-5.04023300	-2.02632600	-1.93684200
H	-6.69946200	-0.01608900	-0.32343800
H	-7.10850800	-1.69331500	-0.63008400
C	-4.56194200	0.78585400	1.59041800
H	-4.99607400	0.62071600	2.58516500
H	-3.67427700	1.41590700	1.70370200
H	-5.29739400	1.34190700	1.00540700
C	-3.19214500	-0.40635500	-2.76781700
H	-3.69174000	-0.22756300	-3.72618900
H	-2.30637500	0.24585000	-2.75502700
H	-2.85407400	-1.44581800	-2.74068200
C	-3.25318000	-1.29795900	1.92179300
H	-2.37380200	-0.68526500	2.16035500
H	-3.77163400	-1.49277200	2.86775500
H	-2.93291800	-2.26091600	1.50719400
C	-4.55346700	1.39434300	-1.72495600
H	-3.68952300	2.04940300	-1.57669300
H	-4.96281400	1.59514200	-2.72300600
H	-5.31448500	1.68452800	-0.99790700

ts5



B3LYP electronic energy: -2415.6891079 a.u.  
 B3LYP enthalpy: -2415.011700 a.u.

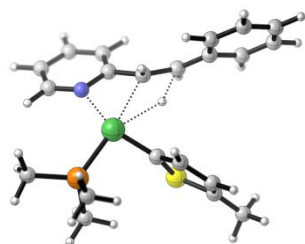
B3LYP free energy: -2415.145150 a.u.  
 M06 SCF energy in solution: -2578.3875286 a.u.  
 M06 enthalpy in solution: -2577.7101206 a.u.  
 M06 free energy in solution: -2577.8435706 a.u.

Cartesian coordinates

ATOM	X	Y	Z
Ni	1.64735900	-0.92362600	-0.12099500
Br	0.31239400	-1.27155200	-2.62858000
P	1.27022700	-2.99682100	0.43669800
C	1.90703000	-3.53041500	2.08048200
H	1.60656700	-4.56291800	2.28526600
H	2.99504200	-3.45248900	2.10223900
H	1.49767900	-2.87801900	2.85633300
C	-0.53184900	-3.37279700	0.56119500
H	-0.99950300	-3.20031500	-0.40964900
H	-0.66875200	-4.41818300	0.85827700
H	-1.00830800	-2.72364900	1.29938700
C	1.87300400	-4.26884500	-0.74137300
H	1.52619200	-5.26045800	-0.43459900
H	1.47979300	-4.02645200	-1.73141500
H	2.96275300	-4.24957300	-0.77805400
C	0.90167600	1.06386800	0.20252800
Zn	-0.96383100	-0.02851700	-0.53019200
H	2.00725000	0.87817800	0.10110300
C	-1.03113400	1.88431100	3.18095900
C	-0.11770000	1.95949100	4.23149900
C	1.22853600	1.73050500	3.94025700
C	1.60132600	1.44579100	2.63009000
C	0.61223800	1.38251600	1.63128400
N	-0.68948400	1.59811800	1.91930000
H	1.98074500	1.78492600	4.72274400
H	-2.09203100	2.05011800	3.36070700
H	-0.45217600	2.18722500	5.23825100
H	2.64245100	1.28166200	2.37051200
C	3.44283400	-1.41406700	-0.11838000
C	4.18251800	-1.70462000	-1.23950800
S	4.51312600	-1.10823600	1.23983200
C	5.59742500	-1.64933400	-1.02104900
H	3.72786700	-1.93033400	-2.19822000
C	5.95421100	-1.34406800	0.26535500
H	6.32971800	-1.83028500	-1.80210200
C	7.32937100	-1.19220800	0.84380100
H	8.07821400	-1.39920500	0.07369700

H	7.50763500	-0.17746500	1.21831500
H	7.50506700	-1.88316600	1.67652200
C	0.65160400	2.26171300	-0.76891800
H	0.70680200	1.89217700	-1.79910400
H	-0.36128100	2.64547200	-0.61137700
C	1.65215500	3.38720200	-0.58380500
C	2.87612500	3.36993600	-1.26896500
C	1.39351900	4.45150700	0.29169300
C	3.81704000	4.38348500	-1.08182100
H	3.08760600	2.55842500	-1.96188000
C	2.33211100	5.46743200	0.48061200
H	0.44692600	4.48431800	0.82502200
C	3.54817600	5.43614500	-0.20428200
H	4.75644500	4.35477200	-1.62726400
H	2.11111700	6.28597900	1.16045900
H	4.27783400	6.22803500	-0.06001200
C	-2.95538800	-0.63615000	-0.22407600
H	-3.18827700	-1.66195100	-0.53730800
C	-2.84623100	2.15164300	-2.59556300
C	-4.09731000	2.21369500	-3.19988500
C	-5.06148900	1.28086300	-2.81131800
C	-4.74927000	0.33690900	-1.83650300
C	-3.46734400	0.33136500	-1.26228500
N	-2.54113900	1.23914200	-1.66219200
H	-6.04802900	1.28962000	-3.26712800
H	-2.05118100	2.83988700	-2.87123000
H	-4.30340600	2.96040700	-3.95945100
H	-5.48201700	-0.39429300	-1.51539100
C	-3.53803200	-0.40717500	1.19537000
H	-3.01644700	-1.08460600	1.88489400
H	-3.29376400	0.60739700	1.52746900
C	-5.03311400	-0.63379200	1.33716700
C	-5.56887400	-1.93130300	1.31625700
C	-5.92200900	0.44119000	1.47502800
C	-6.94228800	-2.14776500	1.42519000
H	-4.89737400	-2.78133200	1.21404900
C	-7.29901100	0.23169700	1.58450400
H	-5.52824800	1.45471700	1.49751500
C	-7.81511000	-1.06428700	1.55935000
H	-7.33275800	-3.16200600	1.41053700
H	-7.96745200	1.08203600	1.69147900
H	-8.88514800	-1.23058900	1.64641500

ts6



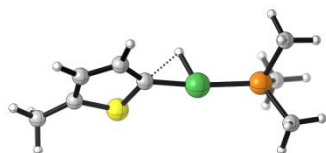
B3LYP electronic energy: -1779.4382976 a.u.  
B3LYP enthalpy: -1778.999777 a.u.  
B3LYP free energy: -1779.090543 a.u.  
M06 SCF energy in solution: -1780.62369499 a.u.  
M06 enthalpy in solution: -1780.18517399 a.u.  
M06 free energy in solution: -1780.27593999 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	0.17996900	1.43381200	0.13313700
C	-0.47646500	2.24754100	1.03393900
C	-1.18196000	3.35459500	0.45773300
C	-1.09121200	3.42187200	-0.90560000
S	-0.10588600	2.08938400	-1.48292700
H	-0.47275900	2.05580800	2.10353400
H	-1.74988200	4.07402300	1.04108900
C	-1.70788900	4.42261800	-1.83691200
H	-0.95495900	4.95882300	-2.42746000
H	-2.40043200	3.95254600	-2.54562300
H	-2.27239500	5.16502400	-1.26451200
Ni	1.17362000	-0.19874300	0.32066000
P	3.14313000	0.88321100	0.59500400
C	3.07907800	2.00371200	2.06151800
H	3.98642300	2.61085900	2.14441200
H	2.20536100	2.65160300	1.96466500
H	2.96464900	1.40696100	2.97116800
C	4.73838800	-0.02053800	0.89172300
H	4.98574100	-0.63283600	0.02000000
H	5.56403200	0.67540000	1.07555200
H	4.63572800	-0.67859300	1.75958200
C	3.62009100	2.02622400	-0.77479800
H	4.50151700	2.62035700	-0.51164800
H	3.83704200	1.44446300	-1.67529400
H	2.77958400	2.68721500	-0.99583500
C	2.63621800	-2.86240800	-0.02872700
C	2.57721600	-3.92349200	-0.91590900
C	1.35234100	-4.19975000	-1.55636200

C	0.24010700	-3.43119600	-1.26296600
C	0.35029100	-2.42818000	-0.27851400
N	1.55823300	-2.12111900	0.29984200
H	1.28040700	-5.01847800	-2.26647200
H	3.56838400	-2.57824000	0.44918100
H	3.46278900	-4.51665200	-1.11569300
H	-0.71970500	-3.61070000	-1.73353000
C	-0.73955200	-1.57448800	0.19520500
H	-0.79582200	-1.50091200	1.27939600
C	-1.99736100	-1.37348500	-0.54170400
H	-0.92218000	-0.43090400	-0.23627100
H	-1.92539600	-1.36813300	-1.62530600
C	-3.28427800	-1.11541100	0.05393400
C	-4.37107300	-0.73785900	-0.77496100
C	-3.54409500	-1.23432200	1.44156600
C	-5.63320700	-0.49451500	-0.24969300
H	-4.20273200	-0.63605300	-1.84442500
C	-4.80791600	-0.97247000	1.96228000
H	-2.75243800	-1.54814800	2.11557100
C	-5.86501100	-0.60256500	1.12654300
H	-6.44360700	-0.21004800	-0.91611700
H	-4.97243100	-1.07087800	3.03242800
H	-6.85078400	-0.40635600	1.53739700

ts7



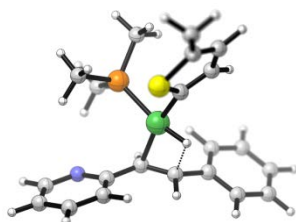
B3LYP electronic energy:	-1222.7270883 a.u.
B3LYP enthalpy:	-1222.505834 a.u.
B3LYP free energy:	-1222.568212 a.u.
M06 SCF energy in solution:	-1224.19148452 a.u.
M06 enthalpy in solution:	-1223.97023052 a.u.
M06 free energy in solution:	-1224.03260752 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	-1.27081200	0.41547400	-0.13451000
C	-2.07093700	1.54342600	-0.06306000
C	-3.46447200	1.27084800	0.06206200
C	-3.77437100	-0.06658200	0.04254900
S	-2.31332400	-1.01133800	-0.13062100

H	-1.66339500	2.54833400	-0.10229800
H	-4.22222300	2.04269600	0.16047800
C	-5.12456900	-0.70705200	0.16778700
H	-5.34823100	-1.36329500	-0.68145400
H	-5.20835800	-1.31399400	1.07748900
H	-5.90060000	0.06314200	0.20913700
Ni	0.53862900	0.16906900	0.06385400
P	2.73931400	-0.07780400	0.04179000
C	3.36084800	-1.41453900	-1.07661500
H	4.45513900	-1.45694200	-1.08759200
H	2.96781700	-2.37965000	-0.74558700
H	2.99568300	-1.23370500	-2.09081900
C	3.68393900	1.39477000	-0.56034000
H	3.49689200	2.24435500	0.10195500
H	4.76058200	1.19779400	-0.59661700
H	3.33229200	1.66397000	-1.55967200
C	3.62313100	-0.47013200	1.62422400
H	4.70311900	-0.56933800	1.47268600
H	3.43840300	0.32353100	2.35377500
H	3.23540200	-1.40507500	2.03868000
H	0.02280200	0.45544000	-1.24756700

ts8



B3LYP electronic energy:	-1779.5026276 a.u.
B3LYP enthalpy:	-1779.063514 a.u.
B3LYP free energy:	-1779.154008 a.u.
M06 SCF energy in solution:	-1780.69768559 a.u.
M06 enthalpy in solution:	-1780.25857259 a.u.
M06 free energy in solution:	-1780.34906559 a.u.

Cartesian coordinates

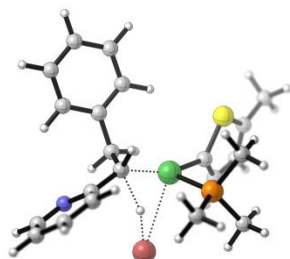
ATOM	X	Y	Z
C	-1.80205500	-0.84223800	-0.24994000
C	-2.38392700	-2.02902000	0.13298500
C	-3.76440200	-2.16708400	-0.23273300
C	-4.26805900	-1.09978500	-0.92343600
S	-3.00444000	0.10493700	-1.12230400



H	-1.83960700	-2.80100700	0.66861600
H	-4.36358300	-3.04086300	0.00852200
C	-5.65139200	-0.90031500	-1.46680900
H	-6.14555200	-0.02156100	-1.03407400
H	-5.65213800	-0.76727100	-2.55558800
H	-6.26987000	-1.77399900	-1.23898400
Ni	-0.05752400	-0.11085600	0.04785300
P	-0.62991300	1.11364300	1.85257800
C	-1.82454600	0.27714500	2.98121300
H	-2.16790200	0.95544800	3.76870500
H	-2.67362500	-0.08495100	2.39847200
H	-1.34019300	-0.58882800	3.44145700
C	0.67277800	1.71227100	3.01976100
H	1.41909600	2.28132300	2.45817600
H	0.24293700	2.33889400	3.80831000
H	1.16842000	0.85462100	3.48517600
C	-1.50558700	2.67150200	1.39190200
H	-1.85702100	3.20761700	2.27943200
H	-0.82324900	3.31511900	0.83062600
H	-2.35669000	2.42386400	0.75277300
C	2.36169400	4.09170100	-0.27868800
C	1.93638700	4.47933500	-1.54871200
C	1.44977700	3.48546200	-2.40029700
C	1.41897100	2.16817700	-1.95823900
C	1.88222400	1.86239100	-0.66124700
N	2.33929900	2.83044800	0.16553900
H	1.09717100	3.73367800	-3.39749000
H	2.74264300	4.83339500	0.42205300
H	1.98066100	5.51956000	-1.85397500
H	1.03284900	1.38652800	-2.60319700
C	1.89352400	0.49645300	-0.10611900
H	2.38826800	0.42199700	0.85654800
C	1.74979500	-0.66762400	-0.89686700
H	-0.02090500	-1.00238500	-1.10331600
H	1.74615600	-0.54883700	-1.97754000
C	2.22437800	-2.00633100	-0.45478300
C	2.57472600	-2.95945300	-1.42381100
C	2.35089700	-2.35802000	0.89998900
C	3.04602200	-4.21905800	-1.05584800
H	2.47732100	-2.70737900	-2.47700400
C	2.82202600	-3.61617300	1.26877800
H	2.07023400	-1.64497700	1.66896700
C	3.17277300	-4.55295600	0.29324000
H	3.31380700	-4.93910700	-1.82384500

H	2.91235900	-3.86802100	2.32173600
H	3.53771300	-5.53395700	0.58294200

ts9



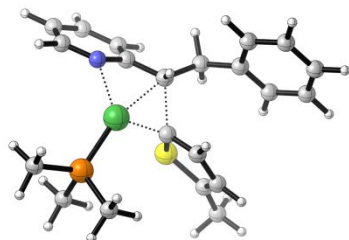
B3LYP electronic energy:	-1793.2736138 a.u.
B3LYP enthalpy:	-1792.822082 a.u.
B3LYP free energy:	-1792.918635 a.u.
M06 SCF energy in solution:	-1794.65901039 a.u.
M06 enthalpy in solution:	-1794.20747839 a.u.
M06 free energy in solution:	-1794.30403139 a.u.

Cartesian coordinates

ATOM	X	Y	Z
Ni	-0.50793000	-0.32667800	-0.05481700
Br	1.04557700	-2.45254000	1.58096700
P	-0.94469200	-1.84854500	-1.55668800
C	-1.93038600	-1.24125300	-2.98772600
H	-2.12616200	-2.05655700	-3.69139900
H	-2.87437200	-0.82892000	-2.62687600
H	-1.38158300	-0.44832100	-3.50288900
C	0.52033200	-2.63245900	-2.35385700
H	1.18041400	-3.03312800	-1.58120500
H	0.20681100	-3.44158100	-3.02138400
H	1.06866800	-1.88622700	-2.93301600
C	-1.88983500	-3.28226100	-0.90827300
H	-2.06232100	-4.01623800	-1.70163800
H	-1.31351400	-3.73866900	-0.10012500
H	-2.83953100	-2.93080000	-0.50293800
C	1.39375800	0.37118700	-0.27673100
H	1.00870500	-1.16643100	0.48321800
C	4.75096700	-0.15308500	1.09973300
C	5.49110800	-0.71211100	0.05939800
C	4.84976900	-0.90008800	-1.16632000
C	3.51313600	-0.54019000	-1.28844400
C	2.83701700	-0.00246600	-0.17751500
N	3.46523000	0.19757500	0.99422200

H	5.38573500	-1.31651100	-2.01482600
H	5.21372900	0.02802100	2.06847700
H	6.53331800	-0.97771700	0.20275100
C	-2.35166300	-0.21979000	0.40781300
C	-2.98467100	-0.81645200	1.47458900
S	-3.47437000	0.89703000	-0.35744100
C	-4.33122100	-0.37499600	1.68926700
H	-2.49638300	-1.55320200	2.10509800
C	-4.76338300	0.55556700	0.78317500
H	-4.95965100	-0.73834200	2.49716900
C	-6.09473200	1.24176900	0.70765800
H	-6.75080500	0.86586500	1.49836900
H	-6.00576700	2.32700100	0.83663700
H	-6.59512900	1.06862700	-0.25246400
C	0.86985200	1.36199900	0.76266000
H	-0.19847600	1.12564400	1.07020100
H	1.44457700	1.21736400	1.68058600
C	0.87017100	2.81090900	0.31618100
C	-0.28092200	3.42547300	-0.19086600
C	2.05895600	3.55201900	0.38875800
C	-0.24403900	4.75239400	-0.62608400
H	-1.21448000	2.86973800	-0.23211100
C	2.09465400	4.87673600	-0.04589200
H	2.95271100	3.08284700	0.79025900
C	0.94353500	5.48136700	-0.55725000
H	-1.14749400	5.21627300	-1.01241300
H	3.02208800	5.43927700	0.01869200
H	0.97174500	6.51405400	-0.89320100
H	2.99200600	-0.66296500	-2.23302500
H	1.18129000	0.69382000	-1.30275800

ts10



B3LYP electronic energy:	-1779.4916788 a.u.
B3LYP enthalpy:	-1779.049190 a.u.
B3LYP free energy:	-1779.137471 a.u.
M06 SCF energy in solution:	-1780.68508891 a.u.
M06 enthalpy in solution:	-1780.24259991 a.u.

M06 free energy in solution: -1780.33088091 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	-0.26567300	-0.68847500	0.11079800
C	-1.08429700	-1.50873700	-0.65423700
C	-1.57032900	-2.66733800	0.02414500
C	-1.18023400	-2.76226800	1.33361800
S	-0.16088200	-1.38740800	1.74647800
H	-1.35079200	-1.26879000	-1.67783900
H	-2.21093300	-3.40789900	-0.44654200
C	-1.49758800	-3.83383500	2.33210000
H	-0.59854700	-4.36012200	2.67712200
H	-1.99746900	-3.43457900	3.22325700
H	-2.16316100	-4.57635900	1.88112100
Ni	1.32388500	0.24302500	-0.43346800
P	2.84931600	-1.22160100	-0.96625600
C	2.23637300	-2.63403300	-1.99331400
H	3.00219500	-3.40457600	-2.13168700
H	1.35871100	-3.06765900	-1.50697800
H	1.92478400	-2.26049600	-2.97307200
C	4.34724600	-0.68823000	-1.92240500
H	4.88331300	0.07789000	-1.35499100
H	5.02612000	-1.52366100	-2.12507500
H	4.03241700	-0.24541900	-2.87163800
C	3.62491700	-2.10652400	0.46497600
H	4.31826100	-2.88733800	0.13362400
H	4.16613700	-1.38757100	1.08658700
H	2.83743600	-2.55405700	1.07689100
C	2.59662600	3.05921500	-0.14987800
C	2.73792700	3.65587200	1.09224700
C	1.76632300	3.38237100	2.07288900
C	0.69015900	2.57065300	1.76418300
C	0.55717600	2.06658900	0.44331700
N	1.54336200	2.28989300	-0.49629200
H	1.85966600	3.80715700	3.06863900
H	3.34678000	3.19550200	-0.92608300
H	3.58524400	4.30045700	1.30018000
H	-0.05791300	2.33393200	2.51265600
C	-0.56140000	1.20758900	-0.01655400
H	-0.70601500	1.33778000	-1.09144700
C	-1.89413400	1.39697400	0.74060300
H	-1.89009500	0.83531200	1.67893200
H	-1.94844700	2.46088900	1.01190500

C	-3.13334000	1.05557700	-0.06158000
C	-3.95921600	-0.01848600	0.29009800
C	-3.49833200	1.84185100	-1.16524600
C	-5.11445000	-0.30433800	-0.44077700
H	-3.68869800	-0.64240700	1.13682600
C	-4.64792700	1.55695200	-1.90176300
H	-2.87874000	2.69092700	-1.44632300
C	-5.46211600	0.48090600	-1.54028700
H	-5.74113200	-1.14335700	-0.15064500
H	-4.91262800	2.17946500	-2.75217200
H	-6.36070300	0.25985500	-2.10949900