

## Supporting Information

### **Computational Mechanism Investigation of Bi(I)/Bi(III) redox catalyzed hydrodefluorination(HDF) of polyfluoroarenes**

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## I. Complete Gaussian 09 Reference

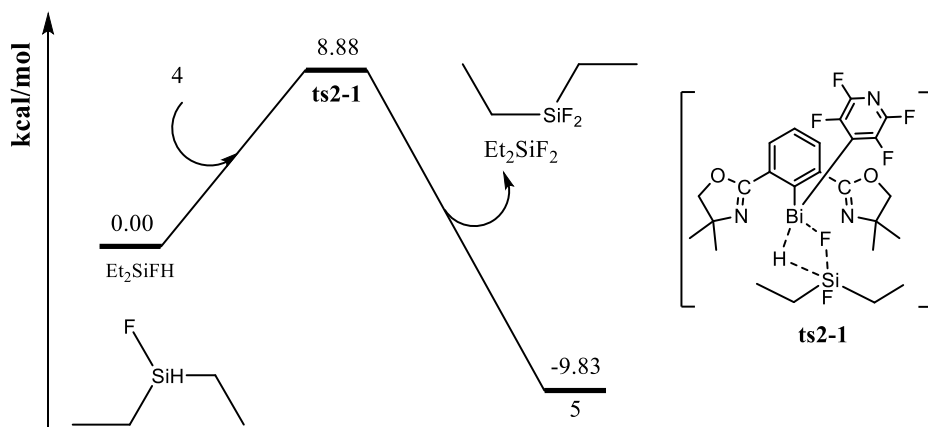
Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, 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-D3 (BJ) (SMD)/def2-SVP method and single point energy corrections were added using B3LYP-D3 (BJ) (SMD)/def2-TZVP method.

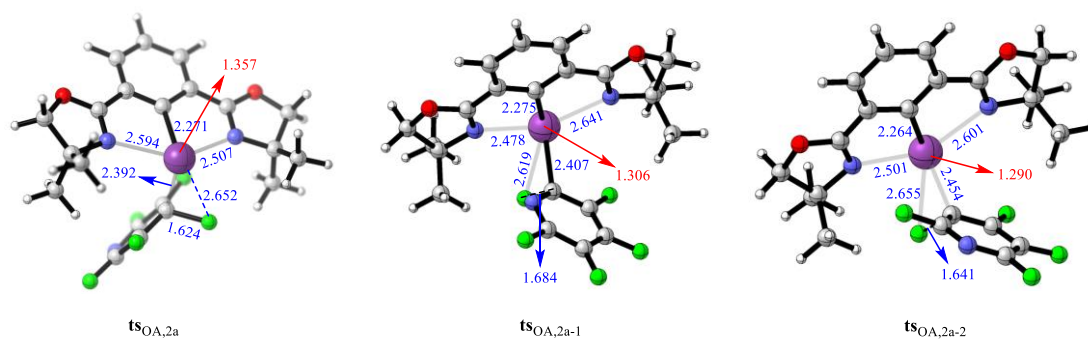
Selected species	Optimized in gas phase without dispersion correction ( <i>kcal/mol</i> )	Optimized in solvent phase with dispersion correction ( <i>kcal/mol</i> )
<b>3a+1a</b>	0.00	0.00
<b>ts1</b>	<b>11.00</b>	<b>9.93</b>
<b>4+Et<sub>2</sub>SiH<sub>2</sub></b>	0.00	0.00
<b>ts2</b>	<b>16.07</b>	<b>17.42</b>

III. Reaction barrier profile for ligand metathesis of **Et<sub>2</sub>SiFH** with intermediate **4**.



**Figure S1.** Reaction barrier profile for ligand metathesis of **Et<sub>2</sub>SiFH** with intermediate **4**.

IV. Comparison of the three oxidative addition transition state structures in Table 1.



**Figure S2.** Calculated structures of transition states with selected bond distances in Angstroms and NPA charge values in a.u..

## V. Frontier Molecular Orbital Analysis of Three Catalysts for Oxidative Addition to Hexafluorobenzene

**Table S2.** Frontier molecular orbital analysis of three catalysts for oxidative addition to hexafluorobenzene.

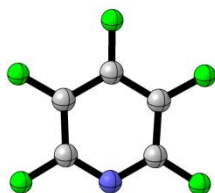
	cat. <b>3a</b> (ev)	cat. <b>3b</b> (ev)	cat. <b>3c</b> (ev)	<b>1b</b> (ev)
LUMO	-1.63	-1.75	-1.69	-0.88
HOMO	-4.20	-4.35	-4.18	7.36
Gap(1b <sub>LUMO</sub> -cat <sub>HOMO</sub> )	3.32	3.47	3.30	

## VI. Cartesian Coordinates\*

\*Among the 6 energy data for each of the following species, the first three energies are calculated with the def2-SVP basis set and then energies 4-6 are calculated with the def2-TZVP basis set.

**The following are the details of the calculation data for each species in Figure 1:**

1a

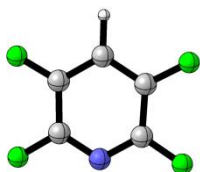


B3LYP electronic energy: -743.8821136 a.u.  
B3LYP enthalpy: -743.823911 a.u.  
B3LYP free energy: -743.867018 a.u.  
B3LYP SCF energy in solution: -744.788476857 a.u.  
B3LYP enthalpy in solution: -744.730273857 a.u.  
B3LYP free energy in solution: -744.773380857 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	-1.13478300	-0.97284300	0.00025900
C	-1.20769800	0.42352600	0.00034100
C	0.00000000	1.12942900	0.00060400
C	1.20769900	0.42354200	0.00038200
C	1.13478200	-0.97283500	0.00044200
N	0.00000700	-1.63123800	0.00024400
F	-2.26162300	-1.66851400	-0.00037900
F	-2.36695300	1.06762200	-0.00019300
F	-0.00002300	2.44995100	-0.00032200
F	2.36695800	1.06762300	-0.00022300
F	2.26163700	-1.66848800	-0.00042400

2a



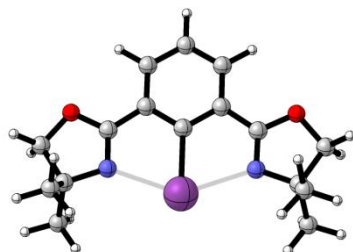


B3LYP electronic energy: -644.7375262 a.u.  
 B3LYP enthalpy: -644.672357 a.u.  
 B3LYP free energy: -644.713236 a.u.  
 B3LYP SCF energy in solution: -645.522838195 a.u.  
 B3LYP enthalpy in solution: -645.457669195 a.u.  
 B3LYP free energy in solution: -645.498548195 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	-1.13528500	-0.70257700	0.00005600
C	-1.19493800	0.69677600	-0.00005000
C	0.00000900	1.41081200	-0.00010900
C	1.19494200	0.69679000	-0.00006700
C	1.13525700	-0.70258400	-0.00002800
N	-0.00000300	-1.35974800	0.00004200
F	-2.26310600	-1.39983700	-0.00002500
F	-2.36829800	1.32323000	0.00005800
F	2.36832300	1.32318800	0.00007200
F	2.26309700	-1.39982200	-0.00000600
H	-0.00003900	2.50209000	0.00000300

3a



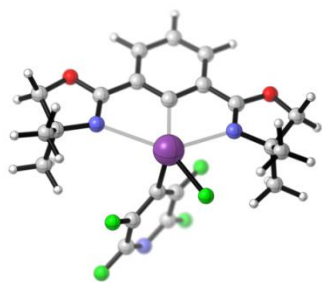
B3LYP electronic energy: -1095.1834881 a.u.  
 B3LYP enthalpy: -1094.837731 a.u.  
 B3LYP free energy: -1094.908824 a.u.  
 B3LYP SCF energy in solution: -1096.26943535 a.u.  
 B3LYP enthalpy in solution: -1095.92367835 a.u.  
 B3LYP free energy in solution: -1095.99477135 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	-1.21909800	1.88942400	-0.01236300
C	-0.00012000	1.16108000	-0.01494400
C	1.21876300	1.88961700	-0.01251100
C	1.21347300	3.29214700	-0.00723700
C	-0.00031500	3.99054400	-0.00389000

C	-1.21402100	3.29192100	-0.00706600
H	2.16309900	3.83301000	-0.00577200
H	-0.00042000	5.08267600	0.00025600
H	-2.16372500	3.83264200	-0.00546000
C	2.42353200	1.08707200	-0.01624400
C	3.77797000	-0.71591100	0.04220100
C	4.60139900	0.59680800	-0.14778700
H	5.39821600	0.72748200	0.59908300
H	5.04194700	0.67026100	-1.15657700
C	-2.42385200	1.08675900	-0.01597900
C	-3.77834800	-0.71613400	0.04211100
C	-4.60187900	0.59672400	-0.14678100
H	-5.04347600	0.67047500	-1.15508300
H	-5.39793400	0.72725900	0.60093700
N	2.39324700	-0.20991900	-0.03240600
N	-2.39361800	-0.21017500	-0.03224600
O	3.64806100	1.66069600	0.00941300
O	-3.64832100	1.66051700	0.00972200
C	-4.05064500	-1.72981300	-1.07417400
H	-3.42522600	-2.62623500	-0.94386100
H	-5.10632600	-2.04743100	-1.06425500
H	-3.82383900	-1.29718100	-2.06025900
C	-4.02199800	-1.34507300	1.42367500
H	-5.05810900	-1.71246300	1.50727000
H	-3.33907100	-2.19225800	1.58693500
H	-3.84649400	-0.61013700	2.22443200
C	4.05021100	-1.73048400	-1.07326300
H	5.10591900	-2.04800000	-1.06320200
H	3.42490900	-2.62687000	-0.94212800
H	3.82324200	-1.29869900	-2.05968100
C	4.02173300	-1.34368000	1.42428700
H	3.33868400	-2.19059800	1.58841300
H	5.05779700	-1.71116300	1.50803600
H	3.84648400	-0.60800600	2.22442400
Bi	0.00033900	-1.03626300	-0.04197900

4-1



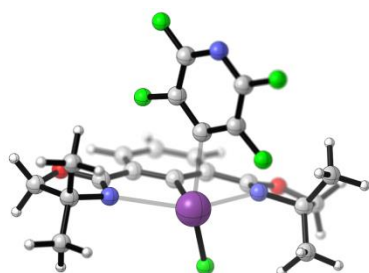
B3LYP electronic energy: -1839.0942677 a.u.  
 B3LYP enthalpy: -1838.689126 a.u.  
 B3LYP free energy: -1838.783677 a.u.  
 B3LYP SCF energy in solution: -1841.11212025 a.u.  
 B3LYP enthalpy in solution: -1840.70697925 a.u.  
 B3LYP free energy in solution: -1840.80152925 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	-0.65975000	-2.47035500	1.06536100
C	0.41221300	-1.70292700	0.58645200
C	1.69595300	-1.99396400	1.06689400
C	1.91896800	-2.98881600	2.03227000
C	0.83257500	-3.72255900	2.51675300
C	-0.45390300	-3.47402100	2.03153100
H	2.93169300	-3.18450100	2.39188700
H	0.98999300	-4.49794800	3.26990900
H	-1.30469400	-4.05422600	2.39494600
C	2.77710500	-1.19724100	0.47843400
C	3.83731800	0.37308000	-0.74971400
C	4.85266400	-0.49278600	0.05700700
H	5.44614900	-1.16387500	-0.58499700
H	5.52861700	0.09610400	0.69191300
C	-1.99595300	-2.20610500	0.50964400
C	-3.71493400	-1.33179700	-0.63346700
C	-4.16034600	-2.62127900	0.12447500
H	-5.01714500	-2.46337200	0.79515400
H	-4.38674800	-3.45986500	-0.55477300
N	2.57396600	-0.35230100	-0.46961600
N	-2.26083000	-1.29380500	-0.35480600
O	4.03226900	-1.32131100	0.91980100
O	-3.01776400	-2.98552300	0.92185900
C	-4.38378500	-0.07748300	-0.04991400
H	-3.97249000	0.82899600	-0.51352100
H	-5.47051600	-0.10092500	-0.23235300
H	-4.21832300	-0.01574600	1.03711400
C	-3.96351500	-1.42828500	-2.14214900

H	-5.04102200	-1.51827800	-2.35572000
H	-3.59026900	-0.52564300	-2.64922700
H	-3.45052000	-2.30289500	-2.57131300
C	3.72535600	1.80184800	-0.19610200
H	4.66211900	2.35487200	-0.37432300
H	2.89414500	2.30366700	-0.71053200
H	3.52480200	1.78827400	0.88662300
C	4.12634400	0.39140600	-2.25227500
H	3.31599300	0.94239300	-2.74998100
H	5.08696800	0.89122900	-2.45677800
H	4.17404100	-0.63167100	-2.65910600
Bi	0.18609000	-0.09222800	-1.18031300
C	-0.35851900	2.88102900	2.34112000
C	0.11065700	1.80734000	1.57307600
C	-0.49243700	1.51840300	0.35485800
C	-1.52727900	2.36266700	-0.02658200
C	-1.93420100	3.40407000	0.81018100
N	-1.35450700	3.64681200	1.96278300
F	0.22021600	3.14748300	3.50935200
F	1.13934300	1.08442200	2.04210500
F	1.28065900	1.60942000	-1.99313800
F	-2.16535300	2.17518100	-1.19875300
F	-2.94618900	4.18624000	0.44288800

4



B3LYP electronic energy: -1839.0880405 a.u.  
 B3LYP enthalpy: -1838.683194 a.u.  
 B3LYP free energy: -1838.779029 a.u.  
 B3LYP SCF energy in solution: -1841.1138232 a.u.  
 B3LYP enthalpy in solution: -1840.7089762 a.u.  
 B3LYP free energy in solution: -1840.8048122 a.u.

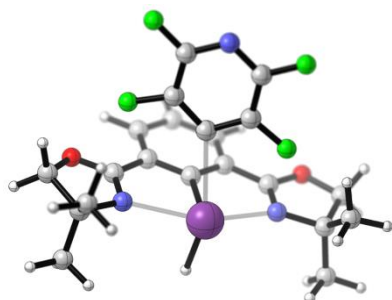
Cartesian coordinates

ATOM	X	Y	Z
C	-0.77801900	-1.87990400	1.69428900
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C	1.60579800	-1.70590300	1.34960900
C	1.83497700	-2.39523100	2.55170600
C	0.74647100	-2.82585300	3.31762100
C	-0.56299300	-2.58011500	2.89271200
H	2.85795800	-2.59570100	2.87696400
H	0.92093000	-3.36453900	4.25157400
H	-1.41463200	-2.92795700	3.48139400
C	2.68112500	-1.23038600	0.47079600
C	3.77221200	-0.22360200	-1.21692800
C	4.77553800	-0.90169300	-0.23184600
H	5.28471200	-1.77294200	-0.67462400
H	5.52812200	-0.21212700	0.17572500
C	-2.10566000	-1.60284500	1.13358800
C	-3.72369400	-0.86252800	-0.25712800
C	-4.28987500	-1.90151400	0.76603400
H	-5.10499000	-1.50013100	1.38512700
H	-4.62138600	-2.83686400	0.28999800
N	2.47149100	-0.66423700	-0.66603700
N	-2.29475800	-0.81789400	0.13052200
O	3.95522400	-1.37211300	0.85912000
O	-3.17858000	-2.22025400	1.63524000
C	-4.36415100	0.51917400	-0.07364900
H	-3.84910200	1.26797400	-0.69044900
H	-5.42605100	0.49023000	-0.36723900
H	-4.30413500	0.84424500	0.97703700
C	-3.84094300	-1.35690600	-1.70568900
H	-4.88772300	-1.60569400	-1.94465100
H	-3.51705800	-0.56886700	-2.40388200
H	-3.19178900	-2.22993200	-1.86696300
C	3.85288100	1.30886100	-1.14031100
H	4.83047100	1.66454700	-1.50410100
H	3.06785000	1.76788000	-1.76021600
H	3.71124500	1.65335700	-0.10517600
C	3.94938400	-0.72004400	-2.65472900
H	3.19376100	-0.26877300	-3.31588900
H	4.94419600	-0.44461700	-3.04069600
H	3.84350800	-1.81413800	-2.71113500
Bi	-0.13723400	-0.45487700	-1.08064900
C	0.61415200	3.56447300	1.62254300
C	0.72297400	2.25445100	1.14076200
C	-0.11996400	1.78923100	0.14177500
C	-1.02822000	2.72884600	-0.32186600
C	-1.08561100	4.01882400	0.21262200
N	-0.27482900	4.41736000	1.16636000

F	1.43866500	3.98772300	2.58304000
F	1.68816900	1.46791100	1.67310800
F	-0.78352900	-2.42098800	-1.73465200
F	-1.89095700	2.40909700	-1.32409700
F	-1.98090100	4.89495400	-0.24681300

5-1



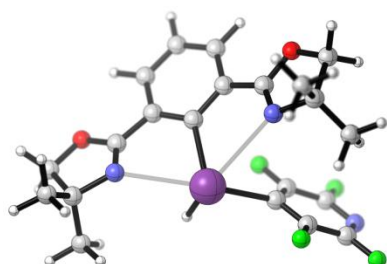
B3LYP electronic energy:	-1739.8639467 a.u.
B3LYP enthalpy:	-1739.456734 a.u.
B3LYP free energy:	-1739.551393 a.u.
B3LYP SCF energy in solution:	-1741.75401673 a.u.
B3LYP enthalpy in solution:	-1741.34680473 a.u.
B3LYP free energy in solution:	-1741.44146273 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	-1.42941400	-0.88804900	1.97149000
C	-0.28304200	-1.07261300	1.19586700
C	0.93868600	-1.36062400	1.80988900
C	1.02303600	-1.45298700	3.20881500
C	-0.12803600	-1.26172500	3.98044800
C	-1.35592400	-0.98034700	3.37178300
H	1.98279300	-1.66927400	3.68286600
H	-0.06718200	-1.32989800	5.06875300
H	-2.25424700	-0.83011400	3.97436000
C	2.07509600	-1.54788300	0.90404700
C	3.28118300	-1.78649300	-0.98899000
C	4.20270300	-1.74500900	0.26894800
H	4.88142400	-2.60552900	0.34709500
H	4.77617800	-0.80886200	0.33882700
C	-2.66434400	-0.59955400	1.23297000
C	-4.12276600	-0.28585500	-0.45419800
C	-4.79942300	-0.01528400	0.92787900
H	-5.05013600	1.04661900	1.07683800
H	-5.69465000	-0.62774300	1.10668400

N	1.95938000	-1.50833800	-0.38037900
N	-2.72333600	-0.55339600	-0.05241700
O	3.29291800	-1.78364000	1.39334900
O	-3.80042500	-0.37708700	1.90708700
C	-4.20242200	0.93459400	-1.37677400
H	-3.70288500	0.73022300	-2.33599200
H	-5.25465700	1.18405800	-1.58969600
H	-3.71032700	1.80617200	-0.92362100
C	-4.69800500	-1.53709300	-1.13459000
H	-5.74825100	-1.37130400	-1.42445500
H	-4.12548100	-1.78111600	-2.04222000
H	-4.65490700	-2.40797400	-0.46210300
C	3.65961300	-0.70912600	-2.00905600
H	4.67683800	-0.88878300	-2.39316600
H	2.97108900	-0.72660700	-2.86835800
H	3.62281700	0.28621000	-1.54743100
C	3.25306100	-3.18122400	-1.63356300
H	2.49543900	-3.22436700	-2.43055400
H	4.23341500	-3.42088500	-2.07610500
H	3.00624500	-3.95587700	-0.89104000
Bi	-0.32664500	-0.83404000	-1.05325300
C	2.18543100	3.50375200	0.55204400
C	1.96138600	2.15142800	0.27502600
C	0.77486200	1.69636800	-0.27205500
C	-0.13743900	2.71174000	-0.49880400
C	0.13634600	4.04897700	-0.19924600
N	1.28317100	4.43120100	0.31794700
F	3.35107900	3.90100800	1.07824500
F	2.98680700	1.28649400	0.56469900
F	-1.36572900	2.42748300	-1.03737000
F	-0.77931100	4.99753300	-0.43430900
H	-0.60558300	-2.73071400	-1.12320600

5



B3LYP electronic energy: -1739.8873245 a.u.

B3LYP enthalpy: -1739.479029 a.u.

B3LYP free energy: -1739.573608 a.u.  
B3LYP SCF energy in solution: -1741.76863037 a.u.  
B3LYP enthalpy in solution: -1741.36033437 a.u.  
B3LYP free energy in solution: -1741.45491437 a.u.

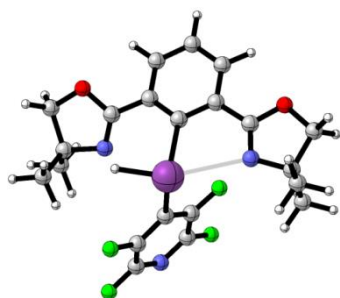
Cartesian coordinates

ATOM	X	Y	Z
C	0.12259000	2.30001600	0.55979200
C	1.03504900	1.23882500	0.39499700
C	2.33473800	1.39809600	0.91796200
C	2.66088800	2.50992800	1.71667700
C	1.71036600	3.49823200	1.96093200
C	0.45681800	3.41048700	1.35823000
H	3.66981500	2.59203200	2.12408800
H	1.95805600	4.35657500	2.58949400
H	-0.27580400	4.20865200	1.48391800
C	3.40587700	0.45676500	0.54606200
C	4.62308800	-1.12456900	-0.46537700
C	-1.14786700	2.33905700	-0.19311800
N	3.34492200	-0.38808400	-0.41263500
N	-1.50656100	1.52035000	-1.10594000
C	-2.47805600	2.42592300	-3.16145400
H	-2.13780500	1.55588900	-3.74291400
H	-3.38738100	2.82762600	-3.63786800
H	-1.69230800	3.19615900	-3.20746500
C	-3.85823900	0.95010800	-1.65059300
H	-4.78666600	1.32509600	-2.11131100
H	-3.54633300	0.04268300	-2.18734900
H	-4.08037700	0.67075300	-0.60998500
C	4.38890600	-2.59862700	-0.10201100
H	5.33958500	-3.15633600	-0.11909300
H	3.94638300	-2.69160100	0.90140900
H	3.70121600	-3.06965700	-0.82043800
C	5.47930300	-0.38902500	0.61648100
H	5.87989700	-1.06146500	1.38976600
H	6.31111900	0.18980800	0.18295200
C	-2.76082100	2.01824200	-1.70701100
C	-3.10110000	3.25236200	-0.81122100
H	-3.99271500	3.09147900	-0.18402600
H	-3.22982600	4.18573500	-1.38018600
C	5.23688300	-1.00236800	-1.86548100
H	5.37522300	0.05403700	-2.14260100
H	6.21710500	-1.50493300	-1.90730300
H	4.57992100	-1.46776500	-2.61575800



O	4.56557200	0.52870700	1.24162800
O	-1.96076000	3.39833100	0.05150900
Bi	0.47852500	-0.74352600	-0.68740100
C	-2.97721300	-1.27779800	2.40852700
C	-1.77392700	-0.88537700	1.80903100
C	-1.53504300	-1.18400100	0.47185900
C	-2.54312900	-1.88567400	-0.17681900
C	-3.71154800	-2.24110400	0.50314300
N	-3.91327200	-1.93618000	1.76387700
F	-3.20086300	-0.97871100	3.68708100
F	-0.87401500	-0.21903500	2.54620400
F	-2.42027500	-2.21946500	-1.47777200
F	-4.67133300	-2.90756300	-0.13724700
H	1.21218000	-1.75504000	0.63868700

5-2



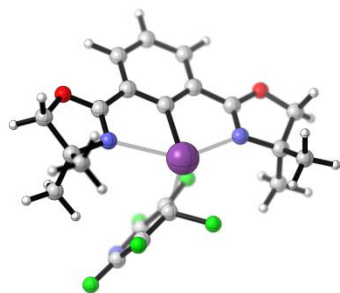
B3LYP electronic energy: -1739.8742377 a.u.  
 B3LYP enthalpy: -1739.466315 a.u.  
 B3LYP free energy: -1739.562157 a.u.  
 B3LYP SCF energy in solution: -1741.7551949 a.u.  
 B3LYP enthalpy in solution: -1741.3472719 a.u.  
 B3LYP free energy in solution: -1741.4431139 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	1.95627700	-1.87648400	0.63389500
C	0.64184500	-1.62494500	0.16816500
C	-0.37436800	-2.53333900	0.54250900
C	-0.05215700	-3.70451200	1.25869500
C	1.25403500	-3.96221200	1.66122300
C	2.25194400	-3.03617400	1.37428600
H	-0.85429000	-4.40056200	1.50802300
H	1.48910900	-4.87123300	2.21968200
H	3.27356700	-3.19558500	1.71966800
C	-1.82467800	-2.30311800	0.32013900
C	-3.87722800	-1.45504600	0.16040700

C	3.05829700	-0.90844300	0.43598700
N	-2.43981500	-1.19078800	0.36750100
N	2.99609200	0.20556300	-0.18418000
C	4.86890800	1.22116300	-1.42798000
H	4.19868700	1.90084900	-1.97573800
H	5.85251100	1.70998500	-1.33475200
H	4.99298100	0.30611600	-2.02774500
C	4.08237400	2.17855500	0.77450600
H	5.04107900	2.69812400	0.93701800
H	3.40256500	2.86408400	0.24640900
H	3.63394600	1.94918200	1.75277400
C	-4.68003400	-0.85766400	1.32200900
H	-5.75334800	-1.08611100	1.21534200
H	-4.33271900	-1.25987100	2.28629800
H	-4.56146600	0.23596100	1.34762100
C	-3.94427300	-3.01593400	0.13833500
H	-4.43854500	-3.43475600	1.03098100
H	-4.43309400	-3.42175100	-0.76023900
C	4.29030200	0.89633900	-0.04542200
C	5.15516800	-0.15575400	0.72111900
H	5.56871800	0.22467000	1.66751100
H	5.97854400	-0.56146000	0.11111800
C	-4.32189100	-0.84317500	-1.17702500
H	-3.77915100	-1.30231700	-2.01755000
H	-5.40235700	-0.99729400	-1.33378600
H	-4.11384600	0.23606100	-1.19749300
O	-2.57012200	-3.43382700	0.13902200
O	4.24305900	-1.22445300	1.02079200
Bi	0.35114400	0.06140000	-1.42514900
C	-0.96301800	2.74980900	2.07787100
C	-0.26151200	1.83161200	1.28739800
C	-0.70129300	1.56072200	-0.00414000
C	-1.82416300	2.26102100	-0.42979900
C	-2.46021000	3.15386700	0.43689500
N	-2.02995400	3.38581400	1.65509900
F	-0.54066000	3.00010100	3.31528500
F	0.81574600	1.22492400	1.80490000
F	-2.32489700	2.07943000	-1.66303900
F	-3.54822600	3.80258100	0.02637300
H	-1.23925500	-0.64917900	-1.98131200

ts1



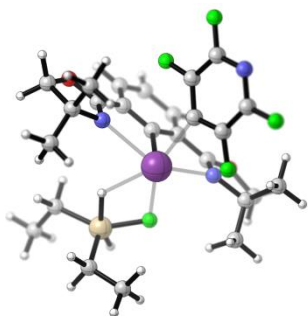
B3LYP electronic energy: -1839.0445142 a.u.  
 B3LYP enthalpy: -1838.640820 a.u.  
 B3LYP free energy: -1838.732478 a.u.  
 B3LYP SCF energy in solution: -1841.06267862 a.u.  
 B3LYP enthalpy in solution: -1840.65898462 a.u.  
 B3LYP free energy in solution: -1840.75064162 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	0.43638700	2.50720900	1.07289000
C	-0.58392400	1.69905700	0.55495200
C	-1.89453700	1.86062100	1.02355500
C	-2.18576600	2.80758900	2.01793800
C	-1.15486100	3.59730000	2.53945500
C	0.15509200	3.45744500	2.06915000
H	-3.21079700	2.92103100	2.37755100
H	-1.37550300	4.33132700	3.31742000
H	0.95915600	4.07907500	2.46890200
C	-2.89477200	0.99052900	0.40210900
C	-3.81574200	-0.66248700	-0.82437200
C	-4.90969900	0.21827400	-0.15241800
H	-5.43440700	0.87094700	-0.87024400
H	-5.64571300	-0.35753600	0.42399700
C	1.76959100	2.30316000	0.49908900
C	3.48094200	1.44775200	-0.69022000
C	3.90104900	2.76540600	0.02850400
H	4.80124900	2.66062100	0.64904800
H	4.03538800	3.60882900	-0.66887000
N	-2.59582000	0.12592900	-0.50729100
N	2.02450000	1.40999600	-0.39677000
O	-4.17981800	1.06907800	0.76442000
O	2.78691100	3.08039100	0.89391700
C	4.17172400	0.22812500	-0.06146700
H	3.79484600	-0.70530500	-0.49756700
H	5.25823300	0.27913800	-0.23864700
H	4.00143000	0.19587700	1.02576100
C	3.72361900	1.49920300	-2.20030000

H	4.79878400	1.60494200	-2.41647100
H	3.37513600	0.56803500	-2.67215200
H	3.19094700	2.34599700	-2.66013300
C	-3.72624100	-2.04560100	-0.16123100
H	-4.63825100	-2.62387800	-0.38273100
H	-2.84565300	-2.58550700	-0.53142000
H	-3.62394800	-1.94966700	0.92973000
C	-4.00266200	-0.78440100	-2.33753800
H	-3.19152600	-1.39026100	-2.76884900
H	-4.95646900	-1.28418100	-2.57044400
H	-4.00055800	0.20463400	-2.82201000
Bi	-0.16386400	0.21219400	-1.11070500
C	0.70464200	-2.75251400	2.28459400
C	-0.08064100	-2.01768000	1.41117200
C	0.32720800	-1.81227100	0.06606100
C	1.61419700	-2.34685700	-0.20260600
C	2.31759000	-3.04583100	0.75911600
N	1.87718000	-3.27616800	1.98028200
F	0.26901600	-2.92764000	3.53807400
F	-1.22904400	-1.44444700	1.85275900
F	-0.74419400	-2.37407000	-1.01862500
F	2.18256900	-2.07889800	-1.41349400
F	3.54292200	-3.49544000	0.45293000

ts2



B3LYP electronic energy: -2288.0491494 a.u.  
 B3LYP enthalpy: -2287.487688 a.u.  
 B3LYP free energy: -2287.604753 a.u.  
 B3LYP SCF energy in solution: -2290.38577416 a.u.  
 B3LYP enthalpy in solution: -2289.82431316 a.u.  
 B3LYP free energy in solution: -2289.94137816 a.u.

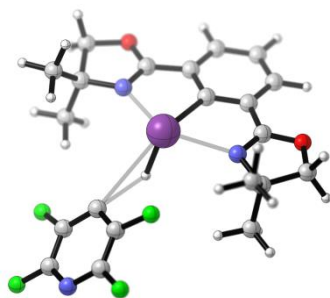
Cartesian coordinates

ATOM	X	Y	Z
C	0.38020200	-0.80439700	2.49594200

C	0.41170000	0.25124800	1.58324800
C	0.66465600	1.55267200	2.02017000
C	0.91621700	1.80247800	3.37921700
C	0.90460900	0.73821200	4.28688700
C	0.63514700	-0.56533800	3.85636100
H	1.11743900	2.82110700	3.71709100
H	1.10365500	0.92764900	5.34389000
H	0.61820900	-1.39461600	4.56658300
C	0.62645300	2.59517300	0.98842100
C	0.34080600	3.63004000	-0.99309900
C	0.84831600	4.63045700	0.09515700
H	1.87142700	4.98839200	-0.09839100
H	0.18319600	5.49314000	0.24148500
C	0.05954800	-2.12686800	1.94130000
C	-0.54010000	-3.75223200	0.49756600
C	-0.08534300	-4.35447800	1.86707500
H	-0.85482500	-4.97382700	2.34988300
H	0.85024100	-4.92913000	1.79123900
N	0.35367200	2.35216600	-0.24628700
N	-0.32611300	-2.30317200	0.72706300
O	0.87104800	3.86585700	1.32154600
O	0.16872000	-3.20999900	2.71520100
C	-2.02730100	-4.01405600	0.22212500
H	-2.35123400	-3.47261800	-0.67771200
H	-2.20354200	-5.09010800	0.06278800
H	-2.65076000	-3.68226000	1.06727100
C	0.33837500	-4.24458800	-0.65853200
H	0.29381400	-5.34360900	-0.72859200
H	-0.01758300	-3.83445400	-1.61626200
H	1.37960200	-3.92343200	-0.51630200
C	-1.09765000	3.94791400	-1.42770000
H	-1.13744900	4.91896400	-1.94705700
H	-1.47372300	3.17552400	-2.11542500
H	-1.76938900	3.98393200	-0.55726500
C	1.28603800	3.56281500	-2.19674200
H	0.93476500	2.81588000	-2.92511600
H	1.32872500	4.53821200	-2.70773800
H	2.30269300	3.28140100	-1.88487900
Bi	0.13647500	-0.17494900	-0.62472100
C	-4.40741100	1.22519500	0.26631200
C	-3.00989000	1.16456600	0.33870200
C	-2.30151400	0.25210000	-0.43300300
C	-3.08843900	-0.54941500	-1.24911400
C	-4.48120600	-0.43501100	-1.25892100

N	-5.11496600	0.44007700	-0.51302100
F	-5.06583400	2.11101700	1.01291100
F	-2.38734500	2.02320200	1.17222500
F	2.24816300	-1.68249800	-0.32360600
F	-2.51097200	-1.47776900	-2.05304500
F	-5.20849600	-1.22857300	-2.04324200
Si	3.64752300	-0.58106600	-0.65489800
H	2.37883100	0.45007200	-0.79998500
H	4.46507400	-1.63886900	0.07983600
C	4.64257200	0.93925900	0.04116500
C	6.14842100	0.71401500	0.20447400
H	4.19408800	1.19913600	1.02005600
H	4.44124400	1.80929800	-0.61329600
H	6.65959400	1.57799700	0.66597300
H	6.35255600	-0.16666700	0.83654900
H	6.63994400	0.52925700	-0.76616900
C	4.07592200	-0.81559700	-2.50248500
C	3.40566500	-2.00864000	-3.19602500
H	5.17420400	-0.92964000	-2.55815800
H	3.84102300	0.11865600	-3.04475200
H	3.73058800	-2.11630100	-4.24566800
H	3.63758800	-2.95537300	-2.68096700
H	2.30652800	-1.91391800	-3.20493300

ts3



B3LYP electronic energy: -1739.8473703 a.u.  
 B3LYP enthalpy: -1739.441069 a.u.  
 B3LYP free energy: -1739.535131 a.u.  
 B3LYP SCF energy in solution: -1741.73457199 a.u.  
 B3LYP enthalpy in solution: -1741.32827099 a.u.  
 B3LYP free energy in solution: -1741.42233299 a.u.

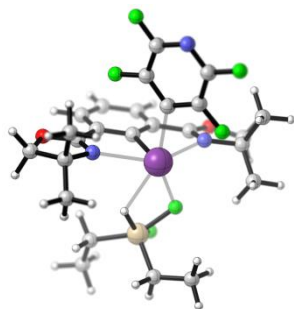
Cartesian coordinates

ATOM	X	Y	Z
C	-3.04011900	-1.48202700	-0.44941200

C	-2.49271300	-0.20599300	-0.26582300
C	-3.24325800	0.92515900	-0.61099200
C	-4.54225700	0.78602800	-1.12786500
C	-5.08239300	-0.49470800	-1.29570200
C	-4.33926100	-1.63321000	-0.96247400
H	-5.12072400	1.67249600	-1.39783700
H	-6.09210900	-0.60680400	-1.69666800
H	-4.75905200	-2.63197800	-1.10245300
C	-2.56677600	2.21285500	-0.41415600
C	-0.95775600	3.73373100	0.03565000
C	-2.15307400	-2.59690100	-0.09979000
N	-1.36296900	2.30813100	0.04053800
N	-0.94946500	-2.42090800	0.33277800
C	0.71810100	-3.90628900	-0.70232800
H	1.50679200	-3.14101300	-0.65813600
H	1.19923000	-4.89620300	-0.64541800
H	0.21242400	-3.82528000	-1.67763600
C	0.40048800	-3.89732000	1.80603500
H	0.81560800	-4.91208500	1.91382800
H	1.23333600	-3.18342300	1.89410600
H	-0.30482500	-3.71992400	2.63282200
C	-0.44604000	4.15193200	1.41806400
H	-0.22096300	5.23043200	1.43406200
H	-1.19408700	3.94149700	2.19822400
H	0.47978400	3.60923600	1.65999200
C	-2.30366200	4.43226900	-0.33894000
H	-2.76395900	4.95769100	0.51284100
H	-2.21660300	5.12529500	-1.18737600
C	-0.28717600	-3.74461500	0.44752700
C	-1.50904900	-4.69877300	0.28627500
H	-1.86086600	-5.10684300	1.24791300
H	-1.33490100	-5.52391500	-0.41741800
C	0.12411600	3.95236700	-1.03275100
H	-0.23507900	3.64635500	-2.02780400
H	0.40489700	5.01703400	-1.07721700
H	1.02130000	3.36785900	-0.78572500
O	-3.19042600	3.35536400	-0.72585300
O	-2.56286300	-3.86162100	-0.24966900
Bi	-0.39754200	0.02031600	0.62086300
C	4.41318600	1.48787000	0.01863800
C	3.12017800	0.97534000	0.12546800
C	2.78250800	-0.30442400	-0.25924900
C	3.85657100	-1.02214400	-0.75525200
C	5.13825300	-0.46443400	-0.83704600

N	5.40454600	0.76810800	-0.45739100
F	4.68662900	2.74349200	0.40191900
F	2.14580800	1.82529100	0.63728400
F	3.70981400	-2.30893400	-1.17767600
F	6.15848300	-1.18687900	-1.31705900
H	0.76146800	-0.14087600	-0.77454100

Ts2-1



B3LYP electronic energy:	-2387.2888377 a.u.
B3LYP enthalpy:	-2386.731452 a.u.
B3LYP free energy:	-2386.850271 a.u.
B3LYP SCF energy in solution:	-2389.75803444 a.u.
B3LYP enthalpy in solution:	-2389.20064844 a.u.
B3LYP free energy in solution:	-2389.31946744 a.u.

Cartesian coordinates

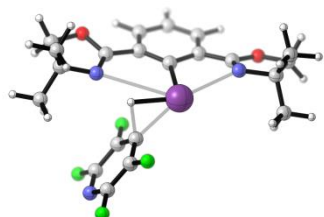
ATOM	X	Y	Z
C	0.50020200	-0.71468700	2.40982500
C	0.36826900	0.33825700	1.50437600
C	0.55757600	1.65668900	1.91992100
C	0.89933300	1.92951100	3.25454400
C	1.04498000	0.86996600	4.15637000
C	0.84774700	-0.45257600	3.74508700
H	1.05061400	2.96136800	3.57792200
H	1.31668700	1.07764800	5.19351400
H	0.96127200	-1.27855500	4.45015600
C	0.36637600	2.68596400	0.89183300
C	-0.13645800	3.68234200	-1.06632200
C	0.38289600	4.72351200	-0.02279400
H	1.36261000	5.14671800	-0.29335500
H	-0.32539000	5.54155400	0.17009400
C	0.25002200	-2.05862800	1.87113000
C	-0.31803400	-3.72639600	0.46102700
C	0.31325200	-4.28794300	1.77596900
H	-0.34302500	-4.98885400	2.31104000



H	1.29482000	-4.75765900	1.61209300
N	0.01781000	2.41411900	-0.31817300
N	-0.21881400	-2.26339300	0.68949400
O	0.54798600	3.97226500	1.20111200
O	0.51717200	-3.12945700	2.61922800
C	-1.79316700	-4.12789400	0.32020100
H	-2.24557700	-3.62970100	-0.54844700
H	-1.87992100	-5.21724500	0.17803100
H	-2.36689600	-3.84985500	1.21831900
C	0.49192600	-4.13009900	-0.77606200
H	0.53426900	-5.22810500	-0.86097700
H	0.01677700	-3.74267800	-1.69070000
H	1.51059300	-3.72215200	-0.72067400
C	-1.62136900	3.90078800	-1.39292300
H	-1.76521600	4.86682600	-1.90304800
H	-1.99361000	3.10544200	-2.05627100
H	-2.22850500	3.89029600	-0.47557500
C	0.71883100	3.66863100	-2.33721200
H	0.36199800	2.89739600	-3.03716000
H	0.66047900	4.64198600	-2.85043700
H	1.77189200	3.45447400	-2.10178400
Bi	-0.02741200	-0.12670100	-0.67445200
C	-4.58066300	0.86273400	0.46079200
C	-3.18088500	0.92067100	0.45444100
C	-2.44615500	0.06151000	-0.35400200
C	-3.20620300	-0.81192400	-1.12103900
C	-4.60178900	-0.81384700	-1.04982500
N	-5.26178100	0.01327100	-0.27280700
F	-5.26676300	1.69815100	1.23811100
F	-2.58470700	1.83298000	1.24564500
F	2.19571000	-1.43968000	-0.53800400
F	-2.59716000	-1.69378600	-1.95093900
F	-5.30290000	-1.67295300	-1.78581800
Si	3.52888100	-0.21785900	-0.66885800
H	2.25152300	0.70968900	-0.93591200
C	4.44734900	1.38961800	-0.09544600
C	5.94414800	1.27641800	0.21362600
H	3.91160200	1.76366400	0.79961900
H	4.26233200	2.15194600	-0.87844100
H	6.38309300	2.23633400	0.54149600
H	6.12106600	0.53448900	1.00715000
H	6.51793700	0.94525800	-0.66910600
C	4.23988400	-0.67949000	-2.36663000
C	3.66402400	-1.91433800	-3.06965600

H	5.32692100	-0.81374900	-2.21725500
H	4.14269000	0.20905800	-3.01809300
H	4.17242500	-2.11880100	-4.02808100
H	3.76550800	-2.81512200	-2.44369700
H	2.58944700	-1.79829700	-3.28789200
F	4.28227300	-1.16808800	0.49381200

ts3-1



B3LYP electronic energy:	-1739.8316558 a.u.
B3LYP enthalpy:	-1739.426027 a.u.
B3LYP free energy:	-1739.520895 a.u.
B3LYP SCF energy in solution:	-1741.71033468 a.u.
B3LYP enthalpy in solution:	-1741.30470668 a.u.
B3LYP free energy in solution:	-1741.39957368 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	-0.02577100	2.45812400	0.24427900
C	-0.96803900	1.39457500	0.19893400
C	-2.27225500	1.67162200	0.69284800
C	-2.59179200	2.89199500	1.31427300
C	-1.63259200	3.89107400	1.41663800
C	-0.37644200	3.68080600	0.85927900
H	-3.60189100	3.04335000	1.69690200
H	-1.86736900	4.84045200	1.90294300
H	0.36743000	4.47563100	0.88940700
C	-3.37756800	0.71598000	0.50925200
C	-4.65730100	-1.00311100	-0.15937600
C	-5.47554500	-0.03875600	0.75663200
H	-6.28117600	0.48317400	0.21488300
H	-5.90267500	-0.53177600	1.64227500
C	1.33156100	2.44112900	-0.36267100
C	3.28175800	1.96716300	-1.35863300
C	3.24065800	3.47549700	-0.96630800
H	3.96364500	3.72799500	-0.17261100
H	3.39584900	4.15559800	-1.81755500
N	-3.36539800	-0.29770400	-0.27604600

N	2.01133000	1.45910800	-0.81063200
O	-4.51986900	0.94054300	1.19921100
O	1.91638900	3.67487600	-0.45821700
C	4.46339500	1.23748500	-0.70834400
H	4.44572300	0.16676000	-0.96108800
H	5.42054400	1.65617000	-1.06039600
H	4.42624400	1.32863400	0.38800400
C	3.28822500	1.76893100	-2.88216500
H	4.22713100	2.14585600	-3.32004100
H	3.19324400	0.70141500	-3.13143900
H	2.44722200	2.30403300	-3.35034100
C	-4.43943200	-2.37232600	0.50259500
H	-5.39622700	-2.90890600	0.60985300
H	-3.76388500	-2.99243900	-0.10589000
H	-3.99120200	-2.25989600	1.50200500
C	-5.29415400	-1.16242000	-1.54467500
H	-4.66399500	-1.79462500	-2.18845900
H	-6.28711200	-1.63466100	-1.46673700
H	-5.41142400	-0.18485900	-2.03693100
Bi	-0.69260800	-0.79681400	-0.60929800
C	3.27665000	-1.15802800	1.93692000
C	2.08415300	-0.63829600	1.43011900
C	1.42659900	-1.30289700	0.38790900
C	2.01753900	-2.51084900	-0.01282300
C	3.19974900	-2.95159300	0.57408400
N	3.81942800	-2.27965500	1.52124500
F	3.91357300	-0.48364800	2.89660400
F	1.58735900	0.48392100	1.96640100
F	1.44183400	-3.22984500	-0.99476400
F	3.74294200	-4.10047200	0.17199800
H	1.16899600	-0.44818400	-0.96772900

The following are the details of the calculation data for each species in Figure 4:

3b



B3LYP electronic energy: -947.2521549 a.u.

B3LYP enthalpy: -946.874346 a.u.

B3LYP free energy: -946.945497 a.u.

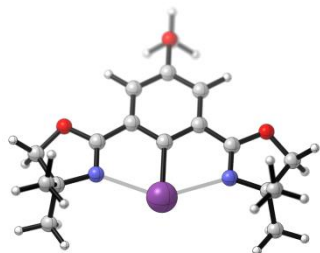
B3LYP SCF energy in solution: -948.1686859 a.u.  
B3LYP enthalpy in solution: -947.790876893 a.u.  
B3LYP free energy in solution: -947.862027893 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	1.22687200	2.09497100	-0.00000100
C	0.00007300	1.38322700	0.00002200
C	-1.22671700	2.09501300	0.00002800
C	-1.21336100	3.50072400	0.00001100
C	0.00012700	4.19985300	-0.00002400
C	1.21362800	3.50062300	-0.00002500
H	-2.15891500	4.05294900	0.00000400
H	0.00018600	5.29219600	-0.00005600
H	2.15919700	4.05282200	-0.00005200
C	-2.44623500	1.31806500	0.00001800
C	-3.64586100	-0.78081200	-0.00004800
C	-4.46876500	-0.47334700	-1.26717300
H	-3.86747800	-0.65832900	-2.17081400
H	-5.36417400	-1.11343200	-1.31012000
C	2.44641900	1.31791900	-0.00002100
C	3.64603700	-0.78091800	-0.00003400
C	4.46825400	-0.47426100	-1.26778700
H	5.36362900	-1.11438900	-1.31080700
H	3.86648900	-0.65979400	-2.17099500
N	-2.39591100	0.02017700	-0.00004300
N	2.39610000	0.02010800	0.00005100
C	4.46928000	-0.47303100	1.26675900
H	3.86822100	-0.65761100	2.17063300
H	5.36465800	-1.11315600	1.30972100
H	4.80578900	0.57492100	1.28924100
C	3.25883900	-2.26772100	0.00083900
H	4.15831300	-2.90271000	0.00089500
H	2.66540500	-2.51788800	0.89418600
H	2.66489900	-2.51879500	-0.89192200
C	-4.46841400	-0.47366900	1.26737100
H	-5.36387600	-1.11367700	1.31035700
H	-3.86691700	-0.65895000	2.17081100
H	-4.80471200	0.57433000	1.29071900
C	-3.25877800	-2.26764100	-0.00029500
H	-2.66485100	-2.51838900	0.89256600
H	-4.15831400	-2.90254500	-0.00005500
H	-2.66538900	-2.51823800	-0.89355100
Bi	-0.00013900	-0.78602500	0.00003700

H	3.40611400	1.85821400	-0.00005000
H	4.80470100	0.57368300	-1.29159500
H	-3.40596400	1.85826300	0.00004900
H	-4.80521400	0.57461200	-1.29016400

3c



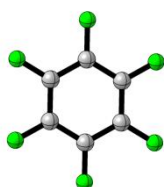
B3LYP electronic energy:	-1209.6140998 a.u.
B3LYP enthalpy:	-1209.234743 a.u.
B3LYP free energy:	-1209.310580 a.u.
B3LYP SCF energy in solution:	-1210.84027125 a.u.
B3LYP enthalpy in solution:	-1210.46091425 a.u.
B3LYP free energy in solution:	-1210.53675125 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	-1.21755300	1.50548000	0.12316900
C	-0.00000100	0.77837400	0.06981900
C	1.21755800	1.50547700	0.12305300
C	1.21571700	2.90419400	0.22308100
C	0.00001400	3.59994400	0.27256400
C	-1.21569600	2.90419400	0.22323200
H	2.15405000	3.46060200	0.27657600
H	-2.15402000	3.46061000	0.27681100
C	2.42319800	0.70485900	0.07553200
C	3.77726200	-1.09829900	0.02521100
C	4.60340000	0.22419400	-0.06170600
H	5.38392000	0.30424400	0.70914400
H	5.06568800	0.36382800	-1.05354600
C	-2.42320700	0.70487500	0.07570600
C	-3.77730300	-1.09825100	0.02510900
C	-4.60342900	0.22427100	-0.06146200
H	-5.06580400	0.36410900	-1.05323300
H	-5.38388000	0.30418100	0.70947400
N	2.39311000	-0.58816800	-0.02426500
N	-2.39315000	-0.58812600	-0.02441900
O	3.64658600	1.27660100	0.14525600

O	-3.64658100	1.27662300	0.14562400
C	-4.05803600	-2.02862300	-1.15966500
H	-3.42904300	-2.93010400	-1.10121000
H	-5.11287200	-2.34923100	-1.16313100
H	-3.84186300	-1.52420400	-2.11354700
C	-4.00894700	-1.82573300	1.35945000
H	-5.04507500	-2.19653100	1.42638000
H	-3.32639900	-2.68360500	1.45412400
H	-3.82403700	-1.15102600	2.20952900
C	4.05784700	-2.02890300	-1.15941600
H	5.11267700	-2.34952900	-1.16293700
H	3.42884400	-2.93036200	-1.10072100
H	3.84157700	-1.52466100	-2.11337000
C	4.00905300	-1.82552600	1.35966600
H	3.32650700	-2.68337200	1.45458900
H	5.04518500	-2.19632300	1.42654800
H	3.82425100	-1.15065100	2.20963500
Bi	0.00000300	-1.41502000	-0.09166700
O	0.00001500	4.96877300	0.41524500
C	0.00009700	5.70825600	-0.79059900
H	-0.89605900	5.49492800	-1.40351800
H	0.00012100	6.77428500	-0.52050000
H	0.89629400	5.49486900	-1.40343700

1b



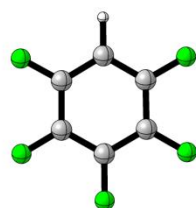
B3LYP electronic energy: -826.987654 a.u.  
 B3LYP enthalpy: -826.925383 a.u.  
 B3LYP free energy: -826.971657 a.u.  
 B3LYP SCF energy in solution: -827.9982371 a.u.  
 B3LYP enthalpy in solution: -827.935966129 a.u.  
 B3LYP free energy in solution: -827.982240129 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	-0.76277100	1.17151100	-0.00040600
C	0.63320200	1.24609500	0.00047000
C	1.39647800	0.07465800	0.00006300

C	0.76261000	-1.17147500	0.00049300
C	-0.63336400	-1.24612200	-0.00039700
F	-1.48672700	2.28388300	-0.00072300
F	1.23456100	2.42950700	-0.00002400
F	2.72172800	0.14547500	0.00007600
F	1.48652200	-2.28403600	-0.00000900
F	-1.23476900	-2.42936100	-0.00074800
C	-1.39603300	-0.07463900	0.00049700
F	-2.72139600	-0.14548500	0.00094800

2b

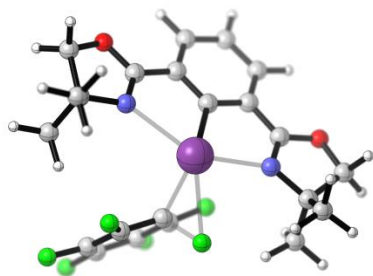


B3LYP electronic energy:	-727.8459993 a.u.
B3LYP enthalpy:	-727.776446 a.u.
B3LYP free energy:	-727.819993 a.u.
B3LYP SCF energy in solution:	-728.735008514 a.u.
B3LYP enthalpy in solution:	-728.665454514 a.u.
B3LYP free energy in solution:	-728.709001514 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	1.21393900	0.42758300	0.00066900
C	1.19992100	-0.97019700	-0.00050700
C	-0.00000100	-1.67666200	-0.00006400
C	-1.19992300	-0.97019900	-0.00049800
C	-1.21393500	0.42758400	0.00066400
F	2.36202200	1.09694500	0.00075500
F	2.36168300	-1.62119100	-0.00013200
F	-2.36168700	-1.62118500	-0.00010400
F	-2.36201900	1.09694400	0.00072500
H	0.00000900	-2.76693100	0.00041200
C	-0.00000100	1.12205200	-0.00068600
F	0.00000000	2.44914800	-0.00100800

ts1a



B3LYP electronic energy: -1922.139979 a.u.  
 B3LYP enthalpy: -1921.732383 a.u.  
 B3LYP free energy: -1921.827574 a.u.  
 B3LYP SCF energy in solution: -1924.25718542 a.u.  
 B3LYP enthalpy in solution: -1923.84958942 a.u.  
 B3LYP free energy in solution: -1923.94478042 a.u.

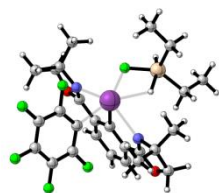
Cartesian coordinates

ATOM	X	Y	Z
C	-0.12496200	2.51167200	1.32167800
C	-0.98802500	1.57067000	0.73974400
C	-2.27661000	1.40311600	1.27099500
C	-2.69556500	2.15153300	2.38195400
C	-1.81838500	3.07487600	2.96202300
C	-0.53620500	3.26357400	2.43487400
H	-3.70030600	2.00812900	2.78569700
H	-2.13844500	3.65549100	3.82988800
H	0.14627100	3.99068800	2.88042800
C	-3.11369300	0.42035700	0.58411400
C	-3.74639500	-1.24290000	-0.80015400
C	-4.95833000	-0.68490700	0.00129700
H	-5.63688000	-0.07582400	-0.61970200
H	-5.53645000	-1.45952900	0.52233200
C	1.18438700	2.66013800	0.68411200
C	2.95249900	2.33782000	-0.67434000
C	3.15151400	3.60462900	0.21280300
H	4.08944800	3.59832000	0.78489600
H	3.08385000	4.54272900	-0.36269100
N	-2.69710600	-0.25663900	-0.43267800
N	1.55890800	1.95765100	-0.33196900
O	-4.36720900	0.18630800	0.99453900
O	2.04945500	3.57590300	1.14561100
C	3.91598000	1.21339700	-0.26525300
H	3.70409900	0.29253800	-0.82334500
H	4.95590400	1.51238000	-0.47452400
H	3.83041700	0.99422800	0.81030700
C	3.07454700	2.64663500	-2.16888800



H	4.08858900	3.00496600	-2.40863500
H	2.88900500	1.73851000	-2.76232200
H	2.35122900	3.41798100	-2.47532200
C	-3.34334700	-2.63982300	-0.30181100
H	-4.12933600	-3.36810400	-0.56091000
H	-2.39225700	-2.94220100	-0.75789300
H	-3.20710200	-2.64060700	0.78967600
C	-3.98447500	-1.24387100	-2.31084000
H	-3.08622700	-1.60991400	-2.83065900
H	-4.82074000	-1.91278300	-2.56990500
H	-4.21925500	-0.23332200	-2.68004900
Bi	-0.37370200	0.40030300	-1.10226000
C	1.32220000	-2.75935900	1.85653600
C	0.36389500	-2.12556000	1.07152800
C	0.63284800	-1.66344000	-0.23575000
C	1.95887400	-1.86446700	-0.67459900
C	2.93402000	-2.48075100	0.09829400
F	1.00940400	-3.16689500	3.09130300
F	-0.84423200	-1.86829700	1.62575100
F	-0.42857500	-2.23159800	-1.35046300
F	2.33124000	-1.30999300	-1.86078000
F	4.18487000	-2.58843600	-0.36699500
C	2.62071200	-2.95943700	1.37445300
F	3.53640400	-3.60222900	2.11285200

ts2a



B3LYP electronic energy: -2371.1557075 a.u.  
 B3LYP enthalpy: -2370.589837 a.u.  
 B3LYP free energy: -2370.709958 a.u.  
 B3LYP SCF energy in solution: -2373.59621487 a.u.  
 B3LYP enthalpy in solution: -2373.03034487 a.u.  
 B3LYP free energy in solution: -2373.15046487 a.u.

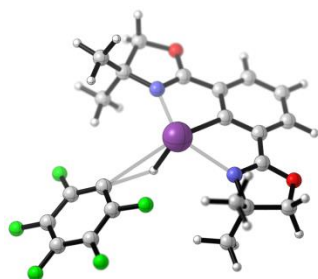
Cartesian coordinates

ATOM	X	Y	Z
C	-0.60773800	0.79276000	2.50142500
C	-0.58638600	-0.26100200	1.58605300

C	-0.82999400	-1.56786600	2.01210300
C	-1.12090700	-1.82629100	3.36157700
C	-1.15863500	-0.76462100	4.27161800
C	-0.90165700	0.54509700	3.85246200
H	-1.31486300	-2.84935800	3.69020800
H	-1.38841400	-0.96069700	5.32117000
H	-0.92547300	1.37284000	4.56430100
C	-0.74340100	-2.60614900	0.97910800
C	-0.38201100	-3.62949300	-0.99551800
C	-0.90629600	-4.64157100	0.07380600
H	-1.91821400	-5.01299100	-0.15095200
H	-0.23362900	-5.49563400	0.23574000
C	-0.30217800	2.12400300	1.95946600
C	0.29364200	3.76794300	0.53560100
C	-0.20468900	4.35474600	1.89672400
H	0.54101900	4.98706400	2.39977700
H	-1.14921100	4.91153000	1.80108100
N	-0.43961600	-2.35465100	-0.24638200
N	0.10976200	2.31385700	0.75618100
O	-0.97521000	-3.88253000	1.30163800
O	-0.45575900	3.20194500	2.73395000
C	1.77951500	4.06654600	0.29187700
H	2.13418900	3.53678500	-0.60333400
H	1.93330700	5.14716800	0.14013700
H	2.39319100	3.74575000	1.14835500
C	-0.57196600	4.24270300	-0.63758900
H	-0.55054400	5.34262800	-0.70508600
H	-0.18787500	3.84181700	-1.58830600
H	-1.60821600	3.89746500	-0.51740200
C	1.07460500	-3.92144800	-1.38592400
H	1.14696700	-4.88999400	-1.90657600
H	1.45867700	-3.13999300	-2.05880400
H	1.71935700	-3.94865400	-0.49496700
C	-1.29023400	-3.57506100	-2.22791500
H	-0.92848500	-2.82132500	-2.94401000
H	-1.30145400	-4.55024200	-2.74099900
H	-2.32021400	-3.30994000	-1.94713200
Bi	-0.25011000	0.17686800	-0.61221000
C	4.28193700	-1.15597600	0.41730900
C	2.88508200	-1.08085400	0.41381500
C	2.17957800	-0.18497300	-0.37949300
C	2.94711000	0.64242800	-1.18716900
C	4.34292100	0.62133200	-1.22132600
F	4.92632200	-2.03347500	1.18919300

F	2.24311500	-1.94277000	1.23081200
F	-2.42202300	1.64012700	-0.36645300
F	2.33219100	1.54693800	-1.99358800
F	5.03608000	1.44799500	-2.00564600
Si	-3.78454300	0.51128800	-0.73590300
H	-2.49512000	-0.49409600	-0.85155000
H	-4.65050800	1.56513200	-0.04882800
C	-4.76285400	-1.01545700	-0.03052200
C	-6.27624100	-0.82119300	0.09896500
H	-4.32854000	-1.24672900	0.96191900
H	-4.52925500	-1.89341300	-0.66337400
H	-6.77739700	-1.68653100	0.56903600
H	-6.51233100	0.06806700	0.70746800
H	-6.75236300	-0.66811500	-0.88483700
C	-4.17316400	0.71123400	-2.59748000
C	-3.47952800	1.88779700	-3.29628800
H	-5.26904800	0.83070100	-2.68133700
H	-3.92956200	-0.23364000	-3.11709200
H	-3.78091800	1.98070100	-4.35444800
H	-3.71466900	2.84482200	-2.80203600
H	-2.38108000	1.78433700	-3.28080900
C	5.01280700	-0.29561300	-0.40697500
F	6.34256100	-0.34964500	-0.41530000

ts3a



B3LYP electronic energy:	-1822.9522953 a.u.
B3LYP enthalpy:	-1822.541625 a.u.
B3LYP free energy:	-1822.638246 a.u.
B3LYP SCF energy in solution:	-1824.94243979 a.u.
B3LYP enthalpy in solution:	-1824.53176979 a.u.
B3LYP free energy in solution:	-1824.62839079 a.u.

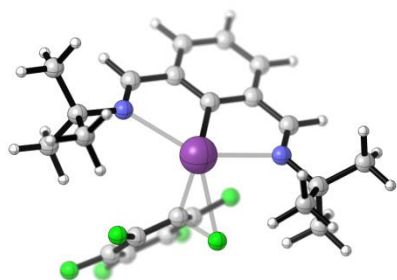
Cartesian coordinates

ATOM	X	Y	Z
C	3.32531900	1.25449700	-0.46291400
C	2.67331800	0.02875500	-0.27763700

C	3.32915100	-1.16109800	-0.61900400
C	4.63562700	-1.13105900	-1.13488100
C	5.27958400	0.10036400	-1.30570600
C	4.63308100	1.29702300	-0.97473700
H	5.13982500	-2.06280000	-1.40142300
H	6.29546700	0.12767200	-1.70589200
H	5.13500000	2.25714700	-1.11486100
C	2.55066500	-2.38880600	-0.41648100
C	0.82595100	-3.77374800	0.04228400
C	2.53545200	2.43965200	-0.11148900
N	1.34209700	-2.38453700	0.03521200
N	1.31867000	2.36687400	0.31405900
C	-0.20683800	4.01113700	-0.70232800
H	-1.06559700	3.32536400	-0.66469700
H	-0.59000000	5.04241600	-0.63520300
H	0.28950200	3.89203200	-1.67854100
C	0.10480500	3.93844600	1.80547900
H	-0.22125500	4.98385300	1.92594700
H	-0.78617000	3.29739600	1.88473500
H	0.79159000	3.69048200	2.62968500
C	0.28398500	-4.13812200	1.42848000
H	-0.02518600	-5.19546300	1.45424900
H	1.04744200	-3.98024500	2.20617000
H	-0.59540800	-3.52144400	1.66555000
C	2.11199100	-4.57997400	-0.32644200
H	2.52747100	-5.13635900	0.52871300
H	1.96998500	-5.26849200	-1.17118000
C	0.77793100	3.74303000	0.44515800
C	2.08011300	4.58684100	0.29513600
H	2.46466900	4.95398600	1.26079300
H	1.98024300	5.43032600	-0.40126200
C	-0.26985800	-3.91694800	-1.02462100
H	0.11188900	-3.64831100	-2.02207200
H	-0.63227500	-4.95708600	-1.06004500
H	-1.11852700	-3.26246900	-0.78266100
O	3.08249200	-3.58003000	-0.71787100
O	3.05657900	3.66483700	-0.24695900
Bi	0.55857800	-0.02187600	0.60350800
C	-4.31825500	-1.20618300	0.12326800
C	-3.00349600	-0.74323900	0.18511000
C	-2.58022100	0.50605400	-0.20228900
C	-3.57580000	1.33302100	-0.68596400
C	-4.91967000	0.95702900	-0.78039800
F	-4.67096300	-2.44144600	0.51305200

F	-2.07356300	-1.65847500	0.67788700
F	-3.28601500	2.60103300	-1.10029300
F	-5.86330000	1.78692400	-1.24907400
H	-0.58941400	0.21398100	-0.79044800
C	-5.28835200	-0.32998500	-0.37179700
F	-6.56572300	-0.71927900	-0.45428100

ts1b



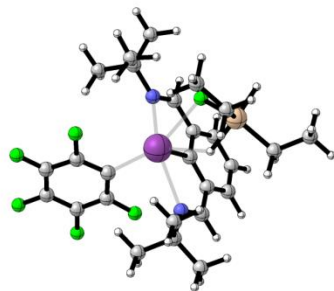
B3LYP electronic energy:	-1774.2004211 a.u.
B3LYP enthalpy:	-1773.760714 a.u.
B3LYP free energy:	-1773.856079 a.u.
B3LYP SCF energy in solution:	-1776.15033317 a.u.
B3LYP enthalpy in solution:	-1775.71062617 a.u.
B3LYP free energy in solution:	-1775.80599117 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	0.04242000	-2.09480000	1.95010300
C	0.96693900	-1.33382100	1.21861900
C	2.19327700	-0.96905800	1.79290800
C	2.48999100	-1.35625700	3.11128100
C	1.56201800	-2.10051400	3.84858700
C	0.34410000	-2.47390200	3.27225100
H	3.44562000	-1.07318600	3.56291300
H	1.79145400	-2.39380400	4.87531700
H	-0.37467800	-3.06376600	3.84928100
C	3.12495800	-0.19257600	0.97310800
C	3.74306200	0.99094400	-1.05250200
C	5.21999000	0.62739500	-0.80985700
H	5.40002700	-0.44785800	-0.97014900
H	5.85264100	1.18624600	-1.51548300
C	-1.19685100	-2.50427600	1.28713300
C	-2.70047800	-2.62033900	-0.60848000
C	-3.08956700	-4.05608700	-0.20538900
H	-3.93724000	-4.39272600	-0.82070500
H	-2.25319300	-4.75464400	-0.36689600

N	2.82354300	0.15919800	-0.22420500
N	-1.45536900	-2.16789900	0.07411400
C	-3.84201100	-1.64697800	-0.25192100
H	-3.62093400	-0.62745800	-0.59318100
H	-4.77389400	-1.97059600	-0.74156400
H	-4.01767700	-1.62568500	0.83515600
C	-2.43249600	-2.57878200	-2.12184600
H	-3.32540200	-2.90468800	-2.67696000
H	-2.19290800	-1.55623400	-2.44754800
H	-1.59978800	-3.24671100	-2.39348700
C	3.48694900	2.47035300	-0.69936200
H	4.12421500	3.11665600	-1.32373800
H	2.43334100	2.71886700	-0.87997500
H	3.72409800	2.66847900	0.35766900
C	3.39489800	0.74295500	-2.52922300
H	2.35871500	1.05031900	-2.73102400
H	4.05553200	1.33929800	-3.17694600
H	3.52731900	-0.31777800	-2.79695100
Bi	0.49995300	-0.68365700	-0.86966900
C	-1.33812800	2.87697400	1.49473900
C	-0.36370500	2.12669800	0.84266100
C	-0.61052800	1.44322500	-0.36585200
C	-1.92130200	1.56732400	-0.86352000
C	-2.91523600	2.29486800	-0.21990400
F	-1.04749500	3.49387100	2.64467800
F	0.84359800	2.00503300	1.43738700
F	0.50100800	1.86552400	-1.56485400
F	-2.26781200	0.85246500	-1.96520800
F	-4.15656100	2.31445800	-0.71913600
H	-1.88602900	-3.13587700	1.86923800
H	-3.40834100	-4.13017800	0.84541200
H	4.09029000	0.07819300	1.42564600
H	5.56225900	0.89187700	0.20236500
C	-2.62852800	2.98018800	0.96423800
F	-3.56466900	3.71692900	1.57581400

ts2b



B3LYP electronic energy: -2223.2136499 a.u.  
 B3LYP enthalpy: -2222.615732 a.u.  
 B3LYP free energy: -2222.736847 a.u.  
 B3LYP SCF energy in solution: -2225.48876728 a.u.  
 B3LYP enthalpy in solution: -2224.89084928 a.u.  
 B3LYP free energy in solution: -2225.01196428 a.u.

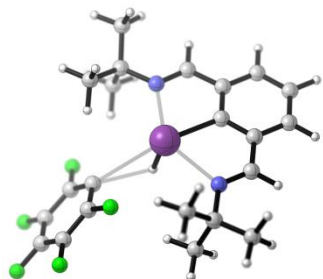
Cartesian coordinates

ATOM	X	Y	Z
C	-0.62465000	0.69946800	2.65223100
C	-0.60116400	-0.32668600	1.70625100
C	-0.82225400	-1.65453500	2.07804600
C	-1.09196800	-1.95883500	3.42497000
C	-1.12913500	-0.93596900	4.37746600
C	-0.89582300	0.38932100	3.99811400
H	-1.27208400	-2.99463300	3.72721200
H	-1.34062100	-1.17335500	5.42235800
H	-0.92359600	1.18556000	4.74783500
C	-0.74913200	-2.69443900	1.04271300
C	-0.32331100	-3.43958800	-1.23188800
C	-0.91672500	-4.80246700	-0.83778200
H	-1.98153900	-4.71754100	-0.56914600
H	-0.84105500	-5.49179900	-1.69158900
C	-0.36943900	2.07923500	2.20697200
C	0.21736500	3.73333400	0.52934000
C	-0.44501300	4.79670300	1.42179800
H	-0.29897300	5.78956000	0.97150600
H	-1.52835900	4.62068600	1.51162700
N	-0.44900300	-2.41346500	-0.16880600
N	-0.02386800	2.34677200	1.00659800
C	1.74317600	3.94992600	0.49183300
H	2.22567900	3.22331100	-0.17494400
H	1.96658100	4.95936300	0.11264000
H	2.18237900	3.85433900	1.49743200
C	-0.36511800	3.82844200	-0.89202900
H	-0.25127500	4.85183200	-1.28074500

H	0.17207000	3.15337700	-1.57633600
H	-1.42913800	3.55429800	-0.89031300
C	1.18212000	-3.59328900	-1.52892200
H	1.33447700	-4.32449100	-2.33790400
H	1.62500400	-2.63614000	-1.84055200
H	1.72296900	-3.94021800	-0.63538400
C	-1.05564400	-2.90926400	-2.47738700
H	-0.61936500	-1.95873400	-2.82250900
H	-0.96957600	-3.63273000	-3.30244500
H	-2.12177400	-2.73753100	-2.26853400
C	4.25472100	-1.11430000	0.55176900
C	2.85841000	-1.03330200	0.55907300
C	2.14840500	-0.15403600	-0.24997500
C	2.91189000	0.64212500	-1.09217900
C	4.30737700	0.61207900	-1.14009500
F	4.90287300	-1.97305000	1.34142600
F	2.21949900	-1.87444400	1.39736200
F	2.29703400	1.52878400	-1.91747100
F	4.99613000	1.41226800	-1.95496000
H	-0.95960600	-3.72530600	1.36242700
H	-0.49239700	2.86857300	2.96359100
H	-0.37660500	-5.26794600	0.00124100
H	-0.00621500	4.83543200	2.43120900
C	4.98129000	-0.28320500	-0.30574300
F	6.31045200	-0.34459500	-0.32609800
Bi	-0.29619000	0.17578600	-0.45883200
F	-2.50009600	1.56776200	-0.18364600
Si	-3.83209800	0.38851100	-0.50680600
H	-2.50925300	-0.56765200	-0.65857300
H	-4.70537900	1.38804200	0.24555000
C	-4.74362800	-1.19157800	0.17510600
C	-6.26051300	-1.05137500	0.33204300
H	-4.28692100	-1.43075700	1.15554300
H	-4.49136200	-2.04627700	-0.48171200
H	-6.72522000	-1.94352400	0.78935200
H	-6.51659200	-0.18476800	0.96484200
H	-6.75714800	-0.89210700	-0.64050700
C	-4.28403700	0.60905400	-2.35106400
C	-3.66402300	1.82686400	-3.04792800
H	-5.38623800	0.68096300	-2.39964900
H	-4.01766500	-0.31522600	-2.89612600
H	-4.00199300	1.92481600	-4.09447300
H	-3.92564200	2.76342200	-2.52855700
H	-2.56240000	1.77201900	-3.06653400



Ts3b



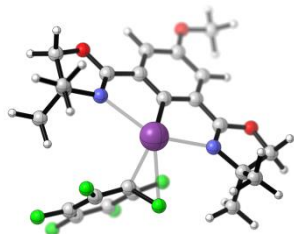
B3LYP electronic energy: -1675.0113139 a.u.  
B3LYP enthalpy: -1674.568580 a.u.  
B3LYP free energy: -1674.665758 a.u.  
B3LYP SCF energy in solution: -1676.83676489 a.u.  
B3LYP enthalpy in solution: -1676.39403089 a.u.  
B3LYP free energy in solution: -1676.49120889 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	3.31835200	-1.54028600	0.62506100
C	2.82530500	-0.24288000	0.44057800
C	3.56627800	0.86560400	0.86781900
C	4.81981800	0.67127100	1.47813600
C	5.31754600	-0.62448600	1.65614700
C	4.57326700	-1.73113900	1.23358000
H	5.40574300	1.53142200	1.81638700
H	6.29006400	-0.77253800	2.13074000
H	4.96620000	-2.74186100	1.38013600
C	2.98645300	2.20088300	0.66874100
C	1.19839200	3.68684900	-0.06012400
C	2.47600000	-2.65584000	0.17712400
N	1.82825800	2.35703400	0.13994900
N	1.31760500	-2.45485100	-0.33723300
C	-0.35950900	-4.01896900	0.51784200
H	-0.96017900	-3.19496300	0.92789100
H	-1.05264900	-4.83301700	0.25468300
H	0.32696400	-4.39041800	1.29593200
C	-0.55667200	-3.03928700	-1.79203200
H	-1.23513100	-3.84116300	-2.12041700
H	-1.17634300	-2.23015000	-1.37115300
H	-0.01780500	-2.66643700	-2.67858700
C	0.74634600	3.75776800	-1.53173300
H	0.27832600	4.73336100	-1.73360800
H	1.60263800	3.63992100	-2.21468900

H	0.00017100	2.98185300	-1.75572800
C	2.14246700	4.86115500	0.24464300
H	3.04629500	4.83872600	-0.38551700
H	1.61910700	5.80614600	0.03909400
H	2.45151500	4.88531100	1.30159800
Bi	0.81996000	0.04216000	-0.55705700
C	-4.10020400	1.29583000	-0.19548500
C	-2.81170200	0.76458300	-0.26599300
C	-2.42211800	-0.45279100	0.23795500
C	-3.42582300	-1.16882600	0.86198800
C	-4.74591300	-0.72097100	0.97608500
F	-4.42060100	2.49652200	-0.70427200
F	-1.86903200	1.57808900	-0.89565500
F	-3.16766400	-2.39415000	1.40783800
F	-5.69817000	-1.44592000	1.58258300
H	-0.29203600	-0.11867400	0.85956400
H	2.87281400	-3.67357700	0.31104900
C	0.42054900	-3.57887600	-0.73660900
C	1.21389200	-4.76195000	-1.32138800
H	1.84801900	-4.44162100	-2.16373500
H	1.85016300	-5.26039300	-0.57367100
H	0.51060000	-5.52004100	-1.69631400
H	3.58856200	3.05936700	1.00116600
C	-0.03111500	3.75039900	0.86783500
H	-0.75405500	2.96275800	0.61702500
H	0.26698000	3.64418100	1.92253200
H	-0.53764500	4.72063900	0.74817800
C	-5.08001700	0.52853300	0.44097300
F	-6.33404400	0.98625400	0.53809400

ts1c



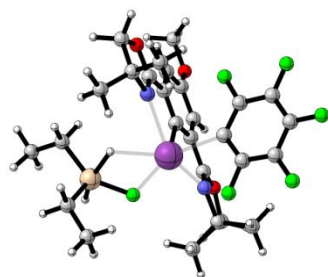
B3LYP electronic energy:	-2036.5768765 a.u.
B3LYP enthalpy:	-2036.134326 a.u.
B3LYP free energy:	-2036.235690 a.u.
B3LYP SCF energy in solution:	-2038.83424074 a.u.
B3LYP enthalpy in solution:	-2038.39169074 a.u.
B3LYP free energy in solution:	-2038.49305474 a.u.

## Cartesian coordinates

ATOM	X	Y	Z
C	-1.09758100	2.30859300	0.28875500
C	-1.38547900	0.97856200	-0.06049900
C	-2.60658100	0.43084000	0.34714400
C	-3.52873900	1.17338800	1.10564900
C	-3.21648300	2.49551900	1.46018700
C	-1.99821700	3.06611800	1.04301100
H	-4.46761700	0.70802400	1.40395700
H	-1.77899200	4.09858100	1.31976100
C	-2.84541600	-0.94707600	-0.08019200
C	-2.49563700	-3.00568700	-0.93059900
C	-3.97561500	-2.82569900	-0.48163400
H	-4.67063600	-2.72960500	-1.33291700
H	-4.33045900	-3.61656600	0.19247000
C	0.17759000	2.83565000	-0.20440400
C	2.20634100	2.96295500	-1.17506900
C	1.71964200	4.36961400	-0.70813400
H	2.43187000	4.88340900	-0.04782600
H	1.46173400	5.03376500	-1.54945800
N	-1.99026700	-1.61744000	-0.77624500
N	1.01094800	2.13014300	-0.89230100
O	-3.98672800	-1.57243900	0.24189600
O	0.51184400	4.11093300	0.03999100
C	3.39453100	2.47524300	-0.33228200
H	3.66519800	1.44444700	-0.59444300
H	4.27173200	3.11879100	-0.50857400
H	3.15436000	2.50731300	0.74171000
C	2.54362500	2.92728000	-2.66823400
H	3.37993100	3.60866500	-2.89293400
H	2.84694200	1.91216900	-2.96619200
H	1.67705300	3.22614800	-3.27800800
C	-1.73294800	-3.94393400	0.01823200
H	-2.11566400	-4.97242800	-0.08741100
H	-0.66003800	-3.92123100	-0.21143900
H	-1.85655100	-3.62681900	1.06430700
C	-2.36978600	-3.46854600	-2.38296700
H	-1.30770500	-3.54643300	-2.66039900
H	-2.82648100	-4.46268900	-2.51380400
H	-2.86302600	-2.76468100	-3.07137900
Bi	0.02890400	-0.23506400	-1.34252600
C	1.96698700	-1.53263700	2.67495000
C	1.07556000	-1.58394900	1.60815500

C	1.47622700	-1.40010100	0.26515900
C	2.85068400	-1.12548500	0.09314200
C	3.75410000	-1.05462400	1.14517000
F	1.52179700	-1.70693600	3.92454600
F	-0.24177200	-1.72971900	1.88795600
F	1.01150900	-2.62023300	-0.71406000
F	3.28574800	-0.78745200	-1.15230200
F	5.03332700	-0.73911800	0.90558600
C	3.32626500	-1.28043800	2.45733800
F	4.19686100	-1.26904400	3.47727900
O	-4.02319100	3.30070900	2.19264800
C	-5.25270700	2.79926900	2.67067800
H	-5.71851300	3.61125400	3.24444800
H	-5.92831100	2.51143800	1.84503400
H	-5.10940000	1.92756300	3.33392400

ts2c



B3LYP electronic energy: -2485.5935451 a.u.  
 B3LYP enthalpy: -2484.992734 a.u.  
 B3LYP free energy: -2485.117905 a.u.  
 B3LYP SCF energy in solution: -2488.1738598 a.u.  
 B3LYP enthalpy in solution: -2487.5730488 a.u.  
 B3LYP free energy in solution: -2487.6982198 a.u.

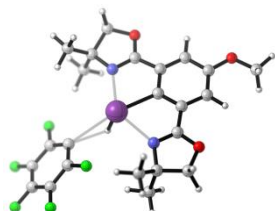
Cartesian coordinates

ATOM	X	Y	Z
C	0.74547100	0.06304600	2.36640900
C	0.68531500	0.65382200	1.10002600
C	1.05893000	1.98584400	0.94692700
C	1.51544500	2.74117300	2.04149100
C	1.58781300	2.13561900	3.30665200
C	1.19818500	0.79103400	3.46936800
H	1.80208300	3.78050100	1.88697400
H	1.25605900	0.34204200	4.46202500
C	0.92493500	2.53580200	-0.40723600

C	0.40702000	2.73078000	-2.59168500
C	1.11742800	4.01975600	-2.06629900
H	2.12075100	4.15964900	-2.49813000
H	0.52807800	4.93590400	-2.21276500
C	0.29979600	-1.33633900	2.44312000
C	-0.55474500	-3.34082400	1.86542500
C	0.06906400	-3.38625300	3.29824800
H	-0.64429300	-3.69326300	4.07645900
H	0.96532700	-4.02269900	3.35360100
N	0.46910600	1.85566400	-1.40053500
N	-0.25817400	-1.94705400	1.45866200
O	1.27273300	3.80543400	-0.64541200
O	0.47792700	-2.02609200	3.57333300
C	-2.07485700	-3.55487700	1.89448500
H	-2.50256200	-3.39403600	0.89499200
H	-2.31038900	-4.58344800	2.21236900
H	-2.56030400	-2.85627400	2.59409400
C	0.12994500	-4.32802300	0.91330500
H	0.02519300	-5.35795400	1.29159900
H	-0.33710000	-4.28680600	-0.08287100
H	1.19394000	-4.07905700	0.79861700
C	-1.06355400	2.99842200	-2.94575900
H	-1.13413300	3.68494300	-3.80487500
H	-1.57297000	2.06029200	-3.21260800
H	-1.59617600	3.44133500	-2.09133600
C	1.15760300	2.09957500	-3.76847800
H	0.66469700	1.16846900	-4.08738200
H	1.17084400	2.78674500	-4.62990400
H	2.19437300	1.85746000	-3.49193200
Bi	0.07119800	-0.57630100	-0.69144400
C	-4.22111300	1.52271200	0.06285900
C	-2.84189200	1.30846600	-0.03027400
C	-2.29090000	0.09897200	-0.43432500
C	-3.19825700	-0.90201400	-0.75175200
C	-4.58429400	-0.75283000	-0.66935500
F	-4.71504300	2.70130000	0.44862800
F	-2.05687100	2.35886800	0.29160400
F	2.14796200	-2.07257800	-0.07623500
F	-2.74104100	-2.11540000	-1.15779500
F	-5.41530100	-1.75129400	-0.97259200
Si	3.52314600	-1.35839500	-1.00189000
H	2.31721500	-0.30917700	-1.36777100
H	4.39583500	-2.18488800	-0.05877400
C	4.71745000	0.17667600	-1.05365200

C	6.21161600	-0.15610000	-1.01926300
H	4.45608100	0.81938400	-0.19012200
H	4.46574700	0.77576000	-1.95007100
H	6.84818000	0.74654100	-0.98530100
H	6.46206500	-0.77035500	-0.13799600
H	6.51948400	-0.73492600	-1.90710400
C	3.61266300	-2.29129300	-2.66925300
C	2.72741400	-3.53985900	-2.77773100
H	4.66993600	-2.57922000	-2.81664400
H	3.37245400	-1.58661300	-3.48653100
H	2.85748300	-4.06083700	-3.74258800
H	2.95442700	-4.26547800	-1.97932300
H	1.65594700	-3.29232200	-2.68626100
C	-5.09558600	0.48080500	-0.25822000
F	-6.41120400	0.66382400	-0.17264400
O	2.01272400	2.76272700	4.42665700
C	2.43070200	4.10992900	4.35336000
H	2.73395100	4.39675200	5.36869300
H	3.29165300	4.23424900	3.67279700
H	1.61299200	4.77444800	4.02184300

ts3c



B3LYP electronic energy:	-1937.3893229 a.u.
B3LYP enthalpy:	-1936.943773 a.u.
B3LYP free energy:	-1937.046507 a.u.
B3LYP SCF energy in solution:	-1939.51936885 a.u.
B3LYP enthalpy in solution:	-1939.07381885 a.u.
B3LYP free energy in solution:	-1939.17655285 a.u.

Cartesian coordinates

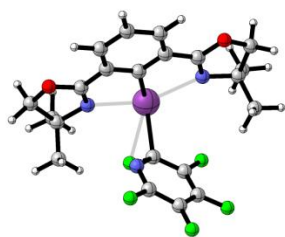
ATOM	X	Y	Z
C	-2.95880700	-1.37281800	-0.16391900
C	-2.32933600	-0.12821800	-0.01485600
C	-3.05428800	1.03103000	-0.29735100
C	-4.39670000	0.97095800	-0.71612200
C	-5.01524600	-0.28328400	-0.84998300
C	-4.29206400	-1.46146800	-0.57454000

H	-4.93030000	1.89606800	-0.93186100
H	-4.79120100	-2.42468600	-0.69354200
C	-2.31026100	2.28693900	-0.14474200
C	-0.60939300	3.73549300	0.18775900
C	-2.10706000	-2.53569900	0.11465300
N	-1.07252200	2.32841800	0.21723300
N	-0.86661200	-2.42373500	0.45384400
C	0.64510000	-3.99524900	-0.68857600
H	1.48016100	-3.27973500	-0.69643600
H	1.06765900	-5.01301500	-0.66560800
H	0.08069100	-3.87880000	-1.62738600
C	0.50010300	-3.96912100	1.83552900
H	0.87242900	-5.00285200	1.91634500
H	1.36979200	-3.29545600	1.86712200
H	-0.13897800	-3.75995300	2.70752600
C	0.03484400	4.11853500	1.52407200
H	0.30622700	5.18651000	1.52765900
H	-0.65315400	3.93184400	2.36331800
H	0.95302300	3.53404200	1.68244500
C	-1.95102500	4.49305800	-0.06673900
H	-2.32086000	5.01774000	0.82870600
H	-1.90358600	5.20050800	-0.90641400
C	-0.26947700	-3.78039500	0.52627400
C	-1.54746300	-4.67026300	0.45033000
H	-1.84848600	-5.06992600	1.43250800
H	-1.46631600	-5.49625500	-0.26911500
C	0.38572100	3.91901900	-0.96804800
H	-0.07068100	3.63899000	-1.93038900
H	0.70850000	4.97097500	-1.02917900
H	1.27319400	3.29272900	-0.80232600
O	-2.90731000	3.45918700	-0.40071800
O	-2.59321600	-3.77657700	-0.00216900
Bi	-0.16703100	-0.00975000	0.71175600
C	4.63825100	1.33902100	-0.08148300
C	3.34050200	0.84105900	0.04067100
C	2.93342600	-0.41868400	-0.32961400
C	3.92681600	-1.21791500	-0.86141700
C	5.25423700	-0.80601300	-1.01821100
F	4.97674100	2.58234800	0.29578900
F	2.41130200	1.72974300	0.58132800
F	3.65228900	-2.49381300	-1.26289200
F	6.19701300	-1.60975200	-1.53265400
H	0.89709800	-0.19728600	-0.75627500
C	5.60698400	0.48997200	-0.62424500

F	6.86849100	0.91355200	-0.76532600
O	-6.29959400	-0.46147600	-1.24177000
C	-7.09575900	0.66409000	-1.54445900
H	-8.08274600	0.27904800	-1.83247500
H	-7.21202900	1.33099300	-0.67136700
H	-6.67914300	1.24691600	-2.38541500

The following are the details of the calculation data for each species in Table 1:

Ts1-2a-1



B3LYP electronic energy:	-1839.0293997 a.u.
B3LYP enthalpy:	-1838.625969 a.u.
B3LYP free energy:	-1838.719229 a.u.
B3LYP SCF energy in solution:	-1841.04365602 a.u.
B3LYP enthalpy in solution:	-1840.64022502 a.u.
B3LYP free energy in solution:	-1840.73348502 a.u.

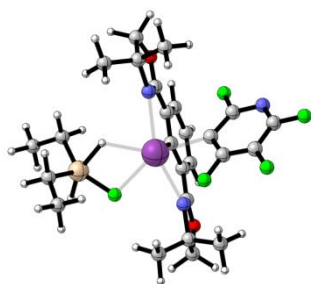
Cartesian coordinates

ATOM	X	Y	Z
C	0.57584000	2.39238400	1.40103000
C	-0.48287600	1.70462900	0.79114900
C	-1.76524600	1.79054800	1.35107800
C	-1.99446400	2.54971600	2.51009000
C	-0.92770000	3.22724400	3.10946200
C	0.35714000	3.15651700	2.55932000
H	-2.99938400	2.60521000	2.93442100
H	-1.09843000	3.81663300	4.01295800
H	1.19055200	3.68759100	3.02442300
C	-2.80920600	1.05598100	0.63512700
C	-3.82116000	-0.32691500	-0.83493800
C	-4.86406000	0.42494100	0.04436800
H	-5.41636200	1.20062400	-0.51238700
H	-5.57745300	-0.24327200	0.54460000
C	1.88598900	2.25793900	0.75851100
C	3.54647900	1.55924700	-0.58645600
C	4.01843900	2.73974500	0.31359100
H	4.93378200	2.52400000	0.88155900



H	4.15340300	3.67788900	-0.25022500
N	-2.56928700	0.36545400	-0.42862100
N	2.09616300	1.51510300	-0.27426400
O	-4.07642200	1.08972600	1.06125200
O	2.93656700	2.93518500	1.24971700
C	4.20272200	0.23706800	-0.15750800
H	3.75785300	-0.61150700	-0.69322000
H	5.28327100	0.26132700	-0.37331400
H	4.07170300	0.06812300	0.92288000
C	3.77133900	1.82925700	-2.07581100
H	4.84620600	1.93496900	-2.29406900
H	3.38566100	0.99227100	-2.67744900
H	3.25917200	2.75054700	-2.39367100
C	-3.74444600	-1.81470100	-0.46076200
H	-4.69153700	-2.31188800	-0.72847700
H	-2.90772600	-2.29110700	-0.98621500
H	-3.56797000	-1.93818200	0.61820500
C	-4.07326900	-0.14830700	-2.33317000
H	-3.29151400	-0.66803300	-2.90716900
H	-5.04521100	-0.58413600	-2.61477900
H	-4.07262100	0.91598200	-2.61642900
Bi	-0.19024100	0.49141400	-1.11186300
C	0.09458900	-1.72949500	-0.22641700
C	1.36078200	-2.31636800	-0.49412100
C	1.88748800	-3.24720700	0.37531600
F	-0.85937000	-1.99623000	-1.58850300
F	2.08256800	-1.88810900	-1.55715200
F	3.09362900	-3.77404000	0.16335700
C	1.14374500	-3.63487700	1.50893200
F	1.62327100	-4.55346300	2.36078600
N	-0.56046500	-2.07750000	0.88581400
C	-0.07631900	-2.99446700	1.69274500
F	-0.80501600	-3.30731400	2.76990400

ts2-2a-1



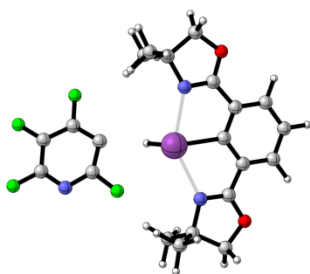
B3LYP electronic energy: -2288.0486981 a.u.  
 B3LYP enthalpy: -2287.487095 a.u.  
 B3LYP free energy: -2287.605005 a.u.  
 B3LYP SCF energy in solution: -2290.38505786 a.u.  
 B3LYP enthalpy in solution: -2289.82345486 a.u.  
 B3LYP free energy in solution: -2289.94136486 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	0.46673000	-0.89707000	2.47152900
C	0.52189300	0.18993300	1.59770700
C	0.87931600	1.45442400	2.06868700
C	1.20683700	1.63526200	3.42236300
C	1.16671700	0.53948300	4.29082400
C	0.79712000	-0.72726200	3.82617100
H	1.48927700	2.62528000	3.78608200
H	1.42424100	0.67473000	5.34350300
H	0.76115600	-1.58147800	4.50547300
C	0.87107800	2.53484700	1.07624300
C	0.58405700	3.65791200	-0.85674700
C	1.20716800	4.57902400	0.24131400
H	2.24592500	4.86723200	0.01696400
H	0.61488500	5.48261900	0.44302400
C	0.04639800	-2.17642100	1.88367500
C	-0.71061900	-3.70773500	0.41324100
C	-0.19915000	-4.38981100	1.72350100
H	-0.95904700	-5.00965900	2.22043200
H	0.71221500	-4.98644500	1.56538700
N	0.53127900	2.35693800	-0.15288500
N	-0.40873100	-2.28235500	0.68553500
O	1.22085400	3.77196600	1.44026800
O	0.13910600	-3.29584100	2.60751400
C	-2.22472300	-3.88466700	0.23038500
H	-2.57982600	-3.28819600	-0.62167500
H	-2.46648400	-4.94243400	0.03800100
H	-2.77269200	-3.56193100	1.12967700
C	0.06274000	-4.18994400	-0.81917800
H	-0.04221100	-5.28116700	-0.93310900
H	-0.33419200	-3.71846300	-1.73171100
H	1.12571000	-3.92485600	-0.73392600
C	-0.84250400	4.09550500	-1.22057200
H	-0.82934800	5.08090800	-1.71366700
H	-1.30382400	3.37309600	-1.91083500
H	-1.47411600	4.15764400	-0.32209400

C	1.47440200	3.56556800	-2.10003100
H	1.03729700	2.87942900	-2.84162400
H	1.57537700	4.55489600	-2.57489400
H	2.47625600	3.19243700	-1.84116200
Bi	0.11421500	-0.12396300	-0.60845600
C	-2.89634300	1.37599300	0.52939900
C	-2.26214700	0.44415100	-0.29362800
C	-3.15713600	-0.27285900	-1.07670200
C	-4.54150400	-0.08259000	-1.02671500
F	-2.14861100	2.15153900	1.33470200
F	2.15165700	-1.78467900	-0.46471200
F	-2.70013500	-1.21282000	-1.93052400
F	-5.37941500	-0.79154100	-1.78255600
Si	3.60714600	-0.76461700	-0.80346700
H	2.41315500	0.35384900	-0.86180900
H	4.37829400	-1.91683400	-0.16287400
C	4.72970700	0.63964900	-0.05770300
C	6.21960200	0.30183300	0.04621000
H	4.32782800	0.87495900	0.94738200
H	4.57304600	1.55730700	-0.65714000
H	6.80439700	1.10219800	0.53447500
H	6.37798000	-0.62326500	0.62575300
H	6.66909200	0.13427700	-0.94780200
C	3.96272400	-0.92511000	-2.67533400
C	3.15744400	-2.00029100	-3.41635200
H	5.04199900	-1.14315600	-2.77430000
H	3.80678100	0.05976400	-3.15274600
H	3.44452700	-2.07716300	-4.47978900
H	3.30194400	-2.99536600	-2.96409600
H	2.07394700	-1.79323300	-3.38832600
N	-4.19406100	1.60667500	0.61651500
C	-4.99618600	0.89500600	-0.13957400
F	-6.30286600	1.12192800	-0.05145500

ts3-2a-1



B3LYP electronic energy: -1739.8451779 a.u.

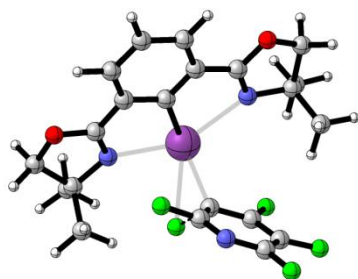
B3LYP enthalpy: -1739.438744 a.u.  
 B3LYP free energy: -1739.532721 a.u.  
 B3LYP SCF energy in solution: -1741.7298091 a.u.  
 B3LYP enthalpy in solution: -1741.3233751 a.u.  
 B3LYP free energy in solution: -1741.4173531 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	3.02084700	1.58937600	-0.44568100
C	2.53320700	0.28926100	-0.26002700
C	3.35025800	-0.80471800	-0.57510800
C	4.65133700	-0.60443900	-1.06603200
C	5.12892300	0.70040400	-1.23773000
C	4.32160200	1.80225900	-0.93230200
H	5.28062800	-1.46289400	-1.31189900
H	6.14018000	0.86011600	-1.61822900
H	4.69329500	2.81983900	-1.07300400
C	2.74063500	-2.12448500	-0.37298500
C	1.20714200	-3.72371600	0.06124500
C	2.07376100	2.66171100	-0.12275700
N	1.53765800	-2.27931400	0.06614400
N	0.87148600	2.43040700	0.28622100
C	-0.84202200	3.82788500	-0.79204000
H	-1.59469900	3.02721100	-0.75200100
H	-1.36856400	4.79541900	-0.75453600
H	-0.31283400	3.76073000	-1.75586200
C	-0.57969800	3.84568900	1.72200900
H	-1.04839300	4.83846000	1.81464700
H	-1.37577400	3.08948700	1.79579600
H	0.11545000	3.70874100	2.56494400
C	0.66921700	-4.15933000	1.42783400
H	0.50196100	-5.24831100	1.44565100
H	1.37664100	-3.90314500	2.23181500
H	-0.29221000	-3.66516400	1.63178300
C	2.59889800	-4.35264100	-0.26210100
H	3.06861000	-4.82246000	0.61693600
H	2.57362300	-5.07612200	-1.08881700
C	0.14500500	3.72092000	0.37990700
C	1.32225000	4.73221900	0.23865700
H	1.63388300	5.16072000	1.20531200
H	1.12272700	5.54539600	-0.47230100
C	0.17643300	-4.00262200	-1.04325100
H	0.55944500	-3.69266600	-2.02823100
H	-0.05725200	-5.07875100	-1.08416300

H	-0.75306500	-3.45363700	-0.83746400
O	3.42861300	-3.23650200	-0.66369000
O	2.42538000	3.94479300	-0.27182900
Bi	0.43112100	-0.03448400	0.59632900
C	-3.01508400	-1.14715200	0.17346700
C	-2.72351600	0.15522400	-0.19633600
C	-3.86155400	0.81026600	-0.63347000
C	-5.12731300	0.20924900	-0.67727300
F	-1.96169500	-1.93163700	0.62390600
F	-3.80568500	2.10194500	-1.04198000
F	-6.21878600	0.86109800	-1.09920800
H	-0.73553700	0.06448500	-0.80062700
C	-5.20453100	-1.12000500	-0.25488200
N	-4.16362900	-1.80075400	0.16902400
F	-6.38899800	-1.73763700	-0.28021800

ts1-2a-2



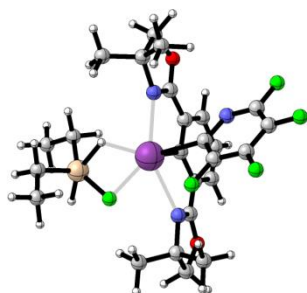
B3LYP electronic energy: -1839.034267 a.u.  
 B3LYP enthalpy: -1838.630996 a.u.  
 B3LYP free energy: -1838.723337 a.u.  
 B3LYP SCF energy in solution: -1841.0471866 a.u.  
 B3LYP enthalpy in solution: -1840.6439156 a.u.  
 B3LYP free energy in solution: -1840.7362566 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	0.08633100	2.54512300	1.14078700
C	-0.83895300	1.61659500	0.64006800
C	-2.13579700	1.58451300	1.17634700
C	-2.50276200	2.45606900	2.21337100
C	-1.56505000	3.36664200	2.71353500
C	-0.27320000	3.42033400	2.17932900
H	-3.51487000	2.41810500	2.62231900
H	-1.84496200	4.04314300	3.52389000
H	0.45717100	4.13675300	2.56172500

C	-3.03884200	0.60560400	0.57274100
C	-3.78650500	-1.12164200	-0.66910100
C	-4.95616100	-0.41468500	0.07515000
H	-5.59201900	0.18400600	-0.59884800
H	-5.58506000	-1.10067500	0.65777600
C	1.40305600	2.54630100	0.50146700
C	3.14907100	1.97943700	-0.80310000
C	3.42349000	3.31657300	-0.05123600
H	4.36275000	3.31725900	0.51857200
H	3.40383200	4.19290100	-0.72022400
N	-2.67059700	-0.18326200	-0.38012700
N	1.73172600	1.72733100	-0.44095400
O	-4.30553900	0.49585900	0.99320100
O	2.32650000	3.44358600	0.87928300
C	4.03430100	0.84556600	-0.26255100
H	3.75718400	-0.11722900	-0.71080300
H	5.09179100	1.04540600	-0.50012200
H	3.93780900	0.75902900	0.83084300
C	3.30077600	2.11802300	-2.31999900
H	4.33792300	2.38000300	-2.58415600
H	3.05710300	1.16602200	-2.81566500
H	2.63253300	2.89811700	-2.71613500
C	-3.48180100	-2.49525400	-0.05096600
H	-4.31222100	-3.18988600	-0.25883500
H	-2.54847000	-2.89663800	-0.46552600
H	-3.35418700	-2.41305000	1.03851300
C	-4.02374000	-1.23317300	-2.17576100
H	-3.15487900	-1.70630400	-2.65774800
H	-4.90645300	-1.85909000	-2.38286600
H	-4.18359400	-0.24291300	-2.63019200
Bi	-0.30648800	0.24281200	-1.07929900
C	0.22847000	-2.08480300	1.38782900
C	0.53587500	-1.77309000	0.03914600
C	1.85538300	-2.13652900	-0.29750500
C	2.71809200	-2.75515600	0.60273300
F	-0.97394400	-1.68139700	1.85879700
F	-0.52551800	-2.40358600	-1.04287600
F	2.33626100	-1.78055200	-1.51225000
F	3.97551200	-3.03966800	0.24649100
N	1.02018700	-2.67376500	2.24568800
C	2.23378600	-3.02534500	1.88358200
F	3.01716800	-3.64398300	2.77672900

ts2-2a-2



B3LYP electronic energy: -2288.026165 a.u.  
B3LYP enthalpy: -2287.464956 a.u.  
B3LYP free energy: -2287.583805 a.u.  
B3LYP SCF energy in solution: -2290.36416183 a.u.  
B3LYP enthalpy in solution: -2289.80295283 a.u.  
B3LYP free energy in solution: -2289.92180183 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	0.40974600	-0.86732800	2.43456500
C	0.35408000	0.21575700	1.55591800
C	0.37547000	1.52231100	2.04673900
C	0.48770500	1.75459300	3.42749300
C	0.57309400	0.66616400	4.30170100
C	0.53319500	-0.64545400	3.81587200
H	0.50851700	2.77818000	3.80710300
H	0.66700200	0.84169100	5.37557000
H	0.59125200	-1.49478700	4.49986500
C	0.27189100	2.58541900	1.04128700
C	0.06080800	3.63785900	-0.94283500
C	0.23589700	4.66587100	0.22376800
H	1.17013500	5.24286800	0.14990300
H	-0.61165700	5.35948800	0.32180200
C	0.31439900	-2.19834000	1.82040000
C	0.01214800	-3.83433100	0.30152600
C	0.55696900	-4.40993000	1.64787500
H	-0.08096100	-5.19373100	2.08042000
H	1.58904100	-4.78329400	1.56346200
N	0.15577800	2.35114100	-0.21963700
N	-0.00590500	-2.37961800	0.58789400
O	0.30177300	3.86495200	1.42424600
O	0.56982000	-3.28467300	2.55643900
C	-1.41778500	-4.31440800	0.01330600
H	-1.83510500	-3.78039800	-0.85192500
H	-1.42309300	-5.39426500	-0.20659100

H	-2.07736700	-4.13454000	0.87720500
C	0.95318000	-4.13766900	-0.86937600
H	1.08112200	-5.22636200	-0.98457800
H	0.53443400	-3.74882600	-1.81086500
H	1.93044800	-3.66181300	-0.70823200
C	-1.32024300	3.75975800	-1.60177500
H	-1.42226800	4.73631700	-2.10223600
H	-1.45929500	2.97246900	-2.35839800
H	-2.11965700	3.65635800	-0.85351800
C	1.18472800	3.75351900	-1.97938100
H	1.07521400	2.98602000	-2.76060000
H	1.15574100	4.74108200	-2.46775400
H	2.17048600	3.61833100	-1.51035000
Bi	0.23936700	-0.14076900	-0.67305200
C	-2.18402600	0.10802000	-0.43821500
C	-3.01187200	-0.75564600	-1.14384900
C	-4.40588600	-0.67944900	-1.03764400
F	2.55388300	-1.44350300	-0.30145200
F	-2.48702000	-1.69961500	-1.95197700
F	-5.20085200	-1.50932200	-1.70057300
Si	3.82642900	-0.18596700	-0.51174900
H	2.47362400	0.71739900	-0.67673100
H	4.74446500	-1.21197000	0.15669600
C	4.61865900	1.35486000	0.37627100
C	6.13074600	1.27670300	0.60383200
H	4.09858600	1.46743500	1.34788600
H	4.35213100	2.25963300	-0.20357500
H	6.52139400	2.13900100	1.17401100
H	6.40241200	0.36291000	1.15883100
H	6.68403400	1.24380800	-0.35075700
C	4.37041800	-0.22075600	-2.34620700
C	3.84999900	-1.40934000	-3.16535900
H	5.47594100	-0.23127500	-2.35000600
H	4.07236600	0.72873500	-2.82773200
H	4.23253500	-1.40307500	-4.20135500
H	4.14527700	-2.37023500	-2.71211300
H	2.74812400	-1.41396600	-3.22713900
C	-4.94466600	0.30481900	-0.21105200
F	-6.26123500	0.43221400	-0.07106500
N	-2.74281500	1.05222600	0.34690500
C	-4.04213300	1.14793500	0.45312200
F	-4.54406800	2.10800900	1.23173500



ts3-2a-2



B3LYP electronic energy: -1739.8238404 a.u.  
B3LYP enthalpy: -1739.417667 a.u.  
B3LYP free energy: -1739.511611 a.u.  
B3LYP SCF energy in solution: -1741.70493359 a.u.  
B3LYP enthalpy in solution: -1741.29876059 a.u.  
B3LYP free energy in solution: -1741.39270459 a.u.

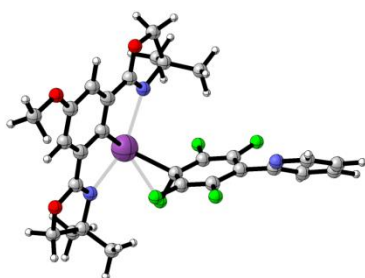
Cartesian coordinates

ATOM	X	Y	Z
C	-3.33434000	-0.94326600	-0.32031600
C	-2.52030600	0.19242300	-0.18317000
C	-3.07580300	1.45691000	-0.43050200
C	-4.42306200	1.59127000	-0.80651700
C	-5.21977200	0.44831700	-0.93510500
C	-4.68262400	-0.82146100	-0.69572700
H	-4.83882500	2.58306200	-0.99846100
H	-6.26735100	0.54759800	-1.22803800
H	-5.30162300	-1.71549300	-0.80099600
C	-2.15890600	2.59250000	-0.28790600
C	-0.27182000	3.78873200	0.01701500
C	-2.67275800	-2.22756500	-0.06882400
N	-0.92320300	2.46018100	0.05411900
N	-1.43621000	-2.31560800	0.27948300
C	-0.10520100	-4.05435800	-0.83528400
H	0.80066700	-3.43028700	-0.78207500
H	0.19314800	-5.11532200	-0.81271500
H	-0.59846900	-3.85452500	-1.79973000
C	-0.39405600	-4.07589200	1.67620600
H	-0.18048200	-5.15480700	1.74401300
H	0.55863600	-3.53492400	1.77774600
H	-1.04596100	-3.79578100	2.51825300
C	0.44376800	4.07906100	1.34050000
H	0.83628900	5.10894900	1.34657900
H	-0.24244100	3.96407200	2.19379600
H	1.29415100	3.39436200	1.47333900
C	-1.49810200	4.72748500	-0.21467300
H	-1.77520800	5.29639800	0.68759200

H	-1.36453000	5.42492400	-1.05372700
C	-1.05281300	-3.74330000	0.33383900
C	-2.44197400	-4.43867100	0.16798800
H	-2.81760300	-4.87170300	1.10930000
H	-2.45487300	-5.21009800	-0.61482900
C	0.71769600	3.83549400	-1.15715700
H	0.20798700	3.62857800	-2.11115200
H	1.18817500	4.83012800	-1.22210300
H	1.50965800	3.08700300	-1.01461900
O	-2.59217300	3.83893700	-0.53412700
O	-3.34458200	-3.37920900	-0.22543200
Bi	-0.32392600	-0.01658700	0.48967400
C	2.43510300	-0.94887400	-0.50232500
C	3.65902300	-1.54767900	-0.78029200
C	4.87223000	-0.88612300	-0.57613600
F	3.71143100	-2.81102200	-1.25062100
F	6.04837100	-1.45053900	-0.84904800
H	0.48735900	-0.60401400	-1.03431200
C	4.84154000	0.41702800	-0.06668900
F	5.97065100	1.09846300	0.14321100
C	3.58622700	0.96153300	0.19997900
N	2.46405500	0.31769300	-0.01521700
F	3.51781200	2.21460200	0.68729400

The following are the details of the calculation data for each species in Table 2:

ts1-2c



B3LYP electronic energy: -2184.3491198 a.u.  
 B3LYP enthalpy: -2183.825649 a.u.  
 B3LYP free energy: -2183.935346 a.u.  
 B3LYP SCF energy in solution: -2186.77980493 a.u.  
 B3LYP enthalpy in solution: -2186.25633393 a.u.  
 B3LYP free energy in solution: -2186.36603093 a.u.

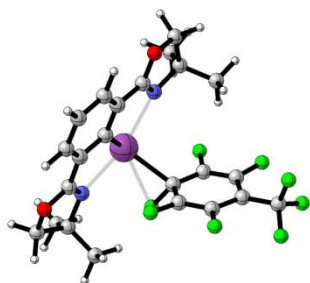
Cartesian coordinates

ATOM	X	Y	Z
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C	-1.78832800	2.02147000	0.99318300
C	-2.02054900	0.72677000	0.50280200
C	-2.86964000	-0.11851000	1.22266000
C	-3.47108400	0.29426200	2.42462300
C	-3.21405200	1.58657600	2.90977100
C	-2.37449600	2.45529800	2.18567400
H	-4.12339400	-0.39712800	2.95684800
H	-2.19431400	3.45868600	2.57460900
C	-3.08193200	-1.44051800	0.63227800
C	-2.85230900	-3.23773000	-0.70913500
C	-4.01092500	-3.44063400	0.31090900
H	-5.00807100	-3.37700200	-0.15660200
H	-3.93418300	-4.37462300	0.88317900
C	-0.92011900	2.86894900	0.17034700
C	0.48576800	3.55412800	-1.45032500
C	0.04082800	4.74864100	-0.55241800
H	0.88036600	5.31623500	-0.12833600
H	-0.64172100	5.44201300	-1.07108600
N	-2.52254900	-1.80853700	-0.47034100
N	-0.36487000	2.45861800	-0.91970900
O	-3.88315100	-2.33144400	1.23182100
O	-0.68943600	4.13783700	0.53396600
C	1.96824000	3.21579300	-1.23169700
H	2.25190100	2.31414600	-1.78886600
H	2.59963600	4.04993700	-1.57848500
H	2.17931900	3.04312700	-0.16508800
C	0.19029900	3.79297100	-2.93317200
H	0.76282800	4.65654900	-3.30809200
H	0.48241400	2.91235500	-3.52511400
H	-0.88082100	3.98643900	-3.09913700
C	-1.64078400	-4.11595200	-0.35858400
H	-1.89110400	-5.17717300	-0.52165000
H	-0.77971000	-3.83721000	-0.97908800
H	-1.35046000	-3.97776900	0.69323000
C	-3.29289600	-3.45614600	-2.15734600
H	-2.45007500	-3.26205800	-2.83778500
H	-3.61710600	-4.49796700	-2.31035900
H	-4.12580300	-2.78841400	-2.42781000
Bi	-1.13368600	0.03647100	-1.46322100
C	2.42501500	-1.37993500	1.11782000
C	1.18518300	-1.44823300	0.50020000
C	0.95411000	-0.99799000	-0.82199500
C	2.09039800	-0.42391700	-1.43777500
C	3.32439700	-0.34405300	-0.82209100

F	2.51515900	-1.87200600	2.35611500
F	0.13427900	-1.92378900	1.21564300
F	0.32536800	-2.15608500	-1.78672700
F	1.91761200	0.18335500	-2.64766600
F	4.30600100	0.29103700	-1.49306400
C	3.56343200	-0.83368100	0.47938900
O	-3.73104800	2.08830100	4.05644900
C	-4.55952700	1.27357100	4.85802600
H	-4.84028400	1.87795400	5.73057100
H	-5.47721700	0.96905800	4.32326700
H	-4.03091900	0.36744500	5.20392200
C	4.89018300	-0.75764800	1.12907200
C	6.08040700	-0.95429400	0.39299000
C	7.30701800	-0.86425300	1.04465900
H	6.03441600	-1.17772300	-0.67281000
C	6.10323000	-0.42437700	3.06282500
C	7.33055000	-0.59470900	2.41586100
H	8.23658200	-1.01416500	0.48843700
H	6.07553600	-0.21243700	4.13958700
H	8.26911900	-0.51922100	2.96979400
N	4.92425200	-0.49342300	2.44809800

ts1-2d



B3LYP electronic energy: -2159.7828687 a.u.  
 B3LYP enthalpy: -2159.359386 a.u.  
 B3LYP free energy: -2159.461379 a.u.  
 B3LYP SCF energy in solution: -2162.19104855 a.u.  
 B3LYP enthalpy in solution: -2161.76756655 a.u.  
 B3LYP free energy in solution: -2161.86955855 a.u.

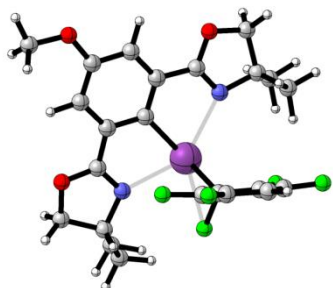
Cartesian coordinates

ATOM	X	Y	Z
C	-1.33902700	2.07444700	1.72089900
C	-1.80090700	0.93285200	1.05307500
C	-2.75857700	0.11595500	1.66966700

C	-3.23963900	0.42218600	2.95220600
C	-2.75714700	1.55561400	3.61611600
C	-1.81248200	2.38775900	3.00635600
H	-3.98396400	-0.22423900	3.42228700
H	-3.12392000	1.79466000	4.61661200
H	-1.44190700	3.27792300	3.51919900
C	-3.19769900	-1.03879900	0.88487300
C	-3.28881400	-2.60464900	-0.73420700
C	-4.44473700	-2.78613800	0.29146100
H	-5.42573700	-2.48348000	-0.11204100
H	-4.51478600	-3.80212600	0.70158800
C	-0.37485400	2.90044800	0.98888800
C	1.05202000	3.63316800	-0.59482700
C	0.86414800	4.70012900	0.52779100
H	1.80839900	5.02419600	0.98627700
H	0.30283200	5.58579000	0.18785700
N	-2.73270700	-1.29854500	-0.29016900
N	0.06205600	2.60209200	-0.18828400
O	-4.11486700	-1.88143000	1.37303700
O	0.07408500	4.03582300	1.53884700
C	2.46940700	3.04201600	-0.56832000
H	2.57010300	2.22761600	-1.29659800
H	3.20625000	3.82221800	-0.81919800
H	2.71412700	2.64628500	0.42948600
C	0.71440900	4.18297600	-1.98349100
H	1.39987100	5.00304900	-2.25114700
H	0.82207300	3.39409300	-2.74322000
H	-0.31709200	4.56622900	-2.02011300
C	-2.22295500	-3.70023700	-0.57318900
H	-2.63754100	-4.67203000	-0.88752400
H	-1.34085400	-3.45993600	-1.17991800
H	-1.89761300	-3.77778400	0.47487000
C	-3.78428400	-2.52244400	-2.17841700
H	-2.93348000	-2.36168500	-2.85752600
H	-4.27640600	-3.46331200	-2.47215100
H	-4.50268700	-1.69818800	-2.30954700
Bi	-1.11323100	0.45700500	-1.05857900
C	2.26351400	-1.86509500	1.02943000
C	1.00396200	-1.63665900	0.50304300
C	0.79804100	-0.96318200	-0.72707500
C	1.98711600	-0.47711800	-1.32333500
C	3.24656400	-0.68684300	-0.79618400
F	2.34059600	-2.48888600	2.21085800
F	-0.07826700	-2.00246900	1.23429500

F	-0.03743400	-1.84779000	-1.80951800
F	1.86120600	0.32835600	-2.41564600
F	4.28300100	-0.11674800	-1.42463500
C	3.44128800	-1.43705700	0.38129000
C	4.79702500	-1.68758800	0.96901200
F	4.86767300	-2.87976600	1.58793900
F	5.76618900	-1.67223000	0.03789900
F	5.14071000	-0.75836500	1.89398900

ts1-2e



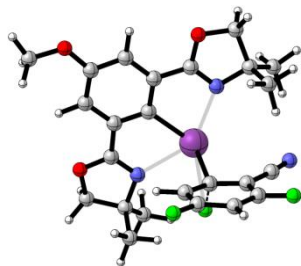
B3LYP electronic energy:	-1937.4348071 a.u.
B3LYP enthalpy:	-1936.985234 a.u.
B3LYP free energy:	-1937.083844 a.u.
B3LYP SCF energy in solution:	-1939.57076922 a.u.
B3LYP enthalpy in solution:	-1939.12119622 a.u.
B3LYP free energy in solution:	-1939.21980622 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	-0.76746800	2.38192400	0.13168100
C	-1.16073600	1.06829200	-0.17302100
C	-2.46766500	0.67551200	0.13370100
C	-3.37507700	1.55570300	0.74888700
C	-2.95960700	2.86006700	1.06058000
C	-1.65158300	3.27512800	0.74402700
H	-4.38274100	1.20732800	0.97301900
H	-1.35034300	4.29567400	0.98565600
C	-2.80966900	-0.69771900	-0.23602900
C	-2.60036500	-2.83548100	-0.91888500
C	-4.08967300	-2.47635600	-0.64207700
H	-4.68257100	-2.37094000	-1.56650000
H	-4.59252500	-3.17824800	0.03642700
C	0.60085400	2.74229600	-0.24996200
C	2.71947700	2.59846600	-1.00145100
C	2.34183400	4.07490800	-0.66949600

H	3.03591900	4.55890600	0.03138500
H	2.24000100	4.70261400	-1.57020600
N	-1.96722500	-1.49747100	-0.79699100
N	1.41797300	1.91259400	-0.80565500
O	-4.03792300	-1.18089600	0.00053700
O	1.04549300	3.98983600	-0.03917800
C	3.75388200	2.04850700	-0.00778600
H	3.93476200	0.97992800	-0.18058300
H	4.70953600	2.58536900	-0.12309800
H	3.40923700	2.17617000	1.03002600
C	3.20364400	2.43009600	-2.44429100
H	4.12966900	3.00363300	-2.61112900
H	3.42107700	1.37146200	-2.65218500
H	2.44451100	2.77833300	-3.16166800
C	-2.04209500	-3.77424400	0.16254100
H	-2.51942700	-4.76450900	0.07854800
H	-0.95497900	-3.87401200	0.05038600
H	-2.23697800	-3.37146400	1.16740700
C	-2.37948100	-3.41191600	-2.31818500
H	-1.30850400	-3.61006700	-2.47563600
H	-2.92046900	-4.36465900	-2.43465000
H	-2.72699200	-2.71565000	-3.09740000
Bi	0.23880600	-0.36818100	-1.22112600
C	1.57456600	-1.54927400	3.04565300
C	0.79043100	-1.59003100	1.89983100
C	1.35441300	-1.54748900	0.60195100
C	2.76323200	-1.42633500	0.56897900
C	3.53763700	-1.36783200	1.71662300
F	0.96454500	-1.58220700	4.24181400
F	-0.56059000	-1.57791400	2.03053400
F	0.87588400	-2.78683600	-0.34392900
F	3.35609800	-1.22880400	-0.64352500
F	4.86515100	-1.19698400	1.58787400
C	2.96782800	-1.45725800	2.98842400
O	-3.74481600	3.78908200	1.65776000
C	-5.06371200	3.44682700	2.02507500
H	-5.49698300	4.33813400	2.49773200
H	-5.67672000	3.17338200	1.14731100
H	-5.08415400	2.61156500	2.74777100
H	3.57672700	-1.45198600	3.89087000

ts1-2f



B3LYP electronic energy: -1831.3098437 a.u.  
 B3LYP enthalpy: -1830.845238 a.u.  
 B3LYP free energy: -1830.943415 a.u.  
 B3LYP SCF energy in solution: -1833.31751871 a.u.  
 B3LYP enthalpy in solution: -1832.85291371 a.u.  
 B3LYP free energy in solution: -1832.95109071 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	-1.28476900	2.21557900	0.22137400
C	-1.40243700	0.84896000	-0.07550500
C	-2.62438200	0.21783400	0.17224600
C	-3.71482900	0.91117000	0.72901300
C	-3.57026400	2.27192600	1.04077700
C	-2.35088300	2.92765500	0.77730400
H	-4.64965500	0.37981100	0.90371900
H	-2.26353600	3.98982600	1.01130000
C	-2.68617400	-1.19380600	-0.21452300
C	-2.05022500	-3.24722500	-0.89354100
C	-3.59671900	-3.15781100	-0.74358700
H	-4.11900100	-3.12823300	-1.71463800
H	-4.02737000	-3.95317400	-0.12098800
C	0.00366100	2.83340300	-0.11498300
C	2.14443700	3.10463800	-0.75832700
C	1.45225600	4.47858000	-0.51795800
H	2.00030800	5.13527400	0.17114000
H	1.24817100	5.02184900	-1.45549000
N	-1.67187800	-1.82222600	-0.70437100
N	0.99063800	2.17471400	-0.61951200
O	-3.82422000	-1.88871000	-0.08201700
O	0.18087900	4.14576200	0.08574600
C	3.17438100	2.80657300	0.34218200
H	3.57531700	1.79051500	0.23711500
H	4.01431600	3.51639200	0.27203000
H	2.72215500	2.90085600	1.34184500
C	2.77382700	2.99782500	-2.14907700
H	3.56158000	3.75920200	-2.26941600



H	3.23666200	2.00879700	-2.28750400
H	2.01966400	3.15454400	-2.93621500
C	-1.42681500	-4.09847300	0.22433200
H	-1.69811500	-5.15778000	0.08569700
H	-0.33477300	-3.98909300	0.20959000
H	-1.79386700	-3.77664900	1.21212800
C	-1.61122000	-3.74663900	-2.27075100
H	-0.51259200	-3.75102600	-2.32991500
H	-1.96552600	-4.77611200	-2.43936300
H	-2.00792100	-3.10639000	-3.07410000
Bi	0.28635300	-0.27583900	-1.11108300
C	1.68265800	-1.56276200	3.06693200
C	0.90052200	-1.50300700	1.93395100
C	1.51060600	-1.30445300	0.65457600
C	2.93168100	-1.03053700	0.65105000
C	3.66156200	-1.11670500	1.85118500
F	1.08034000	-1.77541900	4.25027800
F	1.24550000	-2.59709800	-0.32739800
F	4.98228300	-0.89051900	1.79286000
C	3.07790800	-1.37943500	3.07663900
O	-4.54465000	3.03817800	1.58410400
C	-5.79951900	2.46089000	1.87668900
H	-6.41625400	3.25946800	2.30930900
H	-6.29597000	2.07739500	0.96729700
H	-5.71162700	1.63877400	2.60925400
H	3.65983200	-1.42460600	3.99526700
C	3.57145700	-0.70300800	-0.57165300
N	4.00958700	-0.38377400	-1.60533700
H	-0.17698000	-1.63757500	2.03195800