

Dual reactivity of B(C₆F₅)₃ enables the silylative cascade conversion of N-aryl-piperidines to sila-N-heterocycles: DFT calculations

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Computational Details

Gaussian 16¹ was used for all calculations in this work. Geometric structural optimization and frequency calculation were conducted by B3LYP² functional in gas phase at T = 298.15 K and 1 atm. The all-electron basis set 6-31G** was used in describing the atoms (B, C, H, O, N, F).³ There is no imaginary frequency for all the intermediates, while only-one imaginary frequency is in the structure of transition states. In addition, the intrinsic reaction coordinate (IRC) calculation⁴ which correctly bridges the intermediates, further demonstrates the credibility of transition state structures. Based on the gas-phase optimized geometries, solvation effect of benzene was incorporated with the SMD⁵ model at the level of B3LYP-D3⁶ while 6-311++G** basis set for all main group atoms.³ All 3D molecular structures were generated by using the CYLview (Version) program.⁷ Geometric structural optimization and frequency calculation in benzene as the solvent were conducted for a series of species shown in Figure 1 by using B3LYP functional and 3-21G (opt1), 6-31G (opt2) for all atoms in these calculations. The results were listed in Table S2.

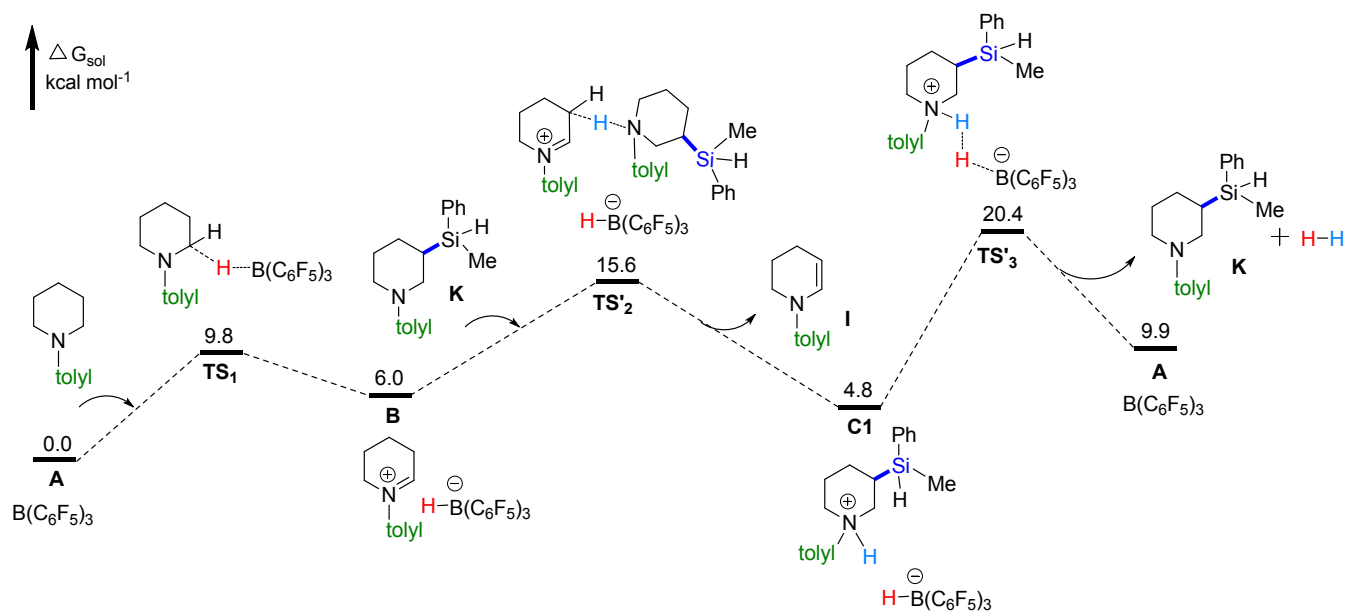


Figure S1. Energy profile for enamine (**I**) formation by intermediate **K** as a hydrogen acceptor.

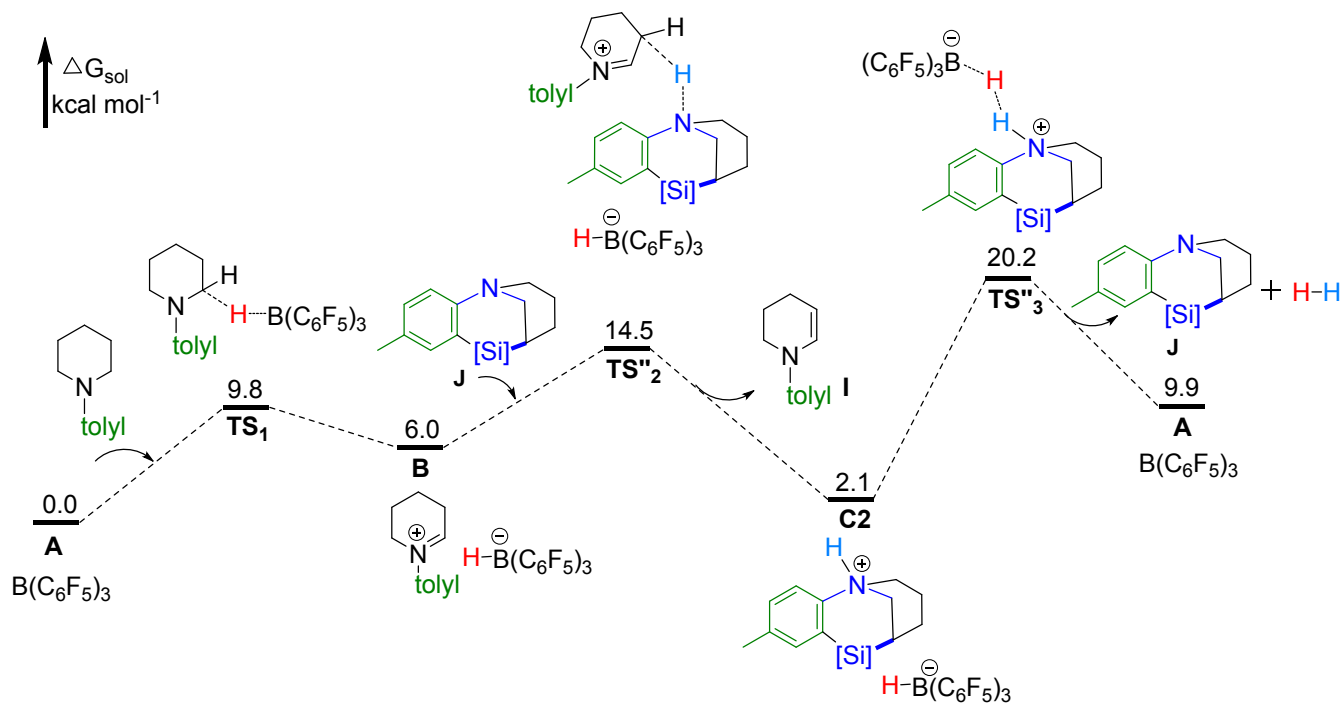


Figure S2. Energy profile for enamine (I) formation by intermediate J as a hydrogen acceptor.

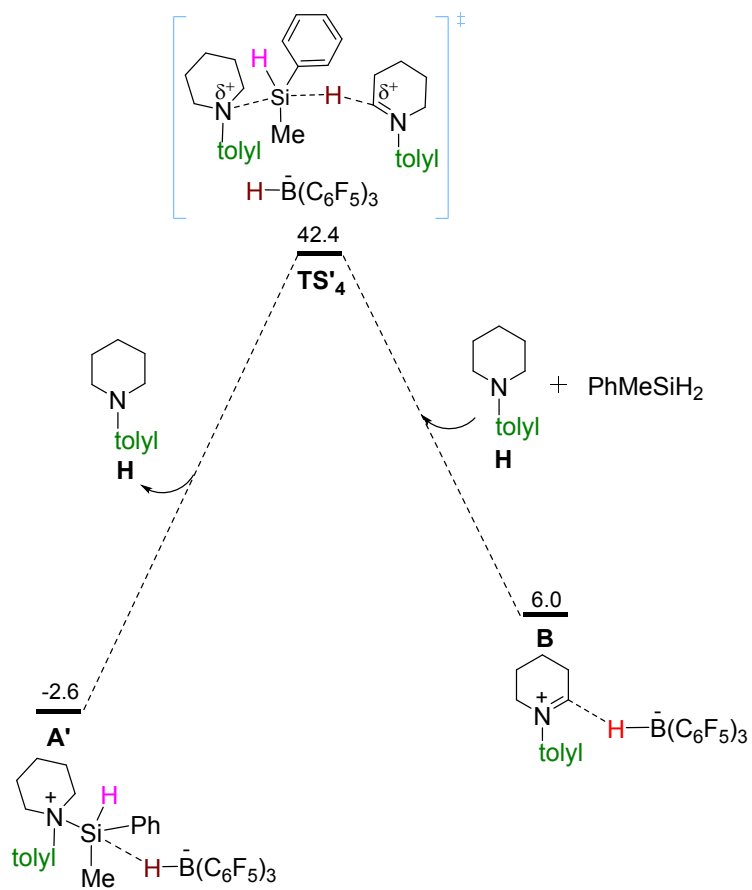


Figure S3. The formation of **A'** from **B** + PhMeSiH_2 + **H** via **TS'**₄.

Table S1. Calculated relative energies of **A'** and **TS₄** by different DFT methods.

DFT Methods	Species	ΔE_{gas}	ΔG_{gas}	ΔE_{sol}	ΔG_{sol}
B3LYP	A'	-0.93	30.58	-34.09	-2.58
	TS₄	30.54	61.95	0.57	31.98
WB97XD	A'	-33.89	-1.07	-34.12	-1.0
	TS₄	28.85	29.08	-0.67	33.46
M062X	A'	-32.01	-1.63	-34.47	-4.09
	TS₄	-4.41	27.62	-1.11	30.92
BP86	A'	-1.16	29.08	-34.23	-4.14
	TS₄	26.58	58.52	0.84	32.78

Table S2. The ΔE_{gas} , ΔG_{gas} and ΔE_{sol} calculated for species in the **Fig. 1**.

Species	ΔG_{gas}	ΔE_{gas}	ΔE_{sol}	$\Delta G_{\text{sol-opt1}}$	$\Delta G_{\text{sol-opt2}}$
A	0	0	0	0	0
TS₁	26.26	12.96	-3.45	12.4	27.5
TS₅	62.00	34.55	6.22		
B	24.29	12.32	-6.01	11.2	20.8
TS₂	42.13	16.64	-6.14	14.2	42.0
C	24.92	10.56	-8.08	7.3	23.4
TS₃	44.45	30.94	18.22		
D	7.25	-3.67	-6.21	-2.5	8.3
TS₄	61.95	30.54	0.57	37.0	33.9
A'	30.58	-0.93	-34.09	2.0	21.0
A	10.39	26.62	25.16		

Table S3. The ΔE_{gas} , ΔG_{gas} and ΔE_{sol} calculated for species in the **Fig. 2**.

Species	ΔG_{gas}	ΔE_{gas}	ΔE_{sol}
A	0	0	0
D	7.62	-3.93	-7.28
TS₆	50.49	20.32	-3.30
E	18.82	-10.79	-34.83
TS₇	27.84	-1.81	-24.94
F	11.57	-17.19	-31.99
TS₈	41.26	5.27	-27.31
G	33.70	-2.12	-29.98
TS₉	53.97	22.80	-17.70
A	5.49	-1.46	-7.83

Table S4. The ΔE_{gas} , ΔG_{gas} and ΔE_{sol} calculated for species in the **Fig. 3**.

Species	ΔG_{gas}	ΔE_{gas}	ΔE_{sol}
A	0	0	0
TS₈	40.00	19.61	-8.36
TS'₈	45.82	26.99	5.44
TS''₈	47.06	27.56	0.44
TS'''₈	35.69	15.47	-11.75
G	32.43	12.22	-11.03
G1	43.22	23.33	-0.50
G2	43.06	24.60	0.63
G3	22.61	2.95	-18.2
TS₉	52.70	37.13	1.25
TS'₉	44.28	30.72	10.51
TS''₉	55.79	41.41	18.88
TS'''₉	40.28	24.16	3.26
J	4.22	12.88	11.12
J1	2.01	11.60	9.35
J2	9.08	18.70	16.74
J3	-2.84	6.85	6.09

Table S5. The ΔE_{gas} , ΔG_{gas} and ΔE_{sol} calculated for species in the **Fig. 4**.

Species	ΔG_{gas}	ΔE_{gas}	ΔE_{sol}
A	0	0	0
TS₁₀	29.91	12.17	-10.24
M	18.16	3.02	-13.24
TS₁₁	26.01	13.71	-1.70
A	-11.09	-0.15	2.68

Table S6. The ΔE_{gas} , ΔG_{gas} and ΔE_{sol} calculated for species in the **Fig. 5**.

Species	ΔG_{gas}	ΔE_{gas}	ΔE_{sol}
A	0	0	0
TS₁₂	16.98	1.19	-8.81
O	10.27	-6.36	-20.44
TS₁₃	29.02	-4.68	-25.03
P	10.33	-8.25	-11.21
TS₁₄	0.20	-32.36	-2.40
R	-10.39	-9.58	-5.16
B	-61.18	-74.48	-35.16
TS₁₅	-57.20	-71.86	-30.44
A	-85.47	-86.80	-29.15

Table S7. The ΔE_{gas} , ΔG_{gas} and ΔE_{sol} calculated for species in the **Fig. S1**.

Species	ΔG_{gas}	ΔE_{gas}	ΔE_{sol}
A	0	0	0
TS₁	26.26	12.96	-3.45
B	24.29	12.32	-6.01
TS'2	39.72	12.94	-10.75
C1	22.47	8.14	-9.51
TS'3	24.35	19.51	15.57
A	10.39	26.62	25.16

Table S8. The ΔE_{gas} , ΔG_{gas} and ΔE_{sol} calculated for species in the **Fig. S2**.

Species	ΔG_{gas}	ΔE_{gas}	ΔE_{sol}
A	0	0	0
TS ₁	26.26	12.96	-3.45
B	24.29	12.32	-6.01
TS'' ₂	36.58	13.26	-8.80
C2	19.24	4.88	-12.20
TS'' ₃	24.90	21.96	17.30
A	10.39	26.62	25.16

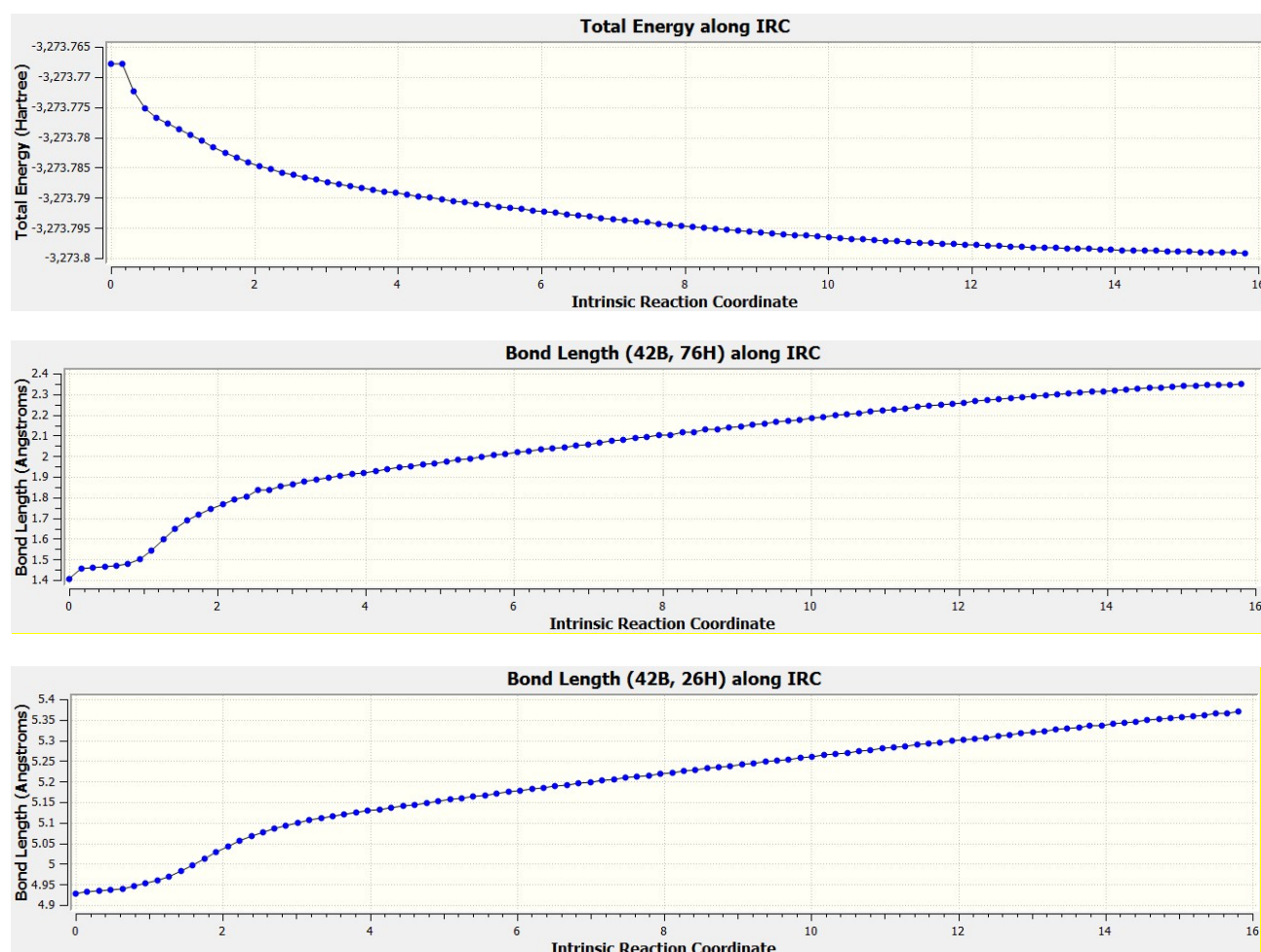
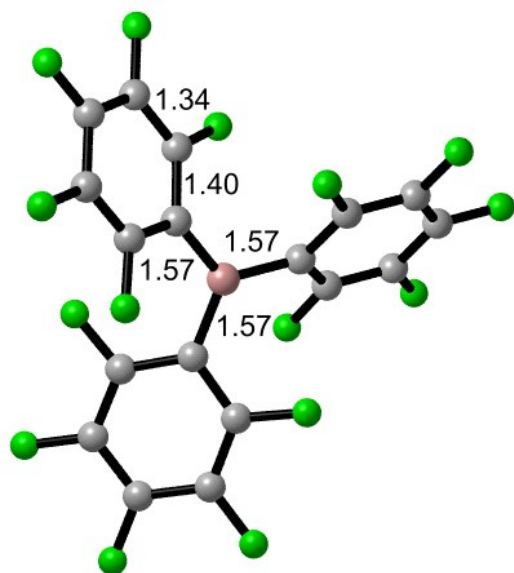


Figure S4. The energy, and (C₆F₅)₃B–H (hydride) and (C₆F₅)₃B–HSi(R)MePh distances along the IRC of TS₇.

Cartesian coordinates and structures of all the compounds optimized in this study



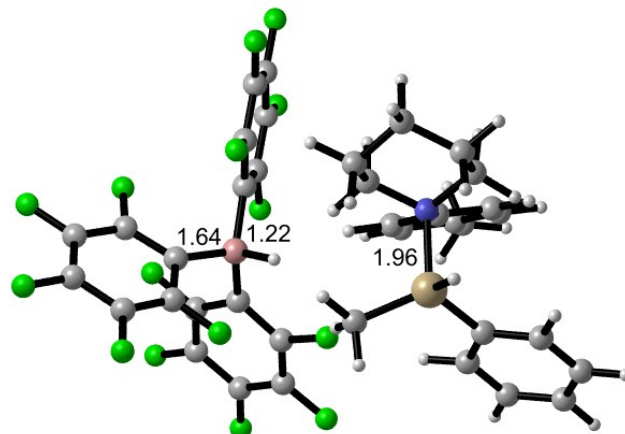
A

G_{gas} = -2208.113272 a.u.

E_{gas} = -2208.20630331 a.u.

B	0.00045200	0.00022800	0.00002800
C	-1.01179600	1.19903000	0.00007600
C	-2.22317500	1.15822600	0.70865400
C	-0.76932400	2.38663500	-0.70840800
C	-3.12750900	2.21391100	0.72882100
C	-1.65922600	3.45451800	-0.72844400
C	-2.84392300	3.36740200	0.00015700
C	1.54491700	0.27702600	0.00003600
C	2.45180200	-0.52757900	-0.70809100
C	2.11586500	1.34650900	0.70813600
C	3.82170000	-0.29164800	-0.72815500
C	3.48242500	1.60108300	0.72820000
C	4.33916600	0.77788600	0.00001700
C	-0.53213700	-1.47567300	-0.00004900
C	-1.68222100	-1.85847100	-0.70845100
C	0.10811300	-2.50487700	0.70839900
C	-2.16301000	-3.16274800	-0.72879500
C	-0.35489200	-3.81558200	0.72826800
C	-1.49590500	-4.14577900	-0.00041200
F	0.35074000	2.52290900	-1.43675300
F	-1.39077400	4.55747300	-1.43406100
F	-3.70328700	4.38449900	0.00020000
F	-4.25970700	2.13338300	1.43459600
F	-2.54427700	0.07672400	1.43726100
F	1.34020100	2.16645600	1.43590200
F	3.97934500	2.62203400	1.43331700
F	5.64978800	1.01295300	-0.00013100
F	4.64225900	-1.07639300	-1.43336800
F	2.00934800	-1.56567100	-1.43624800

F	-2.35976900	-0.95577600	-1.43628900
F	1.20568100	-2.24314000	1.43674400
F	0.28034200	-4.75645700	1.43376100
F	-1.94796700	-5.39823500	-0.00058000
F	-3.25275300	-3.48079600	-1.43433600



A'

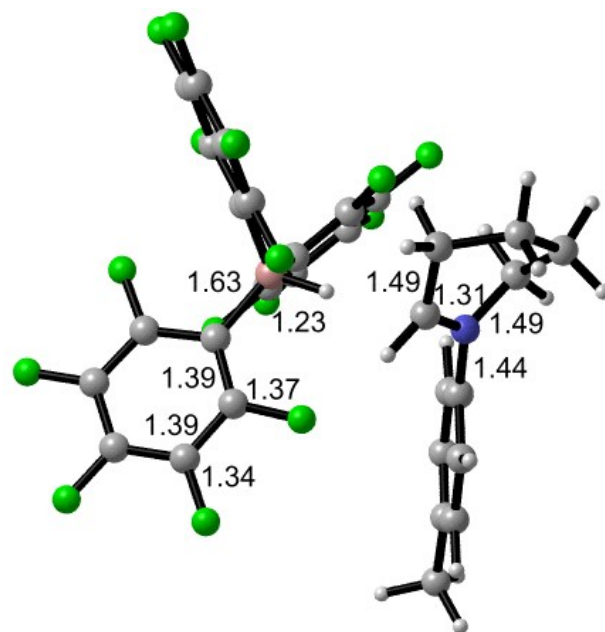
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E_{gas} = -3292.76589819 a.u.

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C	4.49675600	-0.54011400	1.85773900
C	5.85664000	-0.32040500	2.15347600
C	4.10259500	-1.82123400	1.41951700
C	6.79786900	-1.33889900	2.00079100
H	6.18450200	0.64999200	2.51994600
C	5.04414700	-2.83860800	1.27195800
H	3.06241100	-2.03229500	1.18928300
C	6.39052100	-2.59844900	1.55815000
H	7.84205200	-1.15310700	2.23476300
H	4.72513300	-3.82078500	0.93643300
H	7.11997000	-3.39513600	1.44347300
B	-1.55957200	-0.13309200	0.07043000
C	-1.54364900	-1.76584600	-0.10350900
C	-0.46247000	-2.56455300	0.25888600
C	-2.65049000	-2.48309200	-0.56749400
C	-0.44958400	-3.95607400	0.18288900
C	-2.69306900	-3.87133000	-0.66235300
C	-1.57975600	-4.61746100	-0.28143000
C	-1.52691200	0.72914400	-1.32960400
C	-1.48001300	2.12536900	-1.26513900
C	-1.45185800	0.22684000	-2.62991700
C	-1.38794400	2.96661600	-2.36871300
C	-1.36254700	1.02608900	-3.77135700
C	-1.33930700	2.40941400	-3.64347600

C	-2.79286000	0.29368600	1.06371400
C	-4.04156000	0.76291400	0.65125400
C	-2.64406600	0.18296400	2.44771800
C	-5.06517300	1.10814400	1.53323800
C	-3.63611200	0.51465900	3.36700300
C	-4.86167800	0.98211100	2.90342400
F	-3.78675000	-4.49975500	-1.11955900
F	-3.75206900	-1.81824900	-0.96708600
F	-1.59662500	-5.95540300	-0.36739100
F	0.64102500	-4.65559400	0.54805500
F	0.69719500	-2.00136600	0.71630000
F	-1.40963400	-1.10773600	-2.85978900
F	-1.28475600	0.46917600	-4.99083200
F	-1.24562800	3.19511700	-4.72630600
F	-1.33016200	4.30226800	-2.21652500
F	-1.48119800	2.74026800	-0.05096000
F	-1.47598400	-0.26707100	2.97291400
F	-3.42273800	0.39075300	4.68933700
F	-5.83389600	1.30892600	3.76813300
F	-6.24395700	1.56037100	1.07527700
F	-4.31437600	0.91767500	-0.66056900
H	-0.54048800	0.17319200	0.65938500
C	3.88113300	4.13403300	1.23736500
H	4.06976700	3.87741000	2.28429700
H	4.66280700	4.84532100	0.94671600
C	4.06816200	2.90630100	0.34288800
H	4.05061100	3.20533900	-0.70953900
H	5.03459100	2.44145000	0.54549600
C	1.62982200	0.27291500	2.84106700
H	0.93292500	1.09073600	3.03395400
H	1.11603300	-0.46211900	2.21979400
H	1.85317600	-0.20332500	3.80416700
N	2.99954400	1.81859200	0.47881800
C	3.12414800	0.84075000	-0.66605700
C	2.00726700	0.10520700	-1.06998900
C	4.34588500	0.64042000	-1.31696600
C	2.10853500	-0.79328300	-2.13088300
H	1.04745200	0.20628600	-0.58410900
C	4.42944300	-0.26743200	-2.37232600
H	5.24660000	1.16126500	-1.02246400
C	3.31643400	-0.99476200	-2.80799200
H	1.21403800	-1.33048700	-2.43328300
H	5.38821500	-0.40616700	-2.86410400
C	2.48857700	4.75132300	1.09920200
H	2.35478400	5.15975700	0.08894300
H	2.37134400	5.58496000	1.79826100
C	3.40429500	-1.94968000	-3.97249800

H	2.90706800	-2.89784400	-3.74575800
H	2.91077000	-1.53212300	-4.85792100
H	4.44261900	-2.16333000	-4.23979100
C	1.61330400	2.48154500	0.41906200
H	0.86451100	1.72149900	0.63090400
H	1.48576000	2.80072300	-0.61946100
C	1.44162800	3.66885700	1.35961800
H	1.48423000	3.34678300	2.40750900
H	0.42505800	4.03536400	1.18803000



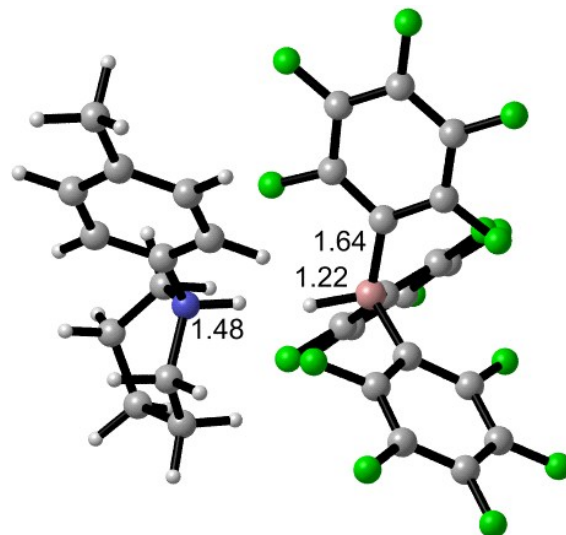
B

$G_{\text{gas}} = -2730.127933 \text{ a.u.}$

$E_{\text{gas}} = -2730.46693512 \text{ a.u.}$

C	3.20102200	-0.81579900	-1.47972400
C	3.74792700	0.09311900	-2.38599400
C	4.78811600	0.92394200	-1.97652200
C	5.29728600	0.86314400	-0.67247600
C	4.73395700	-0.06524300	0.21547700
C	3.69264200	-0.90258700	-0.17499800
H	3.37691200	0.13992500	-3.40500000
H	5.21332400	1.62766500	-2.68619700
H	5.10576500	-0.12618100	1.23425500
H	3.24522100	-1.58844600	0.53691600
N	2.11468700	-1.67142600	-1.88783500
C	1.02681500	-1.19891300	-2.43618500
H	0.97899200	-0.13436800	-2.62846100
C	-0.01273200	-2.15572200	-2.91013600
H	-0.74633900	-1.62535700	-3.51655100
H	-0.54479600	-2.51978000	-2.02301500
C	0.63131300	-3.34802700	-3.66182600
H	0.91243900	-3.02078400	-4.66703500

H	-0.12869300	-4.12306100	-3.78752600
C	1.87617500	-3.90620100	-2.92505800
H	2.75324100	-3.85946500	-3.57765900
H	1.73855600	-4.95726500	-2.65502200
C	2.18267900	-3.13356200	-1.63009800
H	1.45401400	-3.36720200	-0.84967300
H	3.18220000	-3.35726600	-1.25960200
B	-0.65409000	0.13983700	0.09372100
C	-0.54348300	1.76863900	0.03013800
C	-1.33895400	2.59126800	0.83275000
C	0.27915000	2.45451700	-0.85915600
C	-1.32854300	3.98125100	0.76824100
C	0.32692600	3.84369300	-0.96528300
C	-0.48634000	4.61451700	-0.14310400
C	0.04035100	-0.58345500	1.38798000
C	0.18113200	-1.97225200	1.39316200
C	0.59697700	0.04084900	2.50810700
C	0.82744400	-2.70612600	2.38152000
C	1.24885600	-0.64843100	3.53340700
C	1.36777700	-2.03277900	3.47358200
C	-2.20105300	-0.31951400	-0.18058600
C	-2.72705400	-0.25275700	-1.47188000
C	-3.10272800	-0.76380000	0.78895500
C	-4.02848500	-0.61429100	-1.80767400
C	-4.41719100	-1.13297300	0.50404000
C	-4.88489200	-1.05775200	-0.80450300
F	1.11507000	1.78044400	-1.70185000
F	1.14743200	4.43903800	-1.84842000
F	-0.45827300	5.95189100	-0.22381200
F	-2.11361600	4.71678700	1.56932300
F	-2.16383600	2.03267700	1.74072800
F	0.54861100	1.37871200	2.65445400
F	1.76871600	0.01504200	4.57674800
F	1.99653200	-2.70757400	4.44554300
F	0.93883000	-4.04313800	2.28532300
F	-0.31017500	-2.70644100	0.34978800
F	-1.94267900	0.17581000	-2.49990000
F	-2.72520500	-0.86031000	2.07870800
F	-5.23668600	-1.55782200	1.47745600
F	-6.14390900	-1.41154900	-1.09677300
F	-4.46092000	-0.54082400	-3.07809300
H	-0.01795700	-0.29912500	-0.86353200
C	6.40049100	1.79015400	-0.22496500
H	5.98337900	2.69152500	0.24018900
H	7.04963300	1.31294100	0.51472000
H	7.01924300	2.11289400	-1.06672500



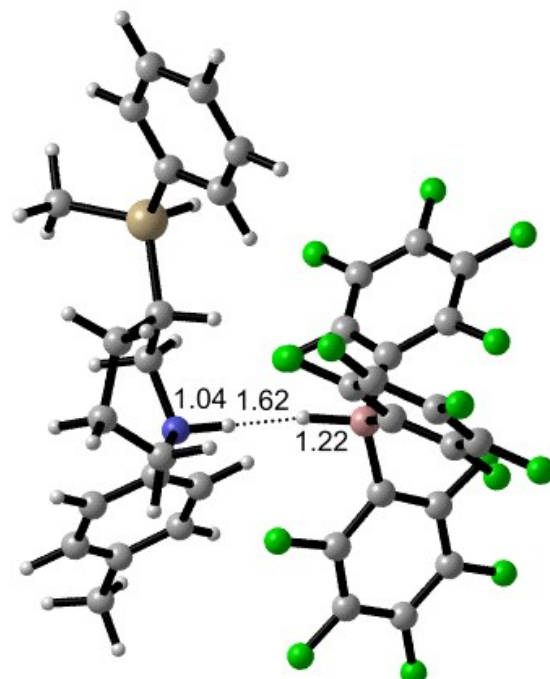
C

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E_{gas} = -2731.68909731 a.u.

H	1.50268900	-1.26791100	-0.38898400
C	3.54625900	-1.19560100	-0.21465100
C	4.70909000	-1.84295200	0.19881900
C	5.88854200	-1.10978800	0.32102600
C	5.92772400	0.26113200	0.03331400
C	4.74492200	0.87824900	-0.39481700
C	3.55582000	0.16238200	-0.52362000
H	4.70918200	-2.90304500	0.42997300
H	6.79289600	-1.61523300	0.64771700
H	4.74744600	1.93875400	-0.62969200
H	2.65258000	0.65527200	-0.86499200
N	2.28724100	-1.95553300	-0.38556000
C	2.24427400	-2.64725400	-1.74636000
H	3.19820500	-3.16630800	-1.86197700
H	2.18680700	-1.84614900	-2.48257500
C	1.05429300	-3.59599100	-1.82791200
H	1.01161800	-3.99099400	-2.84758100
H	0.13554700	-3.02257500	-1.67695900
C	1.14865800	-4.74090800	-0.78752600
H	1.50172000	-5.66378000	-1.25810900
H	0.14906100	-4.94338800	-0.39356600
C	2.09289700	-4.37107100	0.37497100
H	3.13480500	-4.58922200	0.11191300
H	1.87097800	-4.97814600	1.25848400
C	1.94097400	-2.90709600	0.77227100
H	0.90276600	-2.68948800	1.02260200
H	2.56989900	-2.61968500	1.61306400
B	-0.81015300	0.12151600	0.01075000
C	-1.27092700	0.51566200	-1.51373700
C	-2.55449900	0.90944600	-1.90382200

C	-0.35655900	0.45952500	-2.56365400
C	-2.90626800	1.19957900	-3.22183400
C	-0.65145800	0.73843100	-3.89444700
C	-1.94827900	1.11328400	-4.22781900
C	-0.08438500	1.35619400	0.80969900
C	0.97724300	1.11539200	1.68240000
C	-0.44383700	2.70264500	0.70053800
C	1.65667600	2.10532100	2.38760300
C	0.20258300	3.73083100	1.38552000
C	1.26204400	3.43040100	2.23683300
C	-1.98374700	-0.59775600	0.90189800
C	-2.11761600	-1.98454700	0.95274400
C	-2.91182500	0.09220600	1.68820600
C	-3.06708800	-2.65943200	1.71576600
C	-3.88269100	-0.53340300	2.46815400
C	-3.96281100	-1.92302800	2.48244100
F	0.94734400	0.10632700	-2.31933700
F	0.29370300	0.64821600	-4.84590900
F	-2.26902000	1.38942500	-5.49856800
F	-4.15806800	1.56624200	-3.53071600
F	-3.53735700	1.03203100	-0.99368300
F	-1.46393200	3.07205100	-0.09549000
F	-0.18559300	5.00567700	1.23565500
F	1.89696900	4.40573900	2.90127700
F	2.68087400	1.79626600	3.20110600
F	1.42361200	-0.15886600	1.88032400
F	-1.27177300	-2.78706700	0.23848700
F	-2.90541100	1.43764600	1.71973200
F	-4.74285800	0.18754000	3.20193300
F	-4.88874200	-2.54288400	3.22598700
F	-3.12151300	-4.00276600	1.71804600
H	0.04930300	-0.73504600	-0.13410500
C	7.19865000	1.05665500	0.20477600
H	8.08415100	0.41953800	0.13006500
H	7.28046100	1.84559800	-0.54838300
H	7.22389300	1.54172700	1.18801800



C1

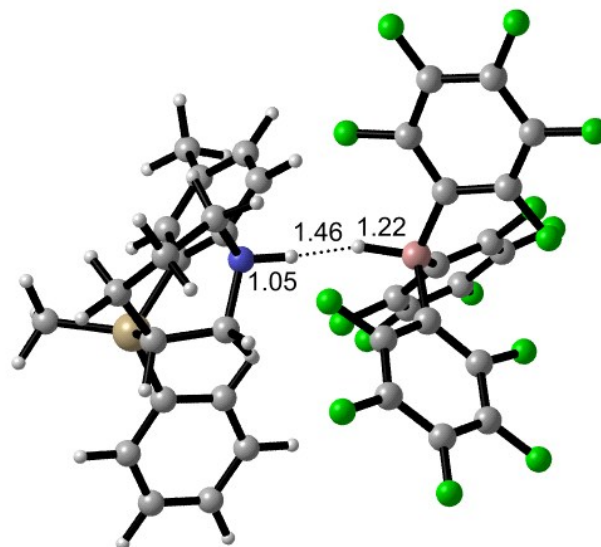
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E_{gas} = -3292.77235166 a.u.

H	0.32766500	1.65951600	-0.40453300
C	1.16342500	3.51744300	-0.60696500
C	2.12569100	3.21835700	0.35485000
C	3.17169900	4.11418300	0.57029100
C	3.27366500	5.30782300	-0.15607300
C	2.28236500	5.58678200	-1.10651900
C	1.22861800	4.70356800	-1.33635400
H	2.05864800	2.30388200	0.93319300
H	3.92335400	3.87424200	1.31683800
H	2.33310700	6.50842000	-1.67936600
H	0.47759900	4.94602200	-2.08057700
N	0.04109800	2.57524800	-0.80672300
C	-1.20525800	3.00272900	-0.01154100
H	-1.34486800	4.06721900	-0.21342800
H	-0.92798900	2.87627600	1.03509400
C	-2.40602200	2.15995000	-0.41959600
H	-2.09449800	1.11316900	-0.32253800
C	-2.78800100	2.42132500	-1.90441500
H	-3.59434000	3.15913700	-1.98793400
H	-3.17258100	1.49219100	-2.33311300
C	-1.57894600	2.91538300	-2.72795100
H	-1.48964200	4.00618400	-2.66521800
H	-1.71490100	2.68552000	-3.78986700
C	-0.28465100	2.25261900	-2.27288600
H	-0.37647600	1.16684900	-2.31636300
H	0.58357500	2.54886700	-2.85915400

B	0.87434800	-1.02686100	0.01789200
C	0.35763500	-1.22977400	1.56342200
C	0.11083100	-2.45861600	2.18345200
C	0.10511300	-0.12883800	2.37884200
C	-0.36628900	-2.58410300	3.48773000
C	-0.37105700	-0.19435600	3.68459100
C	-0.61154100	-1.44321500	4.24645800
C	2.50171800	-0.86206600	-0.10291000
C	3.06604100	0.03599900	-1.00951000
C	3.43613900	-1.56513700	0.66356100
C	4.43403900	0.25147100	-1.15677600
C	4.81460500	-1.38752900	0.55398000
C	5.31909500	-0.47134000	-0.36446300
C	0.25385200	-2.13903100	-1.01810200
C	-0.96073800	-1.92617900	-1.66767100
C	0.85220600	-3.36459000	-1.32791700
C	-1.56208000	-2.82491700	-2.54393500
C	0.30000700	-4.29610900	-2.20598000
C	-0.92064500	-4.02707500	-2.81870100
F	0.32772500	1.14089300	1.90612200
F	-0.59658200	0.92353700	4.39517600
F	-1.06879100	-1.54596700	5.50106800
F	-0.58728500	-3.79358800	4.02203200
F	0.33456500	-3.61115300	1.52637100
F	3.02784100	-2.47433400	1.56759400
F	5.66057700	-2.09021000	1.32163300
F	6.64103500	-0.28529900	-0.48242900
F	4.90159000	1.14427200	-2.04614600
F	2.26493500	0.78594500	-1.82011500
F	-1.65451900	-0.76186700	-1.47177200
F	2.02252100	-3.71116400	-0.76195800
F	0.92734200	-5.45345700	-2.46065700
F	-1.46980000	-4.91328600	-3.65984900
F	-2.74469000	-2.53985400	-3.11831700
H	0.40229200	0.04128700	-0.33872700
Si	-3.87941200	2.31602200	0.79657500
H	-3.35234600	1.93213300	2.13796000
C	-4.50065400	4.09927900	0.88903600
H	-5.31607300	4.19224200	1.61376200
H	-3.70444800	4.77657700	1.21712700
H	-4.87480900	4.45676600	-0.07592800
C	-5.23566700	1.13693900	0.23211100
C	-4.92930000	-0.09779200	-0.37370400
C	-6.59404700	1.45698000	0.41396800
C	-5.93735200	-0.97267000	-0.78112300
H	-3.89689200	-0.38990500	-0.54453600
C	-7.60522600	0.58207500	0.01275200

H	-6.87404400	2.40183300	0.87329000
C	-7.27795600	-0.63493100	-0.58707800
H	-5.67169300	-1.91421600	-1.25336900
H	-8.64652100	0.85202300	0.16542000
H	-8.06328200	-1.31553100	-0.90367100
C	4.43200100	6.25070200	0.06051000
H	4.17616900	7.27379400	-0.22850700
H	4.74868600	6.26022600	1.10740100
H	5.29858600	5.94631400	-0.53876800



C2

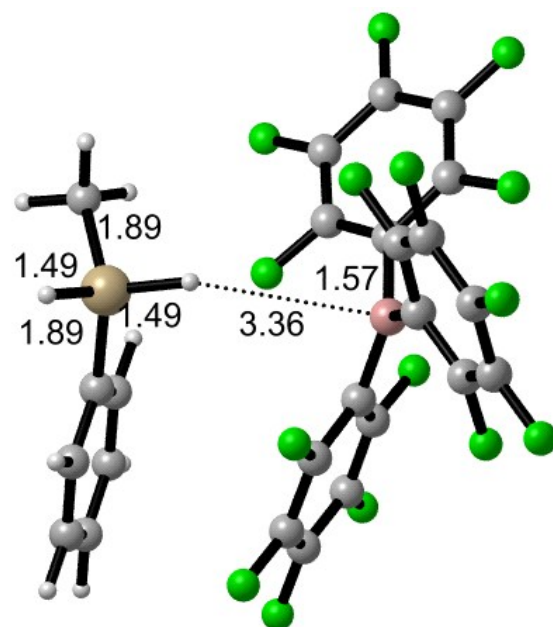
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E_{gas} = -3291.5804317 a.u.

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C	-3.03178100	0.77026500	-0.53597900
C	-4.36475000	0.44626100	-0.26519100
C	-2.87247000	1.81454300	-1.44605900
C	-5.45249600	1.10367000	-0.83528800
C	-3.92488300	2.50394100	-2.04452600
C	-5.23102200	2.14396300	-1.73373800
C	-1.29787600	0.39359900	1.60471200
C	0.02771500	0.21133000	1.99818900
C	-2.10938700	0.94905600	2.59745800
C	0.54216200	0.54670900	3.24529200
C	-1.64434500	1.30548000	3.86440700
C	-0.30780800	1.10283600	4.19495600
C	-1.90545200	-1.65778700	-0.09388900
C	-1.51142100	-2.29075500	-1.27212200
C	-2.42606200	-2.52184800	0.87385300
C	-1.59406100	-3.66149300	-1.49720900
C	-2.53752900	-3.90064400	0.69567300
C	-2.11911400	-4.47682800	-0.50021900

F	-1.62472700	2.22509600	-1.82602100
F	-3.68987100	3.50034600	-2.91519000
F	-6.26315500	2.78888300	-2.29340300
F	-6.70860400	0.74662300	-0.53066500
F	-4.65375100	-0.55069200	0.59129500
F	-3.41569600	1.17660400	2.36982000
F	-2.47501300	1.84074700	4.77072500
F	0.15384200	1.44027400	5.40646600
F	1.84428300	0.34657000	3.53323000
F	0.92728500	-0.32514500	1.12020700
F	-0.97392200	-1.56128800	-2.29829000
F	-2.84655200	-2.04232900	2.05866200
F	-3.04297700	-4.67833200	1.66384300
F	-2.21510700	-5.79978600	-0.68747800
F	-1.16967800	-4.19740500	-2.65512700
H	-0.81383500	0.28853600	-0.62372700
C	2.18985300	1.57604800	-1.05702800
C	3.57884800	1.52942100	-0.88274600
C	4.17206200	2.65582800	-0.28051600
C	3.44476300	3.77497800	0.13374500
C	2.05687100	3.76470400	-0.06733600
C	1.42581000	2.67562900	-0.65861000
H	5.24849400	2.65699300	-0.12287100
H	1.45863600	4.61573300	0.24665400
H	0.35096000	2.68264600	-0.80883200
N	1.42956900	0.46565500	-1.70119000
C	3.14903300	-0.35122100	-3.86276600
H	3.59679100	-1.01101500	-4.61137100
H	3.65116600	0.61839400	-3.97702700
C	1.65559300	-0.15052300	-4.16387300
H	1.12739700	-1.10908200	-4.17683100
H	1.51841400	0.29179700	-5.15639300
C	1.00831900	0.79357300	-3.15051500
H	1.31440600	1.82533100	-3.32501600
H	-0.08031500	0.74512700	-3.16937000
C	3.37340200	-0.93460500	-2.43160600
H	3.67031200	-1.98691700	-2.50024800
Si	4.63091900	0.03176500	-1.37074400
C	5.07949900	-0.93648100	0.18127100
C	4.31963200	-0.82311900	1.36252800
C	6.16893200	-1.82976000	0.18640400
C	4.62784300	-1.57651300	2.49640100
H	3.47411800	-0.14451800	1.41251100
C	6.48277100	-2.58138400	1.31934100
H	6.78720400	-1.94268900	-0.70153600
C	5.71066100	-2.45655800	2.47671600
H	4.01775900	-1.46812700	3.38817600

H	7.32894100	-3.26253300	1.29978300
H	5.95414800	-3.04210200	3.35875500
C	6.16987100	0.55228600	-2.32846100
H	6.82870500	1.16758800	-1.70745300
H	6.74734400	-0.32099400	-2.65038300
H	5.91660700	1.13062200	-3.22207700
C	2.06954600	-0.90355700	-1.62205100
H	2.21930300	-1.12409300	-0.56533800
H	1.30946800	-1.58905200	-1.99735300
H	0.53632100	0.37984700	-1.16031700
C	4.12032000	4.95375900	0.79127800
H	3.84322500	5.89419700	0.30324400
H	3.82596600	5.03765800	1.84374400
H	5.20894100	4.86229500	0.75678600



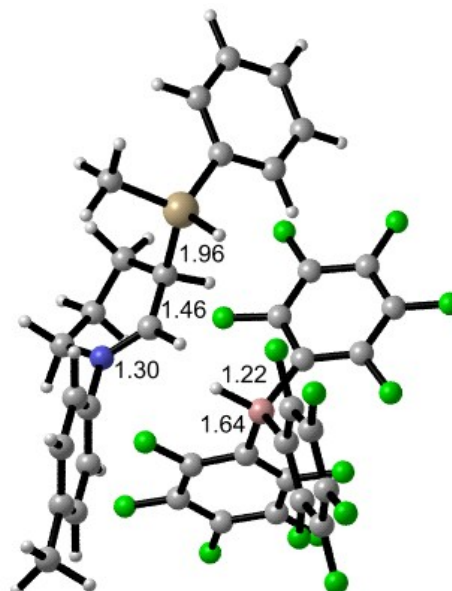
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$E_{\text{gas}} = -2770.49042534 \text{ a.u.}$

B	0.99798000	0.13180300	-0.67681900
C	-0.24872500	0.52425400	-1.54633300
C	-0.28263700	1.67810700	-2.34420900
C	-1.41724800	-0.25130000	-1.56669600
C	-1.38645300	2.04236100	-3.10754600
C	-2.55056500	0.09570400	-2.29161500
C	-2.53149700	1.24819900	-3.07418800
C	1.38196200	-1.38309200	-0.52513300
C	1.78376000	-1.93242100	0.70006900
C	1.31518900	-2.28393200	-1.59756900
C	2.07082300	-3.28165300	0.86879300
C	1.62916200	-3.63321000	-1.47563700

C	2.00177000	-4.13580100	-0.23001800
C	1.84875800	1.23300800	0.04244700
C	1.27728000	2.40373900	0.56853800
C	3.23742900	1.11113100	0.21512600
C	2.01709300	3.37958600	1.22659100
C	4.01179100	2.07606800	0.84920200
C	3.39441900	3.21527500	1.36181400
F	-1.50511300	-1.37079200	-0.82115200
F	-3.65336900	-0.66065900	-2.23745500
F	-3.60302800	1.59043400	-3.78629600
F	-1.36241100	3.14306300	-3.86474000
F	0.79188300	2.47981900	-2.41481400
F	0.95645700	-1.85077900	-2.81796800
F	1.56924800	-4.44946300	-2.53242800
F	2.28587700	-5.42949500	-0.08986300
F	2.39613000	-3.76316100	2.07320500
F	1.85405300	-1.15952600	1.79865000
F	-0.04536000	2.61029900	0.48068500
F	3.88867000	0.04041900	-0.26733100
F	5.33384900	1.92216700	0.97191100
F	4.11922000	4.14530700	1.98000500
F	1.42481900	4.46814800	1.72640700
H	-0.88458900	0.13071800	1.72947300
Si	-1.68700700	-0.55539500	2.78212300
H	-1.31469300	0.05083000	4.09130800
C	-3.51855700	-0.22588500	2.49335700
C	-4.30404900	0.37961300	3.49064400
C	-4.14902500	-0.57295100	1.28265600
C	-5.66400100	0.62779800	3.29099000
H	-3.84860400	0.66460500	4.43607800
C	-5.50598900	-0.32373100	1.07708100
H	-3.57922900	-1.04021200	0.48444400
C	-6.26715800	0.27692000	2.08269200
H	-6.25020100	1.09654400	4.07673700
H	-5.96658400	-0.59511100	0.13108000
H	-7.32421900	0.47169900	1.92378900
C	-1.26494200	-2.39672400	2.78068400
H	-0.19546300	-2.54907300	2.95781700
H	-1.81777500	-2.92545700	3.56343500
H	-1.52030600	-2.85644600	1.82042400



E

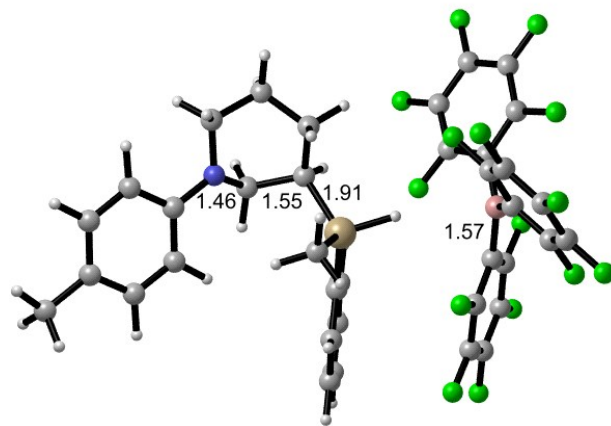
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E_{gas} = -3291.56225959 a.u.

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C	-2.62434900	2.89277300	-1.51628900
C	-3.78997100	3.53947400	-1.11647900
C	-3.75264100	4.75453700	-0.41357100
C	-2.50219200	5.31181100	-0.12037400
C	-1.32184000	4.68060800	-0.51333300
H	-2.66504400	1.93458400	-2.02235400
H	-4.74915600	3.08225600	-1.34289300
H	-2.44652800	6.25272000	0.41940500
H	-0.35728600	5.12846700	-0.29306800
N	-0.16383000	2.81617600	-1.60686300
C	2.32540500	1.62605800	-2.46458000
H	2.96130400	0.74751400	-2.58974300
H	2.90254300	2.49326900	-2.80943300
C	1.05879600	1.49218400	-3.31726800
H	0.54622000	0.55766000	-3.07961300
H	1.30644000	1.47782100	-4.38333000
C	0.10401500	2.65351200	-3.06264700
H	0.49692400	3.60794100	-3.43298300
H	-0.86407500	2.48413300	-3.53698100
C	0.64488700	2.33245000	-0.70512300
H	0.29715900	2.37633100	0.32232200
C	1.96583600	1.77109900	-0.97074700
H	1.95341600	0.79605400	-0.46367400
Si	3.32766600	2.68623200	0.09274500
H	2.74848700	2.80229500	1.45615100
C	4.83453000	1.57387000	0.07351000
C	4.74231900	0.26087200	0.57428100

C	6.06685200	1.99476300	-0.45730800
C	5.83262600	-0.60750000	0.53110200
H	3.80826900	-0.09777400	1.00033700
C	7.16560100	1.13362600	-0.48953200
H	6.17731900	3.00208800	-0.85106800
C	7.04727200	-0.16844100	-0.00113400
H	5.72777200	-1.62390200	0.89758500
H	8.11033100	1.47726900	-0.90127000
H	7.89875200	-0.84186200	-0.03682500
C	3.67374500	4.40671200	-0.59783100
H	4.06513600	4.37771900	-1.61946400
H	2.76787600	5.02243000	-0.60146300
H	4.41269200	4.92052000	0.02597200
B	-0.76429000	-0.94486800	0.11956900
C	0.60561700	-1.80127300	0.43701500
C	0.89595500	-2.47194000	1.62867700
C	1.60511900	-1.90210200	-0.53293900
C	2.09639000	-3.14423600	1.86405400
C	2.81758300	-2.56145600	-0.34954500
C	3.06635200	-3.18580500	0.86769000
C	-1.70577400	-1.79739300	-0.91239800
C	-2.09795100	-1.31535000	-2.15765200
C	-2.11853400	-3.10613800	-0.64755500
C	-2.84747200	-2.04292800	-3.08035800
C	-2.86625200	-3.87765600	-1.53228700
C	-3.23439100	-3.33961700	-2.76370500
C	-1.50048100	-0.38882400	1.47718600
C	-0.82172100	0.52389600	2.28675100
C	-2.78938600	-0.68499200	1.92665400
C	-1.33981100	1.11442900	3.43317400
C	-3.35849700	-0.12282800	3.07143500
C	-2.62985200	0.78155900	3.83479300
F	1.43885300	-1.30426300	-1.74548100
F	3.75214200	-2.57703200	-1.31593500
F	4.24579400	-3.79384400	1.08605800
F	2.32674000	-3.74802000	3.03943200
F	0.00980500	-2.48397800	2.64221600
F	-1.79748200	-3.67611300	0.53071800
F	-3.23710300	-5.12804500	-1.21767100
F	-3.95483000	-4.06350300	-3.63211000
F	-3.19221700	-1.50693900	-4.26524600
F	-1.75343200	-0.05244500	-2.55942100
F	0.44777000	0.91153300	1.94860900
F	-3.58211200	-1.54334900	1.25237200
F	-4.60754200	-0.44686500	3.44128900
F	-3.16354700	1.33400200	4.93417700
F	-0.61809000	1.99699700	4.14588700

H	-0.40498100	0.05215700	-0.47767500
C	-5.03002200	5.42308100	0.03248800
H	-5.77565100	5.43218700	-0.76870600
H	-5.47347000	4.88823000	0.88063200
H	-4.85466200	6.45510000	0.34680800



F

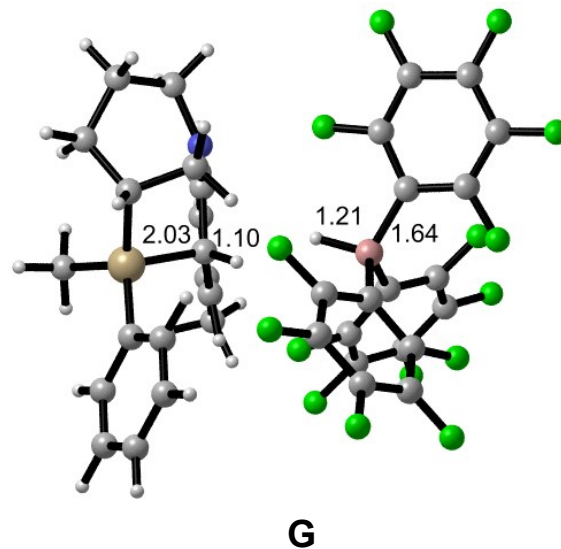
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E_{gas} = -3291.57244913 a.u.

C	5.81062200	-1.11144700	-0.00006600
C	5.94571800	0.27434800	0.25103700
C	7.09842000	0.79133900	0.83060400
C	8.17729300	-0.02441300	1.20098300
C	8.03956400	-1.39309200	0.96139200
C	6.89485500	-1.93249200	0.37278200
H	5.14140600	0.96012800	0.00940500
H	7.15448800	1.86372200	1.00639100
H	8.85017400	-2.06632600	1.23215700
H	6.85853200	-3.00116100	0.20200100
N	4.64059100	-1.65473400	-0.54084700
C	2.07162000	-2.62707800	-0.63579400
H	1.07483900	-2.97225100	-0.93014600
H	2.12403600	-2.74097900	0.45442900
C	3.16192100	-3.50776300	-1.25724800
H	3.12896800	-3.41918900	-2.34987700
H	2.99382100	-4.56568600	-1.02831700
C	4.55000700	-3.10306300	-0.72711200
H	4.71956900	-3.58469800	0.24445300
H	5.33374900	-3.47658500	-1.40974500
C	2.26990100	-1.14032800	-1.05278400
H	1.68278400	-0.96217400	-1.96490800
Si	1.58482300	0.05997500	0.26199000
C	1.76411100	1.84953800	-0.32930300
C	1.53981300	2.20374400	-1.67494800
C	2.10570200	2.88319600	0.56350800
C	1.64516800	3.52675600	-2.10674700

H	1.27024100	1.44002400	-2.39915600
C	2.20860800	4.20989600	0.13869100
H	2.29181400	2.65498100	1.60949900
C	1.97797600	4.53483700	-1.19872800
H	1.46853700	3.77136100	-3.15074800
H	2.46803200	4.98771000	0.85137600
H	2.05870100	5.56558600	-1.53238100
C	2.38401900	-0.16189000	1.95732000
H	3.45774000	0.04783600	1.93245700
H	1.92202200	0.49811600	2.69913200
H	2.25595100	-1.18899000	2.31334100
C	3.75819700	-0.88948500	-1.41739800
H	4.00536300	0.16952500	-1.36182100
H	3.93656400	-1.17733300	-2.46759700
B	-2.58233700	-0.02696400	0.05002500
C	-2.39644300	1.50516600	-0.21966700
C	-2.87141600	2.13028500	-1.38459400
C	-1.73067000	2.35194900	0.68283700
C	-2.70596700	3.48612100	-1.64193700
C	-1.53134100	3.70734200	0.45173200
C	-2.02498700	4.27747200	-0.71917800
C	-2.78763800	-0.55874700	1.51436700
C	-2.21851400	-1.76124600	1.95951200
C	-3.56119700	0.12864800	2.46089300
C	-2.38534600	-2.24733000	3.25138900
C	-3.76868000	-0.33698600	3.75463100
C	-3.17216300	-1.53189600	4.15187200
C	-2.59685300	-1.05487600	-1.14202800
C	-1.73557900	-0.94946900	-2.24300000
C	-3.46154000	-2.15931100	-1.16464800
C	-1.69943500	-1.87725200	-3.27680100
C	-3.47731300	-3.09312600	-2.19599100
C	-2.58498800	-2.95311300	-3.25648500
F	-1.20881000	1.85841200	1.81845200
F	-0.87194600	4.46267300	1.33448000
F	-1.84948900	5.57602500	-0.95555300
F	-3.19012500	4.03507100	-2.76130200
F	-3.54515900	1.42293900	-2.30713300
F	-4.16641900	1.28125400	2.12898400
F	-4.52935300	0.34663800	4.61571400
F	-3.35229800	-1.98877900	5.39035000
F	-1.80454600	-3.38913900	3.63480200
F	-1.44121600	-2.48791200	1.13750400
F	-0.85423900	0.06607500	-2.32008000
F	-4.34710700	-2.34525000	-0.17187800
F	-4.33352400	-4.11935900	-2.17690900
F	-2.57611100	-3.84489800	-4.24608100

F	-0.83042200	-1.74394200	-4.28493200
H	0.13129900	-0.25768700	0.40120100
C	9.42849700	0.55748200	1.81525300
H	10.01518800	1.12538600	1.08183200
H	9.19401500	1.24425500	2.63672200
H	10.07740900	-0.22782600	2.21438400



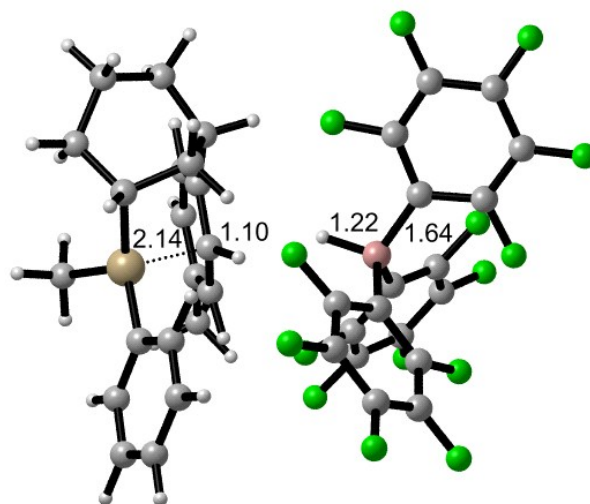
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E_{gas} = -3291.54843718 a.u.

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C	-2.50130500	-1.02433700	0.37190000
C	-2.85260200	-0.85648100	1.78018800
C	-3.23584000	-1.89447000	2.58009600
C	-3.20460800	-3.20523600	2.00208900
C	-2.80492600	-3.46746200	0.71397600
H	-1.63760400	-0.39407200	0.11858100
H	-2.76320100	0.14597400	2.18572900
H	-3.47482600	-4.04931900	2.63311900
H	-2.73604400	-4.49576800	0.38178500
N	-2.00077500	-2.59149600	-1.41101500
C	-4.07378400	-2.05346400	-3.10086600
H	-4.60081300	-1.72330100	-4.00100300
H	-4.85604000	-2.35812600	-2.39688300
C	-3.22017200	-3.29375200	-3.43873300
H	-2.56424300	-3.07641500	-4.28698200
H	-3.86536600	-4.11920400	-3.75553600
C	-2.37400000	-3.76575100	-2.22384300
H	-2.95361200	-4.45487600	-1.61015100
H	-1.46333300	-4.27942100	-2.54834900
C	-3.21685300	-0.86941600	-2.52215300
H	-3.15931600	-0.04925200	-3.24583100
Si	-3.86045400	-0.15297500	-0.85813300
C	-3.72738400	1.70932300	-0.75933400

C	-2.72864200	2.40692100	-1.46809300
C	-4.64731000	2.46123800	-0.00206300
C	-2.65412100	3.79905800	-1.42467100
H	-1.98693200	1.87379400	-2.05420500
C	-4.57236400	3.85336600	0.04550700
H	-5.43638600	1.96287400	0.55468300
C	-3.57637700	4.52339800	-0.66727600
H	-1.87432400	4.30652100	-1.98299500
H	-5.29154600	4.41352500	0.63612800
H	-3.51817500	5.60744700	-0.63148000
C	-5.56888800	-0.76005700	-0.34643400
H	-5.60551000	-1.84930600	-0.25297000
H	-5.85748800	-0.34128000	0.62208300
H	-6.32420200	-0.45671300	-1.07914100
C	-1.78798500	-1.40197400	-2.24750400
H	-1.12079000	-0.69475300	-1.75799900
H	-1.27148400	-1.71813600	-3.15435800
B	1.45406900	0.05002900	0.05081300
C	1.61827700	1.60939500	-0.43452300
C	2.34881800	2.58708300	0.24675900
C	0.96611200	2.07473800	-1.57506700
C	2.41749000	3.92126900	-0.15470700
C	0.99051100	3.39711000	-2.00646200
C	1.72505100	4.33370400	-1.28872000
C	2.54634400	-0.92985900	-0.67709100
C	2.16681300	-2.09775600	-1.33855000
C	3.91499700	-0.65405500	-0.74283900
C	3.05042700	-2.93095600	-2.02257200
C	4.83796200	-1.45406300	-1.41204900
C	4.40077200	-2.60590500	-2.06050400
C	1.35608500	-0.07074800	1.68500500
C	0.24998800	0.49125700	2.32514600
C	2.22577100	-0.74385600	2.54520100
C	-0.02650200	0.36563100	3.68159300
C	2.00217800	-0.88307300	3.91712600
C	0.86353700	-0.32978200	4.49300600
F	0.21589300	1.22504800	-2.33668500
F	0.27581000	3.78606600	-3.08476200
F	1.75816500	5.61596400	-1.68147600
F	3.13211600	4.81486600	0.54678900
F	3.02436200	2.27378300	1.36835400
F	4.40888800	0.43869300	-0.12850000
F	6.14093100	-1.13164100	-1.43813300
F	5.27106400	-3.39186600	-2.71169900
F	2.60771400	-4.04159100	-2.64350400
F	0.86641100	-2.49983300	-1.35278700
F	-0.66911500	1.18587100	1.59553600

F	3.34846400	-1.32447600	2.07784600
F	2.87285900	-1.55432400	4.68740700
F	0.62170500	-0.47032200	5.80555600
F	-1.15905800	0.88589200	4.20716300
H	0.36140900	-0.30684500	-0.34135400
C	-3.60430200	-1.70872200	4.03173100
H	-4.69039700	-1.74932000	4.17930400
H	-3.16321200	-2.49381300	4.65434700
H	-3.24315000	-0.74683700	4.40226400



G1

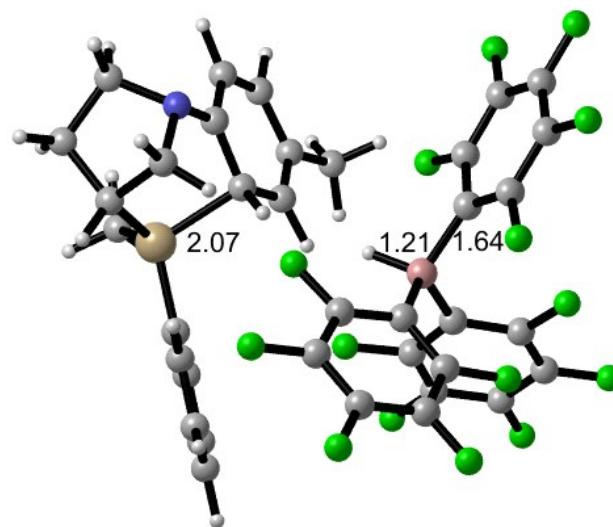
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$E_{\text{gas}} = -3275.50383830 \text{ a.u.}$

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C	-2.51616600	-0.96835600	0.25425300
C	-2.95753200	-0.72926000	1.59160500
C	-3.64267000	-1.69514300	2.31624600
C	-3.83447000	-2.94063700	1.68722100
C	-3.37412400	-3.22136800	0.39816100
H	-1.65831000	-0.36705700	-0.06826500
H	-2.72020600	0.22952500	2.04032900
H	-4.34401000	-3.72889400	2.23715500
H	-3.52977700	-4.21768000	0.00042700
C	-4.37124400	-1.67033500	-3.16610200
H	-4.99439700	-1.23130900	-3.95215100
H	-5.06691000	-1.97295900	-2.37362600
C	-3.67350800	-2.93698100	-3.68244200
H	-3.06184200	-2.68754300	-4.55617400
H	-4.42185700	-3.65600000	-4.03281500
C	-2.79452900	-3.59147700	-2.59162800
H	-3.41468300	-4.25363100	-1.98055000
H	-2.04806200	-4.23502900	-3.06703900
C	-3.34448400	-0.60193700	-2.65207100
H	-3.29305100	0.23081900	-3.36394800

Si	-3.86137900	0.15222300	-0.98435800
C	-3.44034000	1.95421900	-0.76895300
C	-2.39021300	2.54387900	-1.50205300
C	-4.20697200	2.78188400	0.07666500
C	-2.12486700	3.90943100	-1.40205600
H	-1.75577600	1.94432600	-2.14707500
C	-3.93949100	4.14597800	0.18010000
H	-5.02546500	2.36683400	0.65808300
C	-2.89980100	4.71065200	-0.56163100
H	-1.31036000	4.33629600	-1.97716500
H	-4.54173200	4.76682600	0.83683700
H	-2.69088900	5.77347500	-0.48161000
C	-5.60413900	-0.24681900	-0.40349300
H	-5.74999500	-1.31751600	-0.24052900
H	-5.84937800	0.27084300	0.52705500
H	-6.32194100	0.07684400	-1.16570300
C	-1.93128500	-1.22706700	-2.51898700
H	-1.20577000	-0.54168900	-2.07602800
H	-1.52193500	-1.46741000	-3.50416000
B	1.44911400	-0.08792800	0.08754500
C	1.70214700	1.50418900	-0.22880400
C	2.37907700	2.39519500	0.60832000
C	1.23013000	2.07389400	-1.41126300
C	2.57236200	3.74393900	0.30794900
C	1.39192200	3.41359100	-1.74999100
C	2.06905700	4.26119300	-0.88084400
C	2.59938600	-0.98075200	-0.66280400
C	2.30299300	-1.91477200	-1.65358100
C	3.96614700	-0.81458600	-0.42167100
C	3.26457400	-2.64281600	-2.35360900
C	4.96487600	-1.51525400	-1.09147900
C	4.60955800	-2.44019300	-2.07019200
C	1.22889400	-0.37886700	1.68908000
C	0.16583100	0.25618800	2.33475000
C	1.92969400	-1.26974200	2.50524600
C	-0.21258500	0.02462200	3.65174900
C	1.59855200	-1.52490800	3.83896100
C	0.51424200	-0.87789400	4.42024600
F	0.54113100	1.31865200	-2.31161600
F	0.85790100	3.90894300	-2.88812900
F	2.22504600	5.55922700	-1.18266200
F	3.22641300	4.55094800	1.15825600
F	2.87436900	1.98055500	1.79035600
F	4.37354800	0.06310000	0.51677100
F	6.26151000	-1.31246900	-0.80860300
F	5.55376000	-3.12740500	-2.72971400
F	2.90319100	-3.53205100	-3.29676100

F	1.01377100	-2.17526600	-2.00559900
F	-0.61012200	1.13935100	1.64322500
F	2.97963400	-1.96850900	2.03075400
F	2.31085400	-2.40203600	4.56317000
F	0.16473100	-1.12680900	5.69187800
F	-1.30118200	0.63740200	4.17582800
H	0.38222200	-0.37521000	-0.42255700
C	-4.11093600	-1.43654500	3.72722100
H	-5.11414700	-0.99357100	3.73648200
H	-4.15628100	-2.36259700	4.30677600
H	-3.43501600	-0.74468000	4.23570600
C	-2.05692500	-2.53597900	-1.71076000
H	-1.04256800	-2.89519900	-1.49740200



G2

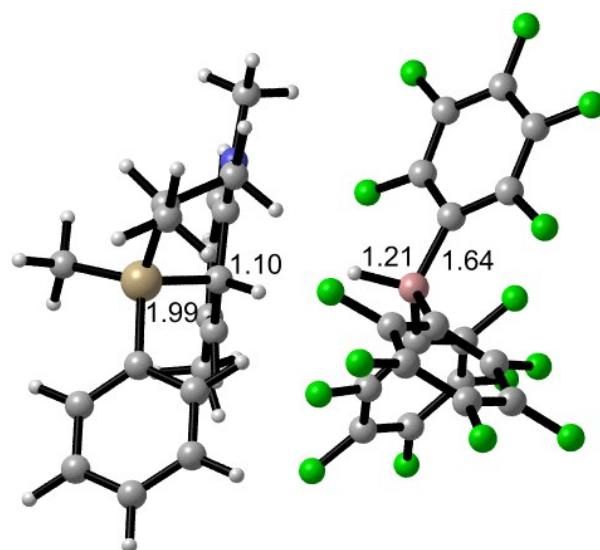
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C	2.62649700	-1.17606400	-0.26544300
C	1.92129800	-1.45219900	-1.50093400
C	2.06808300	-2.63555700	-2.18384700
C	2.90597500	-3.62026600	-1.59352900
C	3.56457200	-3.44630700	-0.38918900
H	2.01524000	-0.56165000	0.40352900
H	1.23980500	-0.68544400	-1.85485800
H	3.01579100	-4.57599200	-2.10158300
H	4.14656300	-4.26154300	0.02571800
N	4.06341400	-2.05341100	1.53690200
C	4.96830500	0.04951100	1.16097200
H	5.25231900	1.03443900	1.54262900
Si	4.09411300	0.25231600	-0.53622100
C	3.30092500	1.92474300	-0.74732300
C	2.95092800	2.70933900	0.36957500

C	3.03950000	2.44289400	-2.03062300
C	2.36432100	3.96328400	0.20925400
H	3.10725700	2.34256400	1.37864100
C	2.45203300	3.69685400	-2.19226300
H	3.28817100	1.86586800	-2.91712300
C	2.11583800	4.45889300	-1.07219300
H	2.09397500	4.54200200	1.08688300
H	2.25039800	4.07426000	-3.19009500
H	1.65304200	5.43337200	-1.19759300
C	5.13289600	-0.25489200	-2.01946200
H	4.55959100	-0.17623400	-2.94742700
H	6.00455100	0.40205000	-2.11098200
H	5.48984400	-1.28559400	-1.93866400
C	3.98395400	-0.69388400	2.10110500
H	2.96485600	-0.31764800	2.14664900
H	4.36420300	-0.73607700	3.12701400
B	-1.33873700	-0.07067100	0.19650100
C	-1.96779800	-1.46485000	0.78350100
C	-2.80279900	-1.60438600	1.89335300
C	-1.64976700	-2.66962700	0.15191900
C	-3.27011100	-2.83349800	2.36000500
C	-2.09288600	-3.91897200	0.57567200
C	-2.91374900	-4.00212800	1.69567000
C	-2.05783300	0.39384100	-1.20705600
C	-1.31267000	0.96316100	-2.24026700
C	-3.41791900	0.24938100	-1.49576700
C	-1.84098800	1.35264200	-3.46849600
C	-3.99582500	0.62553800	-2.70806200
C	-3.20094400	1.18406000	-3.70408400
C	-1.25820300	1.17841100	1.26332300
C	-0.07363700	1.49353700	1.92237300
C	-2.30121200	2.07245700	1.52828200
C	0.11181000	2.60714900	2.73595600
C	-2.17648600	3.19391600	2.34672500
C	-0.95356600	3.47138500	2.95203900
F	-0.85371300	-2.66822800	-0.95156400
F	-1.73509700	-5.03940700	-0.08047800
F	-3.35334700	-5.19399500	2.12881600
F	-4.06380400	-2.90074900	3.44165000
F	-3.20481300	-0.52202500	2.59143300
F	-4.25487500	-0.28232400	-0.58457500
F	-5.31010000	0.45781900	-2.92554000
F	-3.73746800	1.55258000	-4.87742200
F	-1.05397200	1.88577100	-4.42291100
F	0.02984700	1.15827600	-2.09621000
F	1.03624800	0.69857200	1.78395100
F	-3.51167400	1.87803400	0.97544500

F	-3.21690300	4.01578900	2.55272400
F	-0.80373000	4.55643000	3.72664300
F	1.31921300	2.86874300	3.28564900
H	-0.19483700	-0.33118600	-0.08541300
C	1.28620400	-2.94271700	-3.43577200
H	1.87884600	-3.51887200	-4.15324300
H	0.39590200	-3.52909300	-3.18306700
H	0.94577200	-2.02699300	-3.92442800
C	5.52648000	-2.32701000	1.55148900
H	5.78251600	-3.12516600	0.85723200
H	5.81174600	-2.64242400	2.55767400
C	6.17054200	-0.94797000	1.17290800
H	6.90770500	-0.65000200	1.92493000
H	6.69643700	-1.00642600	0.21656600



G3

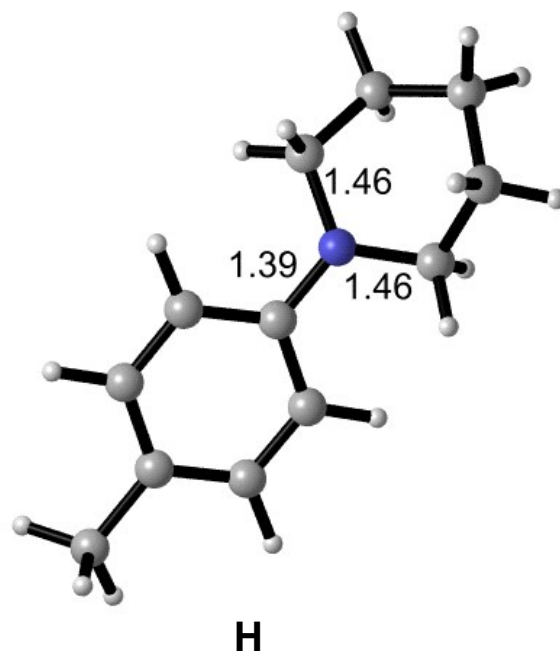
$G_{\text{gas}} = -3253.003190 \text{ a.u.}$

$E_{\text{gas}} = -3253.45676743 \text{ a.u.}$

C	-1.76943400	-2.71157000	-0.53864200
C	-2.27150000	-1.44474900	0.02811000
C	-2.63686000	-1.44661500	1.44740700
C	-2.64898800	-2.57383100	2.21425000
C	-2.21576600	-3.79001600	1.58897500
C	-1.78397100	-3.87327300	0.28895600
H	-1.57556700	-0.61406200	-0.17744700
H	-2.87557500	-0.48268600	1.88494700
H	-2.19799000	-4.69609200	2.19100200
H	-1.42044900	-4.81942600	-0.08970900
N	-1.35968200	-2.74725200	-1.81195600
Si	-3.77017900	-0.84433500	-1.13447800
C	-4.22186100	0.92755700	-0.73737600
C	-3.39643600	1.99255000	-1.15031700
C	-5.40124500	1.23997900	-0.03368000

C	-3.73450500	3.31633200	-0.87179500
H	-2.47343000	1.80321300	-1.68747600
C	-5.74118600	2.56410800	0.24691000
H	-6.06769900	0.44752400	0.29724300
C	-4.90815600	3.60353600	-0.17208500
H	-3.07632400	4.11288000	-1.20568000
H	-6.65581500	2.78392000	0.79014500
H	-5.17362700	4.63398500	0.04621900
C	-5.21989100	-2.02125800	-0.88750400
H	-4.93547600	-3.05623200	-1.10025100
H	-5.58753500	-1.98487900	0.14255400
H	-6.05248300	-1.76048800	-1.54882700
C	-1.44179000	-1.52164400	-2.63279800
H	-0.83239800	-0.74015800	-2.16841100
H	-0.98661900	-1.75095500	-3.59882100
B	1.38740900	0.32510900	-0.02788000
C	1.38463900	1.90525100	-0.45066700
C	2.16468600	2.87716700	0.18118300
C	0.48762600	2.41122300	-1.38712600
C	2.05083500	4.24303000	-0.06882100
C	0.31255900	3.76669900	-1.65208100
C	1.10670700	4.69431400	-0.98845200
C	2.56141500	-0.59945100	-0.69376300
C	2.35208500	-1.97333400	-0.81874000
C	3.77394200	-0.16027200	-1.22940700
C	3.22552000	-2.85151600	-1.44945700
C	4.68946000	-1.00243700	-1.86373700
C	4.41392900	-2.36123000	-1.98005400
C	1.25887700	0.17881200	1.60189700
C	0.04941600	0.50241000	2.21757400
C	2.23794900	-0.29504800	2.47677800
C	-0.21880000	0.31557600	3.56915400
C	2.02464400	-0.48149800	3.84399000
C	0.78307400	-0.18165300	4.39604400
F	-0.32079800	1.57065500	-2.10039500
F	-0.63449200	4.18276500	-2.51871800
F	0.96317100	6.00590300	-1.22775700
F	2.82634400	5.13022500	0.57318400
F	3.07719600	2.50687400	1.09981900
F	4.12225100	1.13985800	-1.16605100
F	5.83379600	-0.51431400	-2.36711700
F	5.27615900	-3.18375300	-2.59537000
F	2.91716800	-4.16150900	-1.56309800
F	1.21582200	-2.53697400	-0.31906300
F	-0.97488500	1.00499500	1.47282200
F	3.46393200	-0.61900400	2.02182300
F	3.00227400	-0.95452900	4.63285500

F	0.55244500	-0.37364000	5.70383800
F	-1.44296300	0.58525800	4.07445300
H	0.35186000	-0.13835400	-0.46239900
C	-3.03094500	-2.56259200	3.67417700
H	-4.03957000	-2.96438700	3.82971100
H	-2.34310200	-3.17591400	4.26527900
H	-2.99973500	-1.54723400	4.07543000
C	-0.73688300	-3.95041900	-2.37661500
H	-1.39622200	-4.81808200	-2.28098100
H	-0.55306600	-3.78170700	-3.43640400
H	0.21759500	-4.15115800	-1.88166000
C	-2.90008900	-1.04064900	-2.82899600
H	-2.82399200	-0.03176100	-3.25350300
C	-3.67053000	-1.93011000	-3.82315300
H	-4.68530300	-1.55882500	-3.99652200
H	-3.16330500	-1.95902700	-4.79500700
H	-3.75886300	-2.96174700	-3.46548400

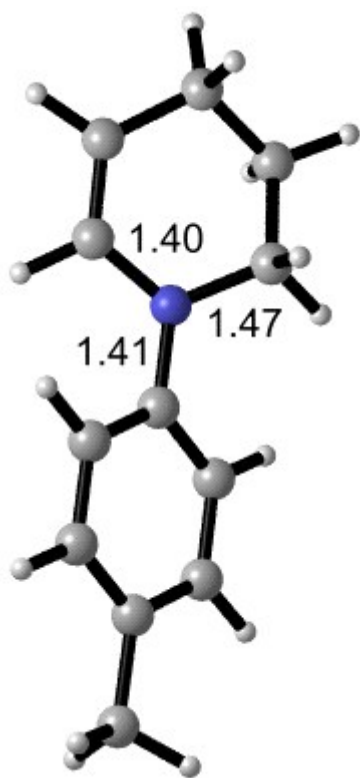


G_{gas} = -522.053370 a.u.

E_{gas} = -522.280258096 a.u.

C	-0.39665600	0.00157500	-0.00244700
C	-1.13497000	1.16362700	0.31410900
C	-2.52739000	1.15387200	0.30177000
C	-3.26062500	0.00255700	-0.00868400
C	-2.52684500	-1.14791100	-0.32144100
C	-1.13452900	-1.15902300	-0.32609700
H	-0.62173700	2.07634300	0.59481500
H	-3.05616400	2.07102500	0.55338600
H	-3.05533200	-2.06201800	-0.58461300
H	-0.62046500	-2.06844900	-0.61587600
N	0.99317800	0.00073100	-0.00049900

C	1.74751300	1.25139900	-0.03004500
H	1.89754500	1.66675800	0.98217600
H	1.17020400	1.99376900	-0.59092600
C	3.10265500	1.04861700	-0.71731300
H	3.62412900	2.00998900	-0.77788700
H	2.91222400	0.73018900	-1.74897800
C	3.97273200	-0.00242500	0.00543800
H	4.62859800	0.48389100	0.73636300
H	4.63104700	-0.48991100	-0.72250100
C	3.09748300	-1.05193800	0.72415400
H	2.90337800	-0.73351800	1.75513900
H	3.61668000	-2.01442800	0.78650000
C	1.74481400	-1.25150200	0.03111800
H	1.89824300	-1.66643800	-0.98079200
H	1.16345600	-1.99302000	0.58895100
C	-4.77105500	-0.00590000	0.01946500
H	-5.18115300	-0.72726500	-0.69500900
H	-5.15926200	-0.27798800	1.01009900
H	-5.18240500	0.97826500	-0.22750900



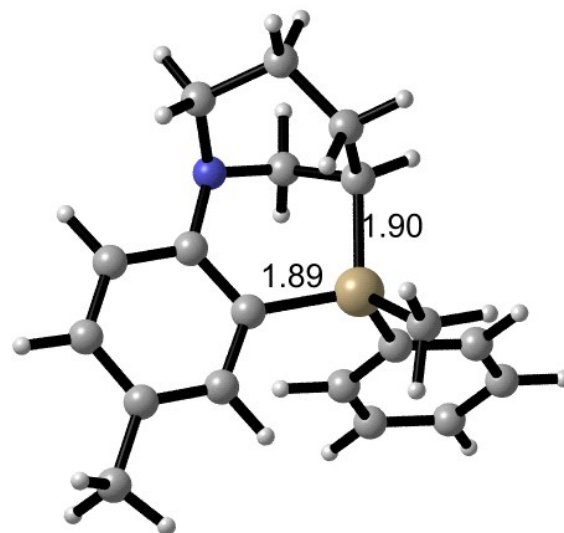
I

$G_{\text{gas}} = -520.856956 \text{ a.u.}$

$E_{\text{gas}} = -521.060895856 \text{ a.u.}$

C	-0.35292500	-0.01280400	-0.09167500
C	-1.05078000	1.15168800	0.26786800
C	-2.44491300	1.16004500	0.31818900
C	-3.19714700	0.01449800	0.04022000

C	-2.49304200	-1.15058800	-0.29844400
C	-1.10446700	-1.16826100	-0.37344400
H	-0.50158900	2.04820800	0.53566000
H	-2.95498500	2.07785100	0.60178200
H	-3.04386300	-2.06099000	-0.52426100
H	-0.59898300	-2.08001900	-0.67553300
N	1.05867000	-0.03925100	-0.18148800
C	3.09310200	1.28146600	-0.29105900
H	3.54836500	2.21820700	-0.59545800
C	3.96350100	0.16946300	0.23592900
H	4.21273200	0.32510100	1.29674100
H	4.92386500	0.15327500	-0.29512000
C	3.24625700	-1.17755700	0.05375000
H	3.75500000	-1.97554300	0.60555200
H	3.25706800	-1.45496400	-1.00674700
C	1.79247800	-1.09680000	0.52781300
H	1.29029800	-2.05254800	0.36341700
H	1.76567200	-0.89911700	1.61184800
C	1.76964600	1.12545600	-0.47154700
H	1.17158200	1.91183900	-0.91910200
C	-4.70696600	0.03033200	0.08256800
H	-5.13741900	0.06726800	-0.92634500
H	-5.10553400	-0.86676700	0.56842300
H	-5.08135900	0.90131800	0.62855900



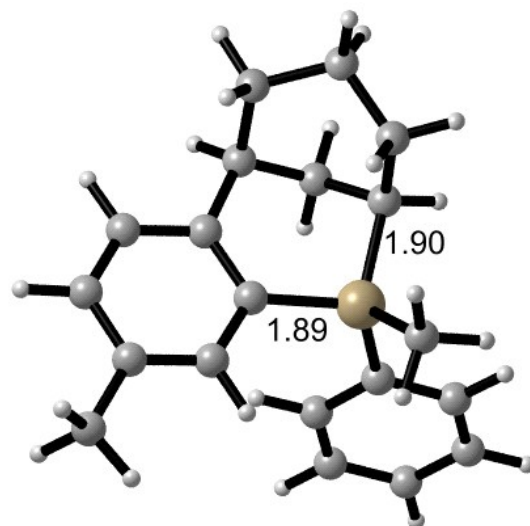
J

$G_{\text{gas}} = -1081.836238 \text{ a.u.}$

$E_{\text{gas}} = -1082.16254552 \text{ a.u.}$

C	1.80118300	0.09741800	-0.68783600
C	0.80436900	0.66135600	0.15049000
C	0.97664500	1.99130800	0.58245400
C	2.08926000	2.76723400	0.25316000
C	3.07668400	2.16784300	-0.54496100
C	2.93445400	0.86887100	-1.01305700

H	0.21703900	2.43591300	1.22476100
H	3.96142900	2.73757900	-0.82185400
H	3.68984400	0.44257000	-1.66715800
N	1.70329700	-1.20462400	-1.23925400
C	1.13966300	-2.71756900	1.01296000
H	0.79159300	-3.49529800	1.70082000
H	1.61174800	-1.95125500	1.64222900
C	2.21738800	-3.28287700	0.07104900
H	1.79625500	-4.11219000	-0.51026900
H	3.05136600	-3.70401700	0.64429900
C	2.75424800	-2.18292400	-0.88141000
H	3.57034600	-1.63962800	-0.39752500
H	3.16516300	-2.64523600	-1.78989400
C	-0.06879600	-2.12340300	0.22070000
H	-0.90582800	-2.83204100	0.21061300
Si	-0.59494700	-0.40311100	0.83872800
C	-2.26987000	0.07984700	0.09771100
C	-2.38185800	1.02395600	-0.93946700
C	-3.45746700	-0.51878800	0.56207200
C	-3.62207400	1.35460500	-1.49102600
H	-1.48646400	1.51071700	-1.31713400
C	-4.69933600	-0.19432400	0.01527100
H	-3.41760900	-1.25221600	1.36531400
C	-4.78357100	0.74535400	-1.01491600
H	-3.68074200	2.08811000	-2.29081400
H	-5.60016000	-0.67157300	0.39197400
H	-5.74943100	1.00111600	-1.44208900
C	-0.68918100	-0.26551300	2.72421900
H	-0.86831700	0.76949400	3.03353400
H	-1.50715200	-0.87349700	3.12620500
H	0.24023100	-0.59814100	3.19690800
C	0.38088500	-1.82544200	-1.23362000
H	-0.32573700	-1.16792700	-1.75323500
H	0.44318000	-2.73960600	-1.83615800
C	2.23085900	4.19450000	0.72759000
H	3.20094500	4.36571900	1.20830800
H	2.15665900	4.90588400	-0.10448700
H	1.45091100	4.45273000	1.44992700



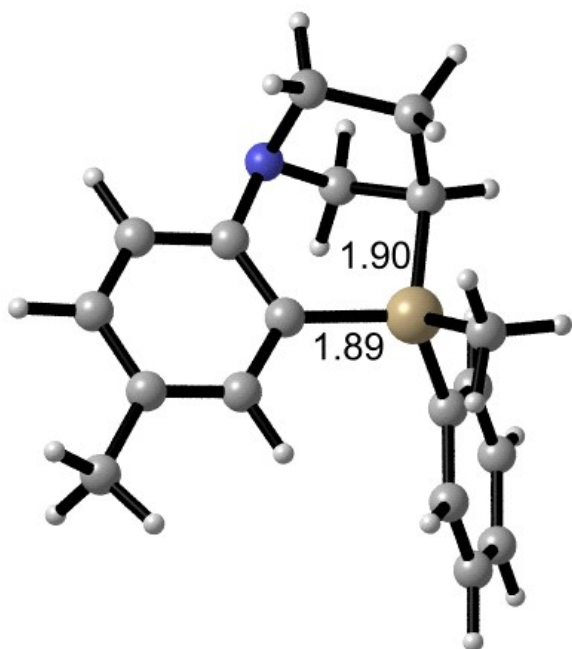
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G_{gas} = -1065.801046 a.u.

E_{gas} = -1066.13769825 a.u.

C	1.76816500	0.22372300	-0.73607900
C	0.82737700	0.65207500	0.22869100
C	0.93484900	1.96109800	0.73931800
C	1.92669900	2.85747000	0.33555900
C	2.84606000	2.41289100	-0.62526900
C	2.76391500	1.12633100	-1.14606500
H	0.21398500	2.29894800	1.48274100
H	3.62929300	3.08381300	-0.97217300
H	3.48729400	0.81055500	-1.89532600
C	1.13694500	-2.83074000	0.97162200
H	0.74908500	-3.67682800	1.54979000
H	1.54164300	-2.12709700	1.71238500
C	2.30280500	-3.28134000	0.08067000
H	1.95926500	-4.05989600	-0.61196400
H	3.08930300	-3.74214900	0.69036700
C	2.88952800	-2.09353300	-0.70358400
H	3.50554200	-1.48939600	-0.02826900
H	3.56420000	-2.46848400	-1.48183000
C	-0.01880600	-2.17843700	0.14427600
H	-0.87721000	-2.86041900	0.11704000
Si	-0.54956800	-0.49129100	0.83397700
C	-2.21606500	0.02713300	0.09292200
C	-3.40741500	-0.59316200	0.51780600
C	-2.31996200	1.01271300	-0.90574200
C	-4.64419900	-0.24981400	-0.02919000
H	-3.37481700	-1.35899300	1.29048900
C	-3.55482400	1.36241300	-1.45752900
H	-1.42292900	1.51815300	-1.25347600
C	-4.71999600	0.73125200	-1.02052700
H	-5.54757500	-0.74467400	0.31755900

H	-3.60656100	2.12820000	-2.22703900
H	-5.68173200	1.00203100	-1.44778500
C	-0.69110400	-0.45731300	2.72228000
H	0.23909500	-0.77392000	3.20396500
H	-0.92554800	0.55084800	3.07976600
H	-1.49064900	-1.12032600	3.07101100
C	0.42454200	-1.89293100	-1.31483500
H	-0.33041800	-1.29127100	-1.83605900
H	0.50419100	-2.82768700	-1.88390700
C	2.01343800	4.25319500	0.90730400
H	2.95368500	4.40600200	1.45056700
H	1.97306800	5.01315200	0.11828200
H	1.19274000	4.45104000	1.60258900
C	1.78684900	-1.17712000	-1.35429800
H	2.05619400	-1.03894000	-2.40836400



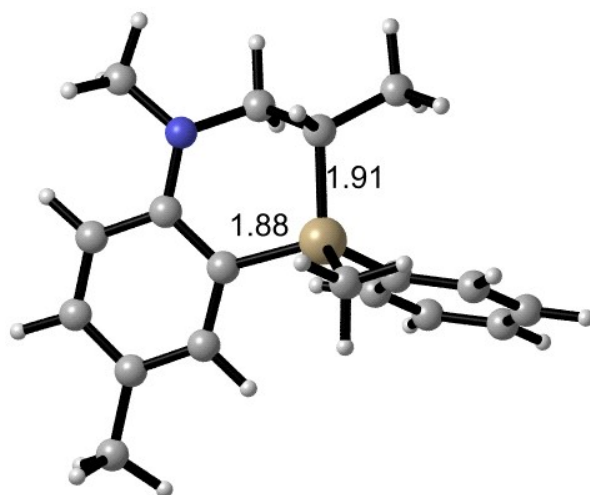
J2

$G_{\text{gas}} = -1042.546744$ a.u.

$E_{\text{gas}} = -1042.84422383$ a.u.

C	1.94879900	-0.31821200	-0.67159000
C	0.99516800	0.39076000	0.09572800
C	1.23895100	1.75139900	0.35635600
C	2.38571500	2.41640200	-0.08748700
C	3.32520900	1.67672600	-0.82064300
C	3.10659800	0.33480200	-1.11469600
H	0.51610400	2.31833500	0.94172800
H	4.23016800	2.16304200	-1.17850200
H	3.82114500	-0.22877200	-1.70741700
N	1.80630700	-1.70977100	-1.02850100
C	-0.13027400	-2.30664400	0.24194600
H	-1.01203700	-2.95422500	0.29399700

Si	-0.48652900	-0.53403800	0.82649000
C	-2.13684500	0.08987600	0.13114900
C	-2.91972400	-0.68111500	-0.74760000
C	-2.63160800	1.35921300	0.48925400
C	-4.13505400	-0.20938500	-1.24894800
H	-2.58296100	-1.66960300	-1.04856600
C	-3.84326100	1.83908700	-0.00858300
H	-2.06626000	1.98918000	1.17266000
C	-4.59927000	1.05381300	-0.88138900
H	-4.71833100	-0.82852600	-1.92530600
H	-4.19852600	2.82318500	0.28521800
H	-5.54399800	1.42379400	-1.27011700
C	-0.52049400	-0.33484400	2.70836500
H	-0.69311200	0.70846100	2.99390300
H	-1.32571400	-0.93255100	3.14922100
H	0.42493800	-0.64508000	3.16423900
C	0.41274600	-2.13944100	-1.20669000
H	-0.13067800	-1.41884900	-1.82466300
H	0.41540100	-3.09959800	-1.74143500
C	2.60420600	3.88431000	0.19643300
H	3.62597100	4.07955700	0.53984100
H	2.44560600	4.49350300	-0.70219100
H	1.91634000	4.24934000	0.96475800
C	2.30568600	-2.63576300	0.01564100
H	3.15655500	-2.19155700	0.53613600
H	2.65286000	-3.55429100	-0.47173900
C	1.09587600	-2.95168700	0.95778300
H	0.96299800	-4.03440000	1.05898600
H	1.25623800	-2.56180200	1.96773100



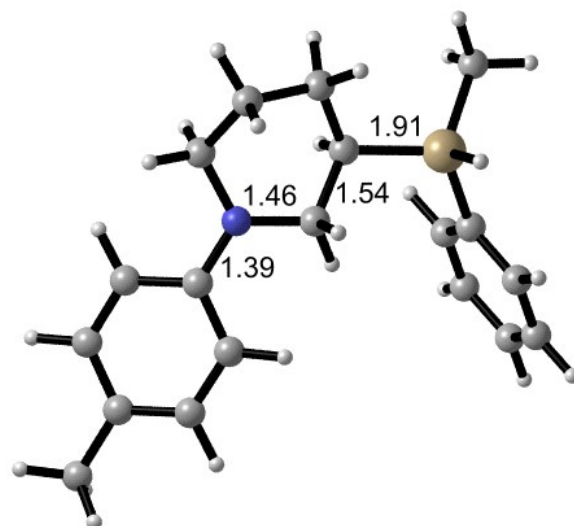
J3

$G_{\text{gas}} = -1043.750692$ a.u.

$E_{\text{gas}} = -1044.06584505$ a.u.

C	2.09953500	-0.50898600	-0.25515100
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C	1.07409500	0.28812400	0.32785700
C	1.31974200	1.65731900	0.52835600
C	2.52398700	2.28412600	0.19976500
C	3.51795500	1.47688900	-0.36585000
C	3.31824400	0.12018300	-0.59570500
H	0.52988900	2.26706900	0.96634500
H	4.47121200	1.91891700	-0.64925900
H	4.11668900	-0.44370500	-1.06168800
N	1.91821800	-1.88319300	-0.47175500
Si	-0.54304000	-0.45138200	0.93223000
C	-2.00975600	0.35762000	0.04443900
C	-1.85204900	0.99281200	-1.20198400
C	-3.30756400	0.31674900	0.59016000
C	-2.93818400	1.55578200	-1.87537600
H	-0.86217400	1.05950800	-1.64568100
C	-4.39785800	0.87750500	-0.07683100
H	-3.47532900	-0.15645600	1.55503200
C	-4.21475600	1.49847600	-1.31403400
H	-2.78706100	2.04249900	-2.83532200
H	-5.38800200	0.83311800	0.36909500
H	-5.06123600	1.93790300	-1.83480600
C	-0.74404000	-0.23551000	2.80235400
H	0.10617600	-0.68259000	3.32810400
H	-0.79131600	0.82220700	3.08104500
H	-1.65508700	-0.71726300	3.17475600
C	0.56452300	-2.38481800	-0.73558100
H	0.11173700	-1.85652600	-1.59456600
H	0.66366800	-3.43367400	-1.03794600
C	2.75357000	3.75499900	0.45595400
H	3.42463400	3.91867000	1.30894300
H	3.21031400	4.24900900	-0.40911200
H	1.81442400	4.27132600	0.67629900
C	2.99837200	-2.63316400	-1.09059300
H	3.92655900	-2.50403300	-0.52569800
H	2.74862900	-3.69619400	-1.07153200
H	3.19517300	-2.34684200	-2.13803500
C	-1.69219600	-3.03895200	0.21796300
H	-1.51371000	-4.09563800	-0.02133100
H	-2.35369700	-3.00985900	1.09039600
H	-2.24264900	-2.59736600	-0.61966600
C	-0.37370400	-2.29533300	0.48187300
H	0.14669000	-2.78132100	1.32000000



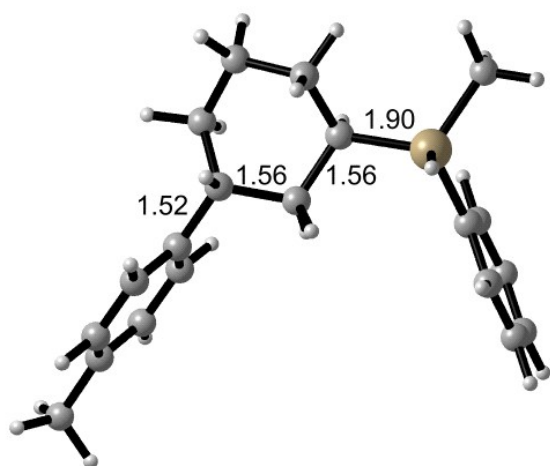
K

$G_{\text{gas}} = -1083.022812$ a.u.

$E_{\text{gas}} = -1083.36160458$ a.u.

C	-2.43107200	-0.43083600	-0.09172500
C	-2.43087300	0.77415900	-0.83044900
C	-3.50614200	1.65535700	-0.76485500
C	-4.63704700	1.39297400	0.01846800
C	-4.64066400	0.19359700	0.73914500
C	-3.57125700	-0.69815100	0.69808800
H	-1.60086600	1.01124300	-1.48626200
H	-3.46685500	2.56847600	-1.35550900
H	-5.49857100	-0.05151900	1.36208400
H	-3.61823900	-1.59681300	1.30248300
C	0.96727200	-3.17188700	-0.08678300
H	1.35164500	-3.67738000	0.80640000
H	1.59297000	-3.51180700	-0.92251700
C	-0.49049000	-3.60423800	-0.35468400
H	-0.65277300	-4.63713800	-0.02721900
H	-0.69467300	-3.58083100	-1.43149500
C	-1.50106500	-2.68660200	0.33850900
H	-2.51552400	-3.03662200	0.11831700
H	-1.37625700	-2.75117700	1.43451000
C	1.08155800	-1.63503800	0.11419400
H	0.93993200	-1.42056700	1.18413300
Si	2.81610800	-0.98389700	-0.34024200
C	2.94245400	0.87716000	-0.06004900
C	2.76481500	1.44219900	1.21789000
C	3.21771600	1.75240800	-1.12665200
C	2.85821300	2.81896100	1.42259600
H	2.54917800	0.80148200	2.07089600
C	3.31447800	3.13147500	-0.92834300
H	3.35966900	1.35180500	-2.12768800
C	3.13436300	3.66699400	0.34754500

H	2.71544600	3.23072900	2.41795000
H	3.52895500	3.78631800	-1.76855900
H	3.20754800	4.73957100	0.50460300
C	-0.04600400	-0.89028000	-0.62422700
H	0.05813200	-1.03387700	-1.71387400
H	0.05185000	0.18336400	-0.43911900
C	-5.78540900	2.37116900	0.10045300
H	-5.61434700	3.13821000	0.86758600
H	-5.93445500	2.89591400	-0.84924900
H	-6.72363300	1.86678700	0.35305400
C	4.12711800	-1.91426400	0.65629100
H	4.00782500	-1.74024800	1.73131100
H	4.06769800	-2.99384400	0.48332900
H	5.13270700	-1.58409100	0.37693900
H	3.04081800	-1.22476200	-1.79709600
N	-1.36307000	-1.31851500	-0.14915700



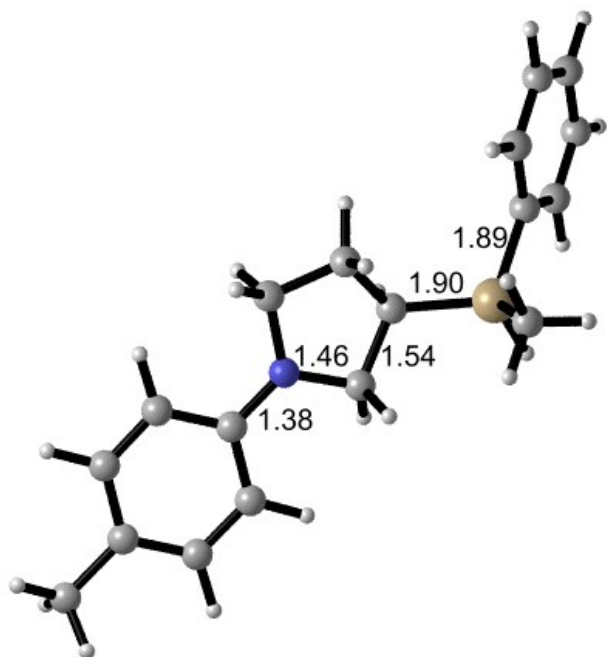
K1

G_{gas} = -1065.801046 a.u.

E_{gas} = -1066.13769825 a.u.

C	1.76816500	0.22372300	-0.73607900
C	0.82737700	0.65207500	0.22869100
C	0.93484900	1.96109800	0.73931800
C	1.92669900	2.85747000	0.33555900
C	2.84606000	2.41289100	-0.62526900
C	2.76391500	1.12633100	-1.14606500
H	0.21398500	2.29894800	1.48274100
H	3.62929300	3.08381300	-0.97217300
H	3.48729400	0.81055500	-1.89532600
C	1.13694500	-2.83074000	0.97162200
H	0.74908500	-3.67682800	1.54979000
H	1.54164300	-2.12709700	1.71238500
C	2.30280500	-3.28134000	0.08067000
H	1.95926500	-4.05989600	-0.61196400
H	3.08930300	-3.74214900	0.69036700

C	2.88952800	-2.09353300	-0.70358400
H	3.50554200	-1.48939600	-0.02826900
H	3.56420000	-2.46848400	-1.48183000
C	-0.01880600	-2.17843700	0.14427600
H	-0.87721000	-2.86041900	0.11704000
Si	-0.54956800	-0.49129100	0.83397700
C	-2.21606500	0.02713300	0.09292200
C	-3.40741500	-0.59316200	0.51780600
C	-2.31996200	1.01271300	-0.90574200
C	-4.64419900	-0.24981400	-0.02919000
H	-3.37481700	-1.35899300	1.29048900
C	-3.55482400	1.36241300	-1.45752900
H	-1.42292900	1.51815300	-1.25347600
C	-4.71999600	0.73125200	-1.02052700
H	-5.54757500	-0.74467400	0.31755900
H	-3.60656100	2.12820000	-2.22703900
H	-5.68173200	1.00203100	-1.44778500
C	-0.69110400	-0.45731300	2.72228000
H	0.23909500	-0.77392000	3.20396500
H	-0.92554800	0.55084800	3.07976600
H	-1.49064900	-1.12032600	3.07101100
C	0.42454200	-1.89293100	-1.31483500
H	-0.33041800	-1.29127100	-1.83605900
H	0.50419100	-2.82768700	-1.88390700
C	2.01343800	4.25319500	0.90730400
H	2.95368500	4.40600200	1.45056700
H	1.97306800	5.01315200	0.11828200
H	1.19274000	4.45104000	1.60258900
C	1.78684900	-1.17712000	-1.35429800
H	2.05619400	-1.03894000	-2.40836400



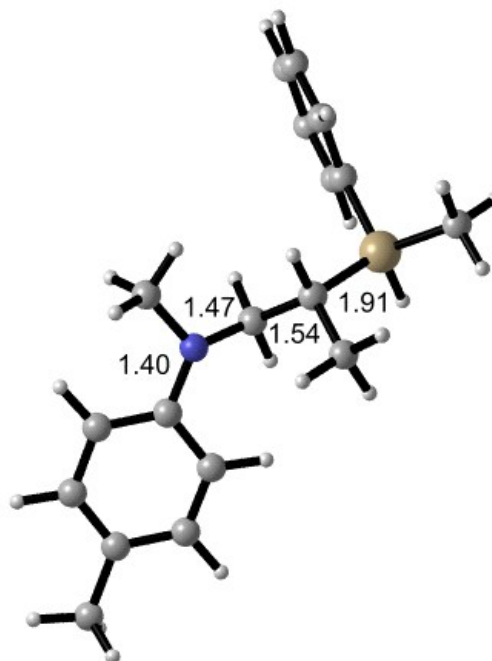
K2

G_{gas} = -1043.741062 a.u.

E_{gas} = -1044.05256228 a.u.

C	4.98865300	-1.10580000	0.43849000
C	3.60625600	-1.01311100	0.30332500
C	2.99006300	0.22405400	0.01175200
C	3.83103400	1.34883700	-0.13850800
C	5.21124900	1.22944100	-0.00141800
C	5.82671500	0.00664600	0.29332000
H	5.42637300	-2.07741600	0.65860300
H	3.00412400	-1.90876900	0.40934300
H	3.40412600	2.32116000	-0.35828200
H	5.82575600	2.11880300	-0.12587200
C	7.32273800	-0.10210300	0.47431600
H	7.85477100	0.63845100	-0.13184200
H	7.62098100	0.06211300	1.51845800
H	7.69018700	-1.09298600	0.18770000
N	1.61960500	0.32774400	-0.12737000
C	0.69508000	-0.76664900	0.15702100
H	0.92613700	-1.24451500	1.11781000
H	0.76394500	-1.55107800	-0.61624000
C	-0.69188500	-0.09124100	0.18143900
H	-0.83859100	0.32663000	1.18789500
C	-0.50317600	1.09414000	-0.79212400
H	-1.23422600	1.89243100	-0.63798900
H	-0.58629700	0.75952000	-1.83338700
C	0.93692200	1.55441700	-0.51838900
H	1.40218400	2.00167800	-1.40632900
H	0.96763300	2.31158800	0.28304100

Si	-2.17283600	-1.24152600	-0.15376600
H	-2.10756100	-2.36355600	0.82869300
C	-3.79227800	-0.32707700	0.16267700
C	-4.29940300	0.61884700	-0.74889800
C	-4.52865500	-0.55725200	1.33919700
C	-5.48552800	1.30875900	-0.49531500
H	-3.76588600	0.82098600	-1.67534500
C	-5.71626000	0.12967600	1.59937400
H	-4.17253200	-1.28726500	2.06245000
C	-6.19646500	1.06522000	0.68186800
H	-5.85663200	2.03316900	-1.21528500
H	-6.26710300	-0.06742000	2.51505600
H	-7.12108900	1.59996500	0.88081200
C	-2.11641600	-1.93944800	-1.91030200
H	-2.22350500	-1.15437000	-2.66628700
H	-1.17246900	-2.45969900	-2.10385000
H	-2.92971800	-2.65639700	-2.06179900



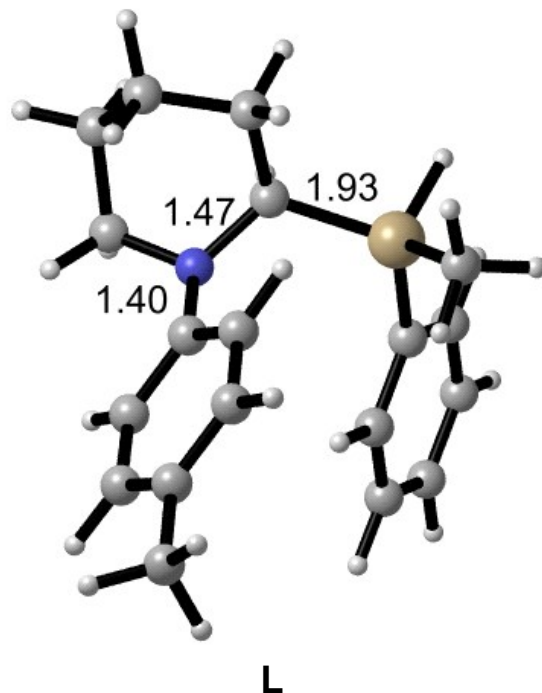
K3

G_{gas} = -1043.750692 a.u.

E_{gas} = -1044.06584505 a.u.

C	2.09953500	-0.50898600	-0.25515100
C	1.07409500	0.28812400	0.32785700
C	1.31974200	1.65731900	0.52835600
C	2.52398700	2.28412600	0.19976500
C	3.51795500	1.47688900	-0.36585000
C	3.31824400	0.12018300	-0.59570500
H	0.52988900	2.26706900	0.96634500
H	4.47121200	1.91891700	-0.64925900
H	4.11668900	-0.44370500	-1.06168800

N	1.91821800	-1.88319300	-0.47175500
Si	-0.54304000	-0.45138200	0.93223000
C	-2.00975600	0.35762000	0.04443900
C	-1.85204900	0.99281200	-1.20198400
C	-3.30756400	0.31674900	0.59016000
C	-2.93818400	1.55578200	-1.87537600
H	-0.86217400	1.05950800	-1.64568100
C	-4.39785800	0.87750500	-0.07683100
H	-3.47532900	-0.15645600	1.55503200
C	-4.21475600	1.49847600	-1.31403400
H	-2.78706100	2.04249900	-2.83532200
H	-5.38800200	0.83311800	0.36909500
H	-5.06123600	1.93790300	-1.83480600
C	-0.74404000	-0.23551000	2.80235400
H	0.10617600	-0.68259000	3.32810400
H	-0.79131600	0.82220700	3.08104500
H	-1.65508700	-0.71726300	3.17475600
C	0.56452300	-2.38481800	-0.73558100
H	0.11173700	-1.85652600	-1.59456600
H	0.66366800	-3.43367400	-1.03794600
C	2.75370000	3.75499900	0.45595400
H	3.42463400	3.91867000	1.30894300
H	3.21031400	4.24900900	-0.40911200
H	1.81442400	4.27132600	0.67629900
C	2.99837200	-2.63316400	-1.09059300
H	3.92655900	-2.50403300	-0.52569800
H	2.74862900	-3.69619400	-1.07153200
H	3.19517300	-2.34684200	-2.13803500
C	-1.69219600	-3.03895200	0.21796300
H	-1.51371000	-4.09563800	-0.02133100
H	-2.35369700	-3.00985900	1.09039600
H	-2.24264900	-2.59736600	-0.61966600
C	-0.37370400	-2.29533300	0.48187300
H	0.14669000	-2.78132100	1.32000000

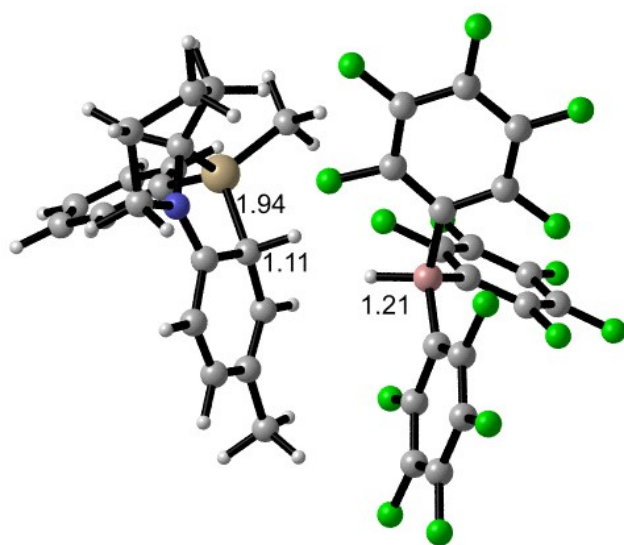


G_{gas} = -1083.009082 a.u.

E_{gas} = -1083.35033278 a.u.

C	-1.40959600	-0.04047400	-0.45164400
C	-1.82704800	-0.30163700	0.86593200
C	-2.60558300	-1.42142100	1.16714200
C	-3.02647400	-2.31623000	0.17973200
C	-2.62452600	-2.04530800	-1.13729100
C	-1.82959500	-0.94855800	-1.44985200
H	-1.57314000	0.38834700	1.66004500
H	-2.91078000	-1.58325600	2.19883700
H	-2.92525400	-2.71951800	-1.93667200
H	-1.50430600	-0.80057400	-2.47481100
N	-0.60056100	1.05009700	-0.79847100
C	-1.78333700	3.41509500	-0.13596600
H	-2.10155800	4.43426000	0.10910900
H	-2.67026400	2.77744900	-0.03820900
C	-1.27067500	3.33486900	-1.58064300
H	-0.36456300	3.94582900	-1.68041700
H	-2.00094900	3.75374600	-2.28176500
C	-0.97645000	1.86080600	-1.97133900
H	-1.87452600	1.42052800	-2.41149500
H	-0.18713900	1.82536300	-2.73687200
Si	1.43305400	0.92501800	1.31944000
C	2.47503000	-0.28669000	0.32028000
C	3.82785300	-0.00475000	0.05449400
C	1.94771200	-1.49427600	-0.17708200
C	4.62407500	-0.88856300	-0.67723700
H	4.26825500	0.91764300	0.42593800
C	2.73931800	-2.38024600	-0.90848700

H	0.90582000	-1.74674900	0.00119100
C	4.07990900	-2.07919400	-1.16012600
H	5.66661800	-0.64834300	-0.86818200
H	2.30987100	-3.30545200	-1.28335500
H	4.69651100	-2.76969900	-1.72927000
C	0.80219200	0.13845900	2.92004400
H	0.28321000	-0.80678400	2.74454200
H	1.65867800	-0.06029200	3.57376600
H	0.12322800	0.80623100	3.46188900
C	0.16768000	1.82820000	0.18118100
H	0.90327400	2.36343500	-0.44125800
H	2.34307800	2.04266000	1.71597500
C	-3.86186300	-3.53045600	0.51071000
H	-3.27490900	-4.45584400	0.44832600
H	-4.26734300	-3.46979600	1.52511200
H	-4.70563900	-3.64041700	-0.17969200
C	-0.69226100	2.93759000	0.85134200
H	-1.16077900	2.59485900	1.78140700
H	-0.03439200	3.77214200	1.12586000



M

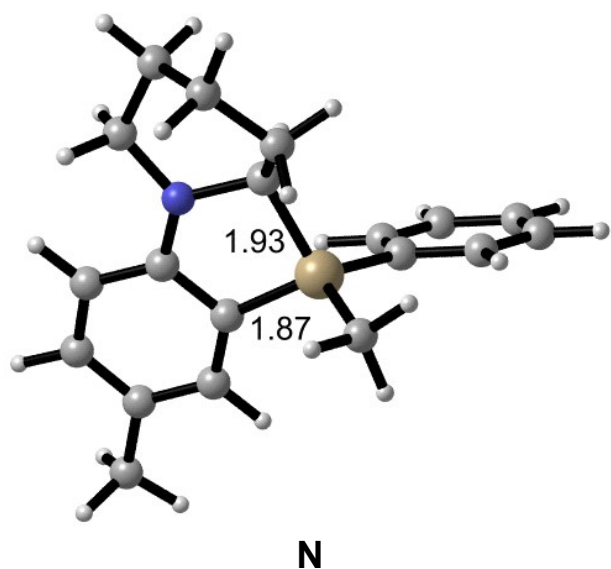
G_{gas} = -3291.093408 a.u.

E_{gas} = -3291.55182845 a.u.

C	-2.58083200	0.35210500	1.82175600
C	-2.31641000	-0.44806200	0.59734300
C	-1.92628800	-1.85650200	0.81464500
C	-1.63771900	-2.35304100	2.04771800
C	-1.71648200	-1.44580000	3.16390700
C	-2.14547300	-0.14481800	3.08146800
H	-1.41222600	0.01648100	0.14189600
H	-1.76797200	-2.46375200	-0.07110200
H	-1.42725300	-1.82595800	4.14157900

H	-2.21790600	0.46223800	3.97582700
N	-3.24760100	1.49251800	1.66132600
C	-3.08630900	4.13964400	0.84753500
H	-3.31510100	5.14819900	0.49121100
H	-2.01047300	4.11616400	1.04681200
C	-3.84809700	3.84544200	2.14580700
H	-4.92964900	3.84440700	1.96505300
H	-3.66056800	4.61923300	2.89677500
C	-3.40399300	2.49709000	2.73372900
H	-2.43215600	2.61463600	3.22387600
H	-4.11884600	2.13010800	3.48214400
Si	-3.66996200	0.13916100	-0.65481600
C	-5.21677400	-0.92212100	-0.60870600
C	-5.65554700	-1.61207300	-1.75407100
C	-5.97440900	-1.05971500	0.57130900
C	-6.80342800	-2.40632200	-1.72355800
H	-5.09874500	-1.53186700	-2.68377000
C	-7.12151300	-1.85117200	0.60666900
H	-5.66831600	-0.54553100	1.48029500
C	-7.53790700	-2.52629500	-0.54342700
H	-7.12307200	-2.92919100	-2.62024600
H	-7.69034100	-1.94225800	1.52759800
H	-8.43147100	-3.14327100	-0.51828700
C	-3.03738400	0.40844200	-2.39644200
H	-2.71453400	-0.53028600	-2.85484200
H	-3.81380100	0.85470000	-3.02652400
H	-2.16797300	1.07049100	-2.39453200
C	-3.91325200	1.76772600	0.35854000
H	-4.97852300	1.88885000	0.59740700
C	-1.17101400	-3.76655000	2.28720600
H	-1.80601800	-4.27529000	3.02148800
H	-1.18848200	-4.34770400	1.36247400
H	-0.14354700	-3.77036800	2.66330400
C	-3.40979100	3.09697400	-0.25272700
H	-2.51790800	2.94847400	-0.86255200
H	-4.19910000	3.46582200	-0.91733300
B	1.65476300	-0.00346000	-0.08082900
C	2.56761200	-0.36428600	1.22998800
C	2.33210500	-1.58286100	1.87101700
C	3.52484300	0.43214100	1.85929400
C	2.95210200	-1.98969700	3.04635100
C	4.18350200	0.06480400	3.03515100
C	3.89621400	-1.15519800	3.63706900
C	1.87148800	-1.07201900	-1.31147800
C	3.08705000	-1.66990800	-1.65659600
C	0.79955300	-1.46307400	-2.11149900
C	3.23042800	-2.57546400	-2.70850000

C	0.88769400	-2.36135600	-3.17021400
C	2.12233900	-2.92387600	-3.47499200
C	1.76447500	1.53399500	-0.64533400
C	0.71395500	2.44027400	-0.53103700
C	2.86922600	2.03311900	-1.34268800
C	0.72529300	3.72987400	-1.05705600
C	2.93492100	3.31539900	-1.88298700
C	1.84888500	4.17609000	-1.74052300
F	3.85899800	1.64117900	1.35950000
F	5.08947500	0.88336500	3.59543700
F	4.51198100	-1.51899200	4.77268100
F	2.63665600	-3.16964300	3.61737200
F	1.42190100	-2.44677300	1.35129500
F	-0.44164600	2.09853900	0.12154300
F	-0.34593500	4.54186200	-0.91330700
F	1.88567900	5.41321200	-2.25582600
F	4.02715900	3.73270000	-2.54039600
F	3.95234200	1.25540600	-1.51898600
F	-0.45276500	-0.96798600	-1.87382100
F	-0.20311000	-2.68803000	-3.89034900
F	2.24141200	-3.79223900	-4.49018300
F	4.42559100	-3.11747200	-2.98972100
F	4.20371000	-1.39859600	-0.95569900
H	0.51541500	-0.14916100	0.29985700

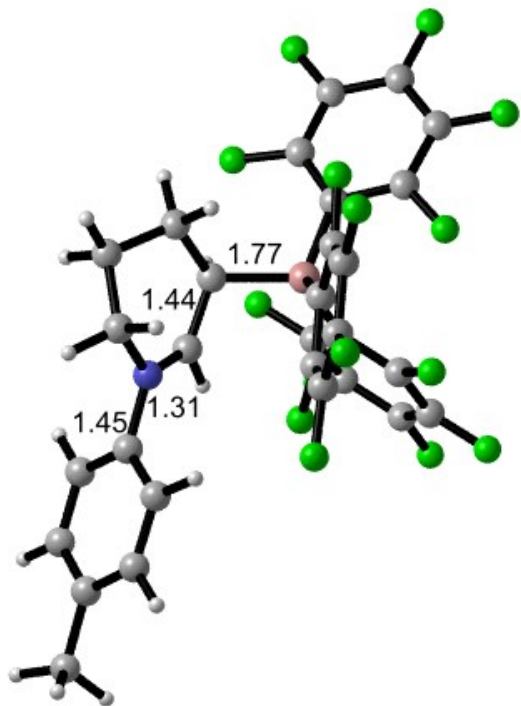


G_{gas} = -1081.846898 a.u.

E_{gas} = -1082.17203611 a.u.

C	1.79419800	0.35851600	-0.18770200
C	0.68471000	1.01877200	0.40519300
C	0.72336000	2.40618900	0.57428200
C	1.81905100	3.17673400	0.16643900
C	2.89546500	2.50093600	-0.42867700

C	2.89957500	1.12074500	-0.61446200
H	-0.12881800	2.91082700	1.02735200
H	3.75876900	3.07303400	-0.76361800
H	3.75506300	0.64689400	-1.08362100
N	1.72298800	-1.02463000	-0.29614300
C	1.86360300	-3.74008100	0.19742900
H	1.69738300	-4.82291200	0.18625300
H	2.68007000	-3.55797800	0.90694700
C	2.30337900	-3.24825500	-1.18626900
H	1.49906800	-3.41635700	-1.91291500
H	3.17015000	-3.81194100	-1.54775000
C	2.66778300	-1.75599000	-1.13586800
H	3.67628300	-1.64673900	-0.71132400
H	2.70613300	-1.33679300	-2.15644300
Si	-0.59930500	-0.26038100	0.84540900
C	-2.29048300	0.02963500	0.05789100
C	-3.47033000	-0.49903000	0.61389700
C	-2.40654600	0.77097600	-1.13369100
C	-4.71142300	-0.30561500	0.00430100
H	-3.42620900	-1.06896000	1.53891000
C	-3.64424500	0.96897900	-1.74718400
H	-1.51697700	1.20763400	-1.58091300
C	-4.80012100	0.42907400	-1.17927800
H	-5.60776700	-0.72448900	0.45390200
H	-3.70794300	1.54756400	-2.66489200
H	-5.76507500	0.58331400	-1.65448700
C	-0.79528200	-0.56760300	2.70101100
H	-1.26369400	0.29490200	3.18704700
H	-1.41090600	-1.44708500	2.91899400
H	0.18297800	-0.72116900	3.16753300
C	0.40729700	-1.64479500	-0.04495500
H	-0.08970500	-1.83045400	-1.01370400
C	1.84584900	4.67689400	0.34847900
H	1.95246300	5.20195500	-0.60875700
H	0.92479600	5.03464800	0.81837200
H	2.68322300	4.99513800	0.98161800
C	0.58553800	-2.99943700	0.67424900
H	0.63615200	-2.86276700	1.75992700
H	-0.30434900	-3.61039500	0.47833700



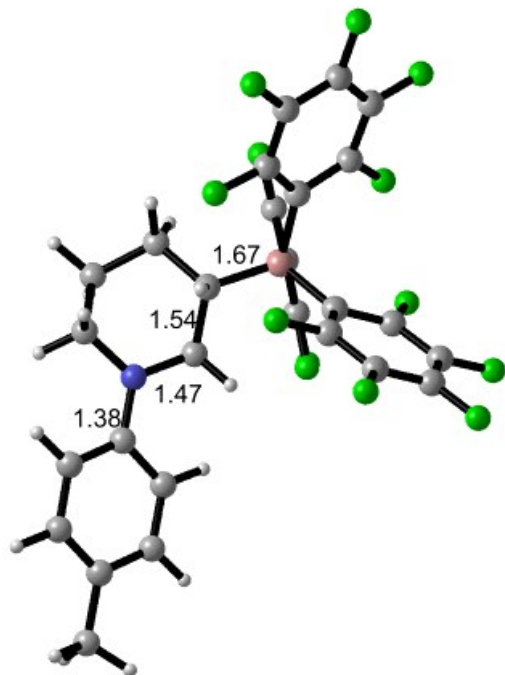
O

$G_{\text{gas}} = -2728.953862 \text{ a.u.}$

$E_{\text{gas}} = -2729.27732804 \text{ a.u.}$

C	3.88867400	0.07991600	-1.34330600
C	4.47865400	1.05858100	-2.14362100
C	5.75299600	1.52868400	-1.82642100
C	6.45459200	1.02887500	-0.72227400
C	5.83937500	0.04108900	0.06154300
C	4.56504200	-0.43644900	-0.23562100
H	3.94863600	1.44207200	-3.01040200
H	6.20817300	2.29171400	-2.45159300
H	6.36112500	-0.35558200	0.92814800
H	4.09535200	-1.17209700	0.40691600
N	2.57467300	-0.41901900	-1.68882500
C	1.50502800	0.32828700	-1.54295800
H	1.69244900	1.32505500	-1.15393200
C	0.15264400	-0.07099400	-1.82027500
H	-0.31661500	0.77731600	-2.31677400
C	0.00442900	-1.37902400	-2.62701700
H	-0.76396300	-1.22862000	-3.38761200
H	-0.35452300	-2.18887500	-1.98759900
C	1.31973100	-1.81065700	-3.28836100
H	1.56703100	-1.14525300	-4.12492100
H	1.23775500	-2.82308500	-3.69622800
C	2.47231600	-1.77725800	-2.28585600
H	2.32419600	-2.50258700	-1.47871200
H	3.43397100	-1.98646500	-2.75859800
B	-0.76254900	-0.05699500	-0.30015500
C	-0.59431400	1.38580400	0.50613000

C	-0.54461700	1.50132700	1.90293300
C	-0.64757800	2.62116600	-0.15064200
C	-0.51935800	2.71819300	2.58371600
C	-0.62185400	3.86055300	0.48481600
C	-0.55733600	3.91149500	1.87196400
C	-0.16062500	-1.35999000	0.51602300
C	-0.73587800	-2.63540800	0.52819600
C	1.07530000	-1.30398600	1.16760900
C	-0.16170500	-3.74895200	1.14386500
C	1.69756000	-2.38678400	1.77913100
C	1.07140500	-3.62879600	1.77389300
C	-2.38248900	-0.14367600	-0.63066700
C	-3.03136500	0.16739300	-1.82865600
C	-3.26336300	-0.42333500	0.42421500
C	-4.41805400	0.17314200	-1.98959500
C	-4.64941000	-0.42969000	0.31390100
C	-5.23770700	-0.12710500	-0.91047200
F	-0.73037600	2.67756100	-1.50734600
F	-0.66237700	4.99532100	-0.22933400
F	-0.53071600	5.08734000	2.50960900
F	-0.45891500	2.74519900	3.92224900
F	-0.51275400	0.41041000	2.69129900
F	1.76897600	-0.13700400	1.20651900
F	2.91291300	-2.24664400	2.34311500
F	1.65225200	-4.68716700	2.35018200
F	-0.77669000	-4.93888800	1.10676800
F	-1.89779500	-2.87646100	-0.11542100
F	-2.33989300	0.48747500	-2.95415200
F	-2.76926800	-0.71233200	1.64610300
F	-5.41976300	-0.71853700	1.37204200
F	-6.56912400	-0.12432500	-1.04380500
F	-4.95990000	0.47264900	-3.17979700
C	7.82365700	1.55501700	-0.36474700
H	7.76013500	2.29007400	0.44666900
H	8.48314900	0.75181500	-0.02240500
H	8.29954600	2.04675200	-1.21733700



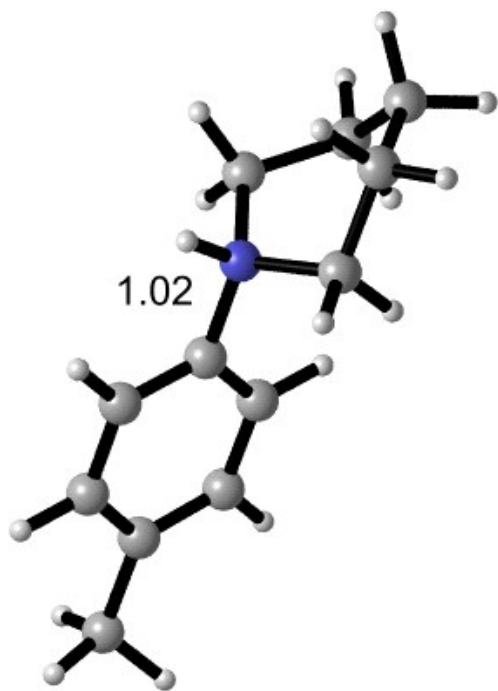
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G_{gas} = -2729.642861 a.u.

E_{gas} = -2729.97556363 a.u.

C	-4.34517200	0.00067900	-1.26948700
C	-4.72272500	-0.27934500	0.06875700
C	-6.02260300	-0.05722400	0.50989300
C	-7.02479400	0.44225300	-0.33296400
C	-6.65193400	0.72448300	-1.65194500
C	-5.35549200	0.51957700	-2.11661300
H	-3.99680400	-0.69124500	0.75965400
H	-6.26481200	-0.29008100	1.54569600
H	-7.39204200	1.13320900	-2.33858900
H	-5.11608600	0.80032600	-3.13601500
N	-3.05808900	-0.21645900	-1.71430500
C	-0.59658200	-0.06177000	-1.36454500
H	-0.73288700	0.96645200	-1.69716700
C	-0.31716800	-0.89853700	-2.64017200
H	0.22903900	-1.81841900	-2.40836000
H	0.33165900	-0.31652900	-3.30094200
C	-1.61572500	-1.27601900	-3.38882600
H	-1.97094200	-2.26076800	-3.05908200
H	-1.43823200	-1.35557800	-4.46888200
C	-2.74525000	-0.27189300	-3.13822100
H	-2.46662600	0.71862100	-3.53738100
H	-3.64032500	-0.59334200	-3.68191900
B	0.65218600	-0.06252800	-0.25084900
C	2.07637900	0.58628700	-0.85939100
C	3.29564300	0.38117700	-0.19751300
C	2.18100700	1.47480200	-1.93479300

C	4.50734400	0.95630900	-0.56789000
C	3.37326200	2.07702400	-2.34461400
C	4.54980300	1.81814900	-1.65771400
C	0.83258300	-1.65347500	0.21680100
C	0.00748100	-2.26026400	1.17044200
C	1.71720300	-2.54855600	-0.39222700
C	0.06391800	-3.60584700	1.52451100
C	1.81359400	-3.90322900	-0.07455400
C	0.98114900	-4.44054300	0.89764700
C	0.36394900	0.96778800	1.04828300
C	-0.18238900	2.24621000	0.86750600
C	0.75853800	0.72519200	2.37210900
C	-0.37325300	3.17934400	1.88626100
C	0.58592900	1.62597400	3.42288900
C	0.01101200	2.86655500	3.18279900
F	1.10703200	1.82141800	-2.68379800
F	3.38843300	2.91326600	-3.40101000
F	5.70741100	2.38995600	-2.03571000
F	5.63580700	0.69423400	0.11912900
F	3.35205300	-0.42422200	0.88566100
F	2.55113700	-2.13725000	-1.37765000
F	2.69845100	-4.69705600	-0.70896700
F	1.05195800	-5.74551900	1.21810100
F	-0.76285000	-4.10810800	2.46177800
F	-0.93359000	-1.53711900	1.82531600
F	-0.54967100	2.68081300	-0.36088500
F	1.35600500	-0.43140600	2.72776400
F	0.98024200	1.30688200	4.67057200
F	-0.16064600	3.74962900	4.18259000
F	-0.91398800	4.38389500	1.62190900
C	-8.44126300	0.64270000	0.15334700
H	-9.02231400	-0.29041800	0.13666100
H	-8.46580600	1.01328100	1.18464300
H	-8.97846300	1.36562900	-0.47036200
C	-1.95653000	-0.46229300	-0.76604400
H	-1.95935300	-1.51579100	-0.44847600
H	-2.14784200	0.13475200	0.12932100



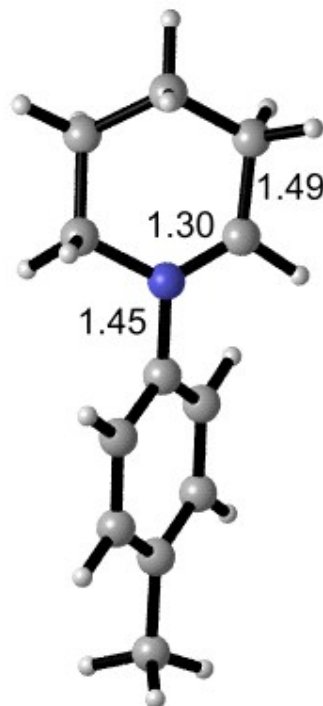
Q

G_{gas} = -522.424491 a.u.

E_{gas} = -522.666080632 a.u.

C	-0.44191800	-0.30052000	0.18244200
C	-0.88127300	0.91668000	-0.33718700
C	-2.25034700	1.12822900	-0.47890500
C	-3.18721500	0.14748500	-0.11282600
C	-2.70809900	-1.06454700	0.40179300
C	-1.34055900	-1.29551700	0.55321000
H	-0.18190400	1.69391600	-0.62896900
H	-2.59709300	2.07411600	-0.88414500
H	-3.40956700	-1.84127700	0.69003000
H	-0.99342700	-2.24466800	0.95631300
C	1.71877600	-0.75217700	-1.01036400
H	1.45005800	0.10882000	-1.62364700
H	1.27492000	-1.64215600	-1.46076800
C	3.22285000	-0.86923900	-0.79790000
H	3.68106500	-1.11539300	-1.75996100
H	3.42639100	-1.72722600	-0.14442300
C	3.82453700	0.43221000	-0.20793300
H	4.28624900	1.02915100	-0.99897200
H	4.62346000	0.17643400	0.49412700
C	2.75318700	1.28503400	0.50226800
H	2.22302300	1.92198700	-0.21431900
H	3.21549900	1.96806100	1.22148400
C	1.75203200	0.42853000	1.26765500
H	2.25735100	-0.18222100	2.02013700
H	0.97875100	1.01716300	1.75998600
C	-4.66616300	0.40577800	-0.25121000
H	-5.23711300	-0.52550000	-0.26058200

H	-5.03207600	1.01026800	0.58712600
H	-4.89009600	0.95532500	-1.16977200
N	1.01091600	-0.56747200	0.33571900
H	1.07325900	-1.47618300	0.80006100



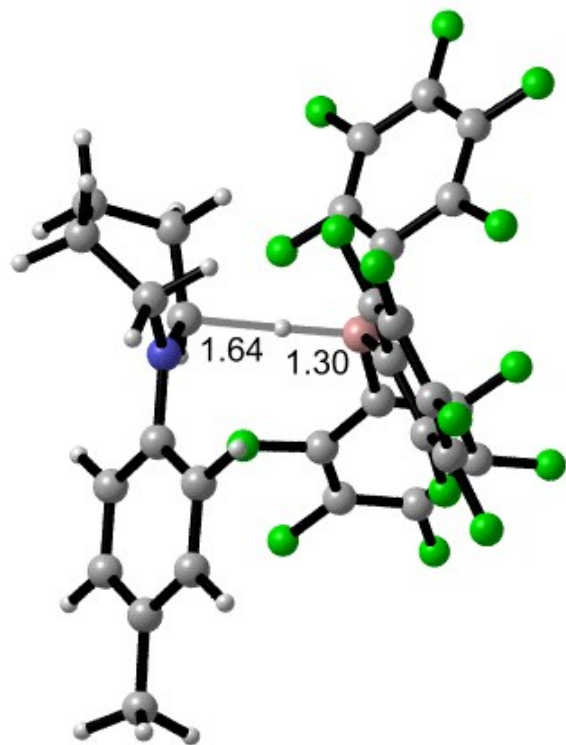
R

G_{gas} = -521.244632 a.u.

E_{gas} = -521.461983475 a.u.

C	0.41410400	-0.01493800	-0.04871500
C	1.09498900	-1.10816800	0.49292300
C	2.48753200	-1.09974800	0.50969800
C	3.21661400	-0.01468200	0.00139600
C	2.50227500	1.07223200	-0.52940700
C	1.11124000	1.08669100	-0.55349800
H	0.54972900	-1.94032000	0.92831300
H	3.01470300	-1.94669700	0.93814700
H	3.04403800	1.91990400	-0.93806800
H	0.58676900	1.93064800	-0.98883800
N	-1.03543700	-0.02241700	-0.08348100
C	-1.68710300	-1.06104600	-0.50218900
H	-1.07918600	-1.88984300	-0.85858800
C	-3.16837500	-1.19288500	-0.51382100
H	-3.40751700	-1.98035100	0.21962200
H	-3.45353000	-1.62405500	-1.48196900
C	-3.91703600	0.11059200	-0.20872600
H	-4.93506100	-0.11637700	0.11578700
H	-4.00107600	0.70889400	-1.12285600
C	-3.16504200	0.90192700	0.86510800
H	-3.13877000	0.34021200	1.80634500

H	-3.66364900	1.85214200	1.07575500
C	-1.73980500	1.20673900	0.41393700
H	-1.72646000	1.93145300	-0.40645700
H	-1.12503200	1.60026300	1.22449800
C	4.72262800	0.00192900	0.05022900
H	5.14440900	0.49736400	-0.82848000
H	5.07285200	0.55059600	0.93280200
H	5.13370800	-1.00878000	0.10674200



TS₁

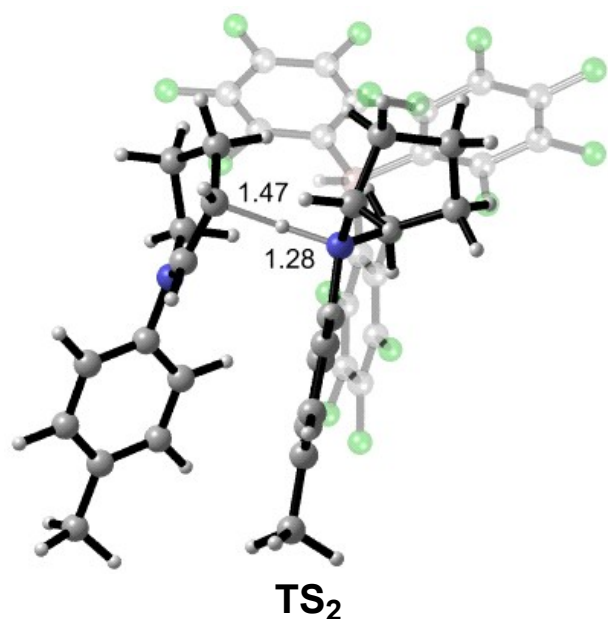
G_{gas} = -2730.124794 a.u.

E_{gas} = -2730.46591480 a.u.

C	3.04565700	-0.63324500	-1.59981700
C	3.49105300	0.37849400	-2.45469200
C	4.60501100	1.13791300	-2.10535600
C	5.30093200	0.90536800	-0.91146800
C	4.84355800	-0.12076000	-0.07317800
C	3.72606400	-0.88333100	-0.40424400
H	2.98188000	0.56136700	-3.39553800
H	4.94402900	1.91953900	-2.77953300
H	5.36040600	-0.31959400	0.86159800
H	3.36952500	-1.65017300	0.27574700
N	1.89629500	-1.42134900	-1.94701800
C	0.74159500	-0.86485500	-2.31764400
H	0.77699300	0.17675300	-2.60694600
C	-0.29009600	-1.78607100	-2.91305800
H	-1.06272800	-1.18998500	-3.39747500

H	-0.77352200	-2.35797800	-2.11536200
C	0.40692400	-2.74833900	-3.90184300
H	0.78632700	-2.16859000	-4.74974900
H	-0.33669700	-3.44044900	-4.30648600
C	1.56756700	-3.51841700	-3.22529700
H	2.44378800	-3.52799300	-3.88035900
H	1.29329300	-4.56281800	-3.04551300
C	1.94907500	-2.89859500	-1.86391600
H	1.25779200	-3.23332100	-1.08794900
H	2.95911500	-3.18158600	-1.56996200
B	-0.63557300	0.08593600	0.10189500
C	-0.58145500	1.71367000	0.16834200
C	-1.31920600	2.37680500	1.15452400
C	0.09982900	2.55535300	-0.70491400
C	-1.38795300	3.76085800	1.27275200
C	0.06190800	3.94716500	-0.63134700
C	-0.69052900	4.55589400	0.36595700
C	0.21179500	-0.70909700	1.23889000
C	0.25470900	-2.10584700	1.23528800
C	0.99715500	-0.12192200	2.23811700
C	1.00040500	-2.88024500	2.11594100
C	1.75477200	-0.85502900	3.15370300
C	1.75945700	-2.24441700	3.09523900
C	-2.17718400	-0.38810900	-0.12791600
C	-2.82628200	-0.06434700	-1.32170800
C	-2.97863000	-1.04814600	0.80748000
C	-4.15080800	-0.38256500	-1.60428400
C	-4.31178100	-1.38304800	0.57311900
C	-4.90341700	-1.04844700	-0.64120600
F	0.86965600	2.04725300	-1.70555300
F	0.74392300	4.69770600	-1.51096400
F	-0.74108100	5.89051000	0.45722200
F	-2.11091900	4.33511300	2.24431000
F	-1.99715000	1.65324300	2.06929300
F	1.07686100	1.21495000	2.36837800
F	2.48486000	-0.22875400	4.08704200
F	2.48521300	-2.96014200	3.96185200
F	0.99908300	-4.21950000	2.02513100
F	-0.44514700	-2.79773500	0.29500500
F	-2.14237900	0.58691200	-2.29916100
F	-2.48503000	-1.39300500	2.01168100
F	-5.03064400	-2.01987500	1.50814100
F	-6.18071900	-1.36662200	-0.88263100
F	-4.70283500	-0.05634000	-2.78316300
H	-0.03656300	-0.29381400	-0.99125500
C	6.48915600	1.75237900	-0.52576600
H	7.20883700	1.18521700	0.07152700

H	7.00750300	2.14050400	-1.40718900
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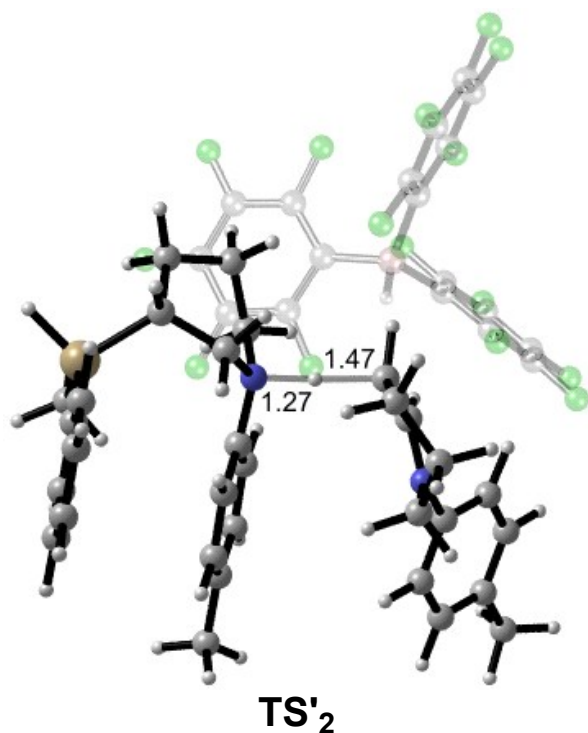
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E_{gas} = -3252.74030795 a.u.

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C	-4.16494700	-3.51216300	0.44463100
C	-5.31755600	-4.01025400	-0.18087300
C	-5.65436300	-3.50127000	-1.44181000
C	-4.86253200	-2.53962400	-2.06995500
H	-2.50535600	-2.14524200	0.34981900
H	-3.88699800	-3.87217700	1.43164100
H	-6.54173300	-3.87103500	-1.94880100
H	-5.12137600	-2.17490800	-3.05968600
N	-2.89933800	-1.06115300	-2.05560400
C	-2.63198900	1.20440400	-2.87303200
H	-2.56486100	2.04340700	-1.66519000
H	-3.22752100	1.91485400	-3.45136400
C	-1.21168400	0.91919000	-3.38846600
H	-0.44519000	1.33907900	-2.72829700
H	-1.07511700	1.40347300	-4.36138800
C	-0.97275800	-0.59233600	-3.52223600
H	0.08911600	-0.81205400	-3.64692100
H	-1.50475300	-0.98079900	-4.39937400
C	-1.45813300	-1.33285000	-2.27524800
H	-1.33973100	-2.41246500	-2.38017100
H	-0.88946300	-1.01104200	-1.39883700
C	-3.39714000	0.12662200	-2.40101300
H	-4.46329000	0.24641500	-2.22673300
C	-3.77724700	2.46305700	0.06788000

C	-5.00758900	3.12617200	-0.00280500
C	-6.11353600	2.63158800	0.69249200
C	-6.03803800	1.46792200	1.46299600
C	-4.80765400	0.79777200	1.49881700
C	-3.69605200	1.27433700	0.81008700
H	-5.13211500	4.02738100	-0.58887600
H	-7.05412400	3.17225600	0.62881100
H	-4.70699600	-0.12261000	2.06737600
H	-2.77623000	0.70599000	0.86413400
N	-2.61342100	2.89791000	-0.70773300
C	-2.79348100	4.20781500	-1.42218600
H	-3.28256700	4.91819600	-0.74902300
H	-3.46488600	4.02644200	-2.26670700
C	-1.45081500	4.78106600	-1.86847200
H	-1.64002200	5.63963600	-2.52032700
H	-0.91541200	4.04398000	-2.47731300
C	-0.60787900	5.18975800	-0.64218300
H	-0.85239500	6.21545200	-0.34534400
H	0.45104000	5.17744600	-0.90686100
C	-0.87544100	4.22881400	0.53976100
H	-1.66131400	4.61963100	1.19750800
H	0.01855900	4.11588800	1.15982600
C	-1.28661000	2.84680100	0.03715200
H	-0.53827200	2.45187200	-0.65192800
H	-1.37963400	2.13519500	0.85167100
B	2.03295900	-0.26658600	0.04524600
C	3.14647900	-1.14773200	-0.78200300
C	4.52973200	-1.10899600	-0.58555000
C	2.74072200	-2.02054800	-1.79372200
C	5.44165800	-1.84738500	-1.33877100
C	3.61041500	-2.78027700	-2.57236700
C	4.97874400	-2.69176100	-2.34245900
C	1.40615300	-1.10629000	1.31696700
C	0.04172800	-1.06968100	1.59128600
C	2.12529000	-1.94888000	2.17228000
C	-0.59074000	-1.79639600	2.59442600
C	1.54366100	-2.69354500	3.19907900
C	0.16957300	-2.62280800	3.41210700
C	2.57991000	1.22913800	0.45706700
C	2.40560900	2.31056800	-0.40957200
C	3.25617400	1.55149800	1.63788000
C	2.87701900	3.59756400	-0.15763600
C	3.72880800	2.82736400	1.94303200
C	3.54038700	3.86380300	1.03432700
F	1.41972600	-2.17517000	-2.08055800
F	3.14259800	-3.59395400	-3.53646700
F	5.83931500	-3.41282200	-3.07662400

F	6.76060100	-1.75819800	-1.10176900
F	5.06281300	-0.32935000	0.37667000
F	3.45465500	-2.08573000	2.03124500
F	2.29179800	-3.48459200	3.98248600
F	-0.41093200	-3.34001500	4.38539400
F	-1.93392400	-1.72941800	2.75077100
F	-0.79622800	-0.29859400	0.82444000
F	1.73007700	2.16235600	-1.58274900
F	3.49500000	0.60548500	2.56510000
F	4.36730000	3.06704500	3.09916200
F	3.99081700	5.09863200	1.30140300
F	2.67755800	4.59406800	-1.04865900
H	1.11629500	-0.08421500	-0.71839000
C	-6.15386700	-5.08190400	0.47668400
H	-6.19316500	-4.94867100	1.56208200
H	-7.17909800	-5.08164800	0.09581800
H	-5.73465700	-6.07799100	0.28887300
C	-7.22760200	0.95383200	2.23644700
H	-8.15843400	1.41348300	1.89325700
H	-7.32749100	-0.13179100	2.13835500
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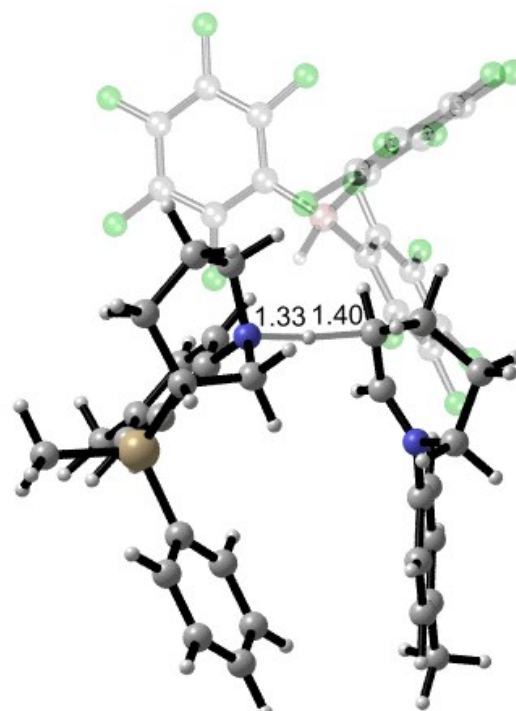
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C	6.42610800	2.12801700	0.28485400
C	6.81111800	0.78726900	0.42303900

C	6.02954800	-0.19021500	-0.20802900
C	4.90194300	0.15211700	-0.95078300
H	4.99822200	3.52888600	-0.52117000
H	7.01766700	2.90537700	0.76165800
H	6.30702100	-1.23844900	-0.14131300
H	4.32952100	-0.61567200	-1.45640000
N	3.37540700	1.85434200	-1.83992400
C	1.02648400	1.60227200	-2.37664200
H	0.32490500	2.55449700	-1.50712600
H	0.26678500	0.82198200	-2.30934900
C	1.19572500	2.29381800	-3.73914100
H	0.75874500	3.30031300	-3.73916300
H	0.64950700	1.72998000	-4.50272400
C	2.67592600	2.39891300	-4.13222000
H	2.81522900	3.11295300	-4.95013300
H	3.04388600	1.42694800	-4.47962500
C	3.52220500	2.83410000	-2.93154500
H	4.58195600	2.89038600	-3.18639800
H	3.20398200	3.82451000	-2.57703000
C	2.17794600	1.28837700	-1.64267200
H	2.11667800	0.57541700	-0.82642700
C	0.54669500	4.22414000	-0.14289800
C	1.30899100	3.65871100	0.89091800
C	2.28061200	4.41758000	1.53945700
C	2.53172300	5.75019000	1.18698400
C	1.77470400	6.29373000	0.14402800
C	0.79771300	5.54896700	-0.51915300
H	1.15305700	2.63201800	1.19935000
H	2.85477600	3.95526800	2.33781300
H	1.94133300	7.32411600	-0.15926000
H	0.23758900	6.02666800	-1.31284000
N	-0.40391500	3.37112300	-0.85008100
C	-1.24573200	2.46055500	0.06584900
H	-1.03103600	2.77009900	1.08997800
H	-0.86976100	1.44557700	-0.07008200
C	-2.74691100	2.53772700	-0.21202300
H	-2.95481500	2.06747200	-1.18292800
C	-3.20247400	4.00921400	-0.24437100
H	-3.03035700	4.45425100	0.74299800
H	-4.27925000	4.07086500	-0.42795000
C	-2.42908900	4.82529100	-1.31590600
H	-2.07625700	5.77142800	-0.89423400
H	-3.08191200	5.08437700	-2.15700700
C	-1.25348600	4.02935400	-1.88881500
H	-1.62072600	3.21813400	-2.52153100
H	-0.61098000	4.64531000	-2.51854800
B	0.15044800	-2.07923900	-0.05471400

C	-0.42857700	-1.57563900	1.40101000
C	-1.40561200	-2.23303800	2.15561500
C	-0.01186900	-0.36303300	1.94601700
C	-1.94114900	-1.72564500	3.33992200
C	-0.53490600	0.19984600	3.10589900
C	-1.50900100	-0.49145900	3.81576700
C	1.47397900	-3.03488600	0.10309500
C	2.58800100	-2.83721700	-0.71276400
C	1.65317500	-4.01727500	1.08131600
C	3.80054500	-3.50407400	-0.55799300
C	2.84027500	-4.72528500	1.26412200
C	3.93105200	-4.45988000	0.44184600
C	-1.05680700	-2.67413100	-0.99009500
C	-1.92792700	-1.79356800	-1.63262900
C	-1.33498100	-4.02271800	-1.22389400
C	-2.98500900	-2.18778300	-2.44563400
C	-2.37582900	-4.46861600	-2.03910700
C	-3.21471500	-3.54339200	-2.65226800
F	0.94324900	0.38481900	1.31506100
F	-0.14833500	1.43023500	3.51414500
F	-2.04235300	0.03973100	4.92710600
F	-2.88304900	-2.40128000	4.01528700
F	-1.89937300	-3.41486100	1.74661000
F	0.65112400	-4.32274600	1.92731800
F	2.94818000	-5.65110300	2.23048000
F	5.09082800	-5.11242800	0.61251800
F	4.85813800	-3.20328100	-1.34395600
F	2.54963000	-1.92367700	-1.72164700
F	-1.78126700	-0.44237200	-1.48149600
F	-0.58503700	-4.98337600	-0.65022700
F	-2.58662500	-5.78061200	-2.22852100
F	-4.22852900	-3.95045500	-3.43048300
F	-3.79639200	-1.27083300	-3.01668700
H	0.53117000	-1.08161100	-0.61881700
Si	-3.76787600	1.47571600	1.02647600
H	-3.16641000	0.12004900	1.04975600
C	-3.72071400	2.22463500	2.76013600
H	-4.28009400	1.59653500	3.46110900
H	-2.69558700	2.28436200	3.13965200
H	-4.15182600	3.23070500	2.79410600
C	-5.52288500	1.36621700	0.35033900
C	-5.77939200	0.63701400	-0.82795600
C	-6.60883800	2.00229000	0.97833600
C	-7.06792400	0.55208200	-1.35620600
H	-4.97218600	0.12136800	-1.34283500
C	-7.90014900	1.91931900	0.45259900
H	-6.45164300	2.56571100	1.89490600

C	-8.13113500	1.19386900	-0.71679700
H	-7.24218700	-0.02053100	-2.26291600
H	-8.72404000	2.41627700	0.95765800
H	-9.13531700	1.12442600	-1.12592600
C	3.55852700	6.57434800	1.92576000
H	3.92712800	7.40126600	1.31197700
H	3.13197100	7.00910400	2.83804500
H	4.41616900	5.96654200	2.22966800
C	8.02081400	0.40240100	1.24070100
H	8.57158100	-0.42038800	0.77474500
H	8.70745000	1.24472000	1.36407500
H	7.72769900	0.06679600	2.24305600



TS''₂

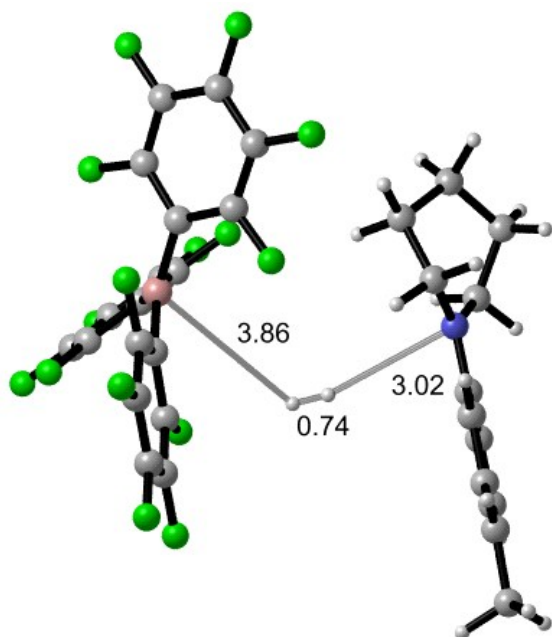
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C	4.24915300	4.86644400	-0.51638800
C	3.18624400	5.46815600	-1.20197000
C	1.89176000	4.98901900	-0.95428900
C	1.65852400	3.95571300	-0.05140000
H	4.88125600	3.35292900	0.87843400
H	5.26356400	5.21605400	-0.69014600
H	1.03908700	5.43634100	-1.45755800
H	0.64244400	3.63147000	0.13899500
N	2.50993200	2.28774600	1.53952200
C	1.35863100	0.23697900	2.14126900
H	0.36209800	-0.16959700	1.98019100

C	1.83370600	0.31791000	3.59881900	C	3.47801600	-1.96488100	-1.35494700
H	2.65389500	-0.38543300	3.79194300	C	3.22144000	-1.75117900	-2.72347800
H	1.01737200	0.01346000	4.26077000	C	1.96390200	-1.40000100	-3.22281300
C	2.30401200	1.73794000	3.93938100	C	0.91189600	-1.26746000	-2.30562900
H	2.84604200	1.75838300	4.89001900	C	1.12427300	-1.45776400	-0.94367700
H	1.44045800	2.40499300	4.04134400	H	4.03607400	-1.88063600	-3.43392700
C	3.21655500	2.28844800	2.83793600	H	-0.08899400	-1.01899300	-2.64607300
H	3.51583100	3.31711200	3.04710700	H	0.28359100	-1.35404400	-0.26531300
H	4.12898800	1.68250900	2.75625100	N	2.51869600	-1.94920300	0.99096800
C	1.61710500	1.32461600	1.29312000	C	3.88197800	-4.42225400	1.06455100
H	1.10201500	1.39269300	0.34131700	H	4.51132200	-5.25865900	1.38287100
B	-2.95847000	-0.19737400	-0.10033300	H	3.49307000	-4.69547500	0.07517800
C	-3.77175400	-1.26754700	-1.03417400	C	2.68663000	-4.26330800	2.01792200
C	-4.84011900	-2.07354800	-0.63719200	H	3.04455600	-4.07863600	3.03751700
C	-3.38193000	-1.44800600	-2.36305400	H	2.10182100	-5.18787900	2.06312200
C	-5.45716100	-3.00588100	-1.47140500	C	1.75240300	-3.12854800	1.56295600
C	-3.96522700	-2.36278200	-3.23503600	H	1.07674900	-3.47499700	0.78093600
C	-5.01756300	-3.15220000	-2.78257200	H	1.13179800	-2.76216500	2.38609400
C	-3.30666400	1.36515000	-0.47696900	C	4.73072400	-3.11491000	0.98939900
C	-2.32819900	2.35174400	-0.36825400	H	5.62668200	-3.20957500	1.61357900
C	-4.53538200	1.83172200	-0.95176000	Si	5.16669400	-2.58859900	-0.78646600
C	-2.51160500	3.68450700	-0.72297500	C	6.42586100	-1.17896100	-0.74800600
C	-4.77068100	3.15688000	-1.31949800	C	6.05895900	0.15328100	-1.01635000
C	-3.74861000	4.09441000	-1.20673500	C	7.77350100	-1.43084400	-0.42325100
C	-3.08242600	-0.45611300	1.51845500	C	6.99437400	1.18946000	-0.96052500
C	-2.10910500	-1.17139000	2.20974600	H	5.03108700	0.38471600	-1.28305400
C	-4.08085300	0.07388700	2.34172300	C	8.71199100	-0.40015600	-0.36431300
C	-2.05517000	-1.30416200	3.59410300	H	8.10258300	-2.44707300	-0.21476900
C	-4.09076300	-0.05128100	3.73044300	C	8.32277900	0.91432300	-0.63310900
C	-3.06158200	-0.74048700	4.36786900	H	6.68406300	2.20749800	-1.18004800
F	-2.36831100	-0.70284100	-2.87863600	H	9.74558400	-0.62122800	-0.11288200
F	-3.52755700	-2.48914400	-4.50113900	H	9.05325000	1.71747100	-0.59196700
F	-5.59960900	-4.04285100	-3.60083400	C	5.78924900	-4.00403400	-1.86686900
F	-6.47556700	-3.75979400	-1.02418800	H	5.91439400	-3.67929500	-2.90479100
F	-5.33891400	-1.98794100	0.61467700	H	6.76296400	-4.36551100	-1.51873600
F	-5.57900500	0.99131800	-1.07880300	H	5.09536700	-4.85018200	-1.86322800
F	-5.97300900	3.54134600	-1.77601500	C	3.90760400	-1.92639600	1.52421600
F	-3.95268300	5.37426700	-1.55363300	H	4.35398600	-0.96147500	1.26088700
F	-1.50689400	4.58285500	-0.59896400	H	3.81795500	-1.94863700	2.61424500
F	-1.09085800	2.03635800	0.11616800	H	1.97855800	-0.84697600	1.50055100
F	-1.08115500	-1.77371000	1.53779000	C	1.73540200	-1.17224200	-4.69739900
F	-5.10540600	0.75973900	1.80205100	H	1.55076700	-0.11227200	-4.90807000
F	-5.07490400	0.49104900	4.46451000	H	2.59912200	-1.48425800	-5.29111800
F	-3.03912300	-0.85273900	5.70480500	H	0.85928000	-1.72437100	-5.05233700
F	-1.01899100	-1.94620800	4.18332700	C	3.41751900	6.61235600	-2.15947200
H	-1.78792500	-0.34324300	-0.37285500	H	3.08087100	7.56258200	-1.72784700
C	2.39649900	-1.79963800	-0.46614400	H	4.47683300	6.71957400	-2.40842200

H	2.86258700	6.46936000	-3.09224500
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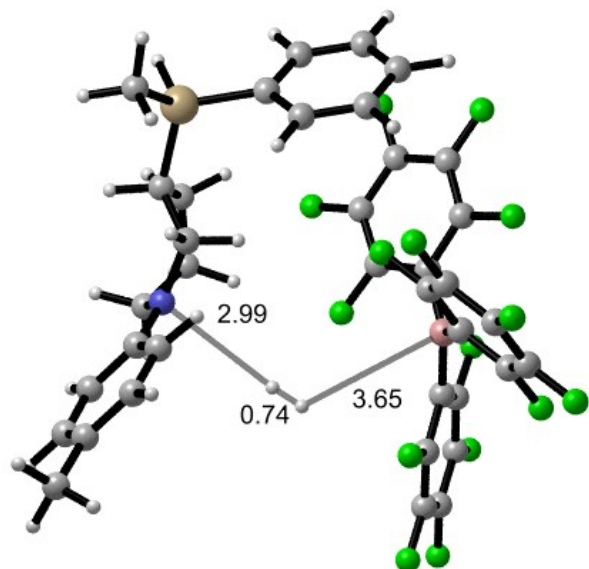
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E_{gas} = -2731.66928116 a.u.

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C	5.00297000	-0.41940200	-0.52843100
C	5.92052000	0.62935700	-0.55050000
C	6.48540100	1.14886200	0.61895000
C	6.08378000	0.56555300	1.82760400
C	5.16148400	-0.47525600	1.87450800
H	4.62517600	-0.80055500	-1.46982200
H	6.21335900	1.04385400	-1.51305600
H	6.49322900	0.94069700	2.76337100
H	4.86105800	-0.86432200	2.84111800
N	3.66554400	-2.03852000	0.73383000
C	2.94339800	-2.42612300	-0.47494800
H	3.58351300	-2.99094900	-1.17668700
H	2.62602800	-1.51944700	-0.99979800
C	1.70189500	-3.25226600	-0.12544600
H	1.16523700	-3.47950000	-1.05142000
H	1.03722300	-2.62860100	0.48438500
C	2.05394200	-4.54983100	0.63711500
H	2.12010800	-5.39527100	-0.05684800
H	1.24673400	-4.78940900	1.33856300
C	3.38984600	-4.40636700	1.39393000
H	4.22244800	-4.69488300	0.74129900
H	3.42173500	-5.08060200	2.25687000
C	3.63425200	-2.96849400	1.86720800
H	2.86448200	-2.68126400	2.60253400

H	4.59740800	-2.92370900	2.38440400
B	-1.71778100	0.57275900	-0.28897900
C	-1.99599300	-0.78349400	-1.03316000
C	-3.21212100	-1.46592400	-0.89540700
C	-1.03917600	-1.40716600	-1.84287700
C	-3.47678500	-2.67774700	-1.52539600
C	-1.25624600	-2.63087900	-2.46367900
C	-2.48558400	-3.26830000	-2.30662000
C	-1.02263500	1.76029400	-1.03255400
C	-0.22838600	2.71140700	-0.36624200
C	-1.14058300	1.95022700	-2.42170100
C	0.41333100	3.75900700	-1.01612900
C	-0.52888000	2.99684200	-3.10184100
C	0.25671600	3.90378900	-2.39335600
C	-2.14980700	0.69180900	1.21442900
C	-1.99438300	-0.37429400	2.11302100
C	-2.73323900	1.85149400	1.74496000
C	-2.37716500	-0.30130200	3.44803600
C	-3.14814900	1.95388600	3.06741700
C	-2.96406200	0.86942600	3.92406400
F	0.17015100	-0.84152700	-2.01119000
F	-0.28958200	-3.21372800	-3.18395200
F	-2.71094600	-4.43961500	-2.89996000
F	-4.66033400	-3.28165000	-1.38088100
F	-4.19841100	-0.93757200	-0.15098600
F	-1.89467300	1.12187700	-3.16039200
F	-0.68685700	3.14126700	-4.42082600
F	0.85497100	4.90679000	-3.03043500
F	1.16945200	4.62569100	-0.33794000
F	-0.02970500	2.62488100	0.95835100
F	-1.42310900	-1.52305000	1.70906400
F	-2.93749200	2.92016200	0.95767200
F	-3.71679900	3.07376600	3.52398600
F	-3.34682700	0.95343700	5.19683800
F	-2.19086100	-1.33676500	4.27246500
H	1.54252600	0.84747800	1.76029700
C	7.46006000	2.30259300	0.58495400
H	7.95053000	2.38188200	-0.39038700
H	6.96216100	3.26247200	0.77598400
H	8.24241400	2.19132400	1.34336100



TS'₃

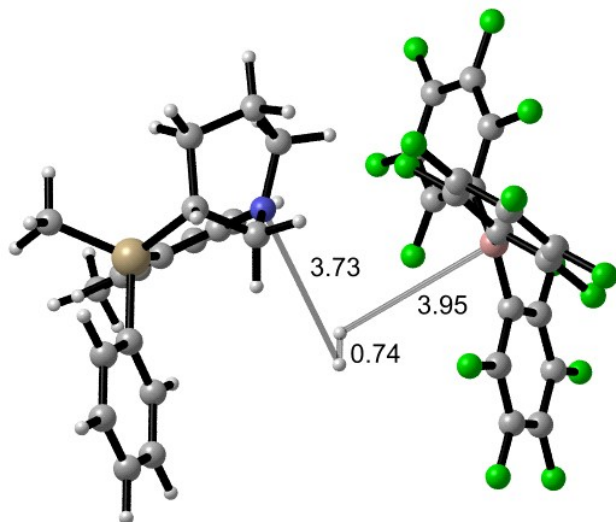
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E_{gas} = -3292.75424034 a.u.

H	-0.24117100	2.58072600	0.20086400
C	-3.18866400	3.40680700	0.55213400
C	-3.38322600	4.59034900	1.29500900
C	-3.50568000	5.82493000	0.65849600
C	-3.45385800	5.95296800	-0.73278600
C	-3.25391100	4.77722400	-1.46873600
C	-3.11723200	3.53725900	-0.85379500
H	-3.45493100	4.55386700	2.37541000
H	-3.65655700	6.71221100	1.26990500
H	-3.18620900	4.83152600	-2.55346900
H	-2.91654200	2.66725600	-1.46957200
N	-3.03653600	2.16400600	1.17028000
C	-2.95122600	2.09198800	2.62768800
H	-3.91125500	2.34853400	3.11189500
H	-2.22133600	2.83446700	2.96857500
C	-2.50521400	0.69664800	3.06903000
H	-2.37206600	0.68916900	4.15620000
H	-1.51919600	0.49908000	2.63719400
C	-3.51160500	-0.39588900	2.63794500
H	-4.21965700	-0.60057600	3.44891400
H	-2.96652800	-1.33220900	2.46872700
C	-4.30651900	0.03056500	1.37716400
H	-5.15792300	0.64593200	1.70688500
C	-3.45064500	0.93546400	0.47007700
H	-2.57522300	0.37943000	0.10075300
H	-4.03229800	1.22928200	-0.40865200
B	2.34611400	-0.49844800	-0.09758000
C	1.54677700	-1.65103100	0.60830000
C	1.42731000	-2.92813600	0.04440800

C	0.85665500	-1.45182400	1.81012700
C	0.68704800	-3.94718500	0.63165000
C	0.07373800	-2.43376600	2.40477200
C	-0.00912500	-3.69103800	1.81019900
C	3.29216600	0.43335700	0.72911400
C	3.51851900	1.77778500	0.38650500
C	3.97297300	-0.01560300	1.87454300
C	4.34287700	2.62240600	1.12026000
C	4.82102600	0.79474100	2.62099200
C	5.00275600	2.12323900	2.24195500
C	2.16025200	-0.31001400	-1.64418100
C	0.91281500	-0.48588600	-2.26232900
C	3.22236200	0.00515100	-2.50417600
C	0.72474700	-0.36806200	-3.63457700
C	3.07410300	0.11879800	-3.88192500
C	1.81462700	-0.06958300	-4.44952300
F	0.89312400	-0.24859600	2.41254300
F	-0.61908900	-2.17636500	3.52134600
F	-0.75782500	-4.64440900	2.36320100
F	0.61211200	-5.15585900	0.06288200
F	2.06367400	-3.21802000	-1.10384000
F	3.84981100	-1.28761600	2.28345300
F	5.45973500	0.31474600	3.69215800
F	5.80416100	2.91469900	2.95058300
F	4.51014400	3.89848600	0.76293100
F	2.89857400	2.32104700	-0.67344700
F	-0.17632700	-0.75473100	-1.52376200
F	4.45823300	0.18102500	-2.00947500
F	4.12055800	0.40116900	-4.66374400
F	1.65388100	0.03787700	-5.76706600
F	-0.48687100	-0.54681500	-4.17782100
H	0.45208000	2.62269400	-0.06444800
Si	-5.11701500	-1.44283100	0.47142100
C	-3.62282700	7.29006200	-1.41516900
H	-4.64251500	7.42517400	-1.79932800
H	-3.42405200	8.11719700	-0.72669200
H	-2.94337200	7.39577600	-2.26800600
C	-3.85460200	-2.55360900	-0.38656000
C	-3.22558900	-2.16584400	-1.58519500
C	-3.50686600	-3.80594300	0.15411200
C	-2.28943300	-2.98603900	-2.21638600
H	-3.46485800	-1.20708200	-2.03996400
C	-2.57206400	-4.63357000	-0.47210500
H	-3.97557200	-4.14303900	1.07564600
C	-1.96207600	-4.22420800	-1.65990200
H	-1.81156300	-2.65030400	-3.13182700
H	-2.31257700	-5.59103900	-0.03001300

H	-1.22863400	-4.86417800	-2.14185700
C	-6.40975700	-0.82138600	-0.76097400
H	-7.14998600	-0.18495800	-0.26419700
H	-5.95895200	-0.23524200	-1.56899400
H	-6.94201300	-1.66056300	-1.22011400
H	-5.78259000	-2.27579600	1.51577400



TS₃

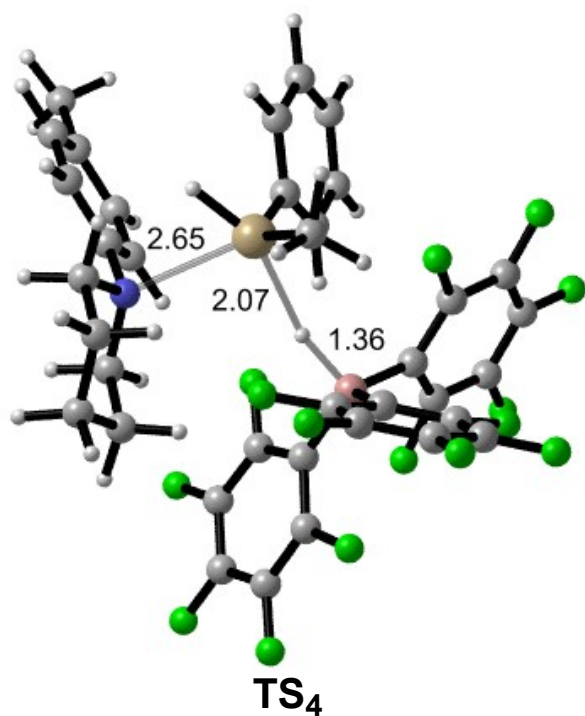
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E_{gas} = -3291.55322062 a.u.

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B	2.72713200	-0.09259300	-0.01279400
C	2.33506900	-1.51172900	-0.55661600
C	2.80248500	-1.99545000	-1.78820300
C	1.48571000	-2.37780500	0.14888300
C	2.47133000	-3.25035000	-2.28731600
C	1.11808500	-3.63024900	-0.32861200
C	1.61478000	-4.06947000	-1.55401500
C	3.01103600	0.11146600	1.51466500
C	2.66471200	1.29148300	2.19313500
C	3.62451300	-0.87670600	2.30214300
C	2.89547200	1.48279300	3.55044800
C	3.88923400	-0.71279900	3.65694800
C	3.51656300	0.47421000	4.28464700
C	2.83579000	1.11732600	-1.00799400
C	1.96376100	1.27547800	-2.09556900
C	3.81379100	2.11560100	-0.87586200
C	2.03093500	2.34543700	-2.97962500
C	3.92902500	3.18783400	-1.75380100
C	3.02746600	3.30463600	-2.81015800
F	0.96676900	-2.00610200	1.32914000
F	0.27955800	-4.40861800	0.36712300
F	1.27517900	-5.26922200	-2.02129300

F	2.95897700	-3.67369500	-3.45762300
F	3.63577700	-1.25006900	-2.53309600
F	4.01604700	-2.03644600	1.74977900
F	4.49294300	-1.67666700	4.35900000
F	3.75407700	0.64464700	5.58342800
F	2.53078900	2.61772900	4.15447400
F	2.05281600	2.29214100	1.54084300
F	0.97363500	0.38695800	-2.30630500
F	4.71450500	2.05110100	0.11761200
F	4.88960500	4.10303000	-1.59463500
F	3.11690800	4.33077600	-3.65377000
F	1.15687600	2.45841100	-3.98474700
H	-0.72940700	0.58966500	2.39401900
C	-3.19064800	-1.46003400	0.05050200
C	-2.91808000	-2.71642800	0.62581500
C	-3.85596500	-3.35633000	1.42487100
C	-5.09897900	-2.76722300	1.70503400
C	-5.36252400	-1.52532900	1.12492000
C	-4.45006900	-0.85242200	0.28833800
H	-1.94473100	-3.17072800	0.46782800
H	-3.61032700	-4.32316000	1.85943800
H	-6.33282600	-1.06830400	1.31667100
N	-2.16733700	-0.85204600	-0.72698100
C	-1.75528800	-1.55576100	-1.96589100
H	-2.20543700	-2.55240200	-1.95186600
H	-0.66567000	-1.68866300	-1.97957500
C	-2.19660900	-0.79712500	-3.24210700
H	-2.24511600	-1.50195300	-4.08036200
H	-1.44053200	-0.05041700	-3.51151100
C	-3.55576900	-0.10899800	-3.03082500
H	-4.30436000	-0.89198800	-2.84971700
H	-3.87106800	0.39796600	-3.94883300
Si	-4.96247500	0.71298300	-0.63413900
C	-5.05411000	2.20692300	0.52702800
C	-4.66117400	2.13100200	1.87581400
C	-5.50892500	3.45274000	0.05207700
C	-4.71714000	3.24785000	2.71328800
H	-4.31097800	1.18374800	2.27733800
C	-5.56618000	4.57257200	0.88223000
H	-5.82563300	3.55578400	-0.98420100
C	-5.16928700	4.47135400	2.21775900
H	-4.40899400	3.16179500	3.75194400
H	-5.92082300	5.52205300	0.48996300
H	-5.21394200	5.34130300	2.86734800
C	-6.64025200	0.48628700	-1.48064100
H	-7.42093000	0.25695000	-0.74785300
H	-6.94428300	1.39717000	-2.00807900

H	-6.61608000	-0.33100300	-2.20813900
C	-2.28415200	0.58909500	-0.95095900
H	-1.34820700	0.92388400	-1.41063200
H	-2.34636500	1.09472100	0.01931800
C	-3.51032000	0.90766300	-1.84577600
H	-3.42875800	1.93327100	-2.22588500
C	-6.10147700	-3.45288300	2.60342700
H	-6.30152800	-4.47938600	2.27502400
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H	-7.05462300	-2.91624200	2.61843300



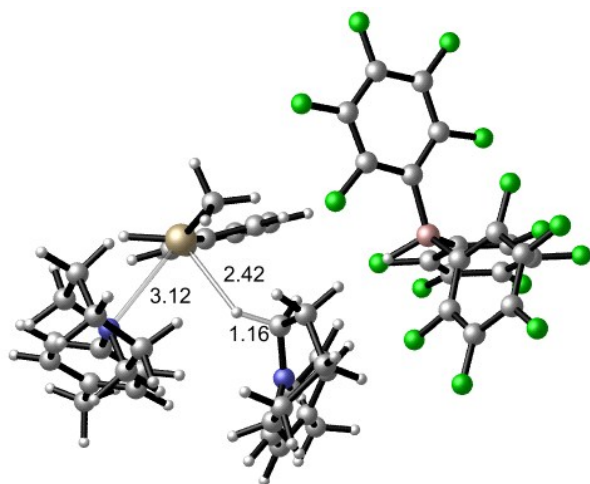
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E_{gas} = -3292.71575531 a.u.

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H	2.51746800	-0.70268200	-2.73368700
C	2.24169300	1.49151900	-1.31507600
C	3.17987100	2.02615900	-2.22251900
C	2.02149700	2.17270000	-0.10833800
C	3.83286200	3.22915600	-1.95461600
H	3.41099600	1.50007900	-3.14576200
C	2.69247700	3.36409200	0.16963700
H	1.33816500	1.76827500	0.62396400
C	3.58996600	3.90016600	-0.75522900
H	4.53930100	3.63187100	-2.67473200
H	2.51163600	3.87416400	1.11138000
H	4.10540400	4.83148300	-0.53819000
B	-1.23274100	0.17173900	0.15437500
C	-1.16019000	-0.79495300	1.46812300

C	-0.03220500	-0.81158900	2.28807800
C	-2.19730200	-1.61903300	1.91997000
C	0.11125000	-1.58972800	3.42857600
C	-2.10870500	-2.41341600	3.06518000
C	-0.94476900	-2.40554900	3.82509600
C	-2.41709900	-0.26207200	-0.88375900
C	-3.61612100	0.43966700	-1.05870300
C	-2.34161300	-1.43729100	-1.63070300
C	-4.63119700	0.02995800	-1.92355800
C	-3.31841300	-1.88641200	-2.51119000
C	-4.48346100	-1.14095000	-2.65912800
C	-1.26050800	1.76801100	0.51321300
C	-1.46485400	2.30448800	1.79003100
C	-1.14355600	2.73472000	-0.49100700
C	-1.51838000	3.67429100	2.05467300
C	-1.18948300	4.10672100	-0.27854000
C	-1.37909400	4.58472800	1.01482400
F	-3.13986400	-3.18292800	3.43782800
F	-3.37457500	-1.68167100	1.26820800
F	-0.83957000	-3.16770600	4.91888300
F	1.25568900	-1.57147700	4.13025000
F	1.03468100	-0.02788000	1.97205600
F	-1.23429200	-2.22000300	-1.52947400
F	-3.14630100	-3.01951300	-3.20928700
F	-5.44594100	-1.54516900	-3.49481400
F	-5.75321300	0.75180900	-2.04340300
F	-3.87135900	1.56466400	-0.36345300
F	-0.96087000	2.34636900	-1.77522300
F	-1.05540600	4.96615400	-1.29814000
F	-1.42587400	5.90042400	1.25161200
F	-1.71190500	4.11573700	3.30561800
F	-1.64397700	1.51173700	2.86675700
H	-0.05712100	-0.06060800	-0.49646900
C	1.39049100	-3.94885100	-2.03066800
H	0.58433500	-3.29507100	-2.37561600
H	1.58088100	-4.66802600	-2.83570600
C	2.67229100	-3.14441800	-1.82385700
H	3.49909800	-3.83025900	-1.58467700
H	2.93329400	-2.62907500	-2.74936800
C	0.07325400	-0.04425700	-3.24465900
H	-0.11840600	-1.05532300	-3.61292500
H	-0.85713600	0.43141200	-2.95423600
H	0.52834600	0.52372100	-4.06854400
N	2.58378200	-2.12921400	-0.73164800
C	3.85855200	-1.45097200	-0.50862700
C	4.02414600	-0.62899400	0.62091100
C	4.93615200	-1.56333200	-1.39725100

C	5.22431300	0.03166200	0.85081800
H	3.21125800	-0.47929200	1.31853400
C	6.13456100	-0.88505800	-1.15610800
H	4.87438600	-2.17972100	-2.28332900
C	6.30929900	-0.07986100	-0.03076600
H	5.31303000	0.65878600	1.73421500
H	6.94922400	-0.99835400	-1.86683200
C	0.96076200	-4.66024100	-0.74614800
H	1.70087400	-5.42975200	-0.48591600
H	0.00404300	-5.17249200	-0.89009400
C	7.60180700	0.65486900	0.22912500
H	8.35960600	0.40850300	-0.51955200
H	7.45129100	1.74056000	0.20747500
H	8.01087000	0.40727300	1.21505000
C	2.13858900	-2.81713000	0.53213400
H	2.01274900	-2.06648800	1.30497900
H	2.96224200	-3.47553800	0.84729200
C	0.85702700	-3.63261600	0.38207800
H	0.01439000	-2.96550700	0.19447700
H	0.66826200	-4.12307800	1.34379400



TS'4

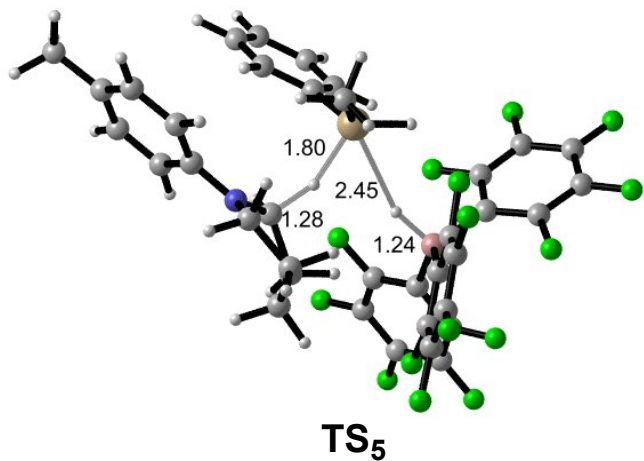
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E_{gas} = -3814.99036222 a.u.

Si	-3.26476100	-1.29828100	1.82307600
H	-4.62352100	-1.44965900	2.36773300
C	-2.57372200	0.32130200	2.31288000
C	-3.47047000	1.31397500	2.77512400
C	-1.18701500	0.59585100	2.31216700
C	-2.98894600	2.53401700	3.23794700
H	-4.54091800	1.12900100	2.76717600
C	-0.71367900	1.82030200	2.77311600

H	-0.47970900	-0.14479500	1.95550600
C	-1.61365000	2.78678700	3.23335400
H	-3.68196800	3.28956200	3.59522300
H	0.34946300	2.02735900	2.74594200
H	-1.23982300	3.74394400	3.58531900
B	2.88758400	-0.14672000	0.13001900
C	3.30361400	-1.07660500	-1.15695600
C	2.59241400	-0.98454200	-2.35521700
C	4.33885700	-2.01528600	-1.17431900
C	2.86294900	-1.75618900	-3.48306600
C	4.64667900	-2.80981200	-2.27802400
C	3.89999500	-2.68110600	-3.44508800
C	2.98253900	-0.97272300	1.54798100
C	4.05838500	-0.97385200	2.44045900
C	1.90876400	-1.75547100	1.96434900
C	4.05800900	-1.66636100	3.65193700
C	1.85202100	-2.46121000	3.16121100
C	2.94553900	-2.41901400	4.01826100
C	3.66873900	1.29747200	0.14403200
C	5.00151100	1.50842200	-0.22227400
C	2.98472800	2.46591100	0.47622400
C	5.59999400	2.76665800	-0.28132700
C	3.53034100	3.74504600	0.42330300
C	4.85706200	3.89922600	0.03964000
F	5.65272100	-3.69850000	-2.22882400
F	5.10836100	-2.19971000	-0.08339100
F	4.17494100	-3.43932100	-4.51759300
F	2.11633500	-1.62905000	-4.59943400
F	1.55218200	-0.11996600	-2.47569200
F	0.78543100	-1.84732400	1.17951500
F	0.75447200	-3.17523800	3.49252300
F	2.92620500	-3.08979700	5.17974700
F	5.12096400	-1.62058900	4.46960300
F	5.17555100	-0.27919300	2.16051700
F	1.67963300	2.41400600	0.87089500
F	2.77873000	4.82347200	0.72398900

F	5.41268300	5.11881300	-0.01912900	H	-4.19416100	-3.47531700	-1.20778400
F	6.88530100	2.90016800	-0.64618700	H	-5.26364400	-3.71568300	-2.58698400
F	5.78985300	0.46700100	-0.54923700	C	-0.72711600	2.13554100	-1.23632900
H	-2.54628400	-0.93620400	-0.45883200	C	-1.77041600	1.59461400	-2.01577100
C	-6.13620900	-3.91447300	0.75947600	C	-2.62162200	2.49129900	-2.68767100
H	-5.14211700	-3.99048000	1.21786300	C	-2.43919500	3.87090500	-2.57063100
H	-6.80805000	-4.53795100	1.35977900	C	-1.41857900	4.41128000	-1.78397400
C	-6.62291800	-2.46536600	0.83473200	C	-0.56824700	3.51039500	-1.12216300
H	-7.67492100	-2.42190800	0.50258100	H	-0.00223400	1.49194100	-0.75282100
H	-6.60222000	-2.11940000	1.87224300	H	-3.43595700	2.12410500	-3.30152200
C	-2.25307700	-2.86274300	1.83294700	H	-3.11133400	4.53582000	-3.10806600
H	-2.62983900	-3.59543200	1.11508600	H	0.25345500	3.88503100	-0.51849400
H	-1.19246300	-2.68750600	1.64936400	C	-0.98842700	-2.05343600	-1.57825800
H	-2.35906900	-3.29644700	2.83687200	H	-1.54978000	-2.88534200	-1.13697300
N	-5.79566900	-1.55303000	0.02365700	H	0.02899100	-2.11797700	-1.18686700
C	-6.12649400	-0.15807400	0.16655200	C	-1.61162100	-0.71001200	-1.10989200
C	-5.30430000	0.80799200	-0.44298100	H	-0.94428100	-0.21398800	-0.40915000
C	-7.21238900	0.29737400	0.92701500	C	-2.61906700	-0.28880600	-3.36507100
C	-5.56799800	2.16545700	-0.30861100	H	-2.23955200	0.30107800	-4.20612100
H	-4.43177600	0.49946500	-1.00807800	H	-3.70319100	-0.09380100	-3.31147300
C	-7.46170800	1.66791300	1.06332900	C	-2.36857200	-1.78295400	-3.63099400
H	-7.88410000	-0.39744300	1.41526700	H	-2.46393300	-1.96124900	-4.70696600
C	-6.65759800	2.62797800	0.44682800	H	-3.13908100	-2.39371400	-3.14524800
H	-4.89802400	2.87480200	-0.78743400	C	-0.99598400	-2.19726500	-3.10404900
H	-8.31253500	1.98596500	1.66088900	H	-0.21586400	-1.56991200	-3.54375700
C	-6.07622400	-4.40873100	-0.68870400	H	-0.77024100	-3.23250500	-3.38006700
H	-7.09405200	-4.46603200	-1.09787200	N	-1.92872000	0.19823500	-2.16651800
H	-5.65878100	-5.42005600	-0.73740700	H	1.71562200	0.11238600	-0.00989000
C	-6.94292500	4.10505500	0.57592000	C	-1.21778600	5.90182900	-1.65793100
H	-6.03884300	4.66603400	0.83583500	H	-1.95951000	6.45702400	-2.23926300
H	-7.31716300	4.52135700	-0.36713600	H	-1.29503200	6.22988500	-0.61460400
H	-7.69567500	4.30199800	1.34428900	H	-0.22403000	6.20084100	-2.01059100
C	-5.75579100	-2.00018000	-1.39181200				
H	-5.11878300	-1.31815000	-1.95539200				
H	-6.76838200	-1.92556300	-1.82499300				
C	-5.24331300	-3.43521100	-1.52801100				



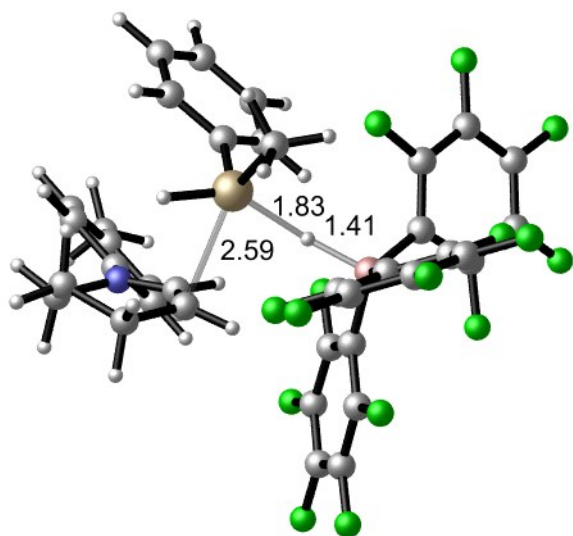
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C	-5.30202900	0.18587500	1.29326400
C	-6.60984500	-0.27105400	1.18181000
C	-7.45704200	0.16574900	0.15133000
C	-6.93439000	1.08158800	-0.76722400
C	-5.61992000	1.54254100	-0.67497100
H	-4.69419800	-0.14630300	2.12841200
H	-6.98693100	-0.96890000	1.92497500
H	-7.56185900	1.44472300	-1.57699000
H	-5.25768500	2.24881500	-1.41320900
N	-3.44675700	1.57247400	0.47867500
C	-2.40651400	0.73902200	0.87189200
H	-2.77438200	-0.21158500	1.25143100
C	-1.32588700	1.37108100	1.76271500
H	-0.34116200	1.08406700	1.39914000
H	-1.42672800	0.92565000	2.75777000
C	-1.43998700	2.89862700	1.82419000
H	-0.49858600	3.31613500	2.19157500
H	-2.22645400	3.19906000	2.52784300
C	-1.76871100	3.42568100	0.42788500
H	-1.00250900	3.08480000	-0.27671200
H	-1.76537000	4.51921300	0.39053800
C	-3.15436600	2.93481800	-0.00967400
H	-3.93698500	3.58802600	0.39168000
H	-3.23174900	2.97038100	-1.10458200
B	1.61434800	0.05840100	0.02278600
C	1.91881800	-0.44490900	1.54769500
C	3.18077700	-0.28921300	2.12627300
C	1.01110800	-1.16967600	2.31813800
C	3.52307800	-0.78142600	3.38169200
C	1.30474000	-1.68225400	3.58125700
C	2.57255700	-1.48686800	4.11689200
C	1.72933700	1.66675900	-0.27861800

C	1.43978900	2.14009200	-1.56300400
C	2.01544700	2.67963300	0.63925400
C	1.46504300	3.47812100	-1.94029400
C	2.05334400	4.03742500	0.31320600
C	1.78625500	4.44292400	-0.98859500
C	2.48602700	-0.88945700	-0.99155500
C	2.17890200	-2.24860000	-1.09161800
C	3.58305800	-0.49425200	-1.76184500
C	2.85472500	-3.15294000	-1.90478400
C	4.29612500	-1.36203700	-2.58900500
C	3.92995800	-2.70232900	-2.66359300
F	-0.25039800	-1.41369900	1.86733100
F	0.37860300	-2.36163500	4.28013300
F	2.87709800	-1.97051600	5.32905400
F	4.74993100	-0.59152900	3.88974600
F	4.13774500	0.37526600	1.44753100
F	2.22304900	2.39873900	1.94477000
F	2.32017500	4.95505600	1.25585000
F	1.80997000	5.74137500	-1.31836700
F	1.17378500	3.84630100	-3.19884000
F	1.07992000	1.25989900	-2.53453900
F	1.15501600	-2.76066300	-0.35575700
F	4.01473900	0.78261900	-1.74144700
F	5.33632800	-0.91828600	-3.31032700
F	4.60371300	-3.54775400	-3.45484000
F	2.48425400	-4.44333500	-1.95778200
H	0.42413200	-0.20154900	-0.20994000
C	-8.88779500	-0.30793800	0.06548900
H	-9.30440500	-0.14408400	-0.93216500
H	-8.97211100	-1.37439500	0.29738500
H	-9.52537300	0.22801600	0.77936000
Si	-1.51418100	-0.77359600	-1.58698000
H	-1.77615200	0.26928900	-0.14205200
H	-0.20015600	-1.24385500	-2.03901500
C	-2.59296300	-2.21972300	-1.14354400
C	-1.98321800	-3.45703600	-0.84627900
C	-4.00066900	-2.15126000	-1.16994400
C	-2.76011800	-4.58606900	-0.58690500
H	-0.90148800	-3.53627300	-0.81993700
C	-4.77310100	-3.28248700	-0.91574200
H	-4.50224200	-1.21404800	-1.39426600
C	-4.15297600	-4.50012000	-0.62132200
H	-2.27693200	-5.53147200	-0.35939500
H	-5.85642700	-3.21443000	-0.94618600
H	-4.75626300	-5.38092300	-0.42017200
C	-2.23726000	0.50178200	-2.75928200
H	-1.54916300	1.34488400	-2.86444800

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H	-3.22180900	0.86219500	-2.45429600



TS₆

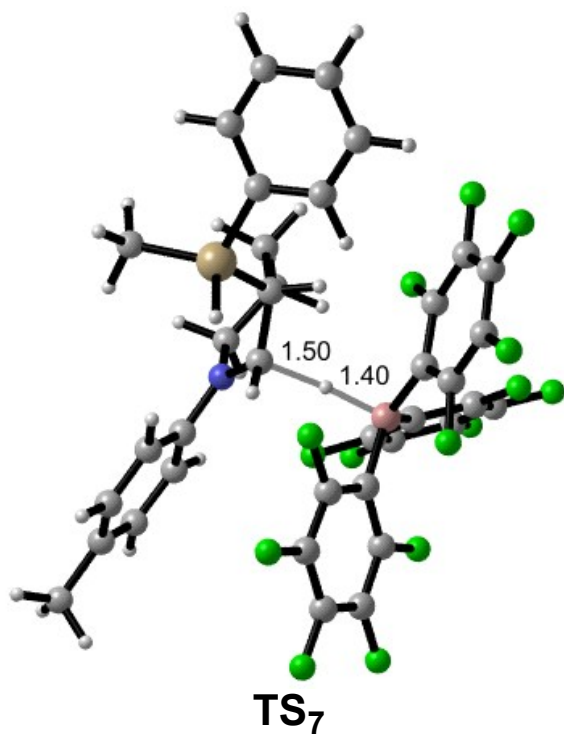
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C	1.57095300	0.75475600	-2.44451400
C	2.38396000	0.71946500	-3.59409700
C	1.78688300	1.78785500	-1.51734600
C	3.36330400	1.68915900	-3.81732600
H	2.25270900	-0.07179700	-4.32919600
C	2.77153300	2.75273300	-1.73309500
H	1.19428200	1.83653700	-0.61133600
C	3.55918000	2.70856300	-2.88475800
H	3.97225200	1.64603700	-4.71626900
H	2.92255600	3.54065700	-1.00070400
H	4.32284000	3.46270900	-3.05282500
B	-1.56315200	0.10180200	0.22336000
C	-0.96339800	-0.70798200	1.50390300
C	0.26347600	-0.33337300	2.06147100
C	-1.58590800	-1.77220100	2.16812100
C	0.86810800	-0.96983100	3.13653300
C	-1.02525700	-2.43139700	3.26425600
C	0.21501800	-2.03513700	3.74995200
C	-2.90889800	-0.51657000	-0.43628300
C	-4.14994500	0.12979000	-0.46416600
C	-2.91572300	-1.78784100	-1.01587000
C	-5.29479200	-0.43030700	-1.03429700
C	-4.02281900	-2.38323400	-1.60393600
C	-5.23294500	-1.69388800	-1.60975800
C	-1.60184500	1.71045700	0.47368800

C	-1.87040000	2.24957900	1.73852400
C	-1.46069500	2.66688500	-0.53273300
C	-1.95191000	3.61539500	1.99740100
C	-1.52616800	4.04234000	-0.32226200
C	-1.77473100	4.52300300	0.95823800
F	-1.67457500	-3.44546100	3.84918400
F	-2.79527700	-2.22220200	1.78857100
F	0.77391700	-2.66575800	4.78677500
F	2.08013600	-0.58208800	3.57232400
F	0.96698400	0.69088500	1.51331900
F	-1.76463400	-2.51108900	-1.04441500
F	-3.93796900	-3.60029200	-2.15943700
F	-6.31900600	-2.24140100	-2.16355500
F	-6.45369000	0.24055500	-1.02556200
F	-4.31478900	1.34860900	0.08306400
F	-1.23932800	2.28154200	-1.80967000
F	-1.36228400	4.89816600	-1.34035800
F	-1.84641300	5.83861200	1.18720300
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F	-2.09655000	1.44152200	2.79522900
H	-0.58559500	-0.14270600	-0.75742100
C	1.26011500	-2.27515000	-0.61591100
H	0.36957400	-2.14682400	-0.01565200
C	2.75695500	-3.57822000	-2.14477400
H	2.64380600	-2.92182100	-3.01430100
H	2.99221800	-4.57880300	-2.52214700
C	3.93290900	-3.08367300	-1.30168500
H	4.17853000	-3.81285300	-0.51680300
H	4.82515400	-2.96275300	-1.91853300
C	2.36371600	-1.52337300	-0.27064200
H	2.25271300	-0.61709200	0.31000400
C	-1.29054200	-0.27139200	-3.35412500
H	-1.84853700	-1.19822900	-3.51087600
H	-1.96008500	0.50576000	-2.99435500
H	-0.89321800	0.03409200	-4.33207100
N	3.63449800	-1.79145300	-0.65336100
C	4.72196200	-0.98318400	-0.19378500
C	4.77608400	-0.54398700	1.13496600
C	5.74883900	-0.62133200	-1.07428100
C	5.83777900	0.25162500	1.56300900
H	3.99459200	-0.81758400	1.83670400
C	6.81148200	0.15897400	-0.62679800
H	5.69999600	-0.91989800	-2.11652700
C	6.87941600	0.60999100	0.69867000
H	5.85963200	0.58755000	2.59642400
H	7.59493000	0.43692600	-1.32722500
C	1.44935500	-3.58914900	-1.34000800

H	1.46281100	-4.41168600	-0.61048200
H	0.60262900	-3.78903000	-2.00547800
C	8.04836300	1.43434400	1.18253200
H	8.86519100	0.79365300	1.53792100
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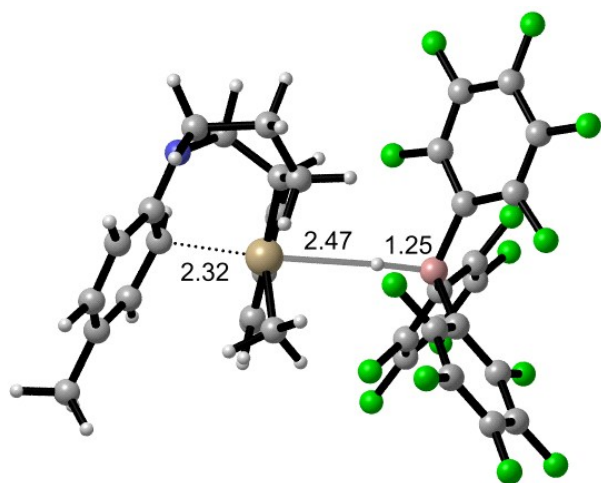
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E_{gas} = -3291.54794388 a.u.

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C	4.33699300	-3.09919200	-1.70285500
C	4.23406100	-4.13005600	-0.76187900
C	2.97474200	-4.36217300	-0.19240300
C	1.86714100	-3.59762200	-0.54534900
H	3.37984000	-1.50497500	-2.76041800
H	5.29825200	-2.89251700	-2.16593200
H	2.85069900	-5.16776300	0.52655200
H	0.90103700	-3.83404600	-0.11096800
N	0.83323300	-1.78795200	-1.83470600
C	-1.75161100	-1.03715200	-2.79450200
H	-2.62133400	-0.38664700	-2.91517100
H	-1.96226200	-1.95499400	-3.35800400
C	-0.50309700	-0.38083400	-3.38959000
H	-0.32892900	0.58333800	-2.90382500
H	-0.63405600	-0.18401800	-4.45878000

C	0.72078600	-1.27907600	-3.21744400
H	0.67588000	-2.14262100	-3.89288500
H	1.62275500	-0.71222100	-3.45882200
C	-0.08466600	-1.42469000	-0.89970300
H	0.11396500	-1.84842600	0.07605600
C	-1.53925600	-1.34491500	-1.29115900
H	-1.99863900	-0.56053600	-0.68551500
Si	-2.49699400	-2.91578400	-0.68732000
H	-1.95101900	-3.23801000	0.66147200
C	-4.30447400	-2.41928900	-0.53752100
C	-4.66288700	-1.39925000	0.36490500
C	-5.32269400	-2.98872000	-1.32131900
C	-5.97832100	-0.94901500	0.46933900
H	-3.90428800	-0.94382800	0.99748200
C	-6.64522200	-2.55176100	-1.21246700
H	-5.08808200	-3.78194500	-2.02692400
C	-6.97328000	-1.52821700	-0.32217700
H	-6.21924100	-0.14359900	1.15713500
H	-7.41750000	-3.00678100	-1.82646000
H	-7.99997200	-1.18181900	-0.24525500
C	-2.24046100	-4.39884400	-1.82561000
H	-2.64615100	-4.23205800	-2.82842100
H	-1.17576200	-4.63227300	-1.93159300
H	-2.73286700	-5.28481100	-1.41110500
B	0.43579900	1.06572700	0.43572200
C	-1.06563700	1.41808700	0.94237600
C	-1.49362600	1.43977400	2.27610000
C	-2.06711200	1.74957900	0.01915000
C	-2.80661900	1.71664100	2.66096300
C	-3.38660900	2.03167100	0.35429500
C	-3.76220400	2.00753100	1.69392600
C	1.06371900	2.15002300	-0.59599900
C	2.05778200	1.79426900	-1.50807400
C	0.70448400	3.50129600	-0.64064300
C	2.63076200	2.66306700	-2.42857000
C	1.25760900	4.41543900	-1.53740700
C	2.22491600	3.99425700	-2.44370000
C	1.47006800	0.46245300	1.53072300
C	1.15942800	-0.68258500	2.27280600
C	2.73594300	0.99212200	1.80731300
C	2.01271400	-1.28732500	3.18576200
C	3.62615000	0.42506200	2.72085400
C	3.26614500	-0.72448000	3.41292300
F	-1.77474700	1.79205900	-1.30405500
F	-4.29351700	2.30925900	-0.59185800
F	-5.03404900	2.24274100	2.04297400
F	-3.15084600	1.70925200	3.95514400

F	-0.63734900	1.20664400	3.28724700
F	-0.20723800	4.00221000	0.21573100
F	0.86562600	5.69660700	-1.53108700
F	2.75950200	4.85567900	-3.31583100
F	3.56507800	2.22992600	-3.29025700
F	2.52227400	0.52064600	-1.52035100
F	-0.05377500	-1.27497300	2.11362400
F	3.16993900	2.11507700	1.20302700
F	4.82504500	0.98355600	2.93576800
F	4.10953400	-1.28370600	4.28724700
F	1.64327400	-2.39290300	3.84829800
H	0.21186400	-0.05291100	-0.38029500
C	5.43618800	-4.94873500	-0.35844500
H	5.15954200	-5.98384400	-0.13594100
H	6.19494500	-4.96147900	-1.14601900
H	5.90752000	-4.53829200	0.54322100



TS₈

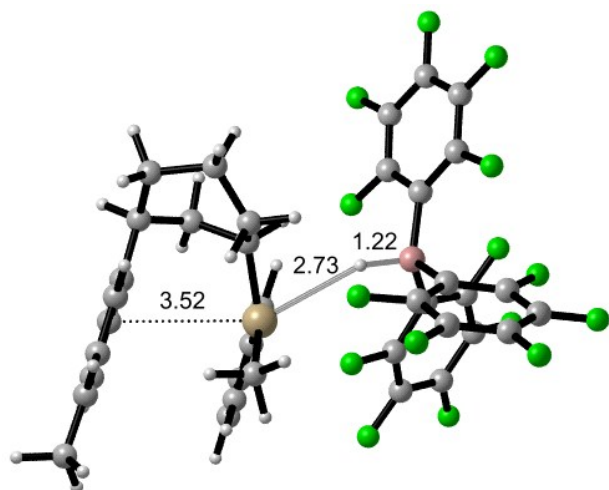
G_{gas} = -3291.072351 a.u.

E_{gas} = -3291.53666076 a.u.

C	4.95019300	-1.07137500	-0.45234700
C	4.58612200	0.32565900	-0.42166200
C	5.14135100	1.18016300	0.58244300
C	5.90590500	0.69786300	1.62053500
C	6.20227700	-0.69274000	1.60036400
C	5.75890500	-1.54977800	0.61495500
H	4.37040800	0.81313800	-1.36783100
H	4.91817100	2.24153900	0.51474900
H	6.82469400	-1.10253500	2.39278200
H	6.07210600	-2.58546300	0.64749600
N	4.49148000	-1.86473200	-1.46515700
C	2.00811100	-2.62254500	-0.60870300
H	0.95524700	-2.90492200	-0.57006700
H	2.32946800	-2.55309000	0.43611900

C	2.84439200	-3.72134900	-1.28444300
H	2.47687400	-3.91140300	-2.29836200
H	2.73735900	-4.66444900	-0.73962600
C	4.34535100	-3.33219100	-1.31768000
H	4.82592000	-3.64724700	-0.39284900
H	4.86547800	-3.82744900	-2.14504900
C	2.15277400	-1.24328200	-1.33704600
H	1.27370700	-1.04347000	-1.95349800
Si	2.29107500	0.22386100	-0.12883200
C	1.95202400	1.91992100	-0.82798300
C	1.60438500	2.11008900	-2.17916400
C	2.08491200	3.05813100	-0.00850000
C	1.40456300	3.39193800	-2.69223800
H	1.45365100	1.25755300	-2.83326000
C	1.88074200	4.33918400	-0.51965600
H	2.32274600	2.94661500	1.04551700
C	1.54378900	4.50728500	-1.86448700
H	1.12424900	3.51767400	-3.73382600
H	1.96464500	5.20171100	0.13395100
H	1.37740000	5.50401200	-2.26239500
C	2.15654800	0.00031800	1.72463800
H	3.11930400	0.12354000	2.22649500
H	1.44941800	0.73913400	2.10847700
H	1.75068100	-0.98511400	1.95628900
C	3.39280100	-1.31626300	-2.26668000
H	3.66569900	-0.35815600	-2.71277900
H	3.21846700	-1.99499000	-3.10394600
B	-1.39440500	-0.13819500	0.16024200
C	-1.84559900	1.41030100	-0.12865900
C	-2.77404700	1.84417700	-1.07727500
C	-1.26228500	2.44393900	0.60628000
C	-3.07648300	3.18739900	-1.30599500
C	-1.52451400	3.79504400	0.41403800
C	-2.44447900	4.17352900	-0.55804500
C	-1.73798800	-0.61684800	1.69094400
C	-1.03190000	-1.65393600	2.29912800
C	-2.73934100	-0.06759100	2.49667200
C	-1.24041900	-2.09890900	3.60025300
C	-2.99276900	-0.47837700	3.80552800
C	-2.23661300	-1.50218100	4.36547200
C	-1.90001800	-1.21062900	-0.97650100
C	-1.42472300	-1.12763600	-2.28654900
C	-2.78725700	-2.27099000	-0.76898700
C	-1.74402400	-2.01414100	-3.30781800
C	-3.14709900	-3.18621200	-1.76108800
C	-2.62168600	-3.06068700	-3.04130000
F	-0.36451300	2.15027300	1.58522400

F	-0.89314600	4.73253300	1.14462700	H	0.66146900	-2.53939200	-0.75895300
F	-2.71408300	5.47051000	-0.77082400	H	2.32416200	-2.69741400	-0.24236900
F	-3.97338100	3.53590100	-2.24284300	C	2.03340300	-3.19994000	-2.31662100
F	-3.45151000	0.96084300	-1.84166600	H	1.37261200	-2.89255900	-3.13646400
F	-3.54088300	0.91141600	2.02909900	H	1.80604500	-4.25435300	-2.12735800
F	-3.96497800	0.09990200	4.52760900	C	3.51312300	-3.04681000	-2.75265600
F	-2.46420900	-1.90946400	5.62233500	H	4.12200300	-3.85662200	-2.34097800
F	-0.49880800	-3.09500400	4.11663300	H	3.57293500	-3.16445400	-3.83994700
F	-0.05445500	-2.30575400	1.60711200	C	1.89443100	-0.85120600	-1.35832700
F	-0.57621400	-0.11624300	-2.62915800	H	0.96645000	-0.44866500	-1.77583700
F	-3.36485400	-2.47136400	0.43304900	Si	2.19177600	0.17583800	0.19212300
F	-3.99873200	-4.18661100	-1.48834700	C	2.58973200	1.95523700	-0.10255300
F	-2.95051900	-3.93374300	-4.00401200	C	2.09056100	2.62927300	-1.23743000
F	-1.22041500	-1.86970100	-4.53844500	C	3.38305400	2.67394500	0.81474500
H	-0.14465200	-0.12809100	0.07069500	C	2.38541900	3.97534500	-1.44781200
C	6.44947300	1.58170400	2.71585000	H	1.45183200	2.11209300	-1.94674900
H	6.05676900	1.28934300	3.69651900	C	3.68613700	4.01540600	0.59490400
H	7.54183600	1.51839400	2.77445800	H	3.76963600	2.18351700	1.70353000
H	6.18303200	2.62841700	2.54919800	C	3.18665700	4.66631900	-0.53601700



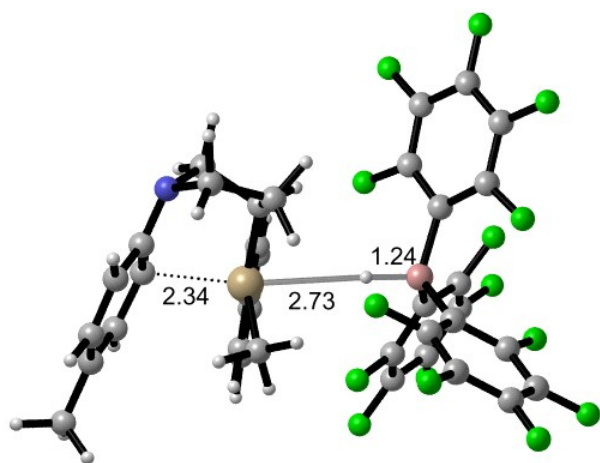
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G_{gas} = -3275.024356 a.u.

E_{gas} = -3275.49801867 a.u.

C	4.91818800	-1.59052600	-1.07735500	C	0.66146900	-2.53939200	-0.75895300
C	5.54079100	-0.37492900	-0.73415700	C	2.32416200	-2.69741400	-0.24236900
C	6.30515800	-0.24364500	0.42572400	C	2.03340300	-3.19994000	-2.31662100
C	6.49090100	-1.32452700	1.29741400	H	1.37261200	-2.89255900	-3.13646400
C	5.87431000	-2.53645800	0.95978600	H	1.80604500	-4.25435300	-2.12735800
C	5.10753500	-2.66795800	-0.20025100	C	3.51312300	-3.04681000	-2.75265600
H	5.45084800	0.48079000	-1.39827900	H	4.12200300	-3.85662200	-2.34097800
H	6.77359700	0.71196900	0.64876500	H	3.57293500	-3.16445400	-3.83994700
H	5.99536100	-3.39686900	1.61353500	C	1.89443100	-0.85120600	-1.35832700
H	4.65437200	-3.63039800	-0.40973200	H	0.96645000	-0.44866500	-1.77583700
C	1.69202500	-2.36594700	-1.07339900	Si	2.19177600	0.17583800	0.19212300
				C	2.58973200	1.95523700	-0.10255300
				C	2.09056100	2.62927300	-1.23743000
				C	3.38305400	2.67394500	0.81474500
				C	2.38541900	3.97534500	-1.44781200
				H	1.45183200	2.11209300	-1.94674900
				C	3.68613700	4.01540600	0.59490400
				H	3.76963600	2.18351700	1.70353000
				C	3.18665700	4.66631900	-0.53601700
				H	1.98658900	4.48506300	-2.31945500
				H	4.30191200	4.55580800	1.30738200
				H	3.41588000	5.71484300	-0.70235700
				C	2.67244400	-0.62286000	1.79674700
				H	3.62893500	-1.14395800	1.68940300
				H	2.74480100	0.11182300	2.60117800
				H	1.90536400	-1.35658500	2.06240600
				C	3.00605000	-0.60579900	-2.43613800
				H	3.42211800	0.40254100	-2.36588500
				H	2.53217000	-0.65874100	-3.42339100
				B	-1.62676900	-0.21541400	0.08443700
				C	-2.30675000	-0.46889300	-1.38140900
				C	-3.38278700	-1.30837200	-1.67940300
				C	-1.76842000	0.17776800	-2.49582800
				C	-3.88190700	-1.49344900	-2.97038400
				C	-2.22426900	0.02650800	-3.80003700
				C	-3.30267600	-0.82002400	-4.03980600
				C	-1.63857600	1.36815200	0.51674100
				C	-0.58188400	1.86996700	1.26150700
				C	-2.62520700	2.31522300	0.22955900
				C	-0.44513200	3.17796200	1.70755500
				C	-2.55266400	3.64309400	0.65348700
				C	-1.45918500	4.07921400	1.39933700
				C	-2.18736200	-1.11129500	1.33350900
				C	-1.42038800	-2.07972200	1.97797800
				C	-3.45197300	-0.91162500	1.89412300
				C	-1.85091200	-2.80570800	3.08774600
				C	-3.93124200	-1.61130400	2.99744900

C	-3.12032300	-2.56929100	3.60176200	H	6.60901900	-2.66299300	1.94317700
F	-0.70062600	1.01602900	-2.33390300	H	5.45408100	-3.65542900	0.04967100
F	-1.64018400	0.68034200	-4.81874300	N	4.10821800	-2.33330700	-1.86163700
F	-3.76825800	-0.98908100	-5.28491400	C	2.06110000	-1.23260400	-1.61753800
F	-4.91738100	-2.31749300	-3.18879900	H	1.19203300	-0.77002400	-2.08670100
F	-4.00477700	-2.01068100	-0.71171200	Si	2.54972700	-0.11521200	-0.15279900
F	-3.70309200	1.97873000	-0.49759300	C	2.45622900	1.71643300	-0.46517600
F	-3.52666100	4.51099000	0.34999500	C	2.10757400	2.22800300	-1.73053000
F	-1.38084000	5.35189200	1.80931600	C	2.76262200	2.62930700	0.56334600
F	0.62851700	3.57072000	2.41201600	C	2.07088100	3.60341500	-1.95802400
F	0.46383100	1.01472000	1.59506300	H	1.82914100	1.55857600	-2.53754700
F	-0.16151100	-2.37451600	1.54494600	C	2.72194000	4.00375200	0.33677600
F	-4.28058900	0.00280700	1.35201400	H	3.01329700	2.26975700	1.55690200
F	-5.15774500	-1.37479300	3.48644500	C	2.37844300	4.49181800	-0.92602800
F	-3.55863800	-3.25367800	4.66711500	H	1.78600400	3.98035100	-2.93562700
F	-1.05376300	-3.72370900	3.66093600	H	2.93822100	4.69177300	1.14780600
H	-0.44452600	-0.49946000	-0.04549800	H	2.33853100	5.56284900	-1.10134500
C	7.35141900	-1.19997900	2.53193800	C	2.45171900	-0.71514500	1.61352100
H	8.39241700	-1.46897100	2.31409900	H	3.36228800	-1.23682500	1.91912000
H	7.35535100	-0.17619200	2.91752600	H	2.28218700	0.13166600	2.28147800
H	7.00616000	-1.86314800	3.33056000	H	1.60078500	-1.38994000	1.72032700
C	4.12613500	-1.66826900	-2.38715100	C	3.24326300	-1.40195200	-2.60442600
H	4.84106900	-1.40509900	-3.17835600	H	3.76584100	-0.49703100	-2.91152500



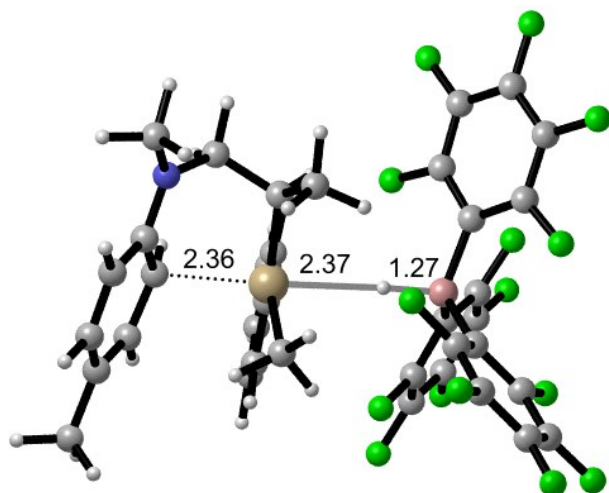
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G_{gas} = -3251.77934 a.u.

E_{gas} = -3252.21494123 a.u.

C	4.79790000	-1.77234300	-0.80193400	C	-3.03153300	-1.63130400	-1.44364400
C	4.83255400	-0.35097800	-0.59769000	C	-1.85725200	-0.71361500	-3.76307600
C	5.58169900	0.19568700	0.48727700	C	-3.47867000	-2.10284600	-2.68010900
C	6.19307800	-0.60242400	1.43190900	C	-2.89001300	-1.64173100	-3.85146700
C	6.11273700	-2.00603000	1.23258200	F	0.21640400	1.44811700	1.93285700
C	5.44535200	-2.57805300	0.16704000	F	0.14834100	4.09991200	2.28106700
H	4.67707200	0.31314000	-1.44108000	F	-1.65613700	5.63557300	0.89582100
H	5.64693500	1.27761900	0.56168700	F	-3.38107200	4.43322600	-0.85548300

F	-3.32438100	1.79251400	-1.22797200
F	-3.83964000	0.47883500	1.68023700
F	-4.68220800	-0.76661200	3.89036100
F	-3.31000300	-2.91423900	4.88584900
F	-1.04841200	-3.78372600	3.59901900
F	-0.18113200	-2.55911200	1.39984300
F	-0.43913700	0.63882700	-2.50207700
F	-3.67292700	-2.13944500	-0.37142300
F	-4.47503200	-2.99942900	-2.74750100
F	-3.30304300	-2.08819500	-5.04653000
F	-1.26327200	-0.25589900	-4.88028800
H	-0.16159600	-0.35331200	0.05974800
C	6.94747000	-0.03707400	2.60938600
H	6.48505500	-0.33544300	3.55716100
H	7.98233700	-0.39620100	2.62829700
H	6.97130100	1.05497500	2.57878400
C	3.16395000	-3.43899900	-1.52550200
H	3.52470700	-4.01796100	-0.67777100
H	3.09898800	-4.10622100	-2.38832900
C	1.80049500	-2.72434000	-1.24233900
H	1.01074500	-3.13129800	-1.88012000
H	1.46915300	-2.86354000	-0.21373800



TS''₈

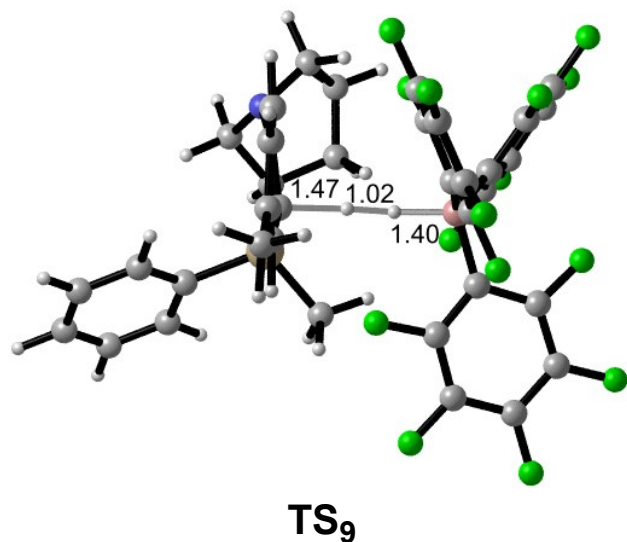
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E_{gas} = -3253.43695488 a.u.

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C	4.61298200	-0.02447000	-0.35850800
C	5.14409000	0.87397600	0.61277400
C	5.86669500	0.43767900	1.70431100
C	6.12287200	-0.95646300	1.78699900
C	5.69324500	-1.86088300	0.83611800
H	4.40079500	0.39816500	-1.33648100
H	4.94026700	1.93300200	0.48237700

H	6.68595500	-1.33307900	2.63813200
H	5.93039700	-2.91039200	0.95764400
N	4.52872400	-2.26357100	-1.27164100
C	2.12615500	-1.52241200	-1.33899200
H	1.39517800	-1.17834900	-2.07779100
Si	2.26569700	-0.06538300	-0.11125900
C	2.07623700	1.65485600	-0.81201000
C	1.81797400	1.87610300	-2.17822800
C	2.25846200	2.77702000	0.02011700
C	1.75160400	3.17111900	-2.69321900
H	1.63809900	1.04054200	-2.84652500
C	2.18890000	4.07148600	-0.49332600
H	2.43102700	2.64435200	1.08398300
C	1.93843900	4.26980400	-1.85289100
H	1.53957200	3.32100300	-3.74768600
H	2.30896300	4.92259700	0.16949600
H	1.87708900	5.27758800	-2.25300400
C	2.14074500	-0.30481400	1.74011800
H	3.11284000	-0.22060100	2.23183300
H	1.46396000	0.45235100	2.14322000
H	1.70441600	-1.27992300	1.96050200
C	3.42741200	-1.81905900	-2.13071000
H	3.74013600	-0.94714000	-2.71818100
H	3.23129400	-2.61884500	-2.84928400
B	-1.35523000	-0.13624900	0.11759300
C	-1.65811000	1.43584900	-0.22770800
C	-2.49804100	1.92327500	-1.23139800
C	-1.04709200	2.43349300	0.53383400
C	-2.69321600	3.28172600	-1.48418800
C	-1.20592700	3.79747800	0.32079500
C	-2.03967700	4.22905800	-0.70521300
C	-1.81787400	-0.52184200	1.64544400
C	-1.23299000	-1.56965100	2.35605800
C	-2.83608300	0.13203500	2.34716200
C	-1.56359600	-1.92733900	3.65911900
C	-3.20904000	-0.18792300	3.65255400
C	-2.56605600	-1.22500400	4.31868500
C	-1.89105100	-1.19887200	-1.01279300
C	-1.38254700	-1.15976500	-2.31285200
C	-2.82776700	-2.21641900	-0.80774800
C	-1.71850100	-2.04779200	-3.32655100
C	-3.20651800	-3.13069400	-1.79409700
C	-2.64771800	-3.05012300	-3.06339900
F	-0.22846800	2.08689200	1.56332500
F	-0.55434100	4.69600400	1.08151700
F	-2.20632000	5.53910600	-0.94024900
F	-3.50856500	3.68205000	-2.47309200

F	-3.19331500	1.08225100	-2.02633000	H	-0.90505300	0.19518100	-0.24713100
F	-3.54013800	1.12953400	1.77336800	H	-2.44984500	1.75099900	1.31698300
F	-4.18901000	0.49079600	4.26846300	H	-1.28682800	3.99687400	-2.13023400
F	-2.90912500	-1.54647700	5.57368800	H	-1.54934800	2.02550800	-3.55834200
F	-0.93462500	-2.94271400	4.27570500	N	-2.52971200	-0.29672300	-2.83812100
F	-0.26767000	-2.33329500	1.77232300	C	-1.64549800	-2.60271700	-1.69666000
F	-0.48133300	-0.19433300	-2.64977400	H	-1.48585400	-3.63948900	-1.38640900
F	-3.43885100	-2.37412100	0.38376400	H	-0.89943500	-2.01946800	-1.15216600
F	-4.10750700	-4.08743900	-1.52470400	C	-1.35248800	-2.44893600	-3.20333900
F	-2.99399100	-3.92309800	-4.01943900	H	-2.02634700	-3.09253100	-3.78051400
F	-1.16167800	-1.94757100	-4.54652400	H	-0.33618500	-2.78961600	-3.42746800
H	-0.09228600	-0.23476000	0.08122400	C	-1.50408800	-0.97142900	-3.66486100
C	6.38862700	1.37809300	2.76304500	H	-0.56286200	-0.43340600	-3.54424300
H	5.95705700	1.15404700	3.74540700	H	-1.78467400	-0.93058000	-4.72512700
H	7.47697800	1.30063300	2.86429500	C	-3.08829600	-2.13581400	-1.31580500
H	6.14829100	2.41700200	2.52345000	H	-3.75925900	-2.99572700	-1.20008700
C	4.88445300	-3.67901900	-1.23913000	Si	-3.16541400	-0.98460900	0.20628200
H	4.38465100	-4.22340200	-0.42733000	C	-4.96785400	-0.56093500	0.59903700
H	4.59486400	-4.13539100	-2.18602000	C	-5.75808700	-1.48607300	1.30982700
H	5.96628200	-3.79571500	-1.12707700	C	-5.58231000	0.63790000	0.19230200
C	1.58688500	-2.81024500	-0.68774800	C	-7.09929600	-1.22983800	1.59619400
H	0.59324100	-2.66004600	-0.26948600	H	-5.32458300	-2.42377900	1.65064100
H	1.52144800	-3.61064800	-1.43480900	C	-6.92381200	0.90177500	0.47761400
H	2.23219000	-3.16542700	0.12296700	H	-5.00586300	1.38435900	-0.34834900

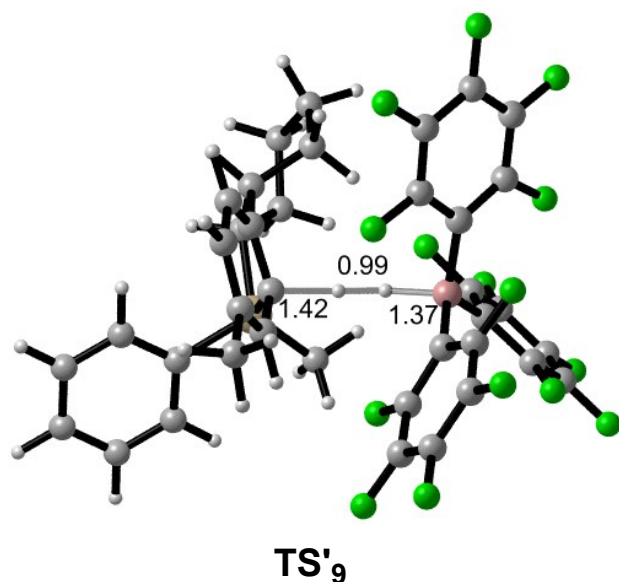


G_{gas} = -3291.052103 a.u.

E_{gas} = -3291.50872757 a.u.

C	-2.18132400	0.72034900	-1.96249500	C	2.97648500	-3.52679400	-1.99367600
C	-2.29255400	0.58249500	-0.51608900	C	1.54234900	-0.20387400	1.85323200
C	-2.25198500	1.80715000	0.25150300	C	0.57994200	0.21916600	2.76722100
C	-1.89749300	3.02373600	-0.29417000	C	2.65483600	-0.82372200	2.43191600
C	-1.59167000	3.05558400	-1.67884100	C	0.66064800	0.01347200	4.14033500
C	-1.71623300	1.94274400	-2.48935300	C	2.78891200	-1.04067700	3.80195900

C	1.77995400	-0.62428800	4.66514300
C	1.78637300	1.51350300	-0.27697900
C	1.55085800	1.86590200	-1.60865600
C	2.29300800	2.55114500	0.51223600
C	1.75058500	3.13472400	-2.13107400
C	2.53032900	3.83984500	0.02625300
C	2.24976800	4.13764700	-1.30156000
F	0.58634200	-2.72384200	0.58089100
F	1.44801900	-4.85694400	-0.76510900
F	3.42025700	-4.59994800	-2.65648400
F	4.48089500	-2.13176800	-3.16344200
F	3.62946200	0.01125100	-1.85282200
F	3.68483000	-1.23086100	1.66304200
F	3.88030000	-1.64199000	4.29419700
F	1.88662700	-0.83063100	5.98230800
F	-0.32561400	0.42438000	4.95199000
F	-0.52474200	0.87137300	2.32836600
F	1.06755100	0.93531100	-2.46537600
F	2.59084300	2.36135300	1.81065500
F	3.01886900	4.79100400	0.83384000
F	2.45319200	5.36985600	-1.78010600
F	1.45068300	3.40940600	-3.41086500
H	0.05567800	-0.03921000	-0.01187500
C	-1.81452000	4.28256100	0.53424200
H	-2.45705100	5.07188200	0.12784200
H	-2.11800400	4.09859000	1.56771700
H	-0.79175200	4.67575400	0.55179800



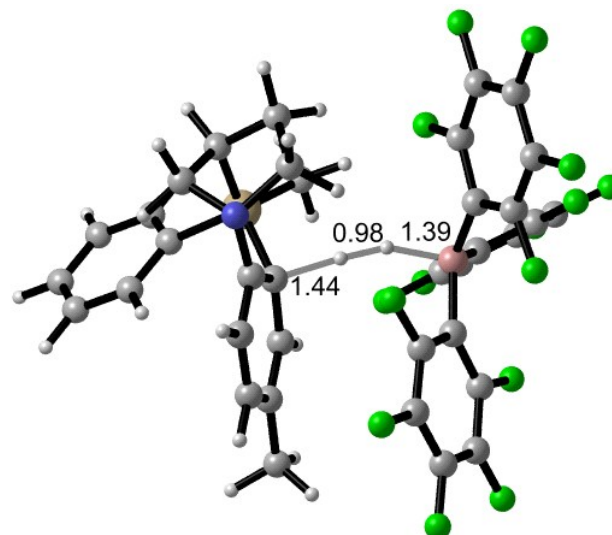
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E_{gas} = -3275.4920616 a.u.

C	2.22107500	-0.72055600	1.88536300
C	2.11573600	0.11870800	0.72473900

C	2.14573700	1.53644400	0.91668200
C	2.18381800	2.11351200	2.17821600
C	2.22889600	1.24904400	3.29032900
C	2.25640800	-0.13808700	3.15143600
H	0.80023900	-0.03367400	0.20755800
H	2.10937400	2.17704100	0.04114900
H	2.26203300	1.67940700	4.28877900
H	2.33416600	-0.76492000	4.03615500
C	2.25002400	-4.87098100	0.56664400
H	3.20730300	-5.10373400	1.05129300
H	1.94192300	-5.78366700	0.04515000
C	1.19561200	-4.48555200	1.63690800
H	1.48424500	-4.90947200	2.60606500
H	0.22485600	-4.92717000	1.38612900
C	1.01228200	-2.95938800	1.77430200
H	0.33846500	-2.59279500	0.99451100
H	0.53346500	-2.72224900	2.73093900
Si	3.03118100	-0.83636900	-0.69314100
C	4.75649300	-0.09346100	-0.87142900
C	5.22949900	0.39028300	-2.10456500
C	5.62294600	-0.01363900	0.23649800
C	6.51293800	0.92748300	-2.22921100
H	4.59233700	0.35091100	-2.98383800
C	6.90537600	0.52034300	0.11865000
H	5.29251300	-0.36946100	1.21036300
C	7.35337300	0.99237100	-1.11782000
H	6.85451500	1.29425500	-3.19311000
H	7.55498100	0.56986200	0.98817700
H	8.35213500	1.40912000	-1.21259000
C	2.16874300	-0.86952300	-2.36229600
H	1.95598700	0.13661500	-2.73358500
H	2.79648000	-1.38087500	-3.10008500
H	1.22496900	-1.41176100	-2.29880700
C	3.05620700	-2.48852300	0.27871500
H	4.11410300	-2.70004000	0.48504100
C	2.16890600	3.61099800	2.36738400
H	2.97641000	3.93919400	3.03041500
H	2.28020600	4.13349700	1.41393900
H	1.22475200	3.93729500	2.81848500
C	2.47759000	-3.73122700	-0.43800400
H	1.53123400	-3.49896000	-0.93784600
H	3.16959300	-4.05216400	-1.22527900
B	-1.45805000	0.24002300	-0.22785000
C	-2.08042900	-0.47862400	1.07851300
C	-1.63588200	-0.11716000	2.35531900
C	-3.04860700	-1.48871800	1.06687000
C	-2.08764900	-0.69909800	3.53377400

C	-3.53452500	-2.09763000	2.22455800
C	-3.04959100	-1.70370200	3.46673200
C	-1.41151100	1.85506900	-0.20679300
C	-2.31321700	2.66108000	0.49400400
C	-0.45072200	2.55718900	-0.93497300
C	-2.25188500	4.05324900	0.49970500
C	-0.33659500	3.94366300	-0.94344800
C	-1.25235600	4.70155300	-0.22074600
C	-1.82873700	-0.40036200	-1.66472100
C	-1.39902900	-1.67568900	-2.03230500
C	-2.61847600	0.24300900	-2.62248300
C	-1.67733300	-2.27677900	-3.25293300
C	-2.93595400	-0.32287800	-3.85768500
C	-2.46015100	-1.58996200	-4.17767700
F	-3.58665100	-1.92402800	-0.08802100
F	-4.46512100	-3.05834600	2.14804500
F	-3.50268900	-2.28000800	4.58489800
F	-1.61079200	-0.30409700	4.72406200
F	-0.70936900	0.85840500	2.48384900
F	-0.63783000	-2.39551800	-1.16680800
F	-1.20404800	-3.49684200	-3.54416500
F	-2.74955400	-2.14348300	-5.35966300
F	-3.69834300	0.34256100	-4.73512300
F	-3.13664200	1.46274600	-2.38212600
F	0.46888000	1.87769400	-1.66801400
F	0.65107400	4.54493800	-1.62513100
F	-1.17005600	6.03652100	-0.21392000
F	-3.14459600	4.77341600	1.19165000
F	-3.31447700	2.10761600	1.20367300
H	-0.13296100	-0.10092500	-0.10396600
C	2.36423100	-2.21516200	1.66641100
H	3.00286000	-2.60424000	2.47134500



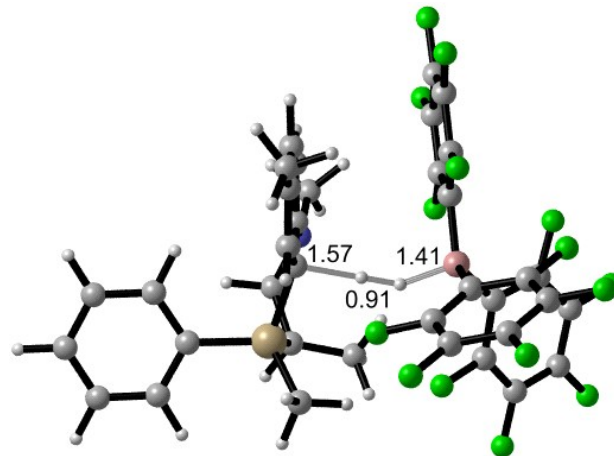
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G_{gas} = -3251.765422 a.u.

E_{gas} = -3252.19287918 a.u.

C	-2.21541500	1.16956400	-1.80088900
C	-2.14544900	0.40085300	-0.57961800
C	-2.39012500	1.11250000	0.64371900
C	-2.62699100	2.48025400	0.69798800
C	-2.63826500	3.18685300	-0.51948200
C	-2.43997800	2.54459500	-1.74046700
H	-0.78062100	0.00432500	-0.36136300
H	-2.36295800	0.55540100	1.57408700
H	-2.80734600	4.26110100	-0.50881500
H	-2.46766800	3.09793600	-2.67287100
N	-2.13416600	0.58449700	-3.10971300
C	-1.28734800	-1.72418400	-3.16401500
H	-1.25993300	-2.25109300	-4.12455500
H	-0.59157400	-2.23987000	-2.50023300
C	-0.90858700	-0.22239800	-3.36838300
H	-0.09671100	0.11457600	-2.72298300
H	-0.59624900	-0.04027600	-4.40185100
C	-2.74387800	-1.66812100	-2.63626600
H	-3.32603300	-2.55146800	-2.92471000
Si	-2.84879000	-1.41648700	-0.75055700
C	-4.64974700	-1.37909800	-0.17811600
C	-5.25638500	-2.55350300	0.30794200
C	-5.44970100	-0.22354400	-0.26532800
C	-6.60085900	-2.57624400	0.68294000
H	-4.67525300	-3.46715900	0.40306100
C	-6.79435300	-0.24025300	0.10754400
H	-5.01809800	0.70944400	-0.61853800
C	-7.37347300	-1.41852200	0.58228300
H	-7.04228900	-3.49557000	1.05742200
H	-7.38843100	0.66628700	0.03170100

H	-8.41927000	-1.43296800	0.87583400
C	-1.89584200	-2.71230300	0.22376600
H	-0.83426100	-2.71473800	-0.03232500
H	-1.98654100	-2.55264200	1.30112400
H	-2.29101100	-3.70849800	-0.00484800
C	-3.24271000	-0.37697100	-3.32340900
H	-4.18422900	0.02457200	-2.93863800
H	-3.36406500	-0.52729200	-4.40451300
B	1.44857200	0.04809400	0.29513400
C	2.32241900	-0.31528600	-1.01583300
C	3.29208200	0.50963300	-1.59479800
C	2.17420800	-1.55819200	-1.63736900
C	4.03544000	0.14587700	-2.71688400
C	2.88364800	-1.96080600	-2.76297400
C	3.82960400	-1.09678400	-3.30771100
C	1.61300700	-1.01469700	1.50357900
C	0.57789000	-1.31566300	2.38736500
C	2.80872600	-1.69313100	1.76082800
C	0.67286600	-2.24076700	3.41989300
C	2.95872200	-2.61857100	2.79297600
C	1.88076400	-2.90074300	3.62618700
C	1.32645500	1.60313600	0.70490400
C	0.94088200	2.55487000	-0.24515500
C	1.52650200	2.11510300	1.99137800
C	0.73557500	3.89854500	0.03531900
C	1.34564600	3.46068500	2.31694000
C	0.93937800	4.35686500	1.33532000
F	1.27828300	-2.45108900	-1.14479100
F	2.66978700	-3.16209200	-3.31766500
F	4.53091900	-1.45742500	-4.38700200
F	4.95018000	0.98057700	-3.22697700
F	3.57186000	1.71731400	-1.07031900
F	3.90322900	-1.46002200	1.01076300
F	4.13085500	-3.23593900	2.98932700
F	2.00381600	-3.79196600	4.61505700
F	-0.38177000	-2.49833900	4.20761600
F	-0.61862100	-0.68935500	2.25514100
F	0.72249300	2.16939100	-1.52279600
F	1.92006200	1.32107900	3.00391600
F	1.54946400	3.89135500	3.56910900
F	0.73724800	5.64484700	1.63531200
F	0.32810000	4.74936800	-0.91865000
H	0.16256100	-0.21135800	-0.17693900
C	-2.86560500	3.19502300	2.00661800
H	-2.13696900	3.99886600	2.15742900
H	-3.86098600	3.65270700	2.03123500
H	-2.79044500	2.50980000	2.85430400



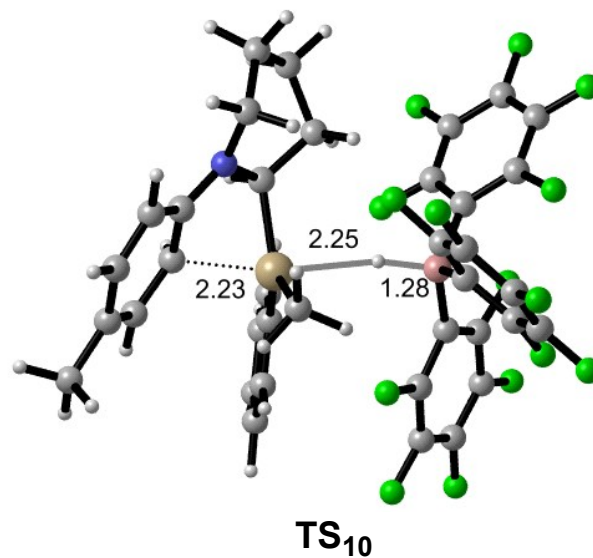
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E_{gas} = -3253.4231059 a.u.

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C	-2.33169400	0.29260700	0.23726000
C	-2.16233700	0.63801200	1.62086300
C	-1.94728000	1.92523400	2.07386700
C	-1.99605600	2.95271100	1.10537700
C	-2.21667000	2.70218600	-0.23593900
H	-0.82955900	-0.12250400	0.05691300
H	-2.13365100	-0.17612300	2.33893100
H	-1.86855600	3.98493000	1.42421600
H	-2.27901600	3.54408400	-0.91292200
N	-2.63851100	1.16660200	-2.06444200
C	-3.06681200	-1.34339100	-2.09563300
H	-3.83405400	-2.03197500	-2.47694700
Si	-3.18238500	-1.35776400	-0.19884000
C	-5.00553800	-1.23801100	0.30225900
C	-5.82789100	-2.38004500	0.22967500
C	-5.60195200	-0.03617200	0.72613200
C	-7.18252800	-2.32469000	0.55894700
H	-5.40908300	-3.33256000	-0.08624600
C	-6.95695600	0.02579100	1.05928800
H	-5.00090900	0.86587800	0.80645900
C	-7.75050700	-1.11882600	0.97542700
H	-7.79309900	-3.22113200	0.49443200
H	-7.39113300	0.96645800	1.38695300
H	-8.80435900	-1.07325500	1.23541700
C	-2.42045700	-2.87823800	0.60297300
H	-1.37438300	-3.01173400	0.32667800
H	-2.47679500	-2.82688900	1.69405600
H	-2.97282700	-3.77075900	0.28789200
C	-3.49657200	0.06035000	-2.54996900
H	-4.53899900	0.25329000	-2.25432300
H	-3.46368100	0.11168600	-3.64289300

B	1.41323900	-0.03501600	0.05393500
C	1.38081000	1.57178500	-0.02045100
C	1.67117800	2.42949400	1.04686900
C	0.99446900	2.22480000	-1.19609700
C	1.61856000	3.81935200	0.95279400
C	0.92891200	3.60565600	-1.33309700
C	1.24430000	4.41522300	-0.24724100
C	1.98612000	-0.84341300	-1.22449900
C	1.60703200	-2.16811300	-1.45344800
C	2.95058100	-0.35024800	-2.10936000
C	2.09157400	-2.94792000	-2.49832000
C	3.47476900	-1.09915700	-3.16138600
C	3.04058700	-2.40653200	-3.36036800
C	1.92355100	-0.71853500	1.42777300
C	1.15945700	-1.43013100	2.34667800
C	3.29022700	-0.65983800	1.71612200
C	1.69317400	-2.04072500	3.48100400
C	3.86829800	-1.24977300	2.83459900
C	3.05863200	-1.95048800	3.72639500
F	0.62008700	1.50282200	-2.27486700
F	0.50909800	4.15947600	-2.48482300
F	1.17048700	5.74590900	-0.35010000
F	1.90725000	4.58450400	2.01440200
F	1.99839300	1.94711900	2.26160600
F	3.43014400	0.89937800	-1.97430700
F	4.39507400	-0.57294800	-3.98024100
F	3.52894700	-3.13429500	-4.36993500
F	1.65618300	-4.20330700	-2.67635000
F	0.70026100	-2.75379900	-0.63629900
F	-0.17677300	-1.56193000	2.17323100
F	4.10759900	0.01594800	0.88181900
F	5.18459700	-1.15255000	3.06217500
F	3.59036200	-2.52780300	4.80947500
F	0.90139300	-2.71095800	4.33081500
H	0.04589800	-0.36401200	-0.03014000
C	-1.63612200	2.23372200	3.51780100
H	-1.90018000	1.39708200	4.17019000
H	-0.56442700	2.42898700	3.64808100
H	-2.17498800	3.12059000	3.86770200
C	-2.51597600	2.28826600	-2.99353200
H	-1.58277800	2.82720000	-2.82839900
H	-2.48979300	1.89410700	-4.01060500
H	-3.35640000	2.99539400	-2.92404400
C	-1.70385000	-1.73236600	-2.69293400
H	-1.35403000	-2.70294600	-2.33185000
H	-1.76277000	-1.78594700	-3.78750200
H	-0.93888800	-0.98867100	-2.44956200



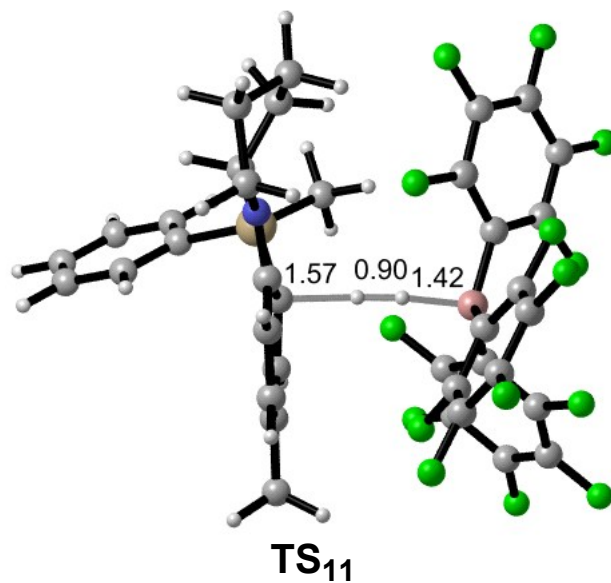
G_{gas} = -3291.074685 a.u.

E_{gas} = -3291.53724174 a.u.

C	-4.48804600	-1.08451500	0.69859700
C	-5.53163800	-1.50715600	-0.16877200
C	-6.33588400	-0.56896800	-0.77613700
C	-6.20149300	0.83739500	-0.57104500
C	-5.24580900	1.24997100	0.32570700
C	-4.34681400	0.33269600	0.96760300
H	-5.67862400	-2.55719700	-0.39021100
H	-7.10852500	-0.91933800	-1.45711200
H	-5.15391100	2.30358200	0.57763400
H	-4.06520100	0.61860000	1.98136000
N	-3.50691700	-1.87790800	1.18281800
C	-1.73016000	-3.30084000	2.87559900
H	-0.90826400	-3.97533500	3.13362100
H	-2.11748400	-2.91024500	3.82432500
C	-1.19114700	-2.12577900	2.04328900
H	-0.69271700	-2.48225800	1.14127900
H	-0.44835300	-1.57352000	2.61638000
C	-2.32724900	-1.15724200	1.71204200
H	-2.61570600	-0.67565600	2.66187000
Si	-2.17153800	0.36154600	0.46954100
C	-1.71273100	2.03365600	1.15825300
C	-1.23689300	2.18965800	2.47390400
C	-1.92139100	3.19130300	0.38304300
C	-0.98206000	3.45783300	2.99610400
H	-1.03214300	1.32029600	3.09040500
C	-1.66300000	4.45894200	0.90404900
H	-2.26044100	3.10666700	-0.64492500
C	-1.19549200	4.59369500	2.21293300
H	-0.60425400	3.55726700	4.00943000
H	-1.81073700	5.33731100	0.28303500

H	-0.98815400	5.58011900	2.61756200
C	-2.35696700	0.12796000	-1.38182800
H	-3.12726700	0.81413000	-1.74713700
H	-1.42791100	0.32716700	-1.90999400
H	-2.67865500	-0.89213600	-1.60207300
B	1.22733500	-0.09318300	-0.27593000
C	2.04011200	-1.04014500	0.78510500
C	1.90613300	-0.84469800	2.16034200
C	2.93322800	-2.05958100	0.44368000
C	2.54954200	-1.59840000	3.13401400
C	3.61115500	-2.84066300	1.38200200
C	3.41832900	-2.61154400	2.73890200
C	1.12799500	-0.76751600	-1.76753500
C	1.91916700	-0.39029200	-2.85771900
C	0.25354500	-1.81787900	-2.04459200
C	1.83079600	-0.97748800	-4.11919800
C	0.12188800	-2.43462300	-3.28470100
C	0.92347100	-2.00924700	-4.33786800
C	1.75949900	1.45896100	-0.29827900
C	2.89303100	1.95182800	0.35715500
C	1.05880700	2.43500300	-1.00936900
C	3.27397900	3.29460800	0.34459700
C	1.38810800	3.78449300	-1.04357100
C	2.51421300	4.22295600	-0.35624000
F	3.20309100	-2.34655200	-0.84666000
F	4.44995200	-3.80885800	0.98354300
F	4.05380500	-3.35597400	3.65361000
F	2.33629700	-1.36428000	4.44007200
F	1.07702400	0.13089500	2.61930300
F	-0.56679700	-2.30201400	-1.06571800
F	-0.76635100	-3.42715600	-3.46840300
F	0.82211600	-2.58344100	-5.54372600
F	2.61761700	-0.56296400	-5.12259800
F	2.84602800	0.57879700	-2.72864100
F	3.71261400	1.13549900	1.05213900
F	-0.04183100	2.08518100	-1.72629000
F	0.62636700	4.66150300	-1.72077300
F	2.85768600	5.51834300	-0.36785500
F	4.37116600	3.69616400	1.00481600
H	0.02316000	-0.03011400	0.15675800
C	-7.11688500	1.79749600	-1.29014800
H	-6.97482800	1.74704600	-2.37609000
H	-8.17065800	1.56980700	-1.09296600
H	-6.93281200	2.82876600	-0.97836500
C	-2.85318900	-4.07051300	2.13390300
H	-3.69347700	-4.25617700	2.81068000
H	-2.50018100	-5.05020100	1.79532100

C	-3.35763700	-3.31012100	0.89633600
H	-2.65919600	-3.43100700	0.05873500
H	-4.32050500	-3.71169600	0.58050700



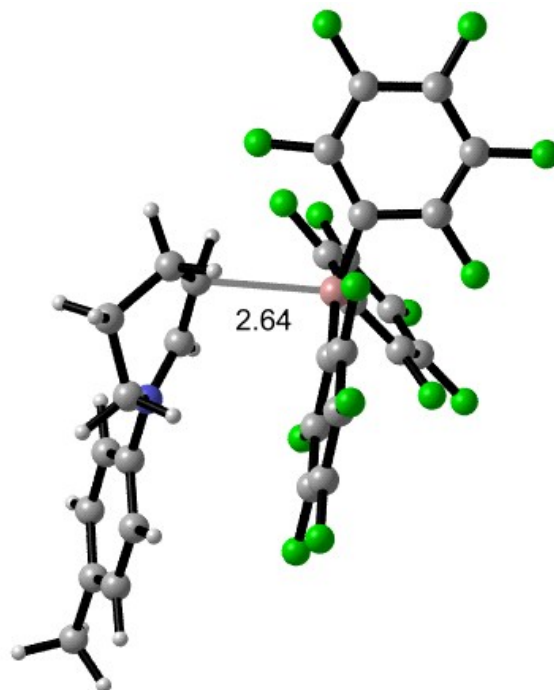
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E_{gas} = -3291.53478863 a.u.

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C	2.04288700	-0.53337200	-1.02299700
C	1.66955900	-1.79898300	-1.57761100
C	1.13567100	-1.91782800	-2.84528400
C	1.00597300	-0.73010000	-3.61165700
C	1.44179000	0.50678400	-3.17413600
H	0.62068300	-0.28445600	-0.39720000
H	1.73974100	-2.67835200	-0.94279100
H	0.54960400	-0.79736900	-4.59695500
H	1.35678700	1.36909200	-3.82523800
N	2.64494500	1.74640500	-1.43429000
C	2.91596500	4.11828900	0.02722300
H	3.34520500	4.97570500	0.55546600
H	1.82866200	4.24183700	0.06024200
C	3.37174400	4.10730400	-1.43574000
H	4.45926900	3.97550000	-1.49361800
H	3.14848500	5.06102700	-1.92501300
C	2.66191600	2.98987500	-2.21158700
H	1.62401900	3.28882800	-2.40991100
H	3.14730300	2.82682600	-3.18602300
Si	3.23784000	-0.16444200	0.40025500
C	4.80835400	-1.19709300	0.27307600
C	5.40684400	-1.77879300	1.40532600
C	5.43459500	-1.39653300	-0.97296900
C	6.58352000	-2.52399200	1.30113500
H	4.95193600	-1.65457900	2.38440600

C	6.61010000	-2.13833300	-1.08312300
H	4.99463700	-0.97386300	-1.87373400
C	7.18750800	-2.70388600	0.05648700
H	7.02573200	-2.96450600	2.19035400
H	7.07366000	-2.27957300	-2.05556000
H	8.10206100	-3.28427100	-0.02705200
C	2.54458700	-0.23683600	2.14738200
H	2.32372300	-1.26684100	2.44057800
H	3.25838300	0.17759800	2.86752300
H	1.61482900	0.33082200	2.23162500
C	3.52303600	1.63529100	-0.24502500
H	4.56085200	1.70124500	-0.60684700
C	0.65705100	-3.23592300	-3.40190800
H	1.11602500	-3.45612300	-4.37250500
H	0.89339700	-4.06131900	-2.72499300
H	-0.42878100	-3.22243600	-3.54884200
C	3.29558100	2.79918500	0.74708100
H	2.51773100	2.56184300	1.47553600
H	4.22455300	2.92799600	1.31505300
B	-1.55328400	-0.02350900	0.34370200
C	-2.24143800	0.64419400	-0.95036200
C	-2.25797600	-0.03775100	-2.17288600
C	-2.83615100	1.91111900	-0.98717800
C	-2.78146200	0.48451400	-3.34985500
C	-3.38844700	2.46653500	-2.14100700
C	-3.35733500	1.75143400	-3.33345000
C	-1.93650200	-1.56231200	0.63105000
C	-3.24202000	-2.03672800	0.47597100
C	-1.01754000	-2.51168900	1.07695800
C	-3.61352100	-3.35521900	0.72516000
C	-1.34031200	-3.84213600	1.33028500
C	-2.65301700	-4.26740600	1.15395500
C	-1.33312700	0.90677600	1.63905100
C	-0.51678300	2.03930600	1.57854400
C	-1.92191300	0.67491600	2.88551000
C	-0.26881700	2.87662800	2.65817200
C	-1.70899500	1.49546500	3.99455000
C	-0.87239200	2.60084700	3.88305400
F	-2.92059700	2.67180200	0.12083200
F	-3.94651200	3.68445800	-2.10982000
F	-3.87296000	2.27452500	-4.45060800
F	-2.73167600	-0.21758300	-4.49235000
F	-1.72132700	-1.27297400	-2.25784500
F	0.09126100	2.35395500	0.40981300
F	0.55123700	3.93440400	2.53492800
F	-0.64988600	3.39180400	4.93724300
F	-2.30216900	1.22585900	5.16432100

F	-2.75547400	-0.36456200	3.07124000
F	0.27870500	-2.16408100	1.27431800
F	-0.40236600	-4.70827300	1.74150000
F	-2.98911000	-5.53916000	1.39547600
F	-4.88227900	-3.75210000	0.56087000
F	-4.22042400	-1.19851000	0.08192000
H	-0.21475700	-0.11698600	-0.11013800



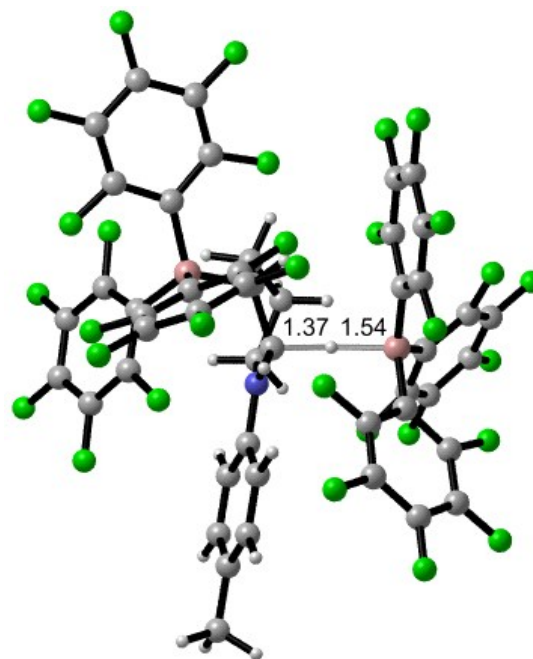
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E_{gas} = -2729.26530460 a.u.

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C	-4.31506600	1.09208100	1.82415300
C	-5.55892500	1.61172100	1.47308500
C	-6.43825000	0.90882900	0.63980200
C	-6.01682200	-0.33698000	0.15747500
C	-4.76955600	-0.86297800	0.48527600
H	-3.67801200	1.64247200	2.50893400
H	-5.85772400	2.57735600	1.87317500
H	-6.66844900	-0.90293700	-0.50338900
H	-4.45903200	-1.80836700	0.05514500
N	-2.62927700	-0.68798400	1.66331400
C	-1.53715100	0.11395500	1.83206700
H	-1.70157000	1.15891700	1.59743300
C	-0.30016500	-0.32651200	2.21210400
H	0.42372000	0.42723200	2.47880800
C	-0.10510800	-1.75091900	2.68571600
H	0.54883600	-1.75901300	3.56305800
H	0.40703500	-2.35916600	1.92858300
C	-1.46016000	-2.38606500	3.03170300

H	-1.83774700	-1.96091100	3.96888400
H	-1.36268800	-3.46630300	3.18069100
C	-2.49283900	-2.13225600	1.92789000
H	-2.19884200	-2.65604700	1.00920600
H	-3.47459600	-2.51033200	2.22295400
B	1.00793900	0.00452800	-0.05373100
C	0.78020500	1.55267200	-0.37033800
C	0.46249100	2.01293400	-1.65630600
C	1.07016400	2.56139800	0.55717800
C	0.37976800	3.36351000	-1.98613100
C	0.98460400	3.92072900	0.27219900
C	0.63550000	4.32524300	-1.01331900
C	0.13455800	-1.12713200	-0.72512400
C	0.57552500	-2.45652100	-0.85697500
C	-1.16024000	-0.89582400	-1.22735800
C	-0.17811300	-3.46520500	-1.45219200
C	-1.94056900	-1.87641700	-1.82769800
C	-1.44706100	-3.17420400	-1.94240200
C	2.54309800	-0.29607100	0.33363800
C	3.19062000	-0.36936200	1.56633200
C	3.38806700	-0.40332400	-0.77878300
C	4.56884800	-0.55507900	1.69123500
C	4.76272100	-0.58627500	-0.70046100
C	5.36092800	-0.66460900	0.55484700
F	1.45238600	2.23884400	1.81163700
F	1.24727200	4.83485000	1.21424200
F	0.55515100	5.62394200	-1.31139900
F	0.06805000	3.74221600	-3.23096600
F	0.24782400	1.14457200	-2.65864300
F	-1.72689500	0.31695000	-1.11478100
F	-3.17240900	-1.59498100	-2.27468700
F	-2.18605300	-4.12677100	-2.51409600
F	0.30549400	-4.70909500	-1.55000700
F	1.77661100	-2.83825700	-0.38655500
F	2.51553400	-0.27146900	2.72942100
F	2.84538000	-0.32554200	-2.01429600
F	5.50771800	-0.68447000	-1.80792900
F	6.68088000	-0.84056900	0.66421500
F	5.13071100	-0.62532800	2.90478700
C	-7.80198400	1.45931900	0.29708500
H	-7.81094900	2.55286800	0.32577700
H	-8.12040900	1.14490100	-0.70147500
H	-8.56290500	1.10848600	1.00573100



TS₁₃

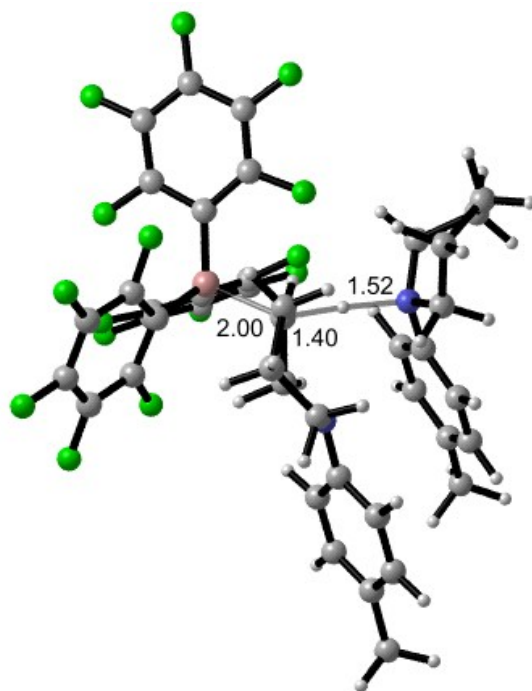
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E_{gas} = -4938.17618497 a.u.

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C	-2.06242100	4.17390600	1.36941400
C	-2.30451300	5.33556000	0.62249300
C	-1.96991400	5.29620300	-0.73124700
C	-1.42719500	4.15519500	-1.32341800
H	-1.34592000	2.17597400	1.43259300
H	-2.30142900	4.15831700	2.43044900
H	-2.12992700	6.17672800	-1.34920300
H	-1.17603300	4.19558700	-2.37484700
N	-0.62648400	1.84721600	-1.18565800
C	-0.26725900	0.70420900	-0.48422500
H	-0.19600800	0.88546800	0.58014700
C	0.89092000	-0.13788200	-1.00752100
H	0.68891800	-1.14903800	-0.67297500
C	0.96777700	-0.14390000	-2.55754000
H	1.13056200	-1.16482400	-2.90520100
H	1.82324800	0.44093900	-2.90708600
C	-0.29665900	0.42571600	-3.19763000
H	-1.14775500	-0.23406500	-3.00724500
H	-0.18851100	0.49927300	-4.28640800
C	-0.59092300	1.82036100	-2.65923100
H	0.17969800	2.52144500	-3.00849600
H	-1.55797100	2.17727000	-3.03036000
B	2.38666500	0.26636000	-0.27991600
C	2.37867400	0.06265500	1.38468600
C	3.03834700	0.88085700	2.31415800

C	1.81440400	-1.07693200	1.97114700
C	3.06242800	0.64271200	3.68836700
C	1.80300800	-1.35426800	3.33605300
C	2.43317700	-0.48019000	4.21107700
C	2.72096600	1.82373300	-0.75860100
C	3.47091500	2.15967900	-1.89044400
C	2.17429100	2.93784200	-0.11339400
C	3.68066500	3.46378400	-2.33878000
C	2.35183100	4.25814000	-0.51695300
C	3.11955600	4.52711700	-1.64421300
C	3.59442500	-0.80524800	-0.72859400
C	3.42871700	-2.11069100	-1.20101400
C	4.93630600	-0.47440700	-0.48757200
C	4.47948400	-2.99635200	-1.45258700
C	6.01574300	-1.31964500	-0.72228000
C	5.78690200	-2.60022900	-1.21305900
F	1.24519800	-2.03703100	1.20165900
F	1.20810100	-2.46662200	3.80154000
F	2.44812700	-0.72092300	5.53184000
F	3.70224400	1.48908900	4.51558400
F	3.72111500	1.97740400	1.92742300
F	1.40055300	2.77242700	0.98497200
F	1.79209000	5.27006400	0.16685400
F	3.30568300	5.79137700	-2.06062700
F	4.41739700	3.69994900	-3.44053200
F	4.04386600	1.19999800	-2.65758400
F	2.20235400	-2.62535300	-1.46288700
F	5.25417400	0.73944100	0.01258900
F	7.27481800	-0.91553800	-0.47358100
F	6.81192900	-3.43692700	-1.44656800
F	4.23216600	-4.23260500	-1.92008200
C	-2.88758900	6.57128300	1.26489500
H	-3.84228100	6.35656400	1.75989800
H	-2.21609200	6.98174500	2.02902600
H	-3.06578700	7.35749400	0.52512200
B	-2.51415600	-1.07981500	-0.07470900
C	-1.70928700	-2.44358900	0.20958400
C	-1.67097700	-3.11632200	1.43966100
C	-0.97301000	-3.07502400	-0.80408200
C	-0.95332400	-4.29057600	1.65558200
C	-0.25011200	-4.24880500	-0.63583900
C	-0.23585200	-4.86143500	0.61264400
C	-3.37168600	-1.01080600	-1.44771000
C	-3.77056600	0.21459400	-1.99145000
C	-3.83850300	-2.12670800	-2.15333900
C	-4.50340800	0.35010000	-3.16538000
C	-4.58643800	-2.03902300	-3.32687100

C	-4.91616200	-0.79188000	-3.84359600
C	-3.23050200	-0.36600800	1.19045800
C	-2.51523500	0.06315400	2.31303700
C	-4.61204900	-0.15930600	1.28469900
C	-3.08357800	0.68602400	3.41674300
C	-5.22949400	0.45203100	2.37625200
C	-4.46099300	0.88453700	3.44863400
F	-0.94969800	-2.54503000	-2.04679400
F	0.42190000	-4.79462800	-1.65706400
F	0.45224400	-5.99360800	0.80376600
F	-0.96571200	-4.88272100	2.85906100
F	-2.36838200	-2.67483100	2.50613400
F	-3.60894400	-3.37765600	-1.71055100
F	-4.99906400	-3.15062900	-3.95715200
F	-5.62871900	-0.69084700	-4.97417800
F	-4.81920200	1.56587200	-3.64101900
F	-3.44763600	1.36246300	-1.36122200
F	-1.17391200	-0.10722900	2.35854700
F	-5.44981400	-0.57214700	0.31119200
F	-6.56175600	0.61898900	2.39934200
F	-5.03631900	1.48087900	4.50142500
F	-2.32348000	1.10030800	4.44123400
H	-1.35019200	-0.12961900	-0.40046800



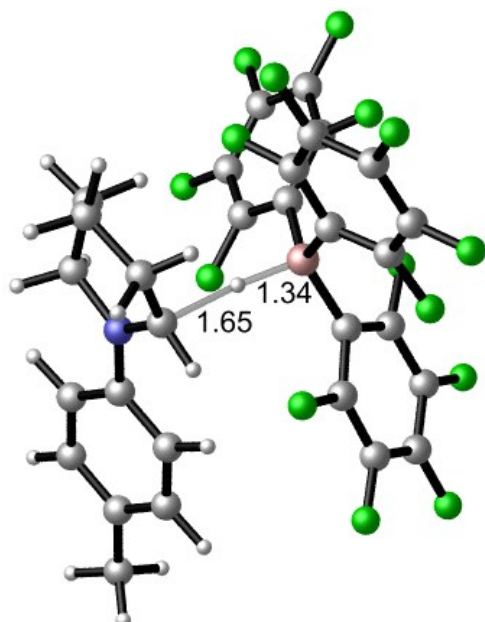
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E_{gas} = -3252.68007541 a.u.

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C	3.71701000	1.92300400	0.24916600

C	4.94019000	2.48196700	0.62031600	F	-1.09315200	5.33136000	-0.05492100
C	5.98063700	2.67118500	-0.29453900	F	-0.40870400	2.98646300	0.92875600
C	5.74424600	2.26439200	-1.61442400	F	-0.18824800	-1.96241700	1.37352900
C	4.53285000	1.70115700	-2.00276500	F	-2.31970200	2.17152200	2.39382300
H	2.94461700	1.83125100	1.00219200	F	-1.69210100	1.84755000	4.93100200
H	5.07494200	2.79580100	1.65329100	F	-0.27697000	-0.33523900	5.77313000
H	6.52648700	2.38833900	-2.36061100	F	0.47608000	-2.23597400	3.92269300
H	4.40945900	1.38673800	-3.03341800	C	7.28558400	3.31739400	0.10793000
N	2.27478000	0.92452500	-1.49422900	H	7.31545900	4.37788600	-0.17370900
C	0.10097100	-0.19204600	-0.97187700	H	7.44032100	3.26593800	1.19002600
H	-0.19852800	-1.06445600	-0.38333800	H	8.14136800	2.83410100	-0.37593200
C	-0.30001400	-0.04098100	-2.45736800	H	0.93902500	-1.31562700	-1.02381900
H	-1.38143000	-0.01202300	-2.59066700	C	3.08520500	-2.13787500	-0.26073700
H	0.05019700	-0.88839800	-3.05501700	C	2.95958000	-2.13565900	1.13793400
C	0.32717100	1.23530900	-3.02679100	C	4.04562700	-1.81675100	1.95015900
H	-0.09437600	2.11459500	-2.53102900	C	5.29067900	-1.47280300	1.41262100
H	0.08521700	1.32985700	-4.09105700	C	5.40030900	-1.45631000	0.01986700
C	1.84684300	1.24012100	-2.87154100	C	4.32379000	-1.77629500	-0.80674500
H	2.27881500	0.51187000	-3.57636200	H	2.01791200	-2.37314100	1.61376800
H	2.23958600	2.22262500	-3.16503400	H	3.91017700	-1.83207600	3.02862900
B	-1.52223500	0.28867400	0.08692800	H	6.34185900	-1.17105100	-0.44127100
C	-2.72494900	-0.82001800	-0.14438000	H	4.47192400	-1.71251700	-1.87562000
C	-3.95699400	-0.56646700	0.47645800	N	1.92711600	-2.46901400	-1.09747900
C	-2.69169900	-2.03291100	-0.82759700	C	2.26494800	-2.58751900	-2.55616500
C	-5.05073300	-1.42501700	0.43231500	H	3.23074700	-3.09417400	-2.66421000
C	-3.75529500	-2.93106300	-0.90134900	H	2.37924700	-1.57653500	-2.94923500
C	-4.95083700	-2.62590600	-0.26491100	C	1.21861700	-3.39961500	-3.32049500
C	-1.90598200	1.76679900	-0.49701400	H	1.42451000	-3.30903500	-4.39193100
C	-1.34570500	2.97334100	-0.04674600	H	0.22108400	-2.98085100	-3.15976100
C	-2.84675600	1.94622800	-1.52406700	C	1.25597000	-4.87709200	-2.87273000
C	-1.67691400	4.23039800	-0.54541400	H	1.97374500	-5.43976300	-3.47966700
C	-3.21014500	3.18353300	-2.05274300	H	0.27584100	-5.33569900	-3.03923200
C	-2.62324100	4.34116700	-1.55802000	C	1.64652300	-4.96801600	-1.38120700
C	-1.15805000	0.19648400	1.69052200	H	2.73028600	-5.08914000	-1.26704800
C	-0.52257300	-0.93378000	2.21010200	H	1.18876700	-5.84296000	-0.90817900
C	-1.57470700	1.09437700	2.68601500	C	1.20185800	-3.71454800	-0.62546100
C	-0.19291800	-1.13384700	3.54452500	H	0.13336300	-3.55168100	-0.76561200
C	-1.28109800	0.93547300	4.04169400	H	1.37623800	-3.82789300	0.44026000
C	-0.57233400	-0.17803300	4.47936700	C	6.45347100	-1.08667800	2.29347000
F	-1.56988000	-2.42696200	-1.49568200	H	6.57483900	0.00301800	2.31802100
F	-3.62625400	-4.08006900	-1.58152100	H	6.30870200	-1.42790800	3.32241700
F	-5.98647200	-3.46973400	-0.31933500	H	7.39413300	-1.50875500	1.92524900
F	-6.19384100	-1.10734900	1.05266700	C	1.21564400	0.75254500	-0.48439100
F	-4.13104900	0.57958800	1.16472400	H	0.82260500	1.72434100	-0.18358200
F	-3.46538700	0.88931800	-2.09866700	H	1.67542000	0.31486100	0.40373200
F	-4.11601500	3.26093800	-3.03693300				
F	-2.95294300	5.53749400	-2.05321300				



TS₁₅

G_{gas} = -2730.121593 a.u.

E_{gas} = -2730.46276222 a.u.

C	2.98874800	0.83469700	-1.98028800
C	3.34274700	-0.49376500	-1.69237500
C	4.65963200	-0.82066100	-1.39125900
C	5.67643100	0.14432700	-1.36713500
C	5.31391100	1.45962900	-1.66572800
C	3.99706900	1.80802000	-1.96610200
H	2.61213600	-1.29008500	-1.68577100
H	4.89589800	-1.85732300	-1.16583500
H	6.07137000	2.23869100	-1.66572400
H	3.78201300	2.84326200	-2.19390900
N	1.64431700	1.20389400	-2.32986300
C	0.65620000	0.30847800	-2.43214400
H	0.95433900	-0.72720100	-2.37742300
C	-0.82368500	2.06010800	-3.58731400
H	-1.90179400	2.23264900	-3.61097700
H	-0.42746900	2.34415700	-4.56934400
C	-0.16848600	2.91968100	-2.50704700
H	-0.63166200	2.71125100	-1.53877600
H	-0.30981000	3.98593900	-2.71044800
C	1.33153900	2.65150500	-2.43374000
H	1.83721700	3.04566300	-3.32342900
H	1.75756300	3.13587200	-1.55248700

C	7.09536000	-0.22647000	-1.01304000
H	7.19878400	-0.40607800	0.06393300
H	7.40816500	-1.14310800	-1.52350900
H	7.79596200	0.56818300	-1.28334900
B	-0.69106500	-0.23128200	0.17109600
C	-2.11777300	-0.80511900	-0.36184200
C	-2.56692500	-2.12541600	-0.23243100
C	-3.02373500	0.03790900	-1.01925400
C	-3.79955900	-2.57282700	-0.71089700
C	-4.25845300	-0.36231200	-1.51630800
C	-4.65283700	-1.68799400	-1.35946400
C	-0.78107300	1.17327900	0.99344500
C	0.32018000	2.02553700	1.07765400
C	-1.89930800	1.61119700	1.71015100
C	0.32767200	3.23650100	1.76250900
C	-1.93864400	2.81044500	2.41967200
C	-0.81749200	3.63424200	2.44456000
C	0.30211700	-1.31336200	0.87852300
C	0.93194300	-2.32721500	0.15615200
C	0.61144900	-1.31690300	2.24298100
C	1.83892700	-3.23376100	0.68766900
C	1.50174400	-2.21738400	2.83131800
C	2.12795600	-3.17969000	2.04845100
F	-2.70957200	1.34513000	-1.20883500
F	-5.06283800	0.50897100	-2.14291600
F	-5.83349000	-2.10317500	-1.82956500
F	-4.16596800	-3.85120300	-0.54938800
F	-1.82448000	-3.05870200	0.39317500
F	-3.01796300	0.86217500	1.76256700
F	-3.04539200	3.17529300	3.08128300
F	-0.84076700	4.79293500	3.11314300
F	1.42214400	4.01497300	1.76589600
F	1.47885800	1.68877700	0.45534600
F	0.68000800	-2.46283400	-1.17786000
F	0.04283600	-0.43254800	3.08530000
F	1.75760100	-2.15899800	4.14500600
F	2.99538400	-4.04131900	2.59124800
F	2.43908800	-4.14473600	-0.09519500
H	-0.06300800	0.11099200	-0.96172100
C	-0.53679400	0.57152800	-3.31652000
H	-0.30844800	0.04643400	-4.25538900
H	-1.39839200	0.05184600	-2.89631600

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