

Alternative mechanistic interpretation for unconventional catalytic behaviour of triisobutylaluminium-activated heterocenes in ethylene polymerization

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S1. Polymerization experiments and polymer analysis

S1.1. Polymerization experiments

Ethylene (polymerization grade) and argon (extra pure) were assessed through oxygen and water scrubbing columns prior to use. TIBA and MMAO-12 were all used as stock solutions stored in glass ampoules connected to a standard Schlenk argon-vacuum line. Catalytic experiments were performed in a Nano-mag NMA1400 autoclave (Nano-Mag Technologies Pvt. Ltd., Mumbai, India) equipped with 400 ml stainless steel ss316 reactor and fluidized jacket (connected to a thermostatic bath). Ethylene was added to the reaction *via* a mass flow controller array BPC 2.0. Solvents and reagents were introduced into the reactor using burettes, and a screw-type syringe was used for the injection of the catalyst solutions after reaching the required pressure. The ethylene uptake data were recorded, along with the reactor pressure, and the reaction mixture temperature.

The rigorously cleaned autoclave was heated (120 °C) under vacuum for 1 h, and then cooled to reaction temperature and back-filled with ethylene (10 bar), which was then vented to 1 bar *via* a septa to purge the inlet valve. *n*-Heptane (200 ml) and TIBA (1 ml of 1 M solution in heptane, 1 mmol) were placed in an autoclave.

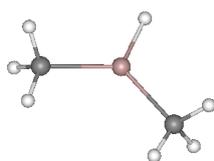
The catalyst solution was prepared by adding TIBA (1 ml, 1 mmol) to a Zr complex (10 µmol) in *n*-heptane (5 ml) and stirring for 10 min at 40 °C. The catalyst was transferred to the autoclave at 40 °C, and the autoclave was pressurized with ethylene (10 bar). After a defined period of time, the reactor was cooled to 20 °C and vented. Polymer was collected, washed successively with 5% HCl (MeOH) and then MeOH, dried in vacuo overnight, and weighed.

S1.3. Polymer analysis

Size exclusion chromatography (SEC) of the polymer samples was performed using an Agilent PL-GPC 220 chromatograph equipped with a PLgel column (Agilent Technologies, Santa Clara, CA, USA), 1,2,4-trichlorobenzene was used as the eluent (1 ml/min). The measurements were recorded with universal calibration based on a polystyrene standard at 135 °C.

Differential scanning calorimetry (DSC) experiments were performed on the TGA/DSC1 apparatus (Mettler Toledo, Columbus, OH, USA).

Me₂AlH

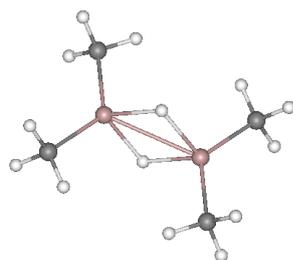


Zero-point vibrational energy	206187.7 (J/mol)
	49.28004 (kcal/mol)
Zero-point correction	0.078533 (Hartree/Particle)
Thermal correction to Energy	0.084839
Thermal correction to Enthalpy	0.085783
Thermal correction to Gibbs Free Energy	0.049544
Sum of electronic and zero-point Energies	-322.675915
Sum of electronic and Thermal Energies	-322.669609
Sum of electronic and Thermal Enthalpies	-322.668665
Sum of electronic and Thermal Free Energies	-322.704904

cartesian

13	0.00000995	0.69409001	0.00005000	1	-2.31759000	0.04249001	-0.87424999
6	-1.71979010	-0.24191001	0.00005000	1	2.31751013	0.04159001	-0.87465000
6	1.71980989	-0.24191001	0.00005000	1	2.31810999	0.04289000	0.87395000
1	-1.62759006	-1.33160996	-0.00025000	1	1.62750995	-1.33160996	0.00085000
1	-2.31788993	0.04209000	0.87424999	1	-0.00009005	2.28389001	-0.00005000

Me₂AlH dimer

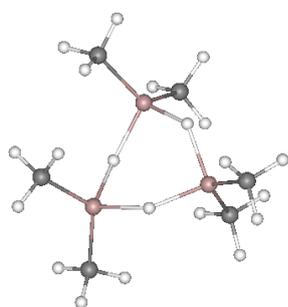


Zero-point vibrational energy	206187.7 (J/mol)
	49.28004 (kcal/mol)
Zero-point correction=	0.078533 (Hartree/Particle)
Thermal correction to Energy=	0.084839
Thermal correction to Enthalpy=	0.085783
Thermal correction to Gibbs Free Energy=	0.049544
Sum of electronic and zero-point Energies=	-322.675915
Sum of electronic and thermal Energies=	-322.669609
Sum of electronic and thermal Enthalpies=	-322.668665
Sum of electronic and thermal Free Energies=	-322.704904

cartesian

1	0.00000000	-0.00010000	-1.14639997	1	2.81500006	1.88979995	-0.87849998
1	-0.00010000	-0.00010000	1.14590001	13	-1.32050002	0.00000000	-0.00020000
13	1.32040000	-0.00010000	-0.00020000	6	-2.17490005	-1.75619996	0.00010000
6	2.17490005	-1.75619996	0.00010000	6	-2.17449999	1.75629997	0.00010000
6	2.17459989	1.75619996	0.00010000	1	-2.80819988	-1.89260006	0.88349998
1	2.81310010	-1.89030004	0.88029999	1	-1.44410002	-2.57110000	-0.00700000
1	2.81509995	-1.88979995	-0.87879997	1	-1.44350004	2.57100010	-0.00700000
1	1.44400001	-2.57110000	-0.00100000	1	-2.81949997	1.88779998	-0.87559998
1	2.81250000	1.89059997	0.88050002	1	-2.80789995	1.89289999	0.88340002
1	1.44360006	2.57100010	-0.00130000	1	-2.81990004	-1.88750005	-0.87550002

Me₂AlH trimer



Zero-point vibrational energy	640581.7 (J/mol)
	153.10270 (kcal/mol)
Zero-point correction=	0.243985 (Hartree/Particle)
Thermal correction to Energy=	0.263940
Thermal correction to Enthalpy=	0.264884
Thermal correction to Gibbs Free Energy=	0.195245
Sum of electronic and zero-point Energies=	-968.123175
Sum of electronic and thermal Energies=	-968.103220
Sum of electronic and thermal Enthalpies=	-968.102276
Sum of electronic and thermal Free Energies=	-968.171914

cartesian

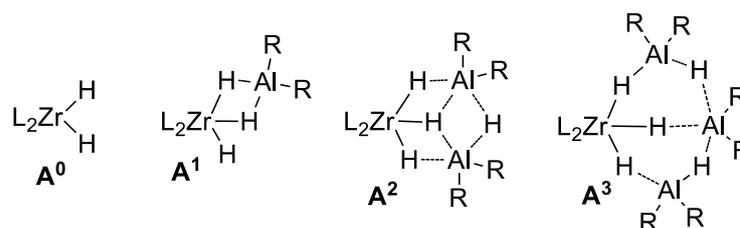
1	-1.00189996	0.11320000	0.76520002	1	0.75209999	2.31599998	2.18379998
1	0.72960001	1.14390004	-0.73250002	1	-2.10960007	1.34309995	-1.98510003
13	-1.02119994	-1.48889995	0.15700001	1	-3.00430012	2.21770000	-0.74390000
6	-0.79879999	-2.66030002	1.70449996	1	-1.79219997	3.05640006	-1.70570004
6	-2.37450004	-1.59909999	-1.25119996	1	-0.89039999	2.94180012	2.34069991
1	-0.66740000	-3.70350003	1.39600003	1	0.49620000	-1.36609995	-0.62989998
1	-1.67470002	-2.63000011	2.36179996	13	1.74460006	-0.20930000	-0.45860001
1	0.07300000	-2.38569999	2.30749989	6	2.27169991	-0.19710000	1.42680001
1	-2.66860008	-2.63619995	-1.44669998	6	2.89269996	-0.37189999	-2.02880001

1	-2.02180004	-1.17869997	-2.19880009	1	2.91930008	0.65679997	1.65750003
1	-3.28360009	-1.05209994	-0.97619998	1	2.83509994	-1.10090005	1.68659997
13	-0.65890002	1.66550004	0.12700000	1	1.41680002	-0.14470001	2.11089993
6	-0.07530000	2.77020001	1.62909997	1	3.61170006	0.45260000	-2.08500004
6	-2.01690006	2.10710001	-1.20679998	1	2.31609988	-0.36680001	-2.95889997
1	0.26150000	3.75550008	1.28750002	1	3.47199988	-1.30130005	-2.00720000

S2.2. Zr-Al complexes $L_2Zr(\mu-H)(H)(Al_xH_xMe_{2x})$ ($x = 0-3$)

As was previously demonstrated experimentally and confirmed by DFT modeling of hydroalumination and carboalumination processes, zirconocene can form different hydride-alkyl complexes with $HAlR_2$ and $ClAlR_2$. Taking into account high TIBA/Zr ratios (200:1) we proposed fully hydride structure for the complexes, and used the simplest model $(HAlMe_2)_x$ for alkyl-hydride aluminium clusters.

In our calculations, we optimized four types of complexes: dihydrides L_2ZrH_2 and adducts of L_2ZrH_2 with one, two and three molecules of Me_2AlH :



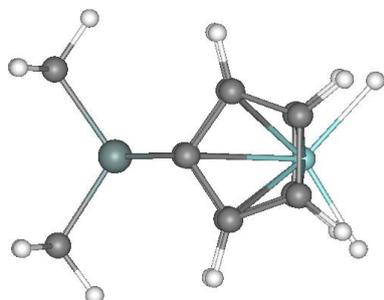
The energies of the formation of these complexes were estimated as a differences between the energies of the adducts and the energies of L_2ZrH_2 plus the energy of trimer $(Me_2AlH)_3$ taken with a factor of 1/3, 2/3 or 1 for A^1 , A^2 and A^3 species, respectively. The results of the calculations are presented in Table S1.

Table S1 The relative energies of the formation of Zr- Al_1 , Zr- Al_2 and Zr- Al_3 complexes ($kcal\ mol^{-1}$)

Zirconocene		1	2	3	4	5	6	7
A^1	ΔG	-16.93	-15.73	-13.05	-16.63	-11.64	-14.18	-14.94
	ΔH	-22.51	-21.07	-18.83	-21.39	-18.05	-20.69	-20.74
A^2	ΔG	-16.97	-11.37	-8.07	-12.24	-4.86	-12.98	-16.51
	ΔH	-26.66	-23.24	-18.22	-23.39	-18.04	-25.22	-25.98
A^3	ΔG	-23.54	-14.68	-9.54	-18.65	-10.57	-10.50	-13.13
	ΔH	-36.54	-33.26	-29.26	-39.27	-30.89	-30.87	-34.14

For **1–7**, **A³** were found to be the most stable in *H* scale and in some cases in *G* scale, so these adducts were chosen as a base for the modeling of ethyl-hydride species (see Section S2.3). Energy parameters and Cartesian coordinates for **A⁰–A³** are presented below.

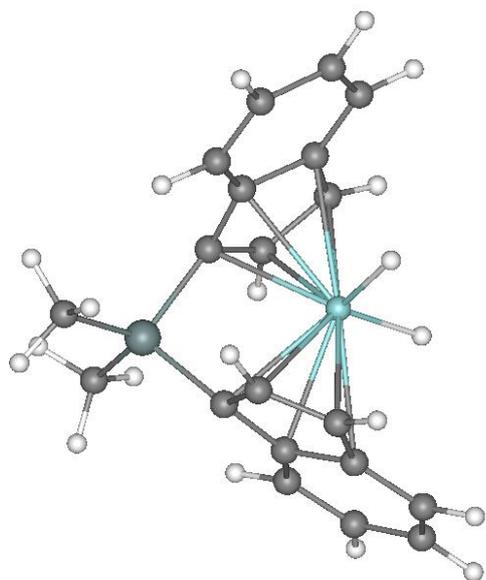
A⁰-1



Zero-point vibrational energy	621553.4 (J/mol)
	148.55482 (kcal/mol)
Zero-point correction=	0.236737 (Hartree/Particle)
Thermal correction to Energy=	0.251700
Thermal correction to Enthalpy=	0.252644
Thermal correction to Gibbs Free Energy=	0.195977
Sum of electronic and zero-point Energies=	-4296.748187
Sum of electronic and thermal Energies=	-4296.733224
Sum of electronic and thermal Enthalpies=	-4296.732280
Sum of electronic and thermal Free Energies=	-4296.788948

				cartesian			
6	1.18490005	-2.48399997	-0.67229998	1	1.97599995	2.83400011	1.38839996
6	-0.00730000	-1.85280001	-1.11090004	1	1.94659996	2.91149998	-1.31149995
6	-0.75430000	-1.41349995	0.02350000	1	-0.28020000	1.69439995	-2.14890003
6	0.02180000	-1.77750003	1.16740000	1	-0.23180000	1.55920005	2.19970012
6	1.20220006	-2.44039989	0.74280000	6	-3.05520010	0.00010000	1.54050004
1	1.97590005	-2.83410001	1.38849998	6	-2.99000001	0.00000000	-1.58120000
1	1.94649994	-2.91160011	-1.31140006	1	-3.63050008	0.88520002	-1.63820004
1	-0.28020000	-1.69439995	-2.14890003	1	-2.34590006	0.00010000	-2.46589994
14	-1.99570000	0.00000000	0.00100000	1	-3.63019991	-0.88550001	-1.63829994
1	-0.23199999	-1.55929995	2.19970012	1	-3.69659996	0.88590002	1.57169998
6	1.18490005	2.48390007	-0.67229998	1	-3.69659996	-0.88559997	1.57200003
6	-0.00720000	1.85280001	-1.11099994	1	-2.44670010	0.00030000	2.45009995
6	-0.75419998	1.41349995	0.02350000	1	2.56040001	0.00000000	1.35430002
6	0.02180000	1.77750003	1.16729999	40	1.30599999	0.00000000	-0.03500000
6	1.20220006	2.44029999	0.74269998	1	2.26929998	0.00000000	-1.63489997

A⁰-2

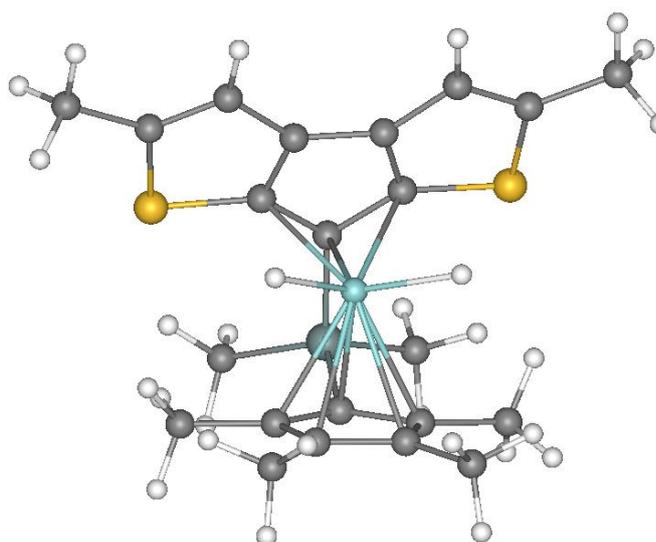


Zero-point vibrational energy	868357.8 (J/mol)
	207.54248 (kcal/mol)
Zero-point correction=	0.330740 (Hartree/Particle)
Thermal correction to Energy=	0.351097
Thermal correction to Enthalpy=	0.352041
Thermal correction to Gibbs Free Energy=	0.283542
Sum of electronic and zero-point Energies=	-4603.814265
Sum of electronic and thermal Energies=	-4603.793908
Sum of electronic and thermal Enthalpies=	-4603.792964
Sum of electronic and thermal Free Energies=	-4603.861463

			cartesian				
1	0.95889997	2.10479999	1.10440004	1	3.50690007	2.72709990	-1.40890002
1	-0.96530002	2.09050012	-1.12179995	6	-3.97950006	0.44440001	-1.09660006
40	-0.00050000	0.96350002	-0.00400000	6	-4.16639996	1.60270000	-0.28889999
6	2.18160009	-0.29229999	-0.33579999	6	-3.36540008	1.84449995	0.79729998
6	2.35509992	0.89679998	-1.13090003	6	-3.00690007	-0.48199999	-0.80879998
6	1.37839997	0.86220002	-2.17650008	1	-2.89809990	-1.37440002	-1.41949999
6	0.65880001	-0.34270000	-2.04010010	1	-4.62550020	0.29179999	-1.95580006
6	1.10350001	-1.07480001	-0.89270002	1	-4.94789982	2.30839992	-0.55140001
6	-1.37129998	0.86940002	2.17309999	1	-3.49979997	2.73410010	1.40559995
6	-1.10189998	-1.07179999	0.89420003	6	-0.91769999	-3.36680007	-1.23769999
6	-2.18199992	-0.29089999	0.33910000	6	0.91500002	-3.36759996	1.24109995
6	-2.35170007	0.90100002	1.13090003	1	0.28040001	-4.20580006	1.54709995
14	-0.00040000	-2.30399990	0.00130000	1	1.18509996	-2.82010007	2.14840007

6	-0.65270001	-0.33629999	2.03769994	1	1.83109999	-3.78169990	0.80860001
6	3.97340012	0.44720000	1.10490000	1	-1.83169997	-3.78329992	-0.80299997
6	4.16520023	1.60189998	0.29290000	1	-0.28259999	-4.20319986	-1.54709995
6	3.36899996	1.84019995	-0.79740000	1	-1.19180000	-2.81809998	-2.14299989
6	3.00139999	-0.47950000	0.81650001	1	-0.17749999	-0.62620002	-2.67230010
1	2.88910007	-1.36940002	1.43019998	1	1.23940003	1.60529995	-2.95090008
1	4.61539984	0.29760000	1.96749997	1	0.18600000	-0.61820000	2.66759992
1	4.94670010	2.30760002	0.55570000	1	-1.22930002	1.61459994	2.94470000

A⁰-3



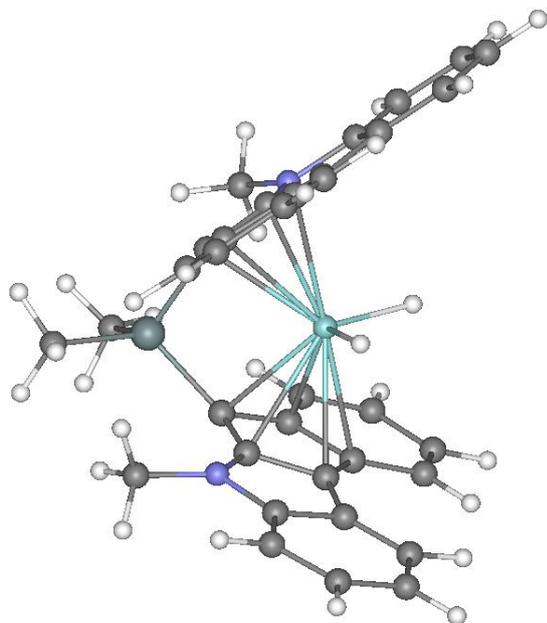
Zero-point vibrational energy	1137292.6 (Joules/Mol)
	271.81945 (Kcal/Mol)
Zero-point correction=	0.433172 (Hartree/Particle)
Thermal correction to Energy=	0.463122
Thermal correction to Enthalpy=	0.464066
Thermal correction to Gibbs Free Energy=	0.376501
Sum of electronic and zero-point Energies=	-5480.974161
Sum of electronic and thermal Energies=	-5480.944211
Sum of electronic and thermal Enthalpies=	-5480.943267
Sum of electronic and thermal Free Energies=	-5481.030832

cartesian

1	1.46669996	-0.13150001	-2.06030011	6	-3.40100002	-1.96700001	-0.60960001
1	-1.46379995	0.45539999	-2.00090003	6	-2.26799989	-2.51670003	-1.11520004
6	0.84630001	-1.50940001	0.66600001	1	-2.27360010	-3.20869994	-1.95000005
6	0.33100000	-2.29410005	-0.40230000	6	-4.81020021	-2.14820004	-1.08519995
6	-1.08190000	-2.06340003	-0.43399999	1	-5.20779991	-1.21550000	-1.49530005
6	-1.36930001	-1.15279996	0.61930001	1	-4.83720016	-2.90569997	-1.87090003

6	-0.18200000	-0.74599999	1.32819998	1	-5.46859980	-2.47149992	-0.27450001
40	0.05080000	0.29449999	-0.91159999	6	3.86730003	-3.54999995	-0.90090001
6	1.26610005	2.51530004	-1.25590003	1	3.68530011	-4.29180002	-1.68079996
6	1.56910002	2.03200006	0.04410000	1	4.55060005	-2.79520011	-1.30040002
6	0.36330000	2.02220011	0.83109999	1	4.36320019	-4.04799986	-0.06340000
6	-0.67979997	2.52559996	-0.02600000	6	-2.11730003	2.79410005	0.34729999
6	-0.12530001	2.81599998	-1.30079997	6	-0.84240001	3.43269992	-2.46910000
16	-3.08800006	-0.86669999	0.72670001	6	2.25979996	2.79439998	-2.34719992
14	0.04950000	0.85579997	2.28590012	6	2.96930003	1.70319998	0.48989999
6	2.56820011	-2.93149996	-0.48269999	1	-1.90240002	3.17429996	-2.46709991
6	1.34029996	-3.10820007	-1.03100002	1	-0.74710000	4.52440023	-2.44899988
16	2.56690001	-1.75979996	0.82999998	1	-0.42550001	3.07890010	-3.41499996
1	1.15999997	-3.78119993	-1.86189997	1	-2.54769993	3.52539992	-0.34070000
6	-1.51359999	1.25800002	3.23510003	1	-2.74990010	1.90230000	0.30849999
6	1.47909999	0.71020001	3.49280000	1	-2.17799997	3.21530008	1.35339999
1	1.93830001	1.68369997	3.69050002	1	1.82710004	2.61500001	-3.33400011
1	2.26399994	0.02920000	3.15149999	1	2.58780003	3.83960009	-2.30850005
1	1.10380006	0.31610000	4.44309998	1	3.13949990	2.15499997	-2.25349998
1	-1.44850004	2.25289989	3.68840003	1	2.98810005	1.19340003	1.45330000
1	-1.63469994	0.52929997	4.04370022	1	3.48370004	1.06449997	-0.23330000
1	-2.42000008	1.22829998	2.62599993	1	3.54629993	2.62930012	0.59469998

A⁰-4



Zero-point vibrational energy

1425841.8 (Joules/Mol)

340.78437 (Kcal/Mol)

Zero-point correction=

0.543074 (Hartree/Particle)

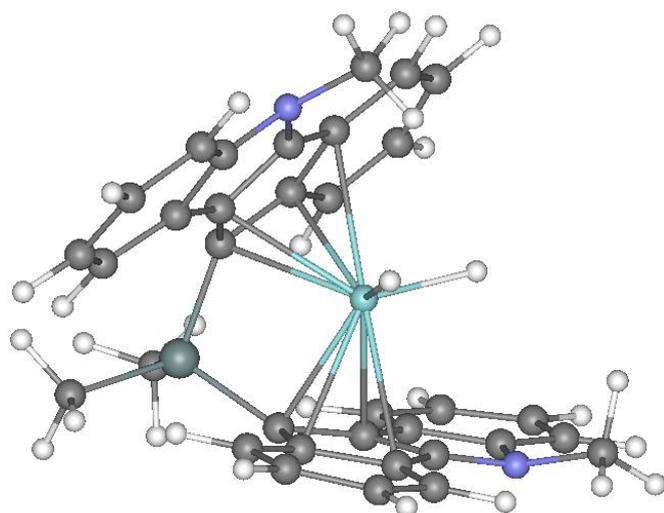
Thermal correction to Energy=	0.575962
Thermal correction to Enthalpy=	0.576907
Thermal correction to Gibbs Free Energy=	0.482451
Sum of electronic and zero-point Energies=	-5252.411840
Sum of electronic and thermal Energies=	-5252.378952
Sum of electronic and thermal Enthalpies=	-5252.378008
Sum of electronic and thermal Free Energies=	-5252.472464

cartesian

6	-0.42960000	-2.04169989	0.86100000	1	-0.23019999	2.03600001	4.30569983
6	-1.15610003	-2.34850001	-0.34840000	1	-1.50109994	0.83999997	4.56209993
6	-2.22909999	-1.40059996	-0.43250000	1	-1.68690002	2.08089995	3.32279992
6	-2.18210006	-0.60200000	0.73989999	6	-4.03719997	-0.01310000	-0.38450000
6	-1.02719998	-0.88499999	1.54859996	6	-3.43269992	-1.04209995	-1.14960003
6	2.24309993	1.31490004	-0.62199998	6	-4.04589987	-1.47660005	-2.32509995
6	2.17459989	0.70050001	0.65579998	6	-5.22809982	0.59219998	-0.78160000
6	1.02639997	1.13110006	1.40869999	6	3.43460011	0.82029998	-1.27660000
6	0.46070001	2.18939996	0.55659997	6	4.00759983	-0.10360000	-0.36739999
6	1.19260001	2.28940010	-0.68510002	6	3.70269990	-0.77819997	2.02300000
7	-3.27060008	0.24900000	0.75279999	6	5.17269993	-0.80510002	-0.66930002
14	-0.01460000	0.21930000	2.69280005	6	4.05819988	1.05299997	-2.50300002
7	3.23850012	-0.17170000	0.79579997	6	-3.74110007	1.02750003	1.87600005
6	1.10270000	-3.84179997	0.31490001	1	-4.82709980	0.92879999	1.95369995
6	0.35010001	-4.16429996	-0.83880001	1	-3.29830003	0.63190001	2.79099989
6	-0.75700003	-3.42120004	-1.18110001	1	-3.48930001	2.08859992	1.77359998
6	0.73610002	-2.80060005	1.14339995	1	-3.59509993	-2.26090002	-2.92549992
1	1.30700004	-2.61039996	2.04390001	6	-5.24289989	-0.88450003	-2.71989989
1	1.98080003	-4.43109989	0.56050003	6	-5.82420015	0.13820000	-1.95669997
1	0.66070002	-4.99329996	-1.46609998	1	-5.67640018	1.39810002	-0.20810001
1	-1.32869995	-3.65319991	-2.07419991	1	-5.72980022	-1.21179998	-3.63290000
6	-1.01479995	3.93449998	-0.25920001	1	-6.75290012	0.59119999	-2.28940010
6	-0.26650000	4.04489994	-1.45400000	1	4.78749990	-0.66009998	2.09689999
6	0.81620002	3.22490001	-1.67799997	1	3.24650002	-0.26100001	2.86770010
6	-0.67670000	3.02340007	0.72140002	1	3.45980000	-1.84549999	2.06979990
1	-1.24590003	2.99979997	1.64289999	1	3.63389993	1.75419998	-3.21499991
1	-1.86950004	4.58589983	-0.10490000	6	5.23089981	0.36489999	-2.80530000
1	-0.56080002	4.77120018	-2.20449996	6	5.77850008	-0.55500001	-1.89929998
1	1.38779998	3.29390001	-2.59840012	1	5.59210014	-1.53240001	0.01960000
6	-0.96980000	1.41059995	3.79180002	1	6.68639994	-1.08870006	-2.16190004
6	0.92409998	-0.77329999	3.98690009	1	5.72300005	0.53420001	-3.75749993
1	1.47819996	-0.08500000	4.63560009	1	1.07959998	-1.05379999	-1.60049999

1	1.62010002	-1.53299999	3.63829994	1	-1.13940001	0.88849998	-1.68970001
1	0.17800000	-1.27890003	4.61100006	40	-0.00920000	-0.01180000	-0.53119999

A⁰-5



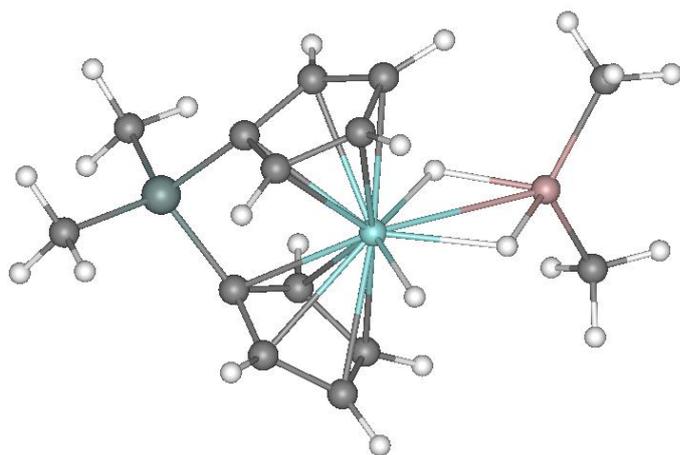
Zero-point vibrational energy	1422820.2 (Joules/Mol)
	340.06220 (Kcal/Mol)
Zero-point correction=	0.541924 (Hartree/Particle)
Thermal correction to Energy=	0.575167
Thermal correction to Enthalpy=	0.576111
Thermal correction to Gibbs Free Energy=	0.480697
Sum of electronic and zero-point Energies=	-5252.413084
Sum of electronic and thermal Energies=	-5252.379841
Sum of electronic and thermal Enthalpies=	-5252.378896
Sum of electronic and thermal Free Energies=	-5252.474311

cartesian

1	1.29639995	0.59280002	-1.87370002	1	-1.92289996	0.04220000	4.11999989
1	-1.29680002	-0.59299999	-1.87259996	1	-1.88619995	-1.54330003	3.32520008
40	0.00010000	0.00030000	-0.66430002	1	-0.71069998	-1.15939999	4.56860018
6	-0.10310000	-2.17880011	0.51899999	1	0.71060002	1.16209996	4.56710005
6	0.60619998	-2.54239988	-0.69510001	1	1.92130005	-0.04230000	4.12179995
6	1.85619998	-1.85350001	-0.62400001	1	1.88810003	1.54190004	3.32439995
6	1.92630005	-1.12500000	0.58759999	6	3.85920000	-0.88400000	-0.62819999
6	0.68879998	-1.26059997	1.32669997	7	3.04670000	-1.76660001	-1.32959998
6	-1.85650003	1.85380006	-0.62360001	6	3.95120001	0.30550000	1.48889995
6	-1.92630005	1.12500000	0.58780003	6	5.11700010	-0.39919999	-0.99610001
6	-0.68870002	1.26059997	1.32690001	7	-3.04690003	1.76670003	-1.32910001
6	0.10300000	2.17899990	0.51920003	6	-3.85929990	0.88370001	-0.62779999

6	-0.60650003	2.54279995	-0.69470000	6	-5.11679983	0.39870000	-0.99580002
6	3.24000001	-0.49759999	0.59079999	6	-3.95059991	-0.30660000	1.48889995
14	0.00010000	0.00000000	2.54760003	1	3.53130007	0.55599999	2.45639992
6	-3.23979998	0.49710000	0.59100002	6	5.21449995	0.76730001	1.13859999
6	-1.98239994	-3.49569988	-0.28000000	6	5.78149986	0.43160000	-0.10180000
6	-1.24450004	-3.90590000	-1.42130005	1	5.57030010	-0.66380000	-1.94610000
6	0.02260000	-3.42750001	-1.64199996	1	5.77089977	1.39199996	1.83000004
6	-1.44210005	-2.64849997	0.65960002	1	6.76230001	0.81650001	-0.36350000
1	-2.03539991	-2.36599994	1.52079999	1	-3.53040004	-0.55769998	2.45609999
1	-2.99839997	-3.85330009	-0.14510000	6	-5.21379995	-0.76870000	1.13839996
1	-1.69739997	-4.58519983	-2.13590002	6	-5.78109980	-0.43270001	-0.10180000
1	0.57529998	-3.72729993	-2.52620006	1	-5.57030010	0.66329998	-1.94570005
6	1.98230004	3.49569988	-0.27990001	1	-6.76170015	-0.81790000	-0.36359999
6	1.24430001	3.90619993	-1.42110002	1	-5.76989985	-1.39400005	1.82959998
6	-0.02300000	3.42790008	-1.64160001	6	-3.15240002	1.96599996	-2.76180005
6	1.44200003	2.64849997	0.65960002	1	-2.78950000	1.08459997	-3.30360007
1	2.03550005	2.36590004	1.52079999	1	-2.56419992	2.83759999	-3.04780006
1	2.99839997	3.85319996	-0.14520000	1	-4.19229984	2.16380000	-3.02710009
1	1.69710004	4.58540010	-2.13569999	6	3.15140009	-1.96490002	-2.76250005
1	-0.57569999	3.72779989	-2.52570009	1	4.19119978	-2.16249990	-3.02859998
6	1.26760006	0.74040002	3.72230005	1	2.78810000	-1.08309996	-3.30340004
6	-1.26750004	-0.74000001	3.72250009	1	2.56299996	-2.83629990	-3.04879999

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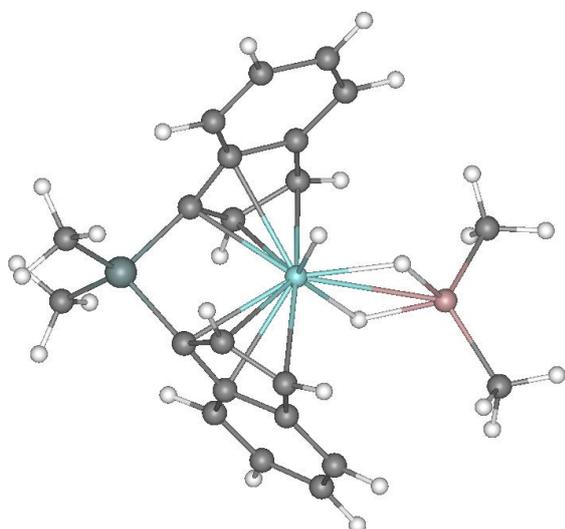


Zero-point vibrational energy	839783.6 (Joules/Mol)
	839783.6 (Kcal/Mol)
Zero-point correction=	0.319857 (Hartree/Particle)
Thermal correction to Energy=	0.340836
Thermal correction to Enthalpy=	0.341781

Thermal correction to Gibbs Free Energy=	0.270792
Sum of electronic and zero-point Energies=	-4619.490830
Sum of electronic and thermal Energies=	-4619.469850
Sum of electronic and thermal Enthalpies=	-4619.468906
Sum of electronic and thermal Free Energies=	-4619.539895

				cartesian			
6	-4.07359982	-1.72940004	0.76590002	14	2.64700007	0.00000000	0.69029999
1	-0.75139999	0.00020000	-2.36640000	1	1.93789995	-1.43990004	-2.08800006
1	-1.60290003	0.00030000	1.05470002	6	-0.49620000	2.50909996	-0.08130000
13	-3.20320010	-0.00010000	0.40830001	6	0.41100001	1.90859997	0.83759999
1	-2.36879992	-0.00030000	-1.09329998	6	1.53960001	1.41129994	0.12310000
6	-4.07439995	1.72899997	0.76450002	6	1.29489994	1.70790005	-1.25619996
1	-4.01550007	2.40450001	-0.09660000	6	0.06080000	2.39400005	-1.37619996
1	-5.13570023	1.61430001	1.01080000	1	-0.38319999	2.74580002	-2.29809999
1	-3.60619998	2.24679995	1.61059999	1	-1.44000006	2.97849989	0.17100000
1	-5.13329983	-1.61450005	1.01890004	1	0.24830000	1.82200003	1.90600002
1	-4.02050018	-2.40260005	-0.09740000	1	1.93750000	1.44060004	-2.08800006
1	-3.60069990	-2.24970007	1.60780001	40	-0.39910001	0.00000000	-0.56639999
6	-0.49630001	-2.50900006	-0.08220000	6	4.27670002	-0.00020000	-0.22360000
6	0.41069999	-1.90880001	0.83710003	6	2.84109998	0.00010000	2.54839993
6	1.53939998	-1.41129994	0.12310000	1	3.38800001	0.88639998	2.88360000
6	1.29509997	-1.70749998	-1.25639999	1	1.87109995	-0.00260000	3.05530000
6	0.06110000	-2.39359999	-1.37689996	1	3.39269996	-0.88349998	2.88319993
1	-0.38270000	-2.74510002	-2.29900002	1	4.86679983	0.88499999	0.03150000
1	-1.44009995	-2.97860003	0.16970000	1	4.86609983	-0.88609999	0.03050000
1	0.24770001	-1.82270002	1.90559995	1	4.13290024	0.00050000	-1.30859995

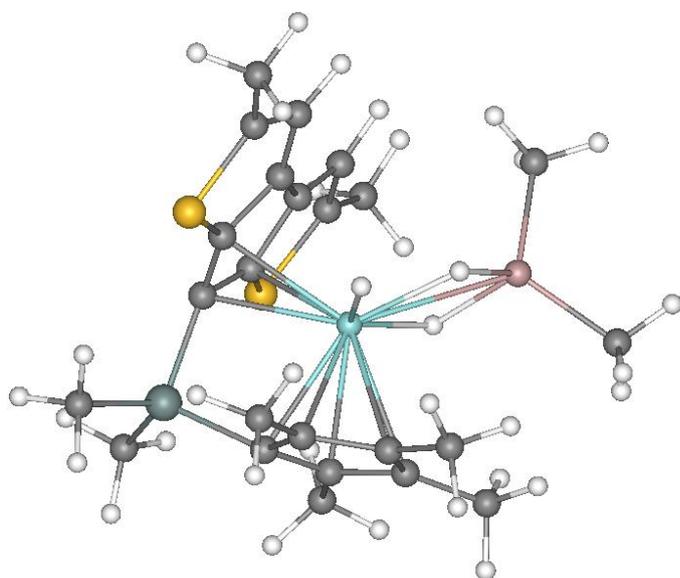
A¹⁻²



Zero-point vibrational energy	1088462.1 (Joules/Mol)
	260.14868 (Kcal/Mol)
Zero-point correction=	0.414573 (Hartree/Particle)
Thermal correction to Energy=	0.441441
Thermal correction to Enthalpy=	0.442385
Thermal correction to Gibbs Free Energy=	0.359169
Sum of electronic and zero-point Energies=	-4926.555105
Sum of electronic and thermal Energies=	-4926.528238
Sum of electronic and thermal Enthalpies=	-4926.527293
Sum of electronic and thermal Free Energies=	-4926.610509

				cartesian			
6	-2.31069994	0.81500000	0.31740001	1	3.95070004	-0.95899999	-1.64950001
6	-1.58959997	1.93980002	0.85240000	6	-1.83239996	-3.38420010	1.70869994
6	-0.69190001	1.44599998	1.84879994	6	-3.38590002	-2.48309994	-0.79159999
6	-0.88669997	0.04870000	1.94099998	1	-3.42880011	-3.55369997	-1.01789999
6	-1.85880005	-0.38560000	0.98140001	1	-3.33270001	-1.95070004	-1.74539995
6	1.08399999	-1.05309999	-2.27099991	1	-4.32429981	-2.20889997	-0.29940000
6	-0.34220001	-2.06200004	-0.71789998	1	-1.40769994	-4.33519983	1.37259996
6	1.00320005	-2.05850005	-0.18940000	1	-2.84290004	-3.58119988	2.08170009
6	1.88189995	-1.45780003	-1.15960002	1	-1.24179995	-3.02699995	2.55690002
14	-1.91289997	-2.14030004	0.31029999	1	-0.32470000	-0.60390002	2.60249996
6	-0.24640000	-1.45739996	-2.01180005	1	-0.01820000	2.04180002	2.45339990
6	-3.55480003	2.31360006	-1.10730004	1	-1.07879996	-1.27779996	-2.68300009
6	-2.82080007	3.42280006	-0.58960003	1	1.43710005	-0.56260002	-3.16969991
6	-1.85080004	3.25250006	0.36289999	6	2.23309994	3.59120011	1.44060004
6	-3.30410004	1.03489995	-0.68519998	1	-0.58270001	1.20109999	-1.72379994
1	-3.87619996	0.20119999	-1.08099997	1	1.83840001	0.67790002	0.73530000
1	-4.32040024	2.49130011	-1.85590005	13	2.44589996	2.16339993	0.10080000
1	-3.04020000	4.41890001	-0.96109998	1	1.08560002	2.02530003	-0.93690002
1	-1.30130005	4.10099983	0.76040000	6	4.13159990	1.93499994	-0.88520002
6	2.89829993	-2.42670012	1.26400006	1	3.98160005	1.48810005	-1.87399995
6	3.76839995	-1.86220002	0.28220001	1	4.63019991	2.89930010	-1.03760004
6	3.28299999	-1.38010001	-0.90410000	1	4.83519983	1.29480004	-0.34000000
6	1.54809999	-2.52509999	1.04639995	1	2.94779992	4.40710020	1.28520000
1	0.90520000	-2.99259996	1.78690004	1	1.23090005	4.03480005	1.42789996
1	3.32060003	-2.79800010	2.19250011	1	2.40330005	3.21309996	2.45650005
1	4.83409977	-1.81840003	0.48449999	40	0.14410000	0.33579999	-0.29690000

A¹-3



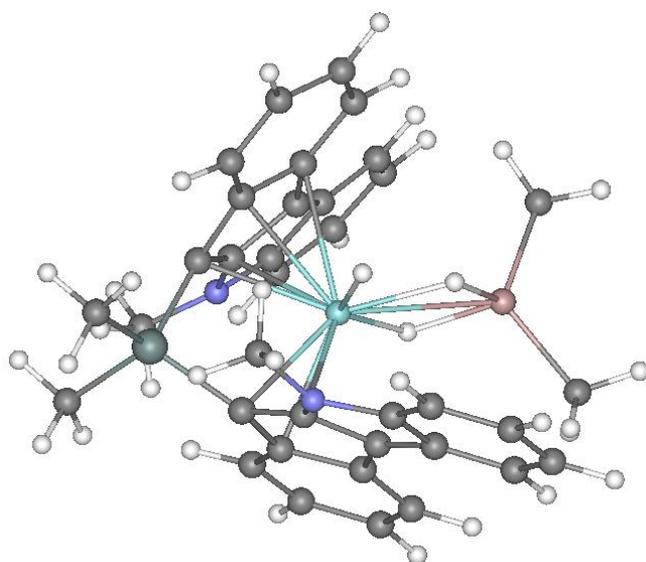
Zero-point vibrational energy	1358312.8 (Joules/Mol)
	324.64454 (Kcal/Mol)
Zero-point correction=	0.517354 (Hartree/Particle)
Thermal correction to Energy=	0.553523
Thermal correction to Enthalpy=	0.554468
Thermal correction to Gibbs Free Energy=	0.452938
Sum of electronic and zero-point Energies=	-5803.714187
Sum of electronic and thermal Energies=	-5803.678018
Sum of electronic and thermal Enthalpies=	-5803.677074
Sum of electronic and thermal Free Energies=	-5803.778604

cartesian

6	1.48399997	-1.52530003	0.12760000	1	2.08949995	-4.15129995	-3.61330009
6	0.38220000	-2.26290011	-0.39289999	1	3.09179997	-2.69970012	-3.76760006
6	-0.71079999	-2.05530000	0.50360000	1	3.63790011	-4.04829979	-2.75950003
6	-0.23780000	-1.18869996	1.53320003	6	-0.90910000	2.67280006	2.09430003
6	1.13709998	-0.81910002	1.33379996	6	-1.75320005	3.64030004	-0.75269997
6	0.58319998	2.65140009	-1.34840000	6	0.60990000	3.00589991	-2.80749989
6	1.65989995	2.07739997	-0.61449999	6	3.01580000	1.79890001	-1.20500004
6	1.26240003	1.95710003	0.76319999	1	-2.62290001	3.17919993	-0.27930000
6	-0.08300000	2.46059990	0.84890002	1	-1.67490005	4.67110014	-0.38800001
6	-0.48449999	2.89610004	-0.44560000	1	-1.94420004	3.68219995	-1.82620001
16	-1.45879996	-0.97530001	2.76959991	1	-1.75049996	3.33419991	1.87440002
14	1.98010004	0.72160000	1.99720001	1	-1.32640004	1.74989998	2.50519991
6	2.04200006	-2.88290000	-1.90240002	1	-0.31009999	3.15170002	2.87369990
6	0.73430002	-3.02320004	-1.56490004	1	-0.37840000	2.89759994	-3.26180005
16	2.92529988	-1.81879997	-0.81699997	1	0.93529999	4.04260015	-2.94970012

1	0.04470000	-3.63890004	-2.13210011	1	1.29499996	2.35459995	-3.35389996
6	1.44990003	1.04470003	3.76419997	1	3.61610007	1.14989996	-0.56739998
6	3.84780002	0.55379999	1.94340003	1	2.93359995	1.31330001	-2.17989993
1	4.33230019	1.52839994	1.82939994	1	3.56450009	2.73970008	-1.32990003
1	4.20190001	-0.09460000	1.13730001	6	-3.71359992	-1.61710000	-1.90090001
1	4.19509983	0.11520000	2.88479996	1	0.81519997	0.02920000	-2.01449990
1	1.79719996	2.02640009	4.10309982	1	-2.17129993	0.49810001	-0.20430000
1	1.90470004	0.28900000	4.41370010	13	-2.82890010	0.13959999	-1.76580000
1	0.36919999	1.00259995	3.91910005	1	-1.18239999	0.05250000	-2.22000003
6	-2.56809998	-2.04069996	1.91090000	6	-3.77500010	1.66289997	-2.58969998
6	-2.04640007	-2.53570008	0.76150000	1	-3.12759995	2.28480005	-3.21810007
1	-2.59209991	-3.21869993	0.12120000	1	-4.57350016	1.28240001	-3.23810005
6	-3.93639994	-2.27460003	2.47440004	1	-4.25070000	2.32929993	-1.86170006
1	-4.51709986	-1.34780002	2.49449992	1	-4.38789988	-1.62370002	-2.76589990
1	-4.46829987	-2.99760008	1.85249996	1	-3.00539994	-2.44160008	-2.03880000
1	-3.88860011	-2.66669989	3.49399996	1	-4.32359982	-1.85020006	-1.02010000
6	2.75979996	-3.47849989	-3.07520008	40	-0.13090000	0.33890000	-0.48789999

A¹⁻⁴



Zero-point vibrational energy	1645737.7 (Joules/Mol)
	393.34076 (Kcal/Mol)
Zero-point correction=	0.626828 (Hartree/Particle)
Thermal correction to Energy=	0.665967
Thermal correction to Enthalpy=	0.666911
Thermal correction to Gibbs Free Energy=	0.559625
Sum of electronic and zero-point Energies=	-5575.151827

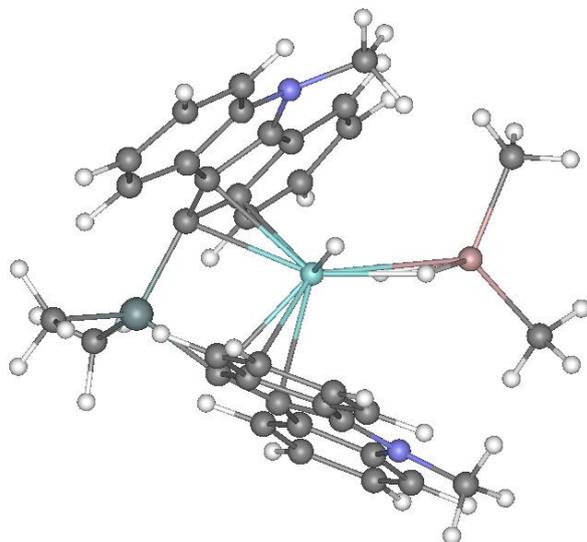
Sum of electronic and thermal Energies=	-5575.112688
Sum of electronic and thermal Enthalpies=	-5575.111744
Sum of electronic and thermal Free Energies=	-5575.219030

cartesian

6	-0.62000000	-1.86730003	-1.71140003	6	-4.16540003	1.44579995	-1.55190003
6	-1.36500001	-0.73790002	-2.21849990	6	-4.98089981	0.59549999	1.02999997
6	-2.27080011	-0.33970001	-1.18030000	6	3.53010011	1.22150004	0.58499998
6	-2.08290005	-1.23239994	-0.09110000	6	4.19119978	0.13740000	-0.04500000
6	-0.99760002	-2.14790010	-0.31779999	6	3.71339989	-2.27509999	-0.54189998
6	2.32550001	0.66020000	1.15480006	6	5.37979984	0.32420000	-0.75059998
6	2.33069992	-0.73220003	0.86610001	6	4.10160017	2.49480009	0.55260003
6	1.16989994	-1.39429998	1.40489995	6	-3.48589993	-1.90670002	1.89950001
6	0.51410002	-0.32390001	2.18099999	1	-4.52950001	-2.18370008	1.71480000
6	1.22580004	0.92159998	2.03090000	1	-2.87739992	-2.80909991	1.84909999
7	-3.03749990	-0.97619998	0.88389999	1	-3.41000009	-1.47560000	2.90319991
14	0.19450000	-2.93449998	0.91890001	1	-3.87059999	1.76970005	-2.54439998
7	3.48709989	-1.04789996	0.18089999	6	-5.28529978	2.00000000	-0.93610001
6	0.42640001	-2.07879996	-3.88689995	6	-5.68440008	1.58249998	0.34140000
6	-0.26870000	-0.93330002	-4.35430002	1	-5.29489994	0.27149999	2.01799989
6	-1.15460002	-0.26870000	-3.54040003	1	-5.85659981	2.76480007	-1.45220006
6	0.27100000	-2.53340006	-2.59899998	1	-6.55830002	2.03189993	0.80260003
1	0.78179997	-3.43549991	-2.28449988	1	4.76160002	-2.33310008	-0.83690000
1	1.09089994	-2.60870004	-4.56239986	1	3.50090003	-3.12319994	0.11050000
1	-0.11320000	-0.59240001	-5.37279987	1	3.08240008	-2.31990004	-1.44060004
1	-1.71650004	0.58440000	-3.90840006	1	3.62100005	3.32990003	1.05280006
6	-1.08350003	0.83429998	3.59270000	6	5.29740000	2.68099999	-0.13440000
6	-0.33770001	2.03480005	3.48490000	6	5.92119980	1.60710001	-0.78609997
6	0.80000001	2.08719993	2.71460009	1	5.87869978	-0.49399999	-1.25989997
6	-0.67320001	-0.31860000	2.95970011	1	6.84600019	1.77600002	-1.32869995
1	-1.23839998	-1.23099995	3.09879994	1	5.74809980	3.66729999	-0.17510000
1	-1.98380005	0.81830001	4.19969988	6	-1.58860004	3.50710011	-2.21539998
1	-0.67110002	2.92100000	4.01560020	1	1.46039999	-0.15510000	-1.48590004
1	1.37619996	3.00340009	2.63549995	1	-0.92869997	1.71959996	0.23880000
6	-0.57110000	-3.79189992	2.41079998	13	-0.33660001	2.96790004	-0.79939997
6	1.16670001	-4.34679985	0.15189999	1	0.69139999	1.70980000	-1.35060000
1	1.82470000	-4.78490019	0.91079998	6	0.58200002	4.37340021	0.22370000
1	1.77260005	-4.11420012	-0.72009999	1	1.59669995	4.08780003	0.51800001
1	0.44790000	-5.12150002	-0.14060000	1	0.66360003	5.29169989	-0.36970001
1	0.24830000	-4.28030014	2.95090008	1	0.03230000	4.62970018	1.13730001
1	-1.24839997	-4.58419991	2.07170010	1	-1.16090000	4.34700012	-2.77740002

1	-1.10220003	-3.17849994	3.13709998	1	-1.79359996	2.71040010	-2.93770003
6	-3.86269999	0.04450000	0.40750000	1	-2.54929996	3.84780002	-1.81309998
6	-3.43540001	0.46770000	-0.87559998	40	0.14460000	0.08650000	-0.25150001

A¹-5



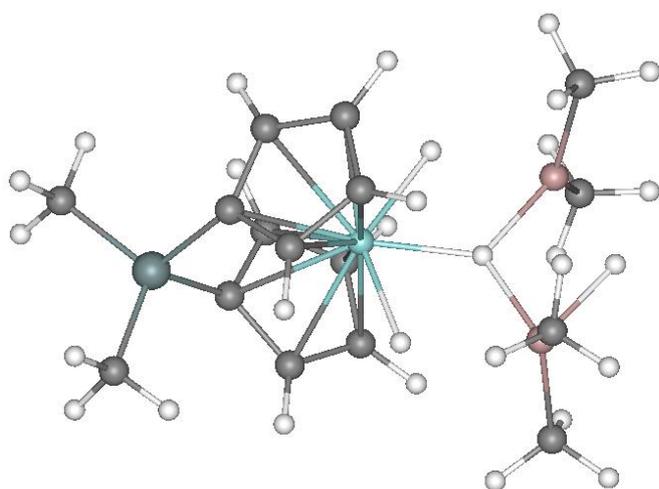
Zero-point vibrational energy	1644057.1 (Joules/Mol)
	392.93908 (Kcal/Mol)
Zero-point correction=	0.626188 (Hartree/Particle)
Thermal correction to Energy=	0.665653
Thermal correction to Enthalpy=	0.666598
Thermal correction to Gibbs Free Energy=	0.558179
Sum of electronic and zero-point Energies=	-5575.148828
Sum of electronic and thermal Energies=	-5575.109363
Sum of electronic and thermal Enthalpies=	-5575.108419
Sum of electronic and thermal Free Energies=	-5575.216838

cartesian

6	-0.34869999	-2.20180011	-0.82010001	6	3.59270000	-1.21819997	1.84619999
6	0.49680001	-1.78709996	-1.91789997	6	5.12669992	-0.58730000	-0.45150000
6	1.73169994	-1.39810002	-1.31620002	7	-3.12150002	2.11199999	0.01440000
6	1.66170001	-1.56739998	0.08840000	6	-3.97560000	1.02349997	-0.14170000
6	0.34130001	-2.03609991	0.45500001	6	-5.15730000	0.95910001	-0.88209999
6	-2.03520012	1.66250002	0.74930000	6	-4.27869987	-1.25119996	0.65460002
6	-2.21269989	0.31209999	1.14769995	1	3.02440000	-1.48559999	2.72939992
6	-1.10169995	-0.11390000	1.96650004	6	4.93389988	-0.87290001	1.95959997
6	-0.26780000	1.06809998	2.08240008	6	5.68959999	-0.55690002	0.81870002
6	-0.84219998	2.17670012	1.33319998	1	5.72590017	-0.34729999	-1.32459998
6	2.99130011	-1.24240005	0.58420002	1	5.40520000	-0.85329998	2.93689990

14	-0.49759999	-1.88629997	2.13240004	1	6.73600006	-0.28900000	0.92699999
6	-3.49510002	-0.09610000	0.58780003	1	-3.97090006	-2.09179997	1.26689994
6	-2.09780002	-2.65899992	-2.43889999	6	-5.47230005	-1.30980003	-0.05770000
6	-1.24090004	-2.28209996	-3.50710011	6	-5.89389992	-0.22020000	-0.83490002
6	0.03400000	-1.83899999	-3.25900006	1	-5.50309992	1.80170000	-1.47239995
6	-1.67890000	-2.60820007	-1.13189995	1	-6.81930017	-0.29010001	-1.39810002
1	-2.36549997	-2.89639997	-0.34650001	1	-6.08389997	-2.20519996	-0.01250000
1	-3.11260009	-2.97729993	-2.65610003	6	-3.03990006	3.20709991	-0.93269998
1	-1.60689998	-2.32990003	-4.52750015	1	-2.48620009	2.90660000	-1.83150005
1	0.68290001	-1.53639996	-4.07499981	1	-2.53870010	4.05420017	-0.46259999
6	1.53980005	2.54229999	2.75720000	1	-4.04549980	3.52659988	-1.20949996
6	0.93400002	3.63369989	2.06879997	6	0.84179997	4.17170000	-1.60459995
6	-0.23050000	3.46329999	1.36790001	1	-1.40429997	0.33219999	-1.55610001
6	0.96780002	1.29750001	2.76570010	1	1.54560006	1.45379996	-0.10720000
1	1.44640005	0.49810001	3.31769991	13	1.61940002	2.35870004	-1.57089996
1	2.47210002	2.70269990	3.28920007	1	0.40329999	1.25489998	-2.04929996
1	1.40040004	4.61320019	2.10610008	6	3.40930009	2.22000003	-2.38319993
1	-0.69139999	4.30530024	0.86240000	1	3.39070010	1.91199994	-3.43499994
6	0.63800001	-2.17910004	3.60050011	1	3.87120008	3.21499991	-2.36199999
6	-1.85109997	-3.16269994	2.40730000	1	4.07999992	1.54480004	-1.84189999
1	-2.57410002	-2.78990006	3.14100003	1	1.03429997	4.61199999	-2.59220004
1	-2.39409995	-3.49530005	1.52450001	1	-0.24180000	4.19649982	-1.45130002
1	-1.37699997	-4.05089998	2.84019995	1	1.29820001	4.84259987	-0.86769998
1	0.00160000	-2.38439989	4.46880007	40	-0.08470000	0.24699999	-0.29650000
1	1.24479997	-3.07399988	3.42309999	6	3.44749999	-0.97970003	-3.08489990
1	1.30299997	-1.36510003	3.88179994	1	4.43550014	-0.52270001	-3.13360000
6	3.77679992	-0.93370003	-0.56290001	1	3.49370003	-1.98670006	-3.51370001
7	3.00009990	-1.02400005	-1.70940006	1	2.76580000	-0.36090001	-3.67409992

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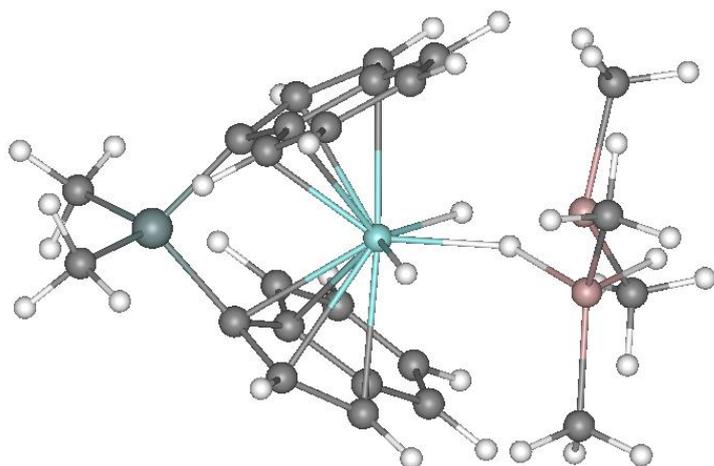


Zero-point vibrational energy	1053597.0 (Joules/Mol)
	251.81572 (Kcal/Mol)
Zero-point correction=	0.401294 (Hartree/Particle)
Thermal correction to Energy=	0.429554
Thermal correction to Enthalpy=	0.430498
Thermal correction to Gibbs Free Energy=	0.342860
Sum of electronic and zero-point Energies=	-4942.205494
Sum of electronic and thermal Energies=	-4942.177235
Sum of electronic and thermal Enthalpies=	-4942.176290
Sum of electronic and thermal Free Energies=	-4942.263928

cartesian

6	2.81060004	1.77429998	2.44910002	6	-1.48889995	1.68770003	-1.33299994
1	1.07650006	0.00060000	-1.76040006	6	-0.26969999	2.38039994	-1.13670003
1	0.49550000	-0.00210000	1.61979997	1	0.40419999	2.72029996	-1.91369998
13	2.66520000	-0.00230000	1.63510001	1	0.77100003	3.00359988	0.73979998
1	3.85450006	-0.00030000	0.34000000	1	-1.31140006	1.87919998	1.99339998
1	1.81159997	-0.00310000	0.11790000	14	-3.30110002	0.00040000	0.22070000
13	2.96059990	0.00190000	-1.24199998	1	-1.89929998	1.41079998	-2.29809999
6	3.38330007	-1.79089999	-1.91180003	6	-0.07400000	-2.52519989	0.25319999
6	3.37840009	1.79929996	-1.90260005	6	-1.18820000	-1.93980002	0.91560000
1	2.92759991	1.98590004	-2.88400006	6	-2.08669996	-1.41180003	-0.05930000
1	2.99830008	2.56669998	-1.21619999	6	-1.48989999	-1.68570006	-1.33599997
1	4.45720005	1.96420002	-1.99570000	6	-0.27120000	-2.37980008	-1.14059997
1	2.93079996	-1.97459996	-2.89299989	1	0.40250000	-2.71880007	-1.91799998
1	4.46239996	-1.95190001	-2.00799990	1	0.76870000	-3.00659990	0.73519999
1	3.00720000	-2.56259990	-1.22800004	1	-1.31330001	-1.88290000	1.99010003
6	2.81150007	-1.78050005	2.44540000	1	-1.89970005	-1.40690005	-2.30069995
1	2.98189998	-2.55550003	1.68920004	40	-0.06030000	-0.00050000	-0.19190000
1	3.66179991	-1.82599998	3.13590002	6	-4.65409994	0.00220000	-1.06690001
1	1.91530001	-2.05340004	3.01340008	6	-3.93759990	-0.00100000	1.97660005
1	3.66039991	1.81799996	3.14030004	1	-4.55100012	-0.88569999	2.17160010
1	2.98180008	2.55100012	1.69480002	1	-3.11579990	-0.00150000	2.69980001
1	1.91400003	2.04600000	3.01699996	1	-4.55100012	0.88349998	2.17300010
6	-0.07200000	2.52340007	0.25720000	1	-5.29400015	-0.87910002	-0.96230000
6	-1.18649995	1.93780005	0.91890001	1	-5.28310013	0.89240003	-0.97140002
6	-2.08559990	1.41209996	-0.05660000	1	-4.24599981	-0.00560000	-2.08240008

A²-2



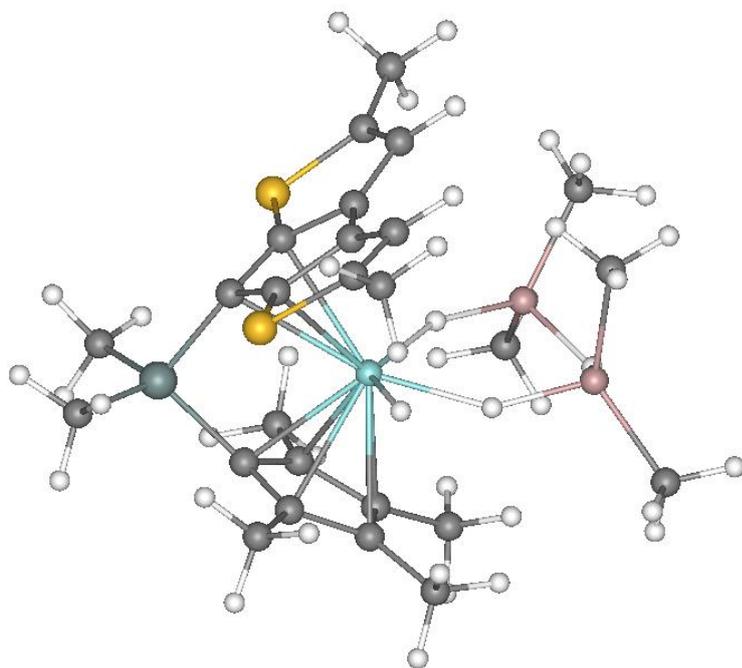
Zero-point vibrational energy	1306813.4 (Joules/Mol)
	312.33590 (Kcal/Mol)
Zero-point correction=	0.497739 (Hartree/Particle)
Thermal correction to Energy=	0.531133
Thermal correction to Enthalpy=	0.532077
Thermal correction to Gibbs Free Energy=	0.436058
Sum of electronic and zero-point Energies=	-5249.265851
Sum of electronic and thermal Energies=	-5249.232456
Sum of electronic and thermal Enthalpies=	-5249.231512
Sum of electronic and thermal Free Energies=	-5249.327532

cartesian

6	-1.14010000	-2.24769998	-0.54060000	1	-4.52990007	-2.35249996	0.91090000
6	0.02770000	-2.21160007	-1.38230002	1	-5.05670023	1.37100005	-0.39969999
6	-0.11840000	-1.10850000	-2.27920008	1	-5.39319992	-0.18850000	-1.16410005
6	-1.36619997	-0.50470001	-2.00920010	1	-4.18860006	0.88480002	-1.86619997
6	-2.01659989	-1.16499996	-0.91610003	1	-1.74179995	0.37470001	-2.52379990
6	-0.21030000	1.39690006	2.20749998	1	0.58029997	-0.81480002	-3.05240011
6	-2.15100002	0.86769998	1.02040005	1	-1.47060001	-0.32710001	2.78760004
6	-1.54020000	2.03550005	0.42559999	1	0.57260001	1.36720002	2.95479989
6	-0.35990000	2.37299991	1.17620003	6	3.15149999	0.35879999	2.89249992
14	-3.31209993	-0.32139999	0.14920001	1	0.95429999	1.24880004	-1.11829996
6	-1.31690001	0.52069998	2.12899995	1	0.62150002	-1.18309999	1.27550006
6	-0.28470001	-4.22879982	0.53759998	13	3.20860004	-0.60409999	1.18620002
6	0.87370002	-4.18699980	-0.29580000	1	4.02050018	0.36989999	0.05460000
6	1.04299998	-3.20070004	-1.23179996	1	1.92219996	-0.06460000	0.14920001
6	-1.26779997	-3.28060007	0.43669999	13	2.77539992	1.09200001	-1.09039998
1	-2.15140009	-3.33100009	1.06560004	6	3.18530011	0.00630000	-2.67549992

1	-0.38229999	-5.02899981	1.26450002	6	3.30530000	2.95519996	-0.78490001
1	1.63419998	-4.95330000	-0.18110000	1	2.65770006	3.66619992	-1.30890000
1	1.91939998	-3.18429995	-1.87339997	1	3.30310011	3.22449994	0.27689999
6	-1.15460002	3.94670010	-0.99900001	1	4.33080006	3.10130000	-1.14639997
6	-0.00960000	4.29990005	-0.22380000	1	2.61109996	0.30989999	-3.55870008
6	0.39449999	3.53259993	0.83670002	1	4.24679995	0.09940000	-2.93309999
6	-1.90740001	2.84139991	-0.69430000	1	2.99449992	-1.06070006	-2.50710011
1	-2.79929996	2.60850000	-1.26900005	6	3.70110011	-2.47519994	0.92420000
1	-1.44019997	4.57630014	-1.83580005	1	3.76799989	-2.74670005	-0.13429999
1	0.55100000	5.19189978	-0.48550001	1	4.68179989	-2.67120004	1.37440002
1	1.26380002	3.80830002	1.42620003	1	2.97700000	-3.14820004	1.39510000
6	-4.59819984	0.52359998	-0.91880000	1	4.11920023	0.27919999	3.40210009
6	-4.12809992	-1.45560002	1.39279997	1	2.95160007	1.42859995	2.76090002
1	-4.96320009	-0.93250000	1.87030005	1	2.39660001	-0.04910000	3.57360005
1	-3.44580007	-1.77199996	2.18639994	40	-0.04020000	0.01250000	0.02820000

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Zero-point vibrational energy	1572065.5 (Joules/Mol)
	375.73267 (Kcal/Mol)
Zero-point correction=	0.598768 (Hartree/Particle)
Thermal correction to Energy=	0.642198
Thermal correction to Enthalpy=	0.643142
Thermal correction to Gibbs Free Energy=	0.524245

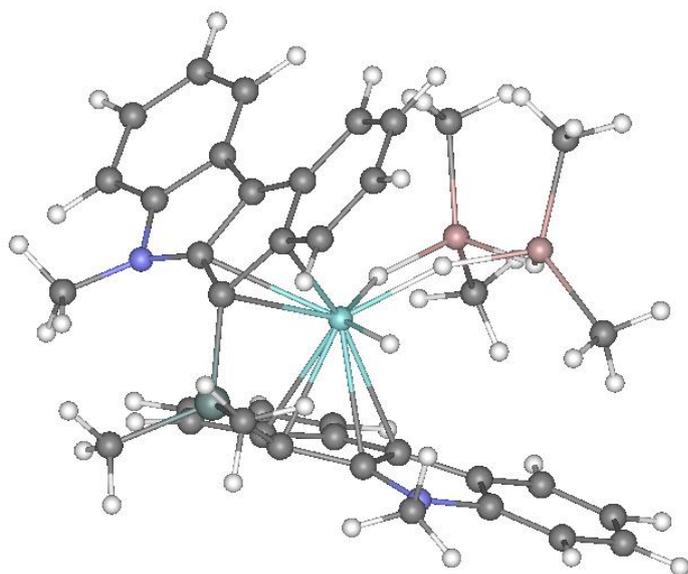
Sum of electronic and zero-point Energies=	-6126.430555
Sum of electronic and thermal Energies=	-6126.387125
Sum of electronic and thermal Enthalpies=	-6126.386181
Sum of electronic and thermal Free Energies=	-6126.505078

cartesian

6	-4.40450001	0.36539999	1.49329996	16	3.27629995	-1.01569998	1.66910005
1	0.91339999	-1.97210002	0.05210000	1	0.37140000	-1.81369996	3.73779988
1	-1.79200006	0.35450000	-0.23100001	6	2.16190004	3.61150002	-1.33529997
13	-3.47119999	0.23140000	-0.23080000	6	4.38549995	1.55289996	-0.94720000
1	-3.53020000	-1.45510006	-0.56779999	1	4.76889992	1.32200003	-1.94579995
1	-1.05949998	-1.94060004	-0.41060001	1	4.70219994	0.75349998	-0.27129999
13	-2.47079992	-2.64350009	0.08530000	1	4.87109995	2.47320008	-0.60589999
6	-2.79150009	-4.24590015	-1.00349998	1	2.48699999	3.87420011	-2.34770012
6	-2.51189995	-2.57870007	2.05069995	1	2.71869993	4.24130011	-0.63309997
1	-1.89049995	-3.38299990	2.46420002	1	1.10459995	3.87240005	-1.24670005
1	-2.10710001	-1.63250005	2.43280005	6	-1.70449996	2.52659988	2.14459991
1	-3.51839995	-2.69460011	2.46849990	6	-1.33850002	1.31780005	2.64100003
1	-1.93830001	-4.93260002	-0.95150000	1	-1.90970004	0.80330002	3.40639997
1	-3.67190003	-4.80109978	-0.66049999	6	-2.88800001	3.36750007	2.51650000
1	-2.95409989	-4.01130009	-2.06180000	1	-3.54049993	3.54380012	1.65559995
6	-4.21150017	1.22749996	-1.76359999	1	-3.46939993	2.86260009	3.29010010
1	-4.54209995	0.57730001	-2.58109999	1	-2.56870008	4.34019995	2.90199995
1	-5.08970022	1.79890001	-1.43920004	6	2.90890002	-3.14499998	3.46199989
1	-3.50110006	1.94830000	-2.18479991	1	2.22070003	-3.54169989	4.21059990
1	-5.37669992	-0.13470000	1.38129997	1	3.07710004	-3.91779995	2.70659995
1	-3.89650011	-0.11330000	2.33480000	1	3.86409998	-2.93409991	3.95029998
1	-4.62120008	1.40180004	1.77279997	6	-0.48390001	2.14050007	-2.72119999
6	1.96379995	0.11110000	1.40869999	6	-1.71780002	-0.72710001	-3.37649989
6	0.85280001	-0.20950000	2.24600005	6	0.47850001	-2.91700006	-2.82990003
6	-0.10800000	0.82929999	2.06669998	6	3.11240005	-1.52839994	-1.89600003
6	0.44459999	1.73870003	1.11409998	1	-2.37989998	0.13370000	-3.27509999
6	1.74810004	1.32860005	0.67299998	1	-1.64390004	-0.97689998	-4.44089985
40	0.15130000	-0.35479999	-0.30660000	1	-2.19910002	-1.57350004	-2.87439990
6	0.63470000	-1.44659996	-2.57640004	1	-1.30079997	2.02069998	-3.43680000
6	1.81519997	-0.80290002	-2.12570000	1	-0.90950000	2.56839991	-1.80789995
6	1.57169998	0.61460000	-2.06590009	1	0.21330000	2.86759996	-3.14369988
6	0.21080001	0.81779999	-2.50070000	1	-0.57309997	-3.21429992	-2.79909992
6	-0.35409999	-0.45199999	-2.80870008	1	0.87570000	-3.18269992	-3.81629992
16	-0.58219999	3.14569998	0.93540001	1	1.01040006	-3.50359988	-2.07719994
14	2.52810001	1.81379998	-0.96329999	1	3.81680012	-0.94669998	-1.30209994

6	2.32389998	-1.91110003	2.84509993	1	2.94810009	-2.47530007	-1.37670004
6	1.08940005	-1.38380003	3.04769993	1	3.58909988	-1.73979998	-2.86030006

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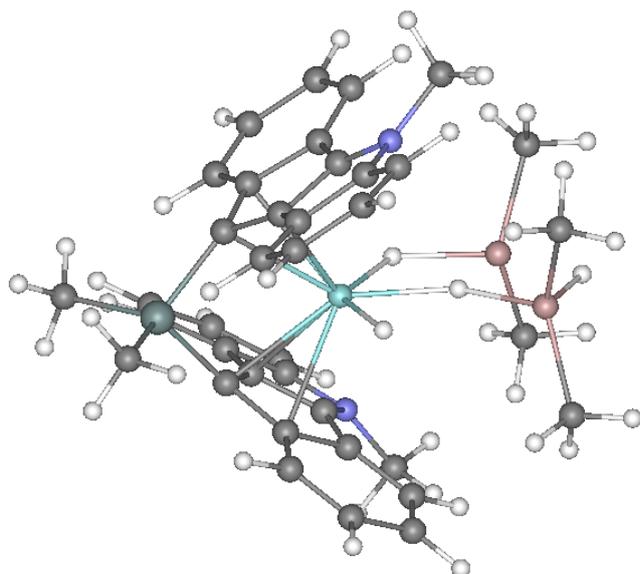


Zero-point vibrational energy	1860867.4 (Joules/Mol)
	444.75799 (Kcal/Mol)
Zero-point correction=	0.708767 (Hartree/Particle)
Thermal correction to Energy=	0.754785
Thermal correction to Enthalpy=	0.755729
Thermal correction to Gibbs Free Energy=	0.634347
Sum of electronic and zero-point Energies=	-5897.866678
Sum of electronic and thermal Energies=	-5897.820660
Sum of electronic and thermal Enthalpies=	-5897.819716
Sum of electronic and thermal Free Energies=	-5897.941098

cartesian

6	0.09090000	1.67620003	1.80890000	6	5.05399990	-0.34700000	1.39059997
6	-0.68709999	0.57810003	2.31290007	6	3.95429993	-2.32710004	-0.32240000
6	-1.90489995	0.55299997	1.55100000	6	-3.53060007	2.77929997	-0.87440002
6	-1.89709997	1.69149995	0.69430000	1	-4.58960009	3.02929997	-0.79060000
6	-0.60890001	2.34349990	0.69090003	1	-2.95499992	3.70099998	-0.78200001
6	2.38910007	-0.34529999	-1.05929995	1	-3.33979988	2.32189989	-1.85319996
6	2.38439989	1.00179994	-0.61900002	1	-3.35010004	-1.65880001	2.90630007
6	1.41470003	1.80550003	-1.32169998	6	-5.26450014	-1.20179999	2.02139997
6	0.99030000	0.90640002	-2.41289997	6	-5.97609997	-0.37480000	1.14010000
6	1.54820001	-0.41090000	-2.22340012	1	-5.91400003	1.28719997	-0.23260000
7	-3.16470003	1.88390005	0.19480000	1	-5.78030014	-2.00699997	2.53419995

14	0.38249999	3.24480009	-0.64399999	1	-7.03350019	-0.55479997	0.97509998
7	3.35879993	1.17519999	0.35150000	1	5.05499983	2.39940000	0.28860000
6	1.78629994	1.14940000	3.45729995	1	3.49850011	3.23950005	0.16310000
6	1.00950003	0.06880000	3.93919992	1	4.04549980	2.61400008	1.73810005
6	-0.21709999	-0.21699999	3.38210011	1	3.54999995	-3.08820009	-0.98150003
6	1.34140003	1.93809998	2.41650009	6	5.01189995	-2.62630010	0.53299999
1	1.92770004	2.79189992	2.09969997	6	5.55289984	-1.64810002	1.38020003
1	2.73990011	1.37090003	3.92810011	1	5.47779989	0.40979999	2.04460001
1	1.38000000	-0.53130001	4.76420021	1	6.37760019	-1.90649998	2.03699994
1	-0.82520002	-1.03199995	3.76169991	1	5.42549992	-3.62960005	0.54290003
6	-0.00810000	0.11770000	-4.47310019	6	-3.89159989	-1.92910004	-1.44519997
6	0.53210002	-1.18120003	-4.26359987	1	0.30930001	-1.57780004	0.77929997
6	1.30170000	-1.44920003	-3.15949988	1	-1.33150005	0.68809998	-1.39789999
6	0.20640001	1.13750005	-3.57809997	13	-2.03920007	-2.55590010	-1.40649998
1	-0.19230001	2.12540007	-3.77670002	1	-1.68690002	-3.20799994	0.15510000
1	-0.59210002	0.31020001	-5.36759996	1	-0.95929998	-1.30359995	-1.18840003
1	0.34760001	-1.96229994	-4.99440002	13	-0.14229999	-3.19029999	0.91030002
1	1.74619997	-2.42950010	-3.01349998	6	1.05320001	-4.26870012	-0.21430001
6	-0.63669997	4.00519991	-2.01979995	6	-0.49930000	-3.63899994	2.79089999
6	1.35560000	4.69339991	0.05870000	1	0.31040001	-3.29780006	3.44700003
1	2.07489991	5.06489992	-0.67979997	1	-1.43579996	-3.21700001	3.17109990
1	1.88660002	4.51469994	0.99440002	1	-0.57130003	-4.72709990	2.90939999
1	0.64139998	5.50209999	0.25279999	1	1.97350001	-4.52939987	0.32170001
1	0.04510000	4.34959984	-2.80609989	1	0.57450002	-5.20489979	-0.52590001
1	-1.17260003	4.88609982	-1.65059996	1	1.34029996	-3.73600006	-1.12790000
1	-1.35930002	3.32450008	-2.47070003	6	-1.37890005	-3.82159996	-2.75620008
6	-3.99079990	0.86979997	0.68739998	1	-0.29730001	-3.98340011	-2.74460006
6	-3.25419998	0.02800000	1.55789995	1	-1.85619998	-4.80049992	-2.61960006
6	-3.90079999	-1.01040006	2.23110008	1	-1.65110004	-3.47440004	-3.76060009
6	-5.35069990	0.66649997	0.45699999	1	-4.50990009	-2.59080005	-2.06380010
6	3.42950010	-1.03349996	-0.32080001	1	-4.35290003	-1.87779999	-0.45420000
6	3.99280000	-0.05470000	0.53549999	1	-3.95309997	-0.92390001	-1.88049996
6	4.02470016	2.42499995	0.65990001	40	-0.04830000	0.14720000	-0.22030000

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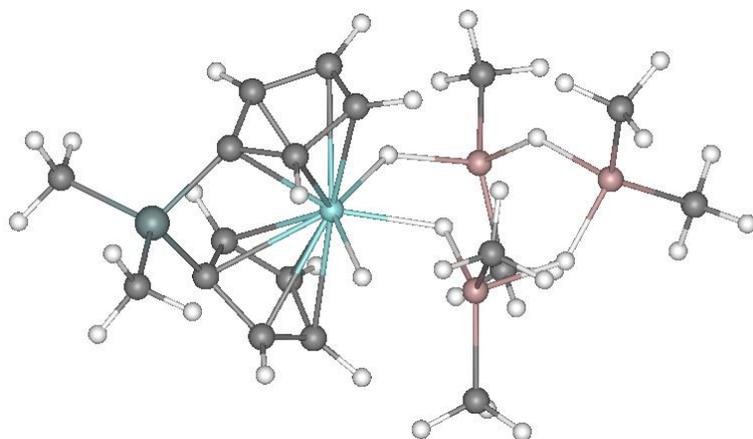
Zero-point vibrational energy	1858212.8 (Joules/Mol)
	444.12352 (Kcal/Mol)
Zero-point correction=	0.707756 (Hartree/Particle)
Thermal correction to Energy=	0.753360
Thermal correction to Enthalpy=	0.754304
Thermal correction to Gibbs Free Energy=	0.633454
Sum of electronic and zero-point Energies=	-5897.855704
Sum of electronic and thermal Energies=	-5897.810100
Sum of electronic and thermal Enthalpies=	-5897.809156
Sum of electronic and thermal Free Energies=	-5897.930006

cartesian

6	0.57590002	-0.53490001	-2.47950006	6	-3.93750000	-2.28379989	-0.96789998
6	1.24360001	0.74559999	-2.34559989	1	3.62590003	-3.05640006	0.45570001
6	2.28369999	0.53700000	-1.39030004	6	5.30459976	-1.88709998	1.10889995
6	2.23569989	-0.80080003	-0.92189997	6	5.93030024	-0.63050002	1.11010003
6	1.13339996	-1.50220001	-1.55019999	1	5.85200024	1.42209995	0.44540000
6	-1.98479998	-0.59020001	1.64690006	1	5.79489994	-2.73009992	1.58510005
6	-1.93920004	-1.52600002	0.58219999	1	6.89099979	-0.51040000	1.60090005
6	-0.64510000	-2.17700005	0.56900001	1	-3.40720010	-3.04180002	-1.53100002
6	0.03990000	-1.64069998	1.73880005	6	-5.28950024	-2.06649995	-1.21010005
6	-0.77920002	-0.65210003	2.40599990	6	-6.00790024	-1.11800003	-0.46630001
6	3.44519997	-0.98040003	-0.12860000	1	-5.96260023	0.33809999	1.12259996
14	0.24869999	-3.00970006	-0.85850000	1	-7.06180000	-0.95980000	-0.67290002
6	-3.28629994	-1.54470003	0.02420000	1	-5.79689980	-2.64070010	-1.97850001
6	-0.72560000	0.39660001	-4.30030012	6	4.08010006	2.28819990	-1.59870005
6	-0.07630000	1.65480006	-4.14489985	1	4.88380003	1.90429997	-2.23760009

6	0.88360000	1.83829999	-3.18479991	1	4.49249983	2.99559999	-0.87680000
6	-0.43090001	-0.66320002	-3.48399997	1	3.36269999	2.82509995	-2.21589994
1	-0.92070001	-1.61619997	-3.63960004	6	-1.62090003	3.92289996	-2.16260004
1	-1.47119999	0.27829999	-5.08010006	1	1.02049994	1.23099995	1.15579998
1	-0.34880000	2.48049998	-4.79460001	1	-1.49070001	0.53659999	-1.08690000
1	1.37240005	2.80180001	-3.08030009	13	-1.82889998	3.26889992	-0.33329999
6	1.74749994	-1.26880002	3.42120004	1	-0.82480001	4.12340021	0.70249999
6	0.89899999	-0.35650000	4.10690022	1	-0.68449998	2.00510001	0.15099999
6	-0.34340000	-0.04680000	3.61660004	13	0.48760000	2.94829988	1.30410004
6	1.33420002	-1.89859998	2.27390003	6	-0.02390000	3.18359995	3.18580008
1	1.98699999	-2.61840010	1.79910004	6	1.95379996	3.87689996	0.39330000
1	2.73519993	-1.48360002	3.81769991	1	2.92860007	3.48609996	0.70529997
1	1.24140000	0.10010000	5.03039980	1	1.88600004	3.77719998	-0.69720000
1	-0.98670000	0.64260000	4.15310001	1	1.92820001	4.94920015	0.61860001
6	1.40369999	-4.39550018	-0.32749999	1	0.62669998	2.64720011	3.88380003
6	-0.92350000	-3.77329993	-2.10209990	1	0.03780000	4.25330019	3.42219996
1	-1.46130002	-4.60480022	-1.63349998	1	-1.05830002	2.88109994	3.38879991
1	-1.66050005	-3.08179998	-2.50839996	6	-3.58330011	2.98589993	0.48480001
1	-0.34660000	-4.18120003	-2.94009995	1	-3.54450011	2.98950005	1.57830000
1	0.86330003	-5.34460020	-0.41429999	1	-4.24679995	3.80660009	0.18400000
1	2.27150011	-4.45109987	-0.99280000	1	-4.05009985	2.05209994	0.15330000
1	1.75730002	-4.33059978	0.70249999	1	-2.21289992	4.84210014	-2.26279998
6	4.11679983	0.26940000	-0.15660000	1	-0.58960003	4.17000008	-2.43039989
7	3.40680003	1.19560003	-0.91520000	1	-2.00009990	3.20510006	-2.89639997
6	4.07359982	-2.06809998	0.48740000	40	-0.02260000	0.09520000	-0.06690000
6	5.35169983	0.45860001	0.46799999	6	-3.71329999	0.67199999	2.93490005
7	-3.23569989	-0.01510000	1.75300002	1	-4.63940001	1.19780004	2.70160007
6	-4.03989983	-0.61280000	0.78899997	1	-3.88960004	-0.02940000	3.75880003
6	-5.39629984	-0.38490000	0.54380000	1	-2.97849989	1.41900003	3.24349999

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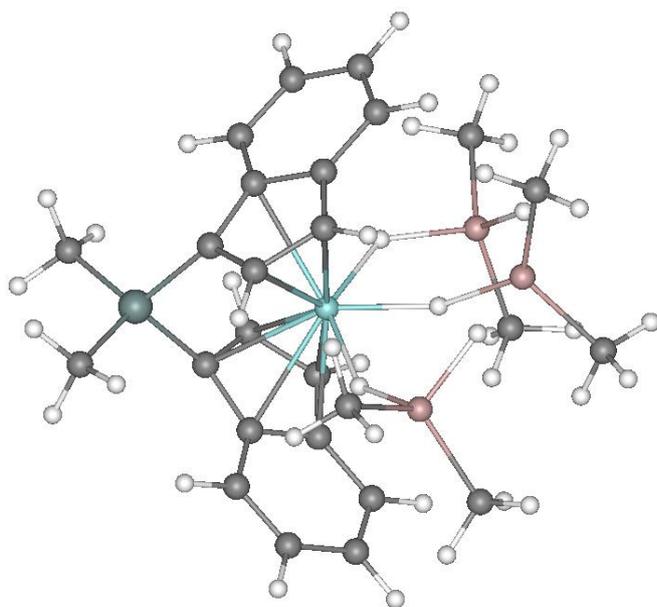


Zero-point vibrational energy	1269873.1 (Joules/Mol)
	303.50696 (Kcal/Mol)
Zero-point correction=	0.483669 (Hartree/Particle)
Thermal correction to Energy=	0.519824
Thermal correction to Enthalpy=	0.520768
Thermal correction to Gibbs Free Energy=	0.415174
Sum of electronic and zero-point Energies=	-5264.929878
Sum of electronic and thermal Energies=	-5264.893724
Sum of electronic and thermal Enthalpies=	-5264.892779
Sum of electronic and thermal Free Energies=	-5264.998373

cartesian

1	-0.43939999	-1.43649995	0.80479997	1	4.27729988	-2.91899991	-1.62249994
1	1.21710002	-0.25150001	0.28110000	1	3.11120009	-1.91260004	-2.47620010
1	3.14860010	-1.22160006	0.81610000	6	-0.63000000	0.10580000	-2.61669993
13	1.46630001	-1.76970005	1.10669994	6	-1.90579998	0.51709998	-2.16540003
6	1.43980002	-1.64870000	3.07089996	6	-2.51799989	-0.55890000	-1.43570006
6	1.47109997	-3.45779991	0.09660000	6	-1.57260001	-1.62919998	-1.44900000
1	2.08929992	-2.41540003	3.50999999	6	-0.41150001	-1.21630001	-2.15969992
1	0.43439999	-1.81130004	3.47909999	1	0.47110000	-1.81729996	-2.34060001
1	1.79620004	-0.68419999	3.44980001	1	0.06560000	0.70260000	-3.19409990
1	2.25580001	-4.12529993	0.47409999	1	-2.34770012	1.49030006	-2.34850001
1	1.66030002	-3.33690000	-0.97570002	14	-3.85940003	-0.26530001	-0.14500000
1	0.51870000	-3.99210000	0.20250000	1	-1.70190001	-2.59739995	-0.98130000
6	4.07310009	-1.89320004	-1.95130002	6	-1.06819999	2.18079996	1.55719995
13	4.08449984	-0.63470000	-0.44330001	6	-2.21440005	1.97399998	0.75410002
1	0.62199998	1.62360001	-0.64139998	6	-2.78600001	0.69480002	1.07029998
1	3.05130005	0.63309997	-0.98470002	6	-1.94700003	0.12950000	2.07820010
13	2.26760006	1.97409999	-0.31130001	6	-0.88450003	1.03219998	2.36420012
6	2.64439988	2.05119991	1.61720002	1	-0.08990000	0.87489998	3.08430004
6	2.63039994	3.46180010	-1.53939998	1	-0.43560001	3.05999994	1.54760003
1	3.69020009	3.74189997	-1.52600002	1	-2.60019994	2.67890000	0.02580000
1	2.37350011	3.21700001	-2.57590008	1	-2.07960010	-0.84039998	2.54150009
1	2.06010008	4.35790014	-1.26789999	40	-0.63919997	0.22030000	-0.05120000
1	3.61969995	2.51970005	1.79770005	6	-4.43979979	-1.87639999	0.59740001
1	1.90810001	2.65050006	2.16739988	6	-5.23689985	0.79589999	-0.82550001
1	2.67280006	1.06120002	2.08859992	1	-5.95839977	1.04760003	-0.04240000
6	5.68699980	0.21890000	0.29699999	1	-4.85599995	1.73559999	-1.23730004
1	6.12820005	0.92729998	-0.41440001	1	-5.77139997	0.27700001	-1.62660003
1	5.47170019	0.77139997	1.21790004	1	-5.12909985	-1.70029998	1.42869997
1	6.46390009	-0.51679999	0.53560001	1	-4.96180010	-2.48490000	-0.14720000
1	4.83729982	-1.63329995	-2.69309998	1	-3.60019994	-2.46609998	0.97930002

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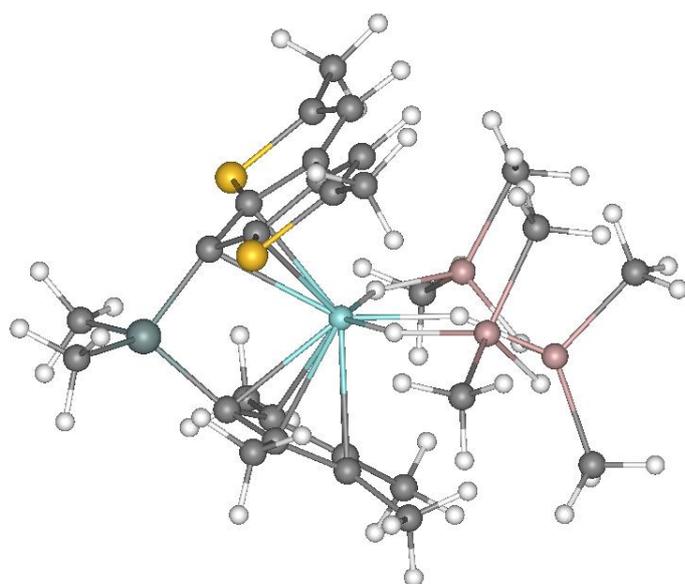


Zero-point vibrational energy	1521672.8 (Joules/Mol)
	363.68852 (Kcal/Mol)
Zero-point correction=	0.579575 (Hartree/Particle)
Thermal correction to Energy=	0.619595
Thermal correction to Enthalpy=	0.620539
Thermal correction to Gibbs Free Energy=	0.512020
Sum of electronic and zero-point Energies=	-5571.989213
Sum of electronic and thermal Energies=	-5571.949193
Sum of electronic and thermal Enthalpies=	-5571.948249
Sum of electronic and thermal Free Energies=	-5572.056768

cartesian							
1	-2.30500007	1.65429997	-1.85339999	6	1.98130000	1.41489995	1.20469999
13	-1.05509996	2.68460011	-1.53110003	6	2.50510001	0.07320000	1.15869999
6	-1.72749996	4.21299982	-0.49700001	6	-0.24590001	-1.92190003	-1.69289994
6	0.08820000	2.93300009	-3.12290001	6	1.93840003	-1.16400003	-1.28859997
1	-0.97649997	5.00000000	-0.36460000	6	1.24779999	-0.23500000	-2.12879992
1	-2.09699988	3.92880011	0.49410000	6	-0.08300000	-0.65979999	-2.34719992
1	-2.57299995	4.66079998	-1.03550005	14	3.44659996	-0.72899997	-0.25310001
1	0.13580000	2.05909991	-3.78360009	6	0.99290001	-2.22490001	-1.02440000
1	1.11740005	3.18639994	-2.83489990	6	4.54979992	0.44970000	-1.19620001
1	-0.27700001	3.76719999	-3.73410010	6	4.40549994	-2.22040009	0.34480000
1	-0.88650000	-1.46340001	0.98240000	1	4.55770016	-2.94630003	-0.45989999
6	-3.80520010	-0.50059998	-2.43980002	1	3.91549993	-2.73300004	1.17729998

1	-0.07530000	1.66740000	-0.52579999	1	5.39160013	-1.90269995	0.69900000
13	-3.22219992	0.41049999	-0.78780001	1	5.18650007	-0.11680000	-1.88370001
1	-1.67499995	0.32550001	0.00810000	1	5.20550013	1.00849998	-0.52100003
1	-3.43379998	-1.14639997	0.24429999	1	3.98499990	1.16980004	-1.79519999
13	-2.53069997	-1.51429999	1.58190000	6	2.37840009	2.61969995	0.54210001
6	-2.71860003	-0.07780000	2.92370009	6	0.19200000	2.67989993	2.38179994
6	-2.73060012	-3.40380001	2.11350012	6	-1.34519994	-2.82730007	-1.60959995
1	-3.30979991	-3.47849989	3.04220009	6	1.09019995	-3.41669989	-0.24180000
1	-3.24880004	-4.00659990	1.36070001	1	3.22040009	2.61689997	-0.14350000
1	-1.75999999	-3.87890005	2.30159998	6	1.71249998	3.78270006	0.82270002
1	-3.78150010	0.14770000	3.07830000	6	0.62089998	3.81299996	1.74619997
1	-2.31320000	-0.36039999	3.90359998	1	-0.63489997	2.70889997	3.08540010
1	-2.24449992	0.86369997	2.62080002	1	2.01710010	4.70599985	0.33939999
6	-4.30079985	1.66349995	0.27070001	1	0.12220000	4.75750017	1.93770003
1	-5.18879986	1.17760003	0.69199997	1	2.01839995	-3.66680002	0.26429999
1	-3.74239993	2.09419990	1.10940003	6	0.01530000	-4.26590014	-0.18390000
1	-4.64429998	2.50079989	-0.34880000	6	-1.19780004	-3.97550011	-0.87629998
1	-4.36310005	-1.42260003	-2.23990011	1	-2.27209997	-2.61019993	-2.13000011
1	-4.49009991	0.18529999	-2.95609999	1	-2.01970005	-4.68109989	-0.81260002
1	-3.01519990	-0.73500001	-3.16120005	1	0.08410000	-5.18279982	0.39309999
40	0.22470000	-0.11850000	0.13890000	1	1.65369999	0.70260000	-2.49670005
6	1.70210004	-0.68390000	2.06949997	1	-0.82580000	-0.14129999	-2.94269991
6	0.70060003	0.13420001	2.64599991	1	-0.04160000	-0.17540000	3.37089992
6	0.87300003	1.45050001	2.12859988	1	1.80690002	-1.74710000	2.26399994

A³-3



Zero-point vibrational energy

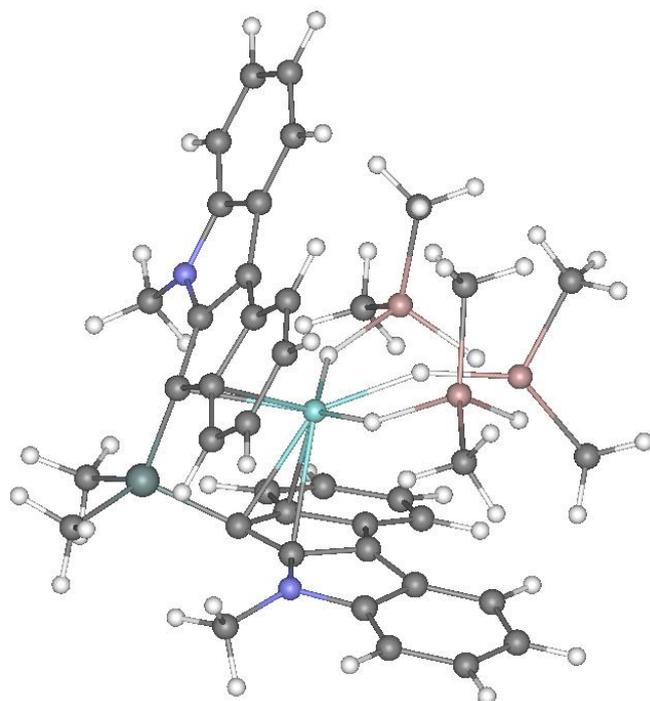
1789584.0 (Joules/Mol)

	427.72085 (Kcal/Mol)
Zero-point correction=	0.681617 (Hartree/Particle)
Thermal correction to Energy=	0.729415
Thermal correction to Enthalpy=	0.730359
Thermal correction to Gibbs Free Energy=	0.606645
Sum of electronic and zero-point Energies=	-6449.148699
Sum of electronic and thermal Energies=	-6449.100900
Sum of electronic and thermal Enthalpies=	-6449.099956
Sum of electronic and thermal Free Energies=	-6449.223670

cartesian							
1	2.62369990	2.45469999	0.75860000	6	0.22620000	0.61489999	2.79690003
13	1.38370001	3.07220006	-0.15629999	16	-2.61579990	2.32290006	-1.24290001
6	2.03469992	3.12540007	-2.01399994	14	-3.25169992	-0.72140002	1.04939997
6	0.52520001	4.64659977	0.67330003	6	-0.05350000	-3.10689998	-2.49959993
1	1.41649997	3.74679995	-2.67070007	6	0.15490000	-1.82900000	-2.90730000
1	2.11969995	2.13199997	-2.46799994	16	-1.24419999	-3.23580003	-1.20910001
1	3.04520011	3.55469990	-2.01710010	1	0.85020000	-1.57330000	-3.69779992
1	0.60750002	4.66610003	1.76639998	6	-4.54850006	0.60949999	1.25880003
1	-0.54640001	4.67920017	0.43470001	6	-4.07060003	-2.39680004	1.24360001
1	0.96530002	5.58129978	0.30440000	1	-4.06659985	-2.72900009	2.28629994
1	1.08029997	-1.58169997	0.04960000	1	-3.60590005	-3.17930007	0.63739997
6	4.32480001	1.09159994	2.31299996	1	-5.11469984	-2.32010007	0.92259997
1	0.14839999	1.88960004	0.15350001	1	-5.01620007	0.52509999	2.24580002
13	3.46190000	0.93049997	0.54040003	1	-5.33360004	0.46329999	0.50889999
1	1.82599998	0.49360001	0.03900000	1	-4.17710018	1.63059998	1.15540004
1	3.57259989	-0.97180003	0.62410003	6	-1.47350001	2.75959992	-2.51099992
13	2.71519995	-2.04040003	-0.31279999	6	-0.69129997	1.72270000	-2.90549994
6	3.24070001	-1.71459997	-2.18160009	1	0.05740000	1.81809998	-3.68319988
6	2.71429992	-3.87100005	0.43220001	6	-1.44140005	4.17740011	-2.99390006
1	3.47830009	-4.49359989	-0.05010000	1	-1.03750002	4.84299994	-2.22329998
1	2.91210008	-3.90100002	1.50979996	1	-0.80309999	4.25000000	-3.87649989
1	1.74849999	-4.36759996	0.26780000	1	-2.44079995	4.53200006	-3.26079988
1	4.33179998	-1.60389996	-2.22959995	6	0.63639998	-4.34660006	-2.98210001
1	2.97049999	-2.54640007	-2.84330010	1	1.21500003	-4.11479998	-3.87859988
1	2.81719995	-0.79589999	-2.60260010	1	1.32379997	-4.73299980	-2.22239995
6	4.55520010	1.28180003	-1.05280006	1	-0.08000000	-5.13509989	-3.22799993
1	5.42640018	0.61400002	-1.04069996	6	-1.80770004	2.16639996	2.44849992
1	4.05950022	1.14810002	-2.01780009	6	1.12779999	1.66129994	3.38599992
1	4.93790007	2.30979991	-1.02349997	6	1.74899995	-1.46749997	3.19610000
1	5.40010023	0.98920000	2.10840011	6	-0.80190003	-2.93700004	2.20900011

1	4.18039989	2.08279991	2.75710011	1	1.27450001	2.51869988	2.72359991
1	4.08860016	0.34240001	3.07380009	1	0.69279999	2.03290009	4.32079983
40	-0.08280000	-0.03790000	0.30070001	1	2.11100006	1.24769998	3.61069989
6	-1.48230004	-1.50109994	-1.20720005	1	-1.12399995	2.91759992	2.85109997
6	-0.63480002	-0.87599999	-2.17330003	1	-2.12210011	2.52500010	1.46500003
6	-0.96420002	0.51190001	-2.17400002	1	-2.68829989	2.12619996	3.09719992
6	-2.01060009	0.68290001	-1.21870005	1	2.63590002	-1.18420005	2.62549996
6	-2.37669992	-0.55690002	-0.59689999	1	1.93859994	-1.21910000	4.24609995
6	0.50139999	-0.77660000	2.72280002	1	1.64069998	-2.55180001	3.12280011
6	-0.68129998	-1.43770003	2.28629994	1	-1.71150005	-3.25320005	1.69959998
6	-1.71519995	-0.45750001	2.10719991	1	0.04540000	-3.38280010	1.68050003
6	-1.12679994	0.82139999	2.40260005	1	-0.83050001	-3.35360003	3.22270012

A³-4



Zero-point vibrational energy	2077474.0 (Joules/Mol)
	496.52819 (Kcal/Mol)
Zero-point correction=	0.791268 (Hartree/Particle)
Thermal correction to Energy=	0.843289
Thermal correction to Enthalpy=	0.844233
Thermal correction to Gibbs Free Energy=	0.712605
Sum of electronic and zero-point Energies=	-6220.582439
Sum of electronic and thermal Energies=	-6220.530418
Sum of electronic and thermal Enthalpies=	-6220.529474

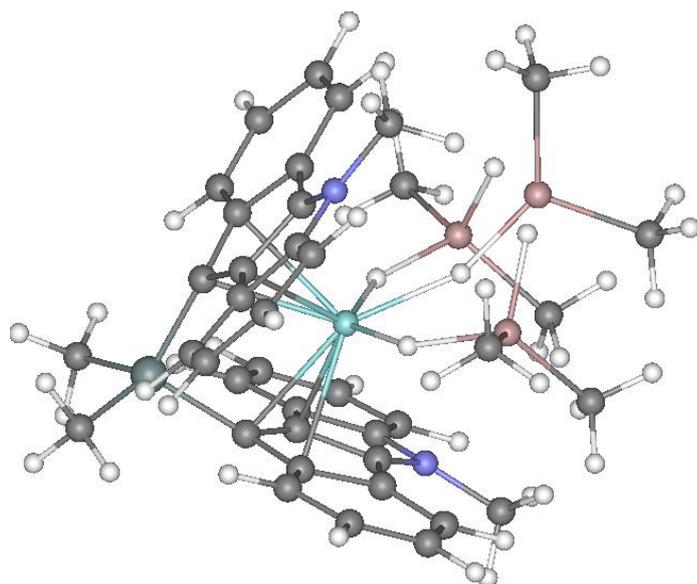
Sum of electronic and thermal Free Energies= -6220.661103

cartesian

6	-0.11700000	-1.81540000	-1.84169996	1	-3.06539989	-1.97210002	1.95369995
6	-0.85589999	-0.73979998	-2.45239997	1	-3.46980000	1.42670000	-3.35249996
6	-2.06189990	-0.59289998	-1.70210004	6	-5.36040020	1.21459997	-2.33870006
6	-2.08470011	-1.61989999	-0.71569997	6	-6.06269979	0.59380001	-1.29470003
6	-0.87190002	-2.38669991	-0.71350002	1	-6.01550007	-0.81410003	0.33550000
6	2.29760003	-0.06720000	1.31260002	1	-5.86520004	1.94299996	-2.96429992
6	2.21560001	-1.38049996	0.77219999	1	-7.10400009	0.84869999	-1.12530005
6	1.08480000	-2.10649991	1.28030002	1	4.80670023	-3.04609990	0.01180000
6	0.56349999	-1.21780002	2.32419991	1	3.15409994	-3.67860007	-0.07240000
6	1.29009998	0.02960000	2.33299994	1	3.91790009	-2.99440002	-1.52919996
7	-3.31669998	-1.62979996	-0.10060000	1	3.79819989	2.48659992	1.66630006
14	0.02620000	-3.47399998	0.52120000	6	5.45340014	1.90269995	0.42019999
7	3.29340005	-1.60469997	-0.06520000	6	6.00489998	0.91680002	-0.40990001
6	1.65180004	-1.43640006	-3.45720005	1	5.75869989	-1.03820002	-1.30190003
6	0.87690002	-0.43509999	-4.09579992	1	6.96649981	1.09089994	-0.88209999
6	-0.36030000	-0.08690000	-3.60680008	1	5.99429989	2.82879996	0.58410001
6	1.17219996	-2.11560011	-2.36039996	1	-1.05659997	2.80590010	2.04200006
1	1.77139997	-2.90120006	-1.92089999	13	-2.33969998	1.82019997	1.66939998
1	2.63369989	-1.68200004	-3.85100007	6	-3.33520007	2.66269994	0.20930000
1	1.27139997	0.06540000	-4.97480011	6	-3.33990002	1.20490003	3.26169991
1	-0.95789999	0.67540002	-4.09429979	1	-4.31510019	2.19700003	0.05690000
6	-0.69520003	-0.44200000	4.24240017	1	-2.81719995	2.66659999	-0.75440001
6	0.02540000	0.77969998	4.23990011	1	-3.51309991	3.71350002	0.47499999
6	1.00610006	1.01760006	3.30730009	1	-2.90669990	1.55089998	4.20679998
6	-0.44659999	-1.41830003	3.30760002	1	-3.40840006	0.11190000	3.32170010
1	-0.96980000	-2.36350012	3.37120008	1	-4.36579990	1.59150004	3.21160007
1	-1.44840002	-0.61199999	5.00500011	1	1.18990004	0.68260002	-1.15499997
1	-0.18810000	1.52960002	4.99520016	6	1.39100003	4.12410021	2.22550011
1	1.58050001	1.93490005	3.33150005	1	-1.53989995	0.33910000	1.13259995
6	-1.02030003	-4.37620020	1.79340005	13	0.20070000	3.42319989	0.80470002
6	0.92220002	-4.91219997	-0.29840001	1	-0.15710001	1.77620006	0.18950000
1	1.56799996	-5.41289997	0.43220001	1	1.63279998	3.15510011	-0.36629999
1	1.51030004	-4.70480013	-1.19149995	13	1.53190005	2.27870011	-1.78110003
1	0.15320000	-5.63609982	-0.59189999	6	0.01280000	2.97370005	-2.83119988
1	-0.34700000	-4.81020021	2.54189992	6	3.28049994	1.97979999	-2.63299990
1	-1.53020000	-5.20879984	1.29630005	1	3.37109995	2.57699990	-3.54929996
1	-1.77460003	-3.79949999	2.32209992	1	4.12020016	2.24210000	-1.98080003
6	-4.11569977	-0.65570003	-0.71139997	1	3.40949988	0.92739999	-2.91499996

6	-3.38409996	-0.00880000	-1.73839998	1	-0.00700000	4.06850004	-2.76920009
6	-4.01830006	0.92449999	-2.56080008	1	0.11400000	2.71790004	-3.89249992
6	-5.45240021	-0.34279999	-0.46370000	1	-0.96939999	2.62360001	-2.48670006
6	3.52679992	0.52050000	0.81129998	6	-0.81910002	4.80740023	-0.14590000
6	4.10179996	-0.46540001	-0.02750000	1	-0.11340000	5.53060007	-0.57639998
6	3.82100010	-2.90059996	-0.44260001	1	-1.48090005	4.47569990	-0.94770002
6	5.33430004	-0.28009999	-0.65020001	1	-1.43470001	5.35419989	0.58069998
6	4.21439981	1.71589994	1.02839994	1	1.61870003	5.15460014	1.91799998
6	-3.64790010	-2.35249996	1.10389996	1	0.87589997	4.18849993	3.19169998
1	-4.70639992	-2.21880007	1.32439995	1	2.35630012	3.64129996	2.39210010
1	-3.45689988	-3.41980004	0.96740001	40	-0.00220000	-0.20990001	0.05890000

A³-5



Zero-point vibrational energy	2076519.4 (Joules/Mol)
	496.30004 (Kcal/Mol)
Zero-point correction=	0.790904 (Hartree/Particle)
Thermal correction to Energy=	0.843172
Thermal correction to Enthalpy=	0.844116
Thermal correction to Gibbs Free Energy=	0.711439
Sum of electronic and zero-point Energies=	-6220.583609
Sum of electronic and thermal Energies=	-6220.531341
Sum of electronic and thermal Enthalpies=	-6220.530397
Sum of electronic and thermal Free Energies=	-6220.663075

cartesian

1	1.71850002	3.23880005	0.28290001	6	1.65600002	-2.07069993	2.16120005
13	1.96550000	2.24239993	1.59979999	1	2.24119997	-2.79049993	1.60590005

6	0.80970001	2.87660003	3.06719995	1	3.26799989	-1.61230004	3.46609998
6	3.89100003	1.96270001	1.92789996	1	1.97409999	0.02310000	4.82950020
1	1.15339994	2.49900007	4.03679991	1	-0.36039999	0.55299997	4.27040005
1	-0.24670000	2.60520005	2.94970012	6	-1.71959996	0.04080000	-3.82470012
1	0.84719998	3.97189999	3.11400008	6	-1.01129997	1.27069998	-3.93779993
1	4.53030014	2.37770009	1.13989997	6	0.18560000	1.45930004	-3.29649997
1	4.14179993	0.89870000	2.01699996	6	-1.23310006	-0.99299997	-3.06999993
1	4.18319988	2.45009995	2.86689997	1	-1.78980005	-1.91919994	-3.00909996
1	-1.69949996	0.57309997	-0.65280002	1	-2.66790009	-0.07530000	-4.33909988
6	0.79310000	4.46780014	-2.02780008	1	-1.42809999	2.07340002	-4.53800011
1	1.47759998	0.68760002	0.98170000	1	0.71139997	2.40129995	-3.39190006
13	0.00580000	3.58960009	-0.43220001	6	-1.18900001	-4.27089977	-1.68889999
1	-0.15140000	1.89940000	0.11200000	6	1.36199999	-4.63570023	-0.29359999
1	-1.52250004	3.08220005	-1.35360003	1	2.08249998	-4.75559998	-1.10920000
13	-2.66709995	2.01320004	-0.79369998	1	1.90789998	-4.49860001	0.63929999
6	-3.24429989	2.69390011	0.96130002	1	0.81919998	-5.58330011	-0.20160000
6	-4.05700016	1.53090000	-2.10520005	1	-0.65189999	-4.92040014	-2.38989997
1	-5.01109982	1.97990000	-1.80009997	1	-1.74300003	-4.92170000	-1.00320005
1	-3.84859991	1.86329997	-3.12770009	1	-1.91079998	-3.70180011	-2.26959991
1	-4.21049976	0.44409999	-2.13170004	6	-3.84039998	-0.68129998	1.31229997
1	-3.43790007	3.77029991	0.86909997	7	-2.93440008	-0.15030000	2.22320008
1	-4.17920017	2.22580004	1.28910005	6	-3.93670011	-2.28160000	-0.51849997
1	-2.49839997	2.57879996	1.75419998	6	-5.19700003	-0.37860000	1.16009998
6	-0.71160001	4.86339998	0.88169998	7	3.15700006	0.86229998	-1.58599997
1	-1.47300005	5.48110008	0.38640001	6	3.99690008	-0.02690000	-0.93099999
1	-1.16480005	4.45149994	1.78550005	6	5.32649994	0.17270000	-0.54619998
1	0.09240000	5.54180002	1.19690001	6	4.05359983	-2.32859993	-0.16080000
1	0.05520000	4.58690023	-2.83039999	1	-3.47300005	-3.02850008	-1.15219998
1	1.05139995	5.47980022	-1.68460000	6	-5.28590012	-1.98459995	-0.66869998
1	1.70560002	4.05749989	-2.46469998	6	-5.90509987	-1.03680003	0.16130000
40	0.00270000	-0.11200000	-0.00270000	1	-5.69080019	0.34840000	1.79729998
6	0.29339999	-1.82089996	1.81270003	1	-5.86670017	-2.48830009	-1.43420005
6	-0.41859999	-0.80500001	2.56349993	1	-6.95769978	-0.81150001	0.02320000
6	-1.71500003	-0.74479997	1.97920001	1	3.59669995	-3.30579996	-0.04950000
6	-1.80980003	-1.68529999	0.91750002	6	5.37540007	-2.13759995	0.21789999
6	-0.55549997	-2.38549995	0.77649999	6	6.00080013	-0.89150000	0.03530000
6	1.95439994	0.22100000	-1.79359996	1	5.81659985	1.13150001	-0.68089998
6	2.00110006	-1.10060000	-1.27139997	1	7.03160000	-0.75870001	0.34830001
6	0.78270000	-1.80490005	-1.60599995	1	5.93540001	-2.96040010	0.65039998
6	0.02700000	-0.86350000	-2.40860009	6	3.56609988	2.15639997	-2.09789991
6	0.72630000	0.40430000	-2.50900006	1	3.42440009	2.94650006	-1.35490000

6	-3.19370008	-1.62570000	0.46750000	1	2.98200011	2.38800001	-2.98920012
14	0.09660000	-3.31089997	-0.71660000	1	4.61770010	2.10640001	-2.38930011
6	3.33459997	-1.26329994	-0.71670002	6	-3.25510001	0.57020003	3.44009995
6	2.23119998	-1.41009998	3.21539998	1	-4.21700001	1.06860006	3.32649994
6	1.49419999	-0.46779999	3.98850012	1	-2.50489998	1.34259999	3.62190008
6	0.19419999	-0.16590001	3.67700005	1	-3.29719996	-0.11120000	4.29699993

S2.3. Zr-Al complexes $L_2Zr(\mu-H)(Et)(Al_xH_xMe_{2x})$

Calculated free activation energies for ethylene insertion are presented in Figure S1.

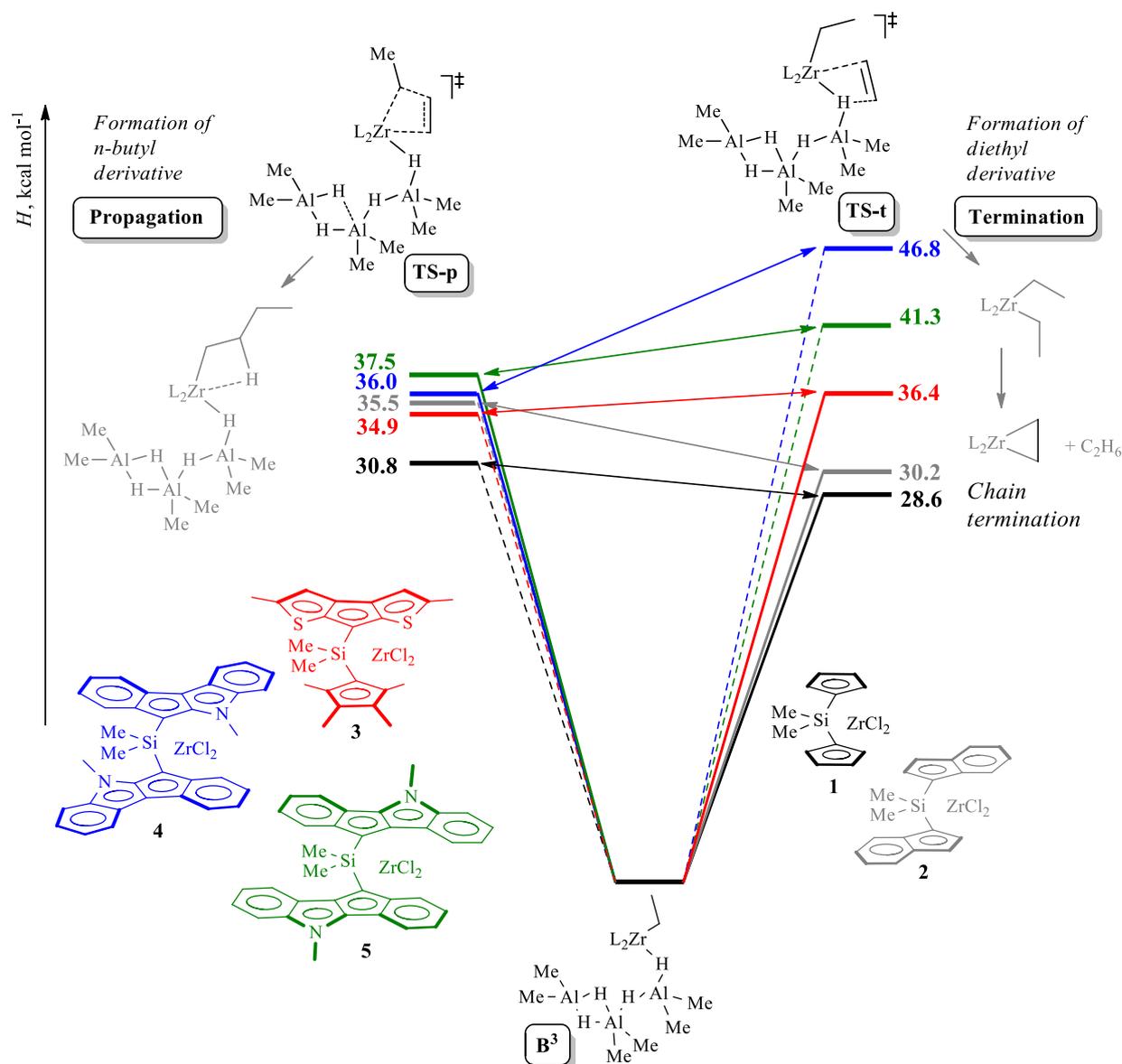
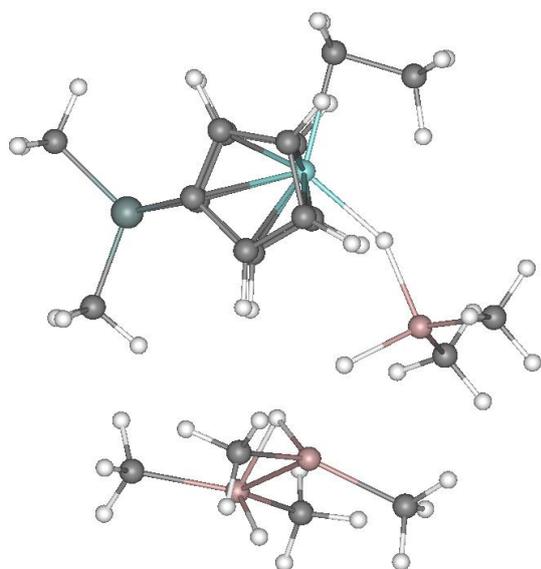


Figure S1. Calculated free activation energies (kcal mol⁻¹, 298.15 K) for ethylene insertion into the Zr–C (left) and Zr–H (right) bonds in B³ model species for zirconocenes 1–5.

B³-1

Zero-point vibrational energy	1422006.0 (Joules/Mol)
	339.86760 (Kcal/Mol)
Zero-point correction=	0.541613 (Hartree/Particle)
Thermal correction to Energy=	0.580888
Thermal correction to Enthalpy=	0.581832
Thermal correction to Gibbs Free Energy=	0.469438
Sum of electronic and zero-point Energies=	-5343.431782
Sum of electronic and thermal Energies=	-5343.392508
Sum of electronic and thermal Enthalpies=	-5343.391563
Sum of electronic and thermal Free Energies=	-5343.503958

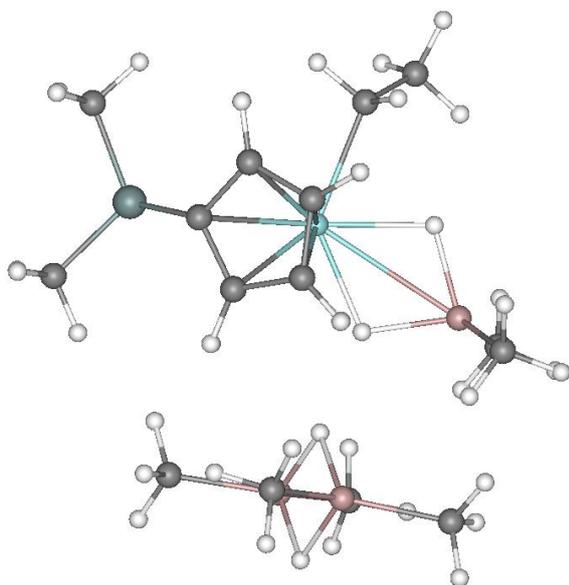
cartesian

40	1.84440005	-0.60100001	0.25369999	1	-3.71790004	0.70859998	-3.43050003
6	3.93969989	-1.29180002	0.77450001	1	-2.33960009	1.47599995	-2.66129994
1	0.42870000	-1.94299996	0.26980001	1	-2.14310002	-0.08910000	-3.46160007
1	4.36549997	-0.91930002	1.70500004	1	-5.32910013	-1.96550000	-1.42929995
6	3.36229992	-2.69610000	0.92269999	1	-3.89229989	-2.96320009	-1.21220005
1	4.68979979	-1.23440003	-0.01290000	1	-4.64519978	-2.16849995	0.17739999
1	3.47830009	-3.10809994	1.92690003	6	2.80879998	-0.89090002	-2.10619998
1	3.76270008	-3.40650010	0.19710000	6	3.05410004	0.43950000	-1.67490005
1	2.24720001	-2.77530003	0.75550002	6	1.80579996	1.11860001	-1.53659999
1	-1.64349997	-1.21270001	-0.94480002	6	0.79400003	0.16670001	-1.87329996
13	-1.18550003	-2.49760008	-0.01330000	6	1.40999997	-1.05840003	-2.23390007
6	-0.92750001	-4.12300014	-1.09389997	1	0.89490002	-1.96150005	-2.54119992
6	-2.05599999	-2.50620008	1.75129998	1	3.56060004	-1.64789999	-2.29620004
1	-1.82959998	-4.74599981	-1.09019995	1	4.03090000	0.85960001	-1.46309996

1	-0.11370000	-4.74599981	-0.70289999	14	1.42809999	2.60750008	-0.45019999
1	-0.69669998	-3.90930009	-2.14380002	1	-0.27640000	0.34259999	-1.84899998
1	-2.96670008	-3.11640000	1.72510004	6	1.93390000	0.06910000	2.73699999
1	-2.35859990	-1.50689995	2.08999991	6	2.37849998	1.16400003	1.95039999
1	-1.41450000	-2.94140005	2.52839994	6	1.28989995	1.63890004	1.15830004
6	-4.38320017	-2.03909993	-0.87940001	6	0.17649999	0.79189998	1.46130002
13	-3.31529999	-0.41190001	-1.16579998	6	0.57080001	-0.15690000	2.44000006
1	-4.78529978	0.77130002	-0.73310000	1	-0.06450000	-0.92180002	2.87080002
1	-2.75230002	0.41249999	0.27090001	1	2.53480005	-0.49800000	3.43799996
13	-4.13630009	1.39080000	0.67360002	1	3.38890004	1.55710006	1.93809998
6	-4.90789986	0.61870003	2.30469990	1	-0.81120002	0.84909999	1.01119995
6	-3.58839989	3.27230000	0.50169998	6	-0.22170000	3.33780003	-0.91270000
1	-2.73200011	3.50830007	1.14530003	6	2.85270000	3.81349993	-0.40950000
1	-3.31559992	3.54020000	-0.52509999	1	2.68099999	4.59989977	0.33109999
1	-4.40199995	3.94210005	0.80449998	1	3.79399991	3.31649995	-0.15410000
1	-4.24230003	0.74970001	3.16589999	1	2.98519993	4.29190016	-1.38440001
1	-5.86159992	1.09099996	2.56690001	1	-0.48510000	4.18230009	-0.26879999
1	-5.09590006	-0.45539999	2.19840002	1	-0.22800000	3.68390012	-1.95089996
6	-2.81999993	0.50449997	-2.83570004	1	-1.01970005	2.59310007	-0.80760002

B³-1'

for zirconocene **1** this more stable structure was considered as a ground state

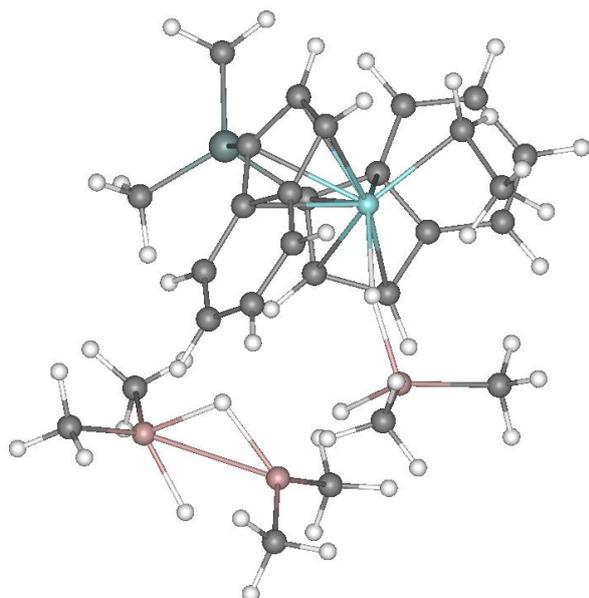


Zero-point vibrational energy	1425033.4 (Joules/Mol)
	340.59115 (Kcal/Mol)
Zero-point correction=	0.542767 (Hartree/Particle)
Thermal correction to Energy=	0.581992
Thermal correction to Enthalpy=	0.582937

Thermal correction to Gibbs Free Energy=	0.471148
Sum of electronic and zero-point Energies=	-5343.440305
Sum of electronic and thermal Energies=	-5343.401079
Sum of electronic and thermal Enthalpies=	-5343.400135
Sum of electronic and thermal Free Energies=	-5343.511924

cartesian

40	1.13629997	-0.75809997	0.14290000	1	-3.04469991	1.02199996	-3.66829991
6	2.74429989	-2.11780000	1.13849998	1	-1.86440003	1.78499997	-2.60660005
1	0.37140000	-2.63450003	0.56110001	1	-1.65989995	0.09450000	-3.09910011
1	3.70219994	-1.57780004	1.12919998	1	-5.28550005	-1.39800000	-1.80649996
6	2.51430011	-2.67269993	2.54920006	1	-3.90619993	-2.30329990	-1.20190001
1	2.87520003	-2.95970011	0.44589999	1	-4.95959997	-1.44830000	-0.07280000
1	2.61199999	-1.89359999	3.31270003	6	2.33610010	-1.63789999	-1.98679996
1	3.24780011	-3.44910002	2.80019999	6	3.12930012	-0.61129999	-1.41450000
1	1.51929998	-3.11730003	2.66000009	6	2.42160010	0.62589997	-1.49339998
1	-0.82539999	-0.98900002	-0.45050001	6	1.16820002	0.32580000	-2.11380005
13	-1.24269998	-2.58170009	0.03850000	6	1.12469995	-1.05690002	-2.42589998
6	-1.50790000	-3.68650007	-1.57060003	1	0.30410001	-1.58050001	-2.90319991
6	-2.48119998	-2.49609995	1.56739998	1	2.60540009	-2.68400002	-2.06520009
1	-2.24340010	-4.48430014	-1.41709995	1	4.10790014	-0.75180000	-0.97200000
1	-0.57470000	-4.16429996	-1.89180005	14	2.67260003	2.11490011	-0.37549999
1	-1.86629999	-3.08809996	-2.41820002	1	0.37110001	1.03450000	-2.30879998
1	-3.20530009	-3.31900001	1.56750000	6	0.77410001	0.02410000	2.60010004
1	-3.06489992	-1.56589997	1.56050003	6	1.93850005	0.65079999	2.08719993
1	-1.94719994	-2.53270006	2.52480006	6	1.56490004	1.53100002	1.02639997
6	-4.48430014	-1.38399994	-1.05719995	6	0.14550000	1.40330005	0.88580000
13	-3.44129992	0.25630000	-1.25730002	6	-0.33390000	0.49059999	1.86039996
1	-4.49849987	1.58980000	-0.78090000	1	-1.36150002	0.17389999	2.00119996
1	-2.64969993	0.70060003	0.21560000	1	0.73360002	-0.69610000	3.40730000
13	-3.68300009	2.01690006	0.69459999	1	2.94970012	0.47330001	2.43630004
6	-4.70849991	1.43009996	2.24850011	1	-0.46750000	1.90699995	0.14430000
6	-2.71180010	3.69569993	0.44250000	6	2.00419998	3.67589998	-1.15380001
1	-1.93280005	3.82290006	1.20280004	6	4.45190001	2.24359989	0.17919999
1	-2.22810006	3.75289989	-0.53939998	1	4.57469988	3.02259994	0.93730003
1	-3.37969995	4.56069994	0.52120000	1	4.80270004	1.30079997	0.61189997
1	-4.07289982	1.36600006	3.13899994	1	5.10780001	2.48589993	-0.66229999
1	-5.51989985	2.12599993	2.48769999	1	2.05320001	4.51440001	-0.45269999
1	-5.15759993	0.44299999	2.09689999	1	2.57270002	3.94530010	-2.04879999
6	-2.39829993	0.84759998	-2.80069995	1	0.95690000	3.55730009	-1.45050001

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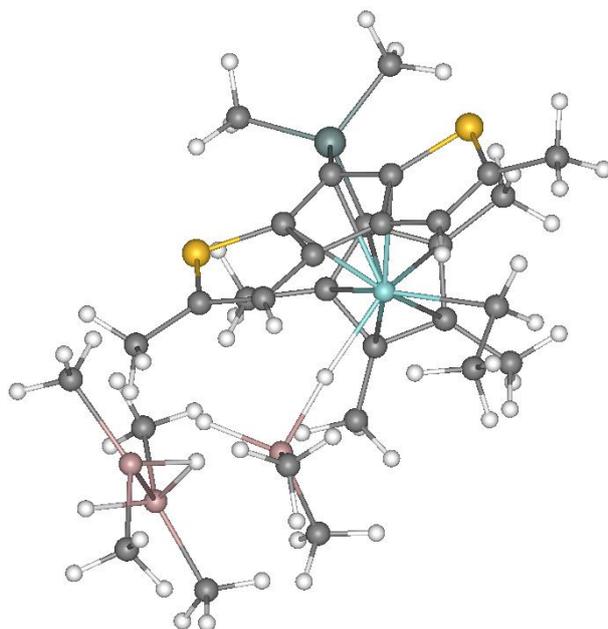
Zero-point vibrational energy	1669950.7 (Joules/Mol)
	399.12779 (Kcal/Mol)
Zero-point correction=	0.636051 (Hartree/Particle)
Thermal correction to Energy=	0.679612
Thermal correction to Enthalpy=	0.680556
Thermal correction to Gibbs Free Energy=	0.560508
Sum of electronic and zero-point Energies=	-5650.503288
Sum of electronic and thermal Energies=	-5650.459727
Sum of electronic and thermal Enthalpies=	-5650.458782
Sum of electronic and thermal Free Energies=	-5650.578830

cartesian

6	-2.43249989	0.75250000	-1.51610005	6	-2.72900009	-2.82060003	0.63050002
6	-1.94630003	-0.47250000	-2.09850001	1	-3.99569988	-1.26170003	1.50380003
6	-0.52829999	-0.50230002	-1.92670000	1	-1.60979998	-2.78139997	0.75360000
6	-0.15290000	0.69620001	-1.28520000	1	-2.86170006	-3.37479997	-0.30250001
6	-1.30929995	1.48409998	-0.97850001	1	-3.03299999	-3.44650006	1.47270000
6	-1.87409997	-0.26660001	3.04399991	1	2.11360002	-1.51269996	-0.85960001
6	-1.18579996	1.59039998	1.80970001	13	1.33120000	-2.70919991	-0.05530000
6	-0.02150000	0.82260001	2.19280005	6	2.40240002	-3.57529998	1.34570003
6	-0.44760001	-0.30700001	2.97460008	6	0.30000001	-3.86630011	-1.28910005
14	-1.28199995	2.79180002	0.36759999	1	2.84599996	-4.49709988	0.94790000
6	-2.30349994	0.90210003	2.37879992	1	1.79799998	-3.86100006	2.21510005
6	-4.66470003	0.17700000	-2.22340012	1	3.22740006	-2.95129991	1.70350003
6	-4.17859983	-1.04170001	-2.78920007	1	-0.01400000	-4.78579998	-0.77810001
6	-2.84829998	-1.37310004	-2.73160005	1	0.91570002	-4.18219995	-2.14120007

6	-3.82319999	1.05550003	-1.58899999	1	-0.60589999	-3.41059995	-1.70760000
1	-4.20359993	1.98839998	-1.18390000	6	2.93560004	-0.73820001	-3.38849998
1	-5.72200012	0.40900001	-2.30550003	13	3.62290001	-0.72039998	-1.54610002
1	-4.87900019	-1.70700002	-3.28460002	1	4.88539982	0.75950003	-1.85109997
1	-2.47709990	-2.28800011	-3.18499994	1	2.95729995	0.59390002	-0.60030001
6	2.26880002	0.09840000	2.44039989	13	4.04519987	1.88989997	-0.97460002
6	1.84189999	-0.98070002	3.27150011	6	3.08629990	3.16950011	-2.13109994
6	0.51419997	-1.20109999	3.52719998	6	4.88700008	2.37879992	0.73509997
6	1.36780000	0.98570001	1.90929997	1	4.16319990	2.77180004	1.46039999
1	1.71619999	1.82360005	1.31099999	1	5.38990021	1.52390003	1.20130002
1	3.32800007	0.22880000	2.23440003	1	5.64529991	3.15879989	0.59990001
1	2.58750010	-1.64610004	3.69440007	1	2.87789989	4.12360001	-1.63399994
1	0.19419999	-2.03200006	4.14949989	1	3.69199991	3.39809990	-3.01600003
6	0.22960000	3.87649989	0.20649999	1	2.13319993	2.77530003	-2.50539994
6	-2.85640001	3.79620004	0.46919999	6	4.94229984	-1.84089994	-0.62029999
1	-2.73760009	4.59119987	1.21249998	1	5.93870020	-1.73580003	-1.06309998
1	-3.72370005	3.19899988	0.76480001	1	5.03000021	-1.55719995	0.43630001
1	-3.08229995	4.27110004	-0.49070001	1	4.67950010	-2.90549994	-0.64080000
1	0.53600001	4.28679991	1.17400002	1	3.72580004	-0.55419999	-4.12440014
1	0.02030000	4.71500015	-0.46610001	1	2.46779990	-1.69840002	-3.64080000
1	1.08099997	3.33690000	-0.22030000	1	2.17490005	0.03960000	-3.53660011
40	-1.39649999	-0.49570000	0.50819999	1	-2.50699997	-0.97570002	3.56430006
6	-3.41689992	-1.45930004	0.60189998	1	-3.34120011	1.19760001	2.26349998
1	0.17560001	-1.65429997	0.65910000	1	0.15130000	-1.25950003	-2.29979992
1	-4.05060005	-1.33749998	-0.27520001	1	0.87110001	0.94450003	-1.01520002

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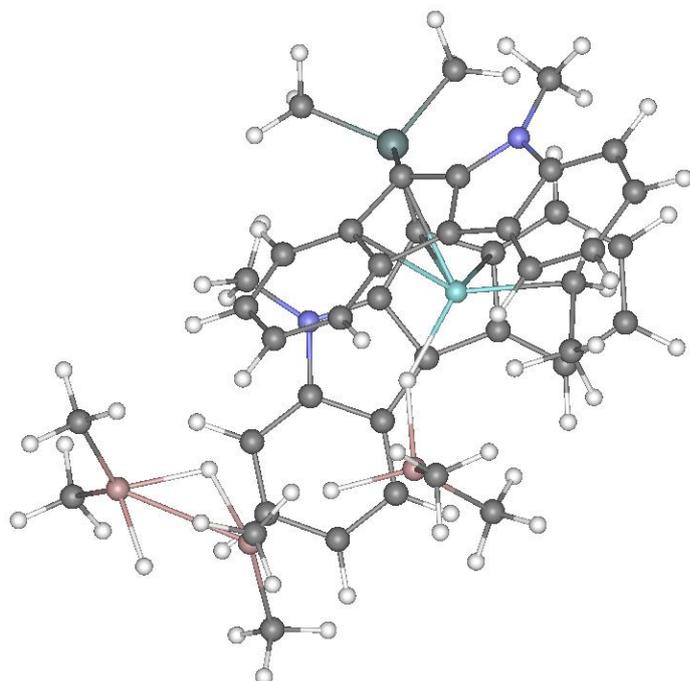


Zero-point vibrational energy	1937874.9 (Joules/Mol)
	463.16322 (Kcal/Mol)
Zero-point correction=	0.738098 (Hartree/Particle)
Thermal correction to Energy=	0.790920
Thermal correction to Enthalpy=	0.791864
Thermal correction to Gibbs Free Energy=	0.655924
Sum of electronic and zero-point Energies=	-6527.665428
Sum of electronic and thermal Energies=	-6527.612605
Sum of electronic and thermal Enthalpies=	-6527.611661
Sum of electronic and thermal Free Energies=	-6527.747601

				cartesian			
40	1.08430004	-0.23180000	-0.60769999	6	-0.31610000	-2.03789997	0.40410000
6	2.44250011	-0.16450000	-2.38459992	6	1.05859995	-2.33550000	0.69389999
1	-0.68419999	0.61260003	-0.96380001	6	1.68470001	-2.67140007	-0.56199998
1	2.44619989	-1.03149998	-3.04430008	6	0.69770002	-2.60780001	-1.58389997
6	1.63650000	0.99879998	-2.97029996	16	4.78889990	0.20200001	0.26830000
1	3.47359991	0.12580000	-2.17249990	14	1.98160005	-1.69180000	2.20479989
1	0.91729999	1.46870005	-2.25169992	6	-0.53310001	2.96779990	1.52269995
1	1.01789999	0.70969999	-3.82380009	6	0.49360001	3.20000005	0.66289997
1	2.26839995	1.84440005	-3.25869989	16	-0.39680001	1.42219996	2.35209990
1	-2.73869991	1.39779997	0.08410000	1	0.56870002	4.10729980	0.07450000
13	-2.05679989	1.57050002	-1.41139996	6	3.67199993	-2.45989990	2.44129992
6	-1.49790001	3.41709995	-1.84749997	6	1.03590000	-1.78869998	3.81900001
6	-3.02290010	0.68419999	-2.88509989	1	0.50389999	-2.74009991	3.91639996
1	-2.06970000	3.75289989	-2.72189999	1	0.30890000	-0.98189998	3.94650006
1	-0.43669999	3.49970007	-2.11450005	1	1.74510002	-1.71580005	4.65010023
1	-1.68669999	4.13940001	-1.04600000	1	3.58100009	-3.53169990	2.64809990
1	-3.64560008	1.44400001	-3.37610006	1	4.15479994	-1.99590003	3.30800009
1	-3.68580008	-0.14129999	-2.60509992	1	4.34280014	-2.34369993	1.58729994
1	-2.33759999	0.30840001	-3.65739989	6	4.89510012	1.63499999	-0.74769998
6	-5.31029987	2.38129997	-0.56860000	6	3.75889993	2.38339996	-0.72869998
13	-4.49709988	1.02590001	0.60360003	1	3.65899992	3.31139994	-1.28180003
1	-6.13460016	-0.03140000	0.75680000	6	6.16120005	1.89769995	-1.50619996
1	-4.07149982	-0.48040000	-0.14370000	1	6.35459995	1.10950005	-2.23920012
13	-5.53160000	-1.39429998	0.00700000	1	6.07940006	2.84759998	-2.03760004
6	-6.20219994	-1.65859997	-1.82009995	1	7.02159977	1.95309997	-0.83420002
6	-5.14480019	-2.85610008	1.26520002	6	-1.71410000	3.85100007	1.78729999
1	-4.45330000	-3.59109998	0.83520001	1	-1.51909995	4.84709978	1.38360000
1	-4.69869995	-2.48309994	2.19440007	1	-2.61479998	3.45549989	1.30579996

1	-6.05319977	-3.40400004	1.54139996	1	-1.91400003	3.94540000	2.85800004
1	-5.50829983	-2.25929999	-2.42090011	6	3.10890007	-3.12439990	-0.76859999
1	-7.16590023	-2.18070006	-1.83350003	6	0.83219999	-2.99880004	-3.02810001
1	-6.34110022	-0.70539999	-2.34229994	6	-1.85870004	-2.19779992	-1.67980003
6	-4.09789991	1.02880001	2.53290009	6	-1.43980002	-1.72440004	1.35769999
1	-5.02209997	1.00450003	3.12140012	1	1.87020004	-3.17260003	-3.31570005
1	-3.51559997	0.14219999	2.81480002	1	0.27300000	-3.92070007	-3.22099996
1	-3.52629995	1.90400004	2.86249995	1	0.42710000	-2.22849989	-3.69230008
1	-6.27190018	2.72740006	-0.17260000	1	3.22679996	-3.57450008	-1.75629997
1	-4.67880011	3.26819992	-0.71340001	1	3.83640003	-2.30990005	-0.69910002
1	-5.51140022	1.96379995	-1.56350005	1	3.37750006	-3.88490009	-0.03040000
6	1.11350000	1.07990003	1.54639995	1	-1.79040003	-1.82519996	-2.70460010
6	1.44529998	2.12229991	0.63679999	1	-2.26679993	-3.21560001	-1.71920002
6	2.73760009	1.80980003	0.10320000	1	-2.57520008	-1.57110000	-1.14419997
6	3.14730000	0.59340000	0.71130002	1	-1.99539995	-0.83219999	1.05060005
6	2.14730000	0.07780000	1.60909998	1	-2.14829993	-2.56080008	1.37979996
6	-0.52759999	-2.21469998	-0.99100000	1	-1.08910000	-1.56229997	2.37730002

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Zero-point vibrational energy	2221985.8 (Joules/Mol)
	531.06736 (Kcal/Mol)
Zero-point correction=	0.846310 (Hartree/Particle)
Thermal correction to Energy=	0.900914
Thermal correction to Enthalpy=	0.901858
Thermal correction to Gibbs Free Energy=	0.761366

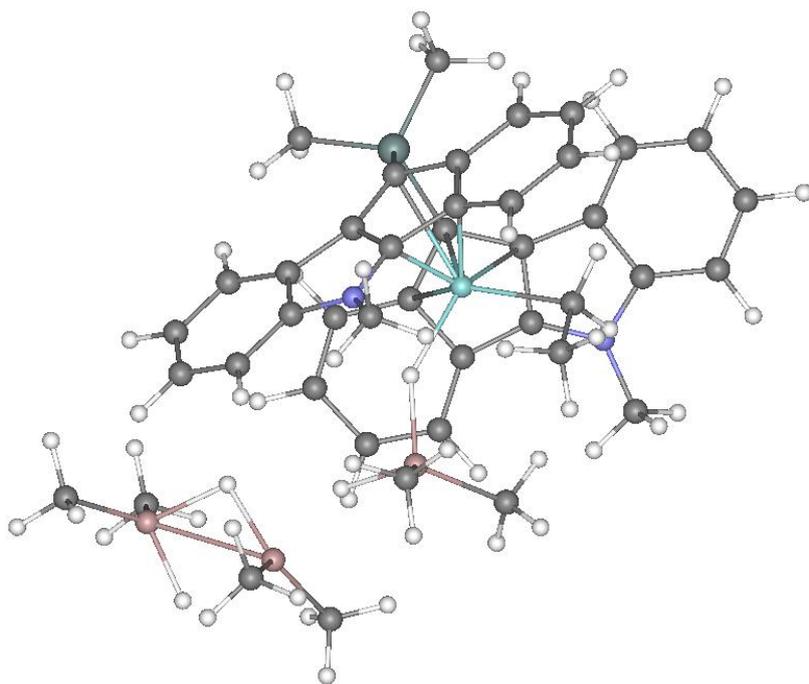
Sum of electronic and zero-point Energies=	-6299.106732
Sum of electronic and thermal Energies=	-6299.052128
Sum of electronic and thermal Enthalpies=	-6299.051184
Sum of electronic and thermal Free Energies=	-6299.191676

cartesian

6	-1.81959999	-2.73900008	0.62400001	6	4.57889986	-2.17729998	1.15789998
6	-0.89440000	-2.50060010	1.70980000	1	4.29540014	-2.27539992	-0.98030001
6	0.38420001	-2.24760008	1.11880004	1	4.59630013	-2.09080005	3.31030011
6	0.23440000	-2.38639998	-0.28810000	1	5.66179991	-2.17429996	1.08389997
6	-1.14059997	-2.57439995	-0.66979998	1	-6.25759983	0.47220001	-1.52400005
6	-2.21819997	1.88730001	-0.90560001	1	-5.09320021	-0.56910002	-2.34759998
6	-2.91420007	0.74790001	-1.38759995	1	-5.38980007	-0.77710003	-0.59500003
6	-2.01719999	-0.20999999	-1.98189998	1	-2.18059993	4.52489996	0.44499999
6	-0.73250002	0.52020001	-2.00920010	6	-4.31010008	4.58690023	0.78789997
6	-0.85689998	1.78989995	-1.34790003	6	-5.53879976	3.92330003	0.63669997
7	1.48000002	-2.34910011	-0.88639998	1	-6.57989979	2.18000007	-0.08750000
14	-2.04150009	-2.07360005	-2.25130010	1	-6.44299984	4.37960005	1.02680004
7	-4.26230001	0.91439998	-1.15709996	1	-4.28009987	5.54850006	1.28970003
6	-3.51670003	-3.26329994	2.27119994	40	-1.19169998	-0.27460000	0.31009999
6	-2.60409999	-3.00359988	3.32730007	6	-2.92589998	0.07760000	1.65709996
6	-1.30879998	-2.62509990	3.05870008	1	0.50840002	0.60030001	0.75260001
6	-3.14569998	-3.12779999	0.95130002	1	-3.16440010	-0.76849997	2.30089998
1	-3.85120010	-3.38280010	0.17050000	6	-2.13739991	1.15579998	2.39429998
1	-4.52349997	-3.59130001	2.51020002	1	-3.84270000	0.46550000	1.21060002
1	-2.92939997	-3.12649989	4.35540009	1	-1.21679997	1.49609995	1.84920001
1	-0.59649998	-2.46359992	3.86249995	1	-1.77429998	0.82749999	3.37159991
6	1.60630000	1.01820004	-2.39569998	1	-2.69289994	2.09319997	2.49569988
6	1.45280004	2.29329991	-1.79729998	1	2.90809989	1.11769998	1.19029999
6	0.23800001	2.68309999	-1.28090000	13	1.47119999	1.42639995	1.92690003
6	0.54130000	0.15230000	-2.50970006	6	0.97570002	3.33649993	2.01139998
1	0.67320001	-0.78990000	-3.02460003	6	1.14400005	0.52700001	3.66039991
1	2.57599998	0.73760003	-2.79719996	1	1.60880005	3.81060004	2.77519989
1	2.30410004	2.96639991	-1.75639999	1	-0.05920000	3.45950007	2.36129999
1	0.10650000	3.66580009	-0.84119999	1	1.09440005	3.93149996	1.10380006
6	-1.26400006	-2.57929993	-3.88590002	1	0.61199999	1.22239995	4.32289982
6	-3.74219990	-2.86409998	-2.35060000	1	2.07299995	0.24620000	4.17019987
1	-4.19229984	-2.62849998	-3.32139993	1	0.52859998	-0.37880000	3.58660007
1	-4.45450020	-2.58410001	-1.57690001	6	5.54129982	1.14390004	2.30979991
1	-3.61529994	-3.95239997	-2.31040001	13	4.57340002	1.82509995	0.73970002
1	-1.98819995	-2.33999991	-4.67299986	1	6.27370024	1.97340000	-0.32949999

1	-1.11049998	-3.66409993	-3.91039991	1	4.29470015	0.79619998	-0.63489997
1	-0.32890001	-2.09430003	-4.16540003	13	5.72419977	1.06229997	-1.59309995
6	2.43319988	-2.23480010	0.13030000	6	6.68940020	-0.64039999	-1.82290006
6	1.80410004	-2.17560005	1.39540005	6	5.17759991	2.11929989	-3.16599989
6	2.58859992	-2.13639998	2.55100012	1	4.78480005	1.49419999	-3.97720003
6	3.81839991	-2.23589993	-0.00600000	1	4.42019987	2.87800002	-2.93759990
6	-3.19289994	2.77659988	-0.32640001	1	6.03940010	2.65630007	-3.58100009
6	-4.44229984	2.12430000	-0.48370001	1	6.19530010	-1.31760001	-2.53049994
6	-5.30590010	-0.04950000	-1.41219997	1	7.69159985	-0.45109999	-2.22679996
6	-5.62389994	2.68569994	0.00510000	1	6.82819986	-1.18210006	-0.88110000
6	-3.13290000	4.01929998	0.31250000	6	4.10750008	3.70980000	0.39330000
6	1.82809997	-2.89190006	-2.18420005	1	4.45009995	4.33339977	1.22950006
1	2.46700001	-3.77259994	-2.05819988	1	4.61189985	4.08790016	-0.50410002
1	0.91880000	-3.19720006	-2.70040011	1	3.03679991	3.90159988	0.28240001
1	2.36290002	-2.15610003	-2.79390001	1	6.16079998	1.94500005	2.73230004
1	2.12980008	-2.11590004	3.53379989	1	4.87120008	0.78560001	3.09990001
6	3.97350001	-2.13120008	2.42240000	1	6.21890020	0.32229999	2.05380011

B³-5



Zero-point vibrational energy	2224782.3 (Joules/Mol)
	531.73574 (Kcal/Mol)
Zero-point correction=	0.847375 (Hartree/Particle)
Thermal correction to Energy=	0.904324
Thermal correction to Enthalpy=	0.905268
Thermal correction to Gibbs Free Energy=	0.760135

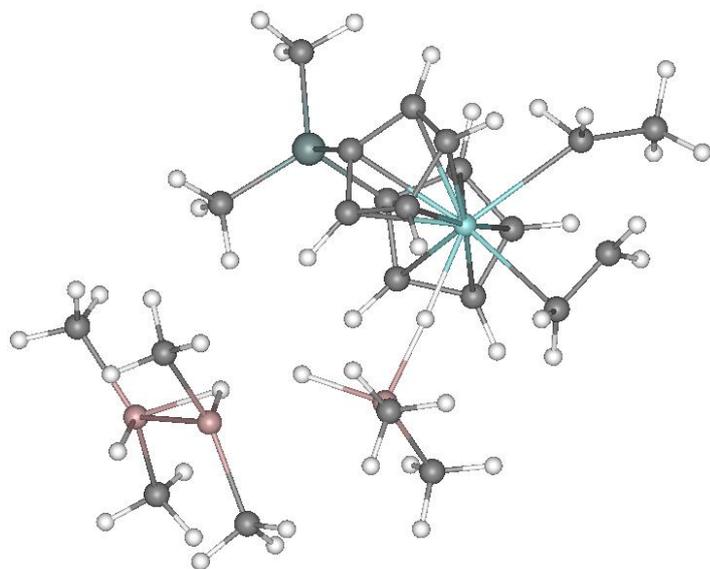
Sum of electronic and zero-point Energies=	-6299.104142
Sum of electronic and thermal Energies=	-6299.047193
Sum of electronic and thermal Enthalpies=	-6299.046249
Sum of electronic and thermal Free Energies=	-6299.191382

cartesian

6	0.38020000	-1.24469995	1.79349995	6	-3.57620001	2.14369988	1.59560001
6	0.45930001	-2.26270008	0.76819998	6	-4.07119989	2.49710011	0.32820001
6	1.84329998	-2.33209991	0.41949999	1	-3.60439992	3.07990003	-1.68929994
6	2.58229995	-1.37170005	1.16320002	1	-5.14389992	2.53469992	0.16540000
6	1.67610002	-0.64270002	2.03950000	1	-4.27190018	1.92589998	2.40009999
6	0.37750000	2.68479991	-0.70850003	6	-0.87459999	3.59699988	-2.66890001
6	0.14129999	2.32870007	0.64579999	1	-1.91330004	3.64010000	-2.99259996
6	1.41639996	2.07100010	1.29740000	1	-0.31720001	3.02509999	-3.41490006
6	2.40930009	2.34789991	0.26980001	1	-0.47409999	4.61469984	-2.61109996
6	1.77929997	2.72119999	-0.97399998	6	2.31500006	-4.13280010	-1.30649996
6	3.96790004	-1.53740001	0.74190003	1	2.95729995	-5.00610018	-1.16439998
14	1.82519996	1.05710006	2.82640004	1	2.40630007	-3.77789998	-2.33890009
6	-1.31149995	2.33649993	0.78810000	1	1.28349996	-4.43319988	-1.13030005
6	-2.00099993	-1.66880000	1.96070004	40	1.09879994	0.17010000	-0.18240000
6	-1.90279996	-2.69779992	0.98199999	6	2.42960000	-0.23260000	-1.93499994
6	-0.70109999	-3.00130010	0.39579999	1	-0.70730001	-0.02740000	-0.96619999
6	-0.89679998	-0.96190000	2.36240005	1	2.71110010	-1.28729999	-2.02539992
1	-0.98750001	-0.22930001	3.15520000	6	1.60169995	0.21080001	-3.16079998
1	-2.96760011	-1.46060002	2.41059995	1	3.36199999	0.34029999	-1.85940003
1	-2.79279995	-3.25430012	0.70490003	1	0.81559998	0.94669998	-2.92120004
1	-0.64150000	-3.80110002	-0.33410001	1	1.09039998	-0.63239998	-3.63299990
6	4.55749989	2.56040001	-0.82870001	1	2.22979999	0.69000000	-3.92070007
6	3.92219996	2.95760012	-2.03699994	1	-2.98860002	-0.98000002	-1.19500005
6	2.55270004	3.04819989	-2.11470008	13	-1.70780003	-0.72570002	-2.17950010
6	3.82979989	2.26290011	0.29890001	6	-2.13809991	0.59100002	-3.58030009
1	4.34460020	2.00449991	1.21689999	6	-0.77840000	-2.37350011	-2.78139997
1	5.64080000	2.50049996	-0.79420000	1	-2.71609998	0.07550000	-4.35960007
1	4.52890015	3.20169997	-2.90310001	1	-1.25489998	1.00460005	-4.08169985
1	2.07279992	3.36069989	-3.03740001	1	-2.76349998	1.42069995	-3.23410010
6	3.51489997	1.41390002	3.56189990	1	-0.63650000	-2.35400009	-3.86949992
6	0.66090000	1.36210001	4.26630020	1	-1.33739996	-3.28760004	-2.54949999
1	1.08710003	2.17459989	4.86530018	1	0.21900000	-2.47979999	-2.33159995
1	-0.35049999	1.66550004	4.00190020	6	-4.55749989	-3.35969996	-1.31320000
1	0.60119998	0.47799999	4.90999985	13	-4.77780008	-1.41139996	-1.10300004
1	3.69580007	2.49379992	3.59270000	1	-6.49480009	-1.69920003	-0.17970000

1	3.50489998	1.05429995	4.59679985	1	-4.51149988	-0.69209999	0.46070001
1	4.36180019	0.93820000	3.07200003	13	-6.06220007	-0.90170002	1.20980000
6	3.96350002	-2.60220003	-0.20080000	6	-5.73330021	-2.08839989	2.74769998
7	2.68039989	-3.09809995	-0.35969999	6	-7.03630018	0.80409998	1.35029995
6	5.19210005	-0.93000001	1.04830003	1	-6.58160019	1.53629994	2.02670002
6	5.12500000	-3.03270006	-0.84850001	1	-7.15409994	1.27709997	0.36849999
7	-0.79689997	2.94639993	-1.37539995	1	-8.04839993	0.61830002	1.73130000
6	-1.83410001	2.72340012	-0.47929999	1	-5.22359991	-1.57470000	3.57200003
6	-3.21059990	2.80040002	-0.71679997	1	-6.67350006	-2.47569990	3.15750003
6	-2.21190000	2.06859994	1.82819998	1	-5.12400007	-2.95889997	2.47589993
1	5.25260019	-0.13460000	1.78020000	6	-5.44519997	-0.09300000	-2.40039992
6	6.35190010	-1.35739994	0.41460001	1	-6.53749990	-0.11910000	-2.48329997
6	6.31720018	-2.39660001	-0.53039998	1	-5.16179991	0.92369998	-2.09910011
1	5.09660006	-3.83340001	-1.58140004	1	-5.03590012	-0.25170001	-3.40520000
1	7.29839993	-0.88360000	0.65380001	1	-5.28700018	-3.73169994	-2.04349995
1	7.23500013	-2.70830011	-1.01880002	1	-3.56349993	-3.66149998	-1.66429996
1	-1.85619998	1.80579996	2.81570005	1	-4.76249981	-3.89829993	-0.37990001

TSP-1



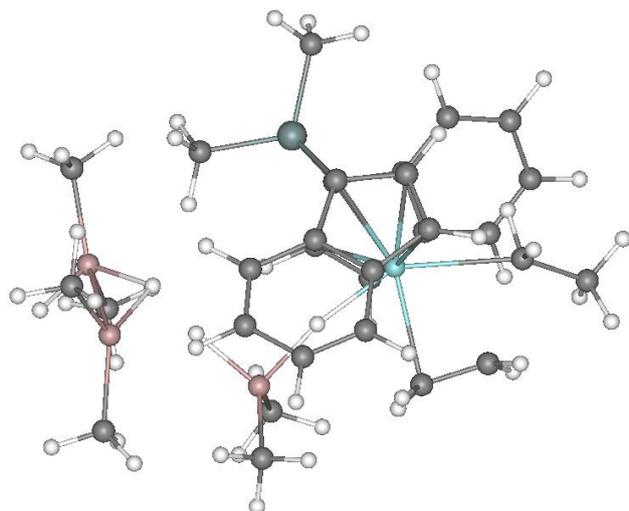
Zero-point vibrational energy	1570261.5 (Joules/Mol)
	375.30150 (Kcal/Mol)
Zero-point correction=	0.598081 (Hartree/Particle)
Thermal correction to Energy=	0.639600
Thermal correction to Enthalpy=	0.640545
Thermal correction to Gibbs Free Energy=	0.524633
Sum of electronic and zero-point Energies=	-5421.903481
Sum of electronic and thermal Energies=	-5421.861962

Sum of electronic and thermal Enthalpies= -5421.861018
 Sum of electronic and thermal Free Energies= -5421.976929

cartesian

40	-1.95410001	-0.23220000	-0.04050000	1	6.85029984	0.42039999	-2.61339998
6	-4.51200008	-0.04020000	-0.29560000	1	5.63219976	-0.85430002	-2.64680004
1	-0.46810001	-1.39170003	0.07540000	6	3.49819994	-0.21089999	2.54920006
6	-2.53449988	-2.55629992	-0.33210000	1	4.43179989	-0.24950001	3.12159991
6	-3.81290007	-2.06979990	-0.63110000	1	3.17589998	0.83789998	2.54419994
1	-2.36269999	-3.05419993	0.61849999	1	2.74749994	-0.77929997	3.11269999
1	-1.89830005	-2.86610007	-1.15610003	1	5.24170017	-2.99550009	0.45330000
1	-4.08610010	-1.98800004	-1.67869997	1	3.57660007	-3.54530001	0.59329998
1	-4.63780022	-2.29040003	0.03850000	1	4.15859985	-2.86350012	-0.92869997
1	-4.15460014	0.99470001	-0.29300001	6	-2.85500002	0.08770000	2.36840010
6	-5.58500004	-0.13760000	-1.37399995	6	-2.56690001	1.36090004	1.80850005
1	-4.95609999	-0.21230000	0.68599999	6	-1.15470004	1.47430003	1.61619997
1	-5.17490005	0.00210000	-2.37899995	6	-0.59530002	0.23559999	2.04439998
1	-6.34709978	0.63459998	-1.22500002	6	-1.63859999	-0.61409998	2.50500011
1	-6.10109997	-1.10259998	-1.35889995	1	-1.51409996	-1.61749995	2.89499998
1	1.90579998	-1.06070006	0.43910000	1	-3.83330011	-0.28070000	2.65109992
13	0.92839998	-2.35879993	0.16490000	1	-3.29940009	2.12829995	1.58200002
6	0.67530000	-3.42589998	1.80040002	14	-0.31740001	2.63989997	0.39860001
6	1.14499998	-3.09470010	-1.64760005	1	0.45930001	-0.02230000	2.01410007
1	1.45690000	-4.18590021	1.91569996	6	-2.23350000	0.48060000	-2.51349998
1	-0.28220001	-3.96219993	1.80350006	6	-2.10809994	1.64590001	-1.71329999
1	0.70670003	-2.80579996	2.70490003	6	-0.79339999	1.68910003	-1.15559995
1	1.86109996	-3.92490005	-1.64779997	6	-0.12860000	0.51490003	-1.61459994
1	1.53279996	-2.34640002	-2.35039997	6	-1.01240003	-0.22640000	-2.44700003
1	0.21190000	-3.48959994	-2.06900001	1	-0.77910000	-1.15939999	-2.94670010
6	4.21150017	-2.75999999	0.16210000	1	-3.10419989	0.18780001	-3.08710003
13	3.74670005	-0.93390000	0.73650002	1	-2.88059998	2.39269996	-1.56389999
1	5.48839998	-0.20010000	0.46830001	1	0.88919997	0.22920001	-1.36500001
1	3.48259997	0.18780001	-0.59060001	6	1.52890003	2.63860011	0.62860000
13	5.08839989	0.83639997	-0.78250003	6	-1.11469996	4.32919979	0.42719999
6	5.77689981	0.22350000	-2.51430011	1	-0.70670003	4.96829987	-0.36140001
6	5.04549980	2.70930004	-0.18810000	1	-2.19779992	4.27050018	0.27869999
1	4.51580000	3.35649991	-0.89679998	1	-0.94019997	4.82469988	1.38680005
1	4.55679989	2.81520009	0.78729999	1	2.02769995	3.23169994	-0.14430000
1	6.05849981	3.11590004	-0.08670000	1	1.81420004	3.04500008	1.60389996
1	5.28249979	0.72700000	-3.35260010	1	1.92929995	1.62010002	0.56360000

TS^p-2

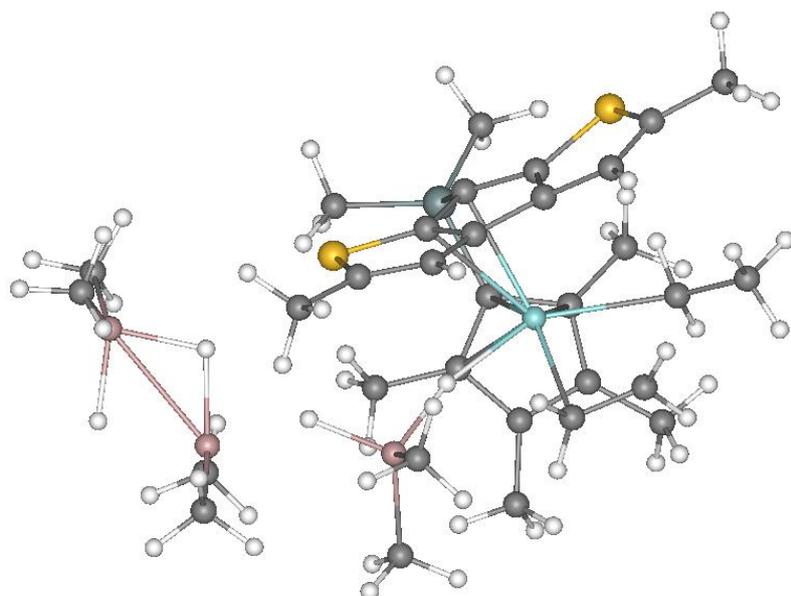


Zero-point vibrational energy	1821856.8 (Joules/Mol)
	435.43421 (Kcal/Mol)
Zero-point correction=	0.693909 (Hartree/Particle)
Thermal correction to Energy=	0.739773
Thermal correction to Enthalpy=	0.740717
Thermal correction to Gibbs Free Energy=	0.617958
Sum of electronic and zero-point Energies=	-5728.968330
Sum of electronic and thermal Energies=	-5728.922465
Sum of electronic and thermal Enthalpies=	-5728.921019
Sum of electronic and thermal Free Energies=	-5729.044280

cartesian							
40	1.57019997	0.40380001	-0.19140001	1	-6.00150013	1.58980000	-1.73580003
6	4.06220007	0.39750001	-0.73130000	1	-4.41120005	2.26200008	-2.08529997
1	-0.17090000	1.12870002	-0.57849997	1	-4.86329985	0.67119998	-2.71210003
6	1.58410001	2.09669995	-1.92719996	6	0.44250000	1.58819997	1.90779996
6	2.93680000	1.78180003	-2.04250002	6	1.49409997	2.49390006	1.53110003
1	1.28240001	3.00580001	-1.41400003	6	2.73029995	1.80299997	1.68149996
1	0.90450001	1.72520006	-2.69059992	6	2.44320011	0.49930000	2.14289999
1	3.25049996	1.17400002	-2.88400006	6	1.02450001	0.31999999	2.25929999
1	3.67950010	2.48119998	-1.67149997	6	0.69669998	-1.43139994	-1.79400003
1	3.93540001	-0.55809999	-0.20500000	6	0.60310000	-1.81879997	0.50749999
6	5.11159992	0.19710000	-1.82290006	6	1.90719998	-2.20409989	0.02210000
1	4.45730019	1.10529995	-0.00560000	6	1.95249999	-1.98790002	-1.39880002
1	4.74709988	-0.40110001	-2.66109991	14	0.18390000	-1.35959995	2.27889991
1	5.98309994	-0.32290000	-1.41009998	6	-0.13130000	-1.41009998	-0.64139998
1	5.46490002	1.15409994	-2.22009993	6	-1.16279995	3.35780001	1.60029995

1	-2.56629992	1.01979995	-0.19710000	6	-0.11580000	4.24879980	1.19959998
13	-1.62300003	1.58089995	-1.42499995	6	1.18879998	3.83829999	1.16180003
6	-1.70760000	3.53340006	-1.68060005	6	-0.90700001	2.05809999	1.93799996
6	-1.76960003	0.44810000	-3.03520012	1	-1.71640003	1.40030003	2.24090004
1	-2.09400010	3.74370003	-2.68610001	1	-2.18330002	3.72770000	1.63279998
1	-0.74390000	4.04640007	-1.59249997	1	-0.37020001	5.26949978	0.93110001
1	-2.39059997	4.01030016	-0.96799999	1	1.98510003	4.52419996	0.88499999
1	-1.98259997	-0.61040002	-2.84010005	6	4.12809992	-3.13720012	-0.05850000
1	-0.89069998	0.49559999	-3.69099998	6	4.15619993	-2.94939995	-1.47280002
1	-2.60920000	0.82709998	-3.63210011	6	3.09750009	-2.38540006	-2.13949990
6	-4.94049978	1.33169997	-1.84050000	6	3.02920008	-2.77880001	0.68320000
13	-4.33010006	0.43619999	-0.19710000	1	3.00040007	-2.97070003	1.75189996
1	-5.72949982	-0.88950002	-0.23540001	1	4.98150015	-3.59780002	0.42919999
1	-3.44490004	-1.06159997	-0.42309999	1	5.03380013	-3.26729989	-2.02780008
13	-4.73880005	-2.22009993	-0.44470000	1	3.11879992	-2.26300001	-3.21900010
6	-4.80810022	-2.96110010	-2.26090002	6	0.97469997	-2.48690009	3.54940009
6	-4.57999992	-3.29099989	1.19679999	6	-1.66610003	-1.27349997	2.48219991
1	-3.66210008	-3.89089990	1.20369995	1	-2.07599998	-2.28749990	2.54209995
1	-4.57460022	-2.66039991	2.09319997	1	-2.15170002	-0.77939999	1.63329995
1	-5.41559982	-3.99280000	1.30120003	1	-1.95350003	-0.74320000	3.39599991
1	-3.91810012	-3.55920005	-2.48760009	1	0.87419999	-3.53979993	3.26780009
1	-5.67549992	-3.61599994	-2.40240002	1	0.47950000	-2.35229993	4.51660013
1	-4.87179995	-2.17079997	-3.01690006	1	2.03640008	-2.27139997	3.70079994
6	-4.63049984	0.96670002	1.67490005	1	3.19070005	-0.26280001	2.34689999
1	-5.70079994	1.11150002	1.86310005	1	3.71190000	2.23650002	1.54349995
1	-4.28599977	0.20860000	2.38879991	1	-1.17060006	-1.09609997	-0.62860000
1	-4.12779999	1.90890002	1.92610002	1	0.38460001	-1.20910001	-2.80669999

TS^p-3



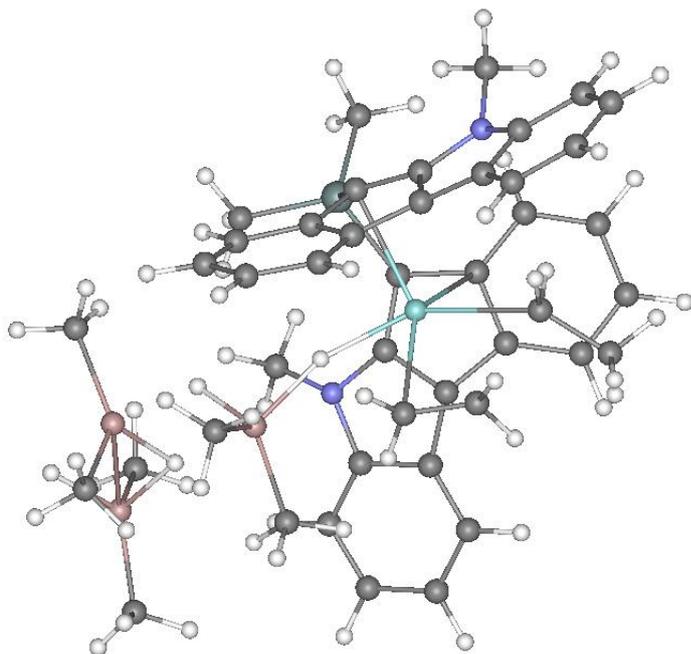
Zero-point vibrational energy	2087459.7 (Joules/Mol)
	498.91485 (Kcal/Mol)
Zero-point correction=	0.795071 (Hartree/Particle)
Thermal correction to Energy=	0.850421
Thermal correction to Enthalpy=	0.851365
Thermal correction to Gibbs Free Energy=	0.710198
Sum of electronic and zero-point Energies=	-6606.121172
Sum of electronic and thermal Energies=	-6606.065823
Sum of electronic and thermal Enthalpies=	-6606.064879
Sum of electronic and thermal Free Energies=	-6606.206046

cartesian

40	1.64961481	0.33636665	0.14415103	1	6.49341488	-2.42873335	1.62295103
6	4.07871485	0.62546664	0.81665105	1	6.02871513	-4.13543320	1.56955111
1	-0.29168510	0.80586666	0.56105101	6	-0.93988508	1.25826669	-2.11174893
6	1.33151484	1.68906665	2.17555118	6	0.63401490	3.80546689	-0.90744901
6	2.70571494	1.57476664	2.30385113	6	3.61681485	3.33056664	-1.08484888
1	0.89311492	2.62406683	1.83185112	6	4.16631508	0.45616668	-2.44674897
1	0.69541490	1.04646659	2.77765107	1	-0.45258510	3.80576682	-0.93744898
1	3.09831500	0.86006671	3.01835108	1	0.98841488	4.58556652	-1.59144890
1	3.34161496	2.43066669	2.09785104	1	0.93871492	4.10166645	0.10155103
1	4.14861488	-0.23563333	0.14375103	1	-1.46298504	2.10496664	-1.66094887
6	5.12071514	0.42866665	1.91835105	1	-1.37648511	0.35706669	-1.67324889
1	4.36981487	1.49856663	0.23745102	1	-1.16828513	1.25946665	-3.18264890
1	4.84421492	-0.34643334	2.63725114	1	3.51851487	3.67856669	-0.05064897
1	6.07881498	0.13366666	1.47385108	1	3.45321488	4.20016670	-1.73134887

1	5.30151510	1.35446668	2.47435117	1	4.64601517	3.00206661	-1.23584890
6	2.48161507	-2.14543343	-0.10724898	1	4.35931492	-0.54863334	-2.06294894
6	2.15911484	-2.06593323	1.28095102	1	4.98021507	1.09156656	-2.09244895
6	0.74581492	-1.87643337	1.36395109	1	4.22921467	0.41166669	-3.53864884
6	0.26311490	-1.85763335	0.02155103	1	-2.83148503	0.60726666	0.45545101
6	1.32221484	-1.98113322	-0.93374896	13	-1.73658514	1.47286677	1.31885111
6	2.61081505	2.26476669	-1.41594887	6	-2.06218505	3.39416671	0.98465103
6	2.82511497	1.00236678	-2.03034902	6	-1.80248499	1.11276674	3.26315117
6	1.54101491	0.43276668	-2.34324884	1	-2.92128491	3.63436675	1.62835109
6	0.54641491	1.36346674	-1.89304888	1	-1.25598502	4.06456661	1.30465102
6	1.21431494	2.48396683	-1.31764889	1	-2.35698509	3.67996669	-0.03044897
16	-1.47398520	-1.95053339	-0.03214897	1	-2.85898495	1.09486675	3.56685114
14	1.24871492	-1.39303327	-2.71104884	1	-1.35098505	0.18676668	3.62965107
6	4.38021517	-2.76043320	1.40745103	1	-1.34478498	1.94646668	3.81255102
6	3.27791500	-2.41253328	2.11925101	6	-5.38718510	1.18716669	1.64415109
16	4.12161493	-2.70283318	-0.33604899	13	-4.60378504	0.59086668	-0.05954897
1	3.25981498	-2.41583323	3.20445108	1	-6.23868513	-0.33883333	-0.64264899
6	-0.40968508	-1.75273323	-3.49614882	1	-4.12688494	-1.08313334	-0.12714897
6	2.59681487	-2.16853333	-3.75614882	13	-5.54808521	-1.84873343	-0.74904901
1	2.74471498	-1.60233331	-4.68164873	6	-6.16938496	-3.09233332	0.64265102
1	3.56491494	-2.24383330	-3.25524902	6	-5.12478495	-2.37593317	-2.59524894
1	2.29261494	-3.18283319	-4.03524923	1	-4.32768488	-3.12823319	-2.62734890
1	-0.49908507	-1.22673333	-4.45264912	1	-4.79068518	-1.51673341	-3.18814898
1	-0.48548508	-2.82583332	-3.70184898	1	-5.98988485	-2.80783319	-3.11114883
1	-1.27308512	-1.47473335	-2.88754892	1	-5.52198505	-3.97373319	0.72385103
6	-1.55488515	-1.96563339	1.72835112	1	-7.17818499	-3.46383333	0.42795104
6	-0.33058506	-1.93083334	2.31935120	1	-6.20828485	-2.61573339	1.62915111
1	-0.20278510	-1.96043324	3.39615107	6	-4.38138485	1.57236671	-1.74994898
6	-2.88978505	-2.00303340	2.40595102	1	-5.35248518	1.76316667	-2.22034883
1	-3.42978501	-1.06103325	2.25955105	1	-3.78088522	1.00646663	-2.47274899
1	-2.74918509	-2.15283322	3.47905111	1	-3.89108515	2.54266667	-1.60554898
1	-3.51658511	-2.81053329	2.01655102	1	-6.40038490	1.57306671	1.48215103
6	5.72861481	-3.14823318	1.93145108	1	-4.81228495	1.98516679	2.12985110
1	5.70451498	-3.17513323	3.02265120	1	-5.47798491	0.36746669	2.36815119

TS^P-4



Zero-point vibrational energy	2378520.2 (Joules/Mol)
	568.47996 (Kcal/Mol)
Zero-point correction=	0.905930 (Hartree/Particle)
Thermal correction to Energy=	0.963600
Thermal correction to Enthalpy=	0.964544
Thermal correction to Gibbs Free Energy=	0.819375
Sum of electronic and zero-point Energies=	-6377.561893
Sum of electronic and thermal Energies=	-6377.504223
Sum of electronic and thermal Enthalpies=	-6377.503279
Sum of electronic and thermal Free Energies=	-6377.648449

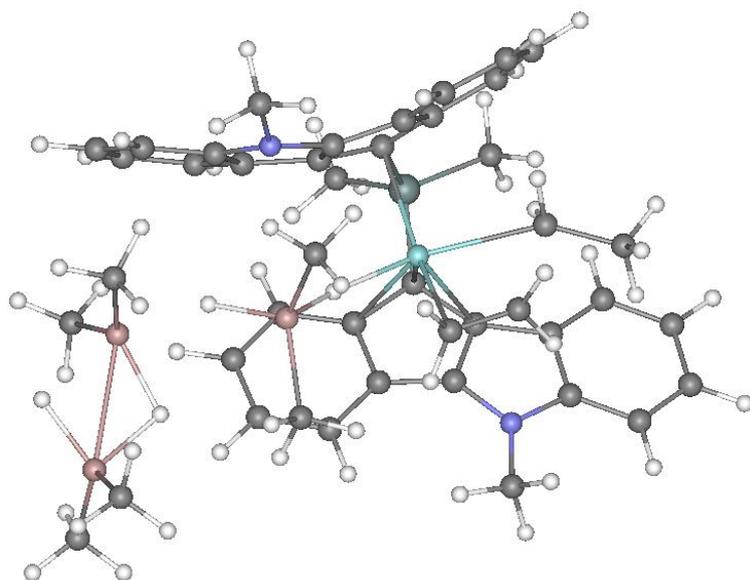
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6	-1.30710006	1.96759999	1.37559998	1	5.27180004	3.77539992	-1.63259995
6	-0.91189998	2.78670001	0.25929999	1	-5.27769995	-0.99910003	3.09910011
6	0.41240001	2.37109995	-0.11230000	1	-3.62059999	-0.48750001	3.45939994
6	0.84600002	1.46379995	0.89670002	1	-4.85340023	0.73060000	3.05450010
6	-0.22920001	1.03939998	1.73829997	1	-5.04530001	-2.14930010	-2.58470011
6	-3.21440005	-1.57579994	-0.31520000	6	-6.74849987	-1.16910005	-1.69570005
6	-2.97440004	-1.05060005	0.97839999	6	-7.24720001	-0.46180001	-0.59170002
6	-1.66369998	-1.39240003	1.46229994	1	-6.82830000	0.38859999	1.35259998
6	-1.18069994	-2.33610010	0.44600001	1	-8.28289986	-0.13740000	-0.58939999
6	-2.09590006	-2.39870000	-0.66159999	1	-7.40450001	-1.38390005	-2.53290009
7	2.21440005	1.35920000	0.89080000	40	-1.10800004	0.15480000	-0.44290000
14	-0.53689998	-0.53109998	2.71079993	6	-3.05419993	1.28069997	-1.53139997
7	-4.12830019	-0.42370000	1.44210005	1	0.68839997	-0.68089998	-0.61919999

6	-3.36369991	3.22679996	1.52970004	6	-0.43950000	-0.13290000	-2.77410007
6	-2.93980002	4.06409979	0.46799999	6	-1.55159998	0.65140003	-3.04509997
6	-1.72800004	3.85859990	-0.15750000	1	-0.48940000	-1.20879996	-2.92479992
6	-2.55819988	2.20490003	1.98720002	1	0.53839999	0.33600000	-2.84800005
1	-2.85509992	1.62769997	2.85409999	1	-1.39400005	1.69760001	-3.28469992
1	-4.31389999	3.42339993	2.01719999	1	-2.44199991	0.20100001	-3.47230005
1	-3.57089996	4.89160013	0.15880001	1	-3.20190001	1.55270004	-0.47229999
1	-1.38849998	4.52860022	-0.94169998	6	-3.45129991	2.47539997	-2.39730000
6	0.03370000	-4.18060017	-0.53450000	1	-3.75419998	0.47830001	-1.74160004
6	-0.85939997	-4.21120024	-1.64110005	1	-2.70050001	3.26850009	-2.41650009
6	-1.90359998	-3.32419991	-1.72029996	1	-4.38149977	2.91359997	-2.02020001
6	-0.09040000	-3.25079989	0.46630001	1	-3.63720012	2.16630006	-3.43079996
1	0.59909999	-3.27110004	1.30009997	1	2.84999990	-1.70239997	-0.00920000
1	0.83600003	-4.90969992	-0.48199999	13	2.14000010	-1.26279998	-1.45169997
1	-0.71179998	-4.94969988	-2.42269993	6	1.86319995	-2.80509996	-2.66090012
1	-2.61069989	-3.36570001	-2.54390001	6	3.09710002	0.17680000	-2.41079998
6	1.02869999	-1.51390004	2.98679996	1	2.61240005	-2.68889999	-3.45580006
6	-1.26180005	-0.22050001	4.41839981	1	0.88700002	-2.86430001	-3.15210009
1	-1.69659996	-1.13890004	4.82849979	1	2.04789996	-3.77740002	-2.19549990
1	-2.00710011	0.57429999	4.48570013	1	4.09539986	0.34720001	-1.98749995
1	-0.43630001	0.06880000	5.07849979	1	2.62579989	1.16159999	-2.49189997
1	0.79089999	-2.51160002	3.37199998	1	3.25000000	-0.18750000	-3.43630004
1	1.64440000	-1.02059996	3.74620008	6	5.05399990	-2.92910004	-1.47889996
1	1.63759995	-1.63080001	2.08520007	13	4.62139988	-2.18090010	0.28870001
6	2.69670010	2.26729989	-0.06760000	1	6.53350019	-1.89890003	0.79130000
6	1.61430001	2.89240003	-0.73570001	1	4.79129982	-0.45100001	0.31349999
6	1.86749995	3.82470012	-1.74259996	13	6.48600006	-0.25240001	0.63129997
6	4.01779985	2.58439994	-0.36849999	6	7.27650023	0.41580001	-1.03880000
6	-4.59630013	-1.31990004	-0.63749999	6	6.60979986	0.69139999	2.35789990
6	-5.11219978	-0.59460002	0.46520001	1	6.37209988	1.76020002	2.28749990
6	-4.49259996	-0.28009999	2.84050012	1	5.94630003	0.25110000	3.11209989
6	-6.43750000	-0.16429999	0.50330001	1	7.62769985	0.62879997	2.76130009
6	-5.42449999	-1.60049999	-1.72739995	1	6.90150023	1.41139996	-1.30649996
6	2.98460007	0.91649997	2.04390001	1	8.36820030	0.49300000	-0.97750002
1	3.91280007	1.48870003	2.09209991	1	7.04419994	-0.25009999	-1.87790000
1	2.40400004	1.11290002	2.95129991	6	4.20650005	-3.06750011	1.99670005
1	3.23539996	-0.14380001	1.98860002	1	5.01149988	-3.75449991	2.28119993
1	1.04900002	4.30280018	-2.27320004	1	4.09520006	-2.35409999	2.82349992
6	3.18939996	4.13259983	-2.05830002	1	3.27769995	-3.64969993	1.94589996
6	4.24879980	3.52390003	-1.37129998	1	6.09730005	-3.26379991	-1.50170004
1	4.84859991	2.10019994	0.13710000	1	4.42819977	-3.78850007	-1.74370003

1 3.40260005 4.85129976 -2.84279990

1 4.94169998 -2.19090009 -2.28410006

TSP-5



Zero-point vibrational energy	2373835.7 (Joules/Mol)
	567.36034 (Kcal/Mol)
Zero-point correction=	0.904146 (Hartree/Particle)
Thermal correction to Energy=	0.962816
Thermal correction to Enthalpy=	0.963760
Thermal correction to Gibbs Free Energy=	0.815397
Sum of electronic and zero-point Energies=	-6377.556960
Sum of electronic and thermal Energies=	-6377.498290
Sum of electronic and thermal Enthalpies=	-6377.497346
Sum of electronic and thermal Free Energies=	-6377.645709

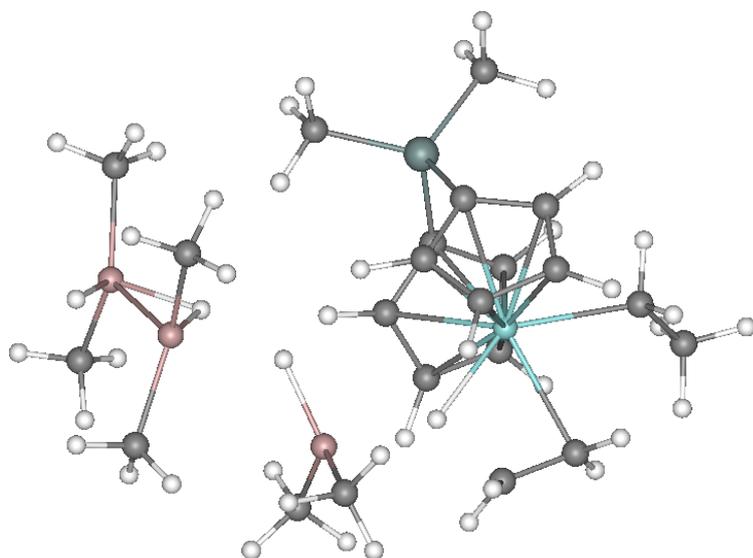
cartesian

40	-1.15740001	-0.10270000	-0.40459999	1	4.20690012	-3.38330007	-0.43250000
6	-0.56129998	0.72259998	1.91229999	1	4.84289980	-3.81839991	1.91639996
6	-0.45989999	1.97759998	1.20850003	1	4.20109987	-0.92379999	2.19779992
6	-1.78820002	2.27370000	0.78100002	6	2.08159995	-3.38260007	-2.30500007
6	-2.67610002	1.26020002	1.21949995	1	3.12599993	-3.11789989	-2.47849989
6	-1.92600000	0.20350000	1.87070000	1	1.52100003	-3.09559989	-3.19199991
6	0.22780000	-2.44930005	-0.90649998	1	1.99899995	-4.46500015	-2.15059996
6	-0.03600000	-2.35270000	0.48210001	6	-1.95630002	4.56010008	-0.32820001
6	-1.46410000	-2.37560010	0.72100002	1	-2.26169991	5.41870022	0.27779999
6	-2.03169990	-2.64960003	-0.57990003	1	-2.30640006	4.70130014	-1.35580003
6	-1.00839996	-2.58450007	-1.61109996	1	-0.86870003	4.51119995	-0.34360000
6	-4.01109982	1.75409997	0.92890000	6	-3.35139990	-0.09730000	-1.56120002

14	-2.33929992	-1.60699999	2.19479990	1	0.76400000	0.26150000	-0.56070000
6	1.23469996	-2.62059999	1.14119995	6	-0.67119998	1.56970000	-2.18249989
6	1.79970002	0.89170003	2.42779994	6	-2.02690005	1.45480001	-2.43980002
6	1.88440001	2.12630010	1.73080003	1	0.02550000	1.12259996	-2.88549995
6	0.77550000	2.67140007	1.13080001	1	-0.29480001	2.39289999	-1.58239996
6	0.61540002	0.20240000	2.51200008	1	-2.72309995	2.19689989	-2.05850005
1	0.57539999	-0.71890002	3.07640004	1	-2.33340001	0.94569999	-3.34730005
1	2.68560004	0.49120000	2.90879989	1	-3.65370011	-0.50480002	-0.58440000
1	2.84019995	2.64150000	1.67610002	6	-4.56909990	0.63620001	-2.12059999
1	0.85270000	3.62249994	0.61409998	1	-3.13360000	-0.93519998	-2.22309995
6	-3.61739993	-3.34870005	-2.26950002	1	-4.80880022	1.55780005	-1.58529997
6	-2.62899995	-3.19810009	-3.28889990	1	-5.44750023	-0.01520000	-2.04920006
6	-1.34440005	-2.83209991	-2.97390008	1	-4.44299984	0.88510001	-3.17880011
6	-3.33969998	-3.06719995	-0.95569998	1	3.21259999	-0.00560000	-0.30680001
1	-4.10169983	-3.21029997	-0.19730000	13	2.20930004	0.64980000	-1.44260001
1	-4.60769987	-3.69889998	-2.54430008	6	2.08710003	-0.29080001	-3.18670011
1	-2.89199996	-3.40700006	-4.32079983	6	2.53309989	2.58260012	-1.71899998
1	-0.59149998	-2.75480008	-3.75230002	1	2.07150006	0.45199999	-3.99559999
6	-4.18650007	-1.91569996	2.11139989	1	1.17700005	-0.89730000	-3.29130006
6	-1.75390005	-2.21460009	3.87229991	1	2.94250011	-0.94569999	-3.38770008
1	-1.57040000	-3.29369998	3.84859991	1	3.42820001	2.65120006	-2.35619998
1	-0.85450000	-1.72000003	4.24399996	1	2.75440001	3.17319989	-0.82550001
1	-2.54340005	-2.02850008	4.60869980	1	1.73189998	3.08610010	-2.27570009
1	-4.38259983	-2.98749995	2.22900009	6	5.56300020	-0.74140000	-1.65929997
1	-4.68279982	-1.40240002	2.94219995	13	5.04530001	0.18470000	0.00280000
1	-4.65430021	-1.58899999	1.17869997	1	6.80380011	1.10169995	0.14410000
6	-3.83249998	3.02500010	0.31500000	1	4.64979982	1.85640001	-0.16300000
7	-2.48300004	3.32699990	0.22139999	13	6.19250011	2.63470006	-0.07250000
6	-5.31099987	1.28900003	1.14769995	6	6.57149982	3.38940001	-1.84739995
6	-4.91209984	3.80329990	-0.10850000	6	6.14809990	3.71219993	1.57470000
7	1.57650006	-2.65820003	-1.14779997	1	5.42770004	4.53539991	1.49609995
6	2.17820001	-2.81960011	0.10390000	1	5.87410021	3.11710000	2.45289993
6	3.48589993	-3.23709989	0.36590001	1	7.12230015	4.16769981	1.78740001
6	1.60850000	-2.90660000	2.45970011	1	5.89720011	4.22119999	-2.08249998
1	-5.48320007	0.34130001	1.64429998	1	7.59420013	3.77789998	-1.91779995
6	-6.39150000	2.06229997	0.73310000	1	6.45609999	2.64120007	-2.63969994
6	-6.19259977	3.30240011	0.10590000	6	5.08750010	-0.36190000	1.89010000
1	-4.76130009	4.76879978	-0.58219999	1	5.96220016	-0.99349999	2.08920002
1	-7.40210009	1.70420003	0.89969999	1	5.18160009	0.51870000	2.53920007
1	-7.05149984	3.88639998	-0.20919999	1	3.19379997	-3.56839991	3.74580002
1	0.88400000	-2.84019995	3.26629996	1	6.57749987	-1.15100002	-1.59500003

6	2.90190005	-3.33839989	2.72620010	1	4.88170004	-1.56449997	-1.90820003
6	3.83349991	-3.49230003	1.68680000	1	5.55289984	-0.05380000	-2.51539993

TS[‡]-1

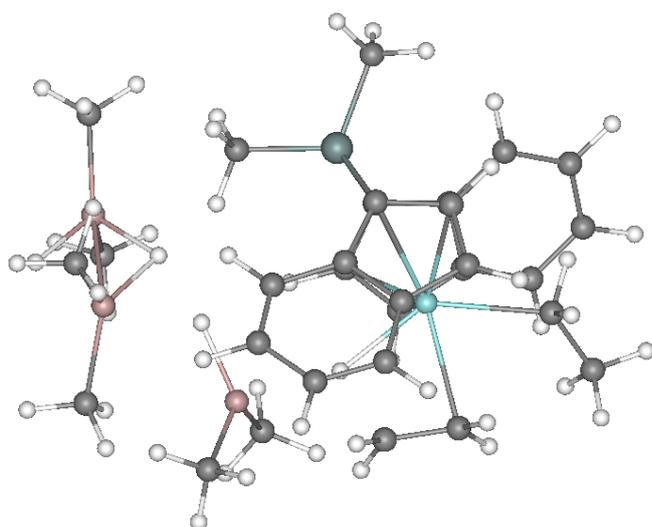


Zero-point vibrational energy	1563922.9 (Joules/Mol)
	373.78654 (Kcal/Mol)
Zero-point correction=	0.595667 (Hartree/Particle)
Thermal correction to Energy=	0.636846
Thermal correction to Enthalpy=	0.637790
Thermal correction to Gibbs Free Energy=	0.523533
Sum of electronic and zero-point Energies=	-5421.908309
Sum of electronic and thermal Energies=	-5421.867130
Sum of electronic and thermal Enthalpies=	-5421.866186
Sum of electronic and thermal Free Energies=	-5421.980443

cartesian							
40	1.97049999	-0.33010000	0.07910000	1	-6.20480013	0.72689998	2.84080005
6	4.27120018	0.12570000	0.41549999	1	-5.15390015	-0.66460001	2.57769990
1	0.73500001	-1.97689998	0.02840000	6	-3.38360000	0.14560001	-2.69639993
6	1.79209995	-3.03710008	0.33199999	1	-4.32810020	0.28780001	-3.23329997
6	3.05559993	-2.48200011	0.57010001	1	-2.89190006	1.12520003	-2.65799999
1	1.60660005	-3.55220008	-0.60799998	1	-2.75320005	-0.50870001	-3.31019998
1	1.21360004	-3.41770005	1.17279994	1	-5.38530016	-2.49920011	-0.81330001
1	3.39610004	-2.39140010	1.59510005	1	-3.80830002	-3.25570011	-0.72710001
1	3.81699991	-2.55789995	-0.19920000	1	-4.49389982	-2.46749997	0.69970000
1	4.38759995	1.18820000	0.15960000	6	2.82960010	-0.30930001	-2.38229990
6	5.00139999	-0.09020000	1.74570000	6	2.71900010	1.03110003	-1.93130004

1	4.81010008	-0.41690001	-0.37290001	6	1.34669995	1.33420002	-1.69309998
1	4.62099981	0.56999999	2.53290009	6	0.61739999	0.14350000	-1.99810004
1	6.07240009	0.12819999	1.65040004	6	1.52830005	-0.85589999	-2.43059993
1	4.92740011	-1.11699998	2.11870003	1	1.26929998	-1.85880005	-2.75009990
1	-1.81149995	-1.08089995	-0.75569999	1	3.74819994	-0.82010001	-2.64389992
13	-1.19739997	-2.45219994	-0.14360000	1	3.54990005	1.70879996	-1.78240001
6	-0.91430002	-3.86459994	-1.47759998	14	0.69510001	2.66179991	-0.53189999
6	-1.65649998	-2.78110003	1.73420000	1	-0.45860001	0.02790000	-1.93019998
1	-1.87720001	-4.17189980	-1.90320003	6	1.89900005	0.29249999	2.60010004
1	-0.46129999	-4.76679993	-1.05100000	6	2.03040004	1.47839999	1.83019996
1	-0.29480001	-3.54990005	-2.32480001	6	0.84619999	1.66460001	1.05639994
1	-2.47259998	-3.51360011	1.76839995	6	-0.00290000	0.55089998	1.35119998
1	-2.02349997	-1.87940001	2.23950005	6	0.64270002	-0.27669999	2.30809999
1	-0.84469998	-3.19860005	2.34109998	1	0.23819999	-1.18330002	2.74219990
6	-4.38089991	-2.38290000	-0.38769999	1	2.63389993	-0.11080000	3.28539991
13	-3.69989991	-0.60720003	-0.91310000	1	2.89890003	2.12669992	1.82439995
1	-5.25250006	0.31389999	-0.44960001	1	-0.99220002	0.38229999	0.93589997
1	-3.13669991	0.37779999	0.41720000	6	-1.09430003	3.05040002	-0.88309997
13	-4.62620020	1.17949998	0.85670000	6	1.82830000	4.14709997	-0.50669998
6	-5.18289995	0.43040001	2.57949996	1	1.51689994	4.86310005	0.25979999
6	-4.45550013	3.08520007	0.42919999	1	2.86240005	3.85899997	-0.29100001
1	-3.74429989	3.58940005	1.09329998	1	1.82179999	4.66219997	-1.47179997
1	-4.12080002	3.24850011	-0.60110003	1	-1.48389995	3.79270005	-0.17980000
1	-5.41669989	3.59929991	0.54479998	1	-1.23329997	3.43519998	-1.89820004
1	-4.53469992	0.77340001	3.39369988	1	-1.71449995	2.15159988	-0.77990001

TS[‡]-2



Zero-point vibrational energy

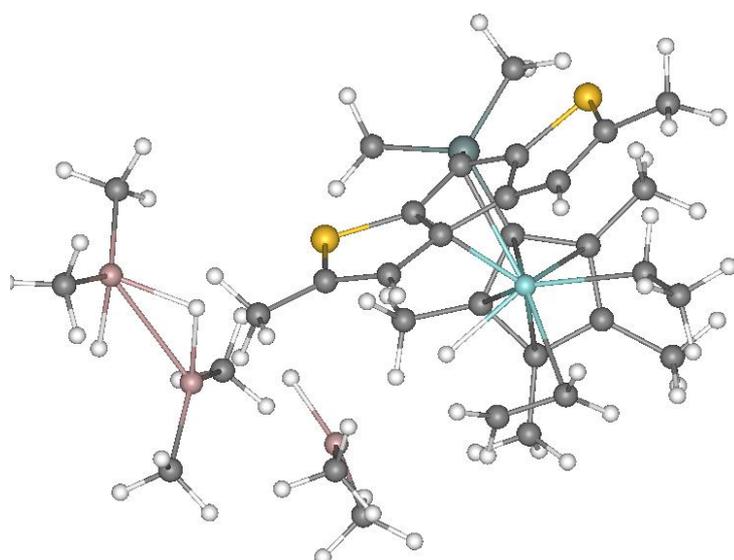
1815791.0 (Joules/Mol)

	433.98447 (Kcal/Mol)
Zero-point correction=	0.691598 (Hartree/Particle)
Thermal correction to Energy=	0.737976
Thermal correction to Enthalpy=	0.738920
Thermal correction to Gibbs Free Energy=	0.615183
Sum of electronic and zero-point Energies=	-5728.968342
Sum of electronic and thermal Energies=	-5728.921964
Sum of electronic and thermal Enthalpies=	-5728.921521
Sum of electronic and thermal Free Energies=	-5729.044757

				cartesian			
40	1.76880002	0.36510000	-0.21950001	1	-5.87729979	1.40489995	-1.88699996
6	4.04750013	0.13339999	-0.70120001	1	-4.33010006	2.13890004	-2.22390008
1	0.19570000	1.47340000	-0.93000001	1	-4.65089989	0.47530001	-2.73350000
6	1.06309998	2.50000000	-1.75569999	6	0.67140001	1.56400001	1.86899996
6	2.41639996	2.16120005	-1.78310001	6	1.82439995	2.38669991	1.59959996
1	0.72710001	3.32209992	-1.13090003	6	2.98210001	1.58080006	1.78450000
1	0.47290000	2.33319998	-2.65490007	6	2.55139995	0.29690000	2.17039990
1	2.80870008	1.68009996	-2.67030001	6	1.11800003	0.24250001	2.21180010
1	3.11640000	2.71670008	-1.16499996	6	0.79200000	-1.34580004	-1.90009999
1	4.27190018	-0.83200002	-0.22499999	6	0.57849997	-1.80170000	0.38090000
6	4.63700008	0.15369999	-2.12069988	6	1.85529995	-2.29279995	-0.07600000
1	4.59800005	0.87470001	-0.11450000	6	1.96689999	-2.04660010	-1.48699999
1	3.95689988	-0.24800000	-2.87919998	14	0.15500000	-1.36489999	2.15420008
1	5.56050014	-0.43439999	-2.17980003	6	-0.06890000	-1.27230000	-0.76920003
1	4.89279985	1.17299998	-2.42659998	6	-0.74460000	3.49780011	1.57389998
1	-2.42230010	0.87349999	-0.21430001	6	0.40540001	4.30980015	1.30509996
13	-1.81930006	1.66030002	-1.50090003	6	1.66670001	3.77589989	1.31210005
6	-2.08850002	3.60419989	-1.49230003	6	-0.62910002	2.15969992	1.84060001
6	-1.70050001	0.61860001	-3.16219997	1	-1.51119995	1.56930006	2.07209992
1	-2.35829997	3.94700003	-2.49930000	1	-1.72599995	3.96300006	1.57879996
1	-1.23570001	4.20539999	-1.16439998	1	0.26640001	5.36940002	1.11140001
1	-2.92720008	3.85960007	-0.83260000	1	2.53929996	4.39909983	1.13469994
1	-1.92379999	-0.44580001	-3.02169991	6	3.97560000	-3.43680000	-0.11330000
1	-0.73229998	0.68650001	-3.67100000	6	4.06220007	-3.22860003	-1.52310002
1	-2.44670010	1.00720000	-3.86649990	6	3.08330011	-2.55340004	-2.20569992
6	-4.80039978	1.19490004	-1.92019999	6	2.89700007	-2.98650002	0.60430002
13	-4.33939981	0.41460001	-0.16370000	1	2.82040000	-3.19260001	1.66789997
1	-5.77570009	-0.75790000	-0.10090000	1	4.76879978	-3.98180008	0.38890001
1	-3.52320004	-1.12370002	-0.27640000	1	4.91669989	-3.62639999	-2.06189990
13	-4.89480019	-2.19860005	-0.19329999	1	3.14820004	-2.42269993	-3.28169990

6	-5.07340002	-3.05629992	-1.94470000	6	0.81739998	-2.58839989	3.41070008
6	-4.86639977	-3.09590006	1.55030000	6	-1.68359995	-1.12730002	2.34509993
1	-4.05670023	-3.83060002	1.62709999	1	-2.19460011	-2.09590006	2.32110000
1	-4.74650002	-2.37980008	2.37100005	1	-2.09570003	-0.52160001	1.53260005
1	-5.80189991	-3.63800001	1.73010004	1	-1.92900002	-0.63919997	3.29430008
1	-4.30380011	-3.82040000	-2.09969997	1	0.64940000	-3.62140012	3.09060001
1	-6.04339981	-3.55369997	-2.05450010	1	0.30030000	-2.44659996	4.36530018
1	-4.98610020	-2.33290005	-2.76239991	1	1.88619995	-2.45840001	3.60260010
6	-4.51240015	1.22549999	1.61380005	1	3.21650004	-0.53920001	2.36809993
1	-5.56069994	1.46150005	1.83010006	1	4.00750017	1.91129994	1.68970001
1	-4.16529989	0.56169999	2.41420007	1	-1.07720006	-0.87220001	-0.76929998
1	-3.94600010	2.16170001	1.69250000	1	0.53619999	-1.07809997	-2.91790009

TS^t-3



Zero-point vibrational energy	2081034.5 (Joules/Mol)
	497.37917 (Kcal/Mol)
Zero-point correction=	0.792624 (Hartree/Particle)
Thermal correction to Energy=	0.848887
Thermal correction to Enthalpy=	0.849831
Thermal correction to Gibbs Free Energy=	0.705483
Sum of electronic and zero-point Energies=	-6606.116785
Sum of electronic and thermal Energies=	-6606.060522
Sum of electronic and thermal Enthalpies=	-6606.059578
Sum of electronic and thermal Free Energies=	-6606.203926

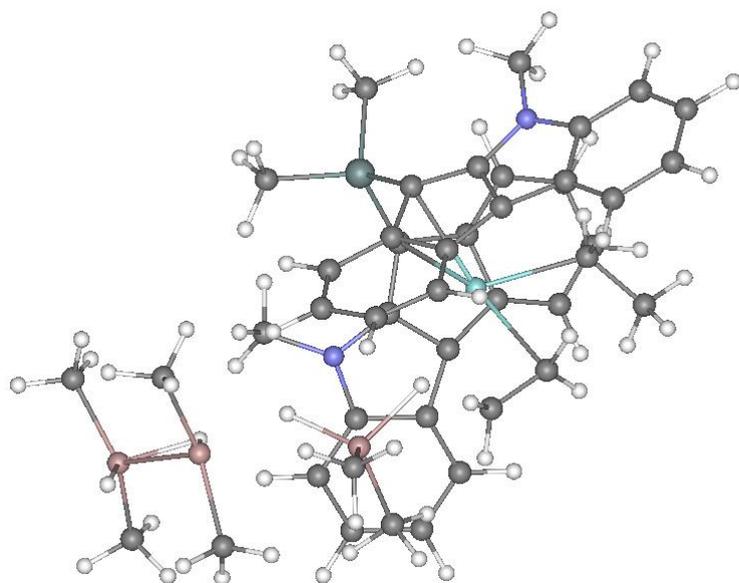
cartesian

6	2.60210729	-2.16076565	-0.00716762	1	4.53640747	-0.58436561	-1.96496761
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6	2.27280712	-2.03986573	1.37423241	1	5.19220734	1.03823447	-2.02046776
6	0.86830723	-1.77626562	1.43923235	1	4.47150707	0.33483434	-3.47426772
6	0.39960724	-1.77116561	0.09233238	40	1.87590718	0.36773437	0.16513237
6	1.45830727	-1.96676564	-0.85026765	6	4.13620758	0.59093434	0.87233233
6	2.83150721	2.26403451	-1.41946757	1	0.07330725	0.96763438	0.67263234
6	3.03740716	0.99363440	-2.01656771	6	0.68810725	1.88503432	2.10013223
6	1.74890721	0.42563438	-2.32256770	6	2.05340719	1.84323430	2.24093223
6	0.76030725	1.36373425	-1.87866759	1	0.20620725	2.77163434	1.69313240
6	1.43510723	2.47933435	-1.30596757	1	0.07290724	1.23983431	2.71793222
16	-1.34169281	-1.80536556	0.02473237	1	2.48850727	1.14403439	2.94433236
14	1.42940724	-1.40306568	-2.63576770	1	2.67980719	2.66043448	1.89423239
6	4.48180771	-2.76656556	1.52813244	1	4.57490730	-0.25926563	0.33483237
6	3.37880731	-2.39336562	2.22573233	6	4.73040771	0.61143434	2.28873229
16	4.22890759	-2.75516558	-0.21576762	1	4.53770733	1.47113442	0.36103237
1	3.35900712	-2.36796570	3.31013227	1	4.26690722	-0.11226565	2.96653223
6	-0.23339278	-1.74406552	-3.42886782	1	5.80300713	0.37783438	2.26783228
6	2.76600718	-2.23866558	-3.64876771	1	4.64160728	1.59853435	2.75553226
1	2.91550732	-1.71566558	-4.59896755	1	-2.88159275	0.63793439	0.16393238
1	3.73420715	-2.29386568	-3.14536762	13	-2.42589283	1.75963449	1.20983243
1	2.45610714	-3.26356554	-3.87866783	6	-2.49659276	3.62053442	0.60223234
1	-0.30449277	-1.24386573	-4.40066767	6	-2.42149282	1.38743424	3.13073230
1	-0.33789277	-2.82066560	-3.60086775	1	-3.46159267	4.01643419	0.94923246
1	-1.08959281	-1.42376566	-2.83006763	1	-1.73249269	4.26243401	1.05453241
6	-1.44369280	-1.78076553	1.78293240	1	-2.47249269	3.76873422	-0.48136762
6	-0.22359276	-1.75886559	2.38573217	1	-2.01019287	2.23793435	3.68723226
1	-0.10759276	-1.78366566	3.46483231	1	-3.45689273	1.25473428	3.47103238
6	-2.79249287	-1.85876560	2.43383217	1	-1.87039280	0.49033433	3.42613220
1	-3.42579269	-1.00626564	2.16483235	6	-5.53419304	1.21973443	1.10313237
1	-2.67959285	-1.87326574	3.52063227	13	-4.72749233	0.36823434	-0.48966762
1	-3.32189274	-2.76726556	2.12853217	1	-6.16849232	-0.69886565	-0.95986760
6	5.82900715	-3.13676548	2.06873226	1	-4.09239292	-1.21066570	-0.16786763
1	5.79300690	-3.15736556	3.15983224	13	-5.43089294	-2.19706559	-0.66616762
1	6.58480740	-2.40576553	1.76563239	6	-6.15149307	-3.04786563	0.94723237
1	6.14870739	-4.12106562	1.71553242	6	-4.90729237	-3.08056569	-2.33266783
6	-0.72779274	1.27773428	-2.09976768	1	-5.75019264	-3.58786559	-2.81446767
6	0.82590723	3.76053452	-0.81706762	1	-4.13459301	-3.83746552	-2.15726781
6	3.85330725	3.31053448	-1.07686758	1	-4.50329304	-2.36256552	-3.05476761
6	4.37680721	0.41153437	-2.38606763	1	-5.55359268	-3.91456556	1.25193238
1	-0.20119277	3.61793447	-0.47976762	1	-7.17329311	-3.41086555	0.78903234
1	0.81110722	4.51153421	-1.61586761	1	-6.18409252	-2.35446548	1.79533243
1	1.39930725	4.18393421	0.01503237	6	-4.27319241	1.13053441	-2.23636770

1	-1.22189271	2.18653440	-1.74426758	1	-5.16779232	1.30543447	-2.84416771
1	-1.19659281	0.43573433	-1.58376765	1	-3.62409282	0.45433438	-2.80606771
1	-0.95189273	1.18483424	-3.16756773	1	-3.74289298	2.08603454	-2.14646769
1	3.78410721	3.62553453	-0.03026762	1	-6.58929253	1.43013430	0.89043236
1	3.69510722	4.20003414	-1.69686759	1	-5.10549259	2.17813444	1.42763245
1	4.87330723	2.96463442	-1.24886763	1	-5.52289295	0.55033433	1.97283232

TS[‡]-4



Zero-point vibrational energy	2372694.5 (Joules/Mol)
	567.08758 (Kcal/Mol)
Zero-point correction=	0.903712 (Hartree/Particle)
Thermal correction to Energy=	0.961786
Thermal correction to Enthalpy=	0.962731
Thermal correction to Gibbs Free Energy=	0.815875
Sum of electronic and zero-point Energies=	-6377.543317
Sum of electronic and thermal Energies=	-6377.485242
Sum of electronic and thermal Enthalpies=	-6377.484298
Sum of electronic and thermal Free Energies=	-6377.631154

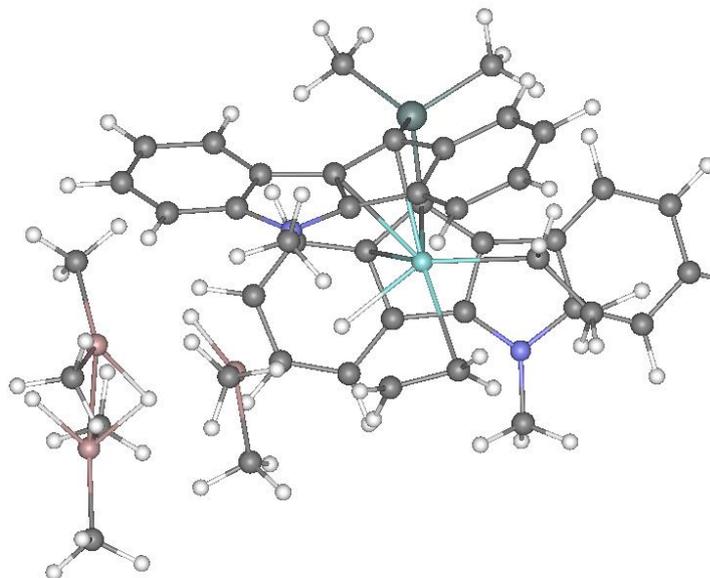
cartesian

6	-1.34730005	2.47550011	0.98769999	1	5.28259993	2.96950006	-2.32800007
6	-0.92330003	2.94169998	-0.30559999	1	-5.80929995	0.08300000	2.73480010
6	0.34279999	2.32229996	-0.57859999	1	-4.17250013	0.05030000	3.39140010
6	0.70980000	1.61010003	0.60390002	1	-4.68830013	1.40880001	2.34389997
6	-0.35110000	1.56309998	1.55739999	1	-4.58589983	-3.22029996	-2.10360003
6	-3.10109997	-1.81470001	0.04400000	6	-6.49130011	-2.33730006	-1.61520004
6	-3.05669999	-0.93620002	1.15450001	6	-7.19140005	-1.45920002	-0.77300000

6	-1.73920000	-0.88249999	1.73810005	1	-7.10260010	-0.07640000	0.88000000
6	-1.00250006	-1.90330005	0.98170000	1	-8.25349998	-1.30170000	-0.93210000
6	-1.83500004	-2.45910001	-0.05280000	1	-7.02050018	-2.85050011	-2.41129994
7	2.06209993	1.33889997	0.59090000	40	-1.28129995	0.22430000	-0.44340000
14	-0.83899999	0.32080001	2.87229991	6	-3.26469994	1.11880004	-1.21630001
7	-4.32609987	-0.43529999	1.37820005	1	0.58090001	-0.85820001	-1.48280001
6	-3.23530006	3.97989988	0.86159998	6	-0.27970001	-1.06789994	-2.80220008
6	-2.80209994	4.44010019	-0.40740001	6	-1.51170003	-0.41630000	-2.78870010
6	-1.65740001	3.93720007	-0.98490000	1	-0.24180000	-2.14580011	-2.68070006
6	-2.52679992	3.02010012	1.55180001	1	0.51920003	-0.63419998	-3.39969993
1	-2.83249998	2.74760008	2.55369997	1	-1.58469999	0.51800001	-3.33170009
1	-4.11990023	4.42019987	1.31190002	1	-2.42070007	-1.00590003	-2.68350005
1	-3.36459994	5.21789980	-0.91409999	1	-3.58430004	1.76909995	-0.39260000
1	-1.30449998	4.32100010	-1.93729997	6	-3.41829991	1.87249994	-2.54839993
6	0.67430001	-3.55990005	0.42840001	1	-3.98720002	0.30070001	-1.23769999
6	-0.18660000	-4.13380003	-0.54670000	1	-2.53360009	2.45180011	-2.83049989
6	-1.41229999	-3.57760000	-0.81419998	1	-4.25500011	2.57890010	-2.50040007
6	0.29650000	-2.46090007	1.16139996	1	-3.63409996	1.18250000	-3.36980009
1	0.97299999	-2.06750011	1.90919995	1	2.99119997	-1.27600002	-0.26960000
1	1.64970005	-4.00150013	0.60420001	13	2.23539996	-1.38100004	-1.74210000
1	0.13730000	-5.01970005	-1.08319998	6	2.20289993	-3.25659990	-2.39330006
1	-2.08019996	-4.01660013	-1.55030000	6	2.91569996	-0.14850000	-3.11919999
6	0.56110001	-0.50019997	3.81979990	1	2.85010004	-3.29029989	-3.27970004
6	-1.84259999	1.06540000	4.27780008	1	1.23420000	-3.65560007	-2.70840001
1	-1.99119997	0.29150000	5.03999996	1	2.62229991	-3.97149992	-1.67410004
1	-2.81609988	1.49220002	4.04820013	1	2.83060002	-0.63220000	-4.10260010
1	-1.23790002	1.85730004	4.73519993	1	3.98449993	0.03520000	-2.95760012
1	0.18810000	-1.43130004	4.26189995	1	2.43849993	0.83389997	-3.19140005
1	0.84719998	0.16050000	4.64610004	6	5.48059988	-2.20619988	-1.68820000
1	1.46930003	-0.73549998	3.26859999	13	4.75169992	-1.94289994	0.11850000
6	2.60630012	1.97370005	-0.53750002	1	6.61579990	-1.85769999	0.85460001
6	1.57579994	2.58349991	-1.29750001	1	4.89839983	-0.33329999	0.68300003
6	1.89820004	3.33599997	-2.42799997	13	6.49090004	-0.29600000	1.38440001
6	3.94549990	2.09520006	-0.90329999	6	7.48250008	1.02030003	0.31099999
6	-4.46280003	-1.87709999	-0.41249999	6	6.19369984	-0.14100000	3.32299995
6	-5.18480015	-0.99500000	0.43270001	1	5.87349987	0.86629999	3.61479998
6	-4.76779985	0.33129999	2.52139997	1	5.42899990	-0.84520000	3.67190003
6	-6.55140018	-0.77289999	0.25600001	1	7.10580015	-0.35560000	3.89190006
6	-5.12659979	-2.54730010	-1.44439995	1	7.17850018	2.04999995	0.53520000
6	2.80879998	1.01730001	1.79270005	1	8.56099987	0.96530002	0.49900001
1	3.77850008	1.51890004	1.75929999	1	7.33869982	0.85879999	-0.76380002

1	2.25349998	1.38619995	2.66100001	6	4.13000011	-3.20530009	1.49810004
1	2.98079991	-0.05840000	1.89059997	1	4.90339994	-3.36450005	2.25720000
1	1.11819994	3.81040001	-3.01629996	1	3.22909999	-2.86039996	2.02080011
6	3.23749995	3.47539997	-2.78530002	1	3.90170002	-4.18959999	1.07060003
6	4.24459982	2.86069989	-2.02920008	1	6.18590021	-3.04570007	-1.65880001
1	4.73839998	1.60889995	-0.34320000	1	4.77629995	-2.40790009	-2.50009990
1	3.50460005	4.05810022	-3.66070008	1	6.06199980	-1.32130003	-1.97730005

TS^t-5



Zero-point vibrational energy	2368266.3 (Joules/Mol)
	566.02924 (Kcal/Mol)
Zero-point correction=	0.902025 (Hartree/Particle)
Thermal correction to Energy=	0.960616
Thermal correction to Enthalpy=	0.961560
Thermal correction to Gibbs Free Energy=	0.813495
Sum of electronic and zero-point Energies=	-6377.551043
Sum of electronic and thermal Energies=	-6377.492453
Sum of electronic and thermal Enthalpies=	-6377.491509
Sum of electronic and thermal Free Energies=	-6377.639573

cartesian

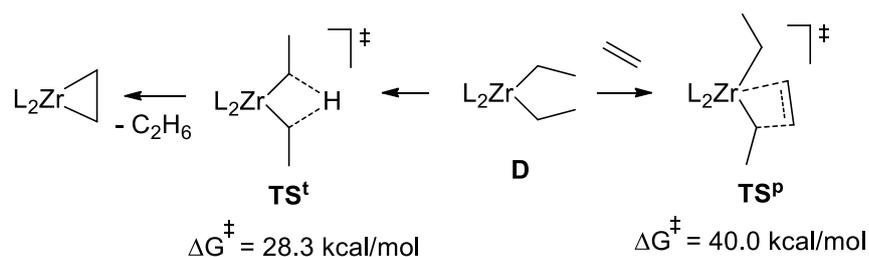
6	-0.39150000	1.23619998	1.37769997	1	4.86030006	-3.57290006	1.53059995
6	-0.45910001	2.23569989	0.33419999	1	3.65269995	-2.62170005	3.47049999
6	-1.84469998	2.40219998	0.05710000	6	1.16059995	-4.18069983	-2.04679990
6	-2.61190009	1.58759999	0.92330003	1	2.21779990	-4.40129995	-2.18770003
6	-1.72669995	0.76090002	1.71920002	1	0.77139997	-3.81139994	-2.99819994
6	-0.24480000	-2.74780011	-0.59429997	1	0.63230002	-5.10090017	-1.77059996

6	-0.20290001	-2.23950005	0.72570002	6	-2.24309993	4.24399996	-1.63530004
6	-1.55330002	-2.04940009	1.21710002	1	-2.12330008	5.25670004	-1.23619998
6	-2.39210010	-2.60389996	0.17200001	1	-2.98609996	4.26039982	-2.43829989
6	-1.59749997	-2.96970010	-0.98199999	1	-1.29550004	3.91479993	-2.06500006
6	-3.98639989	2.04469991	0.77319998	40	-1.30820000	-0.23360001	-0.49360001
14	-2.07189989	-0.87080002	2.58270001	6	-3.48049998	-0.25740001	-1.35090005
6	1.17390001	-2.41860008	1.16330004	1	0.61019999	-0.03840000	-1.24280000
6	1.98199999	1.68509996	1.56210005	6	0.10420000	0.42510000	-2.73210001
6	1.88839996	2.69619989	0.56720001	6	-1.27540004	0.38440001	-2.89210010
6	0.69790000	2.95790005	-0.06170000	1	0.71539998	-0.34840000	-3.19070005
6	0.88520002	0.95080000	1.94029999	1	0.59560001	1.38600004	-2.60290003
1	0.99000001	0.20270000	2.71650004	1	-1.83159995	1.31459999	-2.86820006
1	2.93969989	1.50880003	2.04209995	1	-1.73699999	-0.45660001	-3.40159988
1	2.77449989	3.27270007	0.31729999	1	-4.08249998	-0.34050000	-0.43500000
1	0.63160002	3.74799991	-0.80449998	6	-4.13840008	0.76319999	-2.29040003
6	-4.32989979	-3.51510000	-0.95569998	1	-3.55259991	-1.23549998	-1.83710003
6	-3.54699993	-3.81680012	-2.10940003	1	-3.75950003	1.78299999	-2.18379998
6	-2.19930005	-3.55979991	-2.12709999	1	-5.22020006	0.81660002	-2.11870003
6	-3.77990007	-2.91880012	0.15019999	1	-3.99329996	0.48080000	-3.33839989
1	-4.39610004	-2.72729993	1.02069998	1	3.34920001	-0.27190000	0.00090000
1	-5.38439989	-3.77309990	-0.95370001	13	2.89919996	-0.11930000	-1.55079997
1	-4.02139997	-4.27950001	-2.96889997	6	3.08990002	-1.62419999	-2.80570006
1	-1.60060000	-3.82529998	-2.99320006	6	3.16219997	1.60179996	-2.46269989
6	-3.88709998	-1.07850003	2.99180007	1	3.74270010	-1.26540005	-3.61319995
6	-1.13349998	-1.09389997	4.19689989	1	2.16269994	-1.96190000	-3.27970004
1	-0.93839997	-2.15459991	4.38590002	1	3.57789993	-2.50020003	-2.37069988
1	-0.18799999	-0.55260003	4.25869989	1	2.75539994	1.57140005	-3.48130012
1	-1.76040006	-0.72250003	5.01520014	1	4.24730015	1.74049997	-2.57629991
1	-4.04990005	-2.07159996	3.42589998	1	2.78279996	2.49819994	-1.96589994
1	-4.18480015	-0.33790001	3.74210000	6	5.97399998	-0.87169999	-0.97299999
1	-4.54710007	-0.97530001	2.12859988	13	5.27510023	0.24020000	0.49689999
6	-3.94689989	3.10770011	-0.17000000	1	6.78630018	1.38160002	0.61629999
7	-2.64890003	3.30660009	-0.61140001	1	4.61870003	1.75399995	-0.01910000
6	-5.21689987	1.70650005	1.34580004	13	6.02250004	2.77979994	0.08410000
6	-5.09639978	3.79570007	-0.56449997	6	6.56209993	3.26819992	-1.73710001
7	1.00510001	-3.16750002	-1.01789999	6	5.64510012	4.04829979	1.53429997
6	1.86259997	-3.02090001	0.07630000	1	5.15170002	3.56579995	2.38560009
6	3.19429994	-3.42729998	0.19159999	1	6.56360006	4.50920010	1.91530001
6	1.82669997	-2.28999996	2.39330006	1	4.99660015	4.86740017	1.20290005
1	-5.28410006	0.93210000	2.09969997	1	5.78649998	3.84809995	-2.25049996
6	-6.36670017	2.38649988	0.95700002	1	7.47020006	3.88220000	-1.73529994

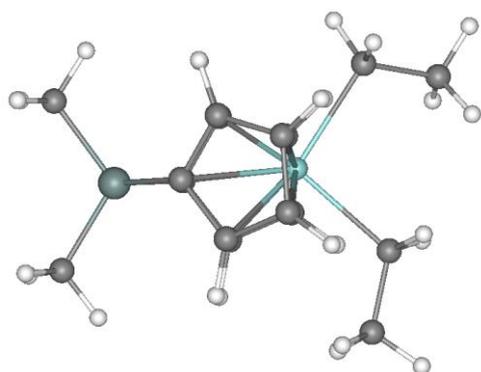
6	-6.30600023	3.41680002	0.00600000	1	6.77220011	2.38520002	-2.35130000
1	-5.05049992	4.60410023	-1.28799999	6	5.10290003	-0.04540000	2.42989993
1	-7.32119989	2.12330008	1.40110004	1	5.74039984	-0.87610000	2.75769997
1	-7.21500015	3.93630004	-0.28060001	1	5.43520021	0.84759998	2.97300005
1	1.29680002	-1.90719998	3.25990009	1	4.08349991	-0.28080001	2.74510002
6	3.14510012	-2.71050000	2.51559997	1	7.05490017	-1.00569999	-0.84579998
6	3.82780004	-3.25559998	1.41740000	1	5.51910019	-1.86889994	-0.99910003
1	3.72230005	-3.89400005	-0.63410002	1	5.84079981	-0.42449999	-1.96790004

S2.4. Transformations of L₂ZrEt₂

Neutral diethyl derivatives of zirconocenes can eliminate ethane with a formation of zirconacyclopropane complexes. However, theoretically these complexes can insert ethylene molecule with a formation of ethyl-butyl derivative (chain propagation). We estimated activation barriers of these processes for diethyl derivatives of **1** and found that elimination of ethane is preferable:



D-1

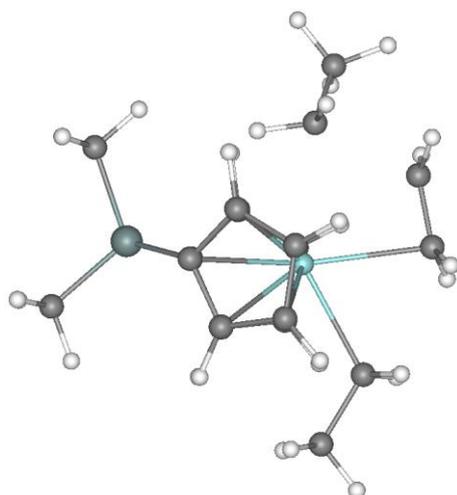


Zero-point vibrational energy	928772.5 (Joules/Mol)
	221.98196 (Kcal/Mol)
Zero-point correction=	0.353751 (Hartree/Particle)
Thermal correction to Energy=	0.375739
Thermal correction to Enthalpy=	0.376684
Thermal correction to Gibbs Free Energy=	0.303322
Sum of electronic and zero-point Energies=	-4453.827711

Sum of electronic and thermal Energies= -4453.805722
 Sum of electronic and thermal Enthalpies= -4453.804778
 Sum of electronic and thermal Free Energies= -4453.878140

cartesian							
6	-0.41339999	2.01370001	-1.78160000	1	4.14120007	-1.76719999	-1.01960003
6	0.71399999	1.15789998	-1.86720002	1	2.93429995	-1.24360001	-2.19720006
6	1.42700005	1.19860005	-0.63110000	1	4.28249979	-0.17919999	-1.78929996
6	0.69099998	2.07870007	0.21940000	1	4.19719982	-0.33870000	1.87080002
6	-0.42750001	2.58450007	-0.48809999	1	4.34130001	1.23459995	1.06959999
1	-1.16620004	3.27620006	-0.10200000	1	3.02419996	0.93680000	2.20740008
1	-1.13810003	2.19219995	-2.56550002	6	-2.34980011	0.84630001	1.26619995
1	0.97549999	0.55150002	-2.72849989	1	-3.00979996	-0.00060000	1.50670004
14	2.57220006	-0.14309999	0.00840000	6	-1.93929994	1.56070006	2.55999994
1	0.93260002	2.30710006	1.25290000	1	-2.95549989	1.52629995	0.64539999
6	-0.72640002	-2.52139997	0.41240001	1	-1.33469999	2.45169997	2.35430002
6	0.49230000	-2.19120002	-0.22980000	1	-1.33840001	0.90850002	3.20429993
6	1.24890006	-1.32560003	0.61369997	1	-2.80229998	1.88870001	3.15229988
6	0.45120001	-1.11740005	1.78129995	40	-0.75580001	0.02600000	-0.13609999
6	-0.75029999	-1.85880005	1.66270006	6	-2.10940003	-0.74119997	-1.81840003
1	-1.54690003	-1.90209997	2.39520001	6	-3.48670006	-1.15269995	-1.25790000
1	-1.49909997	-3.16659999	0.01350000	1	-1.64510000	-1.60189998	-2.31990004
1	0.78570002	-2.52230000	-1.22080004	1	-2.25860000	0.01490000	-2.59829998
1	0.71619999	-0.48269999	2.62109995	1	-4.03319979	-0.28889999	-0.86540002
6	3.62980008	0.48010001	1.41830003	1	-4.12120008	-1.61440003	-2.02480006
6	3.57319999	-0.90270001	-1.37629998	1	-3.40860009	-1.87329996	-0.43489999

TSP-1



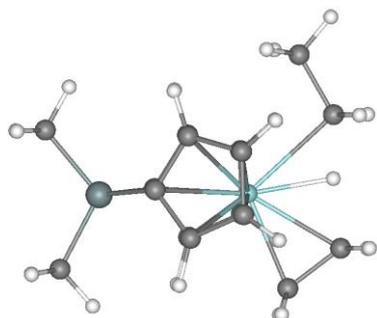
Zero-point vibrational energy

1080636.0 (Joules/Mol)

	258.27821 (Kcal/Mol)
Zero-point correction=	0.411593 (Hartree/Particle)
Thermal correction to Energy=	0.434817
Thermal correction to Enthalpy=	0.435762
Thermal correction to Gibbs Free Energy=	0.362510
Sum of electronic and zero-point Energies=	-4532.279395
Sum of electronic and thermal Energies=	-4532.256170
Sum of electronic and thermal Enthalpies=	-4532.255226
Sum of electronic and thermal Free Energies=	-4532.328477

				cartesian			
6	-0.45060000	-0.36030000	2.65330005	1	4.55840015	-0.63249999	-1.24510002
6	0.62730002	0.43270001	2.17569995	1	4.66779995	-0.98909998	0.48789999
6	1.46659994	-0.35910001	1.34700000	1	3.60820007	-1.94819999	-0.54879999
6	0.88309997	-1.66740000	1.33570004	40	-0.71619999	-0.17110001	0.05300000
6	-0.27370000	-1.66900003	2.14779997	6	-0.92739999	2.42709994	0.63080001
1	-0.92309999	-2.51600003	2.32890010	6	-1.85959995	-2.22959995	-0.29719999
1	-1.24329996	-0.03080000	3.31500006	6	-3.14159989	0.13300000	0.21580000
1	0.77660000	1.48150003	2.39720011	6	-2.88240004	1.49820006	0.28970000
14	2.58699989	0.25909999	-0.02810000	1	-3.44400001	-0.40610000	1.10870004
1	1.26220000	-2.52130008	0.78609997	1	-3.46390009	-0.28310001	-0.73180002
6	-0.72030002	0.66530001	-2.43109989	1	-2.98009992	2.08039999	-0.62129998
6	0.40480000	1.24810004	-1.78620005	1	-3.09739995	2.04099989	1.20420003
6	1.31509995	0.22420000	-1.41040003	1	0.14820001	2.29649997	0.49810001
6	0.72829998	-1.00489998	-1.85580003	6	-1.32400000	3.69420004	-0.12300000
6	-0.50250000	-0.73110002	-2.49200010	1	-1.08539999	2.56030011	1.70439994
1	-1.16799998	-1.46379995	-2.92960000	1	-2.32900000	4.03649998	0.14380001
1	-1.57060003	1.19830000	-2.84109998	1	-2.52889991	-2.09410000	-1.15610003
1	0.54030001	2.30640006	-1.60210001	6	-1.07669997	-3.53010011	-0.52850002
1	1.16190004	-1.99000001	-1.72749996	1	-2.53259993	-2.39150000	0.55479997
6	3.98429990	-0.93699998	-0.36489999	1	-0.40810001	-3.47270012	-1.39520001
6	3.19370008	1.99660003	0.30910000	1	-0.46450001	-3.81349993	0.33460000
1	3.76580000	2.37899995	-0.54200000	1	-1.75339997	-4.37389994	-0.71649998
1	2.37089992	2.69510007	0.49470001	1	-0.63819999	4.51959991	0.10130000
1	3.84640002	2.01559997	1.18729997	1	-1.31219995	3.54600000	-1.20990002

TS[‡]-1



Zero-point vibrational energy	921244.7 (Joules/Mol)
	220.18278 (Kcal/Mol)
Zero-point correction=	0.350884 (Hartree/Particle)
Thermal correction to Energy=	0.371475
Thermal correction to Enthalpy=	0.372420
Thermal correction to Gibbs Free Energy=	0.303548
Sum of electronic and zero-point Energies=	-4453.785781
Sum of electronic and thermal Energies=	-4453.765189
Sum of electronic and thermal Enthalpies=	-4453.764245
Sum of electronic and thermal Free Energies=	-4453.833116

cartesian

6	0.58429998	-2.54679990	-0.68080002	1	-4.23960018	0.84710002	-1.39030004
6	-0.64899999	-1.94029999	-1.03770006	1	-2.98440003	-0.02950000	-2.27270007
6	-1.26349998	-1.41349995	0.13689999	1	-4.22049999	-0.92330003	-1.37989998
6	-0.37130001	-1.70560002	1.22049999	1	-4.13110018	0.88840002	1.81659997
6	0.74940002	-2.40799999	0.71630001	1	-4.13360023	-0.88389999	1.82570004
1	1.59609997	-2.76200008	1.29279995	1	-2.84150004	0.00430000	2.63750005
1	1.27960002	-3.02679992	-1.35920000	6	2.86549997	0.05520000	1.24150002
1	-1.04579997	-1.86880004	-2.04329991	1	3.42339993	0.99760002	1.15559995
14	-2.50909996	-0.00840000	0.16800000	6	2.29320002	-0.03370000	2.66770005
1	-0.52569997	-1.42719996	2.25780010	1	3.62360001	-0.73500001	1.14310002
6	0.56459999	2.55329990	-0.69379997	1	1.77450001	-0.97869998	2.84430003
6	-0.66060001	1.93340003	-1.05929995	1	1.58729994	0.77329999	2.88070011
6	-1.28310001	1.41199994	0.11320000	1	3.09899998	0.03640000	3.40939999
6	-0.40590000	1.72169995	1.20350003	40	0.75489998	0.00600000	-0.24750000
6	0.71399999	2.42910004	0.70700002	6	1.34440005	-0.00920000	-2.45910001
1	1.54849994	2.79629993	1.29289997	6	2.62150002	-0.02830000	-1.73130000
1	1.26180005	3.03670001	-1.36790001	1	1.12109995	0.89940000	-3.01469994
1	-1.04610002	1.85080004	-2.06839991	1	1.09379995	-0.90759999	-3.01950002
1	-0.57429999	1.45500004	2.24149990	1	3.22040009	-0.93650001	-1.81400001
6	-3.49349999	0.00100000	1.75849998	1	3.24469995	0.86369997	-1.81449997
6	-3.58759999	-0.03100000	-1.35930002	1	2.66849995	-0.02540000	-0.17050000