Electronic Supporting Information

For

Coordinative Chain Transfer Polymerization of 1-Decene in the Presence of A Ti-Based Diamine Bis(phenolate) Catalyst: A Sustainable Approach to Produce Low Viscosity PAOs

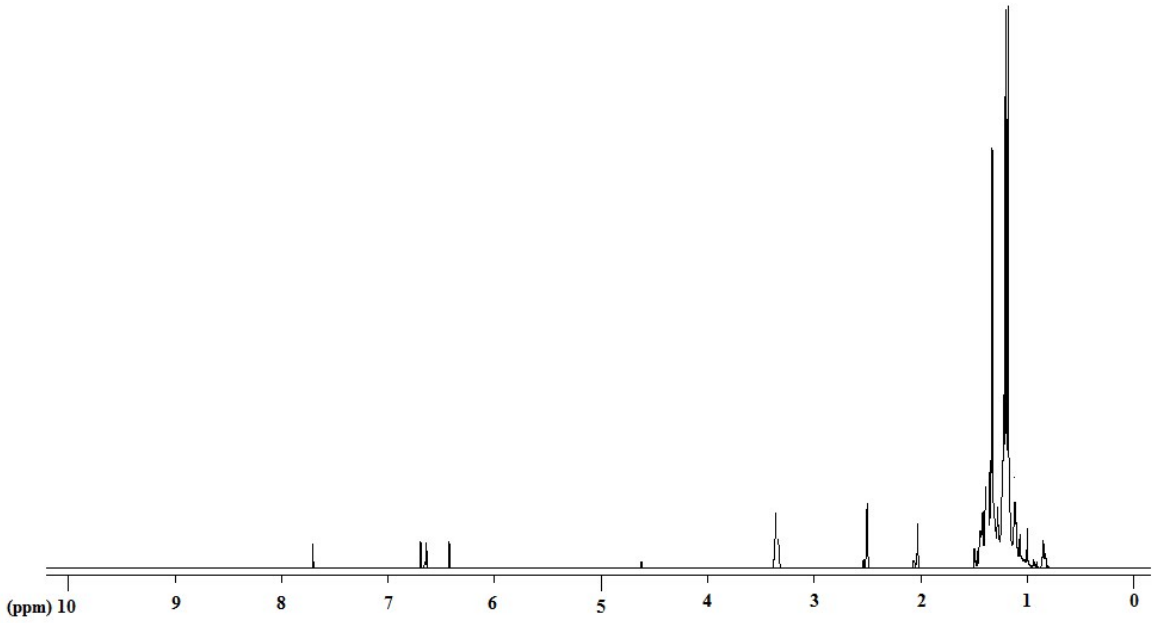


Fig S1. ^{1}H-NMR spectrum of synthesized N,N′-Bis(2-hydroxy-3,5-di-tert-butylphenyl) 4,5-dimethyl-1,2-phenylenediamine ligand, [L_1]

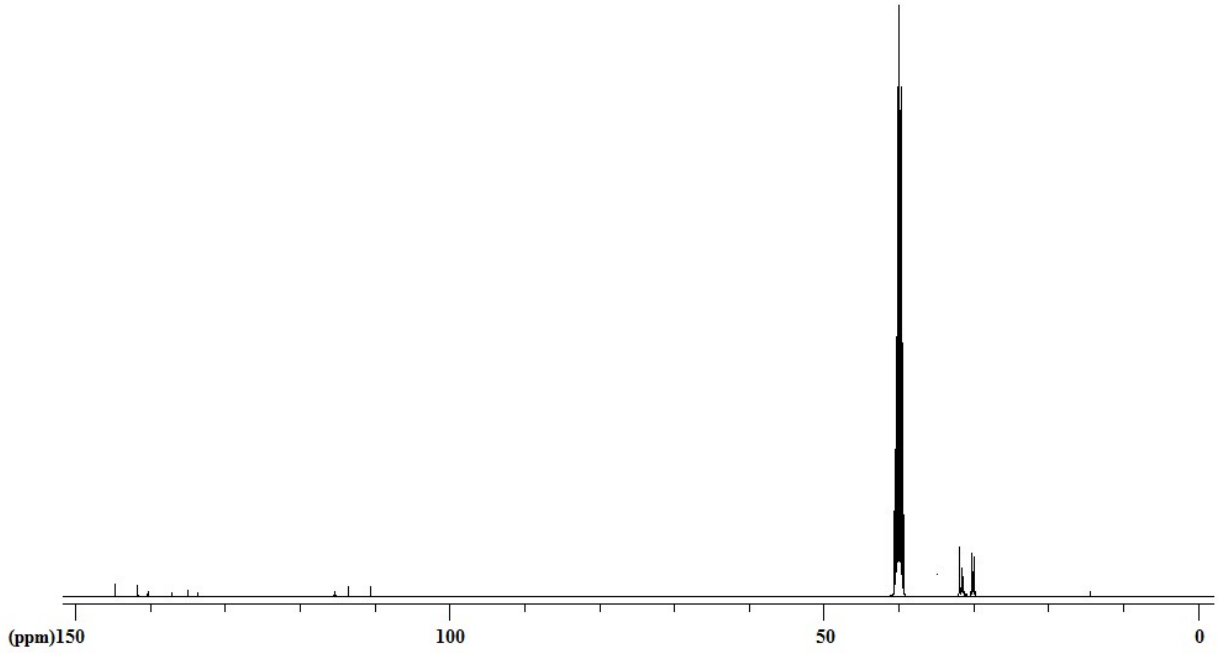


Fig S2. ^{13}C-NMR spectrum of synthesized N,N′-Bis(2-hydroxy-3,5-di-tert-butylphenyl) 4,5-dimethyl-1,2-phenylenediamine ligand, [L_1]

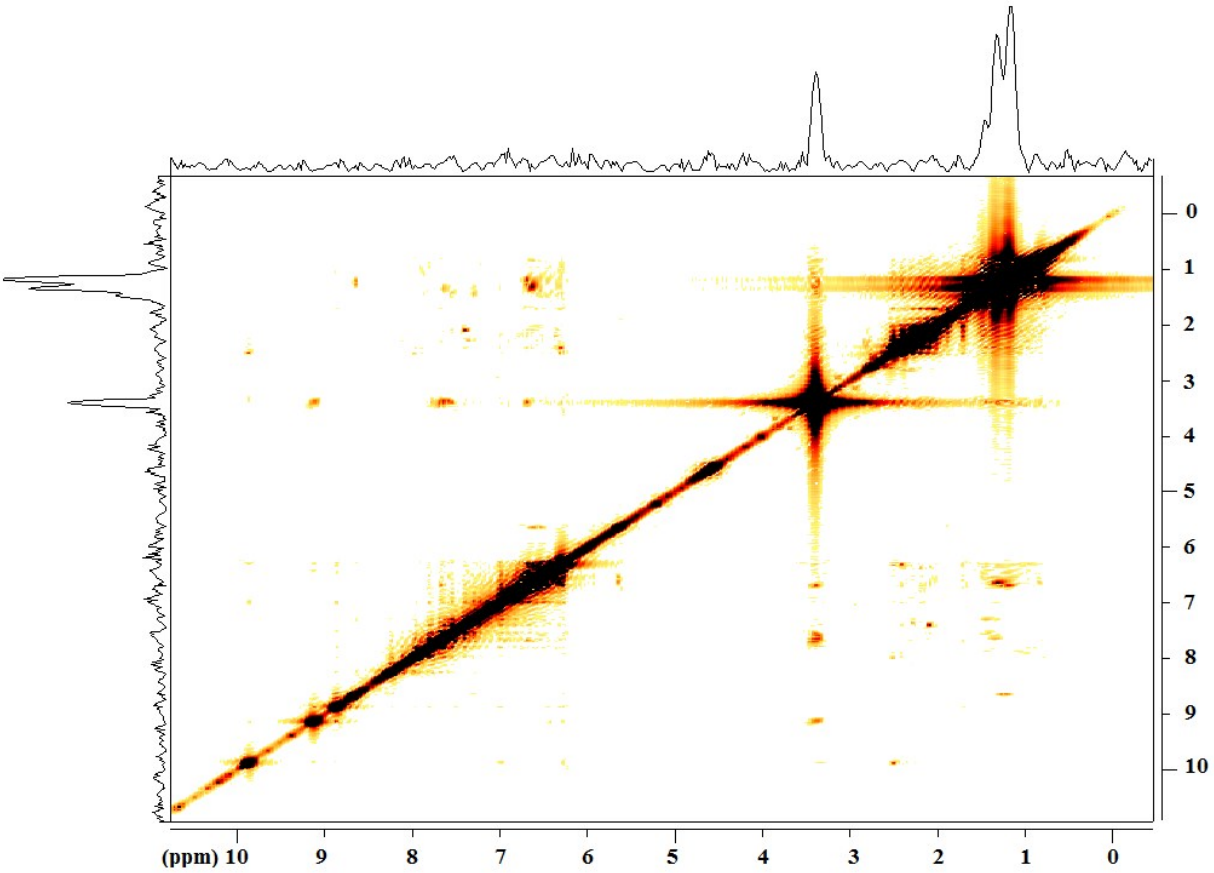


Fig S3. $^{1}H–^{1}H$-COSY spectrum of synthesized N,N′-Bis(2-hydroxy-3,5-di-tert-butylphenyl) 4,5-dimethyl-1,2-phenylenediamine ligand, [L_1]

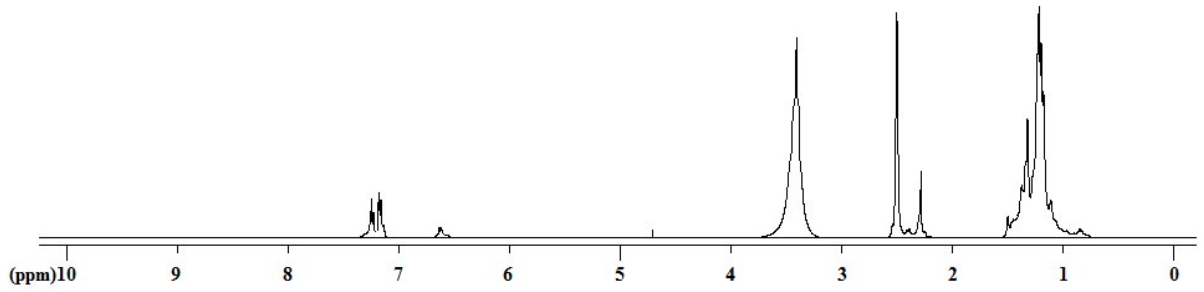


Fig S4. ^{1}H-NMR spectrum of synthesized Ti{2,2′-(OC_6H_2-4,6-$^{t}Bu_2$)$_2$NHMePhMeNH}(Cl_2], [cat]

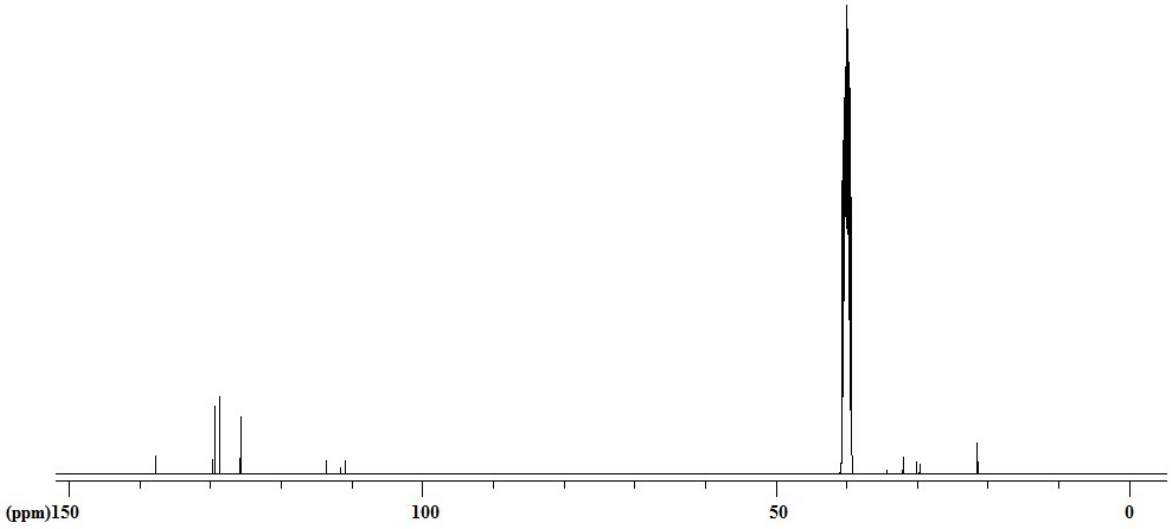


Fig S5. ^{13}C-NMR spectrum of synthesized Ti{2,2′-(OC_6H_2-4,6-$^{t}Bu_2$)$_2$NHMePhMeNH}(Cl_2], [cat]

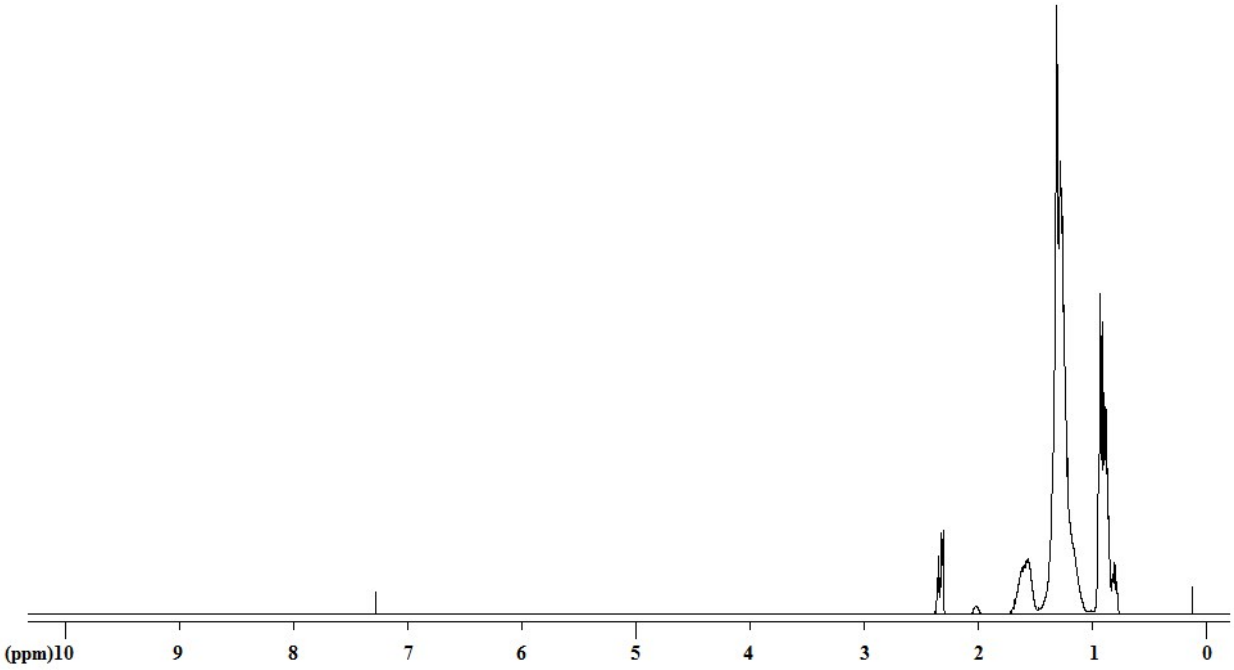


Fig S6. ^{1}H-NMR spectrum of prepared oligomer by Run1, Zn/Ti=0.

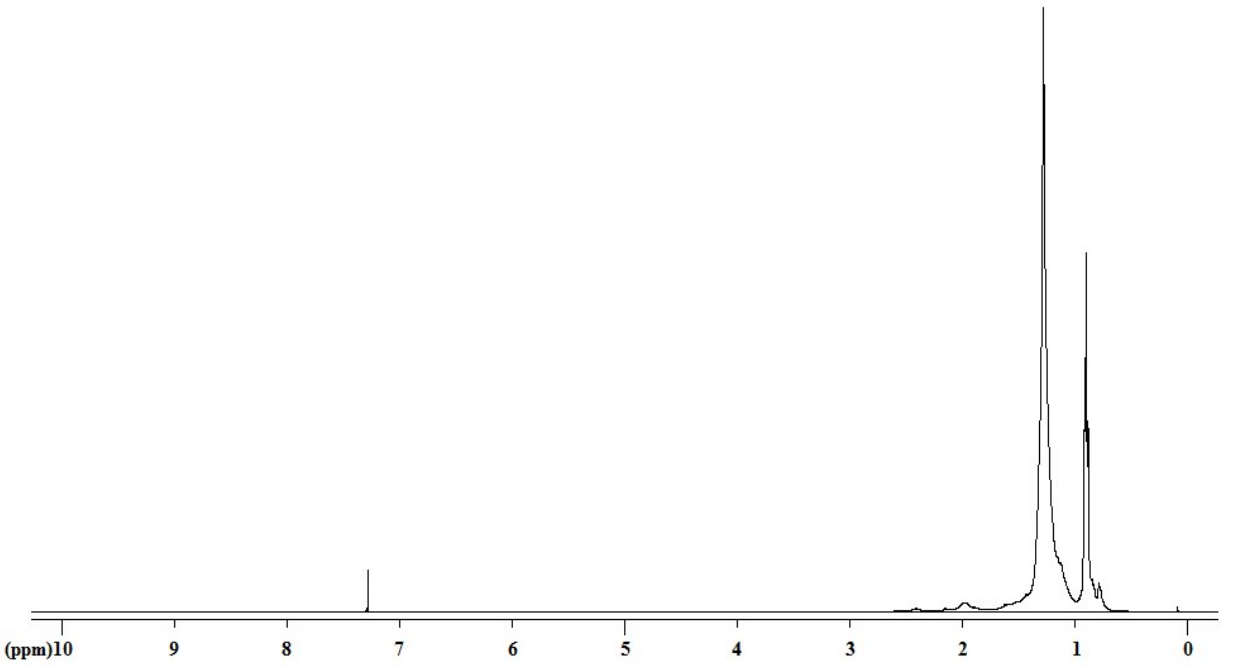


Fig S7. ^{1}H-NMR spectrum of prepared oligomer by Run2, Zn/Ti=30.

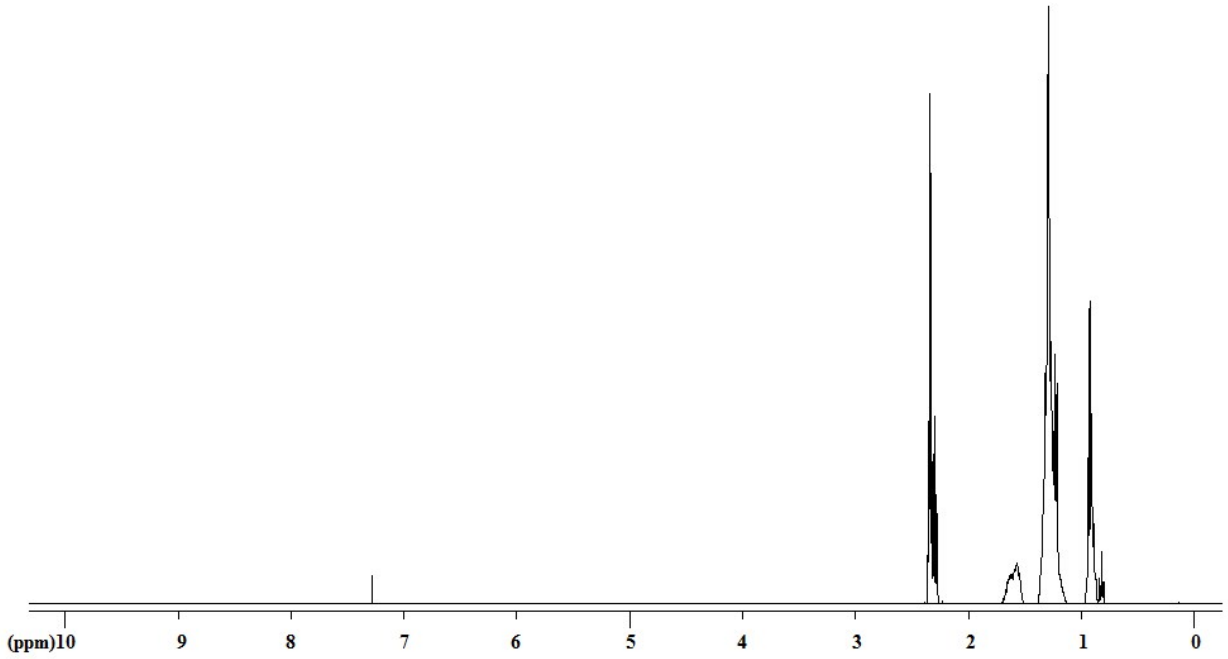


Fig S8. ^{1}H-NMR spectrum of prepared oligomer by Run3, Zn/Ti=90

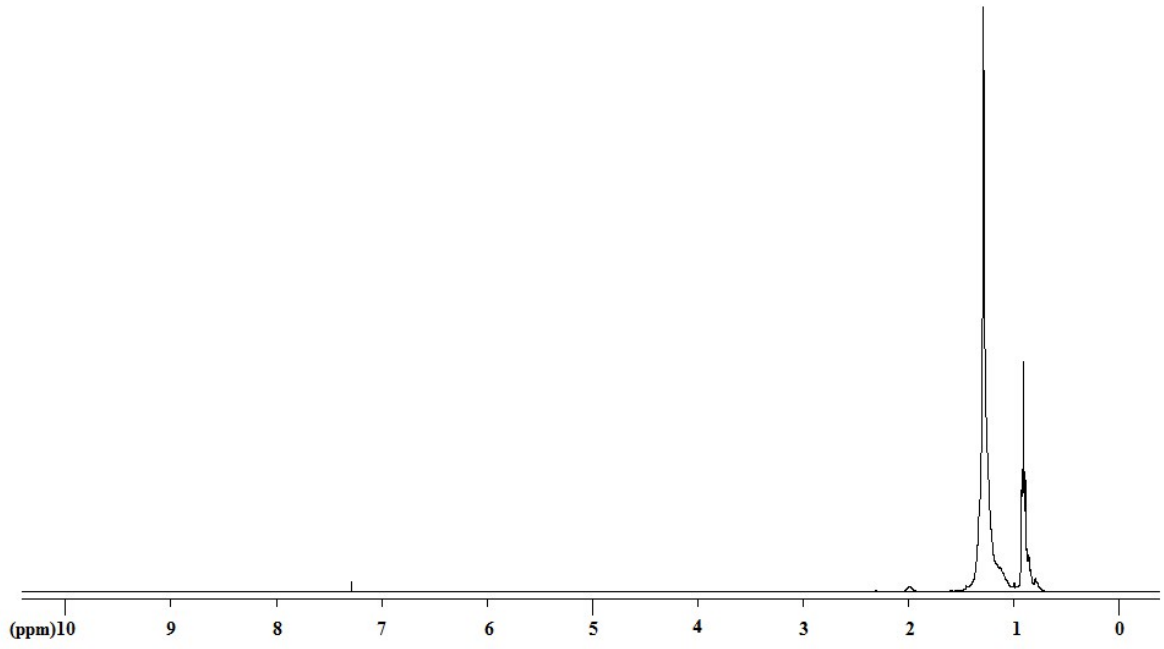


Fig S9. ^{1}H-NMR spectrum of prepared oligomer by Run4, Zn/Ti=120.

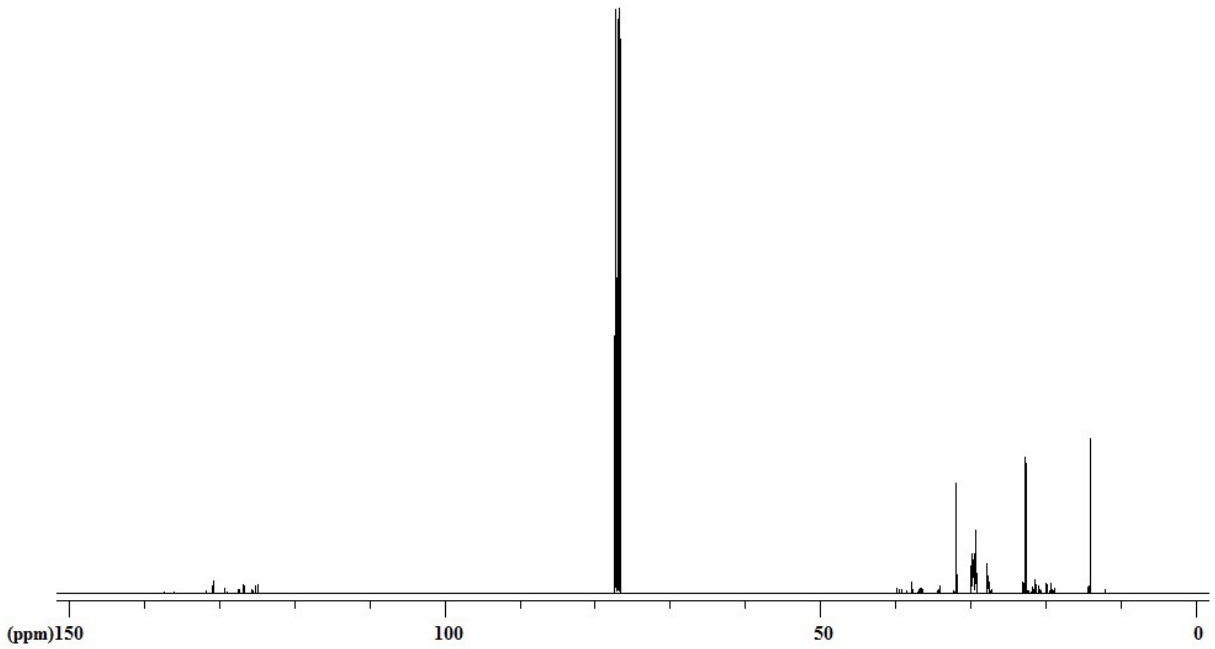


Fig S10. ^{13}C-NMR spectrum of prepared oligomer by Run1, Zn/Ti=0.

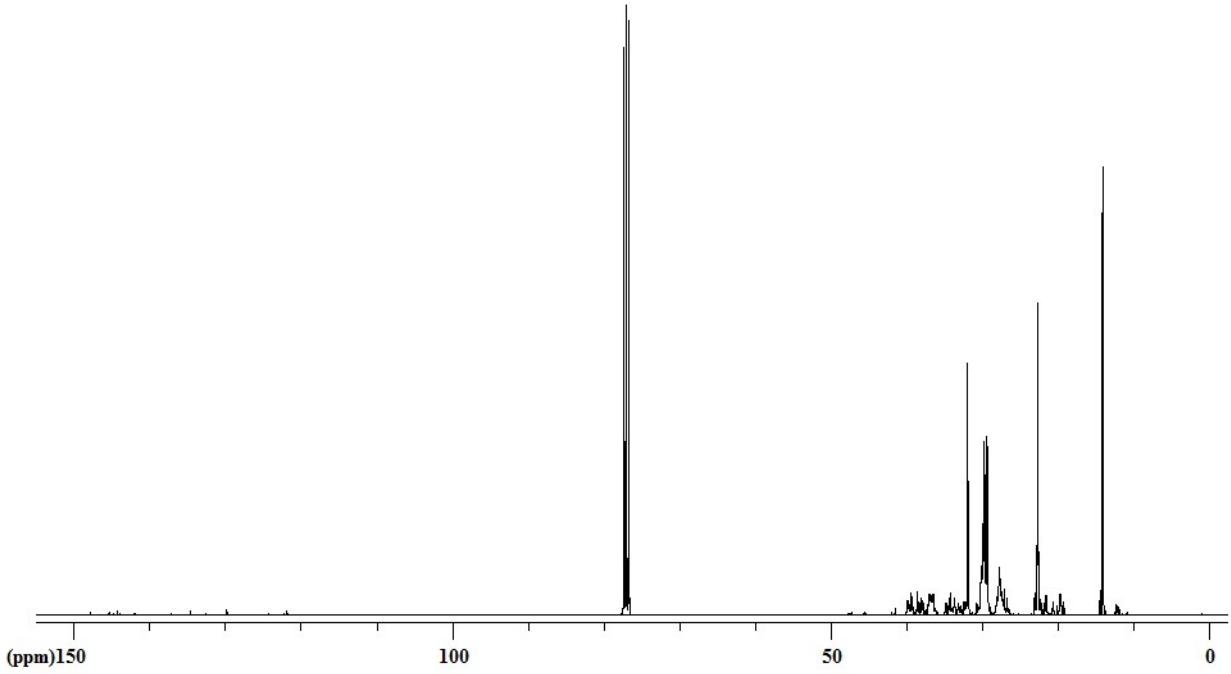


Fig S11. ^{13}C-NMR spectrum of prepared oligomer by Run2, Zn/Ti=30 .

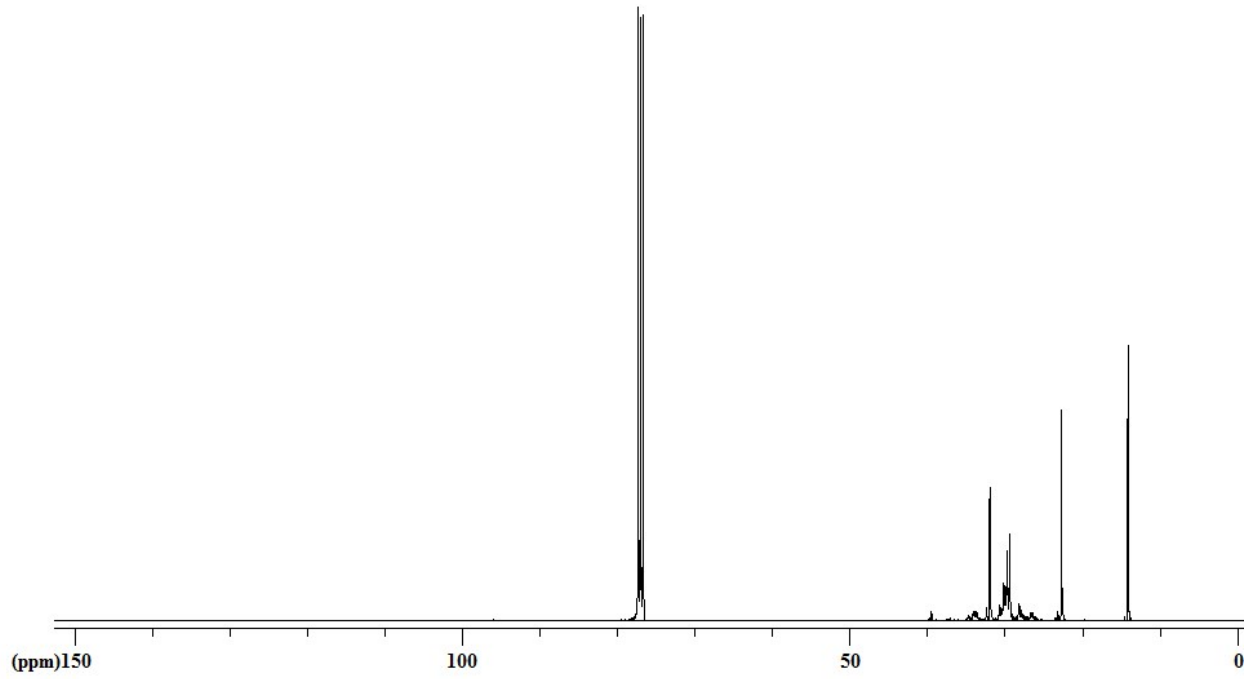


Fig S12. ^{13}C-NMR spectrum of prepared oligomer by Run3, Zn/Ti=90 .

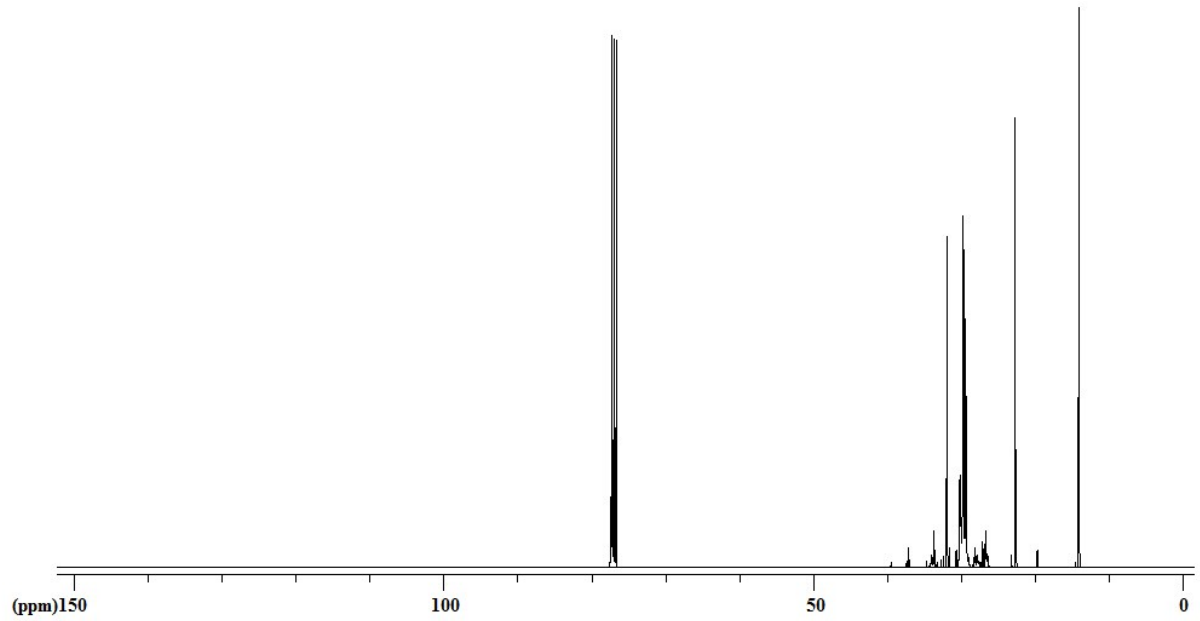
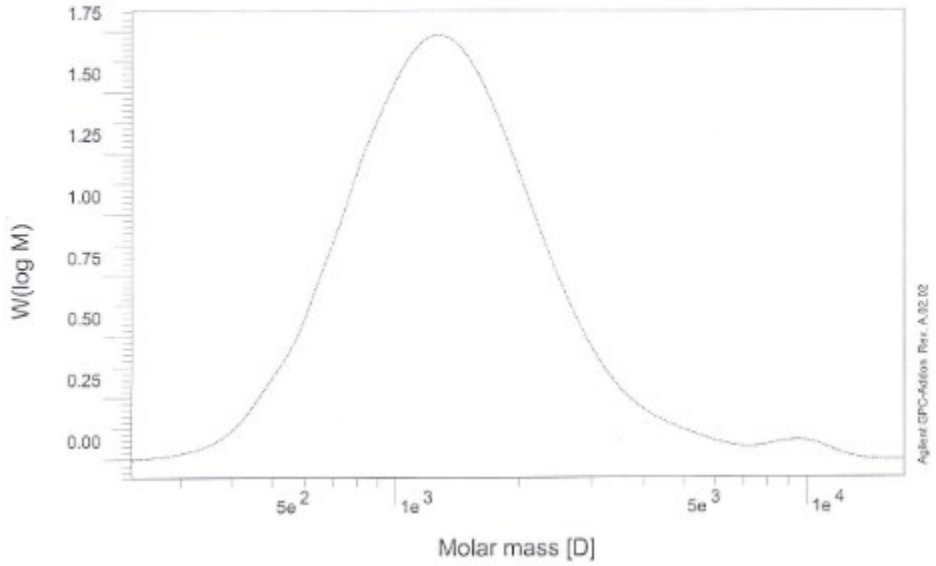


Fig S13. ^{13}C-NMR spectrum of prepared oligomer by Run4, Zn/Ti=120 .

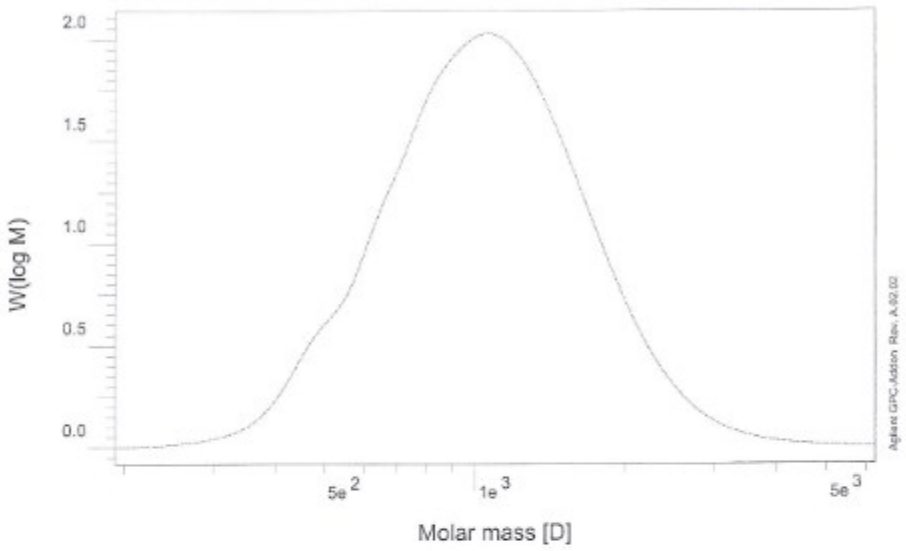


Sample :	1		
Injection Date :	22-Jan-19, 08:45:57		
Calibration File :	G:\GOZARESHAT\CAL-CURVE\CAL-97-07-18.CAL		
Calibration Date :	Thursday 18/10/18 08:02:48		
Baseline from :	15.092 min	**Baseline to :**	19.251 min
Integration from:	15.092 min	**Integration to :**	19.251 min
MHK - A (Cal.):	0.000000E+0	**MHK - K (Cal.):**	1.000000E+0 ml/g
Eluent :	THF	**Flowrate :**	1.000 ml/min
Concentration :	1.000 g/l	**Inject volume :**	20.000 ul
Column 1 :	PLgel OH-MIXED C	**Temperature :**	30.010 C
Detector 1 :	RID A, Refractive Index Signal	**Delay volume :**	0.000 ml
Operator :	IPPI	**Acquisition interval :**	0.430 sec

rid1A

Mn :	1.1620e3	g/mol
Mw :	1.6525e3	g/mol
Mz :	2.7766e3	g/mol
Mv :	0.000000	g/mol
D :	1.4220e0	
[n]:	0.000000	ml/g
Vp :	1.7597e1	ml
Mp :	1.2675e3	g/mol
A :	6.3953e3	ml*V
< 227	0.00	
w% :	100.00	
> 17095	0.00	

Fig S14. GPC curve of prepared oligomer by Run1([Cat]= 5.0 mg, 1-decene=53 mmol, t=120 min, T= 80 °C, Zn/Ti=0, single-stage).

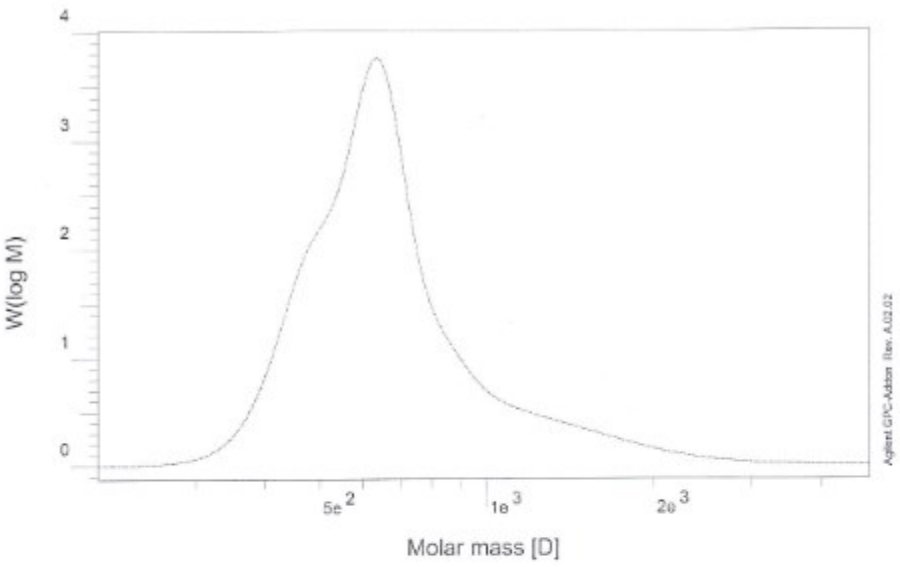


Sample :	2		
Injection Date :	22-Jan-19, 09:19:48		
Calibration File :	G:\GOZARESHAT\CAL-CURVE\CAL-97-07-18.CAL		
Calibration Date :	Thursday 18/10/18 08:02:48		
Baseline from :	16.057 min	**Baseline to :**	19.413 min
Integration from:	16.057 min	**Integration to :**	19.413 min
MHK - A (Cal.):	0.000000E+0	**MHK - K (Cal.):**	1.000000E+0 ml/g
Eluent :	THF	**Flowrate :**	1.000 ml/min
Concentration :	1.000 g/l	**Inject volume :**	20.000 ul
Column 1 :	PLgel OH-MIXED C	**Temperature :**	29.990 C
Detector 1 :	RID A, Refractive Index Signal	**Delay volume :**	0.000 ml
Operator :	IPPI	**Acquisition interval :**	0.430 sec

rid1A

Mn :	9.3882e2	g/mol
Mw :	1.1525e3	g/mol
Mz :	1.4164e3	g/mol
Mv :	0.000000	g/mol
D :	1.2276e0	
[n]:	0.000000	ml/g
Vp :	1.7770e1	ml
Mp :	1.0592e3	g/mol
A :	1.4319e4	ml*V
< 192	0.00	
w% :	100.00	
> 6270	0.00	

Fig S15. GPC curve of prepared oligomer by Run2([Cat]= 5.0 mg, 1-decene=53 mmol, t=120 min, T= 80 °C, Zn/Ti=30, single-stage).

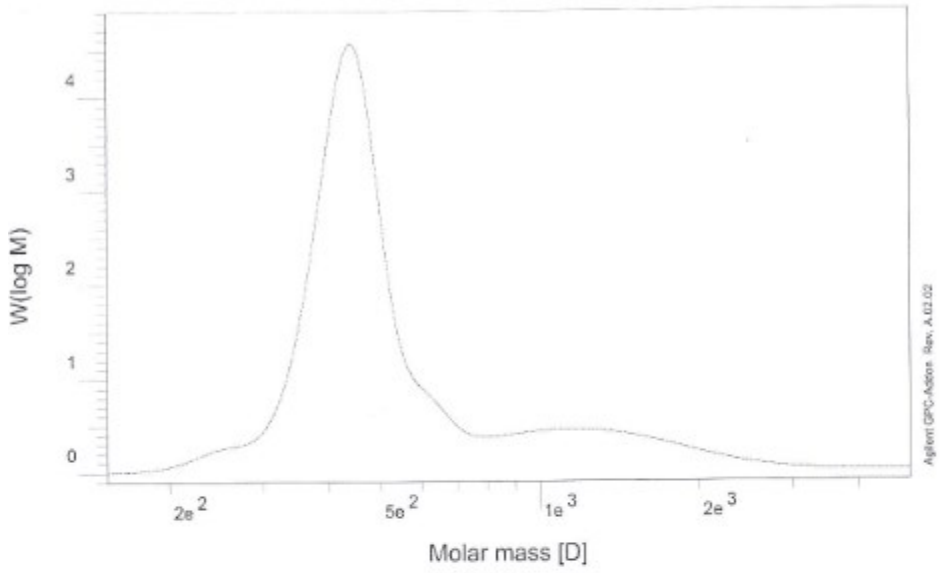


Sample :	3		
Injection Date :	22-Jan-19, 09:55:55		
Calibration File :	G:\GOZARESHAT\CAL-CURVE\CAL-97-07-18.CAL		
Calibration Date :	Thursday 18/10/18 08:02:48		
Baseline from :	16.298 min	**Baseline to :**	19.373 min
Integration from:	16.298 min	**Integration to :**	19.373 min
MHK - A (Cal.):	0.000000E+0	**MHK - K (Cal.):**	1.000000E+0 ml/g
Eluent :	THF	**Flowrate :**	1.000 ml/min
Concentration :	1.000 g/l	**Inject volume :**	20.000 ul
Column 1 :	PLgel OH-MIXED C	**Temperature :**	30.000 C
Detector 1 :	RID A, Refractive Index Signal	**Delay volume :**	0.000 ml
Operator :	IPPI	**Acquisition interval :**	0.430 sec

rid1A

Mn :	6.3021e2	g/mol
Mw :	7.2847e2	g/mol
Mz :	9.0484e2	g/mol
Mv :	0.000000	g/mol
D :	1.1559e0	
[n]:	0.000000	ml/g
Vp :	1.8259e1	ml
Mp :	6.3687e2	g/mol
A :	1.1711e4	ml*V
< 200	0.00	
w% :	100.00	
> 4886	0.00	

Fig S16. GPC curve of prepared oligomer by Run3([Cat]= 5.0 mg, 1-decene=53 mmol, t=120 min, T= 80 °C, Zn/Ti=90, single-stage).

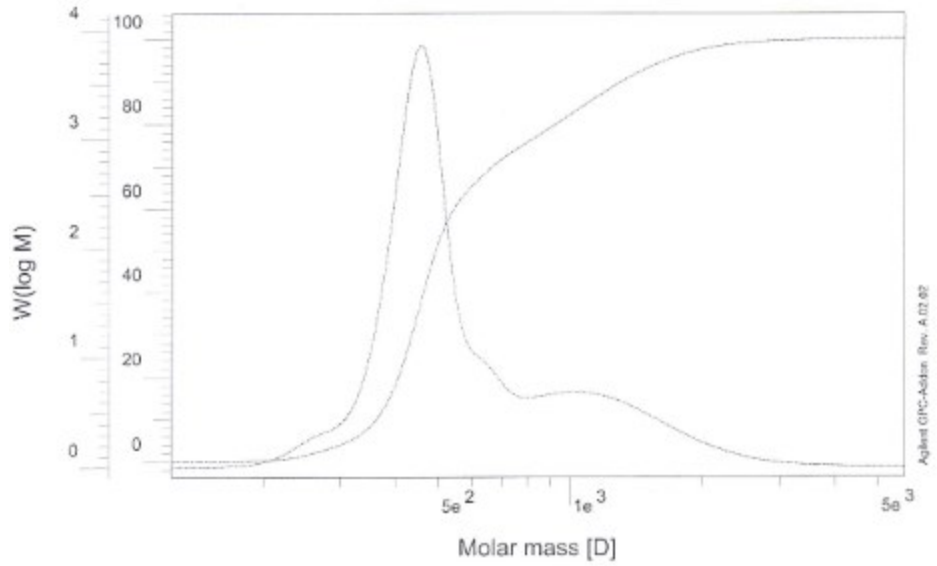


Sample :	3		
Injection Date :	26-Nov-18, 13:23:01		
Calibration File :	G:\GOZARESHAT\CAL-CURVE\CAL-97-07-18.CAL		
Calibration Date :	Thursday 18/10/18 08:02:48		
Baseline from :	16.280 min	**Baseline to :**	19.638 min
Integration from:	16.280 min	**Integration to :**	19.638 min
MHK - A (Cal.):	0.000000E+0	**MHK - K (Cal.):**	1.000000E+0 ml/g
Eluent :	THF	**Flowrate :**	1.000 ml/min
Concentration :	1.000 g/l	**Inject volume :**	20.000 ul
Column 1 :	PLgel OH-MIXED C	**Temperature :**	30.010 C
Detector 1 :	RID A, Refractive Index Signal	**Delay volume :**	0.000 ml
Operator :	IPPI	**Acquisition interval :**	0.430 sec

rid1A

Mn :	4.8267e2	g/mol
Mw :	6.1826e2	g/mol
Mz :	9.2668e2	g/mol
Mv :	0.000000	g/mol
D :	1.2809e0	
[n]:	0.000000	ml/g
Vp :	1.8612e1	ml
Mp :	4.4151e2	g/mol
A :	1.2942e4	ml*V
< 152	0.00	
w% :	100.00	
> 4974	0.00	

Fig S17. GPC curve of prepared oligomer by Run4([Cat]= 5.0 mg, 1-decene=53 mmol , t=120 min, T= 80 °C, Zn/Ti=120, single-stage).

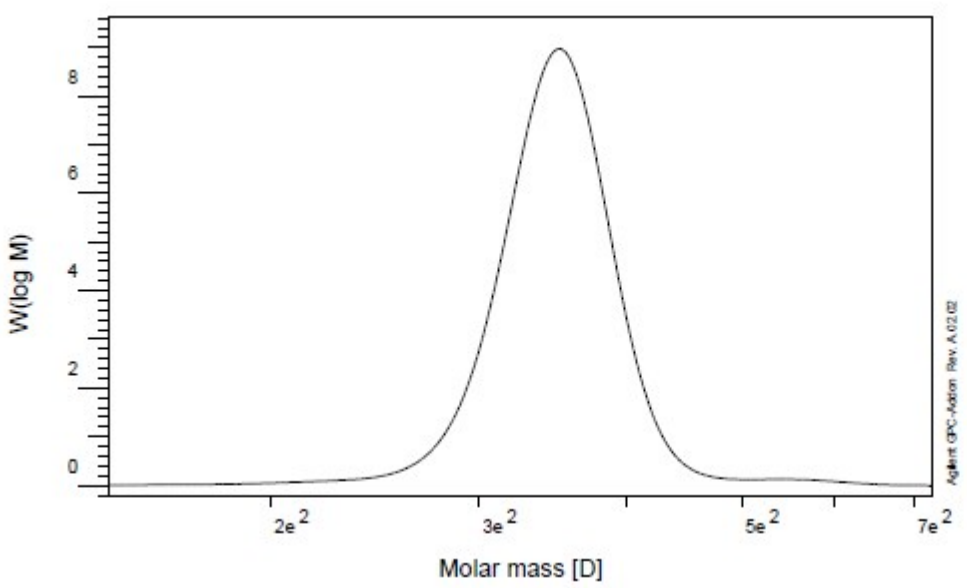


Sample :	4		
Injection Date :	22-Jan-19, 10:30:12		
Calibration File :	G:\GOZARESHAT\CAL-CURVE\CAL-97-07-18.CAL		
Calibration Date :	Thursday 18/10/18 08:02:48		
Baseline from :	16.139 min	**Baseline to :**	19.835 min
Integration from:	16.139 min	**Integration to :**	19.835 min
MHK - A (Cal.):	0.000000E+0	**MHK - K (Cal.):**	1.000000E+0 ml/g
Eluent :	THF	**Flowrate :**	1.000 ml/min
Concentration :	1.000 g/l	**Inject volume :**	20.000 ul
Column 1 :	PLgel OH-MIXED C	**Temperature :**	30.000 C
Detector 1 :	RID A, Refractive Index Signal	**Delay volume :**	0.000 ml
Operator :	IPPI	**Acquisition interval :**	0.430 sec

rid1A

Mn :	5.2580e2	g/mol
Mw :	6.8943e2	g/mol
Mz :	1.0164e3	g/mol
Mv :	0.000000	g/mol
D :	1.3112e0	
[n]:	0.000000	ml/g
Vp :	1.8576e1	ml
Mp :	4.5834e2	g/mol
A :	5.3603e3	ml*V
< 123	0.00	
w% :	100.00	
> 5760	0.00	

Fig S18. GPC curve of prepared oligomer by Run5([Cat]= 5.0 mg, 1-decene=53 mmol, t=120 min, T= 80 °C, Zn/Ti=120, two-stage).

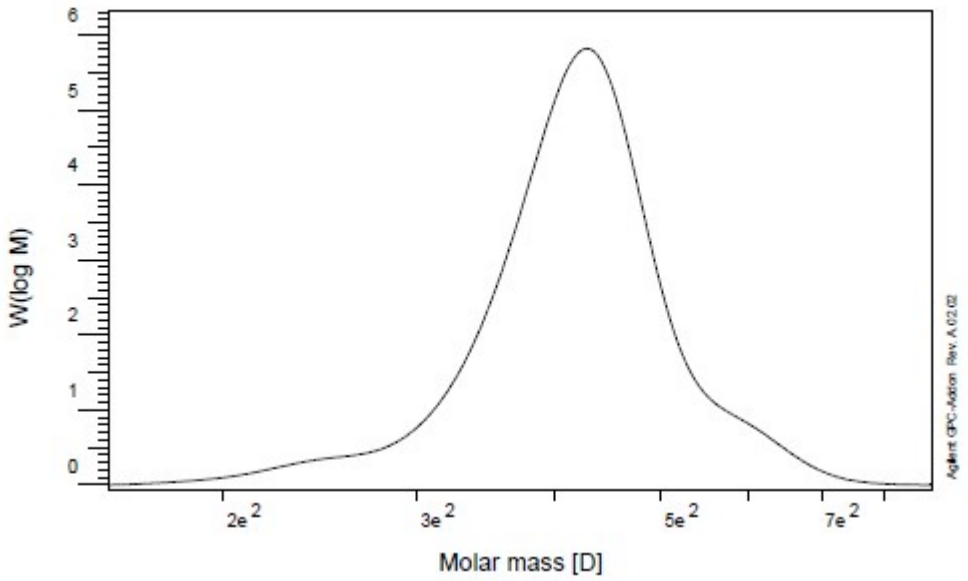


Sample :	PAO2		
Injection Date :	22-Jan-17, 09:18:15		
Calibration File :	C:\HPCHEM\1\DATA\139510\95-10-CAL-L-02.CAL		
Calibration Date :	Monday 17/01/16 14:36:36		
Baseline from :	18.276 min	**Baseline to :**	19.852 min
Integration from:	18.276 min	**Integration to :**	19.852 min
MHK - A (Cal.):	0.000000E+0	**MHK - K (Cal.):**	1.000000E+0 ml/g
Eluent :	THF	**Flowrate :**	1.000 ml/min
Concentration :	1.000 g/l	**Inject volume :**	20.000 ul
Column 1 :	PLgel OH-MIXED C	**Temperature :**	30.010 C
Detector 1 :	RID A, Refractive Index Signal	**Delay volume :**	0.000 ml
Operator :	IPPI	**Acquisition interval :**	0.430 sec

rid1A

$\overline{Mn}$:	3.4524e2	g/mol
$\overline{Mw}$:	3.5101e2	g/mol
$\overline{Mz}$:	3.5694e2	g/mol
$\overline{Mv}$:	0.000000	g/mol
D :	1.0167e0	
[n]:	0.000000	ml/g
Vp :	1.8994e1	ml
Mp :	3.4970e2	g/mol
A :	2.4463e3	ml*V
< 145	0.00	
w% :	100.00	
> 726	0.00	

Fig S19. GPC curve of prepared oligomer by Run3([Cat]= 5.0 mg, 1-decene=53 mmol , t=30 min, T= 80 °C, Zn/Ti=90, single-stage).

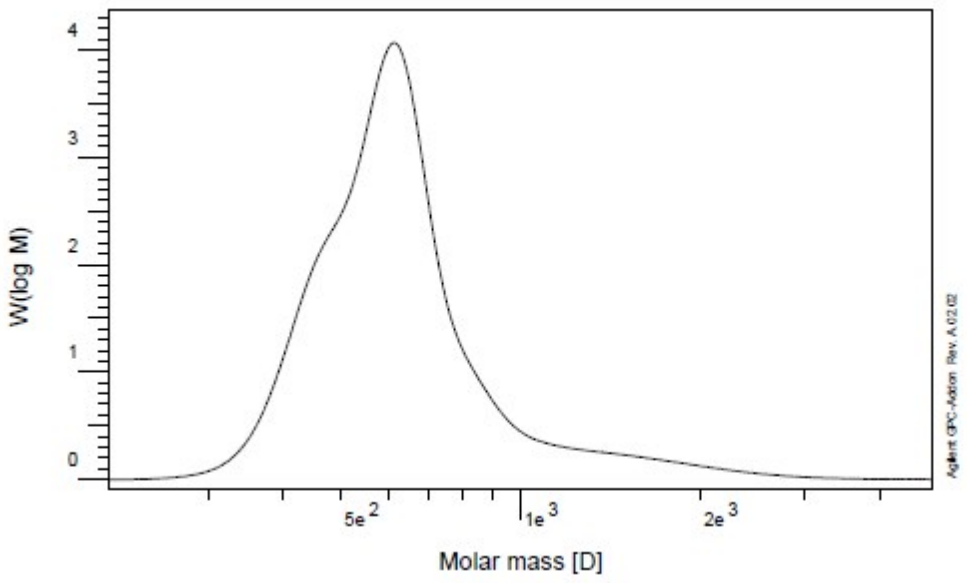


Sample :	131-C		
Injection Date :	14-May-18, 10:46:44		
Calibration File :	G:\GOZARESHAT\CAL\CAL-970120-.CAL		
Calibration Date :	Wednesday 18/04/18 10:32:30		
Baseline from :	18.010 min	**Baseline to :**	19.685 min
Integration from:	18.010 min	**Integration to :**	19.685 min
MHK - A (Cal.):	0.000000E+0	**MHK - K (Cal.):**	1.000000E+0 ml/g
Eluent :	THF	**Flowrate :**	1.000 ml/min
Concentration :	1.000 g/l	**Inject volume :**	20.000 ul
Column 1 :	PLgel OH-MIXED C	**Temperature :**	29.960 C
Detector 1 :	RID A, Refractive Index Signal	**Delay volume :**	0.000 ml
Operator :	IPPI	**Acquisition interval :**	0.430 sec

rid1A

$\overline{Mn}$:	4.0589e2	g/mol
$\overline{Mw}$:	4.2412e2	g/mol
$\overline{Mz}$:	4.4146e2	g/mol
$\overline{Mv}$:	0.000000	g/mol
D :	1.0449e0	
[n]:	0.000000	ml/g
Vp :	1.8713e1	ml
Mp :	4.2879e2	g/mol
A :	4.3542e3	ml*V
< 157	0.00	
w% :	100.00	
> 883	0.00	

Fig S20. GPC curve of prepared oligomer by Run3([Cat]= 5.0 mg, 1-decene=53 mmol , t=60 min, T= 80 °C, Zn/Ti=90, single-stage).



Sample :	1		
Injection Date :	26-Nov-18, 12:16:52		
Calibration File :	G:\GOZARESHAT\CAL-CURVE\CAL-97-07-18.CAL		
Calibration Date :	Thursday 18/10/18 08:02:48		
Baseline from :	16.292 min	**Baseline to :**	19.353 min
Integration from:	16.292 min	**Integration to :**	19.353 min
MHK - A (Cal.):	0.000000E+0	**MHK - K (Cal.):**	1.000000E+0 ml/g
Eluent :	THF	**Flowrate :**	1.000 ml/min
Concentration :	1.000 g/l	**Inject volume :**	20.000 ul
Column 1 :	PLgel OH-MIXED C	**Temperature :**	29.970 C
Detector 1 :	RID A, Refractive Index Signal	**Delay volume :**	0.000 ml
Operator :	IPPI	**Acquisition interval :**	0.430 sec

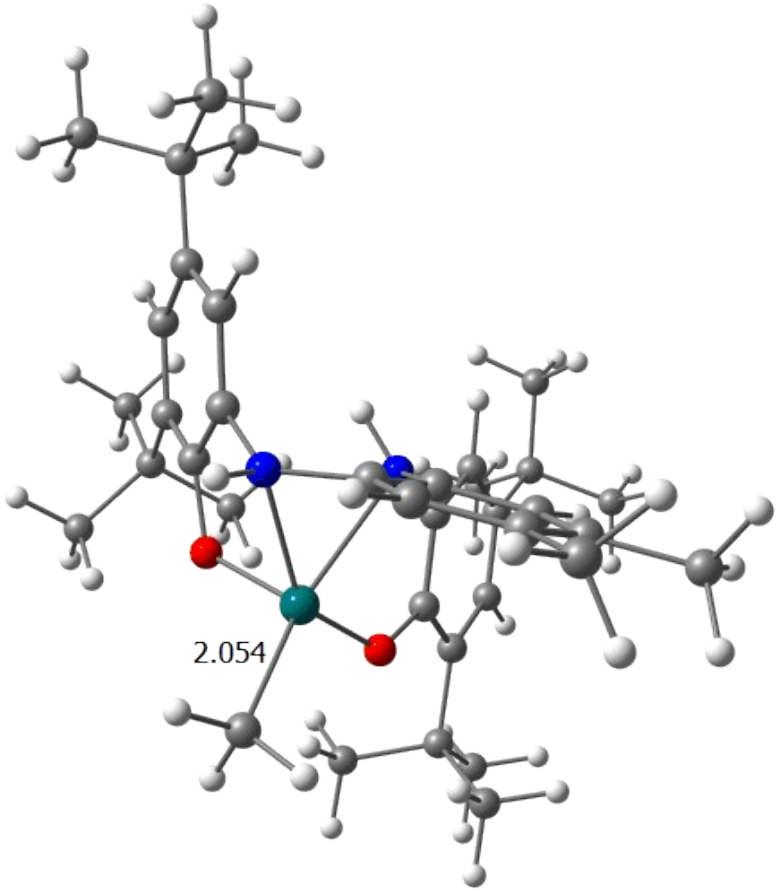
rid1A

$\overline{Mn}$:	5.9474e2	g/mol
$\overline{Mw}$:	6.7552e2	g/mol
$\overline{Mz}$:	8.3210e2	g/mol
$\overline{Mv}$:	0.000000	g/mol
D :	1.1358e0	
[n]:	0.000000	ml/g
Vp :	1.8295e1	ml
Mp :	6.1349e2	g/mol
A :	6.5036e3	ml*V
< 204	0.00	
w% :	100.00	
> 4915	0.00	

Fig S21. GPC curve of prepared oligomer by Run3([Cat]= 5.0 mg, 1-decene=53 mmol, t=90min, T= 80 °C, Zn/Ti=90, single-stage).

Table S1. Cartesian coordinates and energy data of DFT-optimized structures (selected distances in Å), absolute gas and solvent phase energy values (in a.u.).

1



Zero-point correction= 0.799441 (Hartree/Particle)
Thermal correction to Energy= 0.863744
Thermal correction to Enthalpy= 0.864863
Thermal correction to Gibbs Free Energy= 0.697404
Sum of electronic and zero-point Energies= -1758.273361
Sum of electronic and thermal Energies= -1758.209057
Sum of electronic and thermal Enthalpies= -1758.207939
Sum of electronic and thermal Free Energies= -1758.375397

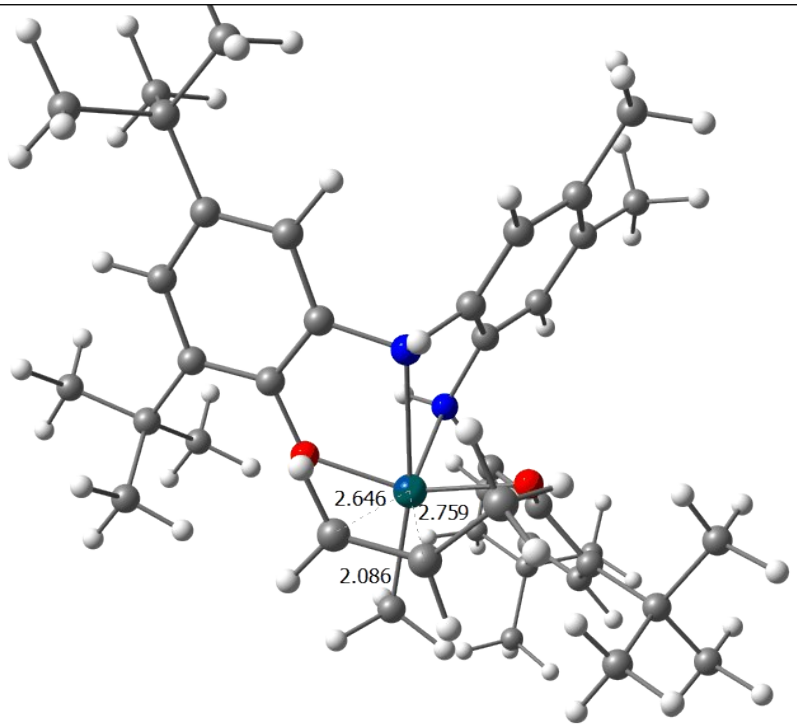
Solvent: -1758.7804031

95
PhTitBuCH3+ SCF Done: -1759.07280123 A.U.

Ti	0.451767	-0.548271	-2.001358
N	-0.209889	0.714779	-0.266536
O	-1.062006	-1.404645	-1.457207
C	-1.952965	-0.916661	-0.543610
C	-1.540535	0.247392	0.138335
C	-2.295423	0.795520	1.183073
H	-1.904227	1.655471	1.741971
C	-3.537454	0.215462	1.510798
C	-3.949036	-0.924043	0.776506
H	-4.917814	-1.372435	1.032528
C	-3.193968	-1.536053	-0.243520
C	0.034429	2.090200	-0.706662
C	-4.439860	0.774300	2.629533
N	1.938623	1.050089	-1.801698
O	1.965316	-1.606670	-2.088319
C	2.527038	-1.146532	-0.921259
C	2.576494	0.268370	-0.741565
C	3.022287	0.853061	0.453919
H	3.004562	1.948425	0.537991
C	3.469698	0.028875	1.500518
C	3.425434	-1.377641	1.300025
H	3.764080	-2.017673	2.124847
C	2.955099	-2.008427	0.136748
C	1.220535	2.258372	-1.455522
C	3.979252	0.593106	2.838727
C	-3.655473	-2.800259	-0.992076
C	2.842121	-3.538206	0.007491
H	0.459114	0.508358	0.502524
H	2.535666	1.166034	-2.634605
H	-0.562706	-0.694529	-4.428282
C	3.962957	2.135568	2.858502
H	4.617212	2.567392	2.072819
H	2.938544	2.543450	2.726749
H	4.337064	2.502384	3.835371
C	3.064955	0.073991	3.979820
H	3.069981	-1.032700	4.050177
H	3.410318	0.470992	4.956763
H	2.014763	0.401490	3.828895
C	5.434900	0.109876	3.070844
H	5.821352	0.511852	4.030178
H	5.506424	-0.995577	3.122092
H	6.104817	0.457348	2.257576
C	3.405552	-4.259439	1.250554
H	4.479134	-4.030694	1.414199
H	2.845610	-4.007375	2.175227
H	3.321783	-5.355398	1.107242
C	3.633761	-4.019819	-1.236396
H	3.249481	-3.570322	-2.171662
H	4.709762	-3.766014	-1.140889
H	3.551922	-5.122519	-1.327729
C	1.339310	-3.912247	-0.129551
H	0.752927	-3.530143	0.732165
H	0.892174	-3.509056	-1.057761
H	1.225752	-5.015446	-0.155706
C	-2.639511	-3.943970	-0.728629
H	-1.624260	-3.683286	-1.084889
H	-2.578911	-4.175224	0.355081
H	-2.961514	-4.865428	-1.256720
C	-3.733711	-2.492605	-2.511113
H	-4.454487	-1.672621	-2.710480
H	-2.748387	-2.197981	-2.922371
H	-4.078348	-3.391631	-3.062985
C	-5.047911	-3.269204	-0.520814
H	-5.056648	-3.537430	0.556070
H	-5.828989	-2.501000	-0.698454
H	-5.342331	-4.175731	-1.087130
C	-4.649010	-0.319869	3.708563
H	-5.296167	0.063803	4.524498
H	-5.137867	-1.224734	3.293781
H	-3.680873	-0.630170	4.153564
C	-5.808415	1.177597	2.021819
H	-6.331932	0.313411	1.564964
H	-6.472329	1.589190	2.810399
H	-5.684215	1.952311	1.236848
C	-3.821955	2.015778	3.305545
H	-2.849861	1.786454	3.790588
H	-3.668620	2.847612	2.585796
H	-4.501566	2.390080	4.097580
C	-0.134226	0.154022	-3.848139
H	0.677885	0.628668	-4.439603
H	-0.943466	0.899044	-3.666775
C	-0.794893	3.192013	-0.473394
C	1.584581	3.525150	-1.923661
C	0.762839	4.647422	-1.682940

	C	-0.450631	4.473513	-0.958339
	H	-1.738021	3.057221	0.073400
	H	2.512698	3.640560	-2.506375
	C	-1.364533	5.647723	-0.708016
	H	-1.687710	6.117384	-1.661520
	H	-2.273343	5.353127	-0.148898
	H	-0.849601	6.442876	-0.127259
	C	1.158396	6.007791	-2.200181
	H	0.394513	6.409873	-2.899726
	H	1.241294	6.744160	-1.372560
	H	2.128082	5.983804	-2.733391

2



Zero-point correction= 0.878974 (Hartree/Particle)
Thermal correction to Energy= 0.950089
Thermal correction to Enthalpy= 0.951207
Thermal correction to Gibbs Free Energy= 0.769186
Sum of electronic and zero-point Energies= -1876.028246
Sum of electronic and thermal Energies= -1875.957131
Sum of electronic and thermal Enthalpies= -1875.956013
Sum of electronic and thermal Free Energies= -1876.138034

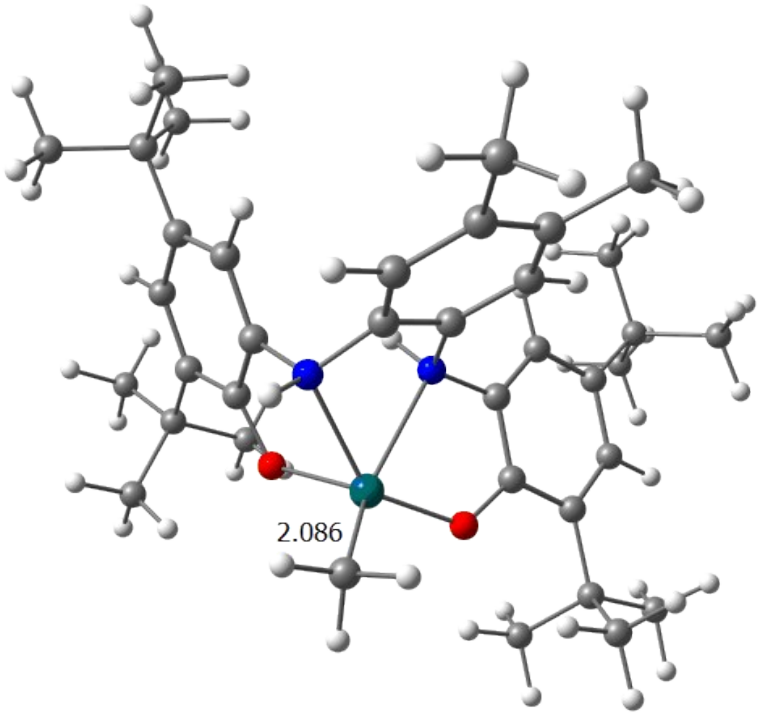
Solvent: -1876.5862019

104
PhTitBuCH3+propTS+PRE SCF Done: -1876.90721981 A.U.

Ti	-0.432700	-0.736111	-1.073663
N	-0.491645	0.106770	0.910979
O	-1.579746	0.796750	-1.356204
C	-2.470133	0.343927	-0.445596
C	-1.912580	-0.130510	0.786067
C	-2.674902	-0.826113	1.743347
H	-2.180666	-1.190741	2.654946
C	-4.042454	-1.020487	1.514560
C	-4.603695	-0.450371	0.333970
H	-5.685676	-0.564729	0.186649
C	-3.883453	0.231190	-0.654659
C	-0.061144	1.504016	0.967473
C	-4.952586	-1.783323	2.494437
N	1.327377	0.961764	-0.965826
O	1.096378	-1.656316	-0.608917
C	2.321622	-1.167618	-0.310807
C	2.503834	0.222650	-0.492469
C	3.730072	0.838272	-0.212480
H	3.821112	1.924346	-0.350639
C	4.813151	0.066165	0.250687
C	4.604417	-1.326004	0.419236
H	5.447904	-1.928328	0.781691
C	3.390028	-1.985480	0.154645
C	0.833881	1.943675	-0.019096
C	6.189085	0.678381	0.580922
C	-4.548038	0.859444	-1.892086
C	3.194030	-3.500594	0.353339
H	-0.057626	-0.470704	1.646945
H	1.546131	1.435986	-1.852993
H	-1.834728	-2.842296	-0.585448
C	6.221347	2.200053	0.327907
H	6.024840	2.447981	-0.736233
H	5.484104	2.741338	0.957341
H	7.224261	2.600999	0.578754
C	6.508784	0.422961	2.076973
H	6.546718	-0.659662	2.314613
H	7.496504	0.856688	2.338520
H	5.743430	0.888634	2.732065
C	7.270736	0.008472	-0.305629
H	8.269348	0.440405	-0.086335
H	7.335684	-1.084443	-0.128355
H	7.056514	0.165639	-1.383083
C	4.482828	-4.185974	0.853979
H	5.319363	-4.076189	0.133150
H	4.812899	-3.789800	1.836766
H	4.298878	-5.271948	0.982038
C	2.793303	-4.148737	-0.999038
H	1.834657	-3.743757	-1.378067
H	3.576539	-3.974108	-1.765651
H	2.675543	-5.245411	-0.875378
C	2.078639	-3.736157	1.407181
H	2.355168	-3.278982	2.380411
H	1.110642	-3.310552	1.076050
H	1.932096	-4.823841	1.571975
C	-4.036352	0.155187	-3.174377
H	-2.938521	0.245017	-3.264327
H	-4.305469	-0.921229	-3.173176
H	-4.495623	0.619036	-4.071689
C	-4.183985	2.367611	-1.938536
H	-4.548262	2.888387	-1.028916
H	-3.090013	2.522363	-2.013092
H	-4.662035	2.845074	-2.818947
C	-6.085057	0.730161	-1.847766
H	-6.418055	-0.328522	-1.858766
H	-6.518967	1.226599	-0.955110
H	-6.521701	1.218691	-2.742215
C	-5.646922	-2.945966	1.737819
H	-6.299403	-3.515312	2.431597
H	-6.285566	-2.583142	0.906832
H	-4.900316	-3.648059	1.312343
C	-6.021974	-0.807318	3.051456
H	-6.657069	-0.381890	2.247944
H	-6.691239	-1.337827	3.760045
H	-5.546839	0.036620	3.593302
C	-4.158412	-2.373837	3.677564
H	-3.379182	-3.087676	3.337164
H	-3.672361	-1.585352	4.289396
H	-4.843142	-2.929931	4.349265
C	-0.236138	-0.280523	-3.787942
C	0.805617	-1.061827	-3.389353
H	-1.206386	-0.774346	-3.983987
H	0.710848	-2.155848	-3.316619
H	1.816748	-0.648504	-3.230588
C	-0.175176	1.190708	-4.065541
H	-0.488081	1.384141	-5.113862
H	-0.882255	1.741554	-3.410769
H	0.846558	1.603121	-3.936993
C	-1.611461	-2.381532	-1.578616
H	-1.089896	-3.139670	-2.199663

	H	-2.577527	-2.107447	-2.051477
	C	-0.587308	2.399106	1.905451
	C	1.193685	3.299349	-0.053623
	C	0.679705	4.218925	0.884258
	C	-0.222195	3.760093	1.888613
	H	-1.314061	2.031359	2.647658
	H	1.885749	3.652640	-0.835554
	C	-0.790693	4.718840	2.905552
	H	-1.343751	5.548455	2.415259
	H	-1.485222	4.214307	3.604615
	H	0.013699	5.192509	3.508206
	C	1.078477	5.672831	0.825527
	H	0.191377	6.329524	0.697444
	H	1.570077	5.993971	1.768819
	H	1.776974	5.878215	-0.008499

1 (triplet)



Zero-point correction= 0.796505 (Hartree/Particle)
Thermal correction to Energy= 0.861917
Thermal correction to Enthalpy= 0.863035
Thermal correction to Gibbs Free Energy= 0.690797
Sum of electronic and zero-point Energies= -1758.207010
Sum of electronic and thermal Energies= -1758.141598
Sum of electronic and thermal Enthalpies= -1758.140479
Sum of electronic and thermal Free Energies= -1758.312718

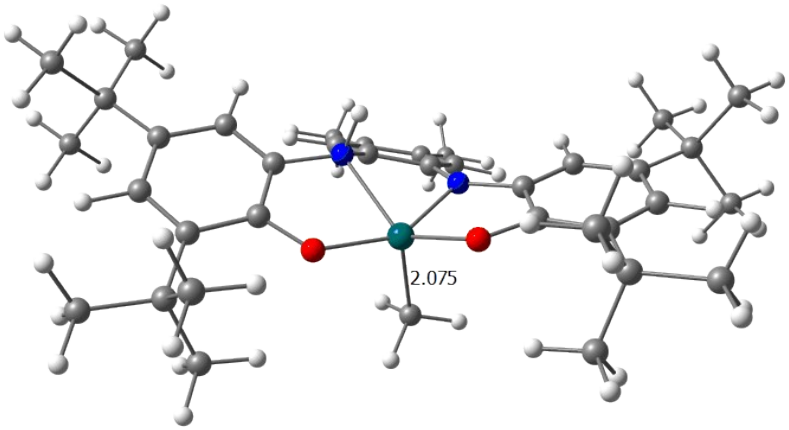
Solvent: -1976.7393619

95
PhTitBuCH3+triplet SCF Done: -1759.00351461 A.U.

Ti	-0.057969	-0.664240	-2.162226
N	-0.384592	0.412023	-0.078467
O	-1.893919	-0.967511	-1.717628
C	-2.501371	-0.644135	-0.583114
C	-1.723460	0.077831	0.375075
C	-2.223505	0.395009	1.634250
H	-1.577684	0.923604	2.349116
C	-3.554934	0.036740	1.973629
C	-4.329218	-0.637636	0.991540
H	-5.361269	-0.904131	1.253017
C	-3.862810	-1.000796	-0.280325
C	-0.102984	1.794814	-0.446836
C	-4.171936	0.360374	3.342026
N	1.647074	0.759211	-1.763334
O	1.326402	-1.846420	-1.375497
C	2.333119	-1.321740	-0.704013
C	2.538315	0.096648	-0.813067
C	3.475286	0.773705	-0.041478
H	3.559323	1.864551	-0.142877
C	4.307660	0.042856	0.845340
C	4.135574	-1.369918	0.907862
H	4.788760	-1.927220	1.591746
C	3.188271	-2.091785	0.171590
C	0.989607	1.969988	-1.324265
C	5.385030	0.716283	1.705825
C	-4.728047	-1.753727	-1.302101
C	3.007505	-3.610945	0.305599
H	0.316632	0.082517	0.605947
H	2.123034	0.906079	-2.667196
H	-0.297156	-1.244781	-4.654212
C	5.400698	2.248816	1.529212
H	5.632146	2.545177	0.485092
H	4.433964	2.710077	1.820805
H	6.184590	2.692230	2.175533
C	5.110308	0.393793	3.200868
H	5.143723	-0.694679	3.408877
H	5.880249	0.877415	3.837002
H	4.116137	0.773375	3.515203
C	6.775351	0.153691	1.300131
H	7.567246	0.627455	1.916511
H	6.844744	-0.942545	1.451532
H	6.994789	0.365785	0.233550
C	4.050968	-4.231431	1.258202
H	5.089363	-4.065682	0.902911
H	3.965159	-3.837382	2.292435
H	3.893036	-5.327270	1.312765
C	3.163110	-4.275428	-1.089549
H	2.405216	-3.906541	-1.806095
H	4.171743	-4.079524	-1.508528
H	3.042085	-5.374290	-0.994331
C	1.591359	-3.899687	0.879604
H	1.467942	-3.432304	1.879273
H	0.796101	-3.522151	0.208657
H	1.451495	-4.994080	0.998281
C	-4.079140	-3.134555	-1.597960
H	-3.064553	-3.026287	-2.026636
H	-4.007866	-3.744154	-0.673318
H	-4.703285	-3.691581	-2.327026
C	-4.823101	-0.918548	-2.608669
H	-5.285795	0.070724	-2.411661
H	-3.828388	-0.757143	-3.065946
H	-5.458516	-1.451003	-3.346276
C	-6.158910	-1.993121	-0.775696
H	-6.170908	-2.618716	0.141061
H	-6.688888	-1.041887	-0.559916
H	-6.748639	-2.530170	-1.545472
C	-4.621601	-0.962757	4.019873
H	-5.069225	-0.745289	5.011826
H	-5.383737	-1.501690	3.421586
H	-3.760167	-1.645273	4.171092
C	-5.404855	1.281635	3.131095
H	-6.185138	0.800135	2.507815
H	-5.864592	1.527746	4.110782
H	-5.112772	2.232251	2.638812
C	-3.176813	1.077763	4.277687
H	-2.282039	0.455448	4.487987
H	-2.840526	2.050633	3.861727
H	-3.664296	1.289961	5.250417
C	0.089435	-0.291167	-4.209365
H	1.070486	-0.081407	-4.690274
H	-0.619324	0.520668	-4.496814
C	-0.856938	2.907266	-0.057814
C	1.334851	3.251734	-1.772695
C	0.583441	4.381695	-1.384736
C	-0.531264	4.203970	-0.517038
H	-1.731482	2.769485	0.594850
H	2.190870	3.371202	-2.456519
C	-1.365041	5.387984	-0.093116
H	-1.817296	5.898454	-0.970551

	H	-2.186289	5.092372	0.587765
	H	-0.748420	6.152055	0.427040
	C	0.952337	5.755282	-1.888258
	H	0.113718	6.216416	-2.452617
	H	1.180729	6.446022	-1.048440
	H	1.835280	5.728421	-2.555604

1 (without H^+)



Zero-point correction= 0.786246 (Hartree/Particle)
Thermal correction to Energy= 0.850322
Thermal correction to Enthalpy= 0.851440
Thermal correction to Gibbs Free Energy= 0.684304
Sum of electronic and zero-point Energies= -1757.893181
Sum of electronic and thermal Energies= -1757.829105
Sum of electronic and thermal Enthalpies= -1757.827987
Sum of electronic and thermal Free Energies= -1757.995123

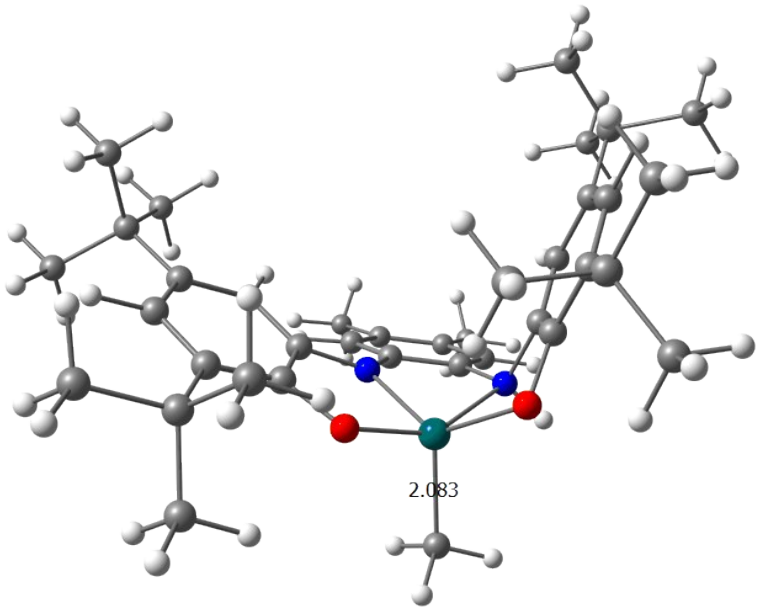
Solvent: -1758.3548091

94
PhTitBuCH3 SCF Done: -1758.67942741 A.U.

Ti	0.110742	-0.910024	-0.515292
N	-1.194450	0.613504	0.535788
O	-1.579899	-1.742300	-0.443123
C	-2.723563	-1.117761	-0.079358
C	-2.581824	0.180666	0.467190
C	-3.676797	0.893990	0.974594
H	-3.501741	1.866174	1.453166
C	-4.970142	0.347029	0.872961
C	-5.096247	-0.930392	0.274606
H	-6.105656	-1.354402	0.186256
C	-4.017349	-1.699940	-0.201609
C	-0.714120	1.885412	-0.002645
C	-6.228708	1.084042	1.376700
N	1.281140	0.630290	-0.021118
O	1.597333	-1.863519	0.016472
C	2.771908	-1.162668	0.153012
C	2.619720	0.259113	0.136913
C	3.746248	1.085666	0.331053
H	3.610623	2.172027	0.366331
C	5.020227	0.510000	0.502314
C	5.133713	-0.899844	0.479135
H	6.131828	-1.339893	0.603214
C	4.035947	-1.773539	0.312405
C	0.697642	1.879003	-0.221740
C	6.289254	1.368531	0.701105
C	-4.195957	-3.096338	-0.827319
C	4.186749	-3.308183	0.297764
H	-0.843353	0.530271	1.508585
H	0.014286	-1.549282	-3.116965
C	5.975859	2.879644	0.712356
H	5.521395	3.213346	-0.243888
H	5.285494	3.152221	1.537643
H	6.911329	3.459640	0.855248
C	6.954687	1.001820	2.052414
H	7.251707	-0.066143	2.089320
H	7.869528	1.611038	2.216548
H	6.259153	1.186549	2.897431
C	7.280647	1.088762	-0.457681
H	8.204983	1.694010	-0.337810
H	7.579676	0.021384	-0.495143
H	6.823562	1.344236	-1.436379
C	5.657268	-3.746476	0.464972
H	6.300927	-3.361134	-0.353181
H	6.084829	-3.409043	1.432210
H	5.719555	-4.854432	0.443305
C	3.670821	-3.861039	-1.056902
H	2.606124	-3.603765	-1.217726
H	4.259696	-3.443214	-1.900156
H	3.768819	-4.967437	-1.083430
C	3.365957	-3.917984	1.464173
H	3.732165	-3.537549	2.440820
H	2.291418	-3.667102	1.374560
H	3.465754	-5.024831	1.467075
C	-3.428793	-4.141652	0.024842
H	-2.347410	-3.909592	0.069545
H	-3.824333	-4.167618	1.061892
H	-3.549195	-5.155054	-0.413917
C	-3.638373	-3.079196	-2.275306
H	-4.189558	-2.344421	-2.898833
H	-2.564274	-2.810932	-2.290769
H	-3.752977	-4.080606	-2.742108
C	-5.679511	-3.518303	-0.886699
H	-6.136166	-3.581808	0.123310
H	-6.287022	-2.821132	-1.501132
H	-5.759919	-4.523600	-1.349325
C	-6.938825	0.218676	2.449438
H	-7.845885	0.735482	2.829194
H	-7.258655	-0.762787	2.043333
H	-6.265016	0.024341	3.309652
C	-7.190899	1.324180	0.184786
H	-7.509505	0.372337	-0.287169
H	-8.106817	1.853239	0.524491
H	-6.704364	1.942183	-0.598316
C	-5.886183	2.451442	2.004850
H	-5.219504	2.346875	2.886267
H	-5.395095	3.129732	1.275899
H	-6.814171	2.952815	2.349561
C	0.379722	-0.659475	-2.557475
H	1.440766	-0.455043	-2.815060
H	-0.240108	0.224412	-2.839742
C	-1.492173	2.998608	-0.320636
C	1.288441	3.058489	-0.726588
C	0.512502	4.197250	-1.029448
C	-0.895515	4.170919	-0.839114
H	-2.582094	2.963356	-0.182142
H	2.364522	3.070478	-0.947041
C	-1.746307	5.370741	-1.186068
H	-1.665282	5.636308	-2.263228
H	-2.817311	5.189331	-0.966637

	H	-1.435233	6.275455	-0.618835
	C	1.178719	5.435556	-1.584755
	H	0.777670	5.699467	-2.587564
	H	0.999381	6.319712	-0.934921
	H	2.274358	5.304442	-1.681937

1 (without H^+) (isomer)



Zero-point correction= 0.786539 (Hartree/Particle)
Thermal correction to Energy= 0.850690
Thermal correction to Enthalpy= 0.851809
Thermal correction to Gibbs Free Energy= 0.684287
Sum of electronic and zero-point Energies= -1757.900818
Sum of electronic and thermal Energies= -1757.836666
Sum of electronic and thermal Enthalpies= -1757.835548
Sum of electronic and thermal Free Energies= -1758.003070

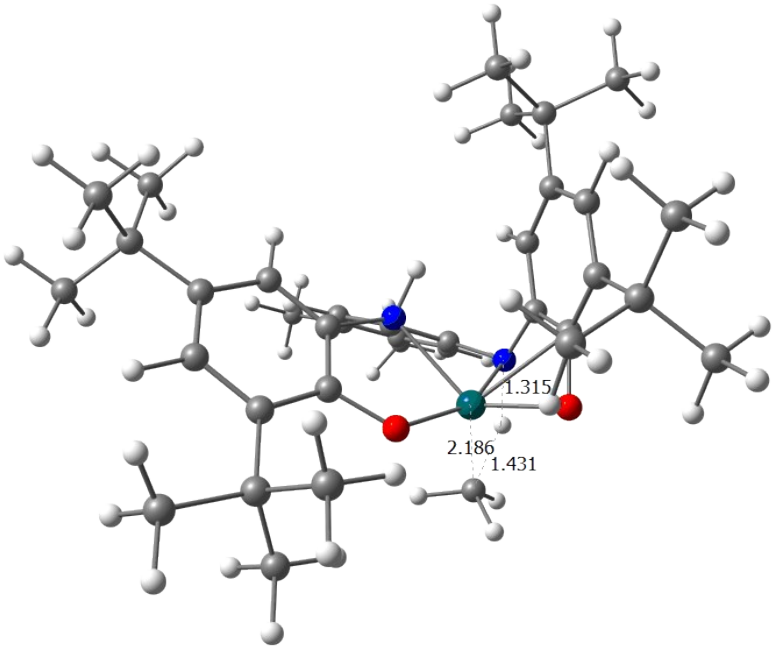
Solvent: -1758.3630473

94
PhTitBuCH3isomer SCF Done: -1758.68735655 A.U.

Ti	-0.008855	-0.684349	-2.133613
N	-0.666306	0.861980	-1.020203
O	-1.595217	-1.378471	-1.516009
C	-2.363401	-0.698735	-0.609646
C	-1.836668	0.584543	-0.286235
C	-2.457920	1.349210	0.720062
H	-2.008714	2.297623	1.031618
C	-3.629676	0.872688	1.347452
C	-4.147802	-0.381236	0.955913
H	-5.063911	-0.740222	1.443008
C	-3.535685	-1.208377	-0.014594
C	0.028359	2.070225	-1.061073
C	-4.352659	1.681685	2.448031
N	1.788552	0.621140	-1.845898
O	1.323202	-1.956536	-1.762059
C	2.150839	-1.520377	-0.769393
C	2.435632	-0.133289	-0.757756
C	3.214204	0.459558	0.240816
H	3.363919	1.546983	0.213628
C	3.761922	-0.345476	1.257420
C	3.478386	-1.733225	1.225243
H	3.894918	-2.357864	2.027250
C	2.675528	-2.360208	0.252556
C	1.362514	1.974753	-1.539179
C	4.631140	0.232332	2.393655
C	-4.087901	-2.594027	-0.404398
C	2.313013	-3.856581	0.301122
H	2.381879	0.598000	-2.690997
H	-0.874060	-1.128258	-4.631040
C	4.815156	1.758594	2.260258
H	5.321884	2.032438	1.311315
H	3.845110	2.296311	2.301908
H	5.442251	2.138206	3.093307
C	3.951072	-0.058317	3.756464
H	3.832470	-1.146456	3.935628
H	4.558462	0.354346	4.590153
H	2.942602	0.402807	3.800414
C	6.030189	-0.434795	2.359539
H	6.672374	-0.034508	3.172905
H	5.966732	-1.534125	2.493115
H	6.537817	-0.241918	1.391473
C	2.993132	-4.577551	1.483768
H	4.100553	-4.523985	1.423328
H	2.676248	-4.162202	2.463165
H	2.711592	-5.650712	1.473492
C	2.766267	-4.544779	-1.012479
H	2.281904	-4.086094	-1.895750
H	3.866970	-4.467580	-1.136335
H	2.498449	-5.622660	-0.990166
C	0.775438	-3.990900	0.469776
H	0.437881	-3.506840	1.409791
H	0.231102	-3.519836	-0.370444
H	0.484044	-5.061855	0.510157
C	-3.036669	-3.680437	-0.057974
H	-2.093088	-3.517582	-0.612408
H	-2.803049	-3.670433	1.027153
H	-3.423072	-4.689059	-0.318967
C	-4.386745	-2.617579	-1.926074
H	-5.147037	-1.852215	-2.187964
H	-3.473392	-2.415014	-2.518731
H	-4.781691	-3.611996	-2.225996
C	-5.393624	-2.927381	0.347475
H	-5.242836	-2.964204	1.446586
H	-6.195614	-2.191059	0.131106
H	-5.761850	-3.924810	0.029067
C	-4.363749	0.861045	3.763176
H	-4.878445	1.422480	4.572468
H	-4.889025	-0.107698	3.638296
H	-3.328571	0.641200	4.097863
C	-5.809644	1.967777	2.002431
H	-6.381647	1.032429	1.834971
H	-6.347636	2.556667	2.776333
H	-5.825717	2.544834	1.054337
C	-3.663461	3.033712	2.729813
H	-2.621306	2.900803	3.087758
H	-3.639521	3.680935	1.828032
H	-4.217477	3.583366	3.519161
C	-0.296957	-0.300233	-4.160119
H	0.675316	-0.199330	-4.695454
H	-0.875627	0.643273	-4.279633
C	-0.455786	3.370310	-0.774652
C	2.169971	3.100971	-1.713739
C	1.685617	4.392551	-1.415096
C	0.349531	4.515371	-0.941915
H	-1.501232	3.500913	-0.465905
H	3.198918	2.972497	-2.089786
C	-0.217193	5.882742	-0.633236
H	-0.184456	6.548392	-1.523066
H	-1.269347	5.824596	-0.291595

	H 0.369178 6.394865 0.160653 C 2.559675 5.610431 -1.601844 H 2.117725 6.329216 -2.326680 H 2.693735 6.171625 -0.650945 H 3.567246 5.337624 -1.974246

1--CH_4



Zero-point correction= 0.794915 (Hartree/Particle)
Thermal correction to Energy= 0.858564
Thermal correction to Enthalpy= 0.859683
Thermal correction to Gibbs Free Energy= 0.693777
Sum of electronic and zero-point Energies= -1758.240085
Sum of electronic and thermal Energies= -1758.176436
Sum of electronic and thermal Enthalpies= -1758.175318
Sum of electronic and thermal Free Energies= -1758.341224

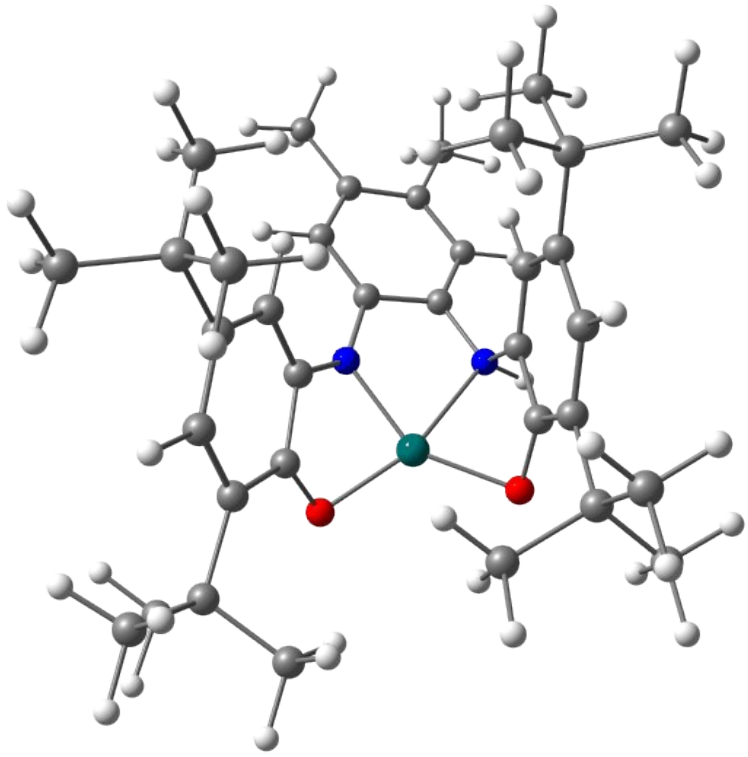
Solvent: -1758.7347477

95
PhTitBu--CH4 SCF Done: -1759.03500044 A.U.

Ti	0.602630	-0.602628	-1.847175
N	-0.152718	0.671571	-0.158710
O	-1.021749	-1.358719	-1.499363
C	-1.926798	-0.901222	-0.580638
C	-1.494695	0.198162	0.190142
C	-2.260556	0.698712	1.250293
H	-1.858473	1.513011	1.867751
C	-3.525150	0.134125	1.512976
C	-3.949272	-0.943314	0.696559
H	-4.932869	-1.384525	0.904191
C	-3.188241	-1.506858	-0.347094
C	0.044812	2.035522	-0.675690
C	-4.437109	0.643117	2.647231
N	1.958511	1.036925	-1.830211
O	2.066951	-1.691154	-2.052650
C	2.581003	-1.146857	-0.898791
C	2.558030	0.292839	-0.789858
C	2.930954	0.906222	0.435806
H	2.888354	2.002570	0.483111
C	3.356952	0.136092	1.520225
C	3.369612	-1.284532	1.377830
H	3.692156	-1.881135	2.240141
C	2.977368	-1.959237	0.219754
C	1.202364	2.210398	-1.475492
C	3.785908	0.764250	2.857774
C	-3.658755	-2.717840	-1.174210
C	2.927444	-3.496296	0.129713
H	0.483887	0.544669	0.653989
H	1.474728	0.615071	-2.977659
H	0.402907	-0.848835	-4.319916
C	3.713461	2.304488	2.825216
H	4.386311	2.735433	2.055266
H	2.681979	2.668610	2.633965
H	4.028640	2.715343	3.805348
C	2.837741	0.248542	3.972913
H	2.875634	-0.854354	4.081777
H	3.123992	0.689099	4.950239
H	1.785328	0.535505	3.764223
C	5.245357	0.341406	3.170471
H	5.572737	0.790949	4.130552
H	5.352616	-0.758197	3.264937
H	5.938745	0.685098	2.375638
C	3.457947	-4.156278	1.420663
H	4.513366	-3.881472	1.625302
H	2.845978	-3.897218	2.309596
H	3.421725	-5.258492	1.309491
C	3.795237	-3.987702	-1.058407
H	3.437547	-3.591127	-2.027366
H	4.853847	-3.683807	-0.924345
H	3.764001	-5.095587	-1.109845
C	1.447493	-3.936533	-0.060812
H	0.805652	-3.535226	0.751556
H	1.032357	-3.604721	-1.031447
H	1.377313	-5.043334	-0.032312
C	-2.675319	-3.897183	-0.944244
H	-1.644779	-3.641927	-1.259130
H	-2.650090	-4.185422	0.127091
H	-3.002698	-4.782265	-1.528294
C	-3.690372	-2.333005	-2.676921
H	-4.385547	-1.486001	-2.852997
H	-2.687436	-2.045145	-3.048434
H	-4.042068	-3.194314	-3.281872
C	-5.073141	-3.178368	-0.763514
H	-5.115164	-3.505704	0.295977
H	-5.831849	-2.382965	-0.916526
H	-5.373837	-4.045182	-1.386065
C	-4.679596	-0.507335	3.658593
H	-5.332504	-0.159962	4.486147
H	-5.176244	-1.378831	3.185704
H	-3.723153	-0.858523	4.098584
C	-5.789626	1.103162	2.043968
H	-6.321049	0.275590	1.531849
H	-6.458334	1.480617	2.845415
H	-5.641228	1.919412	1.306760
C	-3.810328	1.834107	3.401676
H	-2.851319	1.560972	3.889872
H	-3.630378	2.701093	2.731404
H	-4.497481	2.176425	4.201658
C	0.458679	0.175386	-3.884947
H	1.042775	0.794270	-4.599798
H	-0.560562	0.616303	-3.818771
C	-0.813685	3.116794	-0.447020
C	1.492185	3.472489	-2.010309
C	0.647504	4.576578	-1.769384
C	-0.529642	4.390319	-0.987555
H	-1.730161	2.973234	0.142386
H	2.390786	3.581635	-2.636836
C	-1.470068	5.543466	-0.737919
H	-1.852454	5.965545	-1.691866

	H	-2.341731	5.241941	-0.125836
	H	-0.955582	6.376740	-0.212981
	C	0.975623	5.930291	-2.348040
	H	0.168778	6.287484	-3.023429
	H	1.074458	6.696069	-1.549207
	H	1.920456	5.915467	-2.924339

1 (without CH_4)



Zero-point correction= 0.754171 (Hartree/Particle)
Thermal correction to Energy= 0.814160
Thermal correction to Enthalpy= 0.815279
Thermal correction to Gibbs Free Energy= 0.658739
Sum of electronic and zero-point Energies= -1717.819085
Sum of electronic and thermal Energies= -1717.759096
Sum of electronic and thermal Enthalpies= -1717.757977
Sum of electronic and thermal Free Energies= -1717.914517

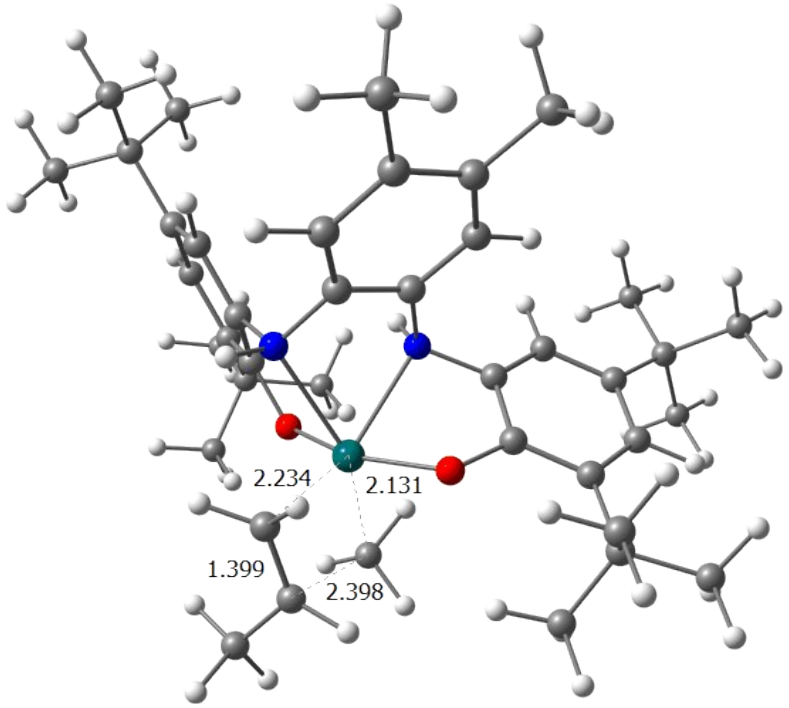
Solvent: -1718.2917541

90
PhTitBu SCF Done: -1718.57325587 A.U.

Ti	0.375295	-0.043625	2.094166
N	-1.841717	-0.565519	2.263685
O	0.430783	-1.869409	2.573243
C	-0.186711	-2.140774	1.386977
C	-1.418628	-1.446015	1.168128
C	-2.104517	-1.526916	-0.056626
H	-3.033868	-0.956320	-0.174800
C	-1.577134	-2.310192	-1.092485
C	-0.357588	-3.002287	-0.855400
H	0.049272	-3.609564	-1.674252
C	0.375900	-2.941766	0.337206
C	-2.692631	0.517280	1.823485
C	-2.252980	-2.412732	-2.471328
N	-0.609275	1.399717	1.273259
O	1.724664	1.180143	2.401999
C	1.754974	1.445621	1.061310
C	0.455271	1.617315	0.416374
C	0.371482	1.792332	-0.991867
H	-0.627617	1.864639	-1.439684
C	1.536819	1.849623	-1.752733
C	2.799337	1.751802	-1.082345
H	3.703789	1.844386	-1.696711
C	2.963296	1.565030	0.291196
C	-1.982384	1.534672	1.136758
C	1.515678	1.995688	-3.284901
C	1.728615	-3.647503	0.522039
C	4.338058	1.606773	0.985104
H	-2.202937	-1.094092	3.073811
C	0.086798	2.199498	-3.829006
H	-0.571931	1.333940	-3.607904
H	-0.385842	3.114676	-3.415739
H	0.116901	2.310874	-4.931600
C	2.375591	3.217244	-3.702412
H	3.438645	3.108015	-3.407266
H	2.352167	3.337002	-4.805044
H	1.988398	4.151632	-3.246438
C	2.105595	0.699804	-3.902678
H	2.107619	0.770841	-5.010198
H	3.150812	0.522726	-3.576086
H	1.502605	-0.186500	-3.614994
C	5.477934	1.839388	-0.028935
H	5.545772	1.022253	-0.777178
H	5.369036	2.803527	-0.567206
H	6.446269	1.871888	0.509604
C	4.620208	0.277296	1.729938
H	3.839787	0.045623	2.479529
H	4.691862	-0.566851	1.016031
H	5.589078	0.350055	2.265490
C	4.334742	2.787851	1.995100
H	4.122311	3.748120	1.481119
H	3.583293	2.645074	2.795624
H	5.331728	2.871412	2.475004
C	1.665673	-4.588103	1.753609
H	1.424792	-4.035542	2.682069
H	0.901534	-5.379055	1.606529
H	2.646872	-5.086089	1.896303
C	2.817287	-2.560546	0.731041
H	2.806489	-1.819403	-0.096555
H	2.681741	-2.022417	1.688728
H	3.823771	-3.026445	0.760888
C	2.112741	-4.483990	-0.716594
H	1.366090	-5.275970	-0.932034
H	2.237154	-3.857861	-1.624611
H	3.082197	-4.988761	-0.531672
C	-2.609999	-3.895364	-2.753477
H	-3.100082	-3.986782	-3.744796
H	-1.712468	-4.546890	-2.765356
H	-3.308111	-4.289853	-1.986796
C	-1.262519	-1.895829	-3.547875
H	-0.334739	-2.501712	-3.592187
H	-1.732586	-1.935135	-4.552121
H	-0.971758	-0.844194	-3.344825
C	-3.542020	-1.568648	-2.546701
H	-4.303469	-1.906052	-1.813167
H	-3.343130	-0.489935	-2.374008
H	-3.993990	-1.663166	-3.554528
C	-4.083904	0.559728	1.930945
C	-2.696848	2.574241	0.511873
C	-4.102645	2.626101	0.606593
C	-4.806623	1.619813	1.337981
H	-4.621469	-0.243977	2.459350
H	-2.147240	3.371824	-0.010532
C	-6.308439	1.680896	1.465994
H	-6.804153	1.677208	0.471477
H	-6.709065	0.829367	2.049025
H	-6.630722	2.617581	1.969762
C	-4.862973	3.756427	-0.043425
H	-5.611824	3.374828	-0.769982
H	-5.430490	4.344655	0.709192

	H -4.190346 4.452374 -0.580619

2-3



Zero-point correction= 0.880691 (Hartree/Particle)
Thermal correction to Energy= 0.949735
Thermal correction to Enthalpy= 0.950853
Thermal correction to Gibbs Free Energy= 0.773694
Sum of electronic and zero-point Energies= -1876.021806
Sum of electronic and thermal Energies= -1875.952761
Sum of electronic and thermal Enthalpies= -1875.951643
Sum of electronic and thermal Free Energies= -1876.128802

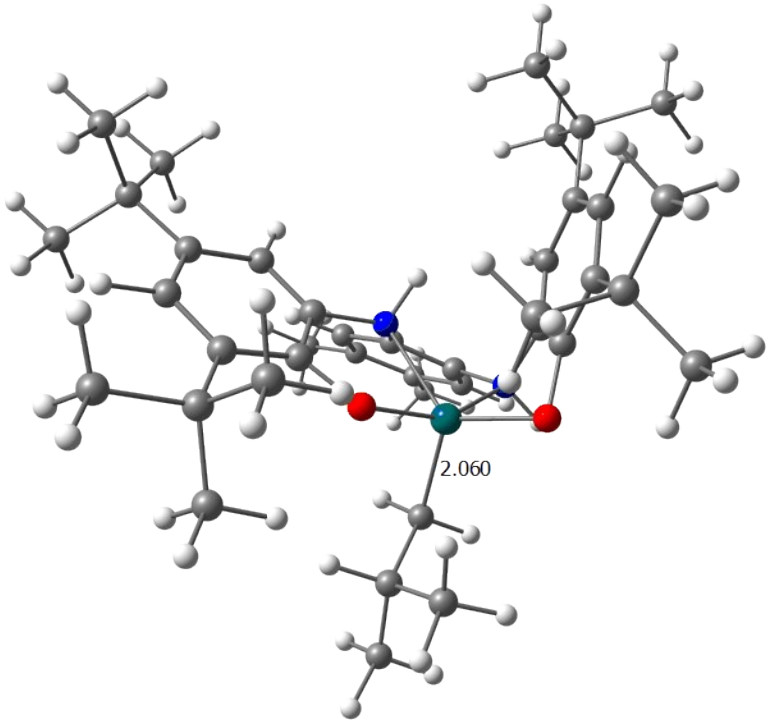
Solvent: -1876.5831899

104
PhTitBuCH3+propTSisomer+ SCF Done: -1876.90249642 A.U.

Ti	-0.133716	-1.237464	-1.324708
N	-0.339251	0.332847	0.324088
O	-1.862094	-0.529451	-1.520081
C	-2.551642	-0.196877	-0.392400
C	-1.737640	0.186343	0.699790
C	-2.260782	0.444630	1.970031
H	-1.581156	0.736511	2.783069
C	-3.653668	0.337011	2.168422
C	-4.454829	-0.000597	1.049614
H	-5.539712	-0.065760	1.204751
C	-3.959673	-0.275143	-0.242902
C	-0.061017	1.614664	-0.337052
C	-4.317380	0.582630	3.538330
N	1.526407	0.353642	-1.690903
O	1.306622	-1.889502	-0.333373
C	2.400949	-1.162039	-0.003951
C	2.598261	0.030090	-0.729664
C	3.697754	0.866727	-0.506823
H	3.788259	1.795129	-1.087816
C	4.646932	0.511126	0.470999
C	4.417867	-0.678706	1.208018
H	5.146771	-0.943881	1.985094
C	3.316474	-1.535675	1.019220
C	0.860222	1.609677	-1.398445
C	5.890303	1.372496	0.771817
C	-4.868709	-0.641915	-1.430148
C	3.067814	-2.793843	1.873145
H	0.302222	0.175042	1.118998
H	1.921095	0.396909	-2.641648
H	-1.184367	-2.607821	-0.111621
C	5.969168	2.611881	-0.143310
H	6.034227	2.330998	-1.215373
H	5.096731	3.285034	-0.007872
H	6.877531	3.200445	0.097559
C	5.830332	1.852548	2.245203
H	5.820046	1.003914	2.959374
H	6.716415	2.477302	2.483430
H	4.920512	2.461750	2.427370
C	7.165853	0.518738	0.551559
H	8.073914	1.123801	0.755093
H	7.198420	-0.364133	1.222205
H	7.223827	0.152278	-0.494353
C	4.169017	-2.997503	2.934191
H	5.168543	-3.138548	2.473491
H	4.226614	-2.146151	3.643758
H	3.948235	-3.907675	3.527960
C	3.033271	-4.046202	0.958227
H	2.229729	-3.971769	0.199799
H	4.000784	-4.174175	0.430105
H	2.853276	-4.957386	1.566282
C	1.708805	-2.635833	2.608452
H	1.721835	-1.743897	3.270045
H	0.868601	-2.535962	1.892563
H	1.509805	-3.524277	3.243328
C	-4.498067	-2.055155	-1.952576
H	-3.456581	-2.078466	-2.327488
H	-4.601215	-2.815450	-1.150405
H	-5.171441	-2.343241	-2.786501
C	-4.662413	0.404549	-2.557073
H	-4.937241	1.420271	-2.204805
H	-3.609421	0.429103	-2.900957
H	-5.305045	0.159619	-3.428559
C	-6.359902	-0.647993	-1.034642
H	-6.581210	-1.402570	-0.251496
H	-6.697161	0.344413	-0.670351
H	-6.977509	-0.900815	-1.920196
C	-5.055961	-0.707603	3.979765
H	-5.539611	-0.555445	4.967174
H	-5.849098	-0.998951	3.261345
H	-4.349557	-1.558829	4.069796
C	-5.330882	1.749404	3.413617
H	-6.135246	1.528180	2.682596
H	-5.816016	1.943680	4.392761
H	-4.824895	2.682516	3.089327
C	-3.283552	0.948462	4.623876
H	-2.539220	0.139395	4.778687
H	-2.739224	1.885411	4.381500
H	-3.797096	1.110354	5.593174
C	-0.399649	-2.826127	-3.369425
C	0.324090	-1.634070	-3.474865
H	-1.486256	-2.774867	-3.557456

	H	1.421454	-1.692526	-3.585479
	H	-0.179772	-0.726486	-3.858723
	C	0.245714	-4.177663	-3.487683
	H	0.353183	-4.400588	-4.572843
	H	1.258469	-4.191028	-3.037921
	H	-0.364385	-4.988627	-3.047286
	C	-0.973514	-3.179255	-1.067661
	H	-0.247586	-3.977847	-0.833410
	H	-1.944422	-3.570175	-1.418391
	C	-0.740065	2.798286	-0.018660
	C	1.097370	2.785391	-2.126071
	C	0.419785	3.981890	-1.816661
	C	-0.509853	3.989097	-0.736180
	H	-1.482413	2.786152	0.793772
	H	1.821796	2.767820	-2.957075
	C	-1.250970	5.252507	-0.372979
	H	-1.863701	5.620243	-1.223976
	H	-1.926595	5.100012	0.490499
	H	-0.548520	6.073989	-0.115942
	C	0.676087	5.236440	-2.613880
	H	-0.260738	5.622944	-3.068993
	H	1.067700	6.050963	-1.967387
	H	1.406462	5.069234	-3.429011

3



Zero-point correction= 0.882636 (Hartree/Particle)
Thermal correction to Energy= 0.952295
Thermal correction to Enthalpy= 0.953413
Thermal correction to Gibbs Free Energy= 0.774574
Sum of electronic and zero-point Energies= -1876.054860
Sum of electronic and thermal Energies= -1875.985201
Sum of electronic and thermal Enthalpies= -1875.984083
Sum of electronic and thermal Free Energies= -1876.162922

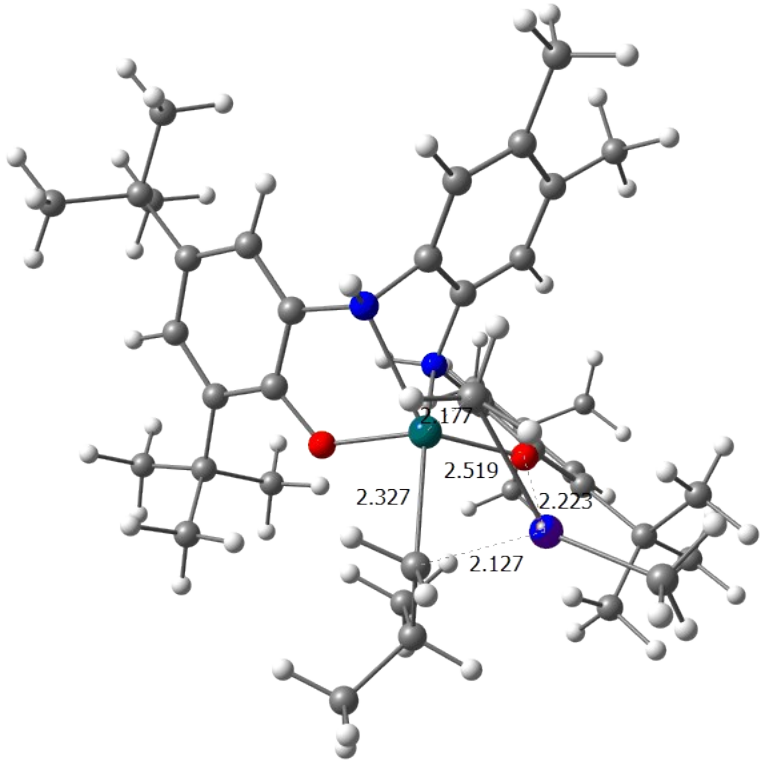
Solvent: -1876.6235381

104
PhTitBuCH3+propTSisomer+POST SCF Done: -1876.93749578 A.U.

Ti	0.384763	0.828374	1.537070
N	-0.161448	-0.811989	0.100766
O	-1.090792	1.514543	0.702670
C	-1.904478	0.823440	-0.147015
C	-1.456166	-0.468020	-0.496504
C	-2.135202	-1.256373	-1.434166
H	-1.712798	-2.223572	-1.736325
C	-3.338803	-0.779540	-1.990619
C	-3.782037	0.507555	-1.598963
H	-4.714639	0.881132	-2.041761
C	-3.098291	1.353720	-0.703298
C	0.050362	-2.045191	0.859405
C	-4.162845	-1.599376	-3.003694
N	1.885902	-0.758032	1.795142
O	1.906639	1.890000	1.504406
C	2.541522	1.199183	0.503392
C	2.589204	-0.221349	0.630102
C	3.103370	-1.044961	-0.383948
H	3.082773	-2.133537	-0.234485
C	3.621212	-0.458456	-1.551511
C	3.584146	0.958830	-1.652718
H	3.983187	1.410973	-2.569603
C	3.049765	1.819694	-0.680311
C	1.190852	-2.022656	1.693418
C	4.205677	-1.290374	-2.707657
C	-3.574382	2.780001	-0.367406
C	2.956810	3.344009	-0.877166
H	0.562126	-0.775194	-0.645098
H	2.429144	-0.671999	2.667518
H	-0.348426	3.227701	2.665046
C	4.146867	-2.804142	-2.416897
H	4.735974	-3.078471	-1.517138
H	3.104644	-3.161012	-2.276797
H	4.572949	-3.366962	-3.271657
C	3.389927	-1.002979	-3.995765
H	3.432306	0.065717	-4.289081
H	3.792318	-1.595858	-4.843118
H	2.322562	-1.277944	-3.861995
C	5.686888	-0.883947	-2.923767
H	6.127826	-1.477417	-3.751180
H	5.791479	0.187372	-3.190390
H	6.288016	-1.067802	-2.009571
C	3.601050	3.788427	-2.207733
H	4.677479	3.523432	-2.259227
H	3.087286	3.353621	-3.090397
H	3.529542	4.890965	-2.299282
C	3.687549	4.065746	0.285417
H	3.243970	3.818628	1.268846
H	4.762701	3.791968	0.305545
H	3.619257	5.164374	0.145291
C	1.457561	3.752797	-0.905338
H	0.907282	3.203849	-1.697844
H	0.956725	3.558577	0.061808
H	1.366163	4.837810	-1.117533
C	-2.501046	3.789496	-0.856177
H	-1.525439	3.619632	-0.360849
H	-2.353270	3.708335	-1.953080
H	-2.824421	4.827013	-0.630601
C	-3.771790	2.920796	1.163974
H	-4.507154	2.179817	1.540534
H	-2.820673	2.779411	1.711217
H	-4.153580	3.934371	1.405527
C	-4.911656	3.115067	-1.060426
H	-4.831517	3.076926	-2.166598
H	-5.727140	2.432176	-0.743354
H	-5.219593	4.145393	-0.790114
C	-4.250758	-0.817992	-4.340098
H	-4.844218	-1.390647	-5.082929
H	-4.740356	0.168753	-4.212315
H	-3.241025	-0.643428	-4.766262
C	-5.587656	-1.823257	-2.433785
H	-6.121131	-0.867154	-2.257202
H	-6.197603	-2.416928	-3.146072
H	-5.550222	-2.372734	-1.470222
C	-3.528515	-2.977947	-3.283927
H	-2.515260	-2.888428	-3.728974
H	-3.455380	-3.596227	-2.364167
H	-4.153735	-3.539744	-4.007038
C	-1.208866	1.626265	3.946228
C	-0.312907	0.476160	3.443250
H	-2.135923	1.616210	3.330732
H	0.566999	0.333207	4.116721
H	-0.858540	-0.497372	3.385874
C	-1.608325	1.420557	5.418960
H	-2.114265	0.444347	5.568221
H	-0.713523	1.443741	6.077807
H	-2.300198	2.219560	5.760318
C	-0.519118	2.990391	3.740351

	H	0.466494	3.021260	4.252254
	H	-1.136830	3.819438	4.142325
	C	-0.775113	-3.173581	0.852068
	C	1.515221	-3.137795	2.472734
	C	0.697593	-4.288775	2.462988
	C	-0.470745	-4.299578	1.649774
	H	-1.687030	-3.177893	0.239396
	H	2.406671	-3.104706	3.119756
	C	-1.380931	-5.502936	1.637959
	H	-1.771947	-5.723203	2.654377
	H	-2.247355	-5.359412	0.964123
	H	-0.839527	-6.415318	1.307770
	C	1.050240	-5.483011	3.313940
	H	0.238303	-5.717515	4.035124
	H	1.187221	-6.393386	2.691935
	H	1.981457	-5.321653	3.890266

4 (isomer)



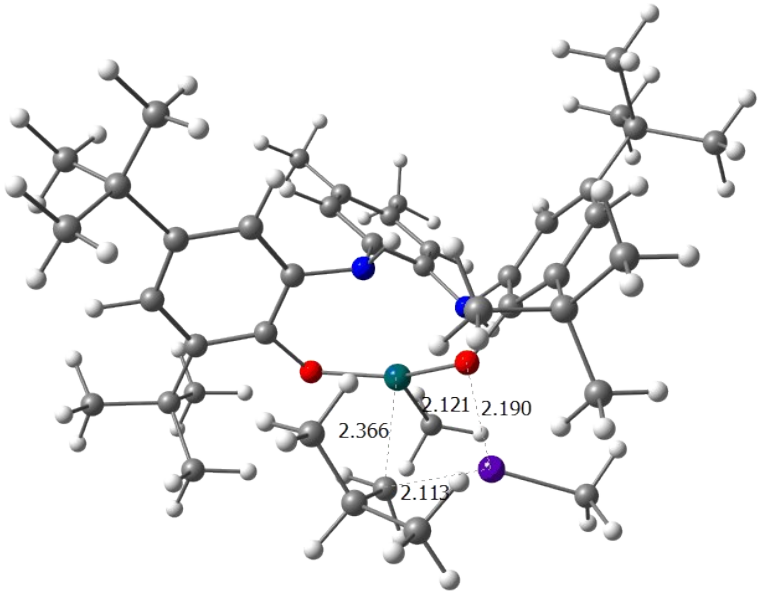
Zero-point correction= 0.954314 (Hartree/Particle)
Thermal correction to Energy= 1.032521
Thermal correction to Enthalpy= 1.033640
Thermal correction to Gibbs Free Energy= 0.837312
Sum of electronic and zero-point Energies= -3735.169392
Sum of electronic and thermal Energies= -3735.091185
Sum of electronic and thermal Enthalpies= -3735.090066
Sum of electronic and thermal Free Energies= -3735.286394

Solvent: -3735.5275297

113
PhTitBuCH3+propTS+POST--ZnMe2min0isomer SCF Done: -3736.12370594 A.U.

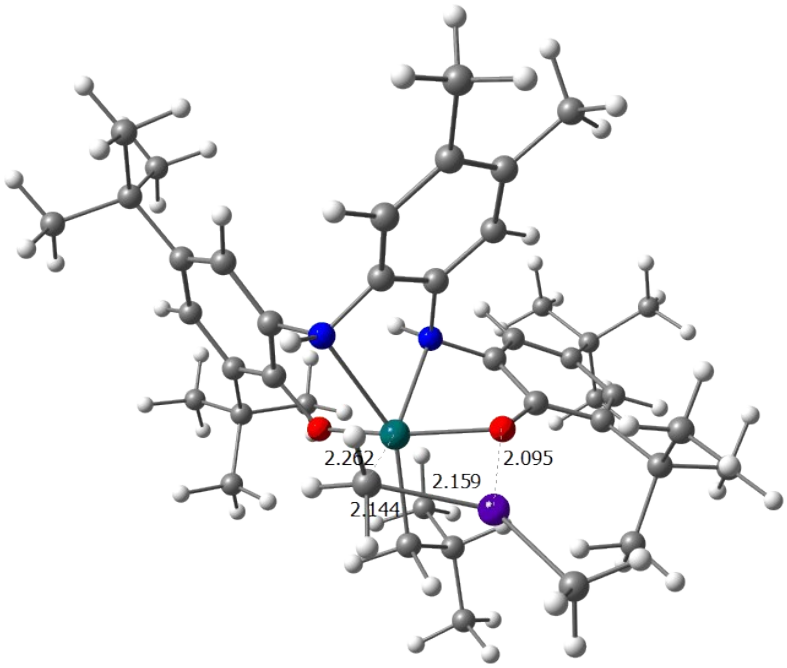
Ti	-0.152051	-1.205246	-1.019760
N	0.205101	0.803350	0.007905
O	-1.885134	-0.415380	-0.772289
C	-2.152167	0.491054	0.229285
C	-0.999894	1.129075	0.736667
C	-1.039784	2.019820	1.812816
H	-0.103563	2.480373	2.157961
C	-2.279965	2.308026	2.416302
C	-3.428196	1.696401	1.861791
H	-4.397466	1.937109	2.316318
C	-3.426704	0.790201	0.778497
C	0.461720	1.617787	-1.175103
C	-2.419887	3.251011	3.627486
N	1.786901	-0.285536	-1.876407
O	1.199079	-1.766174	0.152707
C	2.435502	-1.212921	0.245091
C	2.819568	-0.400615	-0.840311
C	4.055722	0.253513	-0.895647
H	4.285010	0.887036	-1.764196
C	4.963226	0.087733	0.168318
C	4.550050	-0.713358	1.263393
H	5.247520	-0.821986	2.104413
C	3.304671	-1.363664	1.361285
C	1.304161	1.048977	-2.151623
C	6.358954	0.742435	0.185806
C	-4.730225	0.168765	0.242342
C	2.848590	-2.124249	2.618943
H	1.038777	0.762501	0.620543
H	2.099336	-0.740158	-2.747622
H	-1.878067	-1.807963	1.405473
C	6.606999	1.604270	-1.069393
H	6.561187	1.003316	-2.001711
H	5.877853	2.437683	-1.151713
H	7.618352	2.056449	-1.021504
C	6.485286	1.650345	1.436313
H	6.372931	1.078890	2.380242
H	7.483174	2.135640	1.460229
H	5.714309	2.448765	1.427512
C	7.435191	-0.372888	0.239240
H	8.451828	0.072628	0.251054
H	7.335771	-1.001654	1.147740
H	7.361552	-1.039830	-0.644655
C	3.962208	-2.212390	3.683213
H	4.853168	-2.754876	3.304742
H	4.285436	-1.212103	4.038410
H	3.585674	-2.767838	4.566170
C	2.424158	-3.567614	2.244174
H	1.618570	-3.574385	1.485793
H	3.285568	-4.134940	1.835385
H	2.056435	-4.104227	3.143358
C	1.652608	-1.341819	3.228972
H	1.974353	-0.330817	3.555888
H	0.823807	-1.223914	2.502844
H	1.250126	-1.874792	4.115458
C	-4.707964	-1.355715	0.508949
H	-3.847941	-1.848420	0.016632
H	-4.632711	-1.569095	1.594449
H	-5.628038	-1.836017	0.118093
C	-4.849297	0.473447	-1.272701
H	-4.923966	1.567215	-1.442942
H	-3.979783	0.097180	-1.842762
H	-5.757250	-0.004779	-1.693339
C	-5.982803	0.745010	0.938315
H	-6.000844	0.523767	2.025278
H	-6.066700	1.842756	0.800575
H	-6.890351	0.286094	0.496331
C	-3.020218	2.455618	4.816046
H	-3.131663	3.114253	5.702540
H	-4.022994	2.045681	4.577629
H	-2.363844	1.606525	5.098682
C	-3.360613	4.426347	3.257044
H	-4.377093	4.077077	2.983597
H	-3.467849	5.117852	4.118354
H	-2.957131	5.004488	2.399908
C	-1.059251	3.831772	4.065257
H	-0.346518	3.036458	4.368425
H	-0.588880	4.438973	3.263492
H	-1.198482	4.497393	4.941035
C	-1.729951	-3.809290	0.481991
C	-1.064665	-3.338117	-0.836129
H	-2.827287	-3.864809	0.288646
H	0.044950	-3.446207	-0.768506
H	-1.281288	-4.074243	-1.650331
C	-1.251384	-5.223807	0.856916
H	-1.439554	-5.951236	0.040331
H	-0.159944	-5.221363	1.066792
H	-1.768685	-5.592849	1.767268
C	-1.514007	-2.828312	1.644636

	H -0.439740 -2.755281 1.900140 H -2.054843 -3.161498 2.553461 C -0.140766 2.860416 -1.415519 C 1.552871 1.735027 -3.348471 C 0.959761 2.988903 -3.599667 C 0.097108 3.559283 -2.615772 H -0.816092 3.282345 -0.656023 H 2.209676 1.277147 -4.105784 C -0.556914 4.896791 -2.859474 H -1.184708 4.877833 -3.776011 H -1.200689 5.201625 -2.012222 H 0.200622 5.694251 -3.016730 C 1.229457 3.715823 -4.893073 H 0.288513 3.903782 -5.453128 H 1.684809 4.711879 -4.706142 H 1.912024 3.148330 -5.554460 Zn -2.483728 -2.206670 -1.944335 C -0.350320 -1.618412 -3.148181 H -0.121132 -0.658677 -3.661960 H 0.446473 -2.366321 -3.361504 H -1.249656 -2.005136 -3.688820 C -4.124871 -2.507779 -2.973163 H -4.040040 -3.427803 -3.590020 H -5.001107 -2.623266 -2.302906 H -4.328325 -1.654939 -3.654457

4	
 Zero-point correction= 0.954826 (Hartree/Particle) Thermal correction to Energy= 1.032794 Thermal correction to Enthalpy= 1.033912 Thermal correction to Gibbs Free Energy= 0.838435 Sum of electronic and zero-point Energies= -3735.175222 Sum of electronic and thermal Energies= -3735.097254 Sum of electronic and thermal Enthalpies= -3735.096136 Sum of electronic and thermal Free Energies= -3735.291613 Solvent: -3735.5330715	113 PhTitBuCH3+propTS+POST--ZnMe2min0isomer180 SCF Done: -3736.13004807 A.U. Ti -0.121536 -0.888104 -1.329617 N -0.467992 0.849950 0.215772 O -1.922291 -0.448177 -1.407396 C -2.620124 -0.004609 -0.324452 C -1.828531 0.625316 0.661012 C -2.350714 1.015365 1.896752 H -1.690117 1.495019 2.632324 C -3.719592 0.793186 2.160088 C -4.506043 0.220175 1.129888 H -5.575985 0.073941 1.328297 C -4.010720 -0.191738 -0.125593 C -0.328865 2.017651 -0.654100 C -4.373098 1.156874 3.508531 N 1.455164 0.728665 -1.643069 O 1.344183 -1.401808 -0.135784 C 2.320656 -0.512088 0.244536 C 2.424791 0.647636 -0.546577 C 3.346825 1.667451 -0.285746 H 3.350631 2.556030 -0.932546 C 4.226579 1.532996 0.803287 C 4.109806 0.361389 1.590403 H 4.786520 0.259437 2.448462 C 3.184816 -0.678538 1.365252 C 0.656881 1.933472 -1.653210 C 5.274722 2.602327 1.168821 C -4.897982 -0.813405 -1.220598 C 3.116124 -1.914250 2.283340 H 0.216914 0.863884 0.989536 H 1.936838 0.611994 -2.546484 H -2.458414 -2.419895 0.547634 C 5.264116 3.781602 0.174376 H 5.498597 3.453023 -0.859702 H 4.286107 4.306990 0.163282 H 6.032577 4.526064 0.465237 C 4.962578 3.149377 2.585939 H 4.996001 2.351433 3.355648 H 5.706422 3.921387 2.873524 H 3.954692 3.613178 2.619890 C 6.685653 1.959605 1.156027 H 7.454999 2.717579 1.411668 H 6.775616 1.135408 1.892751 H 6.927332 1.548082 0.154244 C 4.092926 -1.814489 3.475208 H 5.151408 -1.759372 3.147779 H 3.877203 -0.936783 4.118999 H 3.993517 -2.720244 4.107219 C 3.495391 -3.169087 1.459852 H 2.837599 -3.289926 0.579834 H 4.536201 -3.099965 1.084060 H 3.406867 -4.086009 2.078450 C 1.681213 -2.047949 2.852112 H 1.414711 -1.156621 3.458178

H	0.933228	-2.155324	2.046204
H	1.605676	-2.939941	3.507926
C	-4.447904	-2.272358	-1.492253
H	-3.393681	-2.315083	-1.829370
H	-4.549899	-2.897858	-0.581417
H	-5.075785	-2.724150	-2.287893
C	-4.758691	0.029656	-2.515762
H	-5.086884	1.075379	-2.341541
H	-3.712488	0.049322	-2.879465
H	-5.394443	-0.398100	-3.318769
C	-6.385804	-0.836169	-0.811430
H	-6.563934	-1.461369	0.087976
H	-6.777004	0.183219	-0.613532
H	-6.989232	-1.267590	-1.635715
C	-4.941681	-0.134694	4.152671
H	-5.413926	0.097438	5.130093
H	-5.713079	-0.611440	3.514138
H	-4.137065	-0.878942	4.327179
C	-5.521727	2.170126	3.267714
H	-6.314340	1.755235	2.612567
H	-5.998679	2.446480	4.231017
H	-5.140796	3.098800	2.794124
C	-3.362891	1.788129	4.489089
H	-2.527425	1.096690	4.726295
H	-2.935284	2.733539	4.093939
H	-3.868798	2.031637	5.445165
C	-1.012656	-3.924117	-0.158356
C	-0.579457	-3.205511	-1.459775
H	-1.851121	-4.607625	-0.430162
H	-0.426054	-3.955239	-2.276277
H	-1.439181	-2.641587	-1.889241
C	0.126454	-4.788932	0.406071
H	0.952960	-4.156479	0.795822
H	-0.219058	-5.413890	1.255230
H	0.544388	-5.476326	-0.361088
C	-1.548781	-2.943734	0.896890
H	-0.790270	-2.173231	1.156711
H	-1.804857	-3.466459	1.840753
C	-1.181880	3.127986	-0.618176
C	0.795291	2.956069	-2.600671
C	-0.056849	4.079122	-2.574802
C	-1.058349	4.167770	-1.562993
H	-1.971571	3.171374	0.147128
H	1.571509	2.873171	-3.378862
C	-1.986159	5.356547	-1.512984
H	-2.567408	5.453653	-2.455017
H	-2.706577	5.283634	-0.675666
H	-1.421246	6.306063	-1.395738
C	0.088875	5.170607	-3.605909
H	-0.848674	5.303433	-4.187134
H	0.301166	6.151140	-3.128471
H	0.905690	4.957167	-4.321899
Zn	1.522651	-3.034447	-1.584565
C	0.336882	-1.090530	-3.390490
H	-0.334161	-1.843574	-3.854509
H	0.067006	-0.094338	-3.815107
H	1.382913	-1.324987	-3.692731
C	3.293407	-3.598575	-2.188022
H	3.314798	-3.778809	-3.283475
H	4.041411	-2.812709	-1.947139
H	3.611939	-4.533612	-1.681057

4-5



Zero-point correction= 0.954910 (Hartree/Particle)
Thermal correction to Energy= 1.031729
Thermal correction to Enthalpy= 1.032847
Thermal correction to Gibbs Free Energy= 0.840421
Sum of electronic and zero-point Energies= -3735.164724
Sum of electronic and thermal Energies= -3735.087905
Sum of electronic and thermal Enthalpies= -3735.086787
Sum of electronic and thermal Free Energies= -3735.279213

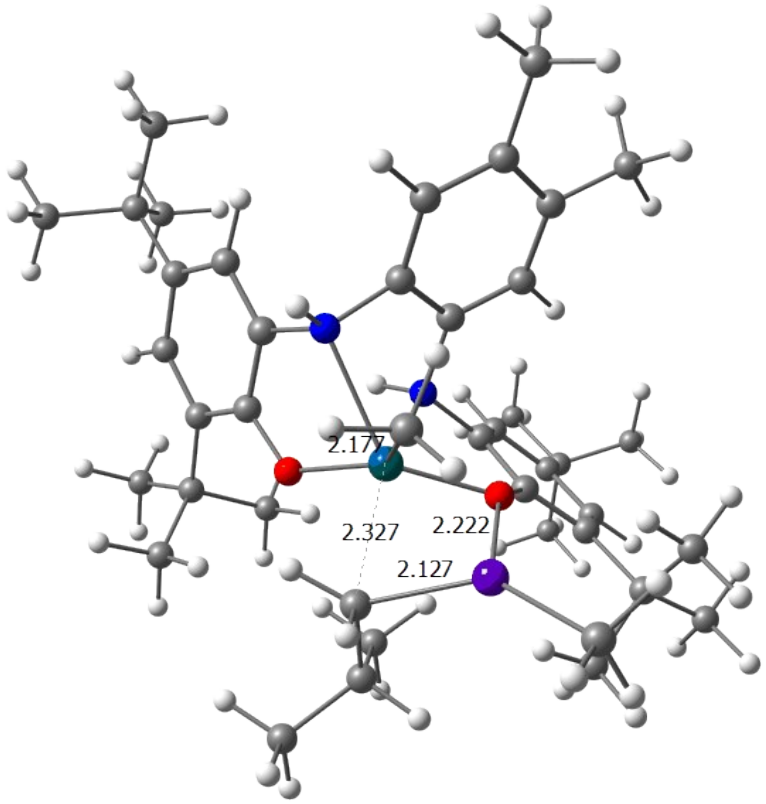
Solvent: - 3735.5260845

113
PhTitBuCH3+propTS+POST--ZnMe2min0TSisomerFllallfllc
SCF Done: -3736.11963406 A.U.

Ti	-0.008614	0.159506	-1.487406
N	0.111608	0.069730	0.747982
O	-1.780037	0.706110	-0.820542
C	-2.241440	0.073389	0.313694
C	-1.201130	-0.391844	1.153267
C	-1.433868	-1.193197	2.273454
H	-0.579120	-1.532320	2.875323
C	-2.759842	-1.539978	2.599885
C	-3.789960	-0.990392	1.800784
H	-4.824618	-1.225366	2.080916
C	-3.594539	-0.172951	0.665323
C	0.376343	1.473954	1.085750
C	-3.112647	-2.468675	3.777359
N	1.795538	1.502423	-0.899464
O	1.428375	-1.026659	-1.432085
C	2.640701	-0.764233	-0.875730
C	2.896970	0.588454	-0.569750
C	4.098109	1.019943	0.004267
H	4.224564	2.087194	0.234622
C	5.106919	0.076383	0.274581
C	4.831860	-1.279700	-0.033496
H	5.613123	-2.019055	0.187500
C	3.626500	-1.751615	-0.589195
C	1.214237	2.206929	0.222334
C	6.467045	0.462489	0.889602
C	-4.783110	0.423731	-0.115344
C	3.347656	-3.249180	-0.812368
H	0.870732	-0.548809	1.080322
H	2.106903	2.180346	-1.610092
H	-0.585898	-2.535905	-0.426538
C	6.569373	1.978627	1.155790
H	6.474927	2.569881	0.220941
H	5.796912	2.327723	1.872861
H	7.558575	2.217672	1.596023
C	6.647845	-0.286156	2.235824
H	6.636963	-1.387485	2.104727
H	7.620018	-0.016415	2.698554
H	5.841236	-0.020658	2.950589
C	7.599851	0.057314	-0.088640
H	8.589367	0.325806	0.336652
H	7.607504	-1.033947	-0.286223
H	7.490600	0.578020	-1.062464
C	4.593991	-4.119577	-0.546684
H	5.433830	-3.854372	-1.221818
H	4.948986	-4.041742	0.501769
H	4.344887	-5.184895	-0.727402
C	2.887962	-3.505246	-2.270981
H	1.965015	-2.947813	-2.518559
H	3.678444	-3.202816	-2.988775
H	2.689163	-4.586991	-2.420160
C	2.237772	-3.665148	0.189085
H	2.592429	-3.551942	1.234930
H	1.328689	-3.048595	0.055989
H	1.949140	-4.726182	0.036893
C	-4.848370	-0.187516	-1.536334
H	-3.909622	-0.035554	-2.100852
H	-5.034629	-1.279623	-1.488870
H	-5.662979	0.281283	-2.124859
C	-4.605460	1.963074	-0.174639
H	-4.599774	2.394629	0.847417
H	-3.661096	2.256012	-0.671319
H	-5.440214	2.426375	-0.739810
C	-6.134692	0.137175	0.575206
H	-6.364650	-0.947223	0.615703
H	-6.169401	0.543452	1.606983
H	-6.949415	0.621426	-0.000448
C	-3.851387	-3.714785	3.222551
H	-4.110757	-4.408741	4.049109
H	-4.795413	-3.443155	2.707379
H	-3.214357	-4.264548	2.498809
C	-4.031697	-1.715034	4.772837
H	-4.983717	-1.394897	4.302330
H	-4.290013	-2.371609	5.629479
H	-3.528046	-0.810514	5.172724
C	-1.854546	-2.942899	4.534321
H	-1.164537	-3.512247	3.876898
H	-1.294347	-2.095676	4.983028
H	-2.146671	-3.617375	5.364336
C	-1.863899	-2.180735	-2.194355
C	-1.017569	-1.095994	-2.902311
H	-2.615738	-1.662016	-1.563499
H	-0.191572	-1.542201	-3.503583
H	-1.672917	-0.580898	-3.649611
C	-2.643189	-3.009256	-3.235008
H	-3.296455	-2.363847	-3.858922
H	-1.947722	-3.547099	-3.913999
H	-3.287668	-3.765557	-2.738131
C	-1.048382	-3.094040	-1.266934

	H	-0.227986	-3.600571	-1.815490
	H	-1.695641	-3.872856	-0.814454
	C	-0.250248	2.122328	2.158778
	C	1.418143	3.577118	0.448883
	C	0.793997	4.240560	1.523628
	C	-0.051678	3.496303	2.398539
	H	-0.922874	1.543879	2.810407
	H	2.075295	4.140901	-0.233509
	C	-0.733608	4.173553	3.561334
	H	-1.385693	5.005150	3.218121
	H	-1.359044	3.467643	4.140845
	H	0.006191	4.624160	4.257043
	C	1.018579	5.715047	1.747987
	H	0.059909	6.276171	1.726403
	H	1.468433	5.905826	2.745891
	H	1.688216	6.154546	0.983862
	Zn	-2.071166	1.534286	-2.722637
	C	0.032112	1.637940	-3.199248
	H	0.452676	2.638974	-2.967894
	H	0.887696	0.929813	-3.361029
	H	-0.387241	1.693357	-4.230041
	C	-3.591936	2.262718	-3.722590
	H	-3.265821	3.080247	-4.399493
	H	-4.046360	1.462508	-4.345235
	H	-4.377262	2.656886	-3.047607

5 (isomer)



Zero-point correction= 0.954321 (Hartree/Particle)
Thermal correction to Energy= 1.032524
Thermal correction to Enthalpy= 1.033642
Thermal correction to Gibbs Free Energy= 0.837342
Sum of electronic and zero-point Energies= -3735.169384
Sum of electronic and thermal Energies= -3735.091182
Sum of electronic and thermal Enthalpies= -3735.090064
Sum of electronic and thermal Free Energies= -3735.286363

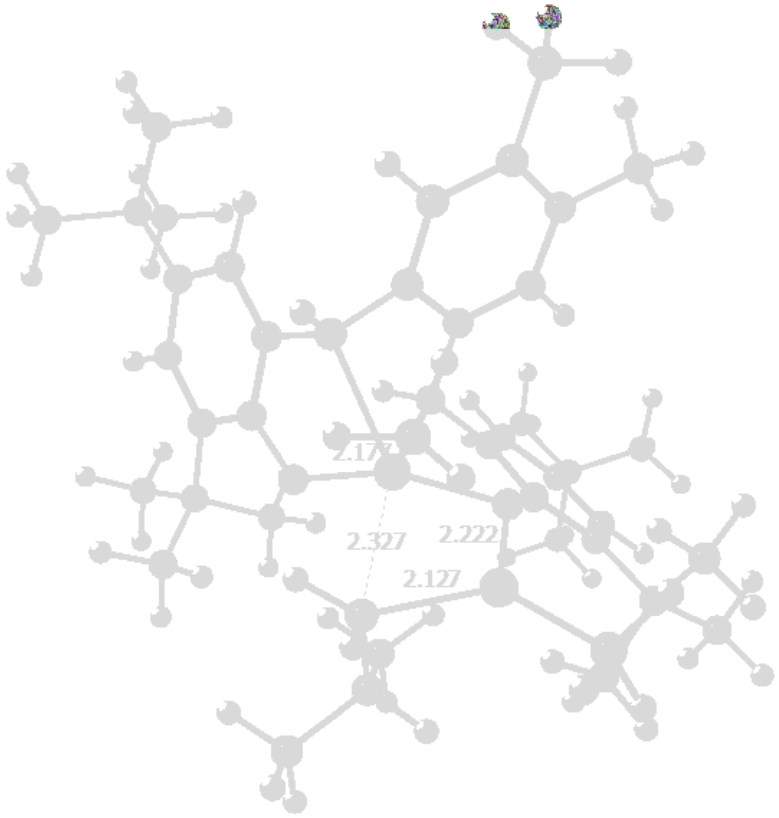
Solvent: -3735.5275321

113
PhTitBuCH3+propTS+POST--ZnMe2minisomer SCF Done: -3736.12370565 A.U.

Ti	-0.152020	-1.205467	-1.019407
N	0.204524	0.803547	0.007589
O	-1.885558	-0.416484	-0.771497
C	-2.152690	0.490680	0.229430
C	-1.000555	1.129463	0.736127
C	-1.040590	2.021029	1.811601
H	-0.104444	2.482080	2.156288
C	-2.280753	2.309336	2.415056
C	-3.428862	1.696873	1.861231
H	-4.398146	1.937593	2.315712
C	-3.427225	0.789737	0.778716
C	0.461594	1.617757	-1.175465
C	-2.420768	3.253215	3.625515
N	1.787217	-0.285607	-1.875994
O	1.198995	-1.765644	0.153428
C	2.435538	-1.212666	0.245742
C	2.819754	-0.400581	-0.839766
C	4.056004	0.253389	-0.895104
H	4.285413	0.886764	-1.763729
C	4.963426	0.087642	0.168932
C	4.550086	-0.713263	1.264090
H	5.247485	-0.821866	2.105173
C	3.304636	-1.363416	1.361986
C	1.304630	1.048932	-2.151446
C	6.359235	0.742162	0.186415
C	-4.730634	0.167327	0.243388
C	2.848452	-2.123984	2.619614
H	1.038072	0.762672	0.620396
H	2.099785	-0.740290	-2.747128
H	-1.876795	-1.809187	1.405693
C	6.607348	1.604017	-1.068753
H	6.561609	1.003081	-2.001086
H	5.878174	2.437403	-1.151089
H	7.618693	2.056205	-1.020799
C	6.485776	1.650001	1.436948
H	6.373396	1.078543	2.380871
H	7.483750	2.135120	1.460821
H	5.714937	2.448555	1.428223
C	7.435299	-0.373347	0.239770
H	8.452015	0.071992	0.251529
H	7.335800	-1.002104	1.148265
H	7.361490	-1.040265	-0.644129
C	3.961944	-2.212115	3.684005
H	4.852951	-2.754603	3.305643
H	4.285141	-1.211830	4.039241
H	3.585313	-2.767558	4.566924
C	2.424129	-3.567370	2.244735
H	1.618791	-3.574158	1.486085
H	3.285682	-4.134692	1.836240
H	2.056115	-4.103970	3.143802
C	1.652384	-1.341601	3.229531
H	1.974095	-0.330610	3.556520
H	0.823644	-1.223660	2.503335
H	1.249795	-1.874591	4.115961
C	-4.707503	-1.357025	0.510756
H	-3.847362	-1.849599	0.018549
H	-4.631854	-1.569732	1.596362
H	-5.627477	-1.837962	0.120450
C	-4.850423	0.471293	-1.271745
H	-4.925956	1.564933	-1.442418
H	-3.980803	0.095485	-1.841953
H	-5.758131	-0.007791	-1.691933
C	-5.983290	0.743198	0.939522
H	-6.000776	0.522538	2.026613
H	-6.067927	1.840814	0.801211
H	-6.890724	0.283476	0.498141
C	-3.020868	2.458685	4.814747
H	-3.132292	3.117989	5.700747
H	-4.023633	2.048441	4.576804
H	-2.364376	1.609878	5.097984
C	-3.361742	4.428097	3.254165
H	-4.378174	4.078390	2.981103
H	-3.469012	5.120314	4.114898
H	-2.958418	5.005549	2.396492
C	-1.060205	3.834561	4.062739
H	-0.347287	3.039589	4.366369
H	-0.590028	4.441315	3.260520
H	-1.199474	4.500760	4.938071
C	-1.728625	-3.810098	0.481151
C	-1.063711	-3.338278	-0.836909
H	-2.825964	-3.865630	0.287813
H	0.045955	-3.446485	-0.769960
H	-1.280952	-4.073897	-1.651394
C	-1.249926	-5.224775	0.855338
H	-0.158434	-5.222359	1.064967
H	-1.767005	-5.594230	1.765651
H	-1.438259	-5.951820	0.038456
C	-1.512812	-2.829704	1.644322

	H	-0.438586	-2.756873	1.900003
	H	-2.053868	-3.163348	2.552850
	C	-0.140873	2.860318	-1.416359
	C	1.553958	1.734915	-3.348208
	C	0.960907	2.988721	-3.599870
	C	0.097606	3.559095	-2.616535
	H	-0.816646	3.282287	-0.657285
	H	2.211194	1.276990	-4.105120
	C	-0.556407	4.896514	-2.860748
	H	-1.183486	4.877478	-3.777770
	H	-1.200872	5.201269	-2.013990
	H	0.201154	5.694069	-3.017416
	C	1.231298	3.715550	-4.893180
	H	0.290690	3.903147	-5.453928
	H	1.686219	4.711767	-4.706072
	H	1.914496	3.148169	-5.554013
	Zn	-2.483839	-2.206475	-1.944182
	C	-0.351012	-1.616742	-3.148173
	H	-0.122448	-0.656212	-3.660730
	H	0.445681	-2.364245	-3.363218
	H	-1.250679	-2.002903	-3.688719
	C	-4.125478	-2.509708	-2.971566
	H	-4.330021	-1.657824	-3.653719
	H	-4.040496	-3.430446	-3.587338
	H	-5.001109	-2.624982	-2.300480

5



Zero-point correction= 0.953820 (Hartree/Particle)
Thermal correction to Energy= 1.032453
Thermal correction to Enthalpy= 1.033572
Thermal correction to Gibbs Free Energy= 0.835052
Sum of electronic and zero-point Energies= -3735.171070
Sum of electronic and thermal Energies= -3735.092437
Sum of electronic and thermal Enthalpies= -3735.091319
Sum of electronic and thermal Free Energies= -3735.289838

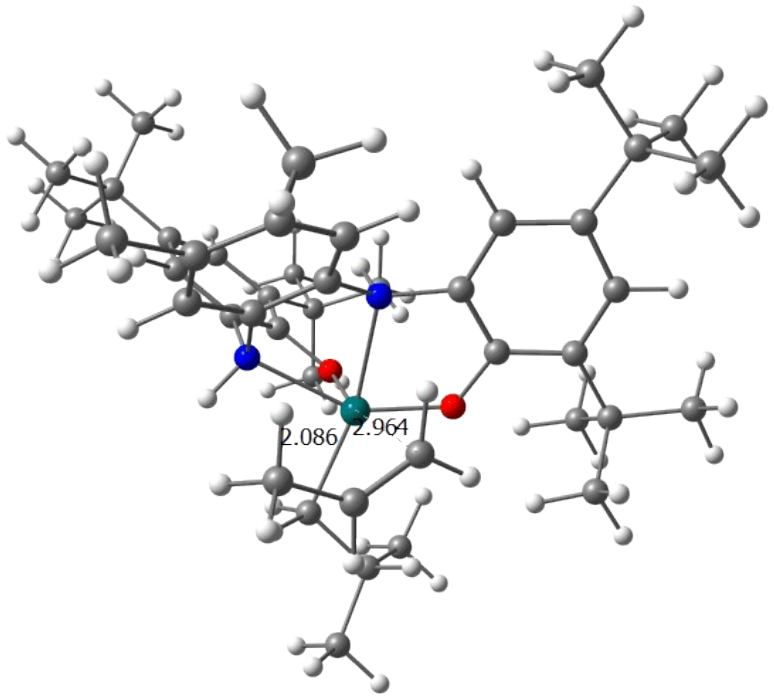
Solvent: -3735.5283354

113
PhTitBuCH3+propTS+POST--ZnMe2minisomer180 SCF Done: -3736.12489029 A.U.

Ti	0.048327	-0.384606	-1.588432
N	-0.348748	0.736390	0.566884
O	-1.485247	0.637364	-1.741572
C	-2.376686	0.712120	-0.710300
C	-1.798843	0.653086	0.579221
C	-2.583466	0.507527	1.727441
H	-2.088004	0.434509	2.704809
C	-3.985399	0.425709	1.596757
C	-4.539255	0.579629	0.302470
H	-5.632789	0.550591	0.209571
C	-3.782865	0.731337	-0.879556
C	0.151931	2.098029	0.401303
C	-4.910222	0.150010	2.798089
N	1.654278	1.141566	-1.272025
O	1.332528	-1.412902	-0.568254
C	2.574283	-0.904461	-0.294933
C	2.781262	0.453121	-0.610955
C	3.995564	1.103147	-0.358106
H	4.089639	2.169951	-0.602521
C	5.063320	0.381280	0.203163
C	4.853648	-0.995660	0.458364
H	5.695611	-1.568244	0.868463
C	3.647430	-1.684629	0.223275
C	1.145700	2.307904	-0.564289
C	6.424398	1.025371	0.533911
C	-4.418290	0.898652	-2.274253
C	3.503849	-3.191792	0.529868
H	0.064395	0.296756	1.404059
H	1.976711	1.447469	-2.203374
H	-3.804581	-1.993623	-0.806022
C	6.459200	2.522190	0.160794
H	6.306556	2.681379	-0.927282
H	5.692828	3.105420	0.713223
H	7.448268	2.951318	0.419805
C	6.685973	0.891485	2.056504
H	6.717702	-0.169038	2.379754
H	7.661154	1.350673	2.321744
H	5.893810	1.401786	2.642949
C	7.542598	0.295969	-0.254672
H	8.529896	0.751934	-0.032779
H	7.607191	-0.778883	0.011007
H	7.368952	0.365607	-1.348494
C	4.877099	-3.860040	0.766845
H	5.548017	-3.746439	-0.109632
H	5.395128	-3.455324	1.659936
H	4.733664	-4.945238	0.943971
C	2.816329	-3.939844	-0.643130
H	1.769258	-3.611662	-0.788360
H	3.358214	-3.772247	-1.597045
H	2.809289	-5.030665	-0.441232
C	2.659889	-3.344312	1.817646
H	3.161727	-2.864871	2.682865
H	1.667424	-2.870033	1.702738
H	2.498124	-4.415828	2.059433
C	-4.018262	-0.279595	-3.202330
H	-2.924452	-0.312569	-3.371337
H	-4.343781	-1.253167	-2.781622
H	-4.505373	-0.162889	-4.192473
C	-3.913643	2.233571	-2.883658
H	-4.203834	3.092535	-2.244009
H	-2.811129	2.238064	-2.994243
H	-4.360247	2.388140	-3.888053
C	-5.958595	0.945803	-2.196730
H	-6.387151	-0.000890	-1.806584
H	-6.316880	1.781356	-1.560734
H	-6.376124	1.101799	-3.212000
C	-5.628886	-1.203956	2.555290
H	-6.295964	-1.446859	3.408573
H	-6.251213	-1.183235	1.637343
H	-4.893359	-2.028365	2.446476
C	-5.958299	1.284430	2.926623
H	-6.595943	1.369121	2.023354
H	-6.629625	1.090405	3.788685
H	-5.465072	2.265211	3.088370
C	-4.124133	0.054929	4.122237
H	-3.382780	-0.771599	4.107542
H	-3.590449	0.999703	4.356989
H	-4.821074	-0.146376	4.960636
C	-2.245069	-3.466415	-1.320764
C	-1.153020	-2.374228	-1.529266
H	-2.662969	-3.689589	-2.330309
H	-0.318978	-2.797306	-2.143166
H	-1.663877	-1.584446	-2.132142
C	-1.644107	-4.774897	-0.776215
H	-1.260424	-4.655182	0.264451
H	-2.410546	-5.575489	-0.736580
H	-0.803590	-5.134106	-1.405125
C	-3.401131	-2.957923	-0.439994

	H	-3.071864	-2.785133	0.608323
	H	-4.229112	-3.694831	-0.408313
	C	-0.378769	3.192847	1.099182
	C	1.601300	3.608456	-0.830341
	C	1.078860	4.716838	-0.135350
	C	0.074992	4.503568	0.855296
	H	-1.182819	3.018615	1.831170
	H	2.371035	3.765747	-1.603563
	C	-0.506226	5.670463	1.614646
	H	-0.985927	6.399715	0.926923
	H	-1.266850	5.347083	2.351135
	H	0.282889	6.229702	2.161297
	C	1.570457	6.110793	-0.437361
	H	0.739275	6.766737	-0.774272
	H	1.999281	6.591212	0.467991
	H	2.347803	6.115225	-1.225586
	Zn	-0.497734	-2.190154	0.439458
	C	0.793098	-0.390376	-3.528896
	H	0.660267	0.601803	-4.015009
	H	1.863658	-0.691454	-3.559757
	H	0.196323	-1.135838	-4.102113
	C	-0.738704	-2.355478	2.381702
	H	-0.100753	-1.650196	2.958073
	H	-1.799481	-2.152297	2.639133
	H	-0.489077	-3.379039	2.732152

6



Zero-point correction= 0.962787 (Hartree/Particle)
Thermal correction to Energy= 1.039190
Thermal correction to Enthalpy= 1.040309
Thermal correction to Gibbs Free Energy= 0.846254
Sum of electronic and zero-point Energies= -1993.811069
Sum of electronic and thermal Energies= -1993.734666
Sum of electronic and thermal Enthalpies= -1993.733548
Sum of electronic and thermal Free Energies= -1993.927603

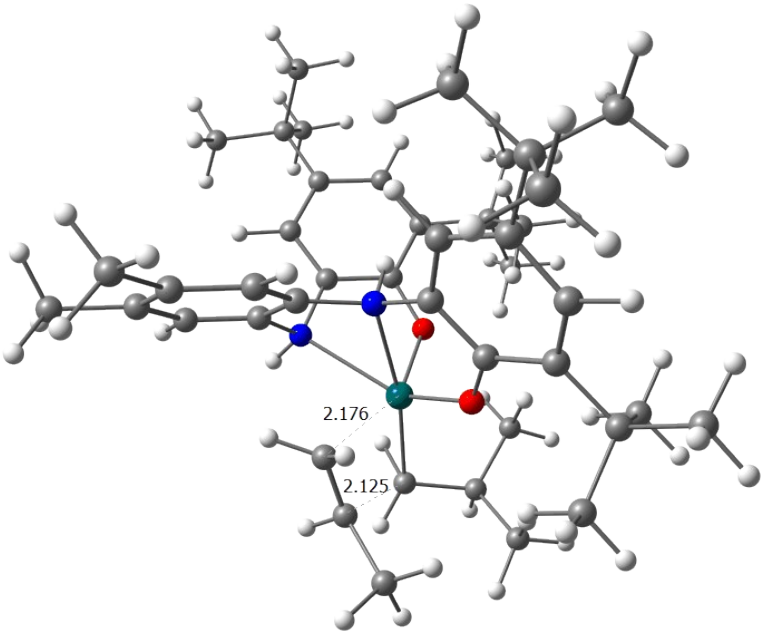
Solvent: -1994.4318219

113
PhTitBuCH3+propTS2+isomerBISrealPRE SCF Done: -1994.77385648 A.U.

Ti	-0.071409	-1.046700	-1.254563
N	-0.381635	0.742955	0.163423
O	-1.724923	-1.383928	-0.554669
C	-2.406664	-0.560807	0.290956
C	-1.738306	0.617378	0.698248
C	-2.320967	1.505675	1.611952
H	-1.743688	2.369312	1.965899
C	-3.626000	1.261028	2.084550
C	-4.285328	0.094095	1.627323
H	-5.302011	-0.094297	1.996105
C	-3.718878	-0.850152	0.748743
C	0.113553	1.933347	-0.504943
C	-4.339931	2.206147	3.072318
N	1.726078	0.337138	-1.383845
O	1.055130	-1.837889	-0.066626
C	2.237318	-1.295416	0.344938
C	2.633528	-0.107883	-0.303951
C	3.791387	0.586773	0.062889
H	4.041421	1.522365	-0.455866
C	4.599448	0.075915	1.097516
C	4.185482	-1.125726	1.726814
H	4.813961	-1.518945	2.536547
C	3.018462	-1.842036	1.397694
C	1.265193	1.714453	-1.289681
C	5.891633	0.775741	1.564301
C	-4.444498	-2.139844	0.316259
C	2.574185	-3.123439	2.127463
H	0.296721	0.482044	0.904262
H	2.188124	0.186842	-2.295782
H	-1.064843	-3.734766	-1.397166
C	6.174132	2.062732	0.761620
H	6.311397	1.855082	-0.320363
H	5.362131	2.811174	0.877094
H	7.109143	2.533979	1.126103
C	5.749997	1.153125	3.061904
H	5.594217	0.261873	3.703267
H	6.669136	1.662941	3.418617
H	4.892237	1.839654	3.219734
C	7.088589	-0.192556	1.379012
H	8.031016	0.294770	1.704832
H	6.970602	-1.119803	1.975873
H	7.202505	-0.485888	0.314890
C	3.581239	-3.536764	3.221345
H	4.585807	-3.751407	2.801439
H	3.687841	-2.761586	4.008480
H	3.227252	-4.462873	3.717695
C	2.460679	-4.285587	1.105333
H	1.715801	-4.068261	0.314872
H	3.439318	-4.480006	0.619733
H	2.146185	-5.215277	1.623514
C	1.197601	-2.868749	2.800336
H	1.264947	-2.037824	3.533607
H	0.415287	-2.619919	2.056288
H	0.869064	-3.777271	3.346440
C	-3.641090	-3.362185	0.835501
H	-2.612757	-3.379413	0.424458
H	-3.571547	-3.346903	1.942675
H	-4.145167	-4.304738	0.536363
C	-4.549322	-2.195564	-1.231486
H	-5.084387	-1.306485	-1.625722
H	-3.551218	-2.250516	-1.708119
H	-5.117375	-3.097419	-1.540303
C	-5.873095	-2.213467	0.895756
H	-5.874127	-2.223419	2.005250
H	-6.506188	-1.369499	0.551162
H	-6.360256	-3.151166	0.559975
C	-4.688979	1.423474	4.364708
H	-5.205262	2.086851	5.089436
H	-5.361844	0.565440	4.162212
H	-3.772871	1.028680	4.850795
C	-5.640971	2.734573	2.414137
H	-6.341577	1.913934	2.157646
H	-6.171636	3.420130	3.107215
H	-5.417798	3.293091	1.481272
C	-3.461042	3.414818	3.455465
H	-2.523703	3.103530	3.962406
H	-3.194378	4.031931	2.571321
H	-4.010946	4.072131	4.158963
C	-0.738006	-2.951256	-3.451063
C	0.392737	-1.963979	-3.069842
H	-1.709780	-2.398980	-3.443155
H	1.344178	-2.521587	-2.887628
H	0.598314	-1.236783	-3.888511
C	-0.538314	-3.504946	-4.875395
H	-0.512235	-2.689806	-5.628691
H	0.421331	-4.060262	-4.946017
H	-1.357127	-4.201443	-5.155000
C	-0.846868	-4.097063	-2.425137

	H	0.101307	-4.674554	-2.382289
	H	-1.662031	-4.799134	-2.694537
	C	-0.462057	3.210272	-0.478742
	C	1.869474	2.776092	-1.973247
	C	1.316303	4.072355	-1.931717
	C	0.119568	4.284480	-1.188643
	H	-1.388504	3.378197	0.086986
	H	2.768981	2.585193	-2.580695
	C	-0.521140	5.649967	-1.153508
	H	-0.764614	6.008404	-2.176413
	H	-1.455208	5.654673	-0.559462
	H	0.165700	6.404872	-0.714240
	C	1.964787	5.206410	-2.686225
	H	1.277076	5.629234	-3.449809
	H	2.229445	6.044592	-2.007040
	H	2.888925	4.883983	-3.203494
	C	-2.073026	0.616050	-2.674317
	C	-1.310592	0.634540	-3.793944
	H	-2.096826	1.472093	-1.980389
	H	-2.778424	-0.204447	-2.479068
	H	-1.381600	-0.228922	-4.480185
	C	-0.420845	1.754701	-4.232649
	H	0.626167	1.409061	-4.378291
	H	-0.755051	2.132663	-5.223478
	H	-0.418586	2.595824	-3.513548

6-7 (isomer)



Zero-point correction= 0.964758 (Hartree/Particle)
Thermal correction to Energy= 1.038806
Thermal correction to Enthalpy= 1.039924
Thermal correction to Gibbs Free Energy= 0.853646
Sum of electronic and zero-point Energies= -1993.787630
Sum of electronic and thermal Energies= -1993.713583
Sum of electronic and thermal Enthalpies= -1993.712464
Sum of electronic and thermal Free Energies= -1993.898743

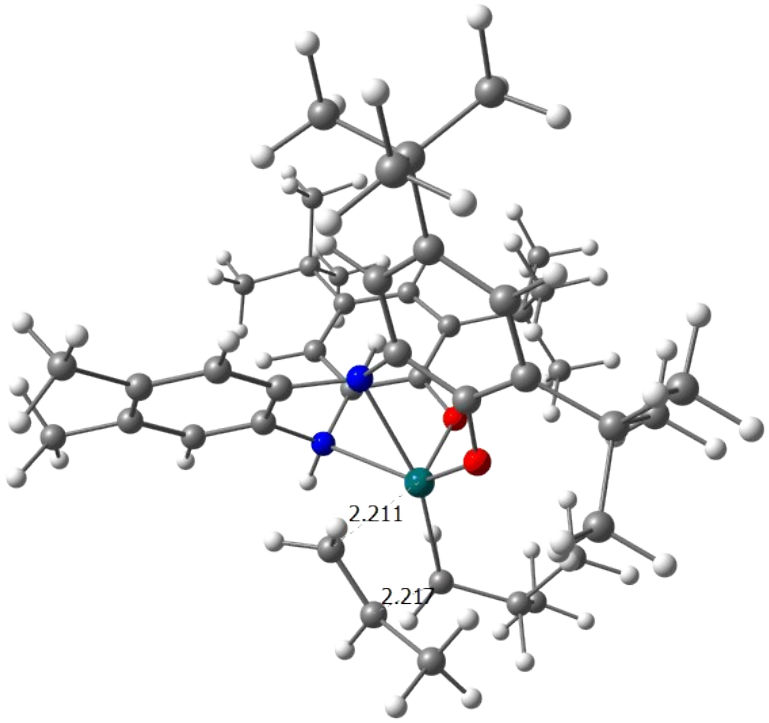
Solvent: -1994.4026829

113
PhTitBuCH3+propTS2isomer+ SCF Done: -1994.75238866 A.U.

Ti	0.439891	-1.450795	1.267512
N	0.010152	0.644517	0.385017
O	2.011974	-1.003268	0.460759
C	2.287801	0.159333	-0.205747
C	1.235242	1.098566	-0.256777
C	1.347700	2.287787	-0.989837
H	0.477739	2.953576	-1.061485
C	2.558743	2.592378	-1.639447
C	3.612111	1.652316	-1.536053
H	4.557865	1.890111	-2.039923
C	3.526334	0.425056	-0.850024
C	-0.713826	1.459732	1.342976
C	2.763388	3.888124	-2.449471
N	-1.843519	-0.653202	1.745751
O	-0.648955	-2.028983	-0.130336
C	-1.855375	-1.548639	-0.506818
C	-2.587091	-0.876051	0.494774
C	-3.859802	-0.344340	0.252192
H	-4.377094	0.189329	1.061336
C	-4.426287	-0.465179	-1.031016
C	-3.641120	-1.076907	-2.040925
H	-4.059750	-1.119334	-3.055019
C	-2.353912	-1.610194	-1.840024
C	-1.718836	0.763490	2.048369
C	-5.824156	0.084561	-1.378240
C	4.692053	-0.580426	-0.798806
C	-1.482666	-2.158302	-2.986009
H	-0.662590	0.368710	-0.359534
H	-2.300169	-1.138777	2.533067
H	1.557221	-3.381174	-0.482265
C	-6.523622	0.700135	-0.148795
H	-6.663810	-0.044298	0.662770
H	-5.959373	1.564469	0.260025
H	-7.529302	1.070212	-0.433666
C	-5.680448	1.182883	-2.463843
H	-5.224426	0.790220	-3.395592
H	-6.675913	1.596037	-2.728993
H	-5.046244	2.018206	-2.100314
C	-6.704669	-1.072248	-1.917800
H	-7.717525	-0.697228	-2.173723
H	-6.278141	-1.528220	-2.834562
H	-6.816101	-1.875403	-1.160134
C	-2.173467	-2.001535	-4.357324
H	-3.122886	-2.572940	-4.413566
H	-2.388081	-0.939448	-4.597889
H	-1.507959	-2.393740	-5.152916
C	-1.200179	-3.662555	-2.749320
H	-0.677475	-3.825353	-1.789283
H	-2.145098	-4.243767	-2.736947
H	-0.559874	-4.065920	-3.561501
C	-0.146323	-1.363407	-3.024811
H	-0.334218	-0.277678	-3.166031
H	0.443617	-1.497672	-2.097219
H	0.478636	-1.709190	-3.874020
C	4.241822	-1.917116	-1.443211
H	3.372644	-2.355799	-0.918949
H	3.961291	-1.763928	-2.505642
H	5.068919	-2.656413	-1.409288
C	5.099750	-0.798411	0.681011
H	5.472282	0.144510	1.131401
H	4.242846	-1.150630	1.286804
H	5.905345	-1.558136	0.753959
C	5.931171	-0.073478	-1.566585
H	5.718366	0.081809	-2.644439
H	6.325687	0.874842	-1.146462
H	6.741685	-0.827064	-1.496148
C	3.106458	3.522142	-3.916634
H	3.259274	4.442347	-4.518293
H	4.035253	2.920204	-3.988829
H	2.286015	2.938059	-4.382785
C	3.931324	4.694947	-1.824983
H	4.884654	4.128274	-1.842434
H	4.094023	5.637269	-2.388698
H	3.713104	4.958562	-0.769156
C	1.501168	4.775361	-2.449727
H	0.631979	4.260861	-2.910487
H	1.217130	5.095071	-1.424944
H	1.688249	5.695138	-3.039969
C	1.668198	-4.227952	1.571990
C	0.826310	-3.270430	2.493287
H	1.406909	-5.229007	1.988807
H	-0.271780	-3.319051	2.229573
H	0.845338	-3.711167	3.501926
C	3.186266	-4.058162	1.718618
H	3.529227	-4.181776	2.763309
H	3.708277	-4.819543	1.104573
H	3.507337	-3.062731	1.357546
C	1.267806	-4.287861	0.086658

	H	0.177759	-4.432284	-0.038714
	H	1.782600	-5.143592	-0.394607
	C	-0.430797	2.785775	1.681382
	C	-2.461267	1.413513	3.038868
	C	-2.205198	2.762770	3.371409
	C	-1.165695	3.452037	2.689169
	H	0.390084	3.313915	1.176579
	H	-3.239661	0.855238	3.584861
	C	-0.844488	4.885614	3.035938
	H	-0.579088	4.993766	4.109433
	H	-0.000067	5.276302	2.435864
	H	-1.719512	5.548602	2.863053
	C	-3.012934	3.454912	4.441869
	H	-2.364469	3.830668	5.262141
	H	-3.544252	4.341900	4.034576
	H	-3.771238	2.783041	4.888733
	C	0.890157	-0.319560	3.070676
	C	1.318053	-1.558131	3.652115
	H	0.011805	0.163103	3.525456
	H	1.673587	0.388487	2.739363
	H	0.622059	-1.947202	4.415384
	C	2.776436	-1.772491	3.979339
	H	3.428122	-1.494952	3.129549
	H	3.023811	-1.095367	4.825425
	H	3.010335	-2.806087	4.294419

6-7



Zero-point correction= 0.964269 (Hartree/Particle)
Thermal correction to Energy= 1.038596
Thermal correction to Enthalpy= 1.039714
Thermal correction to Gibbs Free Energy= 0.852482
Sum of electronic and zero-point Energies= -1993.793540
Sum of electronic and thermal Energies= -1993.719213
Sum of electronic and thermal Enthalpies= -1993.718094
Sum of electronic and thermal Free Energies= -1993.905327

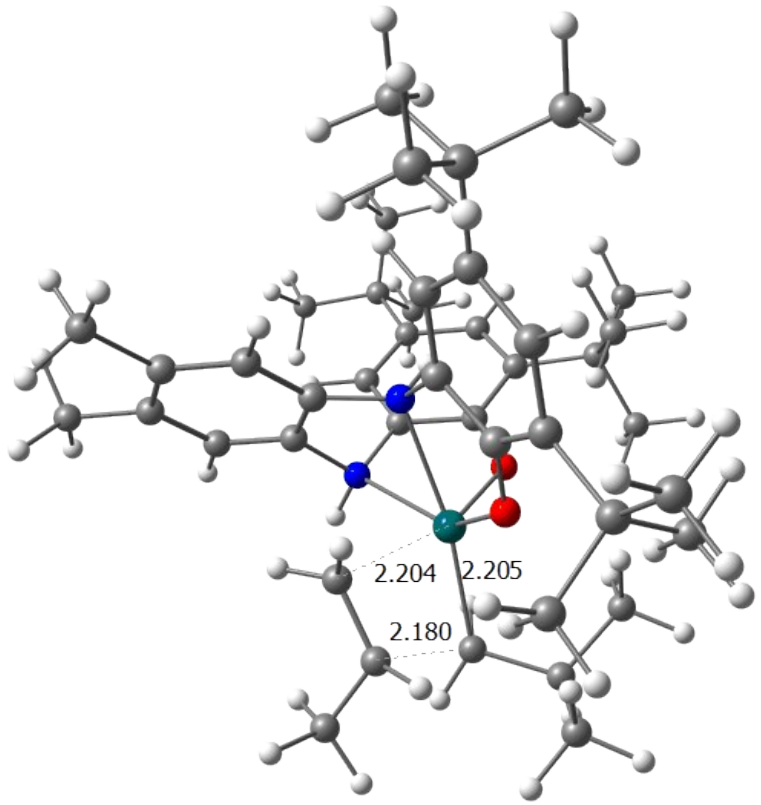
Solvent: -1994.4095826

113
PhTitBuCH3+propTS2+isomer SCF Done: -1994.75780874 A.U.

Ti	0.243098	-1.281095	1.344079
N	0.232750	0.806288	0.352870
O	1.901838	-1.155725	0.594824
C	2.401839	-0.102585	-0.116280
C	1.552357	1.020223	-0.226365
C	1.919796	2.148516	-0.971785
H	1.202128	2.970923	-1.086842
C	3.186207	2.192334	-1.586051
C	4.015196	1.051137	-1.462878
H	4.992115	1.074193	-1.963220
C	3.664026	-0.123296	-0.768830
C	-0.414331	1.766742	1.224460
C	3.675462	3.411154	-2.393791
N	-1.865850	-0.139234	1.613772
O	-0.796776	-1.791406	-0.118835
C	-1.946184	-1.231196	-0.554772
C	-2.585974	-0.352402	0.344424
C	-3.770292	0.315638	0.007277
H	-4.213507	1.011981	0.732488
C	-4.348436	0.100633	-1.258516
C	-3.676786	-0.773648	-2.152219
H	-4.116655	-0.921423	-3.147577
C	-2.478185	-1.448529	-1.856186
C	-1.560411	1.259855	1.871473
C	-5.650955	0.795384	-1.704374
C	4.545859	-1.386339	-0.774519
C	-1.728506	-2.340875	-2.862930
H	-0.424066	0.595148	-0.424793
H	-2.418173	-0.518040	2.398776
H	2.292126	-3.548609	1.205998
C	-6.234534	1.694513	-0.594920
H	-6.485997	1.114786	0.317859
H	-5.537204	2.510905	-0.312331
H	-7.170724	2.170666	-0.950244
C	-5.356064	1.676400	-2.946040
H	-4.973082	1.079272	-3.798707
H	-6.281873	2.186043	-3.285575
H	-4.601130	2.455075	-2.709814
C	-6.704407	-0.283215	-2.066537
H	-7.653390	0.197040	-2.384140
H	-6.367186	-0.933530	-2.899437
H	-6.923258	-0.934496	-1.195038
C	-2.465457	-2.419364	-4.216117
H	-3.479982	-2.856868	-4.111835
H	-2.561301	-1.423784	-4.696943
H	-1.896559	-3.068475	-4.912331
C	-1.603127	-3.777385	-2.290287
H	-1.038150	-3.787897	-1.337652
H	-2.604711	-4.218316	-2.106713
H	-1.069324	-4.429791	-3.012382
C	-0.314908	-1.742793	-3.109621
H	-0.389018	-0.712921	-3.517753
H	0.288854	-1.709299	-2.180696
H	0.235719	-2.360975	-3.848831
C	3.760537	-2.520477	-1.487546
H	2.796856	-2.730413	-0.985168
H	3.544940	-2.244845	-2.540389
H	4.357549	-3.456357	-1.492737
C	4.888993	-1.803941	0.677190
H	5.430860	-0.994023	1.207879
H	3.976140	-2.044034	1.254123
H	5.534918	-2.706221	0.675414
C	5.871505	-1.164089	-1.533073
H	5.705473	-0.903539	-2.598674
H	6.488702	-0.367389	-1.068324
H	6.468640	-2.098260	-1.513862
C	3.962556	2.975558	-3.854163
H	4.312143	3.842535	-4.452711
H	4.749102	2.195559	-3.907988
H	3.048399	2.570102	-4.335318
C	4.975137	3.955623	-1.746117
H	5.784908	3.197806	-1.739025
H	5.346977	4.835418	-2.311559
H	4.795659	4.270726	-0.697192
C	2.630013	4.545571	-2.418346
H	1.683190	4.229614	-2.904331
H	2.394811	4.915344	-1.397995
H	3.022862	5.406215	-2.996633
C	0.525902	-4.309450	2.296413
C	-0.154386	-2.989340	2.705338
H	1.161819	-4.621386	3.153889
H	-1.023695	-2.795930	2.008625
H	-0.659298	-3.111572	3.679035
C	-0.564246	-5.386771	2.101485
H	-1.215184	-5.485828	2.994466
H	-1.207710	-5.137633	1.229961
H	-0.102361	-6.376639	1.904640
C	1.426612	-4.220361	1.052086

	H	0.864576	-3.863780	0.160869
	H	1.829417	-5.220575	0.794539
	C	0.047698	3.046112	1.545624
	C	-2.263274	2.052283	2.783153
	C	-1.825766	3.359254	3.095164
	C	-0.644875	3.854381	2.477265
	H	0.975106	3.421543	1.091355
	H	-3.153928	1.640631	3.286224
	C	-0.130475	5.233073	2.813032
	H	0.067169	5.338095	3.901327
	H	0.807141	5.468231	2.273204
	H	-0.876058	6.015707	2.554938
	C	-2.591309	4.205920	4.082684
	H	-1.957327	4.494101	4.948634
	H	-2.934776	5.155400	3.618849
	H	-3.482872	3.679534	4.475084
	C	0.821387	-0.147906	3.152185
	C	1.015907	-1.424730	3.753878
	H	0.035438	0.498953	3.571132
	H	1.707739	0.388862	2.765497
	H	0.352449	-1.654140	4.601485
	C	2.384722	-2.050674	3.839579
	H	2.970014	-1.879939	2.916238
	H	2.926504	-1.553689	4.674073
	H	2.358174	-3.133648	4.061344

6-7 (isomer)



Zero-point correction= 0.964249 (Hartree/Particle)
Thermal correction to Energy= 1.038579
Thermal correction to Enthalpy= 1.039697
Thermal correction to Gibbs Free Energy= 0.852077
Sum of electronic and zero-point Energies= -1993.791400
Sum of electronic and thermal Energies= -1993.717070
Sum of electronic and thermal Enthalpies= -1993.715952
Sum of electronic and thermal Free Energies= -1993.903572

Solvent: -1994.40801

113
PhTitBuCH3+propTS2+isomerBIS SCF Done: -1994.75564884 A.U.

Ti	0.275129	-1.408807	1.128017
N	0.153869	0.712103	0.179140
O	1.907826	-1.197801	0.345144
C	2.376671	-0.080656	-0.285119
C	1.453767	0.979270	-0.421925
C	1.768695	2.129285	-1.159398
H	0.998289	2.898351	-1.302730
C	3.054888	2.269325	-1.715600
C	3.982430	1.221612	-1.497674
H	4.992777	1.340046	-1.910163
C	3.696970	0.033891	-0.797262
C	-0.442290	1.619279	1.145635
C	3.478701	3.508739	-2.528954
N	-1.791149	-0.345197	1.631986
O	-0.873616	-1.891200	-0.261044
C	-2.063323	-1.323817	-0.569452
C	-2.640857	-0.525747	0.439352
C	-3.875536	0.112261	0.268977
H	-4.268379	0.739766	1.080660
C	-4.567708	-0.041054	-0.947401
C	-3.944569	-0.804480	-1.967418
H	-4.466127	-0.887703	-2.930061
C	-2.698208	-1.445979	-1.838075
C	-1.496495	1.056769	1.893723
C	-5.939477	0.611500	-1.211259
C	4.746034	-1.067642	-0.557086
C	-2.009323	-2.191523	-2.995462
H	-0.541274	0.540320	-0.573616
H	-2.250255	-0.755538	2.460675
H	1.433324	-3.518465	-0.400488
C	-6.453624	1.392031	0.016213
H	-6.582855	0.733585	0.900719
H	-5.774815	2.225467	0.294327
H	-7.443778	1.837513	-0.208950
C	-5.813400	1.596348	-2.402791
H	-5.492987	1.084948	-3.333410
H	-6.791504	2.078879	-2.608887
H	-5.075133	2.395362	-2.182454
C	-6.968962	-0.495569	-1.555787
H	-7.966014	-0.047351	-1.748126
H	-6.680098	-1.065183	-2.462642
H	-7.071065	-1.217780	-0.719456
C	-2.838826	-2.129496	-4.295019
H	-3.829328	-2.616697	-4.180776
H	-2.998929	-1.086706	-4.639517
H	-2.300862	-2.665726	-5.102825
C	-1.814403	-3.679485	-2.610187
H	-1.188970	-3.779830	-1.703395
H	-2.791461	-4.168793	-2.417997
H	-1.312535	-4.227088	-3.435038
C	-0.631335	-1.525330	-3.266880
H	-0.757956	-0.455453	-3.536218
H	0.039876	-1.589681	-2.387434
H	-0.124396	-2.028857	-4.116089
C	4.267855	-2.397534	-1.193954
H	3.310301	-2.740715	-0.760540
H	4.128728	-2.282330	-2.288646
H	5.022694	-3.193884	-1.026452
C	4.935233	-1.236940	0.974079
H	5.329239	-0.304447	1.428122
H	3.978693	-1.483658	1.475163
H	5.654546	-2.054892	1.186532
C	6.115090	-0.707186	-1.171949
H	6.059746	-0.596793	-2.274692
H	6.533260	0.228333	-0.746034
H	6.840307	-1.518687	-0.958899
C	3.883044	3.064112	-3.958509
H	4.190739	3.943065	-4.562541
H	4.734187	2.353232	-3.946658
H	3.035239	2.569114	-4.475823
C	4.687171	4.185006	-1.831065
H	5.563032	3.507920	-1.765653
H	5.004302	5.084721	-2.398370
H	4.425819	4.501752	-0.799937
C	2.339391	4.543299	-2.641927
H	1.451583	4.129587	-3.164408
H	2.018718	4.918312	-1.647132
H	2.684621	5.420095	-3.226507
C	1.182781	-4.339370	1.646717
C	0.353977	-3.234136	2.362966
H	0.754398	-5.288819	2.046854
H	-0.679840	-3.149256	1.910751
H	0.132309	-3.560647	3.388846
C	2.666607	-4.309162	2.044696
H	2.805541	-4.306619	3.145913
H	3.189082	-5.202095	1.645939
H	3.171653	-3.416637	1.622401
C	1.009020	-4.402394	0.118013

	H	-0.058985	-4.476907	-0.165843
	H	1.531726	-5.292879	-0.285223
	C	-0.003609	2.912255	1.447346
	C	-2.130299	1.802138	2.892349
	C	-1.713969	3.118704	3.190046
	C	-0.625719	3.674198	2.463311
	H	0.853685	3.336785	0.906847
	H	-2.948343	1.344663	3.473338
	C	-0.134816	5.067886	2.772247
	H	0.184435	5.159998	3.832565
	H	0.722473	5.355829	2.133610
	H	-0.938136	5.820942	2.622322
	C	-2.403824	3.913411	4.271759
	H	-1.692775	4.215987	5.070120
	H	-2.836224	4.853609	3.867088
	H	-3.224470	3.341236	4.746262
	C	0.966307	-0.326822	2.919604
	C	1.333305	-1.606857	3.433910
	H	0.226190	0.250446	3.498560
	H	1.752737	0.288124	2.445945
	H	2.330569	-1.986773	3.157598
	C	0.880525	-1.980825	4.830001
	H	1.098929	-3.033236	5.097615
	H	1.432330	-1.331410	5.543582
	H	-0.201495	-1.784960	4.979487

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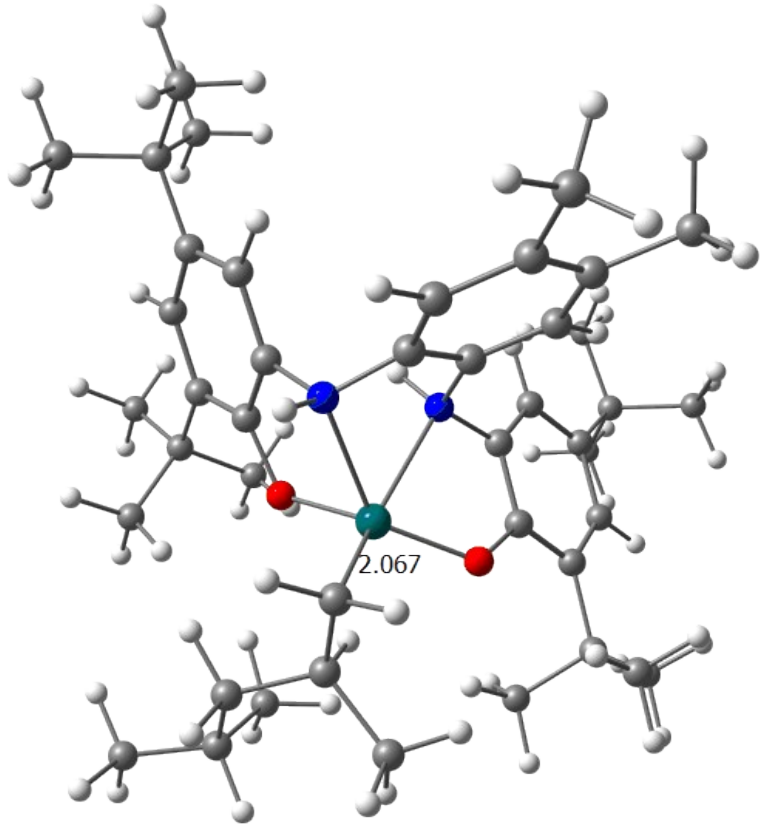


Zero-point correction= 0.966152 (Hartree/Particle)
Thermal correction to Energy= 1.040689
Thermal correction to Enthalpy= 1.041807
Thermal correction to Gibbs Free Energy= 0.852432
Sum of electronic and zero-point Energies= -1993.839934
Sum of electronic and thermal Energies= -1993.765397
Sum of electronic and thermal Enthalpies= -1993.764278
Sum of electronic and thermal Free Energies= -1993.953654

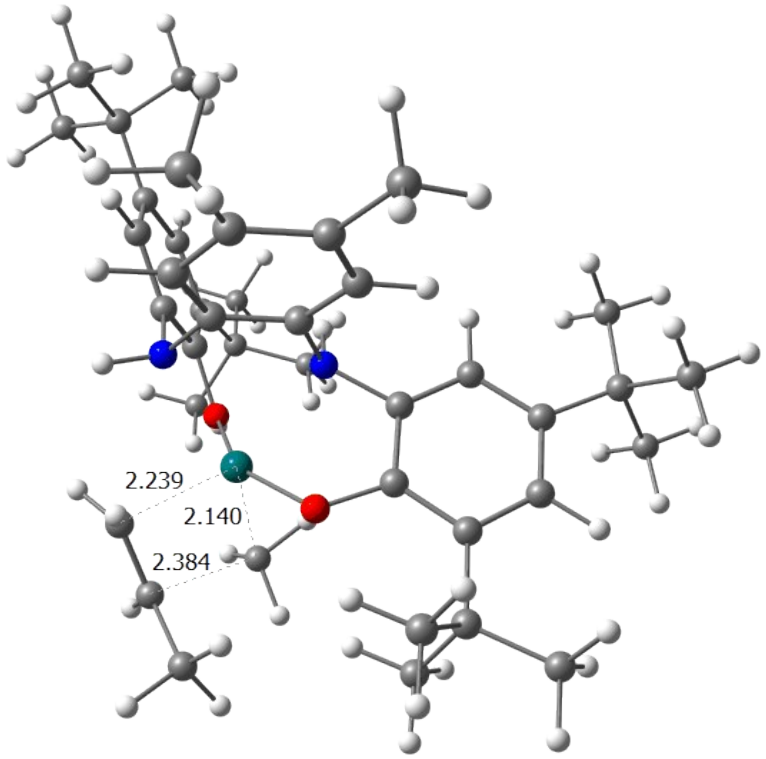
Solvent: -1994.4701497

113
PhTitBuCH3+propTS2+isomerBISrealPOST SCF Done: -1994.80608568 A.U.

Ti	-0.096756	1.014059	1.169391
N	-0.295230	-1.005070	0.098582
O	-1.925608	0.756686	1.016396
C	-2.478795	-0.024109	0.041643
C	-1.617004	-0.996801	-0.507183
C	-2.019650	-1.849296	-1.541457
H	-1.305126	-2.584501	-1.937871
C	-3.330938	-1.739136	-2.048719
C	-4.180389	-0.762723	-1.471981
H	-5.200203	-0.677274	-1.869783
C	-3.804592	0.119899	-0.438366
C	-0.090476	-1.888154	1.238080
C	-3.858756	-2.627192	-3.193465
N	1.630980	-0.275664	1.780250
O	1.170467	1.521291	-0.068975
C	2.256724	0.731903	-0.334650
C	2.529347	-0.280273	0.613699
C	3.556503	-1.214253	0.441089
H	3.701095	-1.990651	1.205695
C	4.367266	-1.135554	-0.708172
C	4.094159	-0.096676	-1.633605
H	4.728544	-0.032757	-2.527410
C	3.062092	0.853768	-1.498332
C	0.945222	-1.505776	2.116801
C	5.517088	-2.124025	-0.986913
C	-4.740261	1.204978	0.126986
C	2.804671	1.969228	-2.528485
H	0.453509	-1.133392	-0.604646
H	2.117713	0.105497	2.604667
H	-1.394337	4.232560	-0.287596
C	5.665495	-3.168420	0.139071
H	5.897988	-2.694383	1.115606
H	4.750894	-3.786897	0.256254
H	6.500105	-3.858958	-0.097188
C	5.229325	-2.870922	-2.315379
H	5.158501	-2.176291	-3.177236
H	6.043903	-3.591980	-2.535532
H	4.276378	-3.436991	-2.254835
C	6.848088	-1.337557	-1.106598
H	7.689810	-2.034208	-1.301352
H	6.825548	-0.603918	-1.937982
H	7.068881	-0.783446	-0.170848
C	3.795328	1.904681	-3.709773
H	4.847919	2.022972	-3.379123
H	3.709069	0.952722	-4.273775
H	3.578498	2.729054	-4.418981
C	2.976849	3.338909	-1.820037
H	2.299038	3.434681	-0.950228
H	4.018367	3.468516	-1.460182
H	2.749617	4.167848	-2.522103
C	1.365754	1.830898	-3.094178
H	1.238871	0.856231	-3.610362
H	0.599008	1.906773	-2.299541
H	1.169839	2.633969	-3.834608
C	-4.106818	2.598946	-0.129491
H	-3.125113	2.696064	0.372538
H	-3.962580	2.775389	-1.215434
H	-4.768751	3.398575	0.263272
C	-4.927654	0.979004	1.650002
H	-5.399511	-0.005668	1.847569
H	-3.960549	1.012415	2.188637
H	-5.587085	1.764896	2.074001
C	-6.129245	1.175585	-0.544607
H	-6.069579	1.368957	-1.635693
H	-6.647418	0.206747	-0.388050
H	-6.769890	1.966507	-0.104401
C	-4.306287	-1.725573	-4.373251
H	-4.687624	-2.347647	-5.209666
H	-5.118496	-1.029393	-4.080730
H	-3.459151	-1.117976	-4.753707
C	-5.067618	-3.451386	-2.679388
H	-5.897541	-2.801988	-2.333570
H	-5.465563	-4.097743	-3.489323
H	-4.772599	-4.104881	-1.832105
C	-2.783180	-3.605970	-3.709025
H	-1.897616	-3.072513	-4.113640
H	-2.441719	-4.304150	-2.916154
H	-3.198824	-4.222995	-4.531253
C	0.142939	5.392933	0.820557
C	0.613091	4.311258	1.820179
H	-0.652898	5.995117	1.315452
H	1.514973	3.808495	1.402607
H	0.929851	4.791481	2.772081
C	1.312510	6.339382	0.498364
H	1.746149	6.780864	1.419825
H	2.125494	5.796173	-0.030382
H	0.985861	7.173919	-0.155136
C	-0.448744	4.788396	-0.466787

	H	0.267165	4.088154	-0.946140
	H	-0.686360	5.582264	-1.203825
	C	-0.878640	-3.006620	1.535959
	C	1.201586	-2.257637	3.271771
	C	0.420672	-3.390395	3.578914
	C	-0.637678	-3.768138	2.698072
	H	-1.698304	-3.278396	0.853758
	H	2.013177	-1.949127	3.950647
	C	-1.492695	-4.971277	3.009516
	H	-1.998158	-4.862296	3.992950
	H	-2.273711	-5.133104	2.242021
	H	-0.880421	-5.896156	3.074486
	C	0.698619	-4.191637	4.826420
	H	-0.190713	-4.224087	5.491594
	H	0.942175	-5.247346	4.580154
	H	1.543382	-3.774151	5.407267
	C	0.177532	2.048022	2.937964
	C	-0.419181	3.216963	2.165646
	H	1.214070	2.218891	3.289963
	H	-0.466013	1.653670	3.752405
	H	-0.747997	2.856935	1.111608
	C	-1.748030	3.729019	2.748536
	H	-2.239316	4.460618	2.077527
	H	-2.454638	2.891123	2.911436
	H	-1.553442	4.223592	3.722004

2-3 (isomer)



Zero-point correction= 0.880961 (Hartree/Particle)
Thermal correction to Energy= 0.949932
Thermal correction to Enthalpy= 0.951051
Thermal correction to Gibbs Free Energy= 0.774129
Sum of electronic and zero-point Energies= -1876.021831
Sum of electronic and thermal Energies= -1875.952859
Sum of electronic and thermal Enthalpies= -1875.951741
Sum of electronic and thermal Free Energies= -1876.128663

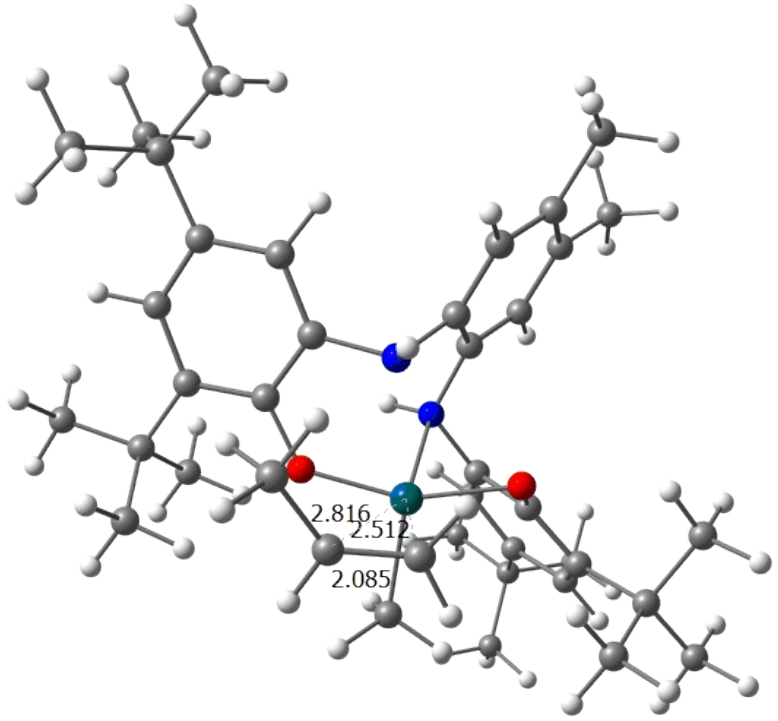
Solvent: -1876.5817636

104
PhTitBuCH3+propTS+ SCF Done: -1876.90279160 A.U.

Ti	-0.151870	-1.007482	-1.627532
N	-0.219518	0.238617	0.306406
O	-1.898625	-0.324505	-1.513511
C	-2.488255	-0.166811	-0.292796
C	-1.579729	0.038205	0.771770
C	-1.987279	0.113380	2.106392
H	-1.232722	0.270865	2.889740
C	-3.361629	0.007142	2.406607
C	-4.260718	-0.145601	1.322637
H	-5.331511	-0.208388	1.556703
C	-3.882178	-0.240172	-0.033157
C	0.029996	1.611362	-0.147285
C	-3.905186	0.073300	3.847767
N	1.565272	0.578991	-1.721486
O	1.285976	-1.867252	-0.806629
C	2.390468	-1.238130	-0.338983
C	2.619139	0.063925	-0.828302
C	3.724148	0.827794	-0.434369
H	3.837001	1.846946	-0.830361
C	4.647611	0.281633	0.477784
C	4.385465	-1.018747	0.979376
H	5.092971	-1.434378	1.709093
C	3.275494	-1.806645	0.619130
C	0.922311	1.776750	-1.221315
C	5.899578	1.045365	0.953966
C	-4.900149	-0.442809	-1.170017
C	2.983058	-3.186337	1.238227
H	0.488769	-0.060859	0.997657
H	1.964835	0.770082	-2.651527
H	-1.127696	-2.681702	-0.758891
C	5.998218	2.446865	0.316489
H	6.072609	2.394839	-0.789987
H	5.128973	3.085071	0.580868
H	6.908583	2.963316	0.682573
C	5.843130	1.210594	2.494858
H	5.824306	0.233273	3.019150
H	6.736233	1.762328	2.855496
H	4.940477	1.778932	2.801846
C	7.162764	0.235491	0.562121
H	8.079567	0.766512	0.893220
H	7.172496	-0.769742	1.030587
H	7.221712	0.098071	-0.537450
C	4.054649	-3.591270	2.272236
H	5.062835	-3.670414	1.815554
H	4.109957	-2.876745	3.119788
H	3.805508	-4.585939	2.694489
C	2.949178	-4.262283	0.121885
H	2.169411	-4.039005	-0.632152
H	3.928456	-4.321819	-0.396528
H	2.733331	-5.259412	0.559380
C	1.609079	-3.124569	1.960440
H	1.619237	-2.351987	2.758323
H	0.787444	-2.893237	1.253433
H	1.381072	-4.100350	2.437599
C	-4.643905	-1.827551	-1.817354
H	-3.613346	-1.889400	-2.211225
H	-4.784241	-2.642673	-1.077615
H	-5.348145	-1.998660	-2.658199
C	-4.722863	0.680276	-2.225038
H	-4.920804	1.675720	-1.776495
H	-3.697478	0.691112	-2.643481
H	-5.438140	0.534664	-3.061291
C	-6.356653	-0.404791	-0.662119
H	-6.570016	-1.220057	0.059652
H	-6.604290	0.563971	-0.180750
H	-7.049174	-0.536178	-1.518284
C	-4.686209	-1.230566	4.156685
H	-5.082258	-1.205537	5.193285
H	-5.549436	-1.369098	3.474614
H	-4.029729	-2.120057	4.060042
C	-4.854207	1.293116	3.974819
H	-5.721627	1.218100	3.287768
H	-5.252656	1.365300	5.008269
H	-4.319679	2.238302	3.744991
C	-2.773616	0.221719	4.886189
H	-2.065796	-0.632908	4.853594
H	-2.198246	1.160617	4.744190
H	-3.203053	0.253786	5.908014
C	-0.579995	-2.015289	-3.991977
C	0.314053	-0.953299	-3.816564
H	-0.154762	-3.023210	-4.125567
H	1.397396	-1.159887	-3.857684
H	-0.019535	0.072879	-4.067460
C	-1.983368	-1.801078	-4.482598
H	-1.931425	-1.686557	-5.588654
H	-2.650419	-2.657111	-4.272042
H	-2.431175	-0.879644	-4.062408
C	-0.976741	-2.970520	-1.843646
H	-0.238408	-3.792574	-1.880025

	H	-1.966501	-3.274634	-2.222748
	C	-0.637514	2.728627	0.372218
	C	1.145904	3.051931	-1.760206
	C	0.481270	4.183296	-1.245585
	C	-0.421947	4.017936	-0.155174
	H	-1.355913	2.587935	1.193802
	H	1.849888	3.166975	-2.600968
	C	-1.146690	5.209070	0.422108
	H	-1.754000	5.726762	-0.351006
	H	-1.824025	4.919055	1.248306
	H	-0.433049	5.964453	0.815660
	C	0.723884	5.548932	-1.838853
	H	-0.218276	5.993452	-2.225289
	H	1.111417	6.256533	-1.074992
	H	1.451709	5.516271	-2.672424

2 (isomer)



Zero-point correction= 0.879223 (Hartree/Particle)
Thermal correction to Energy= 0.950125
Thermal correction to Enthalpy= 0.951243
Thermal correction to Gibbs Free Energy= 0.770710
Sum of electronic and zero-point Energies= -1876.028700
Sum of electronic and thermal Energies= -1875.957799
Sum of electronic and thermal Enthalpies= -1875.956680
Sum of electronic and thermal Free Energies= -1876.137214

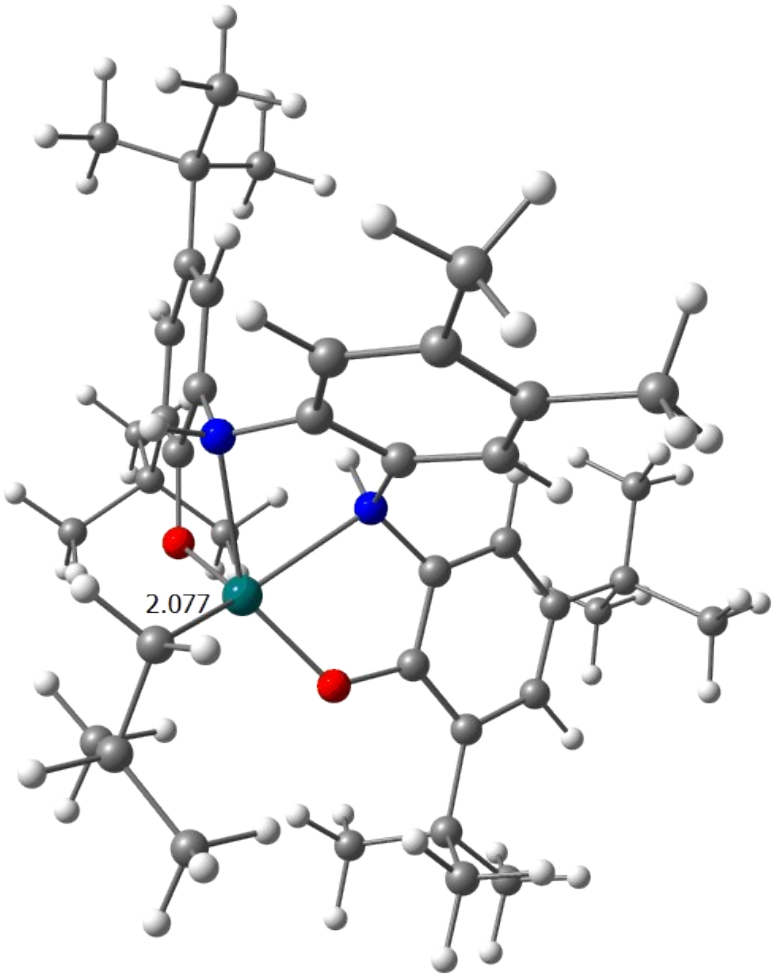
Solvent: -1876.5857653

104
PhTitBuCH3+propTSisomer+PRE SCF Done: -1876.90792337 A.U.

Ti	0.488554	-0.745498	1.099626
N	0.525695	0.303503	-0.797416
O	1.665729	0.734486	1.501669
C	2.528523	0.348880	0.536220
C	1.940080	0.019703	-0.727758
C	2.668197	-0.591306	-1.766022
H	2.150296	-0.840330	-2.702779
C	4.030762	-0.852167	-1.580083
C	4.623923	-0.435204	-0.351267
H	5.701395	-0.608242	-0.230151
C	3.938979	0.163518	0.713182
C	0.129020	1.707766	-0.708963
C	4.899715	-1.545687	-2.645187
N	-1.323749	0.974362	1.102743
O	-1.049847	-1.611671	0.547143
C	-2.250576	-1.098208	0.209180
C	-2.451281	0.276222	0.478410
C	-3.661657	0.906742	0.165296
H	-3.767063	1.979808	0.376507
C	-4.711331	0.166666	-0.413951
C	-4.488562	-1.212156	-0.658583
H	-5.307281	-1.790290	-1.106881
C	-3.289081	-1.885934	-0.364972
C	-0.789053	2.050616	0.294819
C	-6.068413	0.797517	-0.784185
C	4.635840	0.630071	2.003310
C	-3.077598	-3.388416	-0.632343
H	0.058370	-0.191280	-1.572428
H	-1.607745	1.344583	2.020014
H	1.731989	-2.835365	0.267556
C	-6.122558	2.299453	-0.435779
H	-5.990815	2.476973	0.652093
H	-5.351298	2.880773	-0.983149
H	-7.110530	2.715310	-0.719362
C	-6.298632	0.637584	-2.309788
H	-6.321508	-0.427733	-2.617391
H	-7.269623	1.089601	-2.601155
H	-5.496632	1.141384	-2.888311
C	-7.197133	0.071030	-0.007294
H	-8.183531	0.512334	-0.260524
H	-7.244102	-1.009408	-0.253294
H	-7.049922	0.164039	1.088767
C	-4.332475	-4.044679	-1.245227
H	-5.211979	-3.970323	-0.572651
H	-4.601319	-3.596175	-2.223979
H	-4.139587	-5.122764	-1.418380
C	-2.758709	-4.105096	0.707840
H	-1.825449	-3.718786	1.162303
H	-3.589000	-3.971310	1.432550
H	-2.629660	-5.194127	0.537082
C	-1.898103	-3.572203	-1.624991
H	-2.110795	-3.059796	-2.586606
H	-0.951635	-3.172394	-1.210246
H	-1.745713	-4.650069	-1.841429
C	4.083762	-0.159999	3.218179
H	3.000055	0.017255	3.348137
H	4.258004	-1.249664	3.100579
H	4.597698	0.166934	4.145672
C	4.356255	2.145139	2.193391
H	4.755427	2.728970	1.338275
H	3.271739	2.351215	2.282959
H	4.854058	2.508547	3.116387
C	6.162493	0.417355	1.939355
H	6.432470	-0.655077	1.844491
H	6.626102	0.972849	1.097857
H	6.625779	0.790159	2.875110
C	5.465860	-2.859028	-2.043812
H	6.099659	-3.379934	-2.791193
H	6.092729	-2.671672	-1.148314
H	4.646640	-3.546536	-1.747170
C	6.066422	-0.606411	-3.047493
H	6.724693	-0.362789	-2.188866
H	6.697467	-1.092393	-3.820034
H	5.684233	0.347677	-3.465715
C	4.091235	-1.894320	-3.911605
H	3.253683	-2.589141	-3.691916
H	3.678732	-0.988715	-4.403821
H	4.747665	-2.397393	-4.649779
C	-0.874475	-1.522450	3.437910
C	0.207367	-0.705423	3.595556
H	-0.691920	-2.599917	3.270395
H	0.095583	0.367986	3.825993
H	1.223629	-1.125117	3.676408
C	-2.308089	-1.119173	3.529549
H	-2.867213	-1.413446	2.616280
H	-2.783205	-1.668309	4.371633
H	-2.442453	-0.033875	3.708826
C	1.619464	-2.483642	1.321437

	H	1.107063	-3.283513	1.896842
	H	2.634804	-2.309250	1.734409
	C	0.697038	2.692258	-1.524714
	C	-1.129254	3.399748	0.473198
	C	-0.567950	4.409570	-0.336220
	C	0.355987	4.050046	-1.360497
	H	1.437670	2.396244	-2.284981
	H	-1.841321	3.675281	1.268357
	C	0.974453	5.107335	-2.242060
	H	1.545584	5.849222	-1.643601
	H	1.665314	4.669226	-2.988006
	H	0.198626	5.680876	-2.793074
	C	-0.941672	5.855305	-0.120225
	H	-0.045987	6.474751	0.099515
	H	-1.406913	6.291667	-1.030102
	H	-1.654456	5.978714	0.717851

3 (isomer)



Zero-point correction= 0.882951 (Hartree/Particle)
Thermal correction to Energy= 0.952573
Thermal correction to Enthalpy= 0.953691
Thermal correction to Gibbs Free Energy= 0.773603
Sum of electronic and zero-point Energies= -1876.049379
Sum of electronic and thermal Energies= -1875.979758
Sum of electronic and thermal Enthalpies= -1875.978639
Sum of electronic and thermal Free Energies= -1876.158728

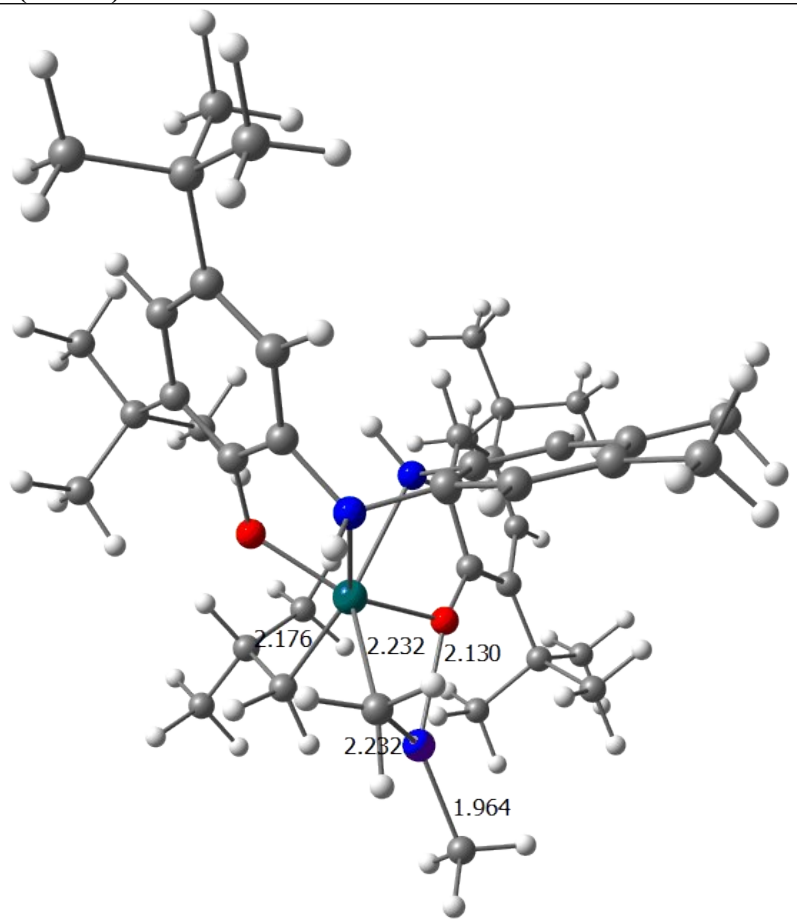
Solvent: -1876.6181862

104
PhTitBuCH3+propTS+POST SCF Done: -1876.93233042 A.U.

Ti	-0.135037	0.609772	1.793262
N	-0.184566	-0.615476	-0.095162
O	-1.897223	0.711592	1.276537
C	-2.367196	0.360303	0.040177
C	-1.457563	-0.360929	-0.756262
C	-1.759483	-0.768038	-2.060681
H	-1.004680	-1.319535	-2.638630
C	-3.023842	-0.453168	-2.597519
C	-3.927238	0.260343	-1.772091
H	-4.913020	0.503411	-2.189469
C	-3.654138	0.689693	-0.456583
C	0.058321	-1.928869	0.479332
C	-3.443553	-0.851248	-4.026970
N	1.714987	-0.682247	1.716003
O	1.101603	1.759784	1.061781
C	2.215294	1.290672	0.420274
C	2.579820	-0.043690	0.712823
C	3.655031	-0.682966	0.086539
H	3.876501	-1.728051	0.345124
C	4.414638	0.032014	-0.861278
C	4.030741	1.368323	-1.139909
H	4.616714	1.918666	-1.887844
C	2.941559	2.036542	-0.543981
C	1.105311	-1.961314	1.425937
C	5.624493	-0.582905	-1.592855
C	-4.679905	1.449020	0.405374
C	2.507326	3.461069	-0.935771
H	0.615790	-0.328514	-0.690820
H	2.184023	-0.703490	2.633968
H	-0.994561	2.741510	2.528243
C	5.861847	-2.051098	-1.182337
H	6.081482	-2.149301	-0.098602
H	4.991886	-2.696945	-1.425316
H	6.735531	-2.457839	-1.730648
C	5.376183	-0.534956	-3.122823
H	5.249532	0.502852	-3.492887
H	6.237343	-0.977049	-3.665635
H	4.466210	-1.108192	-3.397536
C	6.893317	0.237656	-1.243133
H	7.780145	-0.187032	-1.757946
H	6.802322	1.297857	-1.555943
H	7.088875	0.221555	-0.150942
C	3.455502	4.082916	-1.982054
H	4.494644	4.168814	-1.602181
H	3.474072	3.502893	-2.928097
H	3.109538	5.106346	-2.231586
C	2.503339	4.369450	0.321545
H	1.800093	3.998915	1.092382
H	3.516502	4.425417	0.770578
H	2.195783	5.399155	0.044408
C	1.081622	3.390773	-1.549355
H	1.071850	2.743672	-2.451522
H	0.341696	2.994267	-0.826293
H	0.748282	4.404072	-1.855235
C	-4.073103	2.792205	0.889547
H	-3.182880	2.634754	1.527731
H	-3.776871	3.426298	0.028342
H	-4.822830	3.353238	1.485021
C	-5.046805	0.557628	1.620759
H	-5.530578	-0.383215	1.286662
H	-4.150834	0.289747	2.214180
H	-5.753960	1.090319	2.290166
C	-5.972124	1.762511	-0.377827
H	-5.776830	2.405928	-1.260875
H	-6.489289	0.842672	-0.720729
H	-6.678472	2.308546	0.279692
C	-3.761757	0.431771	-4.837698
H	-4.066210	0.168386	-5.872109
H	-4.589763	1.013793	-4.384443
H	-2.873765	1.094482	-4.897893
C	-4.705076	-1.750151	-3.955057
H	-5.563423	-1.226080	-3.487679
H	-5.018287	-2.056111	-4.974993
H	-4.506759	-2.669461	-3.365625
C	-2.330897	-1.629985	-4.759537
H	-1.405371	-1.027112	-4.871514
H	-2.073304	-2.576143	-4.238491
H	-2.670582	-1.900442	-5.779781
C	-0.859668	1.516429	4.410979
C	-0.066026	0.304834	3.847046
H	-0.463257	1.725266	5.430888
H	0.985466	0.330177	4.212296
H	-0.510997	-0.678513	4.124791
C	-2.364591	1.238742	4.538122
H	-2.553970	0.370650	5.201967
H	-2.897100	2.114372	4.962694
H	-2.815421	1.018091	3.549760
C	-0.582597	2.790245	3.569447

	H	0.499375	3.024344	3.501376
	H	-1.094623	3.671905	4.006014
	C	-0.691153	-3.082468	0.219575
	C	1.412616	-3.156283	2.090019
	C	0.673062	-4.329212	1.833051
	C	-0.397706	-4.289130	0.888204
	H	-1.519965	-3.032443	-0.502644
	H	2.228993	-3.171436	2.830050
	C	-1.208995	-5.529134	0.606941
	H	-1.679309	-5.922766	1.533210
	H	-2.013576	-5.338231	-0.128754
	H	-0.569689	-6.346685	0.209855
	C	1.005414	-5.611280	2.554619
	H	0.138928	-5.977101	3.146121
	H	1.257738	-6.421868	1.838046
	H	1.861546	-5.488650	3.245403

4 (isomer)



Zero-point correction= 0.954313 (Hartree/Particle)
Thermal correction to Energy= 1.032545
Thermal correction to Enthalpy= 1.033663
Thermal correction to Gibbs Free Energy= 0.836833
Sum of electronic and zero-point Energies= -3735.168139
Sum of electronic and thermal Energies= -3735.089907
Sum of electronic and thermal Enthalpies= -3735.088789
Sum of electronic and thermal Free Energies= -3735.285619

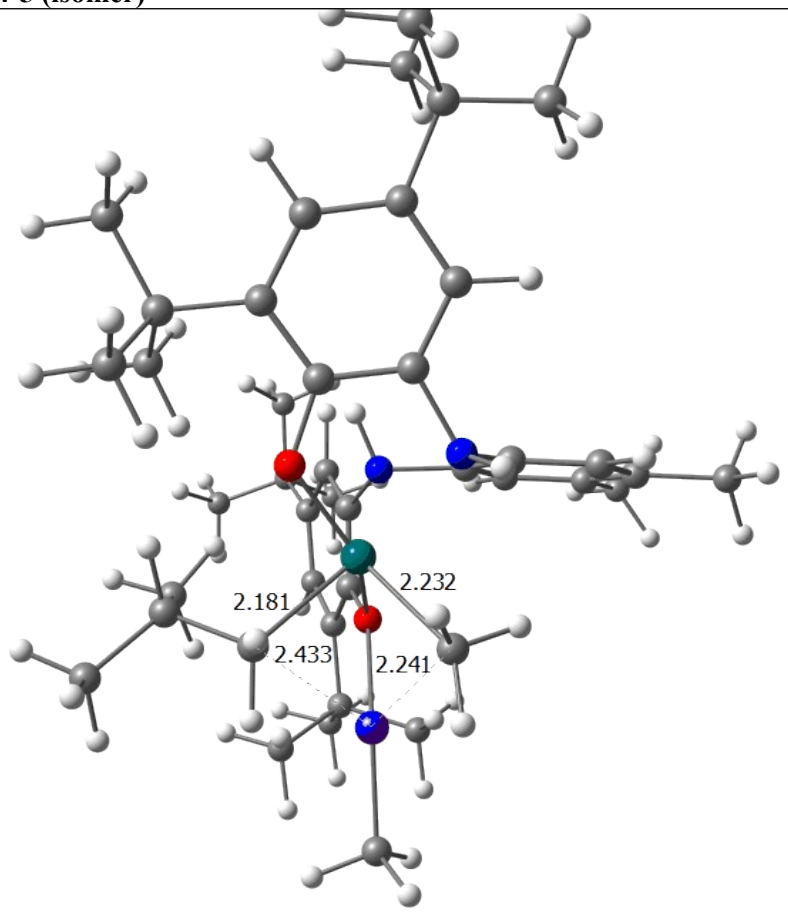
Solvent: -3735.526822

113
PhTitBuCH3+propTS+POST--ZnMe2min0c SCF Done: -3736.12245209 A.U.

Ti	-0.095638	-0.824467	-1.376308
N	0.206704	0.611800	0.348869
O	-1.858675	-0.124776	-0.923043
C	-2.158613	0.283797	0.355459
C	-1.013357	0.588515	1.126405
C	-1.075571	0.885345	2.489693
H	-0.145271	1.106144	3.031266
C	-2.332901	0.907627	3.125762
C	-3.472880	0.691051	2.316657
H	-4.455573	0.752232	2.801456
C	-3.448505	0.391298	0.936163
C	0.393739	1.842211	-0.424603
C	-2.498734	1.178624	4.633714
N	1.766277	0.474566	-1.893961
O	1.351025	-1.737873	-0.624350
C	2.546838	-1.172002	-0.320818
C	2.839006	0.030160	-0.996697
C	4.020647	0.749236	-0.783600
H	4.178433	1.689527	-1.330485
C	4.965241	0.254008	0.136062
C	4.646155	-0.945983	0.821111
H	5.372398	-1.321726	1.553964
C	3.460103	-1.684934	0.642317
C	1.186719	1.761319	-1.588659
C	6.299326	0.969023	0.428551
C	-4.746473	0.216619	0.123459
C	3.127877	-2.949387	1.453970
H	1.046201	0.385972	0.910464
H	2.078356	0.444308	-2.875807
H	-2.744634	-2.806641	0.508859
C	6.461955	2.252419	-0.412325
H	6.456108	2.036951	-1.501312
H	5.665666	2.995325	-0.195905
H	7.432576	2.735337	-0.179073
C	6.350945	1.355343	1.929588
H	6.286534	0.467186	2.590796
H	7.304584	1.873728	2.161671
H	5.515786	2.037388	2.193490
C	7.472558	0.011530	0.094940
H	8.444054	0.508424	0.298182
H	7.439940	-0.915589	0.702964
H	7.453634	-0.283642	-0.974612
C	4.247343	-3.311465	2.452270
H	5.209210	-3.524527	1.941642
H	4.418193	-2.509284	3.200207
H	3.962107	-4.226162	3.010690
C	2.936613	-4.144733	0.484971
H	2.151014	-3.941400	-0.268074
H	3.880504	-4.363544	-0.055307
H	2.645721	-5.054897	1.049610
C	1.827943	-2.686816	2.261876
H	1.975759	-1.852479	2.979887
H	0.978065	-2.433483	1.600864
H	1.545504	-3.588404	2.844132
C	-4.882429	-1.257189	-0.328495
H	-3.993154	-1.603265	-0.888372
H	-5.006774	-1.925303	0.548076
H	-5.760947	-1.384842	-0.992923
C	-4.703754	1.176517	-1.093984
H	-4.635779	2.231144	-0.756171
H	-3.839886	0.975594	-1.755159
H	-5.624850	1.067858	-1.702420
C	-6.003524	0.569101	0.949423
H	-6.138815	-0.106679	1.818571
H	-5.980799	1.615702	1.317214
H	-6.903308	0.460229	0.310496
C	-3.207928	-0.036663	5.286231
H	-3.331057	0.129748	6.376677
H	-4.217204	-0.207259	4.859460
H	-2.617028	-0.965132	5.143515
C	-3.356021	2.454829	4.833809
H	-4.369543	2.349114	4.395955
H	-3.482315	2.668277	5.915679
H	-2.872490	3.336445	4.363837
C	-1.139727	1.385234	5.334220
H	-0.486385	0.492512	5.241542
H	-0.593910	2.264459	4.932097
H	-1.298025	1.566032	6.416594
C	-0.932873	-3.647812	-0.409953
C	-0.968401	-2.791301	-1.702341
H	0.134762	-3.730596	-0.119378
H	-0.254085	-3.197177	-2.455110
H	-1.979820	-2.981971	-2.163380
C	-1.461335	-5.065981	-0.696443
H	-0.912881	-5.543891	-1.534438
H	-1.353044	-5.717739	0.196317
H	-2.540011	-5.042091	-0.965617
C	-1.686308	-3.010409	0.767020

	H	-1.239941	-2.047141	1.090347
	H	-1.674091	-3.679764	1.651070
	C	-0.255925	3.045552	-0.114464
	C	1.322449	2.882717	-2.421384
	C	0.672800	4.095957	-2.119975
	C	-0.125308	4.179111	-0.940003
	H	-0.888216	3.091684	0.784870
	H	1.943574	2.804128	-3.328571
	C	-0.828407	5.465342	-0.583188
	H	-1.522461	5.783302	-1.390429
	H	-1.413832	5.369371	0.351299
	H	-0.104710	6.297591	-0.448239
	C	0.822099	5.291764	-3.026458
	H	-0.164570	5.637174	-3.402740
	H	1.266518	6.153285	-2.483550
	H	1.463746	5.073520	-3.901743
	Zn	-2.409419	-1.072053	-2.749965
	C	-0.402860	-0.538882	-3.568568
	H	-0.211663	0.539108	-3.760154
	H	0.532230	-1.128320	-3.717509
	H	-1.025493	-0.889995	-4.425347
	C	-4.081992	-1.356535	-3.740310
	H	-3.887716	-1.451865	-4.829706
	H	-4.583893	-2.286500	-3.399290
	H	-4.789245	-0.515920	-3.588852

4-5 (isomer)



Zero-point correction= 0.954340 (Hartree/Particle)
Thermal correction to Energy= 1.031433
Thermal correction to Enthalpy= 1.032551
Thermal correction to Gibbs Free Energy= 0.839639
Sum of electronic and zero-point Energies= -3735.168036
Sum of electronic and thermal Energies= -3735.090943
Sum of electronic and thermal Enthalpies= -3735.089825
Sum of electronic and thermal Free Energies= -3735.282738

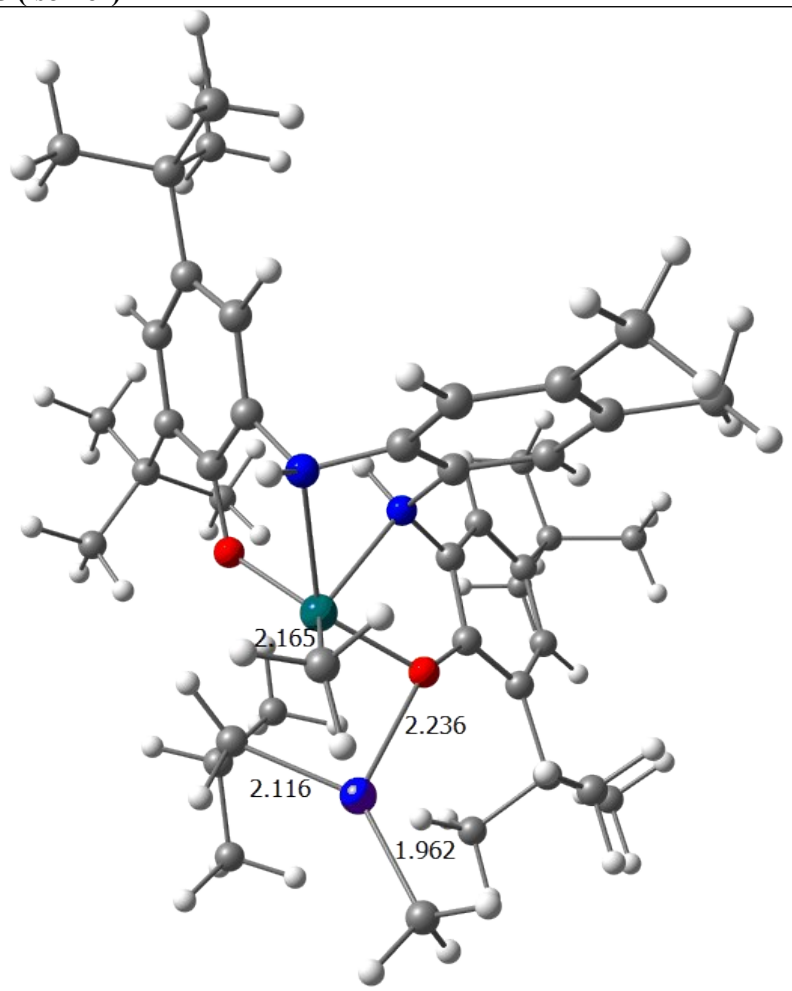
Solvent: -3735.5270891

113
PhTitBuCH3+propTS+POST--ZnMe2min0TS SCF Done: -3736.12237611 A.U.

Ti	-0.071364	-1.142621	-1.108743
N	0.183012	0.684312	0.211794
O	-1.855129	-0.402243	-0.838233
C	-2.177605	0.327273	0.281195
C	-1.048692	0.844835	0.955943
C	-1.137323	1.511497	2.180242
H	-0.218579	1.885679	2.653252
C	-2.406734	1.703281	2.761285
C	-3.529944	1.252704	2.029078
H	-4.521302	1.439099	2.461334
C	-3.478835	0.574947	0.790757
C	0.366047	1.690317	-0.840046
C	-2.604925	2.395689	4.123567
N	1.763716	0.018223	-1.914576
O	1.381462	-1.825760	-0.150482
C	2.573138	-1.193134	0.000850
C	2.841321	-0.176502	-0.937657
C	4.008887	0.594035	-0.907329
H	4.144376	1.386175	-1.657100
C	4.968555	0.338984	0.091069
C	4.681329	-0.684713	1.029812
H	5.424407	-0.876047	1.815227
C	3.508806	-1.465951	1.037681
C	1.171767	1.334494	-1.941357
C	6.290115	1.126640	0.198406
C	-4.761168	0.161491	0.042321
C	3.215455	-2.532987	2.107664
H	1.016415	0.621768	0.822300
H	2.081417	-0.251568	-2.857370
H	-2.644107	-2.523042	1.135069
C	6.408883	2.205536	-0.897942
H	6.397586	1.764597	-1.916729
H	5.594570	2.957338	-0.830720
H	7.368421	2.750118	-0.787380
C	6.357215	1.824013	1.581843
H	6.330255	1.095237	2.417557
H	7.300212	2.401820	1.676389
H	5.508537	2.526992	1.714961
C	7.478832	0.141819	0.051673
H	8.442743	0.687812	0.120894
H	7.476381	-0.632060	0.846035
H	7.446247	-0.377428	-0.928483
C	4.359887	-2.655692	3.135454
H	5.315938	-2.956176	2.659123
H	4.526740	-1.709683	3.691297
H	4.104210	-3.435518	3.881288
C	3.030973	-3.909802	1.418298
H	2.229003	-3.881250	0.655381
H	3.969256	-4.226636	0.918293
H	2.764644	-4.682261	2.169531
C	1.922697	-2.129062	2.866380
H	2.058656	-1.155544	3.383155
H	1.056967	-2.043945	2.183044
H	1.673552	-2.889170	3.635722
C	-4.872938	-1.381873	0.012884
H	-3.978826	-1.856666	-0.433668
H	-4.988421	-1.784821	1.039686
H	-5.748403	-1.700334	-0.588639
C	-4.712636	0.751280	-1.391104
H	-4.672299	1.859412	-1.353859
H	-3.831622	0.399581	-1.960382
H	-5.618797	0.458142	-1.959921
C	-6.035865	0.707725	0.723525
H	-6.179024	0.295725	1.743531
H	-6.031088	1.815414	0.788913
H	-6.923255	0.414036	0.126862
C	-3.327025	1.415696	5.084616
H	-3.470086	1.887419	6.079053
H	-4.328668	1.125440	4.706794
H	-2.734684	0.487839	5.224759
C	-3.468398	3.668809	3.928600
H	-4.472003	3.432772	3.519855
H	-3.617760	4.185302	4.899644
H	-2.976350	4.380475	3.233235
C	-1.262041	2.807030	4.761969
H	-0.604183	1.931416	4.943013
H	-0.709891	3.538846	4.135509
H	-1.444978	3.290130	5.743049
C	-0.881587	-3.669596	0.491175
C	-0.884903	-3.161457	-0.975340
H	0.182525	-3.717721	0.802316
H	-0.112522	-3.691339	-1.578997
H	-1.853314	-3.528882	-1.420052
C	-1.465807	-5.092513	0.564721
H	-0.944622	-5.782895	-0.130308
H	-1.372699	-5.508265	1.590323
H	-2.545863	-5.093437	0.299995
C	-1.607151	-2.728836	1.466151

	H	-1.099498	-1.746982	1.574613
	H	-1.653269	-3.172108	2.481598
	C	-0.296866	2.926338	-0.842819
	C	1.307892	2.215990	-3.024391
	C	0.646540	3.459773	-3.037247
	C	-0.166496	3.822196	-1.922171
	H	-0.940486	3.187829	0.010344
	H	1.938044	1.921540	-3.879507
	C	-0.885622	5.148268	-1.901535
	H	-1.575627	5.246559	-2.766833
	H	-1.478470	5.281431	-0.976339
	H	-0.171113	5.996041	-1.974450
	C	0.797341	4.395017	-4.210418
	H	-0.187165	4.625443	-4.670840
	H	1.228774	5.369026	-3.894700
	H	1.451423	3.972771	-4.997417
	Zn	-2.365530	-1.812692	-2.356144
	C	-0.384789	-1.372611	-3.306442
	H	-0.224649	-0.352545	-3.717941
	H	0.556354	-1.966857	-3.365459
	H	-1.028217	-1.892161	-4.056328
	C	-4.023510	-2.393147	-3.237076
	H	-3.816762	-2.781957	-4.256864
	H	-4.509883	-3.203910	-2.654726
	H	-4.749929	-1.560100	-3.327787

5 (isomer)



Zero-point correction= 0.953928 (Hartree/Particle)
Thermal correction to Energy= 1.032242
Thermal correction to Enthalpy= 1.033360
Thermal correction to Gibbs Free Energy= 0.836112
Sum of electronic and zero-point Energies= -3735.169517
Sum of electronic and thermal Energies= -3735.091204
Sum of electronic and thermal Enthalpies= -3735.090085
Sum of electronic and thermal Free Energies= -3735.287334

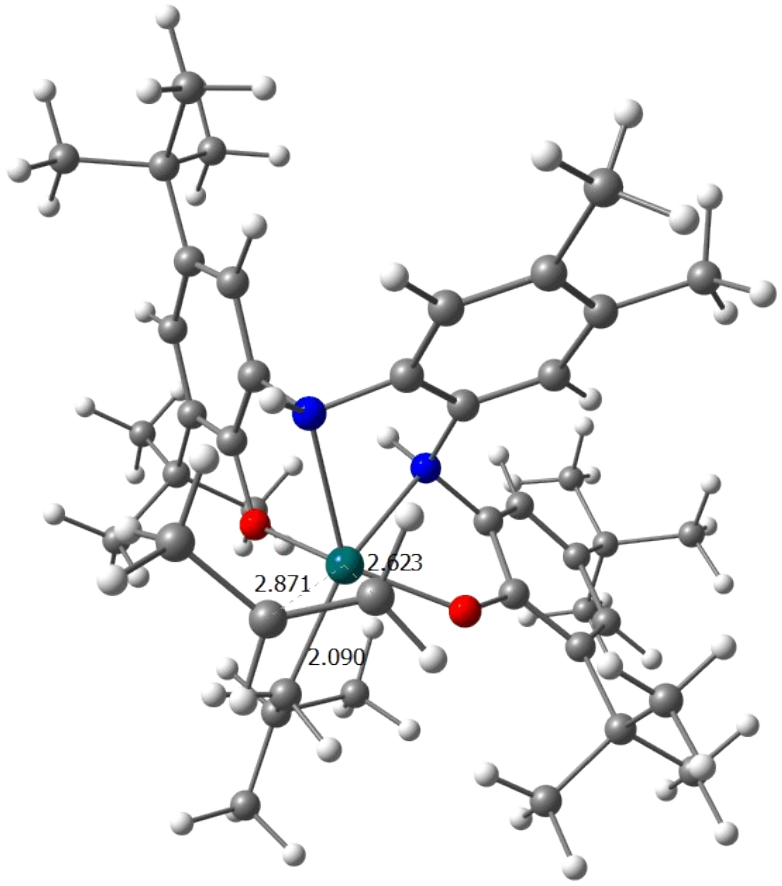
Solvent: -3735.5261814

113
PhTitBuCH3+propTS+POST--ZnMe2min SCF Done: -3736.12344539 A.U.

Ti	-0.137022	-1.305212	-0.908452
N	0.257412	0.756152	-0.027277
O	-1.859179	-0.472819	-0.719529
C	-2.106269	0.517777	0.204719
C	-0.937148	1.145461	0.687325
C	-0.953341	2.099322	1.707924
H	-0.003660	2.542537	2.038742
C	-2.188977	2.476856	2.269989
C	-3.354630	1.899070	1.716125
H	-4.320952	2.221725	2.124110
C	-3.376693	0.931650	0.686562
C	0.503785	1.487860	-1.266126
C	-2.305745	3.493534	3.422012
N	1.798725	-0.471989	-1.849593
O	1.228186	-1.797801	0.285792
C	2.469715	-1.253104	0.322425
C	2.845311	-0.522962	-0.822774
C	4.084889	0.115869	-0.939553
H	4.307234	0.684212	-1.853605
C	5.004239	0.019721	0.122747
C	4.600932	-0.700967	1.276138
H	5.308632	-0.754498	2.114195
C	3.352565	-1.334380	1.434774
C	1.323283	0.843093	-2.214242
C	6.401512	0.670414	0.076287
C	-4.704548	0.383180	0.128110
C	2.905628	-1.995977	2.751040
H	1.099035	0.749743	0.575882
H	2.088995	-0.996089	-2.688765
H	-2.320595	-1.869676	1.512809
C	6.636474	1.435371	-1.242885
H	6.578419	0.766048	-2.126640
H	5.907356	2.261743	-1.378723
H	7.648926	1.887622	-1.240923
C	6.541238	1.669930	1.253425
H	6.439465	1.171245	2.238851
H	7.539121	2.155270	1.229728
H	5.770042	2.465900	1.192539
C	7.477674	-0.438994	0.202415
H	8.494510	0.005277	0.174047
H	7.384832	-1.000058	1.154778
H	7.397059	-1.168562	-0.629917
C	4.048285	-2.058629	3.786168
H	4.907858	-2.653669	3.414007
H	4.417039	-1.051300	4.069743
H	3.682631	-2.545504	4.713071
C	2.409050	-3.441951	2.492702
H	1.546514	-3.463849	1.800103
H	3.219075	-4.062684	2.057063
H	2.096026	-3.911808	3.448137
C	1.759022	-1.127780	3.338409
H	2.126696	-0.111749	3.592601
H	0.919143	-1.021322	2.622429
H	1.354273	-1.587334	4.264196
C	-4.848110	-1.102037	0.531944
H	-4.016697	-1.714503	0.133304
H	-4.847432	-1.218827	1.634540
H	-5.788986	-1.532168	0.131997
C	-4.711734	0.546740	-1.413408
H	-4.656020	1.619944	-1.689764
H	-3.861685	0.025862	-1.891412
H	-5.645259	0.128182	-1.841783
C	-5.929816	1.139831	0.687131
H	-6.040219	1.015433	1.784077
H	-5.887038	2.224622	0.458366
H	-6.851596	0.738340	0.219374
C	-3.020334	2.819145	4.621499
H	-3.115744	3.535623	5.463749
H	-4.042098	2.476966	4.358814
H	-2.448304	1.938753	4.980928
C	-3.131490	4.714754	2.940334
H	-4.158787	4.428522	2.635297
H	-3.222621	5.463761	3.754349
H	-2.644439	5.207435	2.073096
C	-0.923467	3.990527	3.893980
H	-0.288561	3.158009	4.263146
H	-0.373514	4.522380	3.089357
H	-1.046838	4.706018	4.732035
C	-1.495168	-3.808704	0.892128
C	-1.027327	-3.429061	-0.538358
H	-0.745366	-4.523829	1.303515
H	0.086946	-3.460102	-0.607913
H	-1.271558	-4.253007	-1.253440
C	-2.851774	-4.532272	0.838646
H	-2.807486	-5.443665	0.207253
H	-3.189289	-4.831883	1.851718
H	-3.639920	-3.871417	0.412723
C	-1.558186	-2.602445	1.846271

	H	-0.585011	-2.077380	1.914710
	H	-1.828344	-2.919357	2.873947
	C	-0.091950	2.716525	-1.582411
	C	1.553382	1.438270	-3.462358
	C	0.963849	2.675599	-3.792158
	C	0.127031	3.324329	-2.834741
	H	-0.747761	3.199298	-0.842397
	H	2.191231	0.921075	-4.197328
	C	-0.521213	4.646782	-3.161798
	H	-1.172668	4.565438	-4.058229
	H	-1.140205	5.020971	-2.323966
	H	0.238837	5.421978	-3.398029
	C	1.211417	3.304304	-5.140284
	H	0.259888	3.465919	-5.690556
	H	1.684308	4.304355	-5.036164
	H	1.870485	2.681067	-5.774780
	Zn	-2.527863	-2.405267	-1.624417
	C	-0.358134	-1.876231	-2.985226
	H	-0.160350	-0.953957	-3.575754
	H	0.426141	-2.637492	-3.195198
	H	-1.295454	-2.292112	-3.428979
	C	-4.142850	-2.689999	-2.701185
	H	-4.232500	-1.917130	-3.493589
	H	-4.111893	-3.685492	-3.193570
	H	-5.058778	-2.644890	-2.077794

6 (isomer)



Zero-point correction= 0.963588 (Hartree/Particle)
Thermal correction to Energy= 1.039421
Thermal correction to Enthalpy= 1.040540
Thermal correction to Gibbs Free Energy= 0.849925
Sum of electronic and zero-point Energies= -1993.805311
Sum of electronic and thermal Energies= -1993.729478
Sum of electronic and thermal Enthalpies= -1993.728360
Sum of electronic and thermal Free Energies= -1993.918975

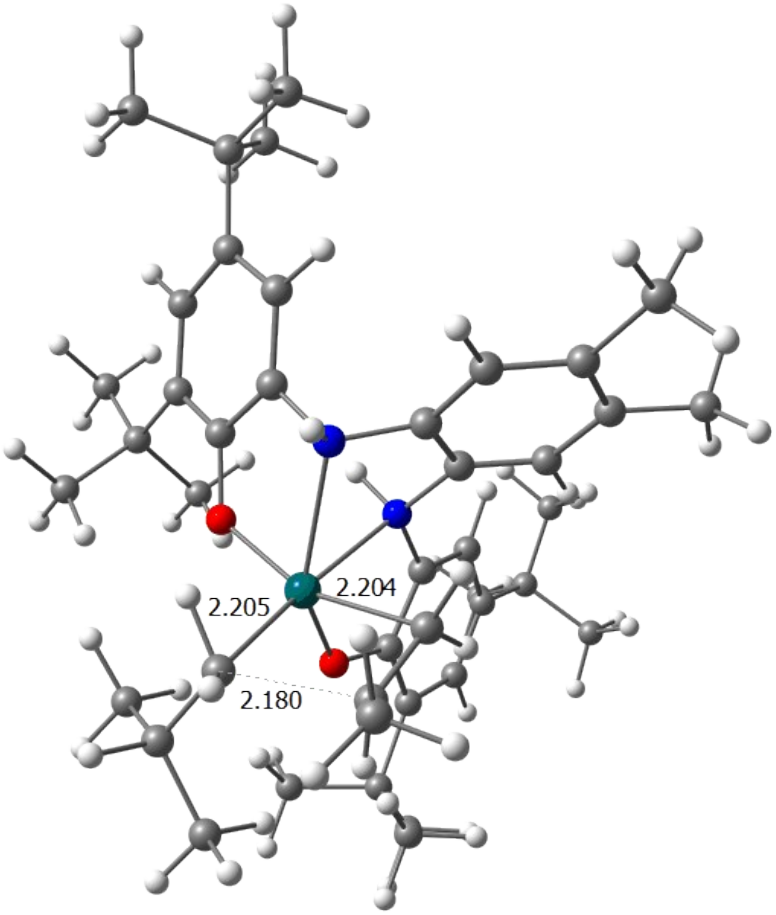
Solvent: -1994.4254334

113
PhTitBuCH3+propTS2+PRE SCF Done: -1994.76889968 A.U.

Ti	-0.073064	-0.372587	-1.717132
N	-0.200369	0.368625	0.484684
O	-1.836601	0.190289	-1.431834
C	-2.452618	0.147896	-0.225623
C	-1.571820	0.126130	0.879642
C	-2.019205	-0.076916	2.187603
H	-1.290415	-0.098132	3.009577
C	-3.403186	-0.234810	2.414484
C	-4.273702	-0.127420	1.300285
H	-5.351741	-0.216517	1.488676
C	-3.854763	0.072648	-0.031212
C	0.094606	1.782392	0.247133
C	-3.988406	-0.499995	3.815873
N	1.741018	1.018899	-1.394873
O	1.238566	-1.496104	-0.978473
C	2.337328	-1.059435	-0.321780
C	2.687847	0.288285	-0.539074
C	3.801609	0.889064	0.058901
H	4.006045	1.951476	-0.136213
C	4.617702	0.119100	0.909232
C	4.240644	-1.229824	1.134429
H	4.866497	-1.824335	1.813129
C	3.118790	-1.859029	0.561212
C	1.061079	2.109968	-0.727134
C	5.870015	0.689015	1.604826
C	-4.830193	0.233737	-1.212789
C	2.721935	-3.312808	0.873775
H	0.493912	-0.073781	1.109659
H	2.229556	1.375696	-2.228504
H	-2.821119	-2.639753	-1.067175
C	6.113161	2.167060	1.235045
H	6.276930	2.300331	0.145027
H	5.268852	2.817854	1.545646
H	7.020992	2.540059	1.751081
C	5.687214	0.591533	3.141663
H	5.556485	-0.456823	3.479384
H	6.578799	0.999349	3.662181
H	4.800078	1.169751	3.474351
C	7.110414	-0.136124	1.174611
H	8.024847	0.260115	1.663414
H	7.018010	-1.204179	1.459106
H	7.258843	-0.089033	0.075915
C	3.682400	-3.970342	1.886585
H	4.721956	-4.023902	1.502200
H	3.695652	-3.433892	2.858254
H	3.352524	-5.009826	2.087542
C	2.749157	-4.142229	-0.436262
H	2.076511	-3.712489	-1.203674
H	3.775623	-4.178168	-0.855811
H	2.422958	-5.184280	-0.236561
C	1.294726	-3.319158	1.484688
H	1.266843	-2.728047	2.424854
H	0.547995	-2.903393	0.782269
H	0.985317	-4.356372	1.729781
C	-4.612676	-0.898584	-2.249234
H	-3.571629	-0.910162	-2.626227
H	-4.833149	-1.891071	-1.805047
H	-5.293790	-0.757018	-3.114160
C	-4.562310	1.610058	-1.879201
H	-4.729710	2.437085	-1.158356
H	-3.521520	1.683203	-2.253076
H	-5.249915	1.759535	-2.737670
C	-6.302279	0.195104	-0.752673
H	-6.570285	-0.779139	-0.293925
H	-6.531570	1.000160	-0.024096
H	-6.968226	0.340884	-1.627392
C	-4.727781	-1.863452	3.798048
H	-5.157621	-2.082099	4.797867
H	-5.561210	-1.873517	3.066169
H	-4.033539	-2.687628	3.532729
C	-4.985154	0.630318	4.180748
H	-5.834389	0.685738	3.469431
H	-5.410330	0.456836	5.191240
H	-4.480872	1.619081	4.185111
C	-2.892291	-0.551925	4.900493
H	-2.159361	-1.364029	4.711539
H	-2.340328	0.408264	4.980061
H	-3.351435	-0.748660	5.890440
C	-0.934074	-3.323149	-1.974340
C	-0.655688	-2.055098	-2.811928
H	0.049747	-3.661786	-1.582364
H	0.186757	-2.258813	-3.514633
H	-1.552871	-1.757623	-3.405296
C	-1.510512	-4.440866	-2.864165
H	-0.848601	-4.656303	-3.728535
H	-1.636814	-5.382862	-2.288873
H	-2.507211	-4.153275	-3.263262
C	-1.846117	-3.067814	-0.762166

	H	-1.397000	-2.364682	-0.028679
	H	-2.042524	-4.010551	-0.211452
	C	-0.624224	2.815652	0.868065
	C	1.300829	3.454600	-1.052395
	C	0.585976	4.496875	-0.430604
	C	-0.392404	4.168617	0.553566
	H	-1.395375	2.551374	1.607429
	H	2.064435	3.693779	-1.811275
	C	-1.173911	5.256080	1.248758
	H	-1.736764	5.879055	0.521025
	H	-1.900157	4.841118	1.973637
	H	-0.501133	5.948763	1.798558
	C	0.855492	5.935322	-0.794639
	H	-0.062497	6.435108	-1.171177
	H	1.185724	6.518438	0.091511
	H	1.637745	6.028031	-1.572646
	C	-0.326813	1.223467	-3.783644
	C	0.515658	0.367927	-4.427479
	H	0.025484	2.168740	-3.332454
	H	-1.416748	1.062736	-3.799932
	H	0.070618	-0.514925	-4.919450
	C	1.996809	0.522061	-4.594393
	H	2.261887	0.450591	-5.670879
	H	2.374425	1.496725	-4.221043
	H	2.545344	-0.305623	-4.091866

6-7 (isomer)



Zero-point correction= 0.964250 (Hartree/Particle)
Thermal correction to Energy= 1.038579
Thermal correction to Enthalpy= 1.039697
Thermal correction to Gibbs Free Energy= 0.852074
Sum of electronic and zero-point Energies= -1993.791399
Sum of electronic and thermal Energies= -1993.717071
Sum of electronic and thermal Enthalpies= -1993.715952
Sum of electronic and thermal Free Energies= -1993.903576

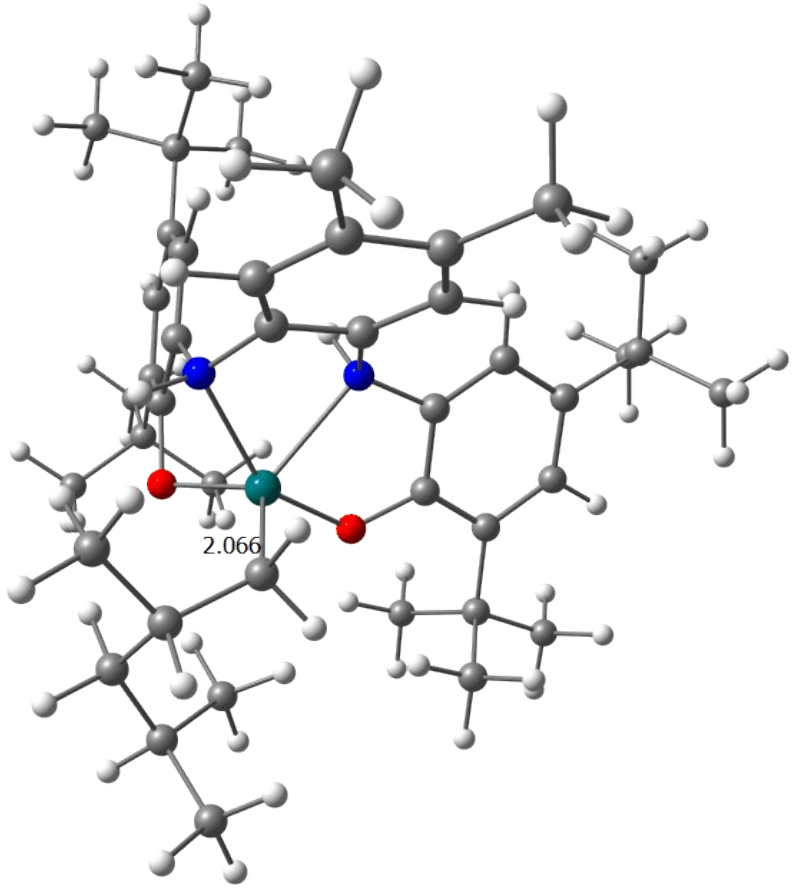
Solvent: -1994.4080054

113
PhTitBuCH3+propTS2+ SCF Done: -1994.75564940 A.U.

Ti	-0.275268	1.409144	1.127807
N	-0.153778	-0.712112	0.179778
O	-1.908182	1.197401	0.345464
C	-2.376723	0.080074	-0.284741
C	-1.453537	-0.979655	-0.421354
C	-1.768011	-2.129827	-1.158766
H	-0.997364	-2.898697	-1.301862
C	-3.054042	-2.270234	-1.715228
C	-3.981870	-1.222731	-1.497556
H	-4.992090	-1.341460	-1.910266
C	-3.696901	-0.034884	-0.797142
C	0.442432	-1.618839	1.146630
C	-3.477308	-3.509699	-2.528780
N	1.791264	0.345915	1.631984
O	0.873243	1.890953	-0.261630
C	2.063060	1.323686	-0.569874
C	2.640826	0.526139	0.439220
C	3.875675	-0.111599	0.269062
H	4.268700	-0.738686	1.080981
C	4.567795	0.041453	-0.947378
C	3.944431	0.804324	-1.967673
H	4.465952	0.887324	-2.930355
C	2.697894	1.445524	-1.838559
C	1.496740	-1.055980	1.894315
C	5.939740	-0.610817	-1.211010
C	-4.746478	1.066232	-0.557284
C	2.008827	2.190462	-2.996221
H	0.541415	-0.540526	-0.572974
H	2.250388	0.756616	2.460483
H	-1.434521	3.515982	-0.401528
C	6.454123	-1.390750	0.016744
H	6.583207	-0.731937	0.900999
H	5.775544	-2.224262	0.295197
H	7.444388	-1.836057	-0.208278
C	5.813927	-1.596132	-2.402181
H	5.493389	-1.085151	-3.332987
H	6.792161	-2.078479	-2.608095
H	5.075867	-2.395258	-2.181560
C	6.968909	0.496418	-1.555951
H	7.966124	0.048427	-1.747974
H	6.679959	1.065508	-2.463106
H	7.070696	1.219053	-0.719947
C	2.838085	2.127718	-4.295899
H	3.828629	2.614938	-4.182112
H	2.998074	1.084735	-4.639869
H	2.299997	2.663556	-5.103882
C	1.814063	3.678624	-2.611666
H	1.189464	3.779414	-1.704348
H	2.791233	4.168171	-2.420670
H	1.311335	4.225675	-3.436362
C	0.630769	1.524174	-3.267065
H	0.757281	0.454015	-3.535343
H	-0.040485	1.589447	-2.387726
H	0.123952	2.026917	-4.116810
C	-4.269243	2.396206	-1.194675
H	-3.311889	2.740371	-0.761556
H	-4.130329	2.280920	-2.289403
H	-5.024621	3.192052	-1.027170
C	-4.935621	1.236011	0.973829
H	-5.328596	0.303317	1.428351
H	-3.979235	1.483908	1.474625
H	-5.655717	2.053332	1.186047
C	-6.115428	0.704817	-1.171851
H	-6.060195	0.594133	-2.274570
H	-6.533020	-0.230805	-0.745595
H	-6.841059	1.515986	-0.958953
C	-3.880053	-3.065128	-3.958806
H	-4.187583	-3.944027	-4.563003
H	-4.730854	-2.353819	-3.947851
H	-3.031510	-2.570609	-4.475369
C	-4.686656	-4.185638	-1.832100
H	-5.562576	-3.508506	-1.767979
H	-5.003171	-5.085520	-2.399483
H	-4.426568	-4.502062	-0.800554
C	-2.338103	-4.544522	-2.640416
H	-1.449762	-4.131180	-3.162282
H	-2.018361	-4.919227	-1.645205
H	-2.682988	-5.421452	-3.224999
C	-1.183837	4.339736	1.644524
C	-0.354963	3.235261	2.361748
H	-0.755204	5.289657	2.043283
H	0.679151	3.150261	1.910235
H	-0.133963	3.562472	3.387550
C	-2.667439	4.309939	2.043306
H	-2.805763	4.310107	3.144611
H	-3.190567	5.201575	1.642529
H	-3.172237	3.415965	1.623791
C	-1.010750	4.400925	0.115654
H	0.057089	4.475913	-0.168686

	H	-1.534310	5.290489	-0.288500
	C	0.003799	-2.911690	1.448945
	C	2.130747	-1.800945	2.893114
	C	1.714494	-3.117402	3.191406
	C	0.626092	-3.673198	2.465124
	H	-0.853578	-3.336441	0.908743
	H	2.948890	-1.343230	3.473774
	C	0.135301	-5.066785	2.774691
	H	-0.183098	-5.158717	3.835276
	H	-0.722523	-5.354756	2.136783
	H	0.938439	-5.819935	2.624224
	C	2.404626	-3.911691	4.273252
	H	1.693798	-4.213942	5.071933
	H	2.836904	-4.852053	3.868832
	H	3.225407	-3.339335	4.747304
	C	-0.965567	0.328173	2.920217
	C	-1.333787	1.608371	3.433357
	H	-0.224994	-0.247871	3.499822
	H	-1.751457	-0.287964	2.447204
	H	-2.331276	1.987185	3.156321
	C	-0.882220	1.983855	4.829437
	H	-1.102265	3.036165	5.096136
	H	-1.433629	1.334186	5.543094
	H	0.199992	1.789723	4.979944

7 (isomer)



Zero-point correction= 0.966116 (Hartree/Particle)
Thermal correction to Energy= 1.040743
Thermal correction to Enthalpy= 1.041862
Thermal correction to Gibbs Free Energy= 0.851610
Sum of electronic and zero-point Energies= -1993.834359
Sum of electronic and thermal Energies= -1993.759732
Sum of electronic and thermal Enthalpies= -1993.758614
Sum of electronic and thermal Free Energies= -1993.948865

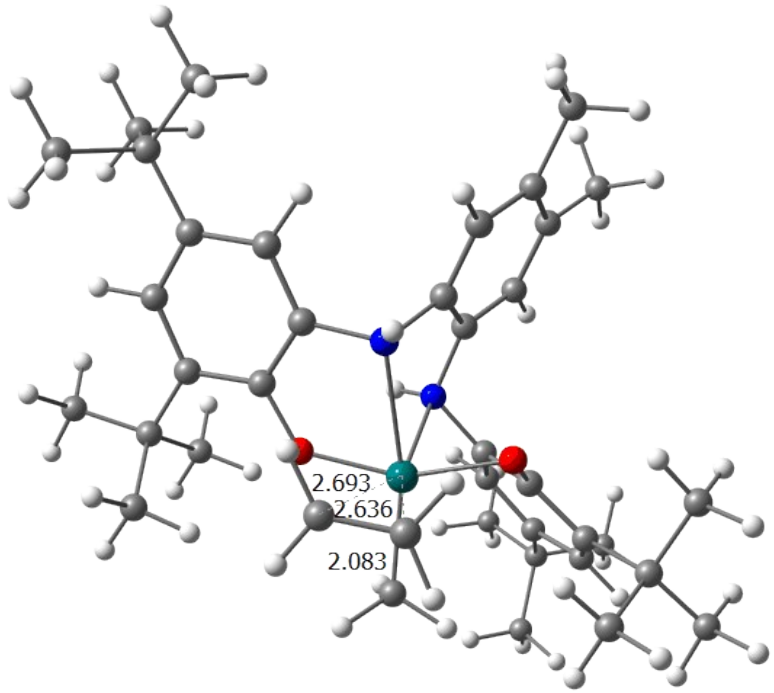
Solvent: -1994.4614209

113
PhTitBuCH3+propTS2+POST SCF Done: -1994.80047521 A.U.

Ti	-0.577354	1.217893	-0.536789
N	0.383252	-0.834600	-0.471024
O	1.022001	1.532083	0.293699
C	2.037360	0.636625	0.444724
C	1.746768	-0.681535	0.038992
C	2.653677	-1.731124	0.234648
H	2.361419	-2.755676	-0.031581
C	3.918335	-1.450226	0.790333
C	4.202802	-0.106564	1.140645
H	5.191480	0.110557	1.565693
C	3.300876	0.966277	1.000054
C	0.102872	-1.388869	-1.792415
C	4.979630	-2.543085	1.029188
N	-1.980065	-0.197234	-1.455093
O	-2.080310	1.652183	0.450247
C	-2.451868	0.391925	0.854748
C	-2.457006	-0.627814	-0.139292
C	-2.724059	-1.968735	0.168688
H	-2.678391	-2.711304	-0.640130
C	-3.036663	-2.321511	1.494773
C	-3.038650	-1.289436	2.470445
H	-3.271031	-1.570062	3.505935
C	-2.736046	0.059458	2.212179
C	-1.194861	-1.098806	-2.267874
C	-3.362114	-3.768266	1.910520
C	3.635691	2.415498	1.398911
C	-2.649008	1.125109	3.320473
H	-0.174802	-1.369426	0.223822
H	-2.701286	0.299270	-2.003394
H	0.542863	3.938517	-0.270883
C	-3.269971	-4.745426	0.720387
H	-3.992818	-4.492206	-0.082881
H	-2.250368	-4.770398	0.281194
H	-3.505834	-5.773786	1.060685
C	-2.353906	-4.221732	2.998780
H	-2.407465	-3.591297	3.909465
H	-2.567390	-5.266359	3.306352
H	-1.311940	-4.182955	2.617486
C	-4.804182	-3.814144	2.479851
H	-5.061535	-4.849258	2.786216
H	-4.919992	-3.164075	3.370674
H	-5.543326	-3.485901	1.720287
C	-3.040536	0.548516	4.697719
H	-4.081747	0.164480	4.706662
H	-2.361132	-0.267249	5.021573
H	-2.978165	1.348557	5.462504
C	-3.604298	2.303032	2.995443
H	-3.341735	2.795683	2.039933
H	-4.655191	1.952464	2.932053
H	-3.548065	3.063947	3.801129
C	-1.181030	1.630211	3.405117
H	-0.483983	0.792643	3.617249
H	-0.853874	2.122712	2.469534
H	-1.082670	2.370327	4.225644
C	2.620695	2.910860	2.464154
H	1.584082	2.914256	2.076339
H	2.652590	2.268735	3.368627
H	2.873700	3.946685	2.771987
C	3.556616	3.309306	0.132511
H	4.296712	2.984898	-0.627813
H	2.549673	3.275686	-0.327977
H	3.773451	4.365438	0.395641
C	5.055544	2.533766	1.990614
H	5.171098	1.930793	2.915134
H	5.837751	2.221682	1.267888
H	5.257808	3.590708	2.258020
C	5.316602	-2.601173	2.541990
H	6.072697	-3.389739	2.738315
H	5.733291	-1.642123	2.911653
H	4.412839	-2.832803	3.142996
C	6.257730	-2.194295	0.222943
H	6.691417	-1.221927	0.532683
H	7.035471	-2.970451	0.379872
H	6.040483	-2.138358	-0.863978
C	4.486557	-3.935942	0.584430
H	3.586965	-4.259259	1.149154
H	4.251150	-3.967233	-0.500432
H	5.277208	-4.691067	0.768975
C	-1.060045	5.219398	-1.112417
C	-2.053563	4.228439	-1.772863
H	-1.704360	6.015070	-0.673689
H	-2.595979	3.680898	-0.968128
H	-2.827762	4.827402	-2.301348
C	-0.129359	5.899116	-2.130301
H	-0.701487	6.357405	-2.964013
H	0.468383	6.701757	-1.651036
H	0.591235	5.178000	-2.574151
C	-0.266726	4.617590	0.063739

	H	-0.925132	4.054645	0.760197
	H	0.233665	5.410618	0.657268
	C	0.993219	-2.102441	-2.600370
	C	-1.601093	-1.551227	-3.527113
	C	-0.715616	-2.281796	-4.349855
	C	0.602746	-2.549874	-3.883032
	H	2.016002	-2.293524	-2.246384
	H	-2.614342	-1.311289	-3.887246
	C	1.579971	-3.304925	-4.750096
	H	1.736448	-2.791746	-5.722904
	H	2.567005	-3.414989	-4.261245
	H	1.203723	-4.322341	-4.991094
	C	-1.159146	-2.757633	-5.710840
	H	-0.514278	-2.341261	-6.514142
	H	-1.086186	-3.863111	-5.793972
	H	-2.205138	-2.469075	-5.929821
	C	-0.392366	2.274940	-2.301853
	C	-1.526817	3.196012	-2.802839
	H	-0.154551	1.482784	-3.055909
	H	0.549087	2.847343	-2.142711
	H	-1.100512	3.771406	-3.658438
	C	-2.718738	2.395795	-3.362783
	H	-3.413656	3.048770	-3.928710
	H	-2.391228	1.582684	-4.045814
	H	-3.326525	1.956707	-2.536729

2 (ethylene)



Zero-point correction= 0.852048 (Hartree/Particle)
Thermal correction to Energy= 0.921051
Thermal correction to Enthalpy= 0.922169
Thermal correction to Gibbs Free Energy= 0.745212
Sum of electronic and zero-point Energies= -1836.757762
Sum of electronic and thermal Energies= -1836.688759
Sum of electronic and thermal Enthalpies= -1836.687641
Sum of electronic and thermal Free Energies= -1836.864598

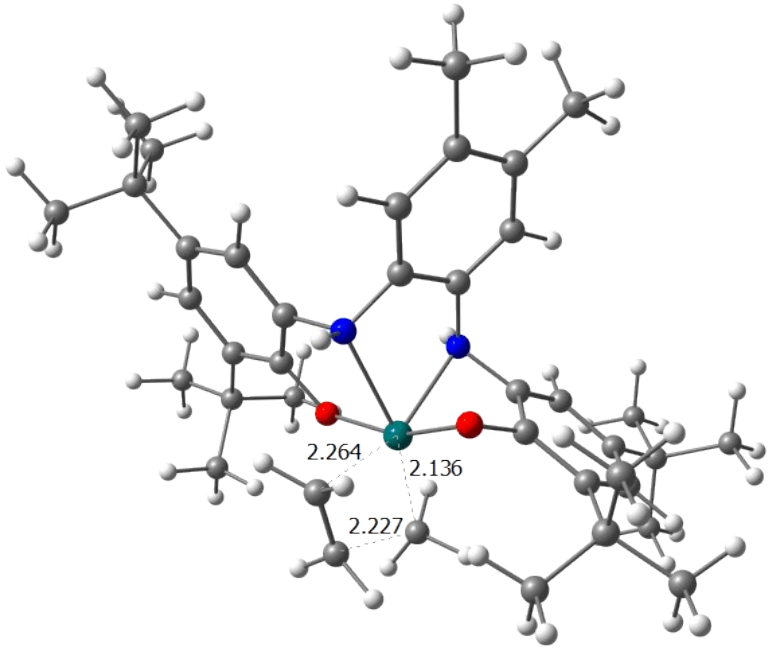
Solvent: -1837.2964238

101
PhTitBuCH3+etileTS+PRE SCF Done: -1837.60981021 A.U.

Ti	0.453713	-0.763007	1.107915
N	0.509856	0.222043	-0.806346
O	1.586934	0.749629	1.513093
C	2.481851	0.363820	0.576831
C	1.931268	-0.017583	-0.690736
C	2.699088	-0.640204	-1.693237
H	2.210014	-0.933444	-2.632948
C	4.063773	-0.857209	-1.470098
C	4.617894	-0.383415	-0.244025
H	5.697177	-0.519444	-0.095191
C	3.893491	0.226501	0.787394
C	0.064714	1.615083	-0.767027
C	4.973790	-1.562842	-2.491649
N	-1.328089	0.932453	1.123423
O	-1.077704	-1.654356	0.588061
C	-2.306390	-1.155575	0.325051
C	-2.500064	0.217743	0.600820
C	-3.733578	0.838350	0.366442
H	-3.836510	1.911252	0.579212
C	-4.810577	0.087918	-0.145127
C	-4.589028	-1.287471	-0.408252
H	-5.427975	-1.871751	-0.808552
C	-3.367885	-1.951370	-0.191177
C	-0.840046	1.977965	0.241771
C	-6.194157	0.705470	-0.429301
C	4.551747	0.748841	2.076189
C	-3.157005	-3.447537	-0.493064
H	0.083618	-0.304968	-1.583598
H	-1.556211	1.352240	2.035757
H	1.739937	-2.867759	0.434480
C	-6.245103	2.204136	-0.065191
H	-6.050401	2.375209	1.014305
H	-5.515878	2.799706	-0.653554
H	-7.253282	2.609678	-0.285385
C	-6.512033	0.555630	-1.939952
H	-6.538965	-0.507242	-2.255438
H	-7.504482	0.996720	-2.169273
H	-5.752222	1.075354	-2.559879
C	-7.266818	-0.040234	0.406473
H	-8.270151	0.397042	0.222099
H	-7.322044	-1.117345	0.148033
H	-7.051453	0.038308	1.492243
C	-4.443928	-4.112105	-1.025373
H	-5.273469	-4.058917	-0.290281
H	-4.788081	-3.654701	-1.976058
H	-4.250413	-5.185062	-1.227391
C	-2.732524	-4.183318	0.806534
H	-1.768657	-3.800945	1.195466
H	-3.503858	-4.066153	1.595897
H	-2.612455	-5.268366	0.606480
C	-2.049790	-3.598262	-1.570965
H	-2.340480	-3.080471	-2.508948
H	-1.083420	-3.184405	-1.220266
H	-1.892588	-4.670909	-1.808916
C	4.019309	-0.047084	3.295452
H	2.923723	0.061747	3.392921
H	4.264560	-1.125784	3.206820
H	4.487532	0.331272	4.227626
C	4.203252	2.252986	2.237228
H	4.582220	2.839175	1.374538
H	3.110387	2.413454	2.316543
H	4.678608	2.653807	3.156457
C	6.087482	0.604873	2.035142
H	6.408249	-0.455474	1.965788
H	6.535782	1.164702	1.188200
H	6.520954	1.016271	2.968975
C	5.550231	-2.844992	-1.834874
H	6.214610	-3.374791	-2.548653
H	6.148510	-2.617173	-0.929188
H	4.737492	-3.540545	-1.539191
C	6.131215	-0.612007	-2.893382
H	6.765276	-0.332101	-2.027596
H	6.788873	-1.106877	-3.637455
H	5.741001	0.322488	-3.346942
C	4.204673	-1.966524	-3.766170
H	3.376245	-2.671920	-3.545796
H	3.786448	-1.084809	-4.295571
H	4.889226	-2.477701	-4.472481
C	0.221032	-0.616470	3.729445
C	-0.880521	-1.326114	3.378603
H	1.168174	-1.119947	3.982737
H	-0.862660	-2.425848	3.315778
H	-1.855970	-0.850360	3.182951
H	0.205951	0.480611	3.838812
C	1.610755	-2.457435	1.466192
H	1.103263	-3.229232	2.082876
H	2.618443	-2.242421	1.878684
C	0.579381	2.575872	-1.644969
C	-1.217865	3.323928	0.361589

	C	-0.714209	4.308894	-0.513132
	C	0.195343	3.927793	-1.542747
	H	1.311341	2.265797	-2.408084
	H	-1.916476	3.617713	1.162081
	C	0.751726	4.957198	-2.495349
	H	1.305026	5.753505	-1.952807
	H	1.442922	4.505606	-3.232874
	H	-0.059339	5.467507	-3.057681
	C	-1.132218	5.750421	-0.360646
	H	-0.252981	6.409963	-0.198744
	H	-1.636495	6.122760	-1.278134
	H	-1.826160	5.893445	0.489951

2-3 (ethylene)



Zero-point correction= 0.854124 (Hartree/Particle)
Thermal correction to Energy= 0.920930
Thermal correction to Enthalpy= 0.922048
Thermal correction to Gibbs Free Energy= 0.750676
Sum of electronic and zero-point Energies= -1836.753613
Sum of electronic and thermal Energies= -1836.686806
Sum of electronic and thermal Enthalpies= -1836.685688
Sum of electronic and thermal Free Energies= -1836.857060

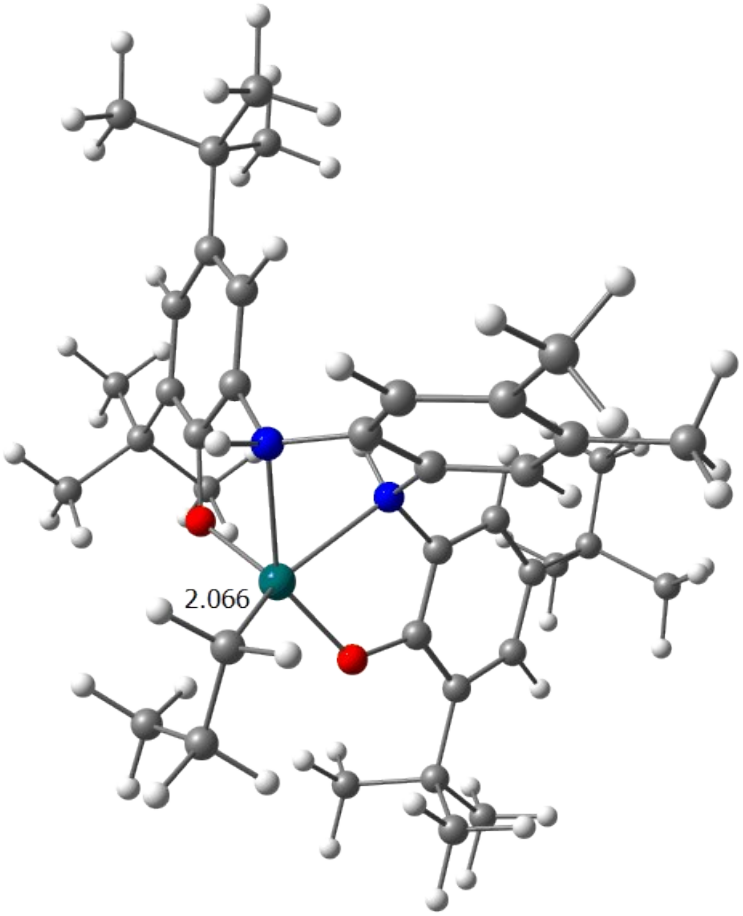
Solvent: -1837.2926268

101
PhTitBuCH3+etileTS+ SCF Done: -1837.60773638 A.U.

Ti	-0.386970	-0.916557	-0.891607
N	-0.618548	0.331600	0.892862
O	-1.515885	0.502527	-1.569630
C	-2.479169	0.280060	-0.646757
C	-2.043177	0.133614	0.706895
C	-2.910587	-0.268982	1.738353
H	-2.509274	-0.384499	2.755182
C	-4.261526	-0.505125	1.447295
C	-4.696508	-0.291125	0.107629
H	-5.761690	-0.449406	-0.106204
C	-3.867288	0.095545	-0.954174
C	-0.123079	1.694828	0.716776
C	-5.275673	-0.966616	2.510550
N	1.262912	0.749838	-1.061919
O	1.124425	-1.729071	-0.210652
C	2.361472	-1.190231	-0.094899
C	2.496951	0.142516	-0.539627
C	3.723264	0.814626	-0.468310
H	3.782949	1.856401	-0.809711
C	4.854027	0.150518	0.046062
C	4.692665	-1.191035	0.474686
H	5.575025	-1.710222	0.871373
C	3.478784	-1.900867	0.424137
C	0.802830	1.910582	-0.312297
C	6.235830	0.826064	0.153347
C	-4.390991	0.333295	-2.382354
C	3.336836	-3.364063	0.886188
H	-0.284493	-0.087382	1.773276
H	1.406938	1.033670	-2.041895
H	-1.317176	-2.497374	0.088592
C	6.208560	2.282533	-0.354927
H	5.925005	2.342651	-1.426738
H	5.507140	2.913234	0.230741
H	7.216397	2.734545	-0.257376
C	6.681747	0.833119	1.638835
H	6.766846	-0.192525	2.052380
H	7.675992	1.316050	1.740430
H	5.959982	1.394314	2.267975
C	7.259629	0.028132	-0.695308
H	8.262490	0.499730	-0.632262
H	7.362549	-1.019661	-0.346487
H	6.957828	0.002341	-1.762947
C	4.673648	-3.936708	1.402188
H	5.457441	-3.936567	0.616726
H	5.056009	-3.374125	2.278856
H	4.528185	-4.988243	1.722849
C	2.865736	-4.232065	-0.311847
H	1.882109	-3.894535	-0.694300
H	3.599074	-4.186016	-1.143477
H	2.768749	-5.293051	-0.000342
C	2.298774	-3.440770	2.037326
H	2.622960	-2.824214	2.901475
H	1.301168	-3.088628	1.707911
H	2.193354	-4.488782	2.387458
C	-3.726930	-0.673562	-3.358655
H	-2.627786	-0.549093	-3.374460
H	-3.969610	-1.720065	-3.076618
H	-4.104607	-0.507598	-4.388644
C	-4.041837	1.784770	-2.806475
H	-4.519837	2.518195	-2.124650
H	-2.948680	1.960282	-2.798371
H	-4.416758	1.979077	-3.832857
C	-5.920730	0.153145	-2.471093
H	-6.237705	-0.879856	-2.217140
H	-6.461698	0.859857	-1.808399
H	-6.255682	0.353018	-3.508995
C	-5.863915	-2.335774	2.078632
H	-6.602803	-2.688493	2.827813
H	-6.384435	-2.276509	1.101026
H	-5.066216	-3.103082	1.995312
C	-6.414518	0.080971	2.618429
H	-6.962939	0.203077	1.662265
H	-7.151686	-0.235032	3.385308
H	-6.016286	1.074127	2.912266
C	-4.624459	-1.128798	3.899341
H	-3.815409	-1.889090	3.892941
H	-4.207164	-0.171906	4.277057
H	-5.383965	-1.466296	4.633058
C	-0.384075	-2.428686	-2.904685
C	0.340624	-1.235766	-3.011198
H	0.162826	-3.365243	-2.719581
H	1.439602	-1.274875	-2.916366
H	-0.098012	-0.378410	-3.548838
H	-1.363594	-2.531921	-3.396472
C	-1.511401	-2.728975	-1.007166
H	-1.304466	-3.807132	-1.110154
H	-2.571954	-2.502521	-1.233482
C	-0.598604	2.766142	1.483287
C	1.235847	3.218134	-0.579832

	C	0.773601	4.310685	0.181697
	C	-0.153641	4.080625	1.240820
	H	-1.346922	2.572568	2.268520
	H	1.943703	3.395343	-1.405582
	C	-0.662610	5.230752	2.074269
	H	-1.175120	5.989951	1.445444
	H	-1.376279	4.894713	2.851031
	H	0.171762	5.759168	2.583344
	C	1.251501	5.709369	-0.121305
	H	0.402766	6.378114	-0.379863
	H	1.749243	6.164246	0.761761
	H	1.969004	5.728970	-0.964122

3 (ethylene)



Zero-point correction= 0.855042 (Hartree/Particle)
Thermal correction to Energy= 0.921884
Thermal correction to Enthalpy= 0.923003
Thermal correction to Gibbs Free Energy= 0.750549
Sum of electronic and zero-point Energies= -1836.789322
Sum of electronic and thermal Energies= -1836.722480
Sum of electronic and thermal Enthalpies= -1836.721362
Sum of electronic and thermal Free Energies= -1836.893815

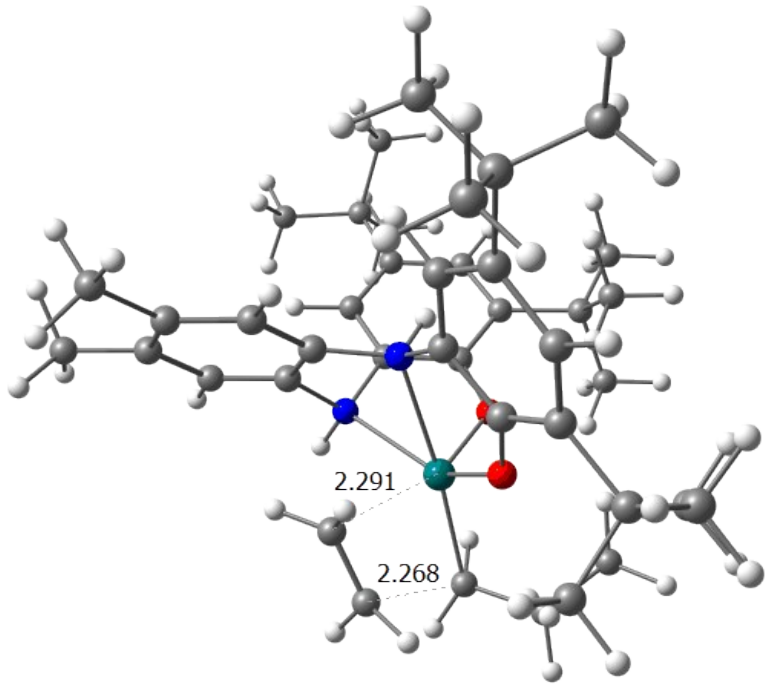
Solvent: -1837.3386826

101
PhTitBuCH3+etileTS+POST SCF Done: -1837.64436421
A.U.

Ti	-0.077267	-0.427907	-1.929238
N	-0.257126	0.566518	0.079563
O	-1.858661	-0.643162	-1.523344
C	-2.403858	-0.432295	-0.288723
C	-1.559360	0.214168	0.633880
C	-1.951814	0.477659	1.951088
H	-1.246765	0.975286	2.631540
C	-3.243594	0.095521	2.366780
C	-4.079776	-0.539631	1.415020
H	-5.085337	-0.836859	1.740881
C	-3.712164	-0.829878	0.085018
C	-0.030463	1.941806	-0.340212
C	-3.762861	0.342230	3.797696
N	1.716071	0.888577	-1.633135
O	1.172591	-1.631114	-1.309206
C	2.247394	-1.210047	-0.572675
C	2.565149	0.163534	-0.677371
C	3.592444	0.756770	0.063667
H	3.778950	1.833866	-0.051246
C	4.351939	-0.045883	0.938580
C	4.020019	-1.421980	1.024447
H	4.605943	-2.044769	1.713232
C	2.980748	-2.048748	0.306370
C	1.052961	2.108791	-1.230303
C	5.507758	0.517068	1.790152
C	-4.644472	-1.539731	-0.914816
C	2.614525	-3.534974	0.476577
H	0.518238	0.242444	0.688712
H	2.212733	1.021755	-2.527113
H	-0.667445	-2.536405	-2.897039
C	5.717678	2.026533	1.550946
H	5.975050	2.246154	0.493616
H	4.820875	2.620527	1.826089
H	6.557363	2.392788	2.175538
C	5.186788	0.295808	3.291129
H	5.071951	-0.779334	3.538151
H	6.006442	0.696502	3.923132
H	4.247779	0.813537	3.578263
C	6.817448	-0.226695	1.420691
H	7.665529	0.168751	2.017445
H	6.748745	-1.315055	1.622463
H	7.061148	-0.094626	0.346262
C	3.566447	-4.252561	1.456469
H	4.618916	-4.230153	1.105154
H	3.527102	-3.815292	2.475800
H	3.270832	-5.317527	1.544986
C	2.701096	-4.249200	-0.897864
H	2.002429	-3.808001	-1.635001
H	3.729413	-4.186223	-1.310229
H	2.445536	-5.323183	-0.783691
C	1.170407	-3.630927	1.040328
H	1.101771	-3.138526	2.032926
H	0.431231	-3.158550	0.363710
H	0.882435	-4.695040	1.168745
C	-3.977069	-2.857317	-1.391375
H	-3.020597	-2.664564	-1.915527
H	-3.774825	-3.531945	-0.533898
H	-4.649811	-3.390850	-2.094694
C	-4.893715	-0.603430	-2.126577
H	-5.382222	0.339079	-1.803228
H	-3.948548	-0.344350	-2.643093
H	-5.561932	-1.099799	-2.860924
C	-6.007349	-1.888732	-0.280810
H	-5.900961	-2.581559	0.579555
H	-6.552004	-0.984516	0.061350
H	-6.646995	-2.392694	-1.033479
C	-4.124883	-1.017803	4.449026
H	-4.497284	-0.862207	5.482973
H	-4.918654	-1.550336	3.886498
H	-3.238578	-1.683799	4.498904
C	-5.024131	1.241952	3.732128
H	-5.842285	0.770783	3.150275
H	-5.411919	1.435684	4.753988
H	-4.791452	2.219675	3.261032
C	-2.709533	1.041939	4.681499
H	-1.787292	0.433446	4.789553
H	-2.428233	2.039455	4.282858
H	-3.118156	1.200352	5.700037
C	-0.941830	-0.944951	-4.470807
C	-0.010841	0.154291	-3.910813
H	-0.914170	-0.927007	-5.583119
H	1.001944	0.093023	-4.368833
H	-0.413725	1.183272	-4.048064
H	-1.996657	-0.741530	-4.187435
C	-0.542963	-2.361343	-3.995794
H	0.512319	-2.595569	-4.243805
H	-1.191186	-3.133024	-4.456725
C	-0.828446	3.038474	0.007317

	C	1.345220	3.377784	-1.748340
	C	0.556493	4.493772	-1.400474
	C	-0.548327	4.319127	-0.512008
	H	-1.685256	2.887634	0.680925
	H	2.189829	3.496753	-2.446008
	C	-1.413229	5.495348	-0.132687
	H	-1.887715	5.951902	-1.027732
	H	-2.218591	5.205581	0.568876
	H	-0.813972	6.298736	0.346517
	C	0.872414	5.855982	-1.965190
	H	0.009126	6.268380	-2.529857
	H	1.092593	6.585072	-1.156200
	H	1.744681	5.830761	-2.646251

6-7 (ethylene)



Zero-point correction= 0.909132 (Hartree/Particle)
Thermal correction to Energy= 0.979970
Thermal correction to Enthalpy= 0.981088
Thermal correction to Gibbs Free Energy= 0.800567
Sum of electronic and zero-point Energies= -1915.269189
Sum of electronic and thermal Energies= -1915.198351
Sum of electronic and thermal Enthalpies= -1915.197233
Sum of electronic and thermal Free Energies= -1915.377754

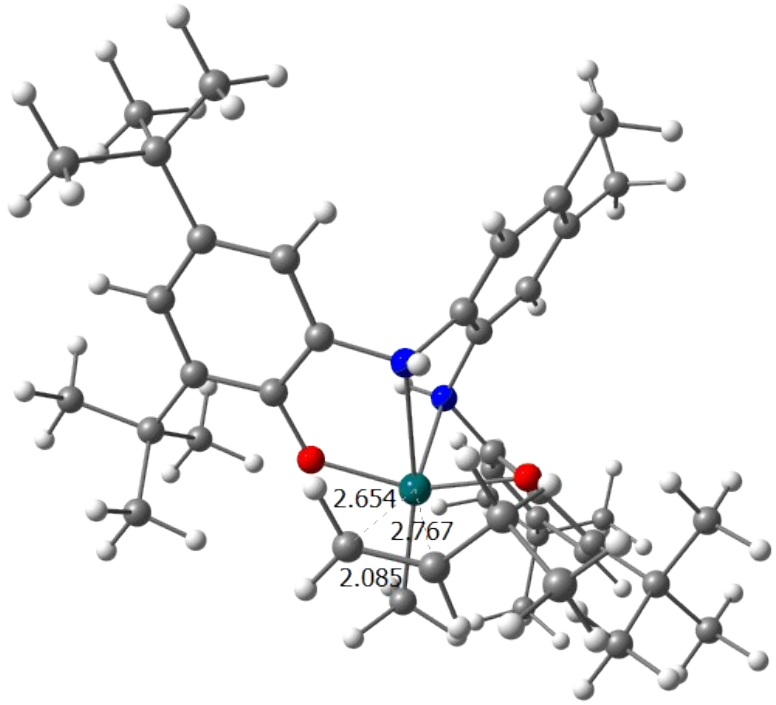
Solvent: -1915.8464998

107
PhTitBuCH3+etileTS2isomer+ SCF Done: -1916.17832125 A.U.

Ti	-0.185375	-1.021365	-1.706332
N	-0.296525	0.715793	-0.142983
O	-1.839301	-1.186499	-0.976914
C	-2.438985	-0.363997	-0.068228
C	-1.639145	0.691170	0.422271
C	-2.102410	1.540261	1.437044
H	-1.427731	2.302453	1.848049
C	-3.413611	1.385947	1.928833
C	-4.208891	0.352511	1.375792
H	-5.233230	0.238891	1.754095
C	-3.770393	-0.549639	0.387385
C	0.279508	1.914959	-0.724853
C	-3.993382	2.283284	3.040558
N	1.787650	0.280535	-1.711106
O	0.938102	-1.869455	-0.493700
C	2.092119	-1.387064	0.026948
C	2.611966	-0.236552	-0.598707
C	3.786585	0.383766	-0.156383
H	4.133621	1.294392	-0.663363
C	4.480973	-0.161101	0.940822
C	3.934004	-1.313033	1.562480
H	4.467431	-1.726155	2.428708
C	2.748795	-1.953829	1.154623
C	1.408558	1.676568	-1.535020
C	5.785814	0.456383	1.483328
C	-4.658510	-1.671635	-0.182367
C	2.154112	-3.176586	1.876728
H	0.371751	0.345186	0.560337
H	2.308091	0.182722	-2.598359
H	-0.804454	-3.850539	-0.837903
C	6.201987	1.713902	0.692533
H	6.392036	1.487378	-0.377554
H	5.434896	2.514423	0.751970
H	7.141769	2.127734	1.111022
C	5.581641	0.855938	2.967841
H	5.338470	-0.018589	3.605147
H	6.507382	1.314686	3.373546
H	4.758074	1.592686	3.071974
C	6.923325	-0.592085	1.375554
H	7.874546	-0.169660	1.761276
H	6.702519	-1.506645	1.962793
H	7.084878	-0.896408	0.320643
C	3.010654	-3.602337	3.086921
H	4.037568	-3.896767	2.786745
H	3.084052	-2.799301	3.849471
H	2.546668	-4.481933	3.577430
C	2.080016	-4.368747	0.887104
H	1.449606	-4.130638	0.009102
H	3.092489	-4.644382	0.526085
H	1.643767	-5.256225	1.391334
C	0.732022	-2.818751	2.389257
H	0.772827	-1.963544	3.096223
H	0.048048	-2.555708	1.558400
H	0.293717	-3.683273	2.929849
C	-4.010648	-3.046022	0.129607
H	-3.001021	-3.134266	-0.313403
H	-3.920692	-3.198928	1.224784
H	-4.638145	-3.865130	-0.279568
C	-4.795185	-1.478288	-1.716056
H	-5.277039	-0.506778	-1.951177
H	-3.808582	-1.503246	-2.219937
H	-5.420872	-2.285673	-2.150129
C	-6.073902	-1.653058	0.432024
H	-6.053051	-1.818637	1.528933
H	-6.604774	-0.699529	0.230889
H	-6.680311	-2.468424	-0.011848
C	-4.321201	1.403984	4.275447
H	-4.745715	2.026480	5.090608
H	-5.063336	0.615279	4.036007
H	-3.408353	0.905023	4.661665
C	-5.287996	2.964499	2.526691
H	-6.069445	2.225366	2.256733
H	-5.713368	3.622706	3.312644
H	-5.083842	3.585978	1.630153
C	-3.001899	3.384422	3.471703
H	-2.066538	2.962242	3.895115
H	-2.734360	4.055434	2.628080
H	-3.460622	4.014976	4.259947
C	-1.309897	-3.517056	-2.959926
C	-0.226077	-2.473288	-3.328256
H	-1.499858	-4.140453	-3.859557
H	0.743112	-2.665691	-2.783328
H	0.061274	-2.525339	-4.391080
H	-2.275707	-3.008587	-2.747031
C	-0.947838	-4.426607	-1.775571
H	-0.008313	-4.985226	-1.968488
H	-1.751086	-5.167650	-1.591041
C	-0.237484	3.211319	-0.637723

	C	2.037695	2.733429	-2.200114
	C	1.542310	4.052327	-2.098001
	C	0.378896	4.288601	-1.315344
	H	-1.151373	3.396443	-0.056953
	H	2.914539	2.528244	-2.836351
	C	-0.198723	5.678805	-1.208475
	H	-0.460119	6.086713	-2.208338
	H	-1.112158	5.700470	-0.583304
	H	0.533846	6.386865	-0.764783
	C	2.227783	5.185673	-2.821149
	H	1.540231	5.687381	-3.535306
	H	2.565670	5.970277	-2.110689
	H	3.113299	4.839490	-3.388561
	C	-0.946517	0.592914	-3.143529
	C	-1.102880	-0.495418	-4.008623
	H	-0.183112	1.353070	-3.368678
	H	-1.796888	0.933372	-2.527122
	H	-2.062635	-1.033215	-4.077030
	H	-0.468620	-0.559884	-4.905035

2 (1-butene)



Zero-point correction= 0.907412 (Hartree/Particle)
Thermal correction to Energy= 0.980074
Thermal correction to Enthalpy= 0.981192
Thermal correction to Gibbs Free Energy= 0.796319
Sum of electronic and zero-point Energies= -1915.286956
Sum of electronic and thermal Energies= -1915.214293
Sum of electronic and thermal Enthalpies= -1915.213175
Sum of electronic and thermal Free Energies= -1915.398048

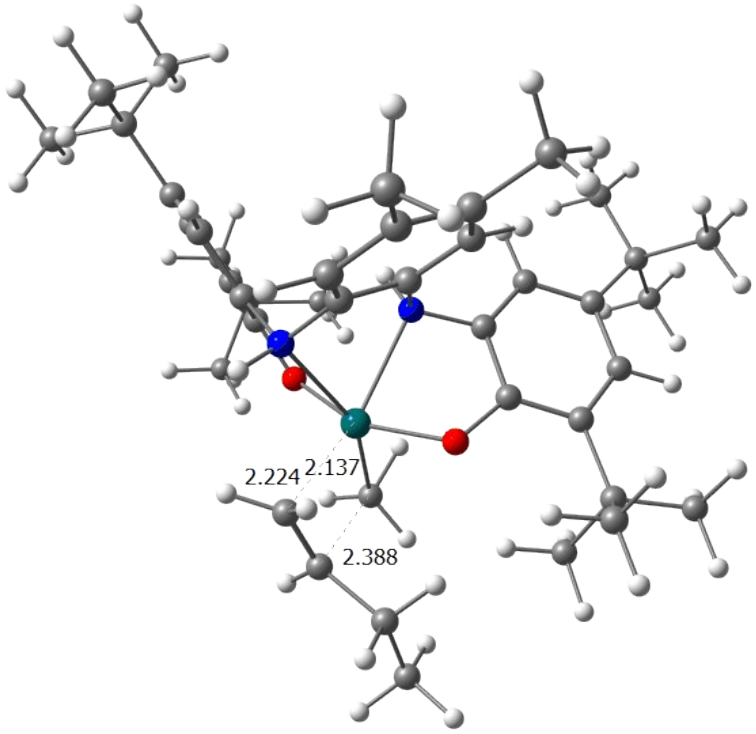
Solvent: -1915.8670269

107
PhTitBuCH3+buteneTS+PRE SCF Done: -1916.19436713 A.U.

Ti	0.412593	-0.644377	1.023927
N	0.494328	-0.107724	-1.063681
O	1.562111	0.910373	1.083881
C	2.461400	0.331769	0.258550
C	1.916359	-0.316860	-0.896159
C	2.693420	-1.130203	-1.741872
H	2.210540	-1.622300	-2.597769
C	4.061342	-1.275483	-1.479155
C	4.607981	-0.543219	-0.383820
H	5.689788	-0.626037	-0.215465
C	3.872622	0.260984	0.495632
C	0.057445	1.264383	-1.327459
C	4.984404	-2.163416	-2.333261
N	-1.319437	1.023981	0.678723
O	-1.121404	-1.614598	0.695806
C	-2.347802	-1.160804	0.349111
C	-2.515588	0.242733	0.341247
C	-3.744815	0.827006	0.012300
H	-3.825769	1.922557	0.005914
C	-4.845090	0.009488	-0.312494
C	-4.647427	-1.394210	-0.301974
H	-5.502471	-2.032325	-0.560226
C	-3.430372	-2.023667	0.018430
C	-0.830702	1.848226	-0.411487
C	-6.229479	0.584556	-0.673092
C	4.516527	1.061302	1.641939
C	-3.246512	-3.553461	0.015926
H	0.068316	-0.788787	-1.710199
H	-1.511315	1.627159	1.491111
H	1.746355	-2.828128	0.883194
C	-6.241924	2.126862	-0.636085
H	-6.001728	2.519430	0.374295
H	-5.526608	2.565176	-1.363298
H	-7.251287	2.501715	-0.901072
C	-6.614772	0.124710	-2.103320
H	-6.676846	-0.979732	-2.183169
H	-7.607515	0.534437	-2.383454
H	-5.872793	0.478627	-2.848911
C	-7.276070	0.059067	0.343615
H	-8.282610	0.460149	0.102614
H	-7.347536	-1.047675	0.331928
H	-7.018742	0.371931	1.376800
C	-4.545216	-4.287538	-0.379695
H	-5.373300	-4.079672	0.329151
H	-4.882685	-4.017412	-1.401828
H	-4.369917	-5.382450	-0.368557
C	-2.833613	-4.022943	1.436599
H	-1.877099	-3.562985	1.752724
H	-3.613998	-3.759782	2.180351
H	-2.705863	-5.125310	1.451011
C	-2.143645	-3.933352	-1.008880
H	-2.420173	-3.593535	-2.029058
H	-1.166178	-3.486970	-0.738013
H	-2.015227	-5.035351	-1.040405
C	3.987044	0.542981	3.003522
H	2.888392	0.642326	3.065066
H	4.255690	-0.522379	3.157953
H	4.433931	1.129703	3.832652
C	4.146021	2.559014	1.471232
H	4.523644	2.951068	0.504215
H	3.050195	2.714512	1.505206
H	4.606002	3.157193	2.285054
C	6.054061	0.934610	1.638122
H	6.388924	-0.110788	1.801091
H	6.500285	1.302617	0.690975
H	6.476765	1.545295	2.461378
C	5.626382	-3.240296	-1.419271
H	6.296767	-3.895411	-2.013425
H	6.235201	-2.791497	-0.608068
H	4.849742	-3.878026	-0.948529
C	6.094080	-1.284103	-2.966969
H	6.717930	-0.780325	-2.200848
H	6.770024	-1.910193	-3.585510
H	5.657187	-0.500132	-3.619591
C	4.215540	-2.875430	-3.465089
H	3.416516	-3.537930	-3.071166
H	3.758620	-2.154934	-4.175522
H	4.911333	-3.511341	-4.048545
C	0.204451	0.221641	3.644088
C	-0.848853	-0.591839	3.358188
H	1.165422	-0.252556	3.922132
H	-0.771175	-1.686668	3.436956
H	-1.852618	-0.190135	3.136284
C	0.174115	1.724164	3.712891
H	0.777875	2.124771	2.868369
H	-0.869102	2.088368	3.578426
C	1.574534	-2.196682	1.789374
H	1.063411	-2.822434	2.551324

	H	2.563715	-1.869701	2.171731
	C	0.569982	2.007442	-2.397101
	C	-1.193624	3.192865	-0.579649
	C	-0.691643	3.959945	-1.650994
	C	0.200517	3.354581	-2.584002
	H	1.290811	1.532083	-3.081595
	H	-1.879563	3.659050	0.146360
	C	0.754981	4.149610	-3.740637
	H	1.316375	5.040633	-3.386417
	H	1.438089	3.544792	-4.367691
	H	-0.057782	4.532334	-4.394575
	C	-1.093078	5.405674	-1.808630
	H	-0.206947	6.075419	-1.781505
	H	-1.587190	5.581742	-2.788048
	H	-1.790122	5.731625	-1.012685
	C	0.754476	2.247909	5.040518
	H	0.180565	1.873345	5.912340
	H	1.810004	1.927362	5.163097
	H	0.734067	3.355695	5.065111

2-3 (isomer) (1-butene)



Zero-point correction= 0.908201 (Hartree/Particle)
Thermal correction to Energy= 0.979120
Thermal correction to Enthalpy= 0.980238
Thermal correction to Gibbs Free Energy= 0.799386
Sum of electronic and zero-point Energies= -1915.280697
Sum of electronic and thermal Energies= -1915.209778
Sum of electronic and thermal Enthalpies= -1915.208660
Sum of electronic and thermal Free Energies= -1915.389512

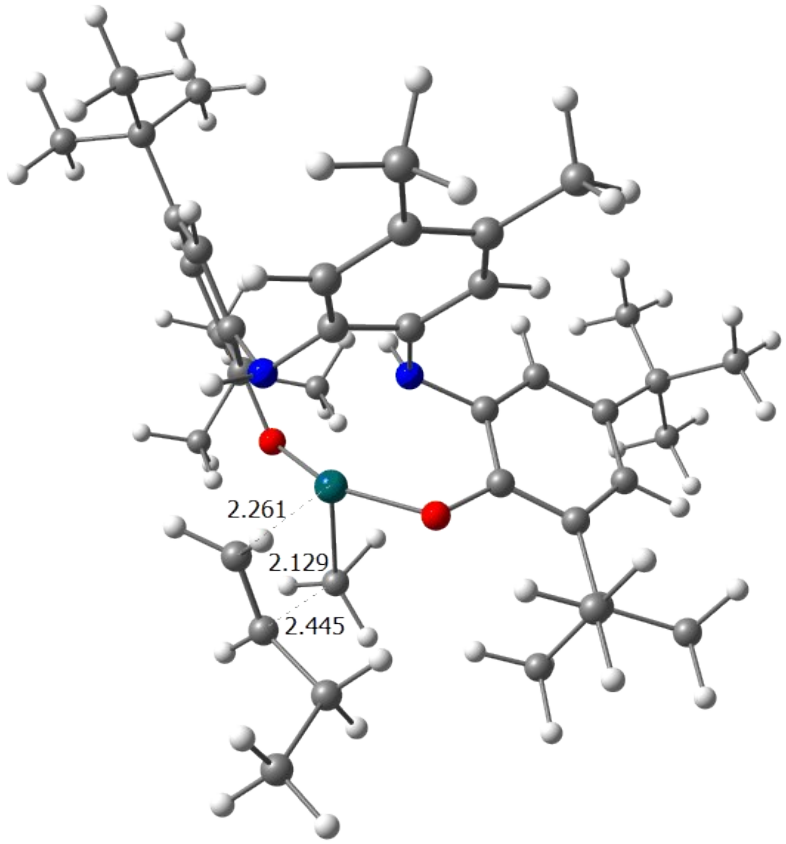
Solvent: -1915.8607013

107
PhTitBuCH3+buteneTS+ SCF Done: -1916.18889756 A.U.

Ti	0.174910	1.679391	-0.547078
N	0.135949	-0.519977	0.127472
O	1.900458	1.005559	-0.876349
C	2.436256	0.072822	-0.036599
C	1.481301	-0.728198	0.631642
C	1.834358	-1.664686	1.607319
H	1.046102	-2.257458	2.092248
C	3.197754	-1.839430	1.924349
C	4.142900	-1.065556	1.207158
H	5.204940	-1.216563	1.440922
C	3.820176	-0.103114	0.227213
C	-0.129935	-1.266649	-1.107140
C	3.680060	-2.843327	2.990263
N	-1.578916	0.600744	-1.669096
O	-1.276547	1.875974	0.609062
C	-2.419082	1.151601	0.541127
C	-2.658237	0.477070	-0.673406
C	-3.806533	-0.294335	-0.886986
H	-3.928631	-0.815100	-1.847264
C	-4.764128	-0.402079	0.139893
C	-4.492309	0.260250	1.364174
H	-5.227639	0.156571	2.172800
C	-3.340503	1.029345	1.618800
C	-0.987538	-0.666420	-2.045629
C	-6.061955	-1.220059	-0.015217
C	4.888117	0.735239	-0.498765
C	-3.046249	1.683173	2.982306
H	-0.591201	-0.703268	0.839204
H	-1.940792	1.070246	-2.511595
H	1.150960	2.350837	1.205866
C	-6.184529	-1.847289	-1.419413
H	-6.201573	-1.075402	-2.217181
H	-5.356003	-2.555015	-1.632393
H	-7.131593	-2.419081	-1.494967
C	-6.071958	-2.361240	1.034940
H	-6.033437	-1.971721	2.072757
H	-6.999189	-2.964036	0.940033
H	-5.204599	-3.039337	0.893684
C	-7.280060	-0.288540	0.214964
H	-8.226406	-0.858525	0.107006
H	-7.275788	0.159020	1.229831
H	-7.291911	0.541357	-0.521697
C	-4.161699	1.400499	4.010527
H	-5.139602	1.812984	3.686697
H	-4.286618	0.315028	4.205124
H	-3.905308	1.881345	4.976424
C	-2.921329	3.219206	2.807254
H	-2.105136	3.481179	2.106309
H	-3.867309	3.648500	2.417324
H	-2.706062	3.697800	3.785485
C	-1.716454	1.102074	3.536284
H	-1.791752	0.001812	3.667775
H	-0.864403	1.321970	2.862479
H	-1.487871	1.545907	4.527502
C	4.694599	2.222525	-0.109706
H	3.678279	2.566514	-0.373319
H	4.837174	2.370401	0.980679
H	5.425468	2.864326	-0.644362
C	4.724339	0.558937	-2.031282
H	4.880406	-0.500156	-2.323467
H	3.716417	0.862517	-2.375681
H	5.475329	1.174722	-2.569030
C	6.321849	0.314518	-0.114555
H	6.527333	0.466263	0.965168
H	6.524343	-0.747453	-0.364377
H	7.051198	0.932445	-0.676783
C	4.480529	-2.083608	4.079617
H	4.836441	-2.789975	4.858267
H	5.372280	-1.573609	3.661610
H	3.849589	-1.315584	4.573063
C	4.592004	-3.900415	2.314678
H	5.485224	-3.440454	1.844781
H	4.951468	-4.635449	3.064669
H	4.042160	-4.455462	1.526226
C	2.503419	-3.573619	3.670289
H	1.822190	-2.867326	4.189539
H	1.907697	-4.168827	2.946661
H	2.888127	-4.279574	4.433928
C	0.751694	3.949230	-1.709773
C	-0.191160	3.064007	-2.249186
H	0.370929	4.830654	-1.166909
H	-1.262645	3.308504	-2.147087
H	0.103669	2.427824	-3.106799
C	2.169246	4.025201	-2.231639
H	2.066889	4.207869	-3.326724
H	2.642547	3.022665	-2.152264
C	1.059000	3.278362	0.561621
H	0.344695	3.968211	1.047158
H	2.073430	3.704512	0.496420

	C	0.498482	-2.478375	-1.424282
	C	-1.221546	-1.286447	-3.281838
	C	-0.597660	-2.506595	-3.611233
	C	0.274370	-3.114824	-2.661766
	H	1.194665	-2.925942	-0.699050
	H	-1.899414	-0.806133	-4.006721
	C	0.960000	-4.420585	-2.981687
	H	1.592112	-4.332771	-3.891321
	H	1.606724	-4.760971	-2.150261
	H	0.222170	-5.224604	-3.190784
	C	-0.850106	-3.159603	-4.947413
	H	0.094755	-3.291510	-5.516941
	H	-1.282871	-4.175403	-4.823360
	H	-1.545339	-2.568433	-5.574282
	C	3.052144	5.115814	-1.619558
	H	4.043257	5.134058	-2.113988
	H	2.595738	6.120008	-1.740126
	H	3.232085	4.955578	-0.537577

2-3 (isomer) (1-butene)



Zero-point correction= 0.908350 (Hartree/Particle)
Thermal correction to Energy= 0.979421
Thermal correction to Enthalpy= 0.980539
Thermal correction to Gibbs Free Energy= 0.798684
Sum of electronic and zero-point Energies= -1915.281244
Sum of electronic and thermal Energies= -1915.210173
Sum of electronic and thermal Enthalpies= -1915.209055
Sum of electronic and thermal Free Energies= -1915.390910

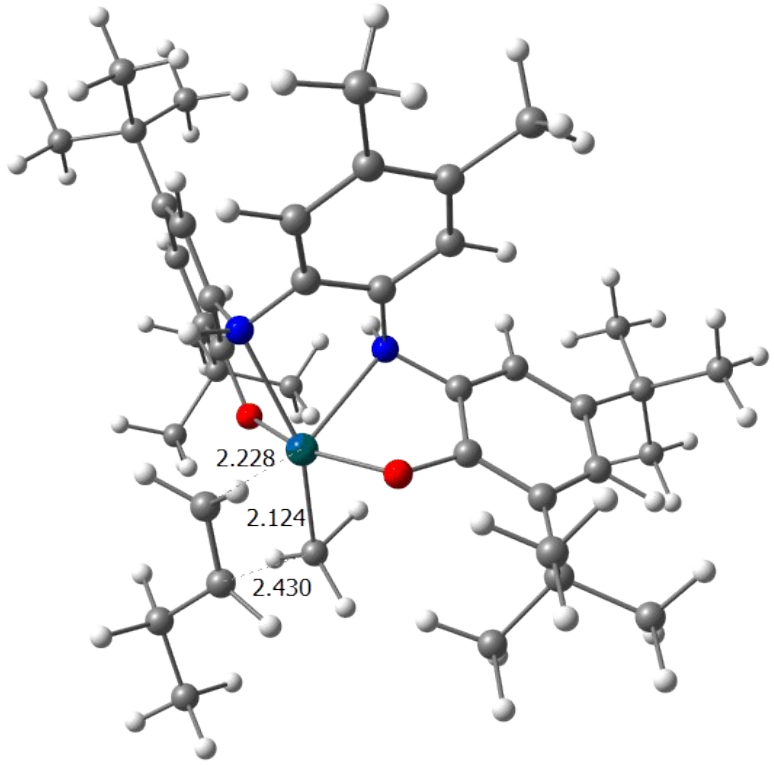
Solvent: -1915.8623721

107
PhTitBuCH3+buteneTS90+ SCF Done: -1916.18959390 A.U.

Ti	-0.185202	1.731187	-0.368170
N	-0.149889	-0.524054	0.078989
O	-1.912806	1.295649	0.230027
C	-2.447756	0.078072	-0.074012
C	-1.492353	-0.944214	-0.280685
C	-1.842784	-2.227207	-0.709809
H	-1.054141	-2.978761	-0.854655
C	-3.204864	-2.526290	-0.923515
C	-4.151058	-1.505888	-0.658115
H	-5.212168	-1.746980	-0.804964
C	-3.830526	-0.197991	-0.236698
C	0.096371	-0.593870	1.524521
C	-3.684615	-3.908692	-1.409062
N	1.547371	1.321967	1.159819
O	1.286366	1.355345	-1.452895
C	2.416204	0.740395	-1.030546
C	2.636179	0.730020	0.361670
C	3.765301	0.134480	0.936043
H	3.869487	0.132756	2.030210
C	4.722504	-0.473076	0.100622
C	4.470164	-0.475657	-1.294993
H	5.204476	-0.971843	-1.943329
C	3.337955	0.098399	-1.904196
C	0.937509	0.385910	2.081094
C	5.995978	-1.148591	0.648134
C	-4.896890	0.885832	0.002132
C	3.059318	0.015933	-3.416857
H	0.582392	-1.028140	-0.449114
H	1.906849	2.131097	1.686206
H	-1.131872	1.469203	-2.273795
C	6.099424	-1.028341	2.182923
H	6.141770	0.030879	2.512745
H	5.249242	-1.523145	2.697803
H	7.027974	-1.520583	2.536602
C	5.971674	-2.653116	0.272835
H	5.946693	-2.806623	-0.825293
H	6.878892	-3.162450	0.659771
H	5.082702	-3.156364	0.707044
C	7.241336	-0.473163	0.017634
H	8.170485	-0.939612	0.406336
H	7.255386	-0.575391	-1.086645
H	7.272097	0.609488	0.258915
C	4.176205	-0.739418	-4.167140
H	5.159597	-0.236484	-4.061144
H	4.279995	-1.787913	-3.818119
H	3.938468	-0.773753	-5.249716
C	2.954204	1.446077	-4.007872
H	2.140036	2.024029	-3.528895
H	3.904966	2.000544	-3.866939
H	2.747856	1.394031	-5.097311
C	1.724471	-0.748641	-3.633625
H	1.787523	-1.776552	-3.217653
H	0.872922	-0.224071	-3.155958
H	1.503365	-0.835833	-4.717800
C	-4.698054	2.008729	-1.047945
H	-3.683790	2.440509	-0.970647
H	-4.832468	1.616249	-2.077109
H	-5.435809	2.823125	-0.889839
C	-4.735106	1.459939	1.434060
H	-4.886299	0.666716	2.195198
H	-3.729209	1.896602	1.589008
H	-5.489711	2.253782	1.614422
C	-6.331051	0.334604	-0.138457
H	-6.538005	-0.042290	-1.161326
H	-6.534455	-0.482453	0.584439
H	-7.059584	1.145812	0.064243
C	-4.470279	-3.736002	-2.735030
H	-4.814696	-4.722450	-3.109668
H	-5.367863	-3.097917	-2.605588
H	-3.833889	-3.273247	-3.517558
C	-4.608485	-4.533538	-0.331695
H	-5.502545	-3.907153	-0.135460
H	-4.966531	-5.530763	-0.662538
H	-4.067068	-4.664042	0.628425
C	-2.506968	-4.873264	-1.661618
H	-1.813515	-4.488586	-2.438593
H	-1.924617	-5.069829	-0.736972
H	-2.891845	-5.849830	-2.018886
C	-0.734168	4.297288	-0.401161
C	0.185142	3.781033	0.509918
H	-0.341858	4.806084	-1.297464
H	1.263360	3.936009	0.333523
H	-0.142347	3.592103	1.551442
C	-2.160606	4.597891	-0.021226
H	-2.809733	4.591279	-0.918842
H	-2.541575	3.811141	0.662268
C	-1.034581	2.586987	-2.123084
H	-0.305834	2.972830	-2.859555
H	-2.042295	3.013741	-2.260584

	C	-0.533736	-1.519229	2.367477
	C	1.146420	0.428504	3.467413
	C	0.517493	-0.496149	4.325109
	C	-0.331449	-1.493239	3.762207
	H	-1.214138	-2.264723	1.929163
	H	1.811486	1.200481	3.888864
	C	-1.016077	-2.503074	4.650455
	H	-1.671182	-2.005997	5.397798
	H	-1.639752	-3.208383	4.068256
	H	-0.277735	-3.098316	5.229353
	C	0.741908	-0.434420	5.815571
	H	-0.214972	-0.288220	6.360876
	H	1.175435	-1.383689	6.196923
	H	1.424816	0.389552	6.099205
	C	-2.238603	5.985042	0.655293
	H	-1.645797	6.012295	1.592251
	H	-1.860103	6.787124	-0.011343
	H	-3.291813	6.223079	0.906411

2-3 (isomer) (1-butene)



Zero-point correction= 0.908261 (Hartree/Particle)
Thermal correction to Energy= 0.979228
Thermal correction to Enthalpy= 0.980347
Thermal correction to Gibbs Free Energy= 0.798437
Sum of electronic and zero-point Energies= -1915.279527
Sum of electronic and thermal Energies= -1915.208560
Sum of electronic and thermal Enthalpies= -1915.207441
Sum of electronic and thermal Free Energies= -1915.389351

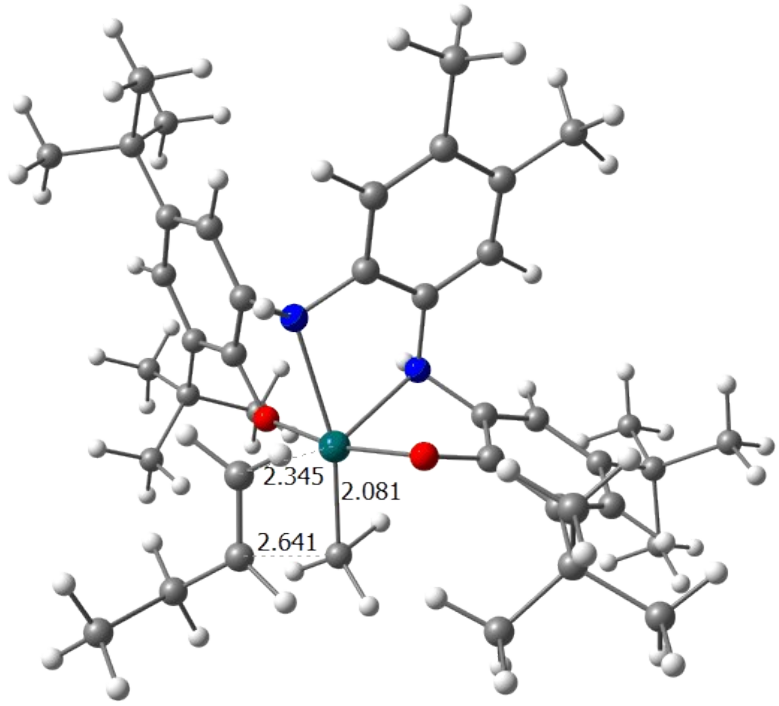
Solvent: -1915.8612312

107
PhTitBuCH3+buteneTSisomer+ SCF Done: -1916.18778794 A.U.

Ti	0.138894	1.407921	-0.896636
N	0.333687	-0.548529	0.277929
O	1.860002	0.763782	-1.277535
C	2.548750	0.140608	-0.280526
C	1.735172	-0.514291	0.674173
C	2.262802	-1.106776	1.825432
H	1.585429	-1.602226	2.535256
C	3.657589	-1.064547	2.036272
C	4.456531	-0.440557	1.046122
H	5.542518	-0.423925	1.206807
C	3.957524	0.171732	-0.122703
C	0.051446	-1.617113	-0.690367
C	4.327904	-1.674316	3.283845
N	-1.516331	-0.040171	-1.684001
O	-1.321971	1.789235	0.202287
C	-2.416638	1.000788	0.321186
C	-2.595945	0.024580	-0.680034
C	-3.688444	-0.850783	-0.680637
H	-3.764346	-1.608653	-1.473076
C	-4.650137	-0.754899	0.343567
C	-4.445425	0.225033	1.347954
H	-5.187328	0.289000	2.155116
C	-3.352421	1.111598	1.387586
C	-0.856293	-1.330872	-1.724076
C	-5.885321	-1.675003	0.412080
C	4.861302	0.842192	-1.173933
C	-3.138475	2.135820	2.518378
H	-0.307115	-0.599776	1.087224
H	-1.902176	0.170183	-2.615952
H	1.173361	2.364924	0.653395
C	-5.916852	-2.685578	-0.753891
H	-5.963368	-2.178792	-1.740597
H	-5.032980	-3.357611	-0.745322
H	-6.817914	-3.326803	-0.672398
C	-5.858233	-2.465939	1.745631
H	-5.889431	-1.795251	2.628407
H	-6.736546	-3.141514	1.810826
H	-4.940651	-3.085778	1.821683
C	-7.168476	-0.806827	0.346111
H	-8.071930	-1.449385	0.400910
H	-7.223197	-0.082897	1.184656
H	-7.211656	-0.231672	-0.601942
C	-4.262012	2.071304	3.573796
H	-5.255963	2.301554	3.137480
H	-4.317732	1.077628	4.065057
H	-4.069223	2.821055	4.367898
C	-3.112257	3.567546	1.920837
H	-2.293644	3.683221	1.183737
H	-4.072599	3.799548	1.415524
H	-2.961306	4.315111	2.727517
C	-1.789643	1.831183	3.225036
H	-1.792991	0.807417	3.655343
H	-0.935731	1.919527	2.524321
H	-1.622539	2.546666	4.056933
C	4.493348	2.344823	-1.294053
H	3.448764	2.471220	-1.638365
H	4.607885	2.861789	-0.318410
H	5.161147	2.844195	-2.026459
C	4.643884	0.138729	-2.539779
H	4.917160	-0.934835	-2.477086
H	3.588598	0.209599	-2.870058
H	5.281658	0.608806	-3.317384
C	6.354749	0.738273	-0.800969
H	6.583436	1.253855	0.154849
H	6.690461	-0.316154	-0.718954
H	6.968438	1.218454	-1.589990
C	5.050353	-0.547853	4.067539
H	5.543878	-0.962476	4.971269
H	5.833249	-0.054612	3.456161
H	4.331826	0.232277	4.393993
C	5.358065	-2.744808	2.839509
H	6.162001	-2.313887	2.208558
H	5.843167	-3.204238	3.725772
H	4.867325	-3.553247	2.258551
C	3.303442	-2.344456	4.223091
H	2.552031	-1.621446	4.604084
H	2.767043	-3.180015	3.725897
H	3.824571	-2.769015	5.104906
C	0.360872	3.518671	-2.429502
C	-0.311203	2.368746	-2.855425
H	1.449356	3.570522	-2.610210
H	-1.409011	2.417105	-2.966310
H	0.229395	1.617986	-3.463045
C	-0.356936	4.828047	-2.190825
H	-0.798523	5.088830	-3.181846
H	-1.230875	4.653842	-1.525333
C	0.986559	3.187458	-0.105318
H	0.280045	3.904468	0.349054

	H	1.970899	3.635008	-0.325840
	C	0.714070	-2.851886	-0.677518
	C	-1.093718	-2.277779	-2.731359
	C	-0.432568	-3.522314	-2.730462
	C	0.482028	-3.817008	-1.677702
	H	1.446139	-3.057356	0.118014
	H	-1.808038	-2.039492	-3.536658
	C	1.205616	-5.140830	-1.642216
	H	1.808773	-5.296163	-2.562351
	H	1.886813	-5.214735	-0.772797
	H	0.491850	-5.990776	-1.589580
	C	-0.690437	-4.528302	-3.824543
	H	0.245906	-4.784766	-4.364969
	H	-1.081550	-5.482131	-3.410221
	H	-1.421338	-4.155805	-4.568080
	C	0.504874	6.000511	-1.709653
	H	1.383811	6.146557	-2.371584
	H	-0.080452	6.941172	-1.722164
	H	0.879140	5.856989	-0.677674

2-3 (1-butene)



Zero-point correction= 0.907569 (Hartree/Particle)
Thermal correction to Energy= 0.978986
Thermal correction to Enthalpy= 0.980104
Thermal correction to Gibbs Free Energy= 0.797832
Sum of electronic and zero-point Energies= -1915.280032
Sum of electronic and thermal Energies= -1915.208615
Sum of electronic and thermal Enthalpies= -1915.207497
Sum of electronic and thermal Free Energies= -1915.389769

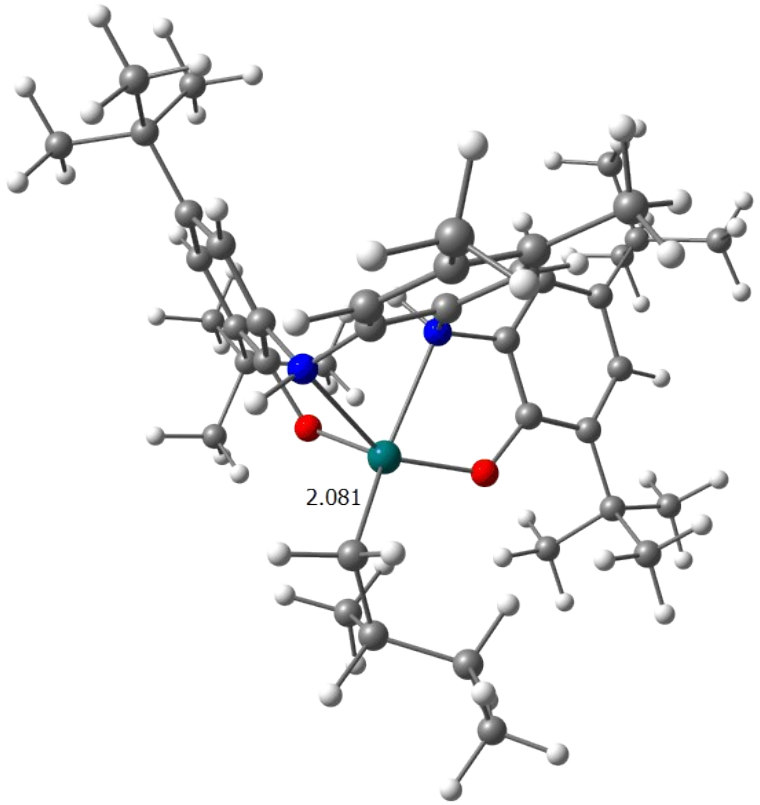
Solvent: -1915.8619526

107
PhTitBuCH3+buteneTS90isomer+ SCF Done: -1916.18760088 A.U.

Ti	0.170502	1.339380	-0.480390
N	0.654939	-0.555803	0.593250
O	1.728895	0.730925	-1.360134
C	2.647504	0.242729	-0.475477
C	2.109139	-0.392919	0.669065
C	2.905481	-0.824617	1.735893
H	2.429711	-1.298656	2.606263
C	4.301278	-0.644429	1.661635
C	4.824789	-0.042538	0.489783
H	5.913712	0.085720	0.430316
C	4.050845	0.421842	-0.593181
C	0.277049	-1.728637	-0.215311
C	5.259400	-1.081898	2.787815
N	-1.329644	-0.275997	-1.374906
O	-1.376260	1.541160	0.524446
C	-2.494078	0.781130	0.484935
C	-2.543667	-0.185110	-0.542380
C	-3.659728	-1.011340	-0.718863
H	-3.650390	-1.762122	-1.520407
C	-4.765871	-0.879243	0.143515
C	-4.687836	0.091745	1.173624
H	-5.547453	0.187181	1.849709
C	-3.582914	0.936789	1.387057
C	-0.659584	-1.561429	-1.245855
C	-6.029584	-1.752650	0.010410
C	4.659661	1.114360	-1.826812
C	-3.521317	1.976377	2.522740
H	0.231240	-0.612911	1.533182
H	-1.588639	-0.145865	-2.363526
H	1.308103	2.228072	1.117085
C	-5.931086	-2.737970	-1.172720
H	-5.817728	-2.211192	-2.143487
H	-5.083597	-3.445615	-1.055042
H	-6.857603	-3.343937	-1.234728
C	-6.219291	-2.571092	1.314214
H	-6.343515	-1.917201	2.201285
H	-7.125812	-3.207425	1.240439
H	-5.347749	-3.232947	1.499099
C	-7.260356	-0.836780	-0.214860
H	-8.180615	-1.448246	-0.321309
H	-7.421776	-0.139493	0.632495
H	-7.141580	-0.230093	-1.136466
C	-4.802113	1.965434	3.383302
H	-5.704392	2.218795	2.789114
H	-4.968634	0.982866	3.871550
H	-4.714096	2.723124	4.188128
C	-3.354823	3.394380	1.914416
H	-2.415804	3.475734	1.332825
H	-4.205536	3.638418	1.244698
H	-3.326736	4.155529	2.721899
C	-2.313884	1.651096	3.442514
H	-2.415681	0.636523	3.881382
H	-1.356613	1.702412	2.886443
H	-2.261054	2.379375	4.278599
C	4.129536	2.571144	-1.907563
H	3.026909	2.589210	-2.008601
H	4.410780	3.144501	-0.999490
H	4.565945	3.088649	-2.787182
C	4.251340	0.330805	-3.101763
H	4.639806	-0.707944	-3.064213
H	3.150821	0.286110	-3.217672
H	4.674990	0.821103	-4.003093
C	6.200195	1.166373	-1.758566
H	6.561124	1.749896	-0.886219
H	6.648806	0.152494	-1.711687
H	6.594587	1.659942	-2.669973
C	6.057302	0.151262	3.285318
H	6.750583	-0.142847	4.100794
H	6.668481	0.604977	2.478638
H	5.376371	0.934815	3.677700
C	6.239627	-2.148166	2.233764
H	6.850388	-1.755186	1.395492
H	6.938709	-2.478914	3.029838
H	5.690726	-3.039310	1.864576
C	4.502674	-1.688554	3.988102
H	3.794197	-0.963893	4.441471
H	3.939183	-2.603061	3.707036
H	5.223769	-1.980240	4.778355
C	-0.077045	3.571573	-1.968714
C	-0.618369	2.387371	-2.423886
H	0.976123	3.791366	-2.219009
H	-1.712092	2.240572	-2.365056
H	-0.038694	1.739419	-3.105241
C	-0.902576	4.697637	-1.410090
H	-1.772621	4.282138	-0.858778
H	-0.304989	5.292090	-0.689826
C	1.016661	3.036784	0.375154
H	0.362639	3.751824	0.906858

	H	1.952851	3.502572	0.014863
	C	0.902520	-2.972119	-0.039761
	C	-0.945804	-2.639325	-2.100244
	C	-0.324813	-3.892283	-1.937857
	C	0.609440	-4.066377	-0.875378
	H	1.659566	-3.081906	0.751752
	H	-1.670763	-2.497741	-2.918660
	C	1.291360	-5.395811	-0.665802
	H	1.857743	-5.706177	-1.569853
	H	1.998685	-5.367357	0.185370
	H	0.552412	-6.201729	-0.467760
	C	-0.645028	-5.033073	-2.871364
	H	0.265106	-5.388013	-3.400719
	H	-1.043308	-5.908304	-2.314854
	H	-1.392991	-4.746166	-3.635423
	C	-1.383655	5.618314	-2.555117
	H	-2.031681	5.068182	-3.267365
	H	-1.965395	6.466191	-2.140997
	H	-0.530005	6.039550	-3.125073

3 (isomer) (1-butene)



Zero-point correction= 0.910397 (Hartree/Particle)
Thermal correction to Energy= 0.981890
Thermal correction to Enthalpy= 0.983009
Thermal correction to Gibbs Free Energy= 0.798449
Sum of electronic and zero-point Energies= -1915.309289
Sum of electronic and thermal Energies= -1915.237796
Sum of electronic and thermal Enthalpies= -1915.236678
Sum of electronic and thermal Free Energies= -1915.421237

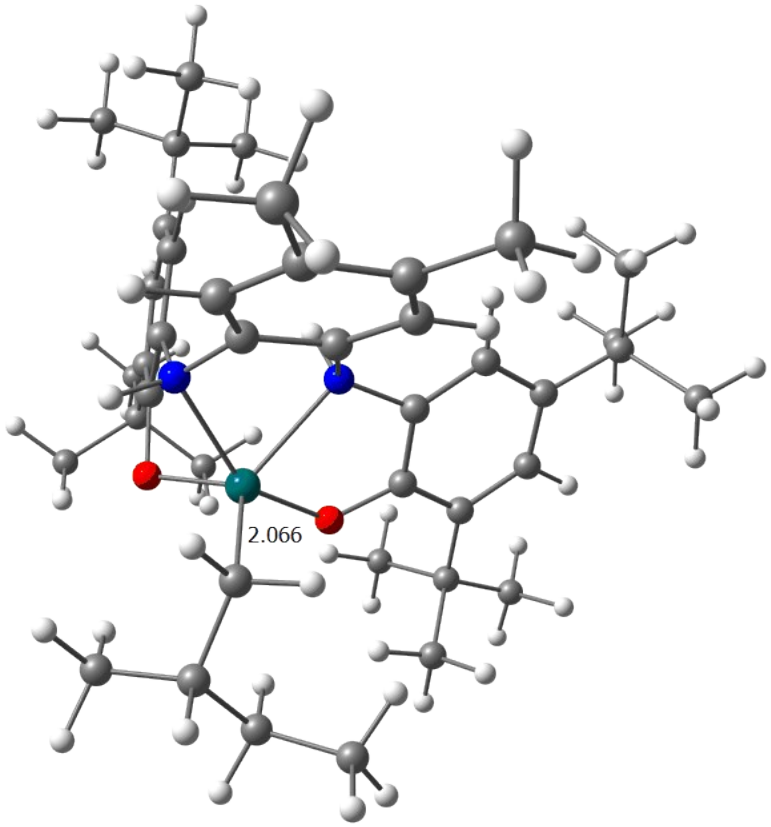
Solvent: -1915.8982504

107
PhTitBuCH3+buteneTS+POST SCF Done: -1916.21968617 A.U.

Ti	0.218673	-1.765852	0.162844
N	0.042116	0.451945	0.537675
O	1.928262	-1.145271	-0.131471
C	2.261671	0.168116	-0.310990
C	1.253644	1.086946	0.037568
C	1.414215	2.469280	-0.108028
H	0.588266	3.137831	0.172494
C	2.632055	2.963091	-0.617725
C	3.634434	2.019597	-0.953235
H	4.580969	2.406346	-1.352638
C	3.504647	0.621129	-0.822523
C	-0.181919	0.397229	1.971631
C	2.896212	4.467726	-0.828733
N	-1.685954	-1.371067	1.307582
O	-1.025996	-1.662994	-1.187867
C	-2.206153	-0.992874	-1.016128
C	-2.601282	-0.775106	0.324210
C	-3.748941	-0.048594	0.659758
H	-3.994417	0.099799	1.720808
C	-4.548974	0.476664	-0.374871
C	-4.133053	0.247058	-1.711013
H	-4.751827	0.669038	-2.513850
C	-2.973877	-0.462954	-2.085320
C	-1.139609	-0.560733	2.372687
C	-5.832063	1.288134	-0.104680
C	4.628022	-0.364504	-1.198837
C	-2.512540	-0.620568	-3.546225
H	-0.803099	0.804498	0.049282
H	-2.076303	-2.249247	1.680678
H	1.277619	-3.123240	-1.469394
C	-6.119437	1.427542	1.404785
H	-6.272766	0.441224	1.890512
H	-5.302540	1.959241	1.936548
H	-7.046613	2.016019	1.557688
C	-5.671338	2.707726	-0.708081
H	-5.506254	2.678176	-1.804439
H	-6.586524	3.308562	-0.525911
H	-4.813229	3.241364	-0.248594
C	-7.034504	0.570251	-0.770882
H	-7.971186	1.135300	-0.583455
H	-6.911821	0.485752	-1.869975
H	-7.162413	-0.453923	-0.363503
C	-3.512085	0.014159	-4.535712
H	-4.515028	-0.456820	-4.473750
H	-3.626432	1.106149	-4.373760
H	-3.145023	-0.126939	-5.572442
C	-2.375927	-2.127008	-3.888948
H	-1.632695	-2.629459	-3.239885
H	-3.349285	-2.647334	-3.773699
H	-2.048232	-2.248009	-4.942389
C	-1.142323	0.093063	-3.711450
H	-1.230763	1.174526	-3.476736
H	-0.366695	-0.345311	-3.052920
H	-0.789422	0.001363	-4.759619
C	4.104516	-1.380929	-2.247201
H	3.269626	-1.985813	-1.845400
H	3.752328	-0.862257	-3.162771
H	4.918417	-2.076670	-2.538634
C	5.080371	-1.111993	0.082145
H	5.492626	-0.403713	0.829814
H	4.238773	-1.657856	0.550384
H	5.869832	-1.852247	-0.164554
C	5.852353	0.358637	-1.798884
H	5.598827	0.903522	-2.731836
H	6.306175	1.076418	-1.084731
H	6.632349	-0.387613	-2.052577
C	3.150634	4.727937	-2.336153
H	3.341596	5.806709	-2.514846
H	4.030867	4.166795	-2.710530
H	2.272619	4.427406	-2.944783
C	4.142801	4.887806	-0.007838
H	5.053635	4.338404	-0.321823
H	4.345591	5.970551	-0.143167
H	3.988585	4.699382	1.075045
C	1.700894	5.332535	-0.377751
H	0.780395	5.102981	-0.954435
H	1.480238	5.204546	0.702948
H	1.929884	6.405057	-0.541285
C	1.269050	-4.391094	0.400475
C	0.294324	-3.536426	1.253558
H	1.028753	-5.465017	0.580441
H	-0.711813	-4.011902	1.295406
H	0.653851	-3.372182	2.295451
C	2.738228	-4.168084	0.823300
H	2.837041	-4.520310	1.873373
H	2.943828	-3.076536	0.850424
C	1.002083	-4.148441	-1.109965
H	-0.059313	-4.333128	-1.373930

	H	1.621705	-4.812738	-1.744096
	C	0.515223	1.139033	2.932947
	C	-1.410103	-0.753003	3.734356
	C	-0.721809	-0.008326	4.714112
	C	0.258033	0.948274	4.306213
	H	1.274734	1.863972	2.603608
	H	-2.155225	-1.505943	4.037901
	C	1.016519	1.747839	5.336447
	H	1.582016	1.084033	6.025019
	H	1.737021	2.445027	4.867815
	H	0.328062	2.343858	5.972884
	C	-1.010927	-0.225878	6.178121
	H	-0.097680	-0.541997	6.726232
	H	-1.356498	0.711768	6.663611
	H	-1.788112	-0.997830	6.337411
	C	3.788995	-4.854198	-0.054980
	H	4.799420	-4.752540	0.390378
	H	3.583602	-5.939701	-0.172614
	H	3.837498	-4.404980	-1.068774

3 (1-butene)



Zero-point correction= 0.910853 (Hartree/Particle)
Thermal correction to Energy= 0.982075
Thermal correction to Enthalpy= 0.983193
Thermal correction to Gibbs Free Energy= 0.800430
Sum of electronic and zero-point Energies= -1915.311662
Sum of electronic and thermal Energies= -1915.240441
Sum of electronic and thermal Enthalpies= -1915.239322
Sum of electronic and thermal Free Energies= -1915.422085

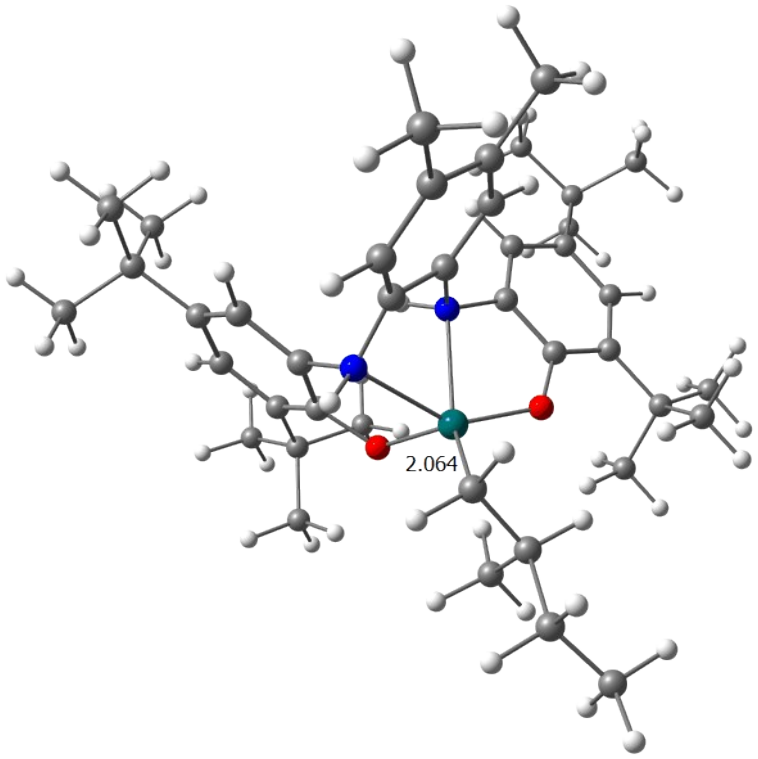
Solvent: -1915.9016739

107
PhTitBuCH3+buteneTS+POST90 SCF Done: -1916.22251532 A.U.

Ti	-0.296339	-0.989715	1.387534
N	0.145903	0.864693	0.219687
O	1.182045	-1.477722	0.418784
C	1.931456	-0.630835	-0.350318
C	1.435559	0.687789	-0.450981
C	2.046015	1.656915	-1.256594
H	1.581196	2.646581	-1.357550
C	3.232192	1.329709	-1.942339
C	3.716574	0.005087	-1.817795
H	4.630845	-0.254346	-2.366674
C	3.098386	-1.014235	-1.065895
C	-0.130933	1.949600	1.155023
C	3.997649	2.347895	-2.810495
N	-1.925836	0.448516	1.792879
O	-1.755766	-2.087248	1.076895
C	-2.450705	-1.296108	0.193672
C	-2.594935	0.076402	0.545158
C	-3.187326	1.012269	-0.313575
H	-3.240264	2.061764	0.007731
C	-3.692282	0.580879	-1.554457
C	-3.563279	-0.795969	-1.878106
H	-3.955560	-1.127217	-2.848265
C	-2.948843	-1.760876	-1.059953
C	-1.295746	1.744351	1.928398
C	-4.357847	1.542958	-2.555999
C	3.619648	-2.464153	-1.055327
C	-2.773952	-3.229221	-1.486301
H	-0.595352	0.884435	-0.509626
H	-2.482202	0.193859	2.623798
H	-0.987067	-3.460766	3.125407
C	-4.429261	2.984854	-2.011868
H	-5.027328	3.047256	-1.078855
H	-3.421531	3.406552	-1.812900
H	-4.916707	3.643476	-2.758625
C	-3.529699	1.550209	-3.867990
H	-3.473373	0.544627	-4.332013
H	-3.992699	2.234054	-4.609254
H	-2.492022	1.898478	-3.681592
C	-5.800202	1.053846	-2.849677
H	-6.298257	1.743124	-3.562539
H	-5.814587	0.041770	-3.302780
H	-6.407466	1.020318	-1.921759
C	-3.420529	-3.507945	-2.859601
H	-4.512324	-3.308742	-2.855122
H	-2.955918	-2.911163	-3.672026
H	-3.282856	-4.576631	-3.120023
C	-3.438786	-4.155282	-0.434164
H	-2.985473	-4.032121	0.568147
H	-4.525684	-3.945931	-0.355754
H	-3.317489	-5.215766	-0.737430
C	-1.255650	-3.538720	-1.592462
H	-0.757776	-2.853601	-2.309795
H	-0.745043	-3.446291	-0.615311
H	-1.103616	-4.576713	-1.953236
C	2.525122	-3.387342	-1.653762
H	1.595772	-3.357190	-1.053594
H	2.278764	-3.088768	-2.693827
H	2.884236	-4.437308	-1.675198
C	3.927683	-2.893593	0.398722
H	4.691287	-2.233106	0.858187
H	3.018039	-2.859740	1.024460
H	4.316695	-3.932797	0.416744
C	4.904740	-2.622516	-1.894608
H	4.743268	-2.371547	-2.963517
H	5.735359	-1.996411	-1.507512
H	5.241848	-3.678088	-1.853142
C	4.140201	1.796183	-4.252403
H	4.680899	2.525571	-4.890543
H	4.711050	0.845845	-4.281325
H	3.145853	1.609473	-4.708306
C	5.403947	2.568206	-2.194320
H	5.989792	1.627385	-2.153286
H	5.981096	3.296184	-2.801820
H	5.328114	2.964928	-1.160491
C	3.273088	3.708273	-2.877938
H	2.262147	3.618314	-3.328296
H	3.171746	4.176057	-1.875963
H	3.851884	4.412658	-3.509038
C	0.558471	-2.236281	4.115988
C	0.352695	-0.914245	3.347521
H	0.795272	-1.962458	5.173204
H	-0.382869	-0.265336	3.880093
H	1.295270	-0.320564	3.254009
C	1.754147	-3.058107	3.589231
H	1.774916	-4.025715	4.136567
H	1.572102	-3.322050	2.520197
C	-0.733474	-3.074735	4.137064
H	-1.601589	-2.479659	4.492170

	H	-0.628937	-3.951154	4.808626
	C	0.650529	3.089331	1.366159
	C	-1.692117	2.700593	2.868550
	C	-0.921833	3.865186	3.080228
	C	0.273153	4.053139	2.328500
	H	1.580531	3.223640	0.796712
	H	-2.601125	2.528393	3.467264
	C	1.132883	5.271671	2.557043
	H	1.473582	5.331938	3.612804
	H	2.030801	5.272739	1.909667
	H	0.567840	6.207374	2.357764
	C	-1.352347	4.887664	4.102243
	H	-0.580616	5.020282	4.890592
	H	-1.496378	5.886011	3.636547
	H	-2.300254	4.604297	4.598622
	C	3.112463	-2.363019	3.733660
	H	3.942698	-3.032289	3.431621
	H	3.184359	-1.454671	3.099425
	H	3.292753	-2.057201	4.786104

4 (isomer) (1-butene)



Zero-point correction= 0.910022 (Hartree/Particle)
Thermal correction to Energy= 0.981705
Thermal correction to Enthalpy= 0.982823
Thermal correction to Gibbs Free Energy= 0.797039
Sum of electronic and zero-point Energies= -1915.310226
Sum of electronic and thermal Energies= -1915.238544
Sum of electronic and thermal Enthalpies= -1915.237425
Sum of electronic and thermal Free Energies= -1915.423210

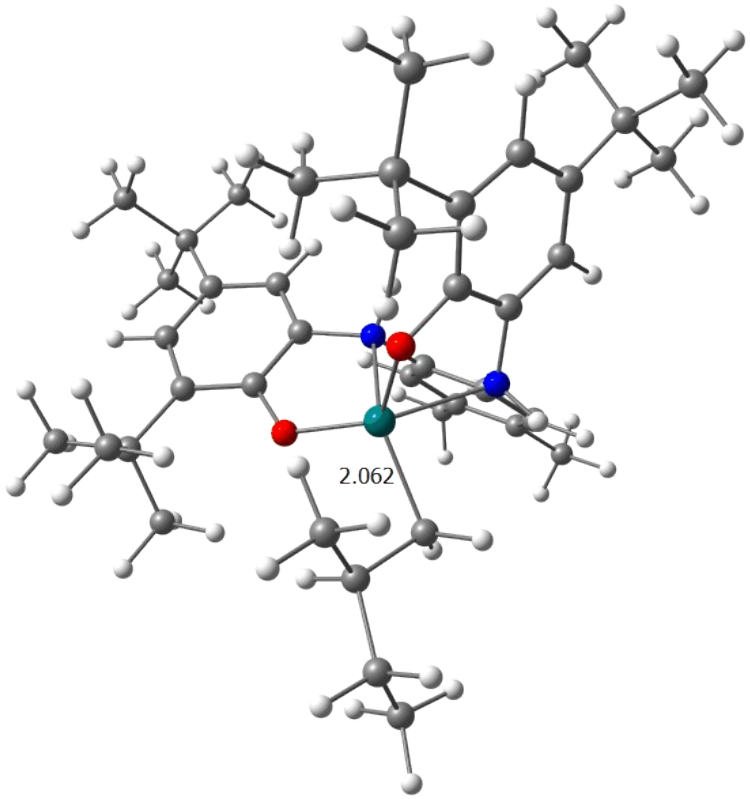
Solvent: -1915.901217

107
PhTitBuCH3+buteneTSisomer+POST SCF Done: -1916.22024870 A.U.

Ti	-0.223842	1.676814	0.155270
N	-0.107494	-0.551356	0.482588
O	-1.952443	1.116981	-0.145498
C	-2.325889	-0.181769	-0.338105
C	-1.341800	-1.138171	-0.024024
C	-1.549629	-2.511036	-0.199492
H	-0.740884	-3.212418	0.049646
C	-2.792251	-2.954483	-0.696415
C	-3.772411	-1.973245	-0.987731
H	-4.739898	-2.320157	-1.373670
C	-3.592418	-0.583235	-0.832132
C	0.118238	-0.546377	1.920091
C	-3.104385	-4.444891	-0.940843
N	1.644744	1.226622	1.321862
O	1.049300	1.608846	-1.178083
C	2.217055	0.918535	-0.999865
C	2.575612	0.650220	0.341187
C	3.703145	-0.105224	0.680927
H	3.917623	-0.294562	1.742200
C	4.523144	-0.605845	-0.350080
C	4.148953	-0.318958	-1.687587
H	4.784286	-0.718480	-2.489013
C	3.009985	0.420729	-2.066428
C	1.084469	0.386360	2.356464
C	5.786962	-1.445174	-0.073862
C	-4.675030	0.454826	-1.184208
C	2.597882	0.646260	-3.533107
H	0.724828	-0.922128	-0.013892
H	2.032857	2.092926	1.724772
H	-0.979032	3.083680	-1.486161
C	6.009028	-1.674020	1.435592
H	6.154460	-0.719690	1.983615
H	5.163390	-2.222502	1.901417
H	6.921643	-2.283876	1.592493
C	5.641860	-2.826978	-0.762712
H	5.528405	-2.735524	-1.862121
H	6.542506	-3.447087	-0.572874
H	4.759054	-3.375481	-0.372924
C	7.021962	-0.702966	-0.647184
H	7.944756	-1.290163	-0.458596
H	6.943148	-0.549681	-1.742811
H	7.144442	0.292897	-0.173222
C	3.618370	0.037117	-4.517291
H	4.625738	0.488956	-4.404821
H	3.711290	-1.062373	-4.397818
H	3.286045	0.226906	-5.557968
C	2.497405	2.168175	-3.814788
H	1.747023	2.657427	-3.163873
H	3.476710	2.664050	-3.652014
H	2.199820	2.339330	-4.870292
C	1.222648	-0.035646	-3.772471
H	1.287257	-1.128111	-3.585529
H	0.434226	0.384925	-3.117559
H	0.903594	0.109900	-4.825345
C	-4.137539	1.397598	-2.293555
H	-3.234722	1.945504	-1.959990
H	-3.880333	0.826392	-3.209426
H	-4.911631	2.145970	-2.562781
C	-5.022854	1.277361	0.084765
H	-5.420162	0.619674	0.885426
H	-4.135805	1.810018	0.480736
H	-5.799957	2.033333	-0.153539
C	-5.966515	-0.213836	-1.699313
H	-5.793282	-0.796138	-2.628011
H	-6.417620	-0.887524	-0.941582
H	-6.718107	0.566422	-1.936042
C	-3.386564	-4.658366	-2.450751
H	-3.609304	-5.726544	-2.654761
H	-4.256299	-4.064115	-2.797696
H	-2.509250	-4.365580	-3.064148
C	-4.351391	-4.850628	-0.113615
H	-5.250571	-4.268462	-0.400910
H	-4.586468	-5.923442	-0.273633
H	-4.177770	-4.694508	0.971447
C	-1.928858	-5.355345	-0.529591
H	-1.010336	-5.137696	-1.113943
H	-1.689261	-5.261301	0.550575
H	-2.191269	-6.416316	-0.716322
C	-1.429545	4.124742	0.476042
C	-0.371569	3.374404	1.320089
H	-2.406050	3.597792	0.575690
H	0.571174	3.966080	1.379094
H	-0.722985	3.140386	2.350970
C	-1.629944	5.573279	0.991762
H	-1.809032	5.517619	2.087711
H	-0.671900	6.127581	0.866141
C	-1.030843	4.101944	-1.020343
H	-0.045963	4.586118	-1.184671

	H	-1.786783	4.613299	-1.648164
	C	-0.585119	-1.316558	2.854266
	C	1.357134	0.525941	3.723889
	C	0.662944	-0.248338	4.676124
	C	-0.325435	-1.180050	4.233579
	H	-1.352667	-2.020595	2.499583
	H	2.109535	1.260291	4.053994
	C	-1.089663	-2.010367	5.234819
	H	-1.651335	-1.367185	5.945739
	H	-1.814191	-2.686725	4.742374
	H	-0.404904	-2.631780	5.850543
	C	0.954762	-0.088749	6.147127
	H	0.045512	0.218752	6.706774
	H	1.287555	-1.048323	6.597444
	H	1.741972	0.666522	6.334584
	C	-2.779775	6.336531	0.322292
	H	-2.596344	6.516896	-0.757168
	H	-3.738651	5.783410	0.414632
	H	-2.919969	7.329429	0.796111

4 (1-butene)



Zero-point correction= 0.910151 (Hartree/Particle)
Thermal correction to Energy= 0.981741
Thermal correction to Enthalpy= 0.982860
Thermal correction to Gibbs Free Energy= 0.797874
Sum of electronic and zero-point Energies= -1915.310760
Sum of electronic and thermal Energies= -1915.239170
Sum of electronic and thermal Enthalpies= -1915.238051
Sum of electronic and thermal Free Energies= -1915.423038

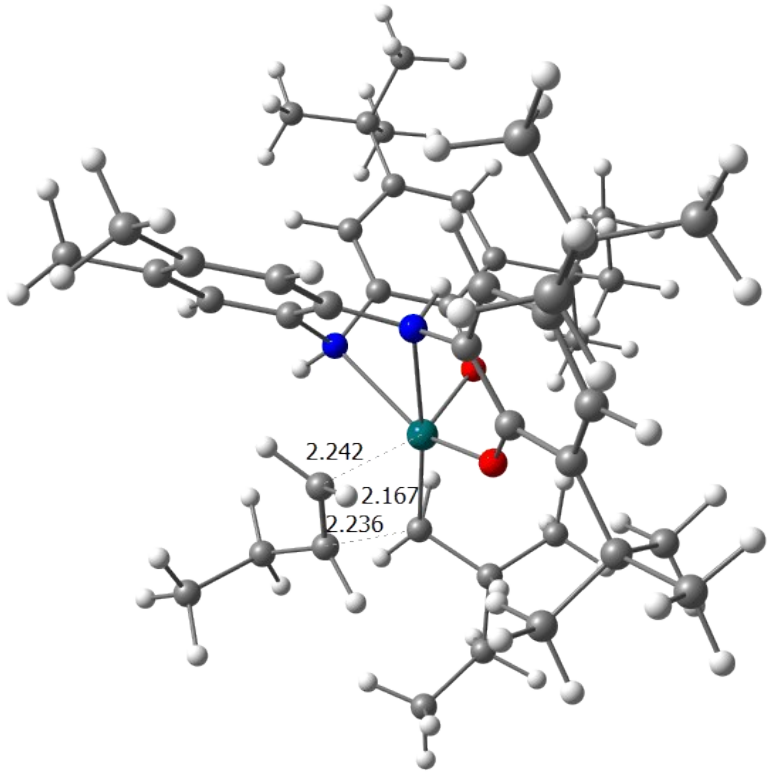
Solvent: -1915.9021278

107
PhTitBuCH3+buteneTS90isomer+POST SCF Done: -1916.22091104 A.U.

Ti	-0.172494	1.687416	-0.231010
N	-0.166409	-0.442913	0.505969
O	-1.906718	1.143163	-0.514242
C	-2.345382	-0.147642	-0.442500
C	-1.418751	-1.063908	0.089083
C	-1.695026	-2.432228	0.190467
H	-0.928926	-3.105473	0.599964
C	-2.951237	-2.907994	-0.237586
C	-3.874602	-1.961821	-0.748375
H	-4.853147	-2.334224	-1.079203
C	-3.623757	-0.580160	-0.876077
C	0.050325	-0.207029	1.927372
C	-3.340958	-4.398736	-0.172472
N	1.640403	1.387155	1.058265
O	1.136731	1.366769	-1.490335
C	2.266934	0.669371	-1.157114
C	2.573088	0.618197	0.221736
C	3.651444	-0.114974	0.727331
H	3.822828	-0.129875	1.812869
C	4.476563	-0.819378	-0.171964
C	4.157604	-0.747952	-1.551926
H	4.796155	-1.305407	-2.249997
C	3.069789	-0.032556	-2.093868
C	1.043842	0.753545	2.213338
C	5.685393	-1.656249	0.292693
C	-4.644899	0.416243	-1.456332
C	2.722346	-0.032655	-3.594364
H	0.653881	-0.927415	0.093505
H	2.050391	2.298993	1.312032
H	-0.867823	2.840088	-2.130685
C	5.858275	-1.617319	1.825214
H	6.039581	-0.586941	2.196638
H	4.974034	-2.031350	2.354029
H	6.733624	-2.230368	2.120632
C	5.478468	-3.131102	-0.140284
H	5.396572	-3.235229	-1.241412
H	6.337515	-3.752165	0.188609
H	4.556557	-3.553380	0.311441
C	6.973719	-1.095220	-0.363012
H	7.857267	-1.684173	-0.039911
H	6.930908	-1.140455	-1.470261
H	7.140177	-0.037214	-0.072728
C	3.746924	-0.837404	-4.420970
H	4.771385	-0.420055	-4.332812
H	3.776454	-1.906833	-4.125627
H	3.466946	-0.801171	-5.493203
C	2.708115	1.426428	-4.121168
H	1.959713	2.047161	-3.590894
H	3.704314	1.899809	-3.998702
H	2.457368	1.436330	-5.202291
C	1.324422	-0.682886	-3.782934
H	1.323275	-1.728815	-3.410619
H	0.533326	-0.119906	-3.249646
H	1.057839	-0.705769	-4.859973
C	-4.044892	1.083734	-2.722489
H	-3.125399	1.654565	-2.486642
H	-3.795179	0.322870	-3.490651
H	-4.779630	1.788301	-3.164904
C	-4.963271	1.497209	-0.389826
H	-5.399641	1.038498	0.521469
H	-4.054176	2.057419	-0.094526
H	-5.698870	2.224485	-0.792544
C	-5.964169	-0.279152	-1.852574
H	-5.812329	-1.044937	-2.641291
H	-6.456464	-0.763215	-0.983691
H	-6.672483	0.473023	-2.255141
C	-3.647879	-4.904903	-1.605925
H	-3.928290	-5.978656	-1.583399
H	-4.488527	-4.350759	-2.071113
H	-2.762047	-4.792956	-2.264938
C	-4.599972	-4.557649	0.718449
H	-5.467807	-3.995294	0.317679
H	-4.895953	-5.625599	0.780162
H	-4.407120	-4.194088	1.749300
C	-2.210476	-5.265551	0.419979
H	-1.287564	-5.221940	-0.195488
H	-1.956026	-4.964093	1.457993
H	-2.529790	-6.326773	0.456337
C	-1.297924	4.209785	-0.378969
C	-0.316699	3.557760	0.625477
H	-2.304295	3.754225	-0.235123
H	0.642151	4.125287	0.658164
H	-0.728297	3.474849	1.656955
C	-1.441430	5.735952	-0.159233
H	-0.454338	6.215610	-0.351184
H	-2.130653	6.128646	-0.940740
C	-0.847249	3.919493	-1.831592
H	0.179670	4.295266	-2.020207

	H	-1.533720	4.394285	-2.561859
	C	-0.678109	-0.793599	2.969178
	C	1.319614	1.104725	3.541247
	C	0.602265	0.514672	4.602430
	C	-0.414628	-0.444570	4.310299
	H	-1.467411	-1.521884	2.730168
	H	2.094956	1.858493	3.753226
	C	-1.203143	-1.080760	5.427790
	H	-1.723172	-0.314620	6.041701
	H	-1.965694	-1.786112	5.045709
	H	-0.539005	-1.638513	6.122416
	C	0.901342	0.898131	6.030190
	H	0.002268	1.314879	6.532426
	H	1.210078	0.013798	6.627615
	H	1.708844	1.652292	6.096900
	C	-1.958653	6.127073	1.228087
	H	-2.931498	5.637384	1.447937
	H	-1.247897	5.840500	2.031029
	H	-2.112309	7.222790	1.300843

6-7 (isomer) (1-butene)



Zero-point correction= 1.019349 (Hartree/Particle)
Thermal correction to Energy= 1.097511
Thermal correction to Enthalpy= 1.098630
Thermal correction to Gibbs Free Energy= 0.901692
Sum of electronic and zero-point Energies= -2072.314845
Sum of electronic and thermal Energies= -2072.236683
Sum of electronic and thermal Enthalpies= -2072.235565
Sum of electronic and thermal Free Energies= -2072.432502

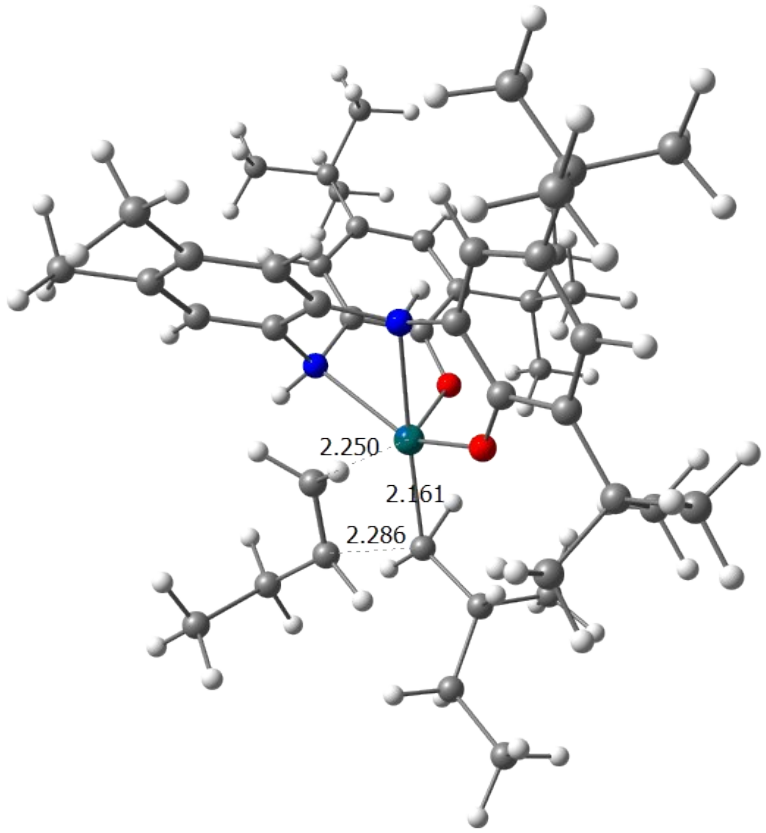
Solvent: -2072.9752228

119
PhTitBuCH3+buteneTS2+isomerBISreal90 SCF Done: -2073.33419430 A.U.

Ti	0.331492	-1.428834	0.451608
N	0.075685	0.891818	0.210915
O	1.877084	-0.890474	-0.334326
C	2.289549	0.386433	-0.571882
C	1.337402	1.397020	-0.315941
C	1.599658	2.735253	-0.641452
H	0.808438	3.483668	-0.505920
C	2.863136	3.093789	-1.151543
C	3.822307	2.065666	-1.322518
H	4.813734	2.348914	-1.699483
C	3.584768	0.703159	-1.058502
C	-0.527274	1.430840	1.417020
C	3.227413	4.546814	-1.517168
N	-1.733919	-0.680443	1.338635
O	-0.875611	-1.564156	-0.965247
C	-2.123018	-1.044521	-1.029169
C	-2.652635	-0.570349	0.187285
C	-3.924038	0.010919	0.268915
H	-4.276521	0.389518	1.238021
C	-4.708161	0.117336	-0.895603
C	-4.150812	-0.355612	-2.111493
H	-4.756489	-0.254838	-3.021961
C	-2.872471	-0.931621	-2.233660
C	-1.505425	0.596791	1.997991
C	-6.119259	0.739332	-0.892625
C	4.646006	-0.395387	-1.260338
C	-2.273445	-1.392128	-3.575549
H	-0.638997	0.898705	-0.542268
H	-2.117698	-1.351249	2.024392
H	1.110528	-3.093745	-1.852522
C	-6.545820	1.194664	0.518359
H	-6.577703	0.347079	1.234712
H	-5.868456	1.974287	0.925913
H	-7.564525	1.631100	0.481688
C	-6.131658	1.973530	-1.831747
H	-5.883003	1.703050	-2.878207
H	-7.138104	2.441511	-1.839730
H	-5.399476	2.736555	-1.494690
C	-7.139239	-0.312783	-1.399647
H	-8.163165	0.115748	-1.406879
H	-6.911947	-0.648103	-2.432196
H	-7.145512	-1.209171	-0.745436
C	-3.245272	-1.152366	-4.749599
H	-4.192986	-1.716371	-4.626497
H	-3.491183	-0.077396	-4.875091
H	-2.777203	-1.496018	-5.694285
C	-1.956010	-2.909136	-3.504366
H	-1.230358	-3.136202	-2.699418
H	-2.879062	-3.496929	-3.320085
H	-1.518884	-3.251924	-4.465469
C	-0.971210	-0.590212	-3.848742
H	-1.181415	0.499077	-3.892751
H	-0.206427	-0.770072	-3.067682
H	-0.537327	-0.891326	-4.824801
C	4.140049	-1.412400	-2.316298
H	3.190282	-1.886144	-2.006060
H	3.973687	-0.914396	-3.293670
H	4.892808	-2.214676	-2.465150
C	4.895844	-1.108762	0.095870
H	5.281291	-0.394656	0.852729
H	3.968557	-1.566553	0.494506
H	5.647556	-1.915899	-0.028198
C	5.989059	0.185073	-1.751294
H	5.889978	0.685243	-2.736773
H	6.418634	0.911313	-1.030496
H	6.724717	-0.635946	-1.871682
C	3.610085	4.612568	-3.018659
H	3.873235	5.652590	-3.303432
H	4.484803	3.972095	-3.252954
H	2.766299	4.282095	-3.659153
C	4.431967	5.000023	-0.651719
H	5.327779	4.368484	-0.821877
H	4.710866	6.045889	-0.897541
H	4.185426	4.954027	0.429507
C	2.054489	5.518090	-1.268386
H	1.165184	5.262665	-1.881851
H	1.750487	5.537909	-0.200470
H	2.355926	6.549653	-1.541602
C	1.894396	-3.966417	0.028005
C	0.705073	-3.510412	0.925087
H	2.710698	-3.212553	0.103770
H	-0.262490	-3.474656	0.342895
H	0.485497	-4.246736	1.714319
C	2.482323	-5.310844	0.520141
H	1.685336	-6.087900	0.479170
H	3.251256	-5.626690	-0.218827
C	1.482076	-4.060531	-1.454649
H	0.674565	-4.810723	-1.593696

	H	2.342790	-4.368423	-2.081887
	C	-0.150542	2.602225	2.081798
	C	-2.124188	0.959811	3.197908
	C	-1.770089	2.153026	3.865769
	C	-0.759596	2.978572	3.301389
	H	0.651507	3.228944	1.668985
	H	-2.879705	0.289886	3.640871
	C	-0.335326	4.248634	3.998293
	H	0.040354	4.042898	5.023583
	H	0.463723	4.777731	3.443969
	H	-1.189820	4.949465	4.114259
	C	-2.442304	2.534742	5.161787
	H	-1.705009	2.641285	5.986201
	H	-2.956053	3.516197	5.075050
	H	-3.195634	1.785573	5.473664
	C	1.130095	-0.865264	2.468918
	C	1.284685	-2.254240	2.682348
	H	0.391912	-0.333639	3.089793
	H	1.999163	-0.261536	2.154737
	H	2.279203	-2.698880	2.506631
	C	0.449938	-2.915514	3.766465
	H	0.449316	-4.019309	3.653210
	H	-0.608963	-2.585760	3.666698
	C	0.983121	-2.549004	5.163951
	H	0.391036	-3.057266	5.951692
	H	2.041139	-2.862910	5.280459
	H	0.933228	-1.455943	5.343018
	C	3.117150	-5.275564	1.914350
	H	2.375465	-5.059416	2.713158
	H	3.579258	-6.251013	2.168001
	H	3.914687	-4.503904	1.974840

6-7 (1-butene)



Zero-point correction= 1.018731 (Hartree/Particle)
Thermal correction to Energy= 1.097241
Thermal correction to Enthalpy= 1.098360
Thermal correction to Gibbs Free Energy= 0.899354
Sum of electronic and zero-point Energies= -2072.314883
Sum of electronic and thermal Energies= -2072.236373
Sum of electronic and thermal Enthalpies= -2072.235255
Sum of electronic and thermal Free Energies= -2072.434261

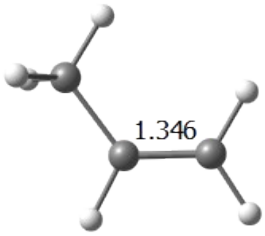
Solvent: -2072.9765152

119
PhTitBuCH3+buteneTS2+isomerBISreal SCF Done: -2073.33361472 A.U.

Ti	0.424352	-1.411292	0.370731
N	-0.099233	0.884772	0.255036
O	1.901136	-0.641805	-0.357637
C	2.151277	0.684174	-0.555690
C	1.081607	1.557888	-0.262242
C	1.169616	2.929327	-0.540094
H	0.290885	3.565188	-0.369752
C	2.371944	3.462946	-1.044123
C	3.451436	2.570394	-1.255331
H	4.395824	2.989050	-1.627252
C	3.391773	1.180574	-1.035500
C	-0.722834	1.285617	1.503048
C	2.547333	4.963309	-1.353188
N	-1.711306	-0.928425	1.321340
O	-0.803091	-1.613964	-1.025284
C	-2.094816	-1.213112	-1.053872
C	-2.651328	-0.848493	0.187454
C	-3.971726	-0.397579	0.308293
H	-4.345987	-0.101417	1.297678
C	-4.777602	-0.313620	-0.842965
C	-4.193169	-0.673885	-2.084711
H	-4.817331	-0.590070	-2.984469
C	-2.866874	-1.116767	-2.245618
C	-1.601839	0.326928	2.049273
C	-6.241669	0.168736	-0.797266
C	4.590436	0.240251	-1.264274
C	-2.244337	-1.449566	-3.614249
H	-0.829383	0.849595	-0.482106
H	-2.015379	-1.672094	1.970950
H	2.170204	-3.477398	-2.064288
C	-6.693638	0.506072	0.638885
H	-6.638883	-0.377513	1.308851
H	-6.087905	1.323084	1.084208
H	-7.748701	0.847176	0.630341
C	-6.383371	1.443968	-1.668131
H	-6.119059	1.254800	-2.728578
H	-7.430643	1.811571	-1.646594
H	-5.725970	2.256011	-1.293370
C	-7.163364	-0.948049	-1.351924
H	-8.224021	-0.622095	-1.321679
H	-6.923723	-1.200708	-2.404794
H	-7.070747	-1.875750	-0.750096
C	-3.257110	-1.266953	-4.763791
H	-4.134999	-1.936621	-4.653196
H	-3.620856	-0.221018	-4.836965
H	-2.771783	-1.515439	-5.729341
C	-1.760862	-2.923867	-3.619616
H	-0.988737	-3.103213	-2.845973
H	-2.608050	-3.616580	-3.435535
H	-1.321868	-3.176855	-4.607269
C	-1.044113	-0.495313	-3.864356
H	-1.376426	0.564142	-3.864585
H	-0.256038	-0.616330	-3.094845
H	-0.588220	-0.706793	-4.854048
C	4.219613	-0.829274	-2.324254
H	3.349090	-1.435231	-2.011592
H	3.975317	-0.351123	-3.295153
H	5.075038	-1.517573	-2.487783
C	4.949976	-0.437793	0.085169
H	5.258434	0.317795	0.836814
H	4.091038	-1.002632	0.499550
H	5.790769	-1.149385	-0.052343
C	5.834819	1.002656	-1.765206
H	5.653214	1.496453	-2.742136
H	6.174834	1.771771	-1.041109
H	6.672887	0.290304	-1.906668
C	2.927234	5.136533	-2.846459
H	3.056047	6.212027	-3.088803
H	3.878702	4.624162	-3.095835
H	2.136577	4.726083	-3.508166
C	3.676589	5.534157	-0.456525
H	4.647925	5.031422	-0.640164
H	3.818320	6.616559	-0.657753
H	3.430148	5.412878	0.618912
C	1.256953	5.764426	-1.082156
H	0.411768	5.416067	-1.711997
H	0.947656	5.708245	-0.017029
H	1.422459	6.835237	-1.317563
C	2.690741	-3.726376	0.061194
C	1.258008	-3.398988	0.525194
H	3.272219	-2.777008	0.070764
H	0.628161	-3.233511	-0.406995
H	0.755305	-4.254804	1.020148
C	3.395900	-4.732858	0.997725
H	3.278852	-4.405374	2.053974
H	2.868668	-5.712196	0.929211
C	2.659841	-4.220525	-1.400624
H	2.102842	-5.177979	-1.486583

	H	3.683627	-4.384429	-1.791978
	C	-0.448287	2.449443	2.229200
	C	-2.232983	0.561738	3.275146
	C	-1.984680	1.745291	4.004446
	C	-1.067662	2.694829	3.476149
	H	0.279548	3.175435	1.841240
	H	-2.911246	-0.202365	3.689773
	C	-0.754708	3.959109	4.239304
	H	-0.350881	3.733914	5.249638
	H	-0.013960	4.588885	3.709824
	H	-1.668638	4.570990	4.398163
	C	-2.668462	1.988686	5.327497
	H	-1.931122	2.118070	6.148626
	H	-3.273188	2.920561	5.302685
	H	-3.343366	1.155775	5.604901
	C	1.111976	-0.943803	2.461329
	C	1.565025	-2.276637	2.492972
	H	0.273687	-0.661963	3.118255
	H	1.823524	-0.131083	2.232508
	H	2.629343	-2.454316	2.265778
	C	0.913518	-3.275928	3.429912
	H	1.146608	-4.315263	3.121866
	H	-0.193136	-3.167104	3.375499
	C	4.891500	-4.913320	0.707360
	H	5.364060	-5.585503	1.451818
	H	5.073249	-5.354507	-0.293614
	H	5.424906	-3.939394	0.746218
	C	1.395860	-3.050040	4.875518
	H	0.943225	-3.797629	5.557795
	H	2.498752	-3.150763	4.948190
	H	1.124951	-2.037931	5.239054

1-propene



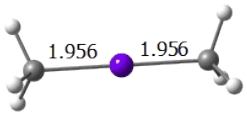
Zero-point correction= 0.076932 (Hartree/Particle)
Thermal correction to Energy= 0.082369
Thermal correction to Enthalpy= 0.083488
Thermal correction to Gibbs Free Energy= 0.046176
Sum of electronic and zero-point Energies= -117.740192
Sum of electronic and thermal Energies= -117.734755
Sum of electronic and thermal Enthalpies= -117.733636
Sum of electronic and thermal Free Energies= -117.770948

Solvent: -117.799473

9
CH2CHMe SCF Done: -117.817123757 A.U.

C	0.129822	0.454947	-0.000017
H	0.160946	1.561871	0.000098
C	-1.240114	-0.164474	-0.000052
H	-1.826665	0.156321	-0.889680
H	-1.194567	-1.273146	0.001261
H	-1.827151	0.157801	0.888793
C	1.294145	-0.220405	0.000028
H	2.264988	0.301283	0.000006
H	1.319337	-1.324544	-0.000231

$Zn(CH_3)_2$



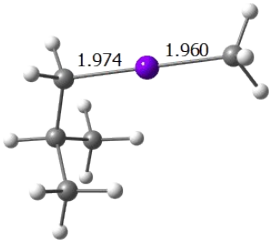
Zero-point correction= 0.068284 (Hartree/Particle)
Thermal correction to Energy= 0.074966
Thermal correction to Enthalpy= 0.076085
Thermal correction to Gibbs Free Energy= 0.034204
Sum of electronic and zero-point Energies= -1859.086433
Sum of electronic and thermal Energies= -1859.079750
Sum of electronic and thermal Enthalpies= -1859.078632
Sum of electronic and thermal Free Energies= -1859.120513

Solvent: -1858.9007194

9
ZnMe2 SCF Done: -1859.15471640 A.U.

C	-1.956198	-0.000027	-0.000080
H	-2.367610	-0.968328	-0.361999
H	-2.367251	0.798101	-0.657290
Zn	-0.000008	0.000002	0.000013
C	1.956179	0.000014	-0.000001
H	2.367376	0.971191	-0.354547
H	2.368083	-0.178663	1.018040
H	2.366731	-0.792790	-0.663967
H	-2.366980	0.170495	1.019867

$Zn(CH_3)(CH_2CH(CH_3)_2)$



Zero-point correction= 0.151371 (Hartree/Particle)
Thermal correction to Energy= 0.164205
Thermal correction to Enthalpy= 0.165323
Thermal correction to Gibbs Free Energy= 0.106594
Sum of electronic and zero-point Energies= -1976.862295
Sum of electronic and thermal Energies= -1976.849461
Sum of electronic and thermal Enthalpies= -1976.848342
Sum of electronic and thermal Free Energies= -1976.907072

Solvent: -1976.7393619

18
ZnMeORG SCF Done: -1977.01366548 A.U.

H	1.022985	-1.276019	-1.311357
C	1.930369	-0.002869	0.222742
C	0.732372	-0.021457	1.195746
H	2.878053	-0.011576	0.815669
H	0.782229	-0.922131	1.851737
H	0.780655	0.855662	1.883069
C	1.933972	1.276805	-0.629904
H	1.938257	2.189043	0.003097
H	2.811568	1.324920	-1.309156
H	1.017822	1.319699	-1.265363
C	1.938299	-1.252235	-0.673686
H	1.944849	-2.185756	-0.072532
H	2.816674	-1.274184	-1.353294
Zn	-0.992720	-0.004993	0.237194
C	-2.705354	0.013044	-0.715912
H	-3.218181	0.996082	-0.622768
H	-2.568317	-0.184332	-1.802471
H	-3.402927	-0.761338	-0.326373