Supporting Information

Mechanism and Stereoselectivity of the Rh(II)-catalyzed cyclopropanation of diazooxindole: A Density Functional Theory Study

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Contents

1. **Table S1.** Energies and relative energies of the stationary points in the $Rh_2(OAc)_4$-catalyzed reaction obtained at different levels of theory. The data reported here is BSSE uncorrected.

B3LYP:

Comp.	SPE[a]	TCH[a]	TCG[a]	H[a]	G[a]	ΔH[b]	ΔG[b]	$\Delta G^{‡}$[b]
1	-547.47317	0.130823	0.086594	-547.342342	-547.386571			
2	-309.74303	0.141445	0.102245	-309.6015836	-309.6407836			
3	-1133.4327	0.233105	0.158468	-1133.199632	-1133.274269			
N2	-109.55442	0.008904	-0.012851	-109.5455193	-109.5672743			
4	-1680.9018	0.366466	0.265346	-1680.53533	-1680.63645	4.2	15.3	0.0
TS9	-1680.8738	0.363761	0.262882	-1680.510045	-1680.610924	20.0	31.3	16.0
10	-1571.3516	0.353361	0.257548	-1570.998264	-1571.094077	-1.1	-0.3	0.0
TS11a	-1881.0872	0.497372	0.384651	-1880.589785	-1880.702506	5.2	20.0	20.3
TS11b	-1881.0857	0.497321	0.38399	-1880.588412	-1880.701743	6.0	20.5	20.8
TS11c	-1881.0828	0.49738	0.384069	-1880.585396	-1880.698707	7.9	22.4	22.7
TS11d	-1881.0764	0.496503	0.38864	-1880.579894	-1880.687757	11.4	29.2	29.5
12a	-747.72934	0.264402	0.208098	-747.4649336	-747.5212376	-41.7	-38.4	
12b	-747.72737	0.264375	0.208383	-747.4629912	-747.5189832	-40.5	-37.0	

[a] in hartree; [b] in kcal/mol; **ΔG:** relative Gibbs free energy with respect to the free reactants; $\Delta G^{‡}$: free energy barrier.

D3-B3LYP:

Comp.	SPE	TCH	TCG	H	G	ΔH	ΔG	$\Delta G^{‡}$
1	-547.4854134	0.130823	0.086594	-547.3545904	-547.3988194			
2	-309.7520696	0.141445	0.102245	-309.6106246	-309.6498246			
3	-1133.466258	0.233105	0.158468	-1133.233153	-1133.30779			
N2	-109.5544237	0.008904	-0.012851	-109.5455197	-109.5672747			
4	-1680.966521	0.366466	0.265346	-1680.600055	-1680.701175	-7.7	3.4	0.0
TS9	-1680.939426	0.363761	0.262882	-1680.575665	-1680.676544	7.6	18.9	15.5
10	-1571.409114	0.353361	0.257548	-1571.055753	-1571.151566	-8.5	-7.7	0.0
TS11a	-1881.174697	0.497372	0.384651	-1880.677325	-1880.790046	-15.4	-0.6	7.1
TS11b	-1881.171175	0.497321	0.38399	-1880.673854	-1880.787185	-13.2	1.2	8.9
TS11c	-1881.168369	0.49738	0.384069	-1880.670989	-1880.7843	-11.4	3.0	10.7
TS11d	-1881.165337	0.496503	0.38864	-1880.668834	-1880.776697	-10.0	7.8	15.5
12a	-747.7583842	0.264402	0.208098	-747.493982	-747.5502862	-46.6	-43.2	
12b	-747.7555484	0.264375	0.208383	-747.491173	-747.5471654	-44.9	-41.3	

M06:

Comp.	SPE	TCH	TCG	H	G	ΔH	ΔG	$\Delta G^{‡}$
1	-547.100898	0.130823	0.086594	-546.9700749	-547.0143039			

2	-309.480371	0.141445	0.102245	-309.3389257	-309.3781257			
3	-1132.84886	0.233105	0.158468	-1132.615754	-1132.690391			
N2	-109.485176	0.008904	-0.012851	-109.476272	-109.498027			
4	-1679.9657	0.366466	0.265346	-1679.599235	-1679.700355	-8.4	2.7	0.0
TS9	-1679.93721	0.363761	0.262882	-1679.573444	-1679.674323	7.8	19.1	16.4
10	-1570.47509	0.353361	0.257548	-1570.121731	-1570.217544	-7.6	-6.8	0.0
TS11a	-1879.96588	0.497372	0.384651	-1879.46851	-1879.581231	-12.6	2.2	9.0
TS11b	-1879.96093	0.497321	0.38399	-1879.463607	-1879.576938	-9.5	4.9	11.7
TS11c	-1879.95758	0.49738	0.384069	-1879.4602	-1879.573511	-7.4	7.1	13.9
TS11d	-1879.95399	0.496503	0.38864	-1879.457482	-1879.565345	-5.6	12.2	19.6
12a	-747.178942	0.264402	0.208098	-746.91454	-746.970844	-51.3	-48.0	
12b	-747.175568	0.264375	0.208383	-746.9111928	-746.9671848	-49.2	-45.7	

wB97XD:

Comp.	SPE	TCH	TCG	H	G	ΔH	ΔG	$\Delta G^{\ddagger}$
1	-547.2731901	0.130823	0.086594	-547.1423671	-547.1865961			
2	-309.6242484	0.141445	0.102245	-309.4828034	-309.5220034			
3	-1133.091044	0.233105	0.158468	-1132.857939	-1132.932576			
N2	-109.5123733	0.008904	-0.012851	-109.5034693	-109.5252243			
4	-1680.379113	0.366466	0.265346	-1680.012647	-1680.113767	-7.7	3.4	0.0
TS9	-1680.34965	0.363761	0.262882	-1679.985889	-1680.086768	9.0	20.3	16.9
10	-1570.859079	0.353361	0.257548	-1570.505718	-1570.601531	-5.6	-4.8	0.0
TS11a	-1880.495771	0.497372	0.384651	-1879.998399	-1880.11112	-11.8	3.0	7.8
TS11b	-1880.490597	0.497321	0.38399	-1879.993276	-1880.106607	-8.6	5.9	10.7
TS11c	-1880.488905	0.49738	0.384069	-1879.991525	-1880.104836	-7.5	7.0	11.8
TS11d	-1880.484263	0.496503	0.38864	-1879.98776	-1880.095623	-5.1	12.8	17.6
12a	-747.476669	0.264402	0.208098	-747.212267	-747.268571	-56.8	-53.5	
12b	-747.4728874	0.264375	0.208383	-747.2085124	-747.2645044	-54.5	-50.9	

2. **Table S2.** Calculated relative free energies with and without BSSE correction of the stationary points at the B3LYP-D3 level.

Comp.	ΔG	ΔG_{CP}	$\Delta G^{\ddagger}$	$\Delta G^{\ddagger}_{CP}$	$\Delta\Delta G^{\ddagger}$	$\Delta\Delta G^{\ddagger}_{CP}$
4	3.4	6.5				
TS9	18.9	22.3	15.5	15.8		
10	-7.7	-5.1				
TS11a	-0.6	1.5	7.1	6.6	0.0	0.0
TS11b	1.2	3.1	8.9	8.2	1.8	1.6
TS11c	3.0	5.1	10.7	10.2	3.6	3.6
TS11d	7.8	10.2	15.5	15.3	8.4	8.7

* **ΔG:** relative Gibbs free energy with respect to the individual reactants; $\Delta G^{\ddagger}$: free energy barrier; $\Delta\Delta G^{\ddagger}$: relative free energy barrier with respect to the most stable TS; CP: counterpoise correction for the BSSE.

It can be seen that although the BSSE correction has some influence on the $\Delta\mathbf{G}$ values (with average 2.5 kcal/mol), only very little influence on the $\Delta\mathbf{G}^{\ddagger}$ and $\Delta\Delta\mathbf{G}^{\ddagger}$, which are responsible for the reaction rate and stereoselectivity of the reaction. Accordingly, only the data without BSSE correction were given and discussed in the manuscript.

3. Table S3. Some donor-acceptor interactions in **TS11a** and **TS11b** and their second order perturbation stabilization energies, *E*(2) (kcal/mol)

TS11a	**Donor NBO (i)**	**Acceptor NBO (j)**	***E*(2) kcal/mol**
	carbene to styrene		
	1. σ(Rh2 - C39)	553. π*(C46 - C48)	3.38
	28. π(C31 - C36)	563. π*(C53 - C56)	0.11
	36. π(C34 - C35)	553. π*(C46 - C48)	0.09
	36. π(C34 - C35)	558. π*(C51 - C52)	0.27
	36. π(C34 - C35)	563. π*(C53 - C56)	0.12
	45. π(C38 - O40)	553. π*(C46 - C48)	0.06
	154. LP*C39	553. π*(C46 - C48)	16.09
	styrene to carbene		
	48. π(C46 - C48)	154. LP*C39	35.83
	48. π(C46 - C48)	541. π*(C34 - C35)	0.09
	48. π(C46 - C48)	550. π*(C38 - O40)	1.73
	53. π(C51 - C52)	541. π*(C34 - C35)	0.07
TS11b	**Donor NBO (i)**	**Acceptor NBO (j)**	***E*(2) kcal/mol**
	carbene to styrene		
	1. σ(Rh2 - C39)	553. π*(C46 - C48)	3.14
	36. π(C34 - C35)	553. π*(C46 - C48)	0.22
	45. π(C38 - O40)	558. π*(C51 - C52)	0.07
	45. π(C38 - O40)	563. π*(C53 - C56)	0.5
	154. LP*C39	553. π*(C46 - C48)	15.23
	styrene to carbene		
	48. π(C46 - C48)	154. LP* C39	33.15
	48. π(C46 - C48)	541. π*(C34 - C35)	0.06
	48. π(C46 - C48)	550. π*(C38 - O40)	1.28
	58. π(C53 - C56)	550. π*(C38 - O40)	0.12

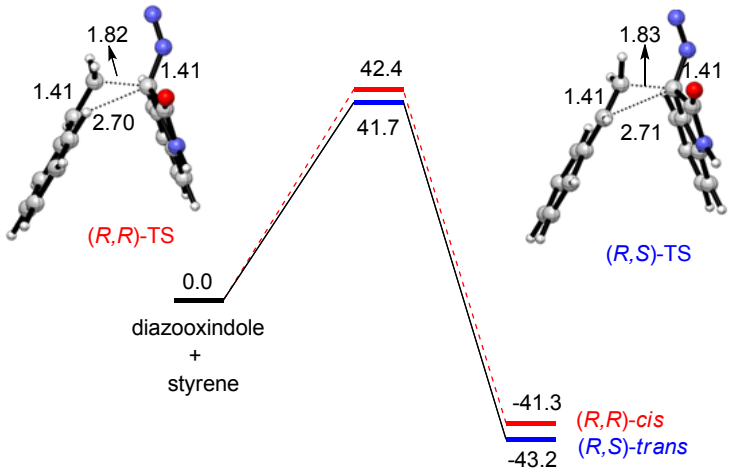
4. **Table S4**. Natural charge on different parts of species in the $Rh_2(OAc)_4$-catalyzed reaction.

Comp.	Rh^1	Rh^2	carboxylate groups	N_2	carbenoid ligand (carbene carbon)	styrene
1				0.13	-0.13 (-0.08)	
3	0.71	0.71	-1.42			
4	0.51	0.67	-1.35	0.26	-0.09 (-0.17)	
TS9	0.47	0.57	-1.33	0.22	0.07 (-0.06)	
10	0.47	0.50	-1.31		0.33 (0.04)	
TS11-a	0.48	0.51	-1.37		0.09 (-0.05)	0.29
TS11-b	0.48	0.51	-1.36		0.09 (-0.04)	0.28
TS11-c	0.48	0.50	-1.39		0.02 (-0.06)	0.38
TS11-d	0.49	0.51	-1.38		-0.01 (-0.07)	0.38

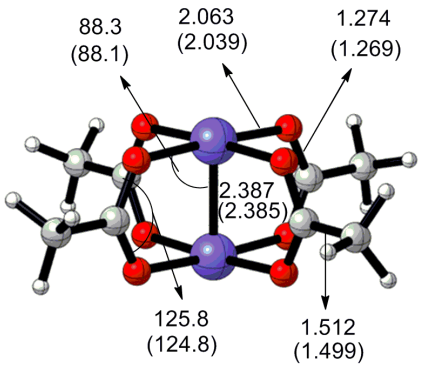
5. **Table S5**. Natural charge on different parts of species in Rh_2(*S*-PTTL)$_4$-catalyzed reaction.

Comp.	Rh^1	Rh^2	carboxylate groups	N_2	carbenoid ligand (carbene carbon)	styrene
1				0.13	-0.13 (-0.08)	
13	0.73	0.74	-1.47			
14	0.54	0.73	-1.45	0.27	-0.08 (-0.17)	
TS15	0.47	0.65	-1.44	0.22	0.09 (-0.06)	
16	0.47	0.59	-1.41		0.36 (0.05)	
TS17-a	0.48	0.61	-1.49		0.10 (-0.05)	0.30
TS17-b	0.48	0.61	-1.49		0.10 (-0.05)	0.30
TS17-c	0.48	0.62	-1.48		0.10 (-0.03)	0.28
TS17-d	0.48	0.61	-1.48		0.11 (-0.04)	0.28
TS17-e	0.49	0.60	-1.51		0.04 (-0.07)	0.38

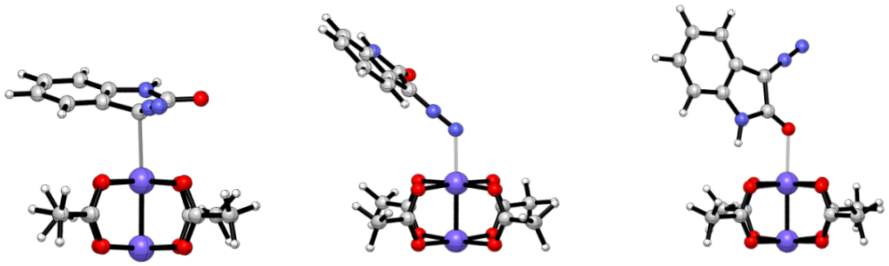
6. **Figure S1.** Energy profile for the uncatalyed cyclopropanation of diazooxindole and styrene for the *Re*-face pathway.



7. **Figure S2.** Comparison between the DFT and x-ray (in parentheses) structure of $Rh_2(OAc)_4$



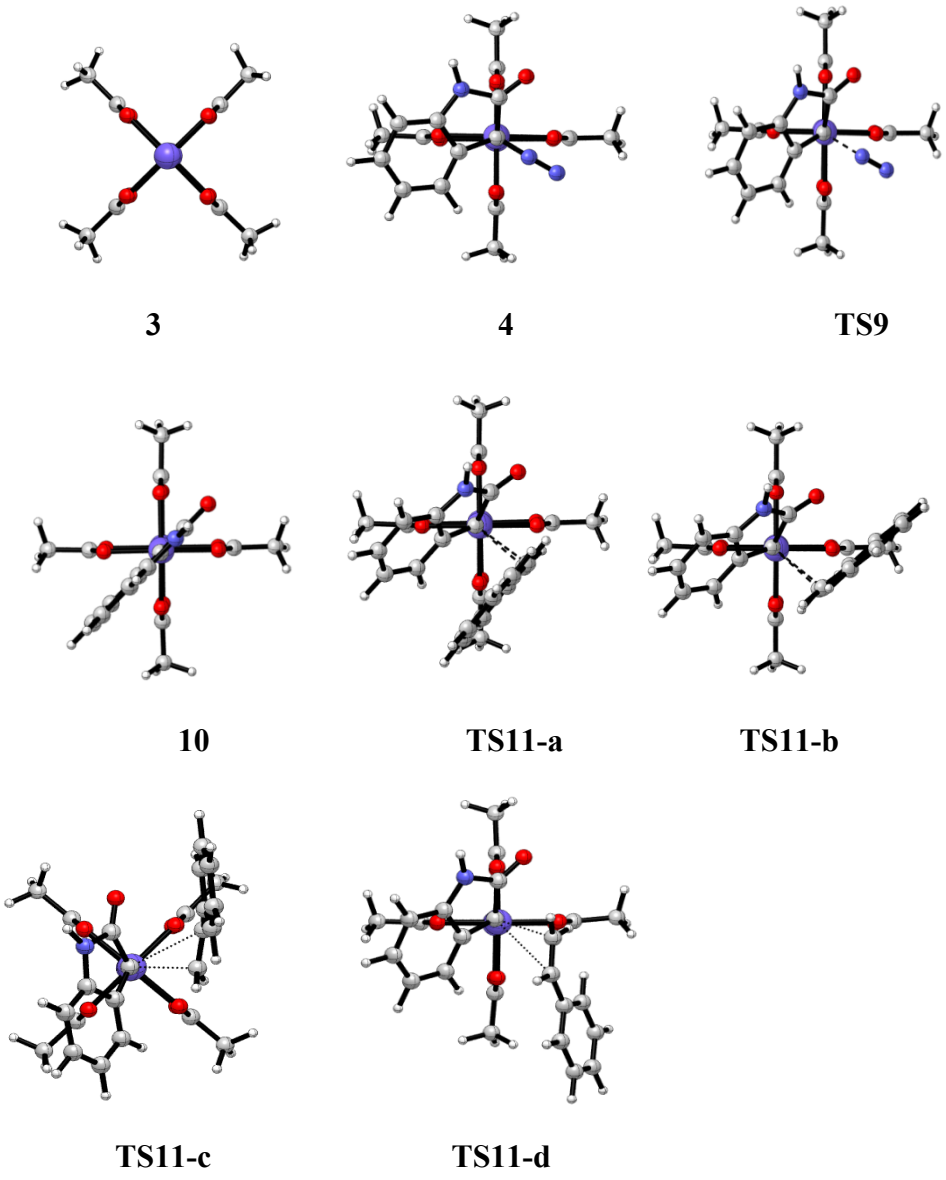
8. **Figure. S3**. Potential complexes formed between diazooxindole **1** and $Rh_2(OAc)_4$ **3 (4, 5** and **6)** or between styrene **2** and **3** (**7** and **8**). Values in parentheses are relative free energies (in kcal/mol) relative to isolated reactants.



4 (3.4) **5** (5.0) **6** (-0.6)

7 (2.8) **8** (4.9)

9. **Figure S4.** Calculated structures (top view) of the stationary points involved in the $Rh_2(OAc)_4$ catalyed cyclopropanation.

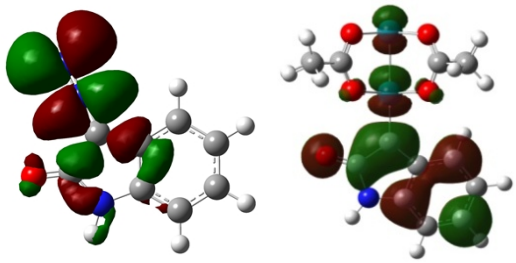


3 **4** **TS9**

10 **TS11-a** **TS11-b**

TS11-c **TS11-d**

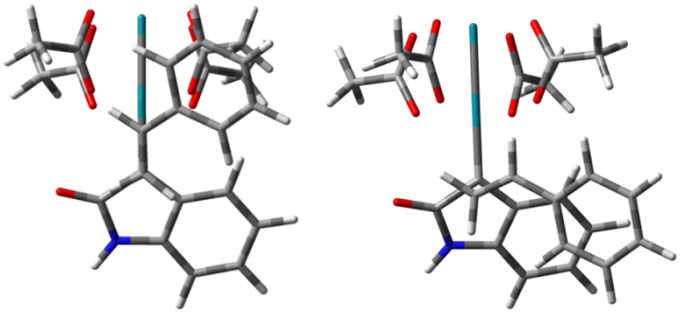
10. Figure S5. Diagram of LUMO of diazooxindole **1** (left) and carbenoid complex **10** (right)



11. Analysis of other four attack models in $Rh_2(OAc)_4$-catalyzed reaction

All our efforts to locate the *endo* transition structures for **TS11-a**, **TS11-b** and **TS11-c** were unsuccessful; instead, the styrene rotated upon optimization around the approach vector (C1-C2 bond) to afford an *exo* orientation. This effect might be due to the steric repulsion with the catalyst. Regarding the *side-on-trans-exo model*, although a suspected TS was located, it was denied by following IRC analysis.

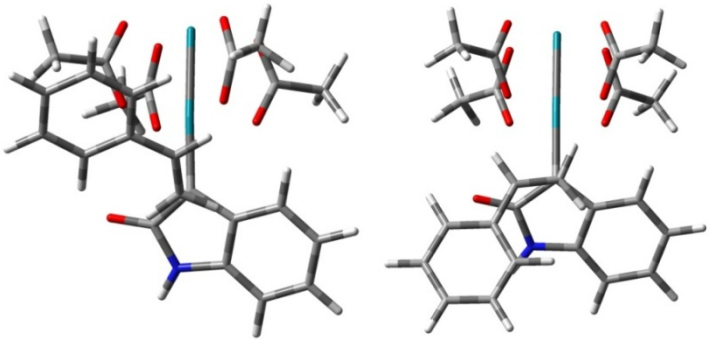
End-on -trans-endo model



Before optimization (*end-on-trans-endo*)

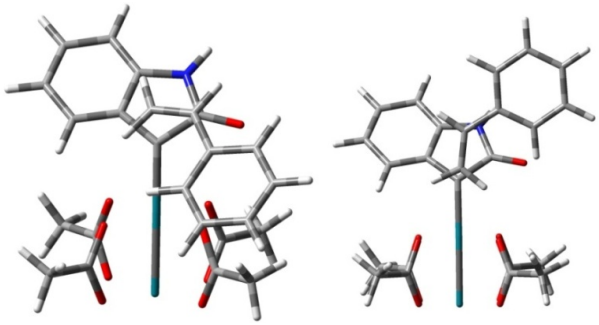
after optimization (*side-on-trans-exo*, -209.58 cm^{-1})

End-on -cis-endo model



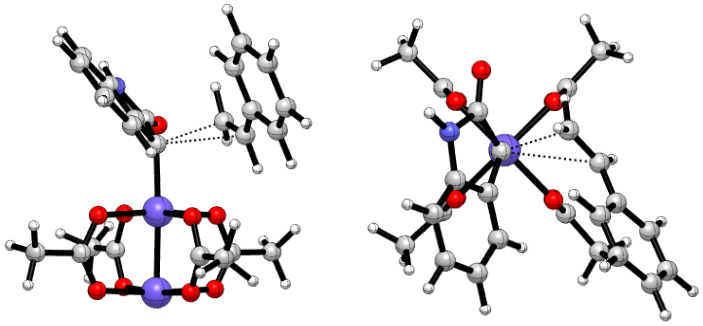
Before opt (*end-on-cis-endo*) after opt (*side-on-cis-exo*, -192.50 cm^{-1})

Side-on -cis-endo model

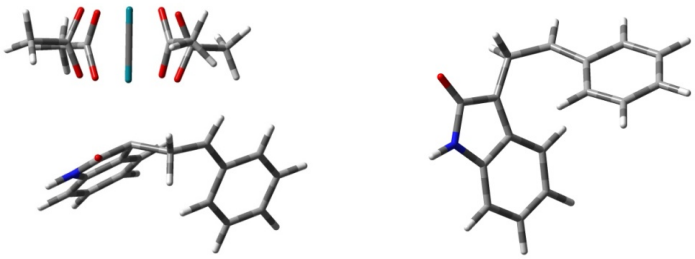


Before opt (*side-on-cis-endo*) after opt (*end-on-cis-exo*, -152.30 cm^{-1})

Side-on -trans-exo model

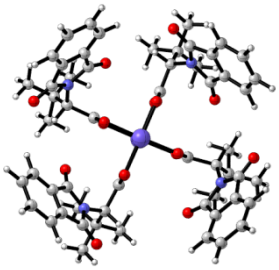


TS (side-view) TS (top-view)

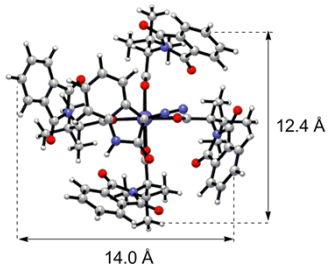


PC Product

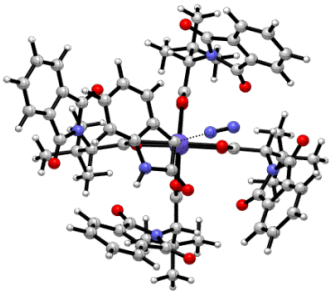
12. Figure S6. Optimized structures (top view) of the stationary points involved in the Rh_2(*S*-PTTL)$_4$ catalyed cyclopropanation.



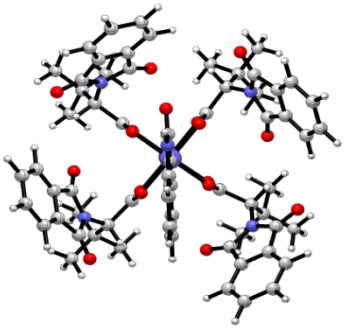
13



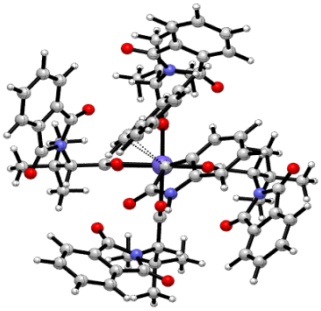
14



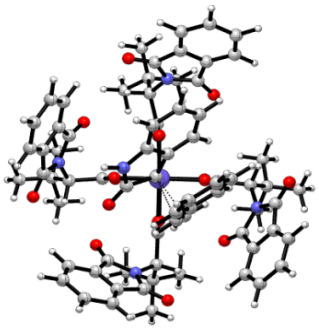
TS15



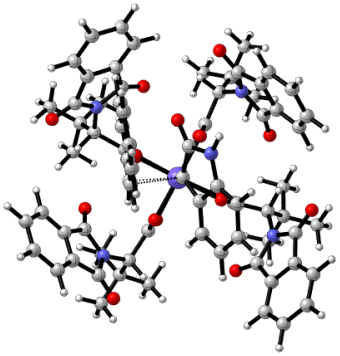
16



TS17-a (*si/trans/end-on*)

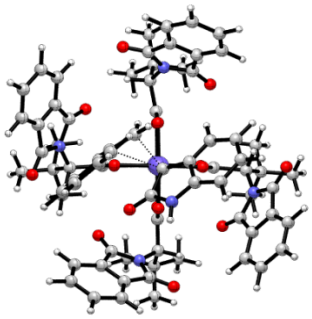


TS17-b (*re/trans/end-on*)



TS17-c (*re/cis/end-on*)

TS17-d (*si/cis/end-on*)



TS17-e (*si/cis/side-on*)

13. Table S6. DFT-Computed Energies at the SMD-(D3)B3LYP/6-311+G** (Lanl2DZ)// B3LYP/6-31G**(Lanl2DZ) level of theory. The data reported here is BSSE uncorrected.

Uncatalyzed Model

No.	SPE[a]	TCH[a]	TCG[a]	H[a]	G[a]	ΔH[b]	ΔG[b]
diazo	-547.4854134	0.130823	0.086594	-547.35459	-547.3988		
styrene	-309.7520696	0.141445	0.102245	-309.61062	-309.6498		
N2	-109.5544237	0.008904	-0.01285	-109.54552	-109.5673		
(*S*,*R*)-TS	-857.1910726	0.271968	0.208823	-856.9191	-856.9822	28.9	41.7
(*S*,*S*)-TS	-857.1906483	0.272103	0.209533	-856.91855	-856.9811	29.3	42.4
(*R*,*S*)-TS	-857.1910637	0.271971	0.208868	-856.91909	-856.9822	28.9	41.7
(*R*,*R*)-TS	-857.1906428	0.272103	0.209533	-856.91854	-856.9811	29.3	42.4
(*S*,*R*)-*trans-P*	-747.7583842	0.264402	0.208098	-747.49398	-747.5503	-46.6	-43.2
(*S*,*S*)-*cis-P*	-747.7555484	0.264375	0.208383	-747.49117	-747.5472	-44.9	-41.3
(*R*,*S*)-*trans-P*	-747.7583855	0.264402	0.208096	-747.49398	-747.5503	-46.6	-43.2
(*R*,*R*)-cis-*P*	-747.7555556	0.26437	0.208362	-747.49119	-747.5472	-44.9	-41.3

[a] in hartree; [b] in kcal/mol.

$Rh_2(OAc)_4$ Model

No.	SPE	TCH	TCG	H	G	ΔH	ΔG
1	-547.4854134	0.130823	0.086594	-547.3545904	-547.3988194		
2	-309.7520696	0.141445	0.102245	-309.6106246	-309.6498246		
3	-1133.466258	0.233105	0.158468	-1133.233153	-1133.30779		
N2	-109.5544237	0.008904	-0.012851	-109.5455197	-109.5672747		
4	-1680.966521	0.366466	0.265346	-1680.600055	-1680.701175	-7.7	3.4
TS9	-1680.939426	0.363761	0.262882	-1680.575665	-1680.676544	7.6	18.9
10	-1571.409114	0.353361	0.257548	-1571.055753	-1571.151566	-8.5	-7.7
TS11-a	-1881.174697	0.497372	0.384651	-1880.677325	-1880.790046	-15.4	-0.6

TS11-b	-1881.171175	0.497321	0.38399	-1880.673854	-1880.787185	-13.2	1.2
TS11-c	-1881.168369	0.49738	0.384069	-1880.670989	-1880.7843	-11.4	3.0
TS11-d	-1881.165337	0.496503	0.38864	-1880.668834	-1880.776697	-10.0	7.8

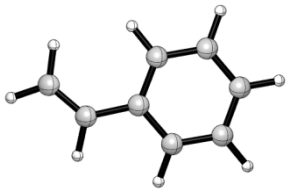
Rh_2(S-PTTL)$_4$ Model

No.	SPE	TCH	TCG	H	G	ΔH	ΔG
1	-547.4854134	0.130823	0.086594	-547.35459	-547.39882		
2	-309.7520696	0.141445	0.102245	-309.61062	-309.64982		
13	-3810.967386	1.128865	0.940747	-3809.8385	-3810.0266		
N2	-109.5544237	0.008904	-0.012851	-109.54552	-109.56727		
14	-4358.485108	1.261212	1.050698	-4357.2239	-4357.4344	-19.3	-5.6
TS15	-4358.45902	1.258354	1.046865	-4357.2007	-4357.4122	-4.7	8.3
16	-4248.923085	1.249153	1.041267	-4247.6739	-4247.8818	-16.5	-14.8
TS17-a	-4558.697398	1.391833	1.167976	-4557.3056	-4557.5294	-29.7	-13.4
TS17-b	-4558.696281	1.391814	1.16782	-4557.3045	-4557.5285	-29.0	-12.8
TS17-c	-4558.692872	1.391739	1.166864	-4557.3011	-4557.5260	-26.9	-11.3
TS17-d	-4558.695065	1.392142	1.169178	-4557.3029	-4557.5259	-28.1	-11.2
TS17-e	-4558.692001	1.39234	1.16889	-4557.2997	-4557.5231	-26.0	-9.5

14. Computed Molecular Cartesian Coordinates and Energies

11.1 Uncatalyzed reaction (Diazooxindole+Styrene)

Styrene:

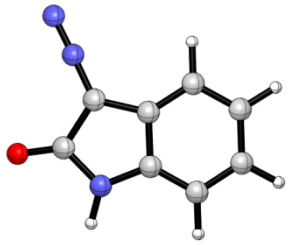


Zero-point correction= 0.133730 (Hartree/Particle)
Thermal correction to Energy= 0.140501
Thermal correction to Enthalpy= 0.141445
Thermal correction to Gibbs Free Energy= 0.102245
Sum of electronic and zero-point Energies= -309.514529
Sum of electronic and thermal Energies= -309.507758
Sum of electronic and thermal Enthalpies= -309.506814
Sum of electronic and thermal Free Energies= -309.546014

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	-1.954787	-0.529189	0.000003
2	1	0	-2.186223	-1.594644	0.000009
3	6	0	-2.977439	0.335025	0.000000
4	1	0	-2.840465	1.413065	-0.000005
5	1	0	-4.004454	-0.016959	0.000004
6	6	0	-0.515243	-0.220389	-0.000002
7	6	0	0.406474	-1.281406	-0.000009
8	6	0	-0.008781	1.092337	0.000003
9	6	0	1.780747	-1.046218	0.000004
10	1	0	0.034889	-2.303863	-0.000011
11	6	0	1.362395	1.329552	-0.000005
12	1	0	-0.693815	1.935298	0.000001
13	6	0	2.265350	0.261853	0.000001
14	1	0	2.471854	-1.885075	0.000016
15	1	0	1.730422	2.352349	0.000001
16	1	0	3.335503	0.450450	0.000003

Diazooxindole

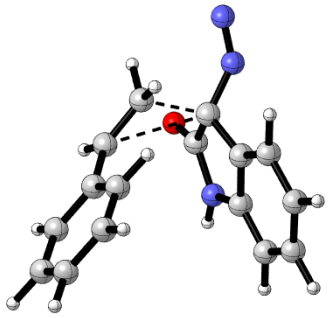


Zero-point correction= 0.120954 (Hartree/Particle)
Thermal correction to Energy= 0.129879
Thermal correction to Enthalpy= 0.130823
Thermal correction to Gibbs Free Energy= 0.086594
Sum of electronic and zero-point Energies= -547.187186
Sum of electronic and thermal Energies= -547.178262
Sum of electronic and thermal Enthalpies= -547.177318
Sum of electronic and thermal Free Energies= -547.221547

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.595592	1.255839	0.000057
2	6	0	3.065842	-0.060635	0.000166
3	6	0	2.181109	-1.146200	0.000146
4	6	0	0.818651	-0.876614	-0.000046
5	6	0	0.333305	0.453382	-0.000175
6	6	0	1.222432	1.524406	-0.000087

7	7	0	-0.263342	-1.758640	0.000026
8	6	0	-1.496978	-1.108263	-0.000363
9	6	0	-1.115437	0.330585	-0.000376
10	8	0	-2.598233	-1.627039	-0.000108
11	1	0	3.301247	2.081148	0.000101
12	1	0	4.135334	-0.250008	0.000305
13	1	0	2.549748	-2.167993	0.000284
14	1	0	0.859982	2.548666	-0.000165
15	1	0	-0.203588	-2.766485	0.000049
16	7	0	-2.005020	1.281324	-0.000282
17	7	0	-2.800774	2.096744	0.000879

Si-trans-ts

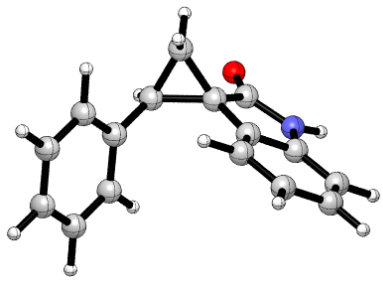


Zero-point correction= 0.254636 (Hartree/Particle)
Thermal correction to Energy= 0.271024
Thermal correction to Enthalpy= 0.271968
Thermal correction to Gibbs Free Energy= 0.208823
Sum of electronic and zero-point Energies= -856.645983
Sum of electronic and thermal Energies= -856.629595
Sum of electronic and thermal Enthalpies= -856.628651
Sum of electronic and thermal Free Energies= -856.691796

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.556284	3.058861	-0.884621
2	6	0	0.316362	3.352093	0.460198
3	6	0	0.579582	2.417570	1.469344
4	6	0	1.088383	1.183766	1.085546
5	6	0	1.318182	0.868728	-0.265093
6	6	0	1.056187	1.804785	-1.256478
7	7	0	1.470126	0.098370	1.886822
8	6	0	1.989002	-0.949039	1.152607
9	6	0	1.783138	-0.549222	-0.332752

10	8	0	2.451844	-1.985317	1.574283
11	1	0	0.350867	3.805006	-1.645924
12	1	0	-0.079932	4.325639	0.734451
13	1	0	0.398160	2.655770	2.513146
14	1	0	1.244794	1.572763	-2.301279
15	1	0	1.426393	0.069902	2.896143
16	7	0	2.957474	-0.796650	-1.080941
17	7	0	3.362916	-1.521540	-1.891006
18	6	0	0.513983	-1.688011	-0.999148
19	1	0	0.324133	-1.201721	-1.958231
20	1	0	1.187944	-2.545313	-1.116149
21	6	0	-0.580042	-1.858064	-0.133371
22	1	0	-0.447195	-2.557778	0.690098
23	6	0	-1.842277	-1.165821	-0.166260
24	6	0	-2.813940	-1.459907	0.823144
25	6	0	-2.195231	-0.209235	-1.150972
26	6	0	-4.058791	-0.842294	0.827161
27	1	0	-2.572374	-2.192696	1.589953
28	6	0	-3.440534	0.406626	-1.141964
29	1	0	-1.481970	0.053472	-1.926087
30	6	0	-4.383661	0.097907	-0.155381
31	1	0	-4.781330	-1.094018	1.599598
32	1	0	-3.681278	1.135962	-1.911601
33	1	0	-5.356341	0.581835	-0.154279

Si-trans-cyclopropane

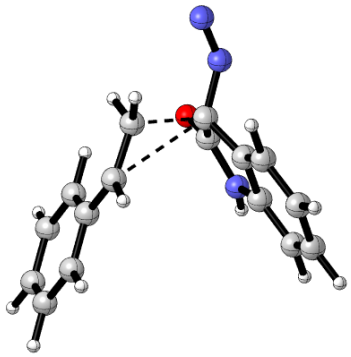


Zero-point correction= 0.249702 (Hartree/Particle)
Thermal correction to Energy= 0.263458
Thermal correction to Enthalpy= 0.264402
Thermal correction to Gibbs Free Energy= 0.208098
Sum of electronic and zero-point Energies= -747.257533
Sum of electronic and thermal Energies= -747.243777
Sum of electronic and thermal Enthalpies= -747.242833
Sum of electronic and thermal Free Energies= -747.299137

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	6	0	1.269674	2.753044	-0.676948
2	6	0	2.514213	2.787172	-0.045811
3	6	0	3.111670	1.615386	0.436105
4	6	0	2.423100	0.421378	0.264870
5	6	0	1.164468	0.367723	-0.370375
6	6	0	0.586984	1.539612	-0.843069
7	7	0	2.799851	-0.873530	0.647083
8	6	0	1.852926	-1.820788	0.292997
9	6	0	0.739683	-1.055484	-0.381052
10	8	0	1.919534	-3.021161	0.497723
11	1	0	0.823492	3.673443	-1.042166
12	1	0	3.032436	3.734473	0.075393
13	1	0	4.081498	1.642150	0.925211
14	1	0	-0.383830	1.520206	-1.328962
15	1	0	3.658276	-1.121857	1.118031
16	6	0	-0.023426	-1.756369	-1.495063
17	1	0	-0.342138	-1.123660	-2.319014
18	1	0	0.341053	-2.741247	-1.773715
19	6	0	-0.689162	-1.602127	-0.172150
20	1	0	-0.674828	-2.497217	0.449717
21	6	0	-1.850158	-0.687121	0.061363
22	6	0	-2.038701	-0.108954	1.325929
23	6	0	-2.786932	-0.416876	-0.944445
24	6	0	-3.130115	0.720635	1.576050
25	1	0	-1.317930	-0.309922	2.114639
26	6	0	-3.880401	0.416289	-0.697265
27	1	0	-2.666947	-0.872500	-1.923670
28	6	0	-4.054573	0.988185	0.563025
29	1	0	-3.258155	1.161687	2.561060
30	1	0	-4.598307	0.612263	-1.489491
31	1	0	-4.905354	1.635958	0.756651

Si-cis-TS

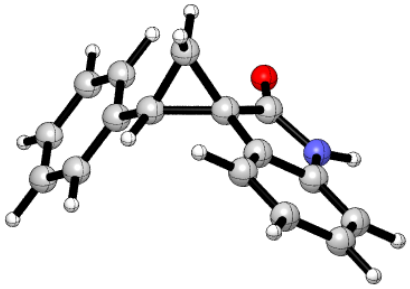


Zero-point correction= 0.254833 (Hartree/Particle)
Thermal correction to Energy= 0.271159
Thermal correction to Enthalpy= 0.272103
Thermal correction to Gibbs Free Energy= 0.209533
Sum of electronic and zero-point Energies= -856.646924
Sum of electronic and thermal Energies= -856.630598
Sum of electronic and thermal Enthalpies= -856.629653
Sum of electronic and thermal Free Energies= -856.692224

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.278056	-2.055444	-0.806225
2	6	0	-2.832817	-2.773585	0.306181
3	6	0	-1.953547	-2.206507	1.237749
4	6	0	-1.539101	-0.899616	1.016485
5	6	0	-1.969270	-0.171012	-0.105926
6	6	0	-2.840454	-0.741879	-1.021860
7	7	0	-0.699196	-0.094064	1.798286
8	6	0	-0.550081	1.176906	1.283276
9	6	0	-1.268665	1.153296	-0.088497
10	8	0	0.062656	2.101831	1.771930
11	1	0	-3.964451	-2.517271	-1.509152
12	1	0	-3.174859	-3.793414	0.458263
13	1	0	-1.615994	-2.769114	2.103037
14	1	0	-3.182174	-0.180001	-1.886844
15	1	0	-0.248152	-0.374970	2.658087
16	7	0	-2.118261	2.272151	-0.250473
17	7	0	-2.305232	3.159804	-0.973722
18	6	0	0.025729	1.314853	-1.351151
19	1	0	-0.641495	1.540276	-2.191666
20	1	0	0.505989	2.224741	-0.984226
21	6	0	0.825129	0.163007	-1.474689
22	1	0	0.431646	-0.649238	-2.083164

23	6	0	2.085111	-0.100860	-0.829722
24	6	0	2.741109	-1.332080	-1.083931
25	6	0	2.735117	0.810414	0.041778
26	6	0	3.971873	-1.632167	-0.513242
27	1	0	2.264988	-2.049947	-1.748314
28	6	0	3.964692	0.502389	0.611600
29	1	0	2.263589	1.757046	0.285072
30	6	0	4.595621	-0.716910	0.340400
31	1	0	4.448922	-2.584080	-0.733420
32	1	0	4.437332	1.220750	1.276862
33	1	0	5.557888	-0.949493	0.788030

Si-cis-cyclopropane

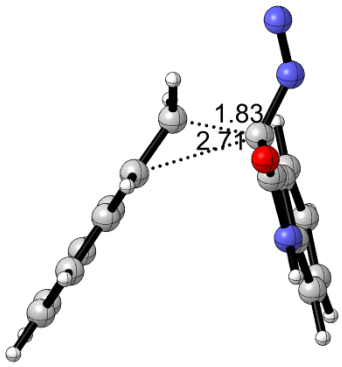


Zero-point correction= 0.249711 (Hartree/Particle)
Thermal correction to Energy= 0.263430
Thermal correction to Enthalpy= 0.264375
Thermal correction to Gibbs Free Energy= 0.208383
Sum of electronic and zero-point Energies= -747.255163
Sum of electronic and thermal Energies= -747.241443
Sum of electronic and thermal Enthalpies= -747.240499
Sum of electronic and thermal Free Energies= -747.296491

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.864012	-1.579005	0.131183
2	6	0	4.380129	-0.669739	-0.794175
3	6	0	3.658720	0.472117	-1.166625
4	6	0	2.413278	0.668811	-0.583391
5	6	0	1.876124	-0.240344	0.350041
6	6	0	2.603525	-1.367379	0.707776
7	7	0	1.502760	1.715568	-0.768788
8	6	0	0.378274	1.587459	0.036088
9	6	0	0.536367	0.263274	0.744690
10	8	0	-0.513065	2.412304	0.142338

11	1	0	4.441939	-2.455885	0.407960
12	1	0	5.357754	-0.845222	-1.234508
13	1	0	4.063235	1.179237	-1.885415
14	1	0	2.207455	-2.078108	1.429645
15	1	0	1.664432	2.544327	-1.323374
16	6	0	-0.134620	0.061621	2.086114
17	1	0	0.428541	-0.468720	2.849923
18	1	0	-0.705356	0.913756	2.445419
19	6	0	-0.671636	-0.711487	0.930222
20	1	0	-0.317995	-1.739787	0.878653
21	6	0	-2.014366	-0.544656	0.298946
22	6	0	-2.449232	-1.546520	-0.583806
23	6	0	-2.874455	0.532170	0.560376
24	6	0	-3.702365	-1.479154	-1.190185
25	1	0	-1.796088	-2.391191	-0.792729
26	6	0	-4.127817	0.600330	-0.047568
27	1	0	-2.559191	1.331645	1.219541
28	6	0	-4.548690	-0.402140	-0.922929
29	1	0	-4.017250	-2.269074	-1.867148
30	1	0	-4.778193	1.444488	0.165840
31	1	0	-5.527584	-0.345025	-1.391532

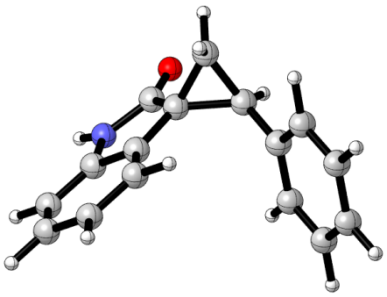
Re-trans-ts



Zero-point correction= 0.254643 (Hartree/Particle)
Thermal correction to Energy= 0.271027
Thermal correction to Enthalpy= 0.271971
Thermal correction to Gibbs Free Energy= 0.208868
Sum of electronic and zero-point Energies= -856.645976
Sum of electronic and thermal Energies= -856.629592
Sum of electronic and thermal Enthalpies= -856.628648
Sum of electronic and thermal Free Energies= -856.691751

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.563363	3.060845	-0.882610
2	6	0	-0.319450	3.352485	0.461843
3	6	0	-0.578064	2.416151	1.470500
4	6	0	-1.086456	1.182203	1.086612
5	6	0	-1.320405	0.868842	-0.263711
6	6	0	-1.062818	1.806637	-1.254621
7	7	0	-1.463977	0.095099	1.887542
8	6	0	-1.983845	-0.951966	1.153535
9	6	0	-1.783508	-0.549653	-0.331917
10	8	0	-2.443997	-1.989414	1.575252
11	1	0	-0.361442	3.808354	-1.643512
12	1	0	0.076417	4.326177	0.736194
13	1	0	-0.393443	2.653078	2.514031
14	1	0	-1.254469	1.575812	-2.299135
15	1	0	-1.416724	0.065151	2.896662
16	7	0	-2.959650	-0.798487	-1.076547
17	7	0	-3.366755	-1.524667	-1.884637
18	6	0	0.580742	-1.857818	-0.140206
19	1	0	0.448406	-2.561077	0.680315
20	6	0	-0.513494	-1.684386	-1.004907
21	1	0	-0.323949	-1.192536	-1.961182
22	1	0	-1.187130	-2.541370	-1.126630
23	6	0	1.842664	-1.164796	-0.170435
24	6	0	2.814824	-1.463011	0.817232
25	6	0	2.194716	-0.203354	-1.150727
26	6	0	4.059378	-0.844807	0.823680
27	1	0	2.573915	-2.199520	1.580676
28	6	0	3.439711	0.413099	-1.139274
29	1	0	1.480981	0.062793	-1.924235
30	6	0	4.383393	0.100166	-0.154547
31	1	0	4.782334	-1.099786	1.594658
32	1	0	3.679770	1.146220	-1.905519
33	1	0	5.355830	0.584576	-0.151539

Re-trans-cyclopropane

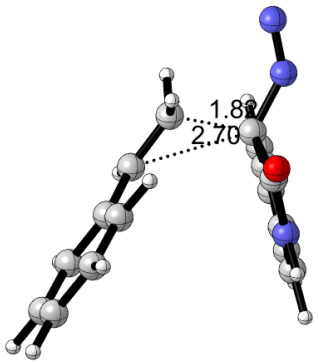


Zero-point correction= 0.249701 (Hartree/Particle)
Thermal correction to Energy= 0.263458
Thermal correction to Enthalpy= 0.264402
Thermal correction to Gibbs Free Energy= 0.208096
Sum of electronic and zero-point Energies= -747.257534
Sum of electronic and thermal Energies= -747.243777
Sum of electronic and thermal Enthalpies= -747.242833
Sum of electronic and thermal Free Energies= -747.299139

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.270303	2.752808	-0.677476
2	6	0	-2.514801	2.786841	-0.046253
3	6	0	-3.111978	1.615029	0.435952
4	6	0	-2.423177	0.421125	0.264893
5	6	0	-1.164605	0.367568	-0.370437
6	6	0	-0.587393	1.539459	-0.843406
7	7	0	-2.799680	-0.873773	0.647428
8	6	0	-1.852769	-1.820952	0.293258
9	6	0	-0.739586	-1.055617	-0.380891
10	8	0	-1.919208	-3.021362	0.497986
11	1	0	-0.824277	3.673190	-1.042919
12	1	0	-3.033191	3.734068	0.074789
13	1	0	-4.081780	1.641649	0.925117
14	1	0	0.383388	1.520205	-1.329376
15	1	0	-3.658383	-1.122265	1.117797
16	6	0	0.689357	-1.601839	-0.172101
17	1	0	0.675239	-2.497122	0.449520
18	6	0	0.023601	-1.756123	-1.495024
19	1	0	0.342124	-1.122964	-2.318716
20	1	0	-0.340440	-2.741035	-1.774101
21	6	0	1.850265	-0.686771	0.061484
22	6	0	2.038160	-0.107595	1.325673
23	6	0	2.787713	-0.417568	-0.943990

24	6	0	3.129651	0.721914	1.575771
25	1	0	1.316861	-0.307706	2.114116
26	6	0	3.881257	0.415484	-0.696833
27	1	0	2.668120	-0.873929	-1.922924
28	6	0	4.054813	0.988363	0.563109
29	1	0	3.257174	1.163771	2.560487
30	1	0	4.599694	0.610634	-1.488779
31	1	0	4.905656	1.636053	0.756734

Re-cis-TS

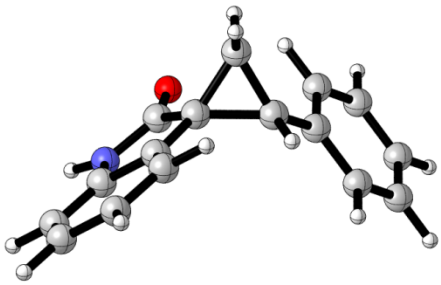


Zero-point correction= 0.254833 (Hartree/Particle)
Thermal correction to Energy= 0.271159
Thermal correction to Enthalpy= 0.272103
Thermal correction to Gibbs Free Energy= 0.209533
Sum of electronic and zero-point Energies= -856.646924
Sum of electronic and thermal Energies= -856.630598
Sum of electronic and thermal Enthalpies= -856.629654
Sum of electronic and thermal Free Energies= -856.692223

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.278150	-2.055300	-0.806793
2	6	0	2.833597	-2.773328	0.305961
3	6	0	1.954723	-2.206233	1.237891
4	6	0	1.539925	-0.899459	1.016603
5	6	0	1.969346	-0.170995	-0.106185
6	6	0	2.840212	-0.741848	-1.022429
7	7	0	0.700388	-0.093874	1.798767
8	6	0	0.550696	1.176943	1.283551
9	6	0	1.268626	1.153259	-0.088563
10	8	0	-0.062043	2.101815	1.772315
11	1	0	3.964274	-2.517125	-1.509985

12	1	0	3.175896	-3.793071	0.458046
13	1	0	1.617742	-2.768732	2.103472
14	1	0	3.181400	-0.180058	-1.887680
15	1	0	0.249552	-0.374825	2.658663
16	7	0	2.118030	2.272234	-0.251073
17	7	0	2.304392	3.159672	-0.974767
18	6	0	-0.825624	0.163130	-1.474367
19	1	0	-0.432203	-0.648943	-2.083107
20	6	0	-0.026274	1.314990	-1.350659
21	1	0	-0.506596	2.224660	-0.983272
22	1	0	0.640678	1.540916	-2.191266
23	6	0	-2.085610	-0.100898	-0.829469
24	6	0	-2.741529	-1.332113	-1.083913
25	6	0	-2.735701	0.810180	0.042172
26	6	0	-3.972288	-1.632382	-0.513311
27	1	0	-2.265345	-2.049833	-1.748411
28	6	0	-3.965270	0.501972	0.611908
29	1	0	-2.264250	1.756805	0.285642
30	6	0	-4.596117	-0.717317	0.340477
31	1	0	-4.449270	-2.584286	-0.733673
32	1	0	-4.437978	1.220189	1.277278
33	1	0	-5.558382	-0.950038	0.788039

Re-cis-cyclopropane



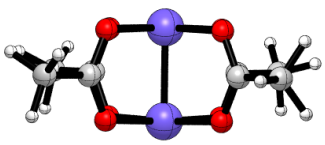
Zero-point correction= 0.249703 (Hartree/Particle)
Thermal correction to Energy= 0.263425
Thermal correction to Enthalpy= 0.264370
Thermal correction to Gibbs Free Energy= 0.208362
Sum of electronic and zero-point Energies= -747.255170
Sum of electronic and thermal Energies= -747.241448
Sum of electronic and thermal Enthalpies= -747.240504
Sum of electronic and thermal Free Energies= -747.296511

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	-3.865294	-1.577175	0.132529
2	6	0	-4.380627	-0.668229	-0.793564
3	6	0	-3.658247	0.472720	-1.166957
4	6	0	-2.412569	0.668853	-0.583977
5	6	0	-1.876283	-0.240016	0.350217
6	6	0	-2.604615	-1.366117	0.708966
7	7	0	-1.501412	1.714861	-0.770050
8	6	0	-0.376836	1.586586	0.035260
9	6	0	-0.536407	0.262900	0.744644
10	8	0	0.515374	2.410321	0.140644
11	1	0	-4.443976	-2.453345	0.409983
12	1	0	-5.358421	-0.843207	-1.233735
13	1	0	-4.062293	1.179570	-1.886284
14	1	0	-2.209062	-2.076605	1.431348
15	1	0	-1.662873	2.542548	-1.326281
16	6	0	0.671656	-0.711558	0.931400
17	1	0	0.318256	-1.740004	0.880841
18	6	0	0.134369	0.062461	2.086479
19	1	0	0.704509	0.914957	2.445808
20	1	0	-0.429247	-0.467640	2.850134
21	6	0	2.014228	-0.544964	0.299637
22	6	0	2.446509	-1.544326	-0.587247
23	6	0	2.876516	0.529164	0.564551
24	6	0	3.699281	-1.476986	-1.194312
25	1	0	1.791561	-2.386941	-0.798798
26	6	0	4.129573	0.597333	-0.044064
27	1	0	2.563501	1.326424	1.227479
28	6	0	4.547822	-0.402540	-0.923590
29	1	0	4.012236	-2.264872	-1.874533
30	1	0	4.781767	1.439376	0.172137
31	1	0	5.526468	-0.345481	-1.392720

14.2 $Rh_2(OAc)_4$-Model (Diazooxindole+Styrene+ $Rh_2(OAc)_4$)

$Rh_2(OAc)_4$:



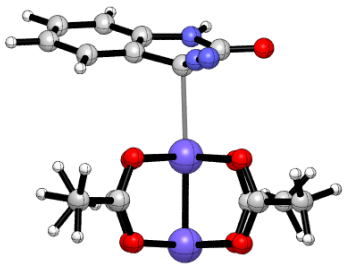
Zero-point correction= 0.211342 (Hartree/Particle)
Thermal correction to Energy= 0.232160

Thermal correction to Enthalpy= 0.233105
Thermal correction to Gibbs Free Energy= 0.158468
Sum of electronic and zero-point Energies= -1132.901655
Sum of electronic and thermal Energies= -1132.880836
Sum of electronic and thermal Enthalpies= -1132.879892
Sum of electronic and thermal Free Energies= -1132.954529

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.000874	-0.003333	-1.191816
2	45	0	0.002379	-0.001670	1.194897
3	8	0	1.483524	-1.436657	-1.133532
4	8	0	1.476389	-1.444783	1.134464
5	8	0	-1.434482	-1.484363	-1.128349
6	8	0	-1.436094	-1.479781	1.139650
7	8	0	-1.483703	1.429415	-1.131365
8	8	0	-1.480329	1.433344	1.136628
9	8	0	1.438297	1.476657	-1.135356
10	8	0	1.442126	1.476021	1.132776
11	6	0	-1.900990	1.831998	0.003039
12	6	0	1.899639	-1.840693	0.000739
13	6	0	-1.838404	-1.898722	0.006701
14	6	0	1.840211	1.895869	-0.002032
15	6	0	-2.895392	-2.979448	-0.001906
16	1	0	-3.802636	-2.593895	-0.478948
17	1	0	-2.546146	-3.827038	-0.599617
18	1	0	-3.122871	-3.304604	1.014167
19	6	0	3.011748	-2.864449	-0.006177
20	1	0	3.951963	-2.366242	-0.269141
21	1	0	3.115434	-3.325565	0.977254
22	1	0	2.814873	-3.623615	-0.767749
23	6	0	2.858863	3.012700	-0.001925
24	1	0	2.330942	3.972447	0.048014
25	1	0	3.505823	2.935113	0.874552
26	1	0	3.447700	2.991007	-0.921043
27	6	0	-2.993328	2.877123	-0.007218
28	1	0	-2.635601	3.770961	-0.528619
29	1	0	-3.855380	2.496756	-0.564407
30	1	0	-3.290420	3.134711	1.010232

Catalyst-Diazooxindole-Complex:

Complex coordination via C

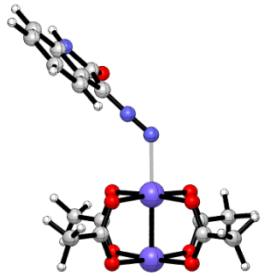


Zero-point correction= 0.332893 (Hartree/Particle)
Thermal correction to Energy= 0.365522
Thermal correction to Enthalpy= 0.366466
Thermal correction to Gibbs Free Energy= 0.265346
Sum of electronic and zero-point Energies= -1680.087099
Sum of electronic and thermal Energies= -1680.054471
Sum of electronic and thermal Enthalpies= -1680.053526
Sum of electronic and thermal Free Energies= -1680.154646

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-2.211781	0.850072	-0.384767
2	45	0	-0.121598	-0.252205	0.114208
3	8	0	-1.140805	2.298524	-1.397580
4	8	0	0.823050	1.248412	-0.963848
5	8	0	-2.330264	-0.276880	-2.110528
6	8	0	-0.368549	-1.316837	-1.643078
7	8	0	-3.173935	-0.659824	0.652343
8	8	0	-1.208525	-1.673353	1.153447
9	8	0	-1.976618	1.910785	1.381128
10	8	0	-0.008254	0.885967	1.849120
11	6	0	-2.480261	-1.579247	1.185825
12	6	0	0.122123	2.179010	-1.477174
13	6	0	-1.399511	-1.106023	-2.360141
14	6	0	-0.949738	1.711662	2.097415
15	6	0	-1.504565	-1.904326	-3.641290
16	1	0	-2.531578	-1.901163	-4.010520
17	1	0	-0.855331	-1.449797	-4.398819
18	1	0	-1.157795	-2.926901	-3.472812
19	6	0	0.862070	3.225876	-2.281781
20	1	0	0.370664	4.196216	-2.179948
21	1	0	1.904725	3.284010	-1.963540
22	1	0	0.835157	2.942946	-3.340813
23	6	0	-0.806178	2.547548	3.351086
24	1	0	-0.367796	1.952150	4.155935

25	1	0	-0.130354	3.385796	3.144182
26	1	0	-1.775229	2.947174	3.654892
27	6	0	-3.218157	-2.681912	1.912159
28	1	0	-4.260685	-2.403832	2.074188
29	1	0	-3.177343	-3.595330	1.308023
30	1	0	-2.725990	-2.894761	2.865126
31	6	0	4.363484	1.723390	0.909226
32	6	0	5.040877	1.440288	-0.280688
33	6	0	4.730206	0.305426	-1.040404
34	6	0	3.730659	-0.536445	-0.569548
35	6	0	3.038999	-0.253203	0.626543
36	6	0	3.345895	0.879670	1.370041
37	7	0	3.251659	-1.732522	-1.112023
38	6	0	2.283136	-2.340744	-0.327637
39	6	0	2.023449	-1.314518	0.761461
40	8	0	1.794329	-3.439934	-0.479947
41	1	0	4.621865	2.610722	1.479450
42	1	0	5.824571	2.108805	-0.625761
43	1	0	5.261474	0.085859	-1.962004
44	1	0	2.791520	1.113748	2.273043
45	1	0	3.586578	-2.171744	-1.957393
46	7	0	1.614633	-1.779874	1.941955
47	7	0	1.192174	-2.170672	2.911913

Complex coordination via N



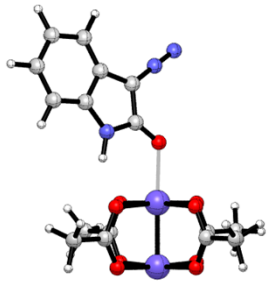
Zero-point correction= 0.333472 (Hartree/Particle)
Thermal correction to Energy= 0.365011
Thermal correction to Enthalpy= 0.365955
Thermal correction to Gibbs Free Energy= 0.265496
Sum of electronic and zero-point Energies= -1680.091960
Sum of electronic and thermal Energies= -1680.060421
Sum of electronic and thermal Enthalpies= -1680.059477
Sum of electronic and thermal Free Energies= -1680.159936

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	45	0	-2.786631	-0.291084	0.726501
2	45	0	-0.705766	0.097306	-0.423266
3	8	0	-1.849613	-1.806216	1.779460
4	8	0	0.114592	-1.443364	0.702840
5	8	0	-2.182530	1.076029	2.152360
6	8	0	-0.213874	1.431634	1.082394
7	8	0	-3.614294	1.240513	-0.381984
8	8	0	-1.655138	1.612640	-1.463609
9	8	0	-3.285911	-1.635856	-0.762960
10	8	0	-1.326389	-1.273198	-1.848018
11	6	0	-2.884426	1.848815	-1.226420
12	6	0	-0.624751	-2.046832	1.549534
13	6	0	-1.048863	1.635263	2.024050
14	6	0	-2.462136	-1.834589	-1.709575
15	6	0	-0.650309	2.654989	3.067723
16	1	0	0.389607	2.496187	3.365781
17	1	0	-0.718433	3.657409	2.630231
18	1	0	-1.310477	2.594928	3.934370
19	6	0	-3.536899	2.937102	-2.049647
20	1	0	-2.826068	3.745214	-2.237263
21	1	0	-3.835453	2.518255	-3.017820
22	1	0	-4.426784	3.315150	-1.543049
23	6	0	0.030871	-3.156816	2.342539
24	1	0	0.355935	-3.948341	1.658955
25	1	0	0.922835	-2.770504	2.845627
26	1	0	-0.664394	-3.567273	3.076059
27	6	0	-2.847711	-2.845963	-2.767012
28	1	0	-2.636225	-2.443283	-3.761383
29	1	0	-2.238632	-3.747930	-2.638720
30	1	0	-3.902752	-3.109537	-2.678274
31	6	0	5.721863	-2.370373	-0.183549
32	6	0	6.872404	-1.666391	0.187264
33	6	0	6.877181	-0.267572	0.264098
34	6	0	5.700629	0.403772	-0.042655
35	6	0	4.533084	-0.300847	-0.419988
36	6	0	4.537904	-1.691517	-0.490409
37	7	0	5.434189	1.775482	-0.049033
38	6	0	4.125740	2.073371	-0.420766
39	6	0	3.527561	0.721014	-0.663662
40	8	0	3.624803	3.175843	-0.522653
41	1	0	5.745455	-3.454647	-0.233783

42	1	0	7.782740	-2.210549	0.421555
43	1	0	7.773629	0.273453	0.552647
44	1	0	3.641383	-2.235507	-0.773877
45	1	0	6.093883	2.505887	0.176326
46	7	0	2.310474	0.566171	-1.069614
47	7	0	1.238996	0.446392	-1.466320

Complex coordination via O

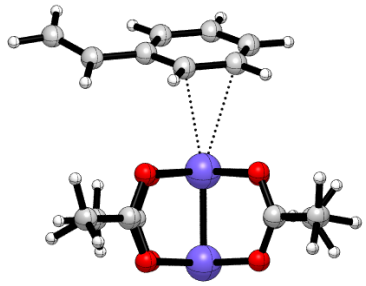


Zero-point correction= 0.334178 (Hartree/Particle)
Thermal correction to Energy= 0.366373
Thermal correction to Enthalpy= 0.367317
Thermal correction to Gibbs Free Energy= 0.265953
Sum of electronic and zero-point Energies= -1680.106896
Sum of electronic and thermal Energies= -1680.074701
Sum of electronic and thermal Enthalpies= -1680.073757
Sum of electronic and thermal Free Energies= -1680.175121

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	2.738019	-0.672843	-0.179097
2	45	0	0.567107	0.345747	0.097493
3	8	0	2.999366	-0.511835	1.865372
4	8	0	0.945733	0.418507	2.132934
5	8	0	1.839924	-2.527190	0.084086
6	8	0	-0.210621	-1.599319	0.316302
7	8	0	2.355583	-0.773979	-2.211456
8	8	0	0.317342	0.191980	-1.954278
9	8	0	3.515247	1.220708	-0.425364
10	8	0	1.475055	2.173813	-0.141151
11	6	0	1.255074	-0.315589	-2.651815
12	6	0	2.062134	-0.015248	2.566391
13	6	0	0.591396	-2.596914	0.258236
14	6	0	2.731812	2.218807	-0.341112
15	6	0	-6.941880	-0.750154	-0.086358

16	6	0	-6.230682	-1.954765	-0.058453
17	6	0	-4.833948	-1.970840	0.035956
18	6	0	-4.172595	-0.750713	0.100801
19	6	0	-4.885069	0.472050	0.073298
20	6	0	-6.274238	0.477345	-0.020474
21	7	0	-2.802833	-0.488180	0.196334
22	6	0	-2.538066	0.856694	0.229512
23	6	0	-3.860452	1.501536	0.156157
24	8	0	-1.429812	1.407639	0.305566
25	1	0	-8.025034	-0.765161	-0.160697
26	1	0	-6.768272	-2.896956	-0.111297
27	1	0	-4.284084	-2.907015	0.056679
28	1	0	-6.829591	1.410757	-0.043369
29	1	0	-2.041422	-1.169107	0.234518
30	7	0	-4.007511	2.798850	0.156570
31	7	0	-4.123171	3.930373	0.158637
32	6	0	-0.025955	-3.971248	0.404924
33	1	0	-0.641745	-4.007897	1.309125
34	1	0	-0.679418	-4.169777	-0.452217
35	1	0	0.750426	-4.735934	0.450985
36	6	0	1.046323	-0.346108	-4.150818
37	1	0	-0.010162	-0.495876	-4.385016
38	1	0	1.351816	0.620165	-4.569343
39	1	0	1.657502	-1.128618	-4.604693
40	6	0	2.284275	0.077749	4.061077
41	1	0	2.240762	1.127445	4.369548
42	1	0	1.480075	-0.449663	4.583938
43	1	0	3.250310	-0.349037	4.334439
44	6	0	3.352685	3.593376	-0.458923
45	1	0	2.626373	4.306611	-0.853911
46	1	0	3.657845	3.929929	0.539002
47	1	0	4.241125	3.553679	-1.092751

Cata- Styrene Complex: coordination via phenyl ring



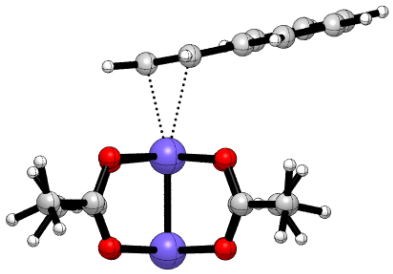
Zero-point correction= 0.346264 (Hartree/Particle)

Thermal correction to Energy= 0.376769
Thermal correction to Enthalpy= 0.377714
Thermal correction to Gibbs Free Energy= 0.278858
Sum of electronic and zero-point Energies= -1442.419080
Sum of electronic and thermal Energies= -1442.388575
Sum of electronic and thermal Enthalpies= -1442.387631
Sum of electronic and thermal Free Energies= -1442.486486

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	1.999189	0.491838	0.557051
2	45	0	-0.143321	-0.212383	-0.277523
3	8	0	2.843717	-0.212755	-1.195417
4	8	0	0.825627	-0.882090	-1.984387
5	8	0	1.687319	2.329060	-0.334464
6	8	0	-0.331376	1.675090	-1.132889
7	8	0	1.054190	1.160849	2.263819
8	8	0	-0.969599	0.494623	1.483733
9	8	0	2.222045	-1.369376	1.414055
10	8	0	0.202266	-2.043229	0.629561
11	6	0	-0.207749	1.021633	2.356298
12	6	0	2.089281	-0.743636	-2.070154
13	6	0	0.608851	2.520810	-0.978889
14	6	0	1.285780	-2.219830	1.273664
15	6	0	0.432480	3.882766	-1.614285
16	1	0	0.429293	4.648899	-0.831883
17	1	0	1.282723	4.090622	-2.271346
18	1	0	-0.498096	3.930455	-2.181625
19	6	0	2.759318	-1.287194	-3.312945
20	1	0	3.185247	-2.271240	-3.084535
21	1	0	2.036434	-1.397054	-4.123347
22	1	0	3.578713	-0.630279	-3.614708
23	6	0	1.461444	-3.556339	1.960676
24	1	0	0.991231	-3.509843	2.950061
25	1	0	0.968430	-4.344805	1.387685
26	1	0	2.521845	-3.780258	2.092457
27	6	0	-0.866619	1.560421	3.606852
28	1	0	-0.185389	1.481289	4.456924
29	1	0	-1.101076	2.620586	3.454853
30	1	0	-1.798125	1.027063	3.806294
31	6	0	-3.944556	1.447954	-0.514571
32	1	0	-3.216285	2.101843	-0.992395

33	6	0	-5.032727	1.994273	0.043162
34	1	0	-5.812158	1.401393	0.515045
35	1	0	-5.184727	3.069478	0.035228
36	6	0	-3.607723	0.016248	-0.571938
37	6	0	-2.625219	-0.414909	-1.493172
38	6	0	-4.210489	-0.948705	0.246561
39	6	0	-2.275875	-1.768293	-1.595950
40	1	0	-2.188001	0.310179	-2.173089
41	6	0	-3.862620	-2.297196	0.142610
42	1	0	-4.948479	-0.644137	0.983040
43	6	0	-2.895993	-2.714110	-0.772256
44	1	0	-1.528788	-2.073839	-2.321632
45	1	0	-4.345563	-3.024523	0.790167
46	1	0	-2.620325	-3.762056	-0.842004

Cata- Styrene Complex: coordination via double bond

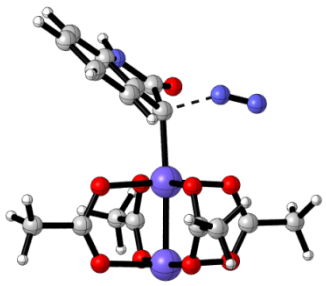


Zero-point correction= 0.347570 (Hartree/Particle)
Thermal correction to Energy= 0.377183
Thermal correction to Enthalpy= 0.378127
Thermal correction to Gibbs Free Energy= 0.284225
Sum of electronic and zero-point Energies= -1442.427489
Sum of electronic and thermal Energies= -1442.397876
Sum of electronic and thermal Enthalpies= -1442.396931
Sum of electronic and thermal Free Energies= -1442.490834

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	1.831057	-0.047633	1.087449
2	45	0	0.100239	0.019877	-0.602733
3	8	0	0.913427	-1.707502	1.900588
4	8	0	-0.713207	-1.663458	0.321008
5	8	0	2.917440	-1.265834	-0.187046

6	8	0	1.290041	-1.217487	-1.769547
7	8	0	2.691821	1.614697	0.215256
8	8	0	1.086002	1.685137	-1.384374
9	8	0	0.641241	1.167781	2.264569
10	8	0	-0.968495	1.257978	0.666786
11	6	0	2.142344	2.112788	-0.814730
12	6	0	-0.144493	-2.146988	1.353208
13	6	0	2.424463	-1.580817	-1.314211
14	6	0	-0.478762	1.553512	1.805847
15	6	0	3.272992	-2.462654	-2.205541
16	1	0	4.169631	-1.910797	-2.507984
17	1	0	3.603193	-3.341755	-1.644263
18	1	0	2.716642	-2.768734	-3.092749
19	6	0	-0.805892	-3.342377	2.005151
20	1	0	-1.374158	-3.000562	2.877964
21	1	0	-1.489666	-3.832669	1.310099
22	1	0	-0.045307	-4.044671	2.355298
23	6	0	-1.303069	2.475447	2.678421
24	1	0	-1.058179	3.514666	2.428569
25	1	0	-2.367853	2.320384	2.491267
26	1	0	-1.067029	2.310933	3.731718
27	6	0	2.782162	3.350490	-1.406146
28	1	0	2.357237	4.236281	-0.919473
29	1	0	3.858366	3.343755	-1.221462
30	1	0	2.574868	3.414422	-2.476719
31	6	0	-2.082457	-0.425147	-2.027484
32	1	0	-1.875928	-1.478560	-2.206537
33	6	0	-1.251517	0.485089	-2.605979
34	1	0	-1.411855	1.555498	-2.526980
35	1	0	-0.470055	0.163426	-3.285502
36	6	0	-3.287461	-0.161961	-1.229948
37	6	0	-4.017744	-1.257420	-0.737150
38	6	0	-3.757870	1.134944	-0.952314
39	6	0	-5.182025	-1.068743	0.005506
40	1	0	-3.660729	-2.263657	-0.940070
41	6	0	-4.919683	1.323897	-0.210638
42	1	0	-3.208483	1.998433	-1.312659
43	6	0	-5.637100	0.223780	0.271428
44	1	0	-5.733054	-1.928998	0.375869
45	1	0	-5.270038	2.332432	-0.007427
46	1	0	-6.545430	0.375614	0.848424

Transition state for loss of N2 (TS-9)

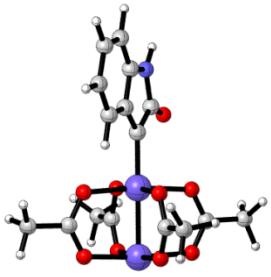


Zero-point correction= 0.330112 (Hartree/Particle)
Thermal correction to Energy= 0.362817
Thermal correction to Enthalpy= 0.363761
Thermal correction to Gibbs Free Energy= 0.262882
Sum of electronic and zero-point Energies= -1680.064708
Sum of electronic and thermal Energies= -1680.032003
Sum of electronic and thermal Enthalpies= -1680.031058
Sum of electronic and thermal Free Energies= -1680.131938

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	2.287797	-0.747153	-0.397487
2	45	0	0.090855	0.219948	0.107350
3	8	0	1.327397	-2.154130	-1.573703
4	8	0	-0.711808	-1.267548	-1.111102
5	8	0	2.400193	0.536583	-2.016740
6	8	0	0.349669	1.408233	-1.571020
7	8	0	3.120219	0.718223	0.809337
8	8	0	1.085289	1.601415	1.282636
9	8	0	2.026930	-1.961365	1.271181
10	8	0	0.004912	-1.050610	1.760481
11	6	0	2.361050	1.560029	1.370179
12	6	0	0.066547	-2.105698	-1.678694
13	6	0	1.426864	1.314584	-2.249063
14	6	0	0.978967	-1.854933	1.969047
15	6	0	1.523888	2.217151	-3.461326
16	1	0	1.168766	3.219598	-3.208087
17	1	0	2.550844	2.254607	-3.828462
18	1	0	0.874953	1.824221	-4.252496
19	6	0	-0.598911	-3.123180	-2.582529
20	1	0	-0.884830	-2.633835	-3.520791
21	1	0	0.087151	-3.942413	-2.803958
22	1	0	-1.511459	-3.501680	-2.114393
23	6	0	0.836517	-2.778259	3.161905

24	1	0	0.445502	-2.226988	4.021508
25	1	0	0.119551	-3.571266	2.919121
26	1	0	1.797595	-3.233079	3.406998
27	6	0	3.001370	2.638361	2.217409
28	1	0	2.506551	2.688976	3.191792
29	1	0	4.067141	2.442351	2.343681
30	1	0	2.863147	3.608568	1.727613
31	6	0	-4.343913	-1.892604	0.774037
32	6	0	-5.283155	-1.377604	-0.128113
33	6	0	-5.095512	-0.142446	-0.761991
34	6	0	-3.948044	0.573478	-0.445594
35	6	0	-2.988715	0.068691	0.464433
36	6	0	-3.178393	-1.179152	1.060948
37	7	0	-3.520488	1.812296	-0.930356
38	6	0	-2.335176	2.216556	-0.324445
39	6	0	-1.840026	0.975570	0.459945
40	8	0	-1.823886	3.310138	-0.409582
41	1	0	-4.518136	-2.857130	1.241031
42	1	0	-6.178465	-1.951275	-0.352384
43	1	0	-5.825279	0.238662	-1.470155
44	1	0	-2.421060	-1.571559	1.730944
45	1	0	-4.065312	2.438965	-1.506303
46	7	0	-1.677507	1.719140	2.088190
47	7	0	-1.065930	1.998093	2.973839

Carbenoid complex (10)



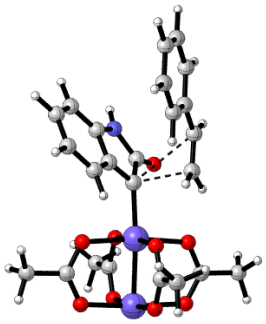
Zero-point correction= 0.322674 (Hartree/Particle)
Thermal correction to Energy= 0.352417
Thermal correction to Enthalpy= 0.353361
Thermal correction to Gibbs Free Energy= 0.257548
Sum of electronic and zero-point Energies= -1570.580363
Sum of electronic and thermal Energies= -1570.550621
Sum of electronic and thermal Enthalpies= -1570.549676
Sum of electronic and thermal Free Energies= -1570.645489

Center Atomic Atomic Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	45	0	-2.341864	-0.529558	0.000424
2	45	0	0.018663	0.182000	-0.000154
3	8	0	-1.823616	-1.908483	1.467967
4	8	0	0.357509	-1.270850	1.451209
5	8	0	-2.692091	0.900581	1.456286
6	8	0	-0.510887	1.538860	1.471728
7	8	0	-2.692934	0.900978	-1.454874
8	8	0	-0.511635	1.538904	-1.471724
9	8	0	-1.824438	-1.908163	-1.467710
10	8	0	0.356761	-1.270764	-1.451761
11	6	0	-1.727165	1.611567	-1.859760
12	6	0	-0.626675	-1.978854	1.864569
13	6	0	-1.726201	1.611431	1.860441
14	6	0	-0.627669	-1.978613	-1.864815
15	6	0	-2.016631	2.670245	2.903527
16	1	0	-1.872036	3.660958	2.459240
17	1	0	-3.041488	2.576840	3.266004
18	1	0	-1.310231	2.576789	3.733668
19	6	0	-0.307175	-2.975470	2.960305
20	1	0	-0.255450	-2.445263	3.918405
21	1	0	-1.087831	-3.735791	3.020367
22	1	0	0.667196	-3.437888	2.782793
23	6	0	-0.308490	-2.975276	-2.960603
24	1	0	-0.250514	-2.444189	-3.917842
25	1	0	0.663224	-3.442090	-2.779857
26	1	0	-1.092065	-3.732255	-3.024417
27	6	0	-2.017587	2.669319	-2.903937
28	1	0	-1.320518	2.565021	-3.740761
29	1	0	-3.046700	2.584402	-3.256245
30	1	0	-1.858167	3.660330	-2.465591
31	6	0	4.576695	-1.918383	-0.000201
32	6	0	5.676874	-1.038155	0.000005
33	6	0	5.530421	0.353628	0.000030
34	6	0	4.235084	0.857577	-0.000151
35	6	0	3.093709	-0.015407	-0.000332
36	6	0	3.283813	-1.416782	-0.000364
37	7	0	3.795705	2.163730	-0.000184
38	6	0	2.386142	2.208383	-0.000327
39	6	0	1.909121	0.750937	-0.000404
40	8	0	1.735852	3.228423	-0.000382
41	1	0	4.750717	-2.989597	-0.000226

42	1	0	6.681720	-1.452884	0.000144
43	1	0	6.398224	1.005980	0.000187
44	1	0	2.413609	-2.061950	-0.000514
45	1	0	4.372674	2.992841	0.000006

End-on transition state leading to *trans* cyclopropane (TS-11a)



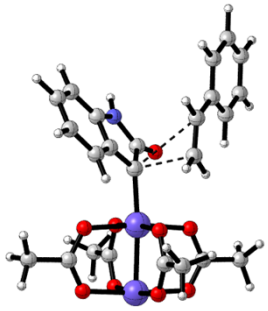
Zero-point correction= 0.458701 (Hartree/Particle)
Thermal correction to Energy= 0.496428
Thermal correction to Enthalpy= 0.497372
Thermal correction to Gibbs Free Energy= 0.384651
Sum of electronic and zero-point Energies= -1880.086983
Sum of electronic and thermal Energies= -1880.049256
Sum of electronic and thermal Enthalpies= -1880.048312
Sum of electronic and thermal Free Energies= -1880.161032

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-3.217948	0.056797	0.524467
2	45	0	-0.838567	-0.081734	-0.120341
3	8	0	-2.985818	2.111515	0.672082
4	8	0	-0.801663	1.994356	0.056441
5	8	0	-3.675690	0.253536	-1.483283
6	8	0	-1.485566	0.123305	-2.081875
7	8	0	-3.314607	-2.004263	0.321590
8	8	0	-1.114958	-2.140625	-0.224376
9	8	0	-2.580381	-0.152360	2.499581
10	8	0	-0.386908	-0.241579	1.911450
11	6	0	-2.270798	-2.640700	-0.001414
12	6	0	-1.862089	2.621699	0.395823
13	6	0	-2.733298	0.232331	-2.329489
14	6	0	-1.348553	-0.242769	2.759042
15	6	0	-3.104036	0.330408	-3.795349

16	1	0	-4.166004	0.554446	-3.907430
17	1	0	-2.499608	1.102254	-4.280911
18	1	0	-2.875877	-0.621855	-4.286510
19	6	0	-1.755083	4.133071	0.436924
20	1	0	-0.753464	4.437945	0.748894
21	1	0	-1.929450	4.526664	-0.571547
22	1	0	-2.511809	4.548159	1.105552
23	6	0	-0.943629	-0.376857	4.214105
24	1	0	-0.472052	-1.352692	4.373679
25	1	0	-0.205092	0.390749	4.466366
26	1	0	-1.815664	-0.282750	4.862781
27	6	0	-2.375924	-4.145262	-0.144223
28	1	0	-1.676041	-4.630192	0.544389
29	1	0	-3.393065	-4.478891	0.066383
30	1	0	-2.090226	-4.435335	-1.160512
31	6	0	3.082172	2.864788	0.687186
32	6	0	3.928974	3.046107	-0.418085
33	6	0	3.863737	2.221179	-1.546658
34	6	0	2.922421	1.197691	-1.538401
35	6	0	2.045307	0.996170	-0.432917
36	6	0	2.134995	1.844301	0.683945
37	7	0	2.636543	0.254113	-2.511500
38	6	0	1.553353	-0.555265	-2.128775
39	6	0	1.122516	-0.064249	-0.734059
40	8	0	1.092402	-1.445814	-2.808882
41	1	0	3.164781	3.530484	1.540974
42	1	0	4.656494	3.853612	-0.402963
43	1	0	4.525121	2.379853	-2.393278
44	1	0	1.458866	1.691242	1.517713
45	1	0	3.069082	0.187050	-3.422047
46	6	0	3.115765	-2.082405	-0.127024
47	1	0	3.186665	-2.682054	-1.033532
48	6	0	1.872554	-1.910940	0.416762
49	1	0	1.712228	-1.407050	1.363607
50	1	0	1.029588	-2.476593	0.037417
51	6	0	4.366394	-1.504314	0.332960
52	6	0	5.536922	-1.717439	-0.427264
53	6	0	4.469320	-0.732320	1.510996
54	6	0	6.757979	-1.181138	-0.032252
55	1	0	5.473550	-2.313582	-1.334463
56	6	0	5.690373	-0.193687	1.902154
57	1	0	3.589944	-0.563692	2.123123
58	6	0	6.838225	-0.414254	1.134058
59	1	0	7.647520	-1.359114	-0.630188

60	1	0	5.750947	0.398268	2.811149
61	1	0	7.790863	0.004993	1.446096

End-on transition state leading to *cis* cyclopropane (TS-11b)

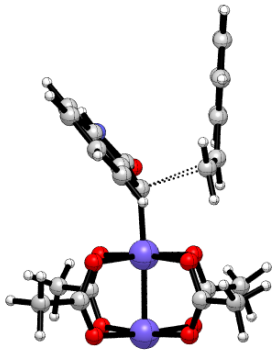


Zero-point correction= 0.458626 (Hartree/Particle)
Thermal correction to Energy= 0.496376
Thermal correction to Enthalpy= 0.497321
Thermal correction to Gibbs Free Energy= 0.383990
Sum of electronic and zero-point Energies= -1880.086876
Sum of electronic and thermal Energies= -1880.049126
Sum of electronic and thermal Enthalpies= -1880.048182
Sum of electronic and thermal Free Energies= -1880.161512

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	3.090547	-0.766999	-0.033105
2	45	0	0.743985	0.004542	0.000618
3	8	0	3.667800	1.192449	0.315269
4	8	0	1.512307	1.910684	0.344485
5	8	0	2.939405	-1.086583	2.005844
6	8	0	0.785387	-0.359763	2.044054
7	8	0	2.368901	-2.683013	-0.365581
8	8	0	0.210932	-1.976688	-0.360568
9	8	0	3.066017	-0.390030	-2.083507
10	8	0	0.912186	0.332803	-2.049390
11	6	0	1.121672	-2.870297	-0.448270
12	6	0	2.775762	2.080965	0.433535
13	6	0	1.844991	-0.822610	2.585672
14	6	0	2.023449	0.065973	-2.629836
15	6	0	1.765133	-1.064503	4.079412
16	1	0	1.636398	-0.107011	4.595784
17	1	0	0.888947	-1.679670	4.305202
18	1	0	2.673027	-1.553162	4.436351

19	6	0	3.236124	3.491043	0.744798
20	1	0	3.266330	3.620484	1.833220
21	1	0	4.241668	3.655270	0.351924
22	1	0	2.535925	4.222555	0.335406
23	6	0	2.062398	0.315783	-4.124526
24	1	0	1.397529	-0.394539	-4.628545
25	1	0	1.695547	1.322911	-4.344777
26	1	0	3.077666	0.193707	-4.504644
27	6	0	0.635379	-4.289196	-0.664407
28	1	0	-0.034367	-4.325652	-1.529389
29	1	0	1.479932	-4.962744	-0.817079
30	1	0	0.061406	-4.611669	0.211049
31	6	0	-1.456655	4.412203	-0.829871
32	6	0	-2.466462	4.745545	0.086357
33	6	0	-3.016638	3.799530	0.960244
34	6	0	-2.529825	2.499722	0.884952
35	6	0	-1.503684	2.136773	-0.033822
36	6	0	-0.964375	3.110012	-0.888512
37	7	0	-2.888883	1.378459	1.617630
38	6	0	-2.131346	0.263578	1.237707
39	6	0	-1.158783	0.749012	0.154497
40	8	0	-2.259035	-0.846517	1.712506
41	1	0	-1.055348	5.177194	-1.487562
42	1	0	-2.832438	5.768324	0.125399
43	1	0	-3.793420	4.077205	1.666704
44	1	0	-0.177636	2.831275	-1.580666
45	1	0	-3.608795	1.330431	2.324711
46	6	0	-3.465140	-0.104906	-1.493650
47	1	0	-3.800030	0.832271	-1.938827
48	6	0	-2.136550	-0.413279	-1.594890
49	1	0	-1.730629	-1.354924	-1.243477
50	1	0	-1.489873	0.159791	-2.249285
51	6	0	-4.509539	-0.878729	-0.845138
52	6	0	-5.837061	-0.399135	-0.895720
53	6	0	-4.262698	-2.098786	-0.176181
54	6	0	-6.879738	-1.109844	-0.311804
55	1	0	-6.039588	0.538977	-1.407495
56	6	0	-5.308416	-2.803428	0.411506
57	1	0	-3.250605	-2.479019	-0.103531
58	6	0	-6.617615	-2.316865	0.344535
59	1	0	-7.895188	-0.727068	-0.366296
60	1	0	-5.101829	-3.736664	0.927675
61	1	0	-7.429868	-2.875054	0.802215

Side -on transition state leading to *trans* cyclopropane (TS-11c)

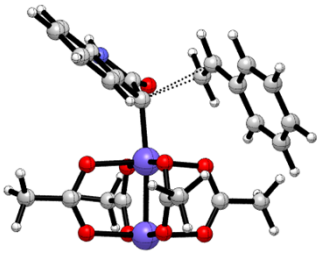


Zero-point correction= 0.458654 (Hartree/Particle)
Thermal correction to Energy= 0.496436
Thermal correction to Enthalpy= 0.497380
Thermal correction to Gibbs Free Energy= 0.384069
Sum of electronic and zero-point Energies= -1880.083183
Sum of electronic and thermal Energies= -1880.045402
Sum of electronic and thermal Enthalpies= -1880.044457
Sum of electronic and thermal Free Energies= -1880.157768

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	3.064829	-0.759933	-0.033235
2	45	0	0.715578	0.007902	0.008436
3	8	0	3.631572	1.207880	0.291430
4	8	0	1.473362	1.920403	0.323049
5	8	0	2.920556	-1.055636	2.010348
6	8	0	0.768829	-0.322445	2.054636
7	8	0	2.336165	-2.680213	-0.344398
8	8	0	0.175806	-1.976926	-0.339098
9	8	0	3.033895	-0.409693	-2.088939
10	8	0	0.874869	0.295372	-2.055279
11	6	0	1.089165	-2.868686	-0.421869
12	6	0	2.736593	2.095010	0.402809
13	6	0	1.831608	-0.779344	2.594626
14	6	0	1.985732	0.026756	-2.637898
15	6	0	1.764509	-0.995102	4.093193
16	1	0	0.872975	-1.578465	4.341446
17	1	0	2.662440	-1.504570	4.446381
18	1	0	1.673558	-0.025408	4.594969
19	6	0	3.194132	3.510842	0.692405
20	1	0	3.211857	3.661547	1.778372

21	1	0	4.203609	3.668256	0.307002
22	1	0	2.497817	4.233783	0.261506
23	6	0	2.016309	0.257786	-4.136005
24	1	0	1.297386	-0.409246	-4.624212
25	1	0	1.713750	1.285922	-4.359001
26	1	0	3.015801	0.069294	-4.530339
27	6	0	0.606251	-4.291707	-0.623782
28	1	0	-0.080552	-4.336173	-1.474975
29	1	0	1.451153	-4.961456	-0.790581
30	1	0	0.053149	-4.614916	0.264959
31	6	0	-1.500107	4.363991	-0.980981
32	6	0	-2.404997	4.766678	0.012279
33	6	0	-2.897353	3.870227	0.969542
34	6	0	-2.465416	2.551395	0.895643
35	6	0	-1.549411	2.119513	-0.101826
36	6	0	-1.059900	3.042051	-1.036137
37	7	0	-2.777197	1.472027	1.712357
38	6	0	-2.119905	0.308574	1.299776
39	6	0	-1.219603	0.723548	0.117959
40	8	0	-2.255527	-0.774297	1.832688
41	1	0	-1.135510	5.089785	-1.701618
42	1	0	-2.730648	5.803028	0.048522
43	1	0	-3.588545	4.199934	1.739846
44	1	0	-0.350223	2.711249	-1.787133
45	1	0	-3.411555	1.482160	2.498488
46	6	0	-2.804509	-1.220325	-1.071593
47	1	0	-2.138805	-2.028531	-0.780025
48	6	0	-2.216203	-0.133192	-1.668682
49	1	0	-2.814827	0.716409	-1.983423
50	1	0	-1.233759	-0.216690	-2.118096
51	6	0	-4.195399	-1.358097	-0.686852
52	6	0	-4.549180	-2.396200	0.201368
53	6	0	-5.215116	-0.505407	-1.165747
54	6	0	-5.870299	-2.571881	0.602885
55	1	0	-3.768590	-3.045327	0.585968
56	6	0	-6.533361	-0.685614	-0.765767
57	1	0	-4.971205	0.285301	-1.868839
58	6	0	-6.865392	-1.718517	0.120226
59	1	0	-6.124862	-3.371718	1.292348
60	1	0	-7.309121	-0.028015	-1.148192
61	1	0	-7.898374	-1.858284	0.427178

Side-on transition state leading to *trans* cyclopropane (TS-11d)



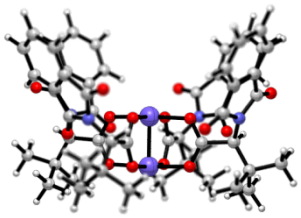
Zero-point correction= 0.458879 (Hartree/Particle)
Thermal correction to Energy= 0.495559
Thermal correction to Enthalpy= 0.496503
Thermal correction to Gibbs Free Energy= 0.388640
Sum of electronic and zero-point Energies= -1880.076673
Sum of electronic and thermal Energies= -1880.039994
Sum of electronic and thermal Enthalpies= -1880.039050
Sum of electronic and thermal Free Energies= -1880.146912

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-2.254363	-1.370994	0.747162
2	45	0	-0.551477	0.144551	-0.209189
3	8	0	-2.671677	0.089786	2.153481
4	8	0	-1.101473	1.484355	1.285414
5	8	0	-3.632685	-0.532731	-0.552006
6	8	0	-2.080550	0.901485	-1.389915
7	8	0	-1.752980	-2.743624	-0.729315
8	8	0	-0.200773	-1.353031	-1.627589
9	8	0	-0.759710	-2.101930	1.995454
10	8	0	0.815502	-0.721794	1.112560
11	6	0	-0.894626	-2.430317	-1.599471
12	6	0	-2.021382	1.174665	2.115847
13	6	0	-3.255519	0.411673	-1.308251
14	6	0	0.405562	-1.616378	1.930413
15	6	0	-4.301662	1.056594	-2.194546
16	1	0	-3.858868	1.345202	-3.150644
17	1	0	-5.142841	0.377223	-2.345075
18	1	0	-4.669765	1.965828	-1.704457
19	6	0	-2.370098	2.237644	3.138185
20	1	0	-2.974967	3.013361	2.654422
21	1	0	-2.942182	1.802920	3.959669
22	1	0	-1.459235	2.712417	3.512303
23	6	0	1.430053	-2.122273	2.926519

24	1	0	2.365790	-2.360663	2.413755
25	1	0	1.641392	-1.331869	3.656090
26	1	0	1.048837	-2.999678	3.451539
27	6	0	-0.663130	-3.401426	-2.739567
28	1	0	0.405414	-3.505894	-2.948859
29	1	0	-1.101812	-4.373005	-2.506307
30	1	0	-1.137192	-3.003108	-3.644022
31	6	0	2.592394	3.339324	1.927871
32	6	0	2.427832	4.644951	1.440822
33	6	0	1.768553	4.899291	0.233010
34	6	0	1.294045	3.805617	-0.483086
35	6	0	1.458792	2.473874	-0.017452
36	6	0	2.098139	2.251809	1.209311
37	7	0	0.599276	3.780963	-1.687240
38	6	0	0.338892	2.469307	-2.094879
39	6	0	0.788468	1.559065	-0.928995
40	8	0	-0.133417	2.166620	-3.170528
41	1	0	3.100755	3.179719	2.874239
42	1	0	2.813293	5.482788	2.016048
43	1	0	1.633448	5.915166	-0.127122
44	1	0	2.198015	1.236343	1.576455
45	1	0	0.427583	4.573681	-2.289852
46	6	0	3.376962	0.208009	-1.407116
47	1	0	4.089172	1.024191	-1.283578
48	6	0	2.245108	0.474260	-2.145185
49	1	0	1.539621	-0.300889	-2.419432
50	1	0	2.293066	1.329311	-2.809139
51	6	0	3.763314	-1.027559	-0.765498
52	6	0	5.008318	-1.084313	-0.099550
53	6	0	2.973834	-2.199271	-0.818145
54	6	0	5.456088	-2.265712	0.482851
55	1	0	5.624494	-0.189535	-0.053661
56	6	0	3.425228	-3.376992	-0.236151
57	1	0	2.001630	-2.162438	-1.295207
58	6	0	4.666831	-3.417428	0.412764
59	1	0	6.418049	-2.292737	0.986744
60	1	0	2.809443	-4.270993	-0.282522
61	1	0	5.014874	-4.343678	0.861850

14.3 Rh_2(*S*-PTTL)$_4$-Model (Diazooxindole+Styrene+ Rh_2(*S*-PTTL)$_4$)

Rh_2(*S*-PTTL)$_4$ (13)



Zero-point correction= 1.053671 (Hartree/Particle)
Thermal correction to Energy= 1.127920
Thermal correction to Enthalpy= 1.128865
Thermal correction to Gibbs Free Energy= 0.940747
Sum of electronic and zero-point Energies= -3808.583069
Sum of electronic and thermal Energies= -3808.508819
Sum of electronic and thermal Enthalpies= -3808.507875
Sum of electronic and thermal Free Energies= -3808.695993

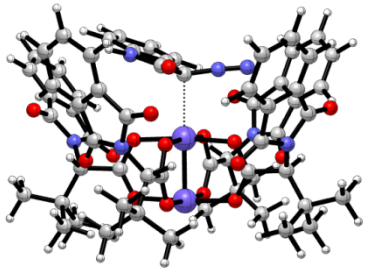
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.025471	-0.132914	0.185449
2	45	0	-0.096019	-0.195755	-2.199157
3	7	0	4.081812	-2.416981	0.138223
4	8	0	2.388484	-3.975519	-0.258601
5	8	0	5.685928	-1.131744	1.244380
6	6	0	3.275025	-3.530799	0.443360
7	6	0	3.734704	-4.012565	1.777861
8	6	0	3.309504	-5.096615	2.532221
9	1	0	2.523182	-5.752968	2.172702
10	6	0	3.931569	-5.301574	3.771249
11	1	0	3.626309	-6.139300	4.391825
12	6	0	4.940443	-4.441695	4.225754
13	1	0	5.402662	-4.626753	5.191328
14	6	0	5.358874	-3.347391	3.456752
15	1	0	6.136515	-2.672609	3.800909
16	6	0	4.737827	-3.154661	2.231052
17	6	0	4.941759	-2.094049	1.202824
18	7	0	2.561292	3.727571	-0.028057
19	8	0	3.786174	1.854746	-0.679754
20	8	0	1.623993	5.395738	1.308834
21	6	0	3.551293	2.739077	0.122824

22	6	0	4.202433	3.001412	1.435286
23	6	0	5.239864	2.328621	2.066287
24	1	0	5.701428	1.455740	1.614276
25	6	0	5.637360	2.807462	3.322643
26	1	0	6.444478	2.309498	3.852459
27	6	0	5.008151	3.912237	3.912116
28	1	0	5.340670	4.256712	4.887409
29	6	0	3.950570	4.571464	3.270390
30	1	0	3.446243	5.418395	3.725253
31	6	0	3.564263	4.093733	2.026508
32	6	0	2.463417	4.535376	1.122099
33	7	0	-3.767517	2.590600	0.198293
34	8	0	-1.852882	3.723426	-0.504593
35	8	0	-5.437503	1.726675	1.580903
36	6	0	-2.714768	3.515838	0.329092
37	6	0	-2.881037	4.145300	1.667725
38	6	0	-2.119167	5.121716	2.294668
39	1	0	-1.239310	5.541979	1.816224
40	6	0	-2.518648	5.514293	3.579791
41	1	0	-1.949274	6.274333	4.107183
42	6	0	-3.635695	4.938872	4.200485
43	1	0	-3.917700	5.265570	5.197515
44	6	0	-4.386519	3.942243	3.561951
45	1	0	-5.244214	3.479664	4.040359
46	6	0	-3.985906	3.560671	2.289699
47	6	0	-4.532558	2.514447	1.378121
48	7	0	-2.941269	-3.733964	0.267708
49	8	0	-3.927325	-1.760389	-0.485296
50	8	0	-2.263364	-5.470989	1.670483
51	6	0	-3.801507	-2.626509	0.361132
52	6	0	-4.487554	-2.743188	1.677714
53	6	0	-5.430281	-1.913672	2.270139
54	1	0	-5.771037	-1.005621	1.781809
55	6	0	-5.895926	-2.282940	3.539810
56	1	0	-6.632037	-1.659828	4.039635
57	6	0	-5.424321	-3.437032	4.179746
58	1	0	-5.806469	-3.694025	5.163756
59	6	0	-4.460596	-4.256991	3.576964
60	1	0	-4.076969	-5.144877	4.069870
61	6	0	-4.005640	-3.885143	2.320220
62	6	0	-2.969735	-4.508396	1.447816
63	8	0	1.871920	-0.918255	0.094200
64	8	0	1.822758	-0.962952	-2.166074
65	8	0	0.775932	1.749248	0.046840

66	8	0	0.693535	1.714860	-2.212922
67	8	0	-1.904380	0.691474	0.154129
68	8	0	-1.990460	0.623667	-2.104853
69	8	0	-0.866681	-2.007227	0.208501
70	8	0	-0.915641	-2.091038	-2.050831
71	6	0	2.396306	-1.125269	-1.045939
72	6	0	3.884831	-1.523271	-1.006083
73	1	0	4.386655	-0.593968	-0.707214
74	6	0	4.573932	-1.995382	-2.331168
75	6	0	6.027011	-2.393563	-1.991277
76	1	0	6.570488	-2.619677	-2.915665
77	1	0	6.067380	-3.286422	-1.358005
78	1	0	6.557929	-1.586317	-1.474099
79	6	0	3.869111	-3.190309	-3.000562
80	1	0	2.837619	-2.948639	-3.267639
81	1	0	3.851016	-4.069493	-2.350474
82	1	0	4.406868	-3.460089	-3.917886
83	6	0	4.626638	-0.801176	-3.310704
84	1	0	3.628763	-0.498584	-3.633263
85	1	0	5.204540	-1.082181	-4.199280
86	1	0	5.114889	0.067439	-2.852779
87	6	0	0.961567	2.264218	-1.101856
88	6	0	1.515935	3.702708	-1.058322
89	1	0	0.694243	4.283556	-0.621045
90	6	0	1.900143	4.407422	-2.399486
91	6	0	2.965249	3.646561	-3.211139
92	1	0	3.902057	3.543728	-2.655698
93	1	0	3.181284	4.199684	-4.133577
94	1	0	2.623850	2.645379	-3.483703
95	6	0	2.440585	5.811972	-2.052150
96	1	0	3.389704	5.758405	-1.507972
97	1	0	1.730965	6.378972	-1.438893
98	1	0	2.618932	6.375703	-2.974946
99	6	0	0.619429	4.583112	-3.245353
100	1	0	-0.158762	5.113362	-2.683510
101	1	0	0.210855	3.622485	-3.564950
102	1	0	0.849393	5.173726	-4.140086
103	6	0	-2.463824	0.917637	-0.966472
104	6	0	-3.855888	1.571526	-0.854678
105	1	0	-4.480116	0.784723	-0.414801
106	6	0	-4.579184	2.039918	-2.159757
107	6	0	-4.890041	0.796558	-3.022445
108	1	0	-5.463001	0.052137	-2.456822
109	1	0	-3.978274	0.317670	-3.384140

110	1	0	-5.490111	1.094661	-3.890224
111	6	0	-5.921321	2.683161	-1.746414
112	1	0	-6.518449	2.009103	-1.121634
113	1	0	-6.505309	2.922406	-2.642386
114	1	0	-5.771162	3.615156	-1.190750
115	6	0	-3.767970	3.058320	-2.982729
116	1	0	-2.813247	2.640606	-3.310156
117	1	0	-3.559634	3.968192	-2.412612
118	1	0	-4.342199	3.343617	-3.872878
119	6	0	-1.174915	-2.552165	-0.898759
120	6	0	-1.900462	-3.908980	-0.753413
121	1	0	-1.167366	-4.565174	-0.267444
122	6	0	-2.372573	-4.647728	-2.047980
123	6	0	-1.125614	-5.020143	-2.880300
124	1	0	-0.605246	-4.134257	-3.250094
125	1	0	-1.427524	-5.624624	-3.743454
126	1	0	-0.415926	-5.614304	-2.291045
127	6	0	-3.069472	-5.957210	-1.617066
128	1	0	-4.005033	-5.761865	-1.081742
129	1	0	-2.429389	-6.564445	-0.967370
130	1	0	-3.315185	-6.550627	-2.505048
131	6	0	-3.350353	-3.821393	-2.904552
132	1	0	-2.893315	-2.893868	-3.255243
133	1	0	-4.255783	-3.561888	-2.348053
134	1	0	-3.651908	-4.410841	-3.779180

Cata-diazo-complex (14)



Zero-point correction= 1.175170 (Hartree/Particle)
Thermal correction to Energy= 1.260267
Thermal correction to Enthalpy= 1.261212
Thermal correction to Gibbs Free Energy= 1.050698
Sum of electronic and zero-point Energies= -4355.769833
Sum of electronic and thermal Energies= -4355.684736
Sum of electronic and thermal Enthalpies= -4355.683791
Sum of electronic and thermal Free Energies= -4355.894305

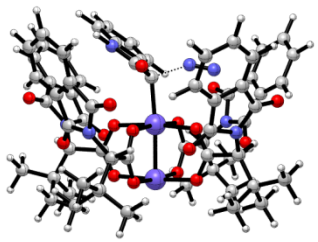
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.122009	0.092742	-0.104315
2	45	0	0.252987	0.131664	-2.518356
3	7	0	-0.838165	-4.448616	-0.245410
4	8	0	-2.683318	-3.209177	-0.949698
5	8	0	0.647109	-5.609249	1.132782
6	6	0	-2.121034	-3.895243	-0.116093
7	6	0	-2.619048	-4.304087	1.226645
8	6	0	-3.825211	-4.017252	1.854220
9	1	0	-4.584610	-3.415405	1.362289
10	6	0	-4.001580	-4.517715	3.153017
11	1	0	-4.931141	-4.322284	3.680777
12	6	0	-2.999407	-5.272438	3.781785
13	1	0	-3.168276	-5.646533	4.787775
14	6	0	-1.784121	-5.543002	3.138522
15	1	0	-0.995452	-6.109055	3.623741
16	6	0	-1.617023	-5.042181	1.855716
17	6	0	-0.440399	-5.104787	0.938009
18	7	0	4.602687	-1.136984	0.030603
19	8	0	3.229414	-2.882497	-0.681029
20	8	0	5.845577	0.272597	1.414238
21	6	0	3.939170	-2.372319	0.164929
22	6	0	4.283478	-2.881385	1.520535
23	6	0	3.886910	-4.046382	2.162429
24	1	0	3.208857	-4.748413	1.686513
25	6	0	4.370501	-4.252894	3.461887
26	1	0	4.081298	-5.149763	4.002173
27	6	0	5.211783	-3.319071	4.081633
28	1	0	5.568041	-3.510543	5.090064
29	6	0	5.588765	-2.137549	3.428443
30	1	0	6.225565	-1.399447	3.906176
31	6	0	5.107591	-1.940795	2.142082
32	6	0	5.273932	-0.783958	1.215755
33	7	0	1.644290	4.479978	-0.082438
34	8	0	3.280735	2.977659	-0.792661
35	8	0	0.346011	5.830463	1.309184
36	6	0	2.836430	3.743037	0.041868
37	6	0	3.399982	4.084325	1.378275
38	6	0	4.551944	3.628816	2.006123
39	1	0	5.202601	2.897927	1.535547
40	6	0	4.816809	4.126292	3.290039

41	1	0	5.705852	3.792431	3.817251
42	6	0	3.952380	5.039183	3.909290
43	1	0	4.188263	5.404824	4.904778
44	6	0	2.783452	5.476685	3.271364
45	1	0	2.097824	6.170309	3.748225
46	6	0	2.528993	4.980562	2.000701
47	6	0	1.363155	5.198786	1.096858
48	7	0	-4.644209	0.728637	-0.565020
49	8	0	-3.705356	2.776461	-1.178467
50	8	0	-5.767428	-0.900920	0.676631
51	6	0	-4.470385	2.123287	-0.497947
52	6	0	-5.407570	2.598258	0.563086
53	6	0	-5.688234	3.884819	0.998936
54	1	0	-5.187205	4.743120	0.562271
55	6	0	-6.641616	4.026720	2.016767
56	1	0	-6.894193	5.018712	2.380758
57	6	0	-7.279739	2.908437	2.571230
58	1	0	-8.018841	3.051000	3.354726
59	6	0	-6.982466	1.612553	2.126642
60	1	0	-7.472030	0.739447	2.547279
61	6	0	-6.039804	1.485133	1.116473
62	6	0	-5.513911	0.265383	0.435352
63	8	0	0.043772	-1.953704	-0.240541
64	8	0	0.202140	-1.943982	-2.496808
65	8	0	2.187516	-0.003581	-0.099159
66	8	0	2.312624	0.038473	-2.356357
67	8	0	0.265619	2.159583	-0.128473
68	8	0	0.350454	2.204087	-2.389982
69	8	0	-1.948912	0.143617	-0.293328
70	8	0	-1.812227	0.145480	-2.552864
71	6	0	0.107994	-2.523237	-1.375148
72	6	0	0.125920	-4.065646	-1.286632
73	1	0	1.102299	-4.285666	-0.838113
74	6	0	0.038618	-4.901255	-2.603800
75	6	0	0.044900	-6.395971	-2.214678
76	1	0	0.095014	-7.011665	-3.120080
77	1	0	-0.864010	-6.678063	-1.672066
78	1	0	0.905816	-6.646398	-1.584464
79	6	0	-1.221035	-4.603819	-3.437813
80	1	0	-1.266296	-3.553291	-3.733810
81	1	0	-2.136776	-4.839028	-2.887574
82	1	0	-1.208576	-5.217604	-4.347124
83	6	0	1.303401	-4.619632	-3.445291
84	1	0	1.331632	-3.585945	-3.795021

85	1	0	1.316753	-5.280322	-4.320374
86	1	0	2.215917	-4.808147	-2.867178
87	6	0	2.822634	-0.046706	-1.203873
88	6	0	4.352831	-0.168194	-1.043563
89	1	0	4.649217	0.794134	-0.610607
90	6	0	5.229229	-0.370319	-2.323204
91	6	0	4.852521	-1.622579	-3.137227
92	1	0	4.971636	-2.538866	-2.551808
93	1	0	5.509858	-1.695529	-4.012556
94	1	0	3.818768	-1.578604	-3.487117
95	6	0	6.701101	-0.490665	-1.870111
96	1	0	6.875051	-1.403658	-1.290390
97	1	0	7.007380	0.363492	-1.255472
98	1	0	7.354021	-0.528137	-2.749586
99	6	0	5.104268	0.888934	-3.209710
100	1	0	5.359512	1.796861	-2.650420
101	1	0	4.092977	1.007111	-3.602959
102	1	0	5.796602	0.808975	-4.056220
103	6	0	0.405971	2.746383	-1.249847
104	6	0	0.629414	4.272793	-1.126342
105	1	0	-0.291194	4.652464	-0.666311
106	6	0	0.849536	5.108785	-2.427818
107	6	0	-0.432972	5.018804	-3.284241
108	1	0	-1.314155	5.347347	-2.718761
109	1	0	-0.613611	4.001568	-3.637282
110	1	0	-0.336381	5.673602	-4.158173
111	6	0	1.047945	6.583576	-2.013698
112	1	0	0.222127	6.946119	-1.390894
113	1	0	1.099607	7.212655	-2.909611
114	1	0	1.979875	6.726711	-1.455930
115	6	0	2.066446	4.654980	-3.256493
116	1	0	1.964216	3.619527	-3.587427
117	1	0	2.997976	4.738156	-2.688820
118	1	0	2.156706	5.294470	-4.143202
119	6	0	-2.451197	0.089426	-1.461191
120	6	0	-3.972564	-0.168721	-1.508681
121	1	0	-4.072039	-1.161429	-1.053618
122	6	0	-4.671993	-0.248343	-2.911885
123	6	0	-4.097246	-1.455609	-3.686584
124	1	0	-3.046387	-1.308763	-3.940677
125	1	0	-4.660567	-1.590544	-4.617767
126	1	0	-4.180315	-2.379294	-3.103382
127	6	0	-6.176754	-0.514998	-2.681860
128	1	0	-6.677830	0.336502	-2.207898

129	1	0	-6.342370	-1.398983	-2.056037
130	1	0	-6.667340	-0.685759	-3.646756
131	6	0	-4.518833	1.032566	-3.754913
132	1	0	-3.468715	1.264661	-3.942949
133	1	0	-4.975461	1.900126	-3.269314
134	1	0	-5.020088	0.890314	-4.720499
135	6	0	-2.377799	2.950757	3.226775
136	6	0	-3.456280	2.137591	3.586098
137	6	0	-3.360847	0.740957	3.539812
138	6	0	-2.152832	0.187549	3.135653
139	6	0	-1.061590	1.002192	2.769573
140	6	0	-1.168075	2.387140	2.805198
141	7	0	-1.779942	-1.157607	3.056743
142	6	0	-0.450473	-1.333528	2.717316
143	6	0	0.016964	0.073666	2.373649
144	8	0	0.184003	-2.368941	2.726083
145	1	0	-2.477021	4.031297	3.259382
146	1	0	-4.391689	2.591901	3.898187
147	1	0	-4.200740	0.111495	3.818209
148	1	0	-0.343083	3.019343	2.496874
149	1	0	-2.384183	-1.948229	3.237856
150	7	0	1.301945	0.340209	2.621755
151	7	0	2.404118	0.534522	2.759040

Transition state for loss of N2 (TS15)



Zero-point correction= 1.172048 (Hartree/Particle)
Thermal correction to Energy= 1.257410
Thermal correction to Enthalpy= 1.258354
Thermal correction to Gibbs Free Energy= 1.046865
Sum of electronic and zero-point Energies= -4355.747749
Sum of electronic and thermal Energies= -4355.662387
Sum of electronic and thermal Enthalpies= -4355.661442
Sum of electronic and thermal Free Energies= -4355.872931

Center	Atomic	Atomic	Coordinates (Angstroms)

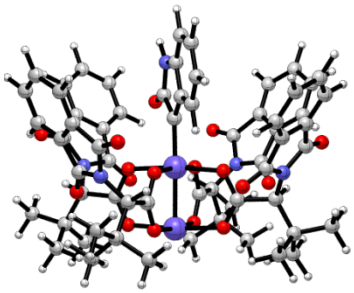
Number	Number	Type	X	Y	Z
1	45	0	0.113195	0.104713	-0.101151
2	45	0	0.288341	0.151815	-2.550311
3	7	0	-1.092149	-4.374332	-0.308063
4	8	0	-2.870254	-3.048720	-1.030044
5	8	0	0.323739	-5.604311	1.083535
6	6	0	-2.345044	-3.751888	-0.187222
7	6	0	-2.863454	-4.114326	1.161657
8	6	0	-4.050460	-3.752559	1.785272
9	1	0	-4.774605	-3.114540	1.286416
10	6	0	-4.250330	-4.220681	3.092121
11	1	0	-5.166928	-3.965966	3.617366
12	6	0	-3.288171	-5.015543	3.734121
13	1	0	-3.475780	-5.365486	4.745733
14	6	0	-2.090405	-5.363839	3.093022
15	1	0	-1.333123	-5.965713	3.585387
16	6	0	-1.901346	-4.896653	1.800366
17	6	0	-0.732610	-5.039429	0.881177
18	7	0	4.513597	-1.386047	0.074205
19	8	0	3.047543	-3.030948	-0.688287
20	8	0	5.834021	-0.088299	1.495210
21	6	0	3.775135	-2.581468	0.176321
22	6	0	4.073219	-3.137881	1.524338
23	6	0	3.596317	-4.286764	2.139614
24	1	0	2.876518	-4.932129	1.645364
25	6	0	4.056107	-4.550734	3.437255
26	1	0	3.705573	-5.437895	3.956980
27	6	0	4.952075	-3.686786	4.081334
28	1	0	5.288527	-3.921989	5.087375
29	6	0	5.409714	-2.519263	3.455124
30	1	0	6.090393	-1.834451	3.951525
31	6	0	4.951871	-2.265642	2.170083
32	6	0	5.198852	-1.102425	1.269622
33	7	0	1.871872	4.418438	-0.044786
34	8	0	3.454483	2.854010	-0.743517
35	8	0	0.609466	5.806228	1.342021
36	6	0	3.035295	3.638725	0.085756
37	6	0	3.606431	3.964818	1.423235
38	6	0	4.743695	3.476743	2.053037
39	1	0	5.372328	2.726501	1.583001
40	6	0	5.022683	3.968126	3.336166
41	1	0	5.901611	3.610038	3.864485

42	6	0	4.184437	4.906607	3.953240
43	1	0	4.430170	5.266927	4.948307
44	6	0	3.029686	5.377559	3.313328
45	1	0	2.364791	6.092368	3.788249
46	6	0	2.762304	4.888061	2.042809
47	6	0	1.607687	5.143265	1.134299
48	7	0	-4.597524	0.951807	-0.608797
49	8	0	-3.581857	2.991455	-1.122849
50	8	0	-5.775551	-0.695867	0.556294
51	6	0	-4.359359	2.330383	-0.464251
52	6	0	-5.246655	2.781628	0.649478
53	6	0	-5.458997	4.051275	1.166898
54	1	0	-4.935726	4.912560	0.763156
55	6	0	-6.375313	4.172730	2.220708
56	1	0	-6.574993	5.151504	2.647992
57	6	0	-7.044721	3.051161	2.729920
58	1	0	-7.754272	3.178193	3.542951
59	6	0	-6.818097	1.772810	2.201409
60	1	0	-7.332972	0.897329	2.585136
61	6	0	-5.912115	1.665851	1.155910
62	6	0	-5.465990	0.468782	0.383698
63	8	0	-0.091249	-1.934895	-0.279357
64	8	0	0.116951	-1.920975	-2.534905
65	8	0	2.168481	-0.097818	-0.079228
66	8	0	2.336959	-0.064591	-2.334401
67	8	0	0.385258	2.165446	-0.120845
68	8	0	0.503629	2.217875	-2.383013
69	8	0	-1.948562	0.287811	-0.359205
70	8	0	-1.779428	0.278917	-2.617510
71	6	0	-0.032868	-2.496187	-1.421302
72	6	0	-0.100888	-4.038989	-1.341130
73	1	0	0.858278	-4.315858	-0.887409
74	6	0	-0.224194	-4.859797	-2.664669
75	6	0	-0.314619	-6.354343	-2.285350
76	1	0	-0.287612	-6.966657	-3.194068
77	1	0	-1.247229	-6.584039	-1.758431
78	1	0	0.519877	-6.660162	-1.643941
79	6	0	-1.452403	-4.480415	-3.512499
80	1	0	-1.425567	-3.428737	-3.806937
81	1	0	-2.387605	-4.656173	-2.973044
82	1	0	-1.468613	-5.092930	-4.422615
83	6	0	1.065896	-4.651580	-3.489036
84	1	0	1.165693	-3.617552	-3.824067
85	1	0	1.045561	-5.300725	-4.372646

86	1	0	1.957308	-4.907430	-2.903815
87	6	0	2.819446	-0.177387	-1.176808
88	6	0	4.337713	-0.384535	-0.984671
89	1	0	4.678599	0.551138	-0.526722
90	6	0	5.226904	-0.610949	-2.251755
91	6	0	4.801769	-1.828786	-3.093845
92	1	0	4.859450	-2.759143	-2.521271
93	1	0	5.473834	-1.923262	-3.955859
94	1	0	3.780079	-1.723797	-3.464951
95	6	0	6.681655	-0.815162	-1.774567
96	1	0	6.796673	-1.745214	-1.207293
97	1	0	7.020843	0.011567	-1.140111
98	1	0	7.347758	-0.873166	-2.643001
99	6	0	5.183048	0.667245	-3.118454
100	1	0	5.473831	1.551635	-2.539148
101	1	0	4.186465	0.843053	-3.527212
102	1	0	5.886018	0.565410	-3.953818
103	6	0	0.570072	2.747478	-1.242108
104	6	0	0.862919	4.261394	-1.102689
105	1	0	-0.045309	4.679929	-0.651754
106	6	0	1.135762	5.096008	-2.395328
107	6	0	-0.140409	5.072010	-3.265479
108	1	0	-1.011513	5.436942	-2.706590
109	1	0	-0.363162	4.066713	-3.628308
110	1	0	-0.004256	5.728394	-4.132949
111	6	0	1.398443	6.556732	-1.967910
112	1	0	0.582927	6.954328	-1.352803
113	1	0	1.491074	7.188661	-2.858523
114	1	0	2.329218	6.651615	-1.397939
115	6	0	2.337861	4.591983	-3.216784
116	1	0	2.191501	3.563560	-3.552758
117	1	0	3.268388	4.631869	-2.642672
118	1	0	2.462425	5.230281	-4.100208
119	6	0	-2.432983	0.257947	-1.538123
120	6	0	-3.965603	0.075922	-1.600000
121	1	0	-4.114707	-0.933069	-1.196796
122	6	0	-4.660460	0.100412	-3.007005
123	6	0	-4.161365	-1.111533	-3.826198
124	1	0	-3.101066	-1.025154	-4.068514
125	1	0	-4.725611	-1.172637	-4.764531
126	1	0	-4.310875	-2.049968	-3.280189
127	6	0	-6.180953	-0.074001	-2.793245
128	1	0	-6.626627	0.789072	-2.285945
129	1	0	-6.408651	-0.969903	-2.204893

130	1	0	-6.676134	-0.172183	-3.765960
131	6	0	-4.415194	1.399829	-3.798146
132	1	0	-3.350920	1.562235	-3.980439
133	1	0	-4.807331	2.278167	-3.277035
134	1	0	-4.924616	1.332874	-4.767672
135	6	0	-2.487895	2.816130	3.211225
136	6	0	-3.374326	1.986866	3.908904
137	6	0	-3.187241	0.599937	3.976352
138	6	0	-2.069032	0.072656	3.345061
139	6	0	-1.164743	0.895508	2.630233
140	6	0	-1.387095	2.271415	2.546598
141	7	0	-1.638173	-1.255041	3.283553
142	6	0	-0.415052	-1.361863	2.636544
143	6	0	-0.183933	0.024927	1.981407
144	8	0	0.296365	-2.341999	2.603501
145	1	0	-2.666653	3.885583	3.170790
146	1	0	-4.239869	2.423910	4.398398
147	1	0	-3.888299	-0.034586	4.510195
148	1	0	-0.713367	2.895983	1.971307
149	1	0	-2.069809	-2.040653	3.751899
150	7	0	1.448658	0.383124	2.671749
151	7	0	2.531284	0.601114	2.543998

Carbenoid complex (16)



Zero-point correction= 1.165152 (Hartree/Particle)
Thermal correction to Energy= 1.248209
Thermal correction to Enthalpy= 1.249153
Thermal correction to Gibbs Free Energy= 1.041267
Sum of electronic and zero-point Energies= -4246.263947
Sum of electronic and thermal Energies= -4246.180889
Sum of electronic and thermal Enthalpies= -4246.179945
Sum of electronic and thermal Free Energies= -4246.387831

Center	Atomic	Atomic	Coordinates (Angstroms)

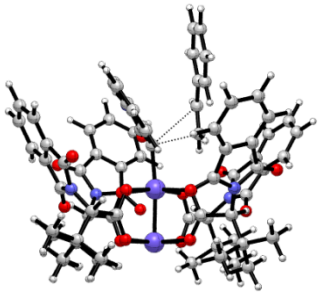
Number	Number	Type	X	Y	Z
1	45	0	-0.048058	-0.081471	-0.107620
2	45	0	-0.177435	0.011189	-2.572581
3	7	0	1.390419	4.358847	-0.111626
4	8	0	3.060944	2.943219	-0.913742
5	8	0	0.104609	5.658294	1.341743
6	6	0	2.618169	3.678584	-0.050622
7	6	0	3.228623	4.038574	1.259473
8	6	0	4.438257	3.647135	1.816963
9	1	0	5.100894	2.961785	1.296613
10	6	0	4.746804	4.153536	3.087426
11	1	0	5.683549	3.873115	3.561006
12	6	0	3.867225	5.012550	3.760436
13	1	0	4.138177	5.388701	4.743218
14	6	0	2.642416	5.387155	3.190693
15	1	0	1.948260	6.042055	3.708321
16	6	0	2.344731	4.882930	1.932938
17	6	0	1.129034	5.056505	1.083918
18	7	0	-4.401422	1.543960	0.066133
19	8	0	-2.915012	3.213466	-0.601014
20	8	0	-5.734595	0.188315	1.420028
21	6	0	-3.670477	2.737492	0.224358
22	6	0	-4.025605	3.261926	1.572309
23	6	0	-3.601879	4.411508	2.222871
24	1	0	-2.884509	5.084326	1.762819
25	6	0	-4.113140	4.644044	3.506796
26	1	0	-3.806714	5.533121	4.050890
27	6	0	-5.008149	3.746862	4.105524
28	1	0	-5.387877	3.958205	5.101545
29	6	0	-5.413506	2.579739	3.443998
30	1	0	-6.096273	1.871080	3.902827
31	6	0	-4.905110	2.360023	2.171913
32	6	0	-5.106726	1.216044	1.236561
33	7	0	-1.894244	-4.328692	-0.313559
34	8	0	-3.408123	-2.663004	-0.923280
35	8	0	-0.700426	-5.857863	0.983088
36	6	0	-3.016303	-3.499284	-0.132143
37	6	0	-3.586611	-3.855992	1.197178
38	6	0	-4.688636	-3.337864	1.864531
39	1	0	-5.279576	-2.531825	1.439753
40	6	0	-4.981147	-3.877090	3.125197
41	1	0	-5.834003	-3.498841	3.681631

42	6	0	-4.190500	-4.890763	3.683532
43	1	0	-4.447121	-5.288263	4.661695
44	6	0	-3.070073	-5.391259	3.006380
45	1	0	-2.441787	-6.165577	3.435760
46	6	0	-2.787578	-4.852842	1.759256
47	6	0	-1.657976	-5.125706	0.824247
48	7	0	4.595625	-1.086300	-0.457391
49	8	0	3.431773	-3.060260	-0.914929
50	8	0	5.855920	0.518983	0.679824
51	6	0	4.232355	-2.427464	-0.253530
52	6	0	5.010093	-2.885796	0.936381
53	6	0	5.083062	-4.137630	1.530989
54	1	0	4.521050	-4.977736	1.134007
55	6	0	5.915594	-4.270874	2.650973
56	1	0	6.005674	-5.236632	3.140523
57	6	0	6.640189	-3.178807	3.147540
58	1	0	7.278311	-3.313994	4.016327
59	6	0	6.558805	-1.919539	2.537739
60	1	0	7.118834	-1.067665	2.910838
61	6	0	5.735608	-1.800696	1.427235
62	6	0	5.448559	-0.620930	0.559082
63	8	0	0.219624	1.962000	-0.151347
64	8	0	0.071084	2.062996	-2.410548
65	8	0	-2.093156	0.206846	-0.118848
66	8	0	-2.221601	0.287977	-2.380452
67	8	0	-0.345821	-2.125908	-0.279160
68	8	0	-0.461796	-2.057844	-2.540545
69	8	0	2.001378	-0.337289	-0.313384
70	8	0	1.891801	-0.207535	-2.572542
71	6	0	0.213300	2.577439	-1.268652
72	6	0	0.349489	4.109337	-1.117822
73	1	0	-0.581089	4.407888	-0.620524
74	6	0	0.470707	4.981147	-2.409647
75	6	0	0.612994	6.455944	-1.972336
76	1	0	0.590550	7.104337	-2.855793
77	1	0	1.560900	6.637053	-1.453712
78	1	0	-0.200855	6.761267	-1.305054
79	6	0	1.674103	4.602990	-3.293224
80	1	0	1.611011	3.567261	-3.633853
81	1	0	2.622013	4.727034	-2.760944
82	1	0	1.697113	5.256008	-4.174651
83	6	0	-0.839535	4.846847	-3.217375
84	1	0	-0.971929	3.835102	-3.604810
85	1	0	-0.819413	5.541790	-4.065481

86	1	0	-1.713019	5.091750	-2.601526
87	6	0	-2.714967	0.357836	-1.223082
88	6	0	-4.230069	0.591309	-1.037169
89	1	0	-4.593271	-0.358190	-0.627747
90	6	0	-5.102292	0.893881	-2.300045
91	6	0	-4.643656	2.136636	-3.086957
92	1	0	-4.693631	3.045080	-2.479433
93	1	0	-5.301144	2.276719	-3.954055
94	1	0	-3.618567	2.027044	-3.447233
95	6	0	-6.557060	1.108970	-1.827832
96	1	0	-6.658064	2.016278	-1.222223
97	1	0	-6.920358	0.263051	-1.233045
98	1	0	-7.213118	1.218464	-2.699042
99	6	0	-5.077101	-0.346106	-3.221246
100	1	0	-5.397476	-1.247362	-2.685137
101	1	0	-4.078822	-0.527984	-3.623039
102	1	0	-5.765055	-0.191064	-4.061044
103	6	0	-0.544361	-2.643514	-1.431242
104	6	0	-0.881918	-4.153469	-1.364623
105	1	0	0.013524	-4.622495	-0.938191
106	6	0	-1.183724	-4.908668	-2.698868
107	6	0	0.089860	-4.878529	-3.572636
108	1	0	0.950003	-5.301537	-3.038048
109	1	0	0.343580	-3.862703	-3.882015
110	1	0	-0.069536	-5.482429	-4.473609
111	6	0	-1.491910	-6.381244	-2.349732
112	1	0	-0.687860	-6.837092	-1.760708
113	1	0	-1.608000	-6.960903	-3.272629
114	1	0	-2.423293	-6.476437	-1.780898
115	6	0	-2.372015	-4.322284	-3.484851
116	1	0	-2.195446	-3.281160	-3.761827
117	1	0	-3.300979	-4.366405	-2.908445
118	1	0	-2.520064	-4.904599	-4.402776
119	6	0	2.516289	-0.282778	-1.481501
120	6	0	4.058115	-0.204052	-1.498656
121	1	0	4.263977	0.805997	-1.123159
122	6	0	4.789391	-0.326755	-2.881549
123	6	0	4.428721	0.905765	-3.741674
124	1	0	3.371401	0.914185	-4.010236
125	1	0	5.019857	0.891281	-4.665301
126	1	0	4.653483	1.839065	-3.212130
127	6	0	6.312216	-0.290565	-2.624691
128	1	0	6.658375	-1.177787	-2.082653
129	1	0	6.606845	0.595629	-2.051536

130	1	0	6.842303	-0.265417	-3.583498
131	6	0	4.442904	-1.617784	-3.648180
132	1	0	3.374094	-1.679707	-3.864476
133	1	0	4.728999	-2.514621	-3.090507
134	1	0	4.987198	-1.629083	-4.600628
135	6	0	1.783763	-3.169479	3.398716
136	6	0	1.520851	-2.825355	4.738658
137	6	0	0.806380	-1.676128	5.097897
138	6	0	0.348851	-0.864787	4.067760
139	6	0	0.601578	-1.189384	2.690030
140	6	0	1.332561	-2.358075	2.368423
141	7	0	-0.374445	0.307941	4.123621
142	6	0	-0.648059	0.776463	2.824431
143	6	0	0.020653	-0.208700	1.859327
144	8	0	-1.293480	1.769878	2.577585
145	1	0	2.343013	-4.072045	3.178128
146	1	0	1.885841	-3.476073	5.529350
147	1	0	0.620050	-1.437586	6.140520
148	1	0	1.514309	-2.599617	1.327920
149	1	0	-0.726714	0.758517	4.956142

End-on transition state leading to *trans* cyclopropane from Si-face (TS-17a)



Zero-point correction= 1.300279 (Hartree/Particle)
Thermal correction to Energy= 1.390888
Thermal correction to Enthalpy= 1.391833
Thermal correction to Gibbs Free Energy= 1.167976
Sum of electronic and zero-point Energies= -4555.770853
Sum of electronic and thermal Energies= -4555.680244
Sum of electronic and thermal Enthalpies= -4555.679299
Sum of electronic and thermal Free Energies= -4555.903156

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

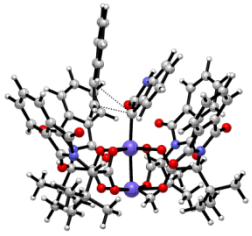
1	45	0	-0.230948	0.001133	-0.418277
2	45	0	-0.727886	0.469356	-2.793948
3	7	0	1.965537	4.188223	-0.257111
4	8	0	3.191076	2.677933	-1.541597
5	8	0	1.254410	5.492665	1.545051
6	6	0	3.073909	3.379037	-0.553461
7	6	0	4.028949	3.553435	0.577577
8	6	0	5.279179	2.986890	0.784273
9	1	0	5.701094	2.284204	0.072160
10	6	0	5.951571	3.341630	1.962381
11	1	0	6.933061	2.921811	2.164318
12	6	0	5.379686	4.225217	2.887644
13	1	0	5.928617	4.479958	3.790101
14	6	0	4.109863	4.778630	2.671790
15	1	0	3.652873	5.455466	3.387178
16	6	0	3.451683	4.424727	1.502871
17	6	0	2.097945	4.806403	1.001493
18	7	0	-4.151539	2.257606	0.705689
19	8	0	-2.520107	3.752640	-0.034531
20	8	0	-5.474471	0.963842	2.129232
21	6	0	-3.219452	3.301951	0.852770
22	6	0	-3.288936	3.717845	2.281383
23	6	0	-2.600625	4.715624	2.954979
24	1	0	-1.863030	5.329426	2.446839
25	6	0	-2.878314	4.875472	4.319363
26	1	0	-2.360900	5.646318	4.883732
27	6	0	-3.809343	4.055315	4.970713
28	1	0	-4.004673	4.207363	6.028857
29	6	0	-4.486182	3.040277	4.280877
30	1	0	-5.202345	2.392588	4.777581
31	6	0	-4.206060	2.891677	2.930450
32	6	0	-4.721672	1.903013	1.939958
33	7	0	-2.873532	-3.807341	-0.812060
34	8	0	-4.111116	-1.833268	-0.915342
35	8	0	-1.859698	-5.739399	0.016420
36	6	0	-3.777799	-2.845181	-0.329113
37	6	0	-4.220772	-3.326066	1.009938
38	6	0	-5.102074	-2.753393	1.917478
39	1	0	-5.571232	-1.793826	1.720581
40	6	0	-5.332163	-3.453391	3.110238
41	1	0	-6.015542	-3.040955	3.847268
42	6	0	-4.695430	-4.674737	3.370016
43	1	0	-4.900861	-5.194553	4.301961
44	6	0	-3.793681	-5.231059	2.452435

45	1	0	-3.285176	-6.169842	2.649182
46	6	0	-3.571083	-4.532207	1.274793
47	6	0	-2.655175	-4.827649	0.134182
48	7	0	4.135617	-1.494633	-1.648518
49	8	0	2.680744	-3.306430	-1.910438
50	8	0	5.804535	-0.108636	-0.780326
51	6	0	3.652578	-2.789416	-1.395311
52	6	0	4.566340	-3.374475	-0.367757
53	6	0	4.577349	-4.637914	0.205558
54	1	0	3.839728	-5.383947	-0.073784
55	6	0	5.580563	-4.909303	1.146756
56	1	0	5.628177	-5.890052	1.611818
57	6	0	6.530032	-3.937695	1.493111
58	1	0	7.298359	-4.179620	2.222102
59	6	0	6.507109	-2.663557	0.908603
60	1	0	7.238414	-1.904091	1.167093
61	6	0	5.512238	-2.408580	-0.024658
62	6	0	5.226989	-1.178869	-0.821361
63	8	0	0.396611	1.974651	-0.282032
64	8	0	-0.101361	2.414579	-2.447245
65	8	0	-2.170603	0.601343	-0.035546
66	8	0	-2.638483	1.037201	-2.211154
67	8	0	-0.942684	-1.917756	-0.792167
68	8	0	-1.382752	-1.500927	-2.974049
69	8	0	1.708074	-0.517591	-1.012213
70	8	0	1.243191	-0.078655	-3.184190
71	6	0	0.308994	2.738691	-1.301085
72	6	0	0.710654	4.205024	-1.020196
73	1	0	-0.039015	4.550852	-0.298899
74	6	0	0.696904	5.222521	-2.209539
75	6	0	1.143012	6.597651	-1.664959
76	1	0	1.047097	7.351606	-2.454679
77	1	0	2.190776	6.589643	-1.344111
78	1	0	0.530970	6.916356	-0.813883
79	6	0	1.625973	4.823222	-3.371864
80	1	0	1.343522	3.857513	-3.795668
81	1	0	2.671792	4.762902	-3.054816
82	1	0	1.561065	5.580915	-4.162759
83	6	0	-0.754312	5.362183	-2.721096
84	1	0	-1.114105	4.434247	-3.168841
85	1	0	-0.798432	6.152701	-3.479991
86	1	0	-1.438152	5.633885	-1.908733
87	6	0	-2.920817	1.006779	-0.982721
88	6	0	-4.323708	1.441686	-0.502725

89	1	0	-4.774936	0.513101	-0.136419
90	6	0	-5.321407	2.039964	-1.548658
91	6	0	-4.789385	3.300587	-2.256122
92	1	0	-4.603510	4.114800	-1.549396
93	1	0	-5.534093	3.650903	-2.981903
94	1	0	-3.857918	3.096947	-2.788218
95	6	0	-6.629263	2.396171	-0.807588
96	1	0	-6.484956	3.218357	-0.098055
97	1	0	-7.028819	1.538414	-0.254642
98	1	0	-7.386473	2.715313	-1.533059
99	6	0	-5.648028	0.950608	-2.594335
100	1	0	-6.022714	0.038429	-2.115149
101	1	0	-4.769670	0.685004	-3.185028
102	1	0	-6.425297	1.318369	-3.275161
103	6	0	-1.409822	-2.218530	-1.939758
104	6	0	-2.021185	-3.642414	-1.998381
105	1	0	-1.179925	-4.319526	-1.805624
106	6	0	-2.674431	-4.115157	-3.338438
107	6	0	-1.573333	-4.174054	-4.420186
108	1	0	-0.747681	-4.828114	-4.111218
109	1	0	-1.166030	-3.184326	-4.635921
110	1	0	-1.990338	-4.584235	-5.347497
111	6	0	-3.215565	-5.546157	-3.126968
112	1	0	-2.440539	-6.224070	-2.752016
113	1	0	-3.584333	-5.943076	-4.079758
114	1	0	-4.050154	-5.562951	-2.417542
115	6	0	-3.828571	-3.210995	-3.810889
116	1	0	-3.492768	-2.185812	-3.977311
117	1	0	-4.645181	-3.185632	-3.083274
118	1	0	-4.232385	-3.602225	-4.753032
119	6	0	2.021265	-0.385207	-2.242313
120	6	0	3.529076	-0.513601	-2.556459
121	1	0	3.939636	0.446506	-2.218302
122	6	0	3.957950	-0.679518	-4.058143
123	6	0	3.660142	0.640133	-4.806014
124	1	0	2.589477	0.842008	-4.855133
125	1	0	4.048120	0.573960	-5.829543
126	1	0	4.147101	1.492116	-4.316510
127	6	0	5.485201	-0.907935	-4.105143
128	1	0	5.770808	-1.873580	-3.672763
129	1	0	6.030098	-0.120633	-3.572308
130	1	0	5.821258	-0.905036	-5.148168
131	6	0	3.253897	-1.851369	-4.769220
132	1	0	2.169341	-1.720506	-4.772955

133	1	0	3.478565	-2.812034	-4.296319
134	1	0	3.596411	-1.901849	-5.810211
135	6	0	0.654737	-4.213555	2.073594
136	6	0	0.040603	-4.310159	3.332828
137	6	0	-0.521452	-3.199778	3.972141
138	6	0	-0.450043	-1.978693	3.312119
139	6	0	0.168976	-1.850227	2.033374
140	6	0	0.723735	-2.987980	1.417921
141	7	0	-0.938899	-0.740761	3.698287
142	6	0	-0.747353	0.212136	2.686133
143	6	0	0.016784	-0.503268	1.556048
144	8	0	-1.135970	1.358762	2.746547
145	1	0	1.054852	-5.105185	1.602341
146	1	0	-0.009894	-5.278111	3.824767
147	1	0	-1.000662	-3.295302	4.941855
148	1	0	1.171427	-2.902456	0.434331
149	1	0	-1.509714	-0.555909	4.511209
150	6	0	2.092588	0.487152	3.324373
151	1	0	1.623134	1.296568	3.881494
152	6	0	2.023860	0.544505	1.959620
153	1	0	2.536035	-0.159593	1.314078
154	1	0	1.643537	1.435104	1.474380
155	6	0	2.669658	-0.570245	4.135462
156	6	0	2.527766	-0.505937	5.538985
157	6	0	3.362918	-1.670716	3.586329
158	6	0	3.049614	-1.499388	6.360534
159	1	0	1.999567	0.338331	5.975684
160	6	0	3.880883	-2.665343	4.409369
161	1	0	3.504605	-1.740870	2.513501
162	6	0	3.726287	-2.585643	5.797049
163	1	0	2.930804	-1.430020	7.438363
164	1	0	4.411312	-3.503036	3.965885
165	1	0	4.135772	-3.363092	6.436409

End-on transition state leading to *trans* cyclopropane from Re-face (TS-17b)



Zero-point correction= 1.300301 (Hartree/Particle)
Thermal correction to Energy= 1.390870

Thermal correction to Enthalpy= 1.391814
Thermal correction to Gibbs Free Energy= 1.167820
Sum of electronic and zero-point Energies= -4555.769247
Sum of electronic and thermal Energies= -4555.678678
Sum of electronic and thermal Enthalpies= -4555.677734
Sum of electronic and thermal Free Energies= -4555.901728

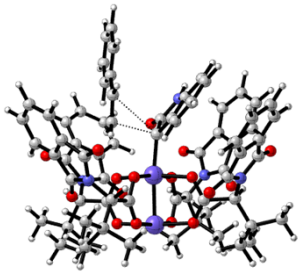
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.028298	0.080815	-0.452983
2	45	0	-0.043841	0.626765	-2.864085
3	7	0	1.608931	4.339154	0.445868
4	8	0	3.307323	3.036795	-0.482742
5	8	0	0.226445	5.374205	2.018838
6	6	0	2.789412	3.577829	0.475926
7	6	0	3.246990	3.572663	1.894093
8	6	0	4.356059	2.967463	2.470086
9	1	0	5.047145	2.379160	1.873062
10	6	0	4.521471	3.127484	3.853056
11	1	0	5.376287	2.672067	4.345443
12	6	0	3.602996	3.865203	4.613820
13	1	0	3.764763	3.975941	5.682873
14	6	0	2.481487	4.460831	4.018869
15	1	0	1.760210	5.028395	4.599056
16	6	0	2.324719	4.296857	2.649638
17	6	0	1.237007	4.760565	1.736758
18	7	0	-4.265764	1.983970	-0.125743
19	8	0	-2.630247	3.621615	-0.413245
20	8	0	-5.754208	0.504903	0.895986
21	6	0	-3.441931	3.050728	0.288390
22	6	0	-3.785302	3.307006	1.714390
23	6	0	-3.275310	4.245708	2.599615
24	1	0	-2.481794	4.924405	2.302445
25	6	0	-3.803077	4.249193	3.897909
26	1	0	-3.431922	4.968302	4.622844
27	6	0	-4.795599	3.337221	4.282204
28	1	0	-5.184692	3.369137	5.296384
29	6	0	-5.287007	2.380854	3.383022
30	1	0	-6.046689	1.661307	3.672988
31	6	0	-4.762710	2.387579	2.097990
32	6	0	-5.036097	1.488488	0.939375
33	7	0	-2.236380	-3.898983	-1.522530

34	8	0	-3.565443	-2.012812	-1.871800
35	8	0	-1.297241	-5.778566	-0.506099
36	6	0	-3.316686	-3.036184	-1.263786
37	6	0	-4.052808	-3.626719	-0.109852
38	6	0	-5.186768	-3.175369	0.552153
39	1	0	-5.673840	-2.246827	0.269689
40	6	0	-5.651391	-3.952216	1.622892
41	1	0	-6.534346	-3.633057	2.169176
42	6	0	-4.993893	-5.128916	2.006335
43	1	0	-5.381447	-5.707816	2.839997
44	6	0	-3.839200	-5.563113	1.340682
45	1	0	-3.314130	-6.465627	1.638152
46	6	0	-3.386704	-4.789271	0.281472
47	6	0	-2.181558	-4.947525	-0.583525
48	7	0	4.612160	-1.122587	-0.947220
49	8	0	3.464587	-2.885012	-1.965025
50	8	0	5.854604	0.092144	0.615164
51	6	0	4.254696	-2.467146	-1.141854
52	6	0	5.030570	-3.245918	-0.130078
53	6	0	5.101038	-4.615151	0.083677
54	1	0	4.541331	-5.306569	-0.538877
55	6	0	5.922704	-5.062513	1.127957
56	1	0	6.010039	-6.127671	1.323532
57	6	0	6.638684	-4.156647	1.922934
58	1	0	7.269889	-4.533939	2.722798
59	6	0	6.558013	-2.775564	1.697101
60	1	0	7.110309	-2.064946	2.304299
61	6	0	5.745400	-2.345204	0.658231
62	6	0	5.454612	-0.965676	0.166099
63	8	0	0.415292	2.069751	-0.152519
64	8	0	0.324676	2.609011	-2.352043
65	8	0	-2.046576	0.546948	-0.483159
66	8	0	-2.073569	1.021286	-2.696375
67	8	0	-0.497636	-1.881346	-0.969707
68	8	0	-0.479562	-1.391543	-3.183317
69	8	0	2.017883	-0.285576	-0.664021
70	8	0	1.998660	0.283124	-2.857904
71	6	0	0.466819	2.885620	-1.129453
72	6	0	0.664964	4.352999	-0.681561
73	1	0	-0.295378	4.613201	-0.220163
74	6	0	0.953412	5.441699	-1.764594
75	6	0	1.153730	6.789702	-1.037523
76	1	0	1.245251	7.595103	-1.775379
77	1	0	2.065424	6.792209	-0.430052

78	1	0	0.308697	7.024806	-0.380324
79	6	0	2.197836	5.141492	-2.620331
80	1	0	2.094966	4.194061	-3.154393
81	1	0	3.105742	5.089553	-2.012393
82	1	0	2.332741	5.940995	-3.359614
83	6	0	-0.288616	5.569029	-2.675187
84	1	0	-0.455268	4.659983	-3.255951
85	1	0	-0.147697	6.404087	-3.372054
86	1	0	-1.193228	5.768800	-2.088353
87	6	0	-2.611787	0.932203	-1.562101
88	6	0	-4.113136	1.252392	-1.389503
89	1	0	-4.570766	0.276653	-1.190056
90	6	0	-4.891388	1.867384	-2.598999
91	6	0	-4.296946	3.195368	-3.104853
92	1	0	-4.317050	3.970141	-2.332885
93	1	0	-4.888062	3.554497	-3.956590
94	1	0	-3.262371	3.071450	-3.431822
95	6	0	-6.349147	2.108499	-2.148507
96	1	0	-6.414239	2.883423	-1.376912
97	1	0	-6.806850	1.195502	-1.750283
98	1	0	-6.947110	2.442711	-3.004186
99	6	0	-4.911137	0.833334	-3.746867
100	1	0	-5.318252	-0.127981	-3.411411
101	1	0	-3.910555	0.656395	-4.145085
102	1	0	-5.547342	1.203215	-4.559850
103	6	0	-0.670907	-2.159085	-2.205279
104	6	0	-1.128760	-3.619430	-2.448780
105	1	0	-0.309997	-4.239595	-2.063931
106	6	0	-1.381895	-4.084146	-3.920145
107	6	0	-0.046523	-3.997707	-4.691938
108	1	0	0.739266	-4.580947	-4.194943
109	1	0	0.299920	-2.966760	-4.785731
110	1	0	-0.177534	-4.410064	-5.699400
111	6	0	-1.819959	-5.564824	-3.883738
112	1	0	-1.101222	-6.189861	-3.341910
113	1	0	-1.900561	-5.948119	-4.907359
114	1	0	-2.799409	-5.686920	-3.408214
115	6	0	-2.463743	-3.262502	-4.646746
116	1	0	-2.195845	-2.205801	-4.701211
117	1	0	-3.434970	-3.341039	-4.148537
118	1	0	-2.581999	-3.644367	-5.668403
119	6	0	2.577279	-0.023126	-1.780033
120	6	0	4.121709	0.013872	-1.733588
121	1	0	4.333730	0.885283	-1.102021

122	6	0	4.901148	0.237159	-3.077659
123	6	0	4.568963	1.648676	-3.612935
124	1	0	3.522422	1.730445	-3.909982
125	1	0	5.194187	1.862140	-4.488355
126	1	0	4.770578	2.417399	-2.858218
127	6	0	6.414434	0.199935	-2.767060
128	1	0	6.747031	-0.797673	-2.458610
129	1	0	6.684877	0.909102	-1.976631
130	1	0	6.977664	0.467267	-3.668350
131	6	0	4.588292	-0.816237	-4.157969
132	1	0	3.525898	-0.825744	-4.410027
133	1	0	4.870764	-1.824744	-3.841661
134	1	0	5.156451	-0.581022	-5.066714
135	6	0	2.592987	-2.999980	2.504818
136	6	0	3.002780	-2.434709	3.723646
137	6	0	2.469896	-1.232963	4.201244
138	6	0	1.499896	-0.610415	3.423758
139	6	0	1.073013	-1.156848	2.177931
140	6	0	1.636283	-2.361172	1.720917
141	7	0	0.806460	0.565854	3.657107
142	6	0	-0.052608	0.864954	2.588465
143	6	0	0.118949	-0.274613	1.565135
144	8	0	-0.759288	1.848539	2.535540
145	1	0	3.039445	-3.930191	2.170159
146	1	0	3.761911	-2.942019	4.313241
147	1	0	2.801188	-0.808746	5.144346
148	1	0	1.320839	-2.767324	0.765259
149	1	0	0.970241	1.211921	4.416565
150	6	0	-2.005785	-1.195333	3.316372
151	1	0	-2.432730	-0.280495	3.724808
152	6	0	-1.918486	-1.292015	1.955266
153	1	0	-1.585102	-2.196576	1.459664
154	1	0	-2.402839	-0.558009	1.322926
155	6	0	-1.535838	-2.156939	4.298146
156	6	0	-1.588018	-1.813556	5.666840
157	6	0	-1.018525	-3.423245	3.947736
158	6	0	-1.134992	-2.691703	6.645558
159	1	0	-1.988258	-0.843007	5.950178
160	6	0	-0.561144	-4.297700	4.927847
161	1	0	-0.985603	-3.724636	2.906461
162	6	0	-0.615608	-3.936884	6.278074
163	1	0	-1.184717	-2.408989	7.693526
164	1	0	-0.164650	-5.267280	4.639939
165	1	0	-0.261523	-4.625702	7.040274

End -on transition state leading to *cis* cyclopropane from Re-face (TS-17c)



Zero-point correction=	1.300049 (Hartree/Particle)
Thermal correction to Energy=	1.390795
Thermal correction to Enthalpy=	1.391739
Thermal correction to Gibbs Free Energy=	1.166864
Sum of electronic and zero-point Energies=	-4555.767291
Sum of electronic and thermal Energies=	-4555.676545
Sum of electronic and thermal Enthalpies=	-4555.675601
Sum of electronic and thermal Free Energies=	-4555.900475

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.129427	0.220840	-0.375592
2	45	0	-0.374499	0.534263	-2.814560
3	7	0	-0.755725	-4.352593	-0.948856
4	8	0	-2.791500	-3.241093	-1.191945
5	8	0	1.028680	-5.514062	0.011311
6	6	0	-2.036742	-3.941712	-0.544352
7	6	0	-2.254214	-4.525933	0.808921
8	6	0	-3.348555	-4.424703	1.657410
9	1	0	-4.223788	-3.845585	1.376434
10	6	0	-3.256218	-5.077039	2.894971
11	1	0	-4.090059	-5.026170	3.589777
12	6	0	-2.106088	-5.794969	3.253588
13	1	0	-2.069455	-6.294247	4.218271
14	6	0	-1.004426	-5.878159	2.389863
15	1	0	-0.105434	-6.423146	2.661091
16	6	0	-1.104155	-5.229884	1.166949
17	6	0	-0.110167	-5.091367	0.060654
18	7	0	4.406539	-0.700128	-1.168881
19	8	0	3.011076	-2.400310	-1.943442
20	8	0	5.874190	0.513475	0.180622
21	6	0	3.865132	-1.999269	-1.177026
22	6	0	4.559894	-2.742212	-0.088142

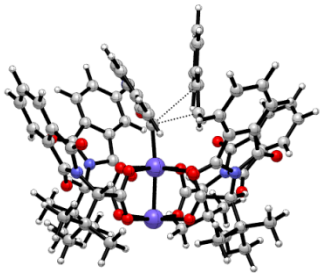
23	6	0	4.411092	-4.056718	0.330665
24	1	0	3.667257	-4.708451	-0.117141
25	6	0	5.239199	-4.489815	1.375664
26	1	0	5.157720	-5.512900	1.731755
27	6	0	6.169302	-3.626698	1.971737
28	1	0	6.804785	-3.998053	2.771379
29	6	0	6.289211	-2.292410	1.556769
30	1	0	6.994707	-1.610878	2.022034
31	6	0	5.468228	-1.873281	0.519241
32	6	0	5.330826	-0.532680	-0.123797
33	7	0	1.073538	4.734818	-0.098960
34	8	0	2.689105	3.467914	-1.208600
35	8	0	-0.060432	5.871051	1.594552
36	6	0	2.333015	4.129218	-0.251807
37	6	0	3.101079	4.452039	0.984683
38	6	0	4.390990	4.095155	1.353694
39	1	0	5.010927	3.477161	0.711035
40	6	0	4.844567	4.540731	2.602892
41	1	0	5.846840	4.280454	2.930849
42	6	0	4.025407	5.310323	3.440084
43	1	0	4.408213	5.640372	4.401819
44	6	0	2.719526	5.651197	3.061824
45	1	0	2.071846	6.235384	3.708287
46	6	0	2.279187	5.206522	1.823350
47	6	0	0.950619	5.353977	1.161185
48	7	0	-4.948620	0.414367	-0.103605
49	8	0	-4.338137	2.625002	-0.547398
50	8	0	-5.676667	-1.487100	1.043417
51	6	0	-4.897318	1.796399	0.143446
52	6	0	-5.651856	2.011442	1.414710
53	6	0	-5.958950	3.186658	2.085447
54	1	0	-5.645310	4.150101	1.695208
55	6	0	-6.687928	3.076191	3.277935
56	1	0	-6.953144	3.973625	3.829922
57	6	0	-7.084745	1.824579	3.769089
58	1	0	-7.651899	1.771294	4.694333
59	6	0	-6.767016	0.644587	3.082406
60	1	0	-7.070684	-0.330044	3.451968
61	6	0	-6.049535	0.766912	1.901258
62	6	0	-5.566976	-0.278780	0.951012
63	8	0	-0.117728	-1.801352	-0.776452
64	8	0	-0.272370	-1.533519	-3.021597
65	8	0	1.920222	0.276434	-0.707851
66	8	0	1.694845	0.610508	-2.936550

67	8	0	-0.120147	2.294175	-0.188277
68	8	0	-0.402825	2.587440	-2.417840
69	8	0	-2.223391	0.157662	-0.311076
70	8	0	-2.417206	0.351421	-2.558982
71	6	0	-0.168963	-2.230114	-1.975560
72	6	0	-0.020147	-3.766701	-2.078305
73	1	0	1.032932	-3.940377	-1.827844
74	6	0	-0.272547	-4.460113	-3.456474
75	6	0	-0.106126	-5.982463	-3.256624
76	1	0	-0.172284	-6.489847	-4.226015
77	1	0	-0.889999	-6.395686	-2.612482
78	1	0	0.863750	-6.229362	-2.809729
79	6	0	-1.670391	-4.180576	-4.039303
80	1	0	-1.832886	-3.111110	-4.191049
81	1	0	-2.464632	-4.554112	-3.386317
82	1	0	-1.767052	-4.684707	-5.009001
83	6	0	0.811605	-3.986334	-4.450157
84	1	0	0.717604	-2.921101	-4.667934
85	1	0	0.713876	-4.542538	-5.390276
86	1	0	1.818757	-4.164704	-4.055130
87	6	0	2.372836	0.427293	-1.892331
88	6	0	3.916260	0.422242	-1.978741
89	1	0	4.220947	1.313309	-1.418528
90	6	0	4.580846	0.531767	-3.392045
91	6	0	4.176658	-0.605711	-4.349563
92	1	0	4.480602	-1.585453	-3.968166
93	1	0	4.672512	-0.456616	-5.316832
94	1	0	3.097734	-0.626920	-4.514316
95	6	0	6.113957	0.500413	-3.202538
96	1	0	6.460152	-0.470109	-2.830164
97	1	0	6.453796	1.272043	-2.502779
98	1	0	6.604434	0.675703	-4.166912
99	6	0	4.208108	1.897389	-4.011035
100	1	0	4.476123	2.724006	-3.342777
101	1	0	3.139776	1.966411	-4.221629
102	1	0	4.756191	2.032239	-4.951324
103	6	0	-0.205966	3.004945	-1.248111
104	6	0	-0.084009	4.526628	-0.981498
105	1	0	-0.940338	4.769966	-0.340686
106	6	0	-0.153272	5.503004	-2.200992
107	6	0	-1.549665	5.371638	-2.848668
108	1	0	-2.347321	5.557219	-2.118048
109	1	0	-1.703698	4.380369	-3.279020
110	1	0	-1.653981	6.114129	-3.648598

111	6	0	-0.006848	6.944848	-1.666713
112	1	0	-0.743528	7.167656	-0.886577
113	1	0	-0.155627	7.655683	-2.487505
114	1	0	0.990664	7.125816	-1.251326
115	6	0	0.940400	5.249017	-3.256067
116	1	0	0.873725	4.240176	-3.667429
117	1	0	1.943892	5.380085	-2.840003
118	1	0	0.823036	5.967466	-4.076741
119	6	0	-2.879729	0.146042	-1.404125
120	6	0	-4.361663	-0.268852	-1.260303
121	1	0	-4.298964	-1.317248	-0.944434
122	6	0	-5.267975	-0.242594	-2.541121
123	6	0	-4.737821	-1.293774	-3.542221
124	1	0	-3.750638	-1.026170	-3.922065
125	1	0	-5.426785	-1.366694	-4.392462
126	1	0	-4.667338	-2.284063	-3.078205
127	6	0	-6.695018	-0.667810	-2.128218
128	1	0	-7.171235	0.071851	-1.474590
129	1	0	-6.698174	-1.633106	-1.609584
130	1	0	-7.320229	-0.762754	-3.023348
131	6	0	-5.339111	1.137605	-3.223183
132	1	0	-4.350182	1.482108	-3.532311
133	1	0	-5.772994	1.897538	-2.566504
134	1	0	-5.974095	1.066456	-4.115095
135	6	0	-2.839995	1.594942	3.602108
136	6	0	-3.051360	0.567718	4.533987
137	6	0	-2.321844	-0.627931	4.498603
138	6	0	-1.357367	-0.757733	3.507878
139	6	0	-1.127923	0.268318	2.548226
140	6	0	-1.890338	1.443906	2.592632
141	7	0	-0.481502	-1.806664	3.259216
142	6	0	0.371726	-1.507490	2.195743
143	6	0	-0.092723	-0.153786	1.635913
144	8	0	1.289935	-2.214398	1.829668
145	1	0	-3.432268	2.501745	3.660960
146	1	0	-3.807952	0.697435	5.303294
147	1	0	-2.503158	-1.415799	5.223740
148	1	0	-1.720742	2.218086	1.851719
149	1	0	-0.387577	-2.649715	3.808056
150	6	0	1.839874	0.892683	3.591046
151	1	0	1.233666	1.619441	4.131726
152	6	0	1.850035	0.986203	2.228073
153	1	0	2.459906	0.354869	1.593338
154	1	0	1.415773	1.854741	1.747851

155	6	0	2.502995	-0.084881	4.437066
156	6	0	2.301437	-0.010175	5.833265
157	6	0	3.341069	-1.105155	3.935204
158	6	0	2.908072	-0.916310	6.696454
159	1	0	1.659649	0.772229	6.231602
160	6	0	3.939253	-2.014330	4.801636
161	1	0	3.513515	-1.190626	2.869104
162	6	0	3.728717	-1.924516	6.181438
163	1	0	2.742766	-0.839754	7.767668
164	1	0	4.574089	-2.795802	4.395100
165	1	0	4.204541	-2.634891	6.852297

End -on transition state leading to *cis* cyclopropane from Si-face (TS-17d)



Zero-point correction= 1.300958 (Hartree/Particle)
Thermal correction to Energy= 1.391197
Thermal correction to Enthalpy= 1.392142
Thermal correction to Gibbs Free Energy= 1.169178
Sum of electronic and zero-point Energies= -4555.771329
Sum of electronic and thermal Energies= -4555.681090
Sum of electronic and thermal Enthalpies= -4555.680145
Sum of electronic and thermal Free Energies= -4555.903109

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.167458	-0.288323	-0.332147
2	45	0	-0.427647	-0.674197	-2.760676
3	7	0	3.390624	2.665760	-1.459130
4	8	0	3.971077	0.475474	-2.010786
5	8	0	3.236617	4.681842	-0.292569
6	6	0	4.153056	1.487749	-1.360791
7	6	0	5.177805	1.744966	-0.309238
8	6	0	6.184960	0.922124	0.175532
9	1	0	6.309018	-0.090547	-0.194016
10	6	0	7.005170	1.447080	1.184374

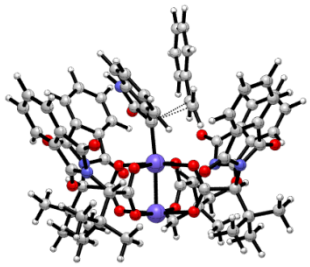
11	1	0	7.806262	0.836709	1.591798
12	6	0	6.806380	2.741266	1.683464
13	1	0	7.458696	3.116187	2.467303
14	6	0	5.773716	3.554462	1.196769
15	1	0	5.598738	4.550957	1.589631
16	6	0	4.971241	3.030739	0.193523
17	6	0	3.788527	3.617246	-0.501345
18	7	0	-3.282933	3.200630	-0.669100
19	8	0	-1.236955	3.894411	-1.555972
20	8	0	-5.046647	2.884674	0.827463
21	6	0	-2.110616	3.979377	-0.715210
22	6	0	-2.190215	4.905124	0.451109
23	6	0	-1.328147	5.914462	0.851633
24	1	0	-0.421358	6.126765	0.293861
25	6	0	-1.672887	6.635093	2.002955
26	1	0	-1.024903	7.435838	2.348458
27	6	0	-2.840569	6.340089	2.719330
28	1	0	-3.081472	6.918545	3.607070
29	6	0	-3.700251	5.312804	2.307869
30	1	0	-4.607586	5.074961	2.854905
31	6	0	-3.350967	4.608650	1.164640
32	6	0	-4.037943	3.474693	0.481876
33	7	0	-3.919937	-3.016718	0.275583
34	8	0	-4.457838	-0.991510	-0.746697
35	8	0	-3.613675	-4.655379	1.909180
36	6	0	-4.498870	-1.737647	0.213199
37	6	0	-5.148101	-1.510247	1.535059
38	6	0	-5.856251	-0.412079	2.004657
39	1	0	-5.987451	0.477615	1.396044
40	6	0	-6.362322	-0.492098	3.309795
41	1	0	-6.923456	0.344846	3.715955
42	6	0	-6.155280	-1.630020	4.101349
43	1	0	-6.565902	-1.660995	5.106996
44	6	0	-5.421627	-2.723098	3.620149
45	1	0	-5.244081	-3.604407	4.228719
46	6	0	-4.925117	-2.636888	2.327639
47	6	0	-4.086796	-3.594886	1.549625
48	7	0	3.416921	-3.410349	-0.208910
49	8	0	1.418342	-4.584331	0.106145
50	8	0	5.480783	-2.404270	0.219392
51	6	0	2.508941	-4.216936	0.498470
52	6	0	3.158006	-4.510641	1.811205
53	6	0	2.717938	-5.287091	2.873482
54	1	0	1.761185	-5.798470	2.832004

55	6	0	3.558163	-5.385072	3.991052
56	1	0	3.250186	-5.985360	4.842544
57	6	0	4.792671	-4.722776	4.028466
58	1	0	5.422219	-4.819489	4.908549
59	6	0	5.226950	-3.941622	2.948968
60	1	0	6.181689	-3.425179	2.965815
61	6	0	4.387382	-3.853467	1.847775
62	6	0	4.556132	-3.118241	0.561006
63	8	0	1.107518	1.278880	-0.829402
64	8	0	0.819880	0.958196	-3.053130
65	8	0	-1.804432	0.969078	-0.495700
66	8	0	-2.045161	0.620313	-2.722867
67	8	0	-1.479330	-1.884409	-0.083905
68	8	0	-1.704866	-2.252114	-2.306657
69	8	0	1.484646	-1.564272	-0.396672
70	8	0	1.233033	-1.920878	-2.618799
71	6	0	1.299486	1.563542	-2.058836
72	6	0	2.177029	2.819287	-2.273956
73	1	0	1.619827	3.622179	-1.776901
74	6	0	2.445853	3.296019	-3.739246
75	6	0	3.312036	4.573536	-3.673304
76	1	0	3.437873	4.981339	-4.682786
77	1	0	4.312007	4.367892	-3.275087
78	1	0	2.851365	5.346725	-3.048400
79	6	0	3.173591	2.247564	-4.601997
80	1	0	2.597279	1.323853	-4.681018
81	1	0	4.159343	2.000015	-4.195190
82	1	0	3.323279	2.651066	-5.611204
83	6	0	1.094660	3.668132	-4.389323
84	1	0	0.459894	2.791057	-4.526830
85	1	0	1.274896	4.121568	-5.371457
86	1	0	0.543841	4.392787	-3.778296
87	6	0	-2.365068	1.152559	-1.625503
88	6	0	-3.596663	2.081439	-1.563635
89	1	0	-4.335562	1.494100	-1.006799
90	6	0	-4.282886	2.503412	-2.907024
91	6	0	-3.332982	3.214376	-3.889863
92	1	0	-2.933566	4.142896	-3.471638
93	1	0	-3.883523	3.468467	-4.804390
94	1	0	-2.489271	2.577057	-4.163215
95	6	0	-5.452036	3.454095	-2.566573
96	1	0	-5.098374	4.406224	-2.155556
97	1	0	-6.141296	3.006844	-1.841239
98	1	0	-6.017934	3.678981	-3.477786

99	6	0	-4.876801	1.242605	-3.575059
100	1	0	-5.551845	0.712088	-2.893285
101	1	0	-4.096025	0.547057	-3.886873
102	1	0	-5.453367	1.535944	-4.460719
103	6	0	-1.983087	-2.469653	-1.098358
104	6	0	-3.002555	-3.576193	-0.726431
105	1	0	-2.422014	-4.314852	-0.160337
106	6	0	-3.704722	-4.356371	-1.885103
107	6	0	-2.624302	-5.120590	-2.682568
108	1	0	-2.037738	-5.778163	-2.028054
109	1	0	-1.938711	-4.438923	-3.189540
110	1	0	-3.104526	-5.751110	-3.440059
111	6	0	-4.655654	-5.396653	-1.253187
112	1	0	-4.134134	-6.046473	-0.541411
113	1	0	-5.083262	-6.027419	-2.040924
114	1	0	-5.488664	-4.919270	-0.725514
115	6	0	-4.514006	-3.450190	-2.832274
116	1	0	-3.880992	-2.694072	-3.300249
117	1	0	-5.323883	-2.935676	-2.306072
118	1	0	-4.965648	-4.064001	-3.621507
119	6	0	1.835195	-2.057412	-1.520383
120	6	0	3.187930	-2.803929	-1.525059
121	1	0	3.926301	-1.993220	-1.572042
122	6	0	3.494063	-3.757646	-2.736195
123	6	0	3.709215	-2.896416	-4.001631
124	1	0	2.798627	-2.369769	-4.290247
125	1	0	4.016291	-3.541322	-4.833853
126	1	0	4.499291	-2.151940	-3.844708
127	6	0	4.816936	-4.500854	-2.446576
128	1	0	4.719820	-5.205156	-1.612808
129	1	0	5.630305	-3.804736	-2.212476
130	1	0	5.110456	-5.078442	-3.330379
131	6	0	2.382335	-4.792996	-2.992677
132	1	0	1.433174	-4.307166	-3.230980
133	1	0	2.222326	-5.442439	-2.127340
134	1	0	2.665056	-5.426195	-3.842770
135	6	0	-0.920749	-3.154835	3.699459
136	6	0	-1.553078	-2.513933	4.776331
137	6	0	-1.700321	-1.122342	4.829476
138	6	0	-1.190073	-0.385645	3.767684
139	6	0	-0.536882	-1.010246	2.664922
140	6	0	-0.412135	-2.409684	2.638183
141	7	0	-1.207138	0.984635	3.558603
142	6	0	-0.640051	1.310052	2.321299

143	6	0	-0.168192	-0.010026	1.695301
144	8	0	-0.572857	2.437139	1.874866
145	1	0	-0.852639	-4.237502	3.684358
146	1	0	-1.950370	-3.113487	5.591341
147	1	0	-2.202914	-0.644205	5.665074
148	1	0	0.060933	-2.893105	1.791029
149	1	0	-1.646824	1.674961	4.150758
150	6	0	2.175018	0.868775	3.299885
151	1	0	2.197643	0.143286	4.113429
152	6	0	2.098292	0.387339	2.022121
153	1	0	2.145011	1.038788	1.157826
154	1	0	2.239845	-0.667613	1.822304
155	6	0	2.234278	2.259510	3.714919
156	6	0	2.401540	2.554262	5.086013
157	6	0	2.158725	3.335354	2.802692
158	6	0	2.506482	3.868322	5.528410
159	1	0	2.458775	1.735064	5.799403
160	6	0	2.266603	4.648865	3.248425
161	1	0	1.997718	3.145502	1.749114
162	6	0	2.442936	4.920958	4.608443
163	1	0	2.640479	4.075533	6.586720
164	1	0	2.219105	5.456606	2.524326
165	1	0	2.530177	5.948376	4.952102

Side -on transition state leading to *trans* cyclopropane from Si-face (TS-17e)



Zero-point correction= 1.301108 (Hartree/Particle)
Thermal correction to Energy= 1.391396
Thermal correction to Enthalpy= 1.392340
Thermal correction to Gibbs Free Energy= 1.168890
Sum of electronic and zero-point Energies= -4555.767218
Sum of electronic and thermal Energies= -4555.676930
Sum of electronic and thermal Enthalpies= -4555.675986
Sum of electronic and thermal Free Energies= -4555.899437

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	45	0	-0.157651	-0.278639	-0.331552
2	45	0	-0.379508	-0.643683	-2.769165
3	7	0	3.318697	2.807785	-1.376448
4	8	0	3.985506	0.647688	-1.948021
5	8	0	3.076877	4.798566	-0.180700
6	6	0	4.123535	1.657894	-1.284475
7	6	0	5.129135	1.939209	-0.220627
8	6	0	6.158644	1.146680	0.267443
9	1	0	6.320572	0.141828	-0.108811
10	6	0	6.950274	1.689877	1.289614
11	1	0	7.767260	1.103176	1.700111
12	6	0	6.703004	2.972155	1.797568
13	1	0	7.335001	3.362302	2.590543
14	6	0	5.647679	3.753998	1.307561
15	1	0	5.437007	4.741898	1.705103
16	6	0	4.873050	3.211915	0.292197
17	6	0	3.673253	3.760771	-0.404897
18	7	0	-3.335717	3.142845	-0.661302
19	8	0	-1.299479	3.878116	-1.536701
20	8	0	-5.094927	2.783984	0.831101
21	6	0	-2.178549	3.943323	-0.699520
22	6	0	-2.280166	4.864008	0.468871
23	6	0	-1.439450	5.889046	0.874502
24	1	0	-0.535458	6.121336	0.319993
25	6	0	-1.801563	6.599137	2.027139
26	1	0	-1.171193	7.412522	2.376007
27	6	0	-2.965094	6.278730	2.739295
28	1	0	-3.220366	6.849720	3.627891
29	6	0	-3.802864	5.235587	2.322323
30	1	0	-4.706692	4.977996	2.866248
31	6	0	-3.436490	4.541988	1.178087
32	6	0	-4.098127	3.396134	0.489669
33	7	0	-3.847450	-3.104820	0.202820
34	8	0	-4.417246	-1.077083	-0.797989
35	8	0	-3.540705	-4.766165	1.813691
36	6	0	-4.455400	-1.839181	0.149383
37	6	0	-5.133786	-1.647983	1.462600
38	6	0	-5.876611	-0.574497	1.935729
39	1	0	-6.015822	0.322259	1.339338
40	6	0	-6.408089	-0.688685	3.228143
41	1	0	-6.996954	0.127985	3.636385

42	6	0	-6.192434	-1.835866	4.003994
43	1	0	-6.624135	-1.894261	4.999573
44	6	0	-5.424289	-2.903595	3.519707
45	1	0	-5.240465	-3.791857	4.116206
46	6	0	-4.902136	-2.783100	2.240089
47	6	0	-4.027694	-3.709165	1.462810
48	7	0	3.538656	-3.300940	-0.249718
49	8	0	1.589234	-4.580866	-0.079408
50	8	0	5.520812	-2.207460	0.326255
51	6	0	2.648637	-4.193485	0.372988
52	6	0	3.268575	-4.540839	1.686658
53	6	0	2.833966	-5.405655	2.680756
54	1	0	1.908280	-5.962133	2.570479
55	6	0	3.638433	-5.531294	3.821599
56	1	0	3.333886	-6.200330	4.621517
57	6	0	4.832766	-4.809092	3.947917
58	1	0	5.435168	-4.929185	4.843980
59	6	0	5.261544	-3.938372	2.936881
60	1	0	6.185172	-3.374421	3.023155
61	6	0	4.457922	-3.823663	1.811511
62	6	0	4.629454	-2.996198	0.582158
63	8	0	1.083509	1.329490	-0.791122
64	8	0	0.821776	1.034374	-3.022745
65	8	0	-1.822758	0.934241	-0.492954
66	8	0	-2.035494	0.604516	-2.726045
67	8	0	-1.427041	-1.912328	-0.110203
68	8	0	-1.613120	-2.264094	-2.340111
69	8	0	1.540350	-1.503385	-0.402469
70	8	0	1.321081	-1.838377	-2.630479
71	6	0	1.273257	1.638487	-2.014676
72	6	0	2.109700	2.927061	-2.205372
73	1	0	1.518249	3.704270	-1.707354
74	6	0	2.382533	3.429569	-3.661422
75	6	0	3.204238	4.734585	-3.570029
76	1	0	3.326793	5.159490	-4.572790
77	1	0	4.206707	4.558452	-3.163755
78	1	0	2.710647	5.483862	-2.940969
79	6	0	3.155630	2.415315	-4.525495
80	1	0	2.611459	1.473759	-4.619632
81	1	0	4.144611	2.197164	-4.109628
82	1	0	3.303100	2.833548	-5.528996
83	6	0	1.028664	3.764321	-4.326224
84	1	0	0.423872	2.868892	-4.478973
85	1	0	1.207430	4.231579	-5.302147

86	1	0	0.447442	4.465695	-3.716512
87	6	0	-2.376417	1.117597	-1.625982
88	6	0	-3.625828	2.022820	-1.563478
89	1	0	-4.355747	1.419149	-1.012553
90	6	0	-4.314856	2.440560	-2.906444
91	6	0	-3.375466	3.177008	-3.880685
92	1	0	-2.996396	4.110566	-3.454768
93	1	0	-3.927419	3.426285	-4.795729
94	1	0	-2.518213	2.558373	-4.154664
95	6	0	-5.504416	3.365148	-2.564908
96	1	0	-5.172022	4.321683	-2.146325
97	1	0	-6.187211	2.899235	-1.845243
98	1	0	-6.071288	3.584376	-3.476924
99	6	0	-4.880073	1.172598	-3.585489
100	1	0	-5.549644	0.625530	-2.911449
101	1	0	-4.084124	0.493551	-3.895380
102	1	0	-5.455755	1.459913	-4.473710
103	6	0	-1.902802	-2.498509	-1.137300
104	6	0	-2.903734	-3.631209	-0.793021
105	1	0	-2.316342	-4.365217	-0.228060
106	6	0	-3.574085	-4.410491	-1.971555
107	6	0	-2.467990	-5.147166	-2.759443
108	1	0	-1.884740	-5.806416	-2.103668
109	1	0	-1.782652	-4.448277	-3.242692
110	1	0	-2.924629	-5.772522	-3.535582
111	6	0	-4.517229	-5.474195	-1.367409
112	1	0	-3.997550	-6.119686	-0.650474
113	1	0	-4.916642	-6.106368	-2.168773
114	1	0	-5.370050	-5.017634	-0.853001
115	6	0	-4.383529	-3.508044	-2.922135
116	1	0	-3.754258	-2.741717	-3.378341
117	1	0	-5.204928	-3.006217	-2.401754
118	1	0	-4.819127	-4.122301	-3.720064
119	6	0	1.924695	-1.959571	-1.532728
120	6	0	3.319432	-2.625081	-1.533619
121	1	0	4.006655	-1.770090	-1.500334
122	6	0	3.730177	-3.475612	-2.787515
123	6	0	3.898384	-2.527731	-3.996933
124	1	0	2.949839	-2.075729	-4.289464
125	1	0	4.290875	-3.093529	-4.850501
126	1	0	4.606327	-1.720470	-3.774146
127	6	0	5.105238	-4.120621	-2.505044
128	1	0	5.052167	-4.871877	-1.709102
129	1	0	5.853318	-3.372693	-2.218614

130	1	0	5.462517	-4.626800	-3.409004
131	6	0	2.717311	-4.584378	-3.132409
132	1	0	1.732166	-4.167841	-3.354809
133	1	0	2.604875	-5.304155	-2.316301
134	1	0	3.065669	-5.131033	-4.017497
135	6	0	-0.810998	-3.245672	3.628545
136	6	0	-1.574576	-2.672738	4.655347
137	6	0	-1.831315	-1.295984	4.705140
138	6	0	-1.291071	-0.507590	3.697712
139	6	0	-0.503814	-1.062568	2.651694
140	6	0	-0.276234	-2.445841	2.619107
141	7	0	-1.408730	0.861680	3.490599
142	6	0	-0.754751	1.260852	2.323587
143	6	0	-0.137056	-0.016650	1.713870
144	8	0	-0.737613	2.403075	1.910593
145	1	0	-0.658682	-4.319745	3.607582
146	1	0	-1.992064	-3.312447	5.428469
147	1	0	-2.441676	-0.869369	5.495722
148	1	0	0.292279	-2.879253	1.803820
149	1	0	-1.965732	1.501318	4.039388
150	6	0	2.101176	1.520876	2.266976
151	1	0	2.074442	2.014538	1.299862
152	6	0	2.002507	0.151179	2.252660
153	1	0	2.022718	-0.417272	3.177533
154	1	0	2.226881	-0.402433	1.348424
155	6	0	2.121419	2.392545	3.424093
156	6	0	2.016084	3.785194	3.215713
157	6	0	2.245097	1.915497	4.748615
158	6	0	2.027542	4.666844	4.293410
159	1	0	1.925135	4.163624	2.201934
160	6	0	2.254481	2.799072	5.820105
161	1	0	2.345014	0.850056	4.932449
162	6	0	2.144646	4.177892	5.596391
163	1	0	1.943894	5.735381	4.116882
164	1	0	2.353466	2.419528	6.833417
165	1	0	2.156346	4.865813	6.437649

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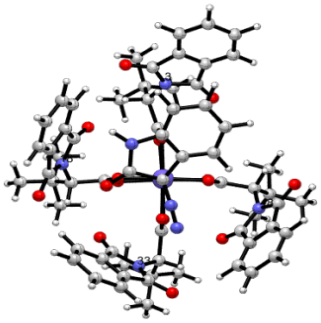
15. Possible complexes of catalyst and diazooxindole

C1:



E=-4334.4457363 a.u (E_{rel}=0.0)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.144083	0.158887	-0.128620
2	45	0	0.284153	0.180367	-2.548935
3	7	0	-4.553170	1.154326	-0.550318
4	8	0	-3.460472	3.145398	-1.148788
5	8	0	-5.796838	-0.445745	0.641039
6	6	0	-4.288034	2.541661	-0.471182
7	6	0	-5.217239	3.053512	0.582719
8	6	0	-5.420763	4.342906	1.038153
9	1	0	-4.864840	5.173257	0.620434
10	6	0	-6.367846	4.530252	2.058173
11	1	0	-6.558394	5.527640	2.436311
12	6	0	-7.072746	3.444593	2.594042
13	1	0	-7.799776	3.616392	3.378863
14	6	0	-6.852540	2.139716	2.123424
15	1	0	-7.393793	1.292797	2.527659
16	6	0	-5.921918	1.971973	1.113913
17	6	0	-5.465889	0.724325	0.425712
18	7	0	-1.396541	-4.155587	-0.213306
19	8	0	-3.026771	-2.682526	-1.034112
20	8	0	-0.058935	-5.418252	1.245570
21	6	0	-2.583841	-3.403875	-0.136325
22	6	0	-3.133489	-3.652527	1.225410
23	6	0	-4.266424	-3.125561	1.827294
24	1	0	-4.904747	-2.418403	1.306437
25	6	0	-4.514323	-3.504947	3.158561
26	1	0	-5.389848	-3.120334	3.668431
27	6	0	-3.646960	-4.372642	3.838423
28	1	0	-3.865529	-4.646966	4.863633

29	6	0	-2.491986	-4.873575	3.217793
30	1	0	-1.799030	-5.517283	3.744781
31	6	0	-2.253551	-4.493328	1.909370
32	6	0	-1.088079	-4.785417	1.016653
33	7	0	4.292503	-1.727152	0.085532
34	8	0	2.582008	-3.177220	-0.612293
35	8	0	5.780044	-0.503132	1.424914
36	6	0	3.355542	-2.775019	0.259013
37	6	0	3.522448	-3.230018	1.665814
38	6	0	2.823787	-4.195952	2.369367
39	1	0	1.998835	-4.738242	1.921090
40	6	0	3.195975	-4.402565	3.708413
41	1	0	2.673147	-5.148193	4.295177
42	6	0	4.218151	-3.653047	4.302580
43	1	0	4.480634	-3.836260	5.337890
44	6	0	4.894214	-2.654573	3.582514
45	1	0	5.669071	-2.051491	4.039726
46	6	0	4.526290	-2.460641	2.263475
47	6	0	4.991357	-1.440588	1.277116
48	7	0	2.418722	4.118573	-0.030302
49	8	0	3.676457	2.250544	-0.693504
50	8	0	1.454231	5.830606	1.252096
51	6	0	3.389430	3.110750	0.142009
52	6	0	3.951758	3.324467	1.506390
53	6	0	4.913457	2.600029	2.191850
54	1	0	5.363144	1.707110	1.771243
55	6	0	5.244788	3.041433	3.484200
56	1	0	5.991153	2.500680	4.053648
57	6	0	4.622992	4.160062	4.051797
58	1	0	4.901401	4.475516	5.050326
59	6	0	3.634400	4.869501	3.350895
60	1	0	3.133414	5.725363	3.786518
61	6	0	3.315785	4.430277	2.078618
62	6	0	2.286486	4.934428	1.121012
63	8	0	-1.887778	0.483393	-0.301522
64	8	0	-1.751355	0.412077	-2.589655
65	8	0	-0.240577	-1.825708	-0.259970
66	8	0	-0.000464	-1.868657	-2.536504
67	8	0	2.143208	-0.247260	-0.120776
68	8	0	2.307867	-0.173620	-2.402466
69	8	0	0.615285	2.156594	-0.122346
70	8	0	0.658550	2.210042	-2.414778
71	6	0	-2.416611	0.427222	-1.483660
72	6	0	-3.939800	0.241686	-1.522976

73	1	0	-4.087363	-0.761461	-1.102525
74	6	0	-4.628431	0.258360	-2.927258
75	6	0	-6.159158	0.151783	-2.707121
76	1	0	-6.650624	0.003385	-3.674614
77	1	0	-6.556869	1.068669	-2.259051
78	1	0	-6.403768	-0.692631	-2.052722
79	6	0	-4.318094	1.527134	-3.754180
80	1	0	-3.244991	1.602137	-3.935047
81	1	0	-4.649269	2.433561	-3.241737
82	1	0	-4.840764	1.459397	-4.715907
83	6	0	-4.165641	-1.000273	-3.707015
84	1	0	-3.096073	-0.945682	-3.912714
85	1	0	-4.712232	-1.055892	-4.655242
86	1	0	-4.361800	-1.908142	-3.127850
87	6	0	-0.203648	-2.439535	-1.400495
88	6	0	-0.373420	-3.960050	-1.259113
89	1	0	0.563659	-4.284941	-0.788256
90	6	0	-0.570011	-4.794790	-2.553521
91	6	0	-1.747016	-4.301012	-3.422919
92	1	0	-2.692760	-4.356732	-2.878566
93	1	0	-1.818492	-4.929450	-4.318486
94	1	0	-1.582423	-3.265266	-3.725741
95	6	0	-0.812305	-6.265058	-2.132214
96	1	0	-1.782485	-6.370340	-1.635888
97	1	0	-0.030834	-6.607118	-1.443310
98	1	0	-0.805804	-6.904343	-3.021745
99	6	0	0.750386	-4.719826	-3.363374
100	1	0	1.594169	-5.071677	-2.758281
101	1	0	0.946856	-3.691423	-3.671468
102	1	0	0.666931	-5.353105	-4.253714
103	6	0	2.800458	-0.377859	-1.234019
104	6	0	4.270207	-0.778197	-1.042434
105	1	0	4.750217	0.127098	-0.649997
106	6	0	5.063764	-1.229059	-2.302792
107	6	0	5.234311	0.006122	-3.224090
108	1	0	5.739266	0.819882	-2.689997
109	1	0	4.259935	0.360044	-3.564492
110	1	0	5.841314	-0.270603	-4.093437
111	6	0	6.464129	-1.694459	-1.832269
112	1	0	6.936520	-0.933772	-1.199490
113	1	0	7.099360	-1.872484	-2.706759
114	1	0	6.391501	-2.624950	-1.260297
115	6	0	4.371484	-2.370734	-3.080028
116	1	0	3.395113	-2.042213	-3.441114

117	1	0	4.227011	-3.249911	-2.448360
118	1	0	4.995176	-2.649251	-3.937706
119	6	0	0.861968	2.735428	-1.257190
120	6	0	1.426423	4.164548	-1.121832
121	1	0	0.616093	4.779743	-0.705749
122	6	0	1.912783	4.869840	-2.422627
123	6	0	0.665825	5.136991	-3.303753
124	1	0	0.182671	4.195257	-3.571163
125	1	0	0.972162	5.654403	-4.219574
126	1	0	-0.053678	5.772972	-2.772817
127	6	0	2.535822	6.228643	-2.016545
128	1	0	3.482533	6.077131	-1.487972
129	1	0	1.859894	6.792261	-1.362959
130	1	0	2.733144	6.819428	-2.917544
131	6	0	2.951109	4.045431	-3.216743
132	1	0	2.510296	3.105570	-3.551558
133	1	0	3.828223	3.818025	-2.606781
134	1	0	3.269783	4.624998	-4.091132
135	6	0	-1.957295	3.240843	2.995617
136	6	0	-3.154940	2.568113	3.256217
137	6	0	-3.230756	1.170604	3.190580
138	6	0	-2.079987	0.464914	2.873266
139	6	0	-0.867041	1.144158	2.618509
140	6	0	-0.796987	2.528755	2.665879
141	7	0	-1.873937	-0.915628	2.779716
142	6	0	-0.545490	-1.253087	2.523386
143	6	0	0.117479	0.099368	2.302312
144	8	0	-0.051118	-2.380083	2.514774
145	1	0	-1.924436	4.322698	3.037012
146	1	0	-4.047052	3.132182	3.497433
147	1	0	-4.164157	0.656787	3.382126
148	1	0	0.121618	3.043917	2.418571
149	1	0	-2.601101	-1.620472	2.842434
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151	7	0	2.559148	0.269208	2.588844

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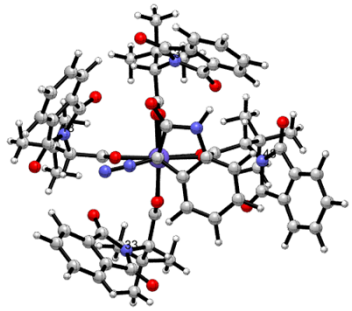

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5	8	0	-0.060144	-5.418729	1.244798
6	6	0	-2.584379	-3.403315	-0.136844
7	6	0	-3.134342	-3.652338	1.224693
8	6	0	-4.267249	-3.125333	1.826570
9	1	0	-4.905297	-2.417770	1.305920
10	6	0	-4.515493	-3.505196	3.157644
11	1	0	-5.391012	-3.120558	3.667505
12	6	0	-3.648493	-4.373395	3.837312
13	1	0	-3.867310	-4.648090	4.862370
14	6	0	-2.493504	-4.874354	3.216699
15	1	0	-1.800836	-5.518472	3.743566
16	6	0	-2.254721	-4.493640	1.908483
17	6	0	-1.089104	-4.785575	1.015907
18	7	0	4.292186	-1.727866	0.085519
19	8	0	2.581506	-3.177581	-0.612667
20	8	0	5.779904	-0.504416	1.425240
21	6	0	3.355040	-2.775637	0.258755
22	6	0	3.521861	-3.230988	1.665441
23	6	0	2.823012	-4.196957	2.368761
24	1	0	1.997841	-4.738827	1.920392
25	6	0	3.195226	-4.404034	3.707729
26	1	0	2.672260	-5.149709	4.294310
27	6	0	4.217592	-3.654899	4.302055
28	1	0	4.480087	-3.838463	5.337299
29	6	0	4.893806	-2.656340	3.582246
30	1	0	5.668787	-2.053522	4.039595
31	6	0	4.525861	-2.461965	2.263280

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35	8	0	1.455302	5.830917	1.252552
36	6	0	3.389572	3.110367	0.142582
37	6	0	3.952079	3.324027	1.506889
38	6	0	4.913655	2.599381	2.192295
39	1	0	5.363035	1.706296	1.771700
40	6	0	5.245245	3.040808	3.484576
41	1	0	5.991543	2.499920	4.053983
42	6	0	4.623793	4.159640	4.052153
43	1	0	4.902396	4.475108	5.050622
44	6	0	3.635303	4.869280	3.351300
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46	6	0	3.316453	4.430047	2.079091
47	6	0	2.287207	4.934402	1.121541
48	7	0	-4.552911	1.155260	-0.550263
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50	8	0	-5.796719	-0.444790	0.640939
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52	6	0	-5.216345	3.054341	0.583282
53	6	0	-5.419589	4.343747	1.038857
54	1	0	-4.863270	5.173898	0.621323
55	6	0	-6.366538	4.531225	2.058935
56	1	0	-6.556858	5.528604	2.437203
57	6	0	-7.071658	3.445633	2.594713
58	1	0	-7.798612	3.617490	3.379591
59	6	0	-6.851777	2.140760	2.123929
60	1	0	-7.393245	1.293941	2.528090
61	6	0	-5.921249	1.972894	1.114343
62	6	0	-5.465598	0.725258	0.425766
63	8	0	-0.241214	-1.825411	-0.260143
64	8	0	-0.000566	-1.868193	-2.536628
65	8	0	2.143076	-0.247616	-0.120576
66	8	0	2.307898	-0.173567	-2.402237
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68	8	0	0.658811	2.210474	-2.414555
69	8	0	-1.887702	0.484188	-0.301566
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72	6	0	-0.373976	-3.959679	-1.259540
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74	6	0	-0.570491	-4.794227	-2.554111
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79	6	0	-1.747384	-4.300259	-3.423548
80	1	0	-1.582648	-3.264516	-3.726303
81	1	0	-2.693162	-4.355881	-2.879248
82	1	0	-1.818881	-4.928639	-4.319155
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84	1	0	0.946457	-3.690796	-3.671878
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88	6	0	4.270074	-0.778597	-1.042217
89	1	0	4.750143	0.126535	-0.649483
90	6	0	5.063704	-1.229147	-2.302646
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92	1	0	4.227240	-3.250073	-2.448883
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94	1	0	3.394997	-2.042105	-3.441020
95	6	0	6.464057	-1.694647	-1.832187
96	1	0	6.391413	-2.625301	-1.260486
97	1	0	6.936409	-0.934127	-1.199178
98	1	0	7.099336	-1.872415	-2.706696
99	6	0	5.234280	0.006254	-3.223633
100	1	0	5.739236	0.819874	-2.689330
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106	6	0	1.913551	4.870000	-2.422012
107	6	0	0.666728	5.137318	-3.303272
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109	1	0	0.183502	4.195637	-3.570744
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115	6	0	2.951875	4.045511	-3.216054
116	1	0	2.511023	3.105661	-3.550842
117	1	0	3.828959	3.818090	-2.606058
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131	6	0	-4.317753	1.528643	-3.753993
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143	6	0	0.117401	0.098163	2.301644
144	8	0	-0.051334	-2.381276	2.513772
145	1	0	-1.924353	4.321532	3.037299
146	1	0	-4.046705	3.130992	3.498480
147	1	0	-4.163998	0.655758	3.382852
148	1	0	0.121569	3.042657	2.418017
149	1	0	-2.601048	-1.621673	2.842349
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151	7	0	2.559036	0.268035	2.588815

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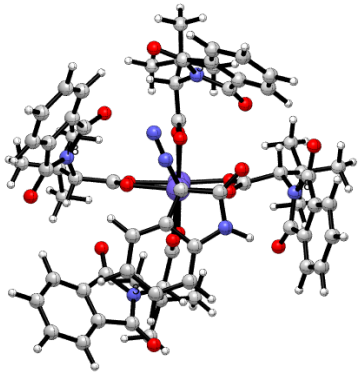

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7	6	0	4.558594	2.163040	1.273835
8	6	0	5.407410	1.296301	1.939770
9	1	0	5.690084	0.345944	1.502204
10	6	0	5.833882	1.680100	3.222186
11	1	0	6.499898	1.030231	3.777370
12	6	0	5.404962	2.879542	3.802927
13	1	0	5.751698	3.146464	4.794360
14	6	0	4.519581	3.732605	3.124857
15	1	0	4.164167	4.653069	3.571742
16	6	0	4.110351	3.351576	1.859907
17	6	0	3.143085	4.005840	0.930156
18	7	0	-2.994267	3.305100	0.074686
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22	6	0	-1.711835	4.487589	1.590178
23	6	0	-0.704671	5.173211	2.248407
24	1	0	0.260929	5.342010	1.782996
25	6	0	-0.971108	5.587327	3.564541
26	1	0	-0.210525	6.126820	4.116097
27	6	0	-2.197161	5.306389	4.179712
28	1	0	-2.371822	5.639552	5.195890
29	6	0	-3.197162	4.586486	3.505176

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36	6	0	-4.332337	-1.474635	-0.183352
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40	6	0	-6.684182	-0.701464	2.731029
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42	6	0	-6.797787	-2.012030	3.213139
43	1	0	-7.422484	-2.210135	4.076184
44	6	0	-6.098677	-3.067309	2.604768
45	1	0	-6.156700	-4.080123	2.984847
46	6	0	-5.318817	-2.764414	1.503841
47	6	0	-4.398092	-3.637254	0.713514
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52	6	0	3.370319	-4.348451	1.346879
53	6	0	2.868095	-5.362384	2.147180
54	1	0	2.059774	-5.994663	1.798726
55	6	0	3.453074	-5.541573	3.411813
56	1	0	3.089185	-6.325553	4.065183
57	6	0	4.506801	-4.722347	3.838495
58	1	0	4.940934	-4.881527	4.818245
59	6	0	5.003862	-3.699098	3.016206
60	1	0	5.813162	-3.055941	3.338458
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62	6	0	4.708791	-2.535274	0.697889
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64	8	0	0.954268	1.624883	-2.543571
65	8	0	-1.609515	1.071072	-0.084260
66	8	0	-1.829080	1.026786	-2.368579
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76	1	0	3.782499	5.817984	-3.120675
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78	1	0	2.953643	5.915636	-1.544168
79	6	0	3.556612	3.045248	-3.434410
80	1	0	2.967222	2.180211	-3.745050
81	1	0	4.412473	2.689936	-2.855695
82	1	0	3.923289	3.566196	-4.326703
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84	1	0	0.860248	3.625745	-3.742643
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87	6	0	-2.173618	1.432823	-1.197925
88	6	0	-3.354778	2.396922	-1.026520
89	1	0	-4.154293	1.767942	-0.620013
90	6	0	-3.913536	3.094873	-2.301527
91	6	0	-2.831872	3.844555	-3.110581
92	1	0	-2.347435	4.615536	-2.507378
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94	1	0	-2.068235	3.145107	-3.454772
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97	1	0	-5.740896	3.604031	-1.198536
98	1	0	-5.521436	4.493280	-2.727291
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101	1	0	-3.825333	1.295873	-3.532921
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103	6	0	-1.744802	-2.210496	-1.337341
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107	6	0	-2.355063	-4.489605	-3.411406
108	1	0	-1.997768	-5.353402	-2.836969
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117	1	0	-4.786183	-2.016303	-2.939277

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136	6	0	-2.451008	-2.923783	3.659782
137	6	0	-1.123695	-3.265150	3.371124
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139	6	0	-0.730247	-0.933219	2.793004
140	6	0	-2.047497	-0.599159	3.074041
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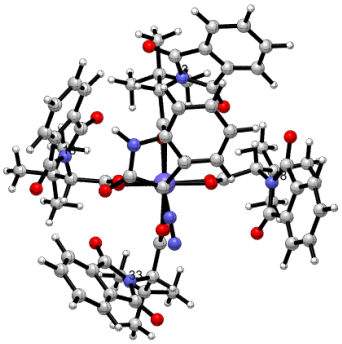
151	7	0	0.772524	2.269872	2.426167

C4:



E= -4334.4428038 a.u. (E_{rel}=1.8 kcal/mol)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
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2	45	0	0.524799	0.398029	-2.516523
3	7	0	-3.111313	-2.903346	-0.715514
4	8	0	-3.753438	-0.766682	-1.426909
5	8	0	-2.846495	-4.842499	0.583671
6	6	0	-3.928600	-1.756358	-0.712205
7	6	0	-4.990436	-2.030327	0.296098
8	6	0	-6.046904	-1.234209	0.699747
9	1	0	-6.151788	-0.221666	0.327565
10	6	0	-6.916811	-1.767753	1.665573
11	1	0	-7.762045	-1.180988	2.005373
12	6	0	-6.703656	-3.043002	2.205274
13	1	0	-7.394604	-3.430772	2.944756
14	6	0	-5.599194	-3.818858	1.813858
15	1	0	-5.412254	-4.794854	2.245249
16	6	0	-4.756112	-3.290082	0.853494
17	6	0	-3.483551	-3.830969	0.278187
18	7	0	3.062427	-3.264730	0.051232
19	8	0	0.999358	-3.783397	-0.945539
20	8	0	4.731873	-2.878315	1.656903
21	6	0	1.767234	-3.815348	0.019737
22	6	0	1.540818	-4.399095	1.372516
23	6	0	0.414190	-5.023043	1.887930
24	1	0	-0.489179	-5.152301	1.299185
25	6	0	0.469135	-5.426125	3.233991
26	1	0	-0.387857	-5.918989	3.677765
27	6	0	1.612714	-5.197234	4.013966
28	1	0	1.623605	-5.518680	5.048634
29	6	0	2.732611	-4.540658	3.479389

30	1	0	3.607360	-4.328742	4.081228
31	6	0	2.670176	-4.147262	2.154475
32	6	0	3.648581	-3.363052	1.336186
33	7	0	4.090490	2.833391	0.243853
34	8	0	4.366134	0.594929	-0.400737
35	8	0	4.002455	4.814713	1.496229
36	6	0	4.440331	1.483079	0.452084
37	6	0	4.901849	1.402158	1.865607
38	6	0	5.299765	0.300360	2.603812
39	1	0	5.276995	-0.701142	2.189703
40	6	0	5.682862	0.529863	3.935734
41	1	0	5.997806	-0.306507	4.548040
42	6	0	5.651222	1.815016	4.490294
43	1	0	5.953120	1.958581	5.521125
44	6	0	5.216592	2.916429	3.735690
45	1	0	5.165198	3.911495	4.160494
46	6	0	4.843859	2.682850	2.424463
47	6	0	4.284164	3.621213	1.408019
48	7	0	-3.482936	3.150671	-0.314202
49	8	0	-1.602614	4.557910	-0.470597
50	8	0	-5.369772	2.010876	0.508824
51	6	0	-2.606916	4.173526	0.123370
52	6	0	-3.174938	4.642722	1.423347
53	6	0	-2.731269	5.637057	2.276538
54	1	0	-1.842656	6.211648	2.045054
55	6	0	-3.473963	5.868556	3.445264
56	1	0	-3.157084	6.639373	4.137448
57	6	0	-4.620310	5.116315	3.729834
58	1	0	-5.175903	5.315530	4.638334
59	6	0	-5.057405	4.108233	2.855823
60	1	0	-5.942810	3.521191	3.067449
61	6	0	-4.316374	3.890157	1.707786
62	6	0	-4.512591	2.893566	0.609083
63	8	0	-0.950964	-1.280264	-0.336466
64	8	0	-0.638548	-1.281673	-2.609816
65	8	0	1.850971	-0.967725	-0.095550
66	8	0	2.184759	-0.826153	-2.357310
67	8	0	1.622197	1.899422	-0.037291
68	8	0	1.776649	2.032573	-2.315021
69	8	0	-1.337825	1.569431	-0.263289
70	8	0	-1.197458	1.526116	-2.551319
71	6	0	-1.125875	-1.773836	-1.522314
72	6	0	-1.929650	-3.079774	-1.570431
73	1	0	-1.296245	-3.804739	-1.047526

74	6	0	-2.253702	-3.670281	-2.978954
75	6	0	-3.122307	-4.937265	-2.774619
76	1	0	-3.246127	-5.447406	-3.736027
77	1	0	-4.115562	-4.671209	-2.397289
78	1	0	-2.652619	-5.627726	-2.064985
79	6	0	-3.009693	-2.680423	-3.893927
80	1	0	-2.412487	-1.781775	-4.050966
81	1	0	-3.971477	-2.392017	-3.460640
82	1	0	-3.197211	-3.162422	-4.860780
83	6	0	-0.919274	-4.094183	-3.644281
84	1	0	-0.296055	-3.219332	-3.831041
85	1	0	-1.134722	-4.595750	-4.594498
86	1	0	-0.364838	-4.781009	-2.996317
87	6	0	2.456946	-1.299378	-1.191896
88	6	0	3.582458	-2.317742	-0.957399
89	1	0	4.348014	-1.744116	-0.421555
90	6	0	4.253059	-2.964442	-2.199086
91	6	0	3.246805	-3.652223	-3.148572
92	1	0	2.704561	-4.453843	-2.641824
93	1	0	3.792503	-4.077966	-3.998885
94	1	0	2.521463	-2.925065	-3.518549
95	6	0	5.283642	-4.002385	-1.690640
96	1	0	4.778997	-4.855116	-1.224918
97	1	0	5.958114	-3.551957	-0.952823
98	1	0	5.877077	-4.369561	-2.535041
99	6	0	5.008275	-1.844699	-2.960875
100	1	0	5.731065	-1.348726	-2.302672
101	1	0	4.303114	-1.098662	-3.330932
102	1	0	5.547182	-2.283245	-3.808217
103	6	0	2.160542	2.349832	-1.129605
104	6	0	3.319729	3.341746	-0.904431
105	1	0	2.871179	4.269790	-0.521270
106	6	0	4.169613	3.730378	-2.151661
107	6	0	3.271024	4.570965	-3.094488
108	1	0	2.909321	5.471509	-2.582422
109	1	0	2.416601	3.980371	-3.430336
110	1	0	3.853943	4.883507	-3.968001
111	6	0	5.341648	4.617039	-1.661619
112	1	0	4.979456	5.429065	-1.020704
113	1	0	5.855778	5.047586	-2.527735
114	1	0	6.061935	4.021558	-1.091647
115	6	0	4.733845	2.508775	-2.912247
116	1	0	3.920438	1.890981	-3.295750
117	1	0	5.357335	1.891595	-2.261639

118	1	0	5.341844	2.864098	-3.752517
119	6	0	-1.811556	1.794765	-1.448735
120	6	0	-3.257330	2.309148	-1.497726
121	1	0	-3.857584	1.406288	-1.313420
122	6	0	-3.749459	2.929460	-2.844403
123	6	0	-3.894284	1.780001	-3.875793
124	1	0	-2.920765	1.331564	-4.076520
125	1	0	-4.308624	2.179781	-4.808323
126	1	0	-4.565010	1.001863	-3.494294
127	6	0	-5.149969	3.544998	-2.601254
128	1	0	-5.082284	4.432969	-1.964428
129	1	0	-5.816902	2.819685	-2.120633
130	1	0	-5.584075	3.841935	-3.562072
131	6	0	-2.793193	4.011744	-3.394539
132	1	0	-1.821715	3.568823	-3.623926
133	1	0	-2.642028	4.815649	-2.670448
134	1	0	-3.218277	4.434367	-4.312583
135	6	0	-3.558929	0.191207	2.871272
136	6	0	-3.592835	-1.163302	3.215447
137	6	0	-2.423503	-1.932687	3.253308
138	6	0	-1.220462	-1.310116	2.953308
139	6	0	-1.183869	0.061624	2.618391
140	6	0	-2.344994	0.818012	2.566431
141	7	0	0.077840	-1.828635	2.943440
142	6	0	1.049688	-0.867499	2.663815
143	6	0	0.226739	0.372353	2.345360
144	8	0	2.270595	-1.014776	2.704408
145	1	0	-4.481701	0.751118	2.791014
146	1	0	-4.542475	-1.636563	3.426783
147	1	0	-2.458937	-2.985969	3.502349
148	1	0	-2.314714	1.853432	2.257252
149	1	0	0.313377	-2.803815	3.086731
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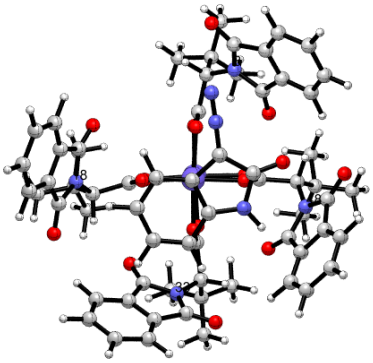
151	7	0	1.279630	2.587054	2.592598

C5:



E= -4334.4406062 a.u. (E_{rel}=3.2 kcal/mol)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
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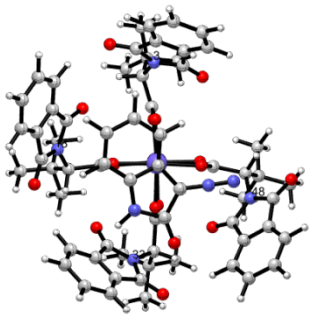
4	8	0	-4.002792	-1.020296	-0.746473
5	8	0	-3.841802	-5.128745	1.402880
6	6	0	-4.222668	-1.880232	0.111889
7	6	0	-5.053558	-1.793329	1.344075
8	6	0	-5.697963	-0.702619	1.904536
9	1	0	-5.625422	0.291343	1.479479
10	6	0	-6.409930	-0.927259	3.095405
11	1	0	-6.925365	-0.099487	3.566913
12	6	0	-6.447766	-2.192127	3.693028
13	1	0	-7.004371	-2.330645	4.612396
14	6	0	-5.753671	-3.276930	3.132733
15	1	0	-5.746322	-4.252026	3.604021
16	6	0	-5.061271	-3.050464	1.957629
17	6	0	-4.166618	-3.964476	1.186759
18	7	0	4.047233	-2.724099	-0.078054
19	8	0	2.284922	-4.286705	-0.037523
20	8	0	5.861184	-1.374910	0.549886
21	6	0	3.250834	-3.745032	0.493947
22	6	0	3.850638	-3.995864	1.840757
23	6	0	3.484069	-4.902078	2.819527
24	1	0	2.643217	-5.568851	2.671777
25	6	0	4.241277	-4.922770	4.002000
26	1	0	3.983045	-5.618535	4.791257
27	6	0	5.328035	-4.057041	4.175909
28	1	0	5.896924	-4.095053	5.097130
29	6	0	5.689914	-3.143133	3.173282

30	1	0	6.531039	-2.471737	3.295932
31	6	0	4.933801	-3.131672	2.014319
32	6	0	5.059950	-2.281849	0.791297
33	7	0	2.973584	3.202649	-0.624779
34	8	0	3.951183	1.175989	-1.283340
35	8	0	2.244187	4.989903	0.716325
36	6	0	3.901145	2.141280	-0.519396
37	6	0	4.729439	2.459285	0.679143
38	6	0	5.773445	1.750103	1.247416
39	1	0	6.086473	0.794541	0.842265
40	6	0	6.351030	2.285404	2.411714
41	1	0	7.172298	1.762445	2.887367
42	6	0	5.875346	3.475230	2.977134
43	1	0	6.339689	3.861260	3.876838
44	6	0	4.793086	4.163700	2.404316
45	1	0	4.399763	5.070408	2.847725
46	6	0	4.239640	3.636622	1.252087
47	6	0	3.046154	4.084423	0.470314
48	7	0	-3.247863	2.962163	-0.222784
49	8	0	-1.121232	3.598102	-0.980142
50	8	0	-5.186466	2.689797	1.074103
51	6	0	-2.027655	3.649536	-0.143331
52	6	0	-2.080464	4.412873	1.135571
53	6	0	-1.104700	5.200769	1.728005
54	1	0	-0.129367	5.331624	1.267992
55	6	0	-1.419491	5.774952	2.971957
56	1	0	-0.687642	6.397253	3.472804
57	6	0	-2.661653	5.547757	3.579719
58	1	0	-2.873640	6.001297	4.540571
59	6	0	-3.626037	4.723931	2.975568
60	1	0	-4.574430	4.516040	3.454754
61	6	0	-3.312010	4.163329	1.750915
62	6	0	-4.080418	3.195222	0.902072
63	8	0	-1.188701	-2.042090	0.071968
64	8	0	-1.208661	-2.270925	-2.204404
65	8	0	1.766152	-1.375306	-0.175792
66	8	0	1.662799	-1.474717	-2.461454
67	8	0	1.049670	1.375716	-0.359815
68	8	0	0.819842	1.271797	-2.637684
69	8	0	-1.715150	0.783927	-0.146992
70	8	0	-1.910670	0.529325	-2.413144
71	6	0	-1.624050	-2.583281	-1.023017
72	6	0	-2.692443	-3.689657	-0.856924
73	1	0	-2.210949	-4.513034	-0.311300

74	6	0	-3.281530	-4.291369	-2.172373
75	6	0	-4.383712	-5.309694	-1.783316
76	1	0	-4.686327	-5.867663	-2.676193
77	1	0	-5.264294	-4.792467	-1.388116
78	1	0	-4.027675	-6.012822	-1.023521
79	6	0	-3.896097	-3.225498	-3.108708
80	1	0	-3.128813	-2.532965	-3.454471
81	1	0	-4.674097	-2.653099	-2.597137
82	1	0	-4.344137	-3.729982	-3.972933
83	6	0	-2.145617	-5.053652	-2.900281
84	1	0	-1.339168	-4.369217	-3.167881
85	1	0	-2.543503	-5.511147	-3.812845
86	1	0	-1.746307	-5.852052	-2.262238
87	6	0	2.278639	-1.629872	-1.335388
88	6	0	3.757833	-2.036476	-1.344035
89	1	0	4.296069	-1.079719	-1.263908
90	6	0	4.284225	-2.769195	-2.620808
91	6	0	3.381772	-3.948643	-3.048793
92	1	0	3.261666	-4.671547	-2.238678
93	1	0	3.831764	-4.451022	-3.913005
94	1	0	2.393194	-3.578383	-3.328715
95	6	0	5.713386	-3.285246	-2.320545
96	1	0	5.689272	-4.110776	-1.601797
97	1	0	6.338553	-2.483273	-1.911243
98	1	0	6.166657	-3.649125	-3.248918
99	6	0	4.374017	-1.729465	-3.767740
100	1	0	5.040186	-0.904632	-3.487675
101	1	0	3.385487	-1.324695	-3.987892
102	1	0	4.774569	-2.213852	-4.665454
103	6	0	1.208698	1.852586	-1.554225
104	6	0	1.863264	3.237831	-1.588582
105	1	0	1.113543	3.894623	-1.130642
106	6	0	2.228857	3.833632	-2.979115
107	6	0	0.906587	4.097952	-3.744619
108	1	0	0.236678	4.730150	-3.151180
109	1	0	0.396934	3.156762	-3.954954
110	1	0	1.130146	4.606436	-4.689258
111	6	0	2.938681	5.188940	-2.737542
112	1	0	2.339466	5.834363	-2.084567
113	1	0	3.085704	5.696506	-3.697016
114	1	0	3.918551	5.036339	-2.273363
115	6	0	3.146367	2.913702	-3.815283
116	1	0	2.655989	1.955404	-3.993312
117	1	0	4.096800	2.730001	-3.307583

118	1	0	3.352519	3.395936	-4.778145
119	6	0	-2.296475	1.013709	-1.283493
120	6	0	-3.541920	1.908338	-1.207123
121	1	0	-4.295895	1.276036	-0.726626
122	6	0	-4.143182	2.419514	-2.550405
123	6	0	-4.714093	1.199136	-3.318079
124	1	0	-3.911747	0.513135	-3.591808
125	1	0	-5.217380	1.548332	-4.226744
126	1	0	-5.439604	0.658254	-2.699514
127	6	0	-5.312689	3.377078	-2.209138
128	1	0	-4.935910	4.308670	-1.773810
129	1	0	-6.003007	2.915761	-1.494413
130	1	0	-5.858293	3.621616	-3.126757
131	6	0	-3.115300	3.162712	-3.432819
132	1	0	-2.290167	2.498138	-3.693181
133	1	0	-2.708699	4.036366	-2.917047
134	1	0	-3.610060	3.497330	-4.352313
135	6	0	2.489071	-0.387519	2.926236
136	6	0	2.605046	1.008344	2.928031
137	6	0	1.479865	1.834178	2.834380
138	6	0	0.230272	1.234629	2.755978
139	6	0	0.104944	-0.181863	2.756043
140	6	0	1.235692	-0.996685	2.840753
141	7	0	-1.039423	1.798499	2.728276
142	6	0	-2.062307	0.834907	2.724565
143	6	0	-1.324054	-0.451937	2.799287
144	8	0	-3.274883	1.069658	2.677922
145	1	0	3.376945	-1.003959	2.984060
146	1	0	3.585492	1.460110	2.994533
147	1	0	1.580237	2.912345	2.818982
148	1	0	1.141330	-2.076414	2.831355
149	1	0	-1.236218	2.781587	2.584560
150	7	0	-1.868208	-1.622490	2.920081
151	7	0	-2.317710	-2.673112	3.040471

C6:



E= -4334.4405931 a.u. (E_{rel}=3.2 kcal/mol)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
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3	7	0	4.040277	-2.730479	-0.079679
4	8	0	2.273096	-4.287749	-0.047319
5	8	0	5.855686	-1.387237	0.556882
6	6	0	3.239109	-3.750131	0.488060
7	6	0	3.834065	-4.005286	1.836182
8	6	0	3.461574	-4.911902	2.812373
9	1	0	2.619084	-5.575794	2.660975
10	6	0	4.214936	-4.936705	3.997206
11	1	0	3.952031	-5.632849	4.784585
12	6	0	5.303810	-4.074603	4.175925
13	1	0	5.869587	-4.115812	5.098922
14	6	0	5.671698	-3.160252	3.175909
15	1	0	6.514395	-2.491517	3.302261
16	6	0	4.919280	-3.144676	2.014576
17	6	0	5.051451	-2.292717	0.793647
18	7	0	2.977988	3.200492	-0.622185
19	8	0	3.951260	1.173283	-1.285880
20	8	0	2.252419	4.985229	0.724400
21	6	0	3.903727	2.137241	-0.520010
22	6	0	4.733942	2.451163	0.678160
23	6	0	5.776982	1.738537	1.243797
24	1	0	6.087377	0.782977	0.836721
25	6	0	6.356869	2.270090	2.408734
26	1	0	7.177583	1.744368	2.882274
27	6	0	5.884030	3.459516	2.977288
28	1	0	6.349944	3.842591	3.877448
29	6	0	4.802518	4.151474	2.407093
30	1	0	4.411295	5.057773	2.853183
31	6	0	4.246963	3.628172	1.254228

32	6	0	3.052994	4.079407	0.475108
33	7	0	-3.245983	2.965470	-0.220343
34	8	0	-1.119303	3.601277	-0.978083
35	8	0	-5.183364	2.691565	1.078024
36	6	0	-2.025168	3.651926	-0.140631
37	6	0	-2.076541	4.413184	1.139565
38	6	0	-1.099773	5.199281	1.732737
39	1	0	-0.124493	5.329955	1.272561
40	6	0	-1.413301	5.771579	2.977877
41	1	0	-0.680595	6.392381	3.479328
42	6	0	-2.655212	5.544282	3.586108
43	1	0	-2.866187	5.996314	4.547891
44	6	0	-3.620600	4.722141	2.981240
45	1	0	-4.568783	4.514047	3.460759
46	6	0	-3.307837	4.163454	1.755385
47	6	0	-4.077371	3.196976	0.905575
48	7	0	-3.708205	-3.185466	0.083039
49	8	0	-4.003754	-1.016154	-0.745521
50	8	0	-3.838551	-5.128777	1.395611
51	6	0	-4.222015	-1.877799	0.111561
52	6	0	-5.050881	-1.793403	1.345274
53	6	0	-5.694898	-0.703920	1.908490
54	1	0	-5.623264	0.290704	1.484872
55	6	0	-6.404940	-0.930847	3.100082
56	1	0	-6.920076	-0.104111	3.573733
57	6	0	-6.441218	-2.196691	3.695714
58	1	0	-6.996324	-2.336982	4.615720
59	6	0	-5.747577	-3.280294	3.132528
60	1	0	-5.739202	-4.256178	3.602168
61	6	0	-5.057161	-3.051609	1.956676
62	6	0	-4.163971	-3.964138	1.182399
63	8	0	1.764272	-1.374739	-0.177442
64	8	0	1.662658	-1.470356	-2.463421
65	8	0	1.050591	1.377093	-0.359116
66	8	0	0.820418	1.276849	-2.637127
67	8	0	-1.714691	0.786916	-0.147525
68	8	0	-1.910731	0.534267	-2.413863
69	8	0	-1.190270	-2.039054	0.067952
70	8	0	-1.208467	-2.266226	-2.208604
71	6	0	2.277144	-1.628601	-1.337092
72	6	0	3.755311	-2.038888	-1.344502
73	1	0	4.295737	-1.083656	-1.261132
74	6	0	4.282173	-2.769561	-2.622141
75	6	0	5.710002	-3.288688	-2.320856

76	1	0	6.164081	-3.651460	-3.249271
77	1	0	5.683369	-4.115619	-1.603806
78	1	0	6.335937	-2.488645	-1.908930
79	6	0	3.378356	-3.946458	-3.054185
80	1	0	2.390710	-3.573921	-3.334391
81	1	0	3.256042	-4.671271	-2.246111
82	1	0	3.828602	-4.447384	-3.919115
83	6	0	4.375324	-1.727317	-3.766527
84	1	0	3.387674	-1.320892	-3.987567
85	1	0	4.776988	-2.210119	-4.664586
86	1	0	5.041809	-0.903841	-3.483287
87	6	0	1.210059	1.855528	-1.552792
88	6	0	1.866758	3.239804	-1.584831
89	1	0	1.118567	3.896815	-1.124741
90	6	0	2.232005	3.838069	-2.974349
91	6	0	3.148281	2.919046	-3.812851
92	1	0	4.099031	2.733902	-3.306252
93	1	0	3.353975	3.402853	-4.775019
94	1	0	2.657190	1.961356	-3.992173
95	6	0	2.943076	5.192309	-2.730448
96	1	0	3.922911	5.037979	-2.266772
97	1	0	2.344576	5.837043	-2.076133
98	1	0	3.090317	5.701539	-3.689011
99	6	0	0.909478	4.104933	-3.738543
100	1	0	0.239914	4.735477	-3.142972
101	1	0	0.399552	3.164456	-3.951378
102	1	0	1.132775	4.616127	-4.681780
103	6	0	-2.296151	1.017828	-1.283673
104	6	0	-3.541213	1.912860	-1.205739
105	1	0	-4.295055	1.280313	-0.725284
106	6	0	-4.143077	2.425677	-2.548029
107	6	0	-4.714896	1.206232	-3.316520
108	1	0	-5.440581	0.665323	-2.698178
109	1	0	-3.912981	0.519997	-3.590945
110	1	0	-5.218196	1.556404	-4.224801
111	6	0	-5.311951	3.383366	-2.205036
112	1	0	-6.002013	2.921555	-1.490375
113	1	0	-5.858025	3.629152	-3.122041
114	1	0	-4.934469	4.314301	-1.768909
115	6	0	-3.115406	3.169332	-3.430335
116	1	0	-2.290739	2.504642	-3.691879
117	1	0	-2.708075	4.042257	-2.913905
118	1	0	-3.610576	3.505127	-4.349175
119	6	0	-1.624844	-2.579376	-1.027761

120	6	0	-2.693624	-3.685465	-0.863292
121	1	0	-2.212086	-4.510674	-0.320441
122	6	0	-3.284673	-4.283309	-2.179669
123	6	0	-2.150481	-5.045691	-2.910143
124	1	0	-1.343091	-4.361913	-3.176586
125	1	0	-2.549689	-5.500318	-3.823563
126	1	0	-1.752087	-5.846273	-2.274270
127	6	0	-4.388054	-5.300804	-1.791869
128	1	0	-5.267644	-4.783119	-1.395068
129	1	0	-4.032422	-6.005879	-1.033670
130	1	0	-4.692038	-5.856663	-2.685596
131	6	0	-3.898149	-3.214352	-3.113179
132	1	0	-3.129844	-2.522548	-3.458189
133	1	0	-4.674514	-2.641438	-2.599746
134	1	0	-4.347891	-3.716135	-3.978096
135	6	0	2.494830	-0.378178	2.930055
136	6	0	2.606304	1.018027	2.933058
137	6	0	1.478549	1.840231	2.838893
138	6	0	0.230990	1.236725	2.759458
139	6	0	0.110042	-0.180094	2.758980
140	6	0	1.243343	-0.991297	2.843493
141	7	0	-1.040261	1.796874	2.730441
142	6	0	-2.060302	0.830468	2.725090
143	6	0	-1.318384	-0.454423	2.799783
144	8	0	-3.273451	1.061968	2.676963
145	1	0	3.384712	-0.991776	2.988061
146	1	0	3.584796	1.473661	3.001210
147	1	0	1.575578	2.918738	2.823459
148	1	0	1.152524	-2.071316	2.833307
149	1	0	-1.239699	2.779427	2.586978
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151	7	0	-2.308026	-2.677972	3.035932

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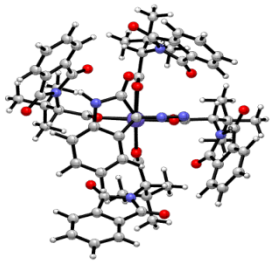

E= -4334.4451766 a.u. (E_{rel}=0.4 kcal/mol)

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
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5	8	0	5.648482	-0.824136	1.339431
6	6	0	3.115207	-3.006220	0.250781
7	6	0	3.284106	-3.448877	1.661423
8	6	0	2.570671	-4.392497	2.381867
9	1	0	1.734842	-4.928889	1.945297
10	6	0	2.947409	-4.591759	3.720808
11	1	0	2.415467	-5.321128	4.320010
12	6	0	3.992914	-3.859168	4.295562
13	1	0	4.260178	-4.035240	5.330895
14	6	0	4.688041	-2.888709	3.555868
15	1	0	5.480194	-2.298362	3.999218
16	6	0	4.312702	-2.699711	2.239270
17	6	0	4.807505	-1.717395	1.229035
18	7	0	2.546157	3.940381	-0.290270
19	8	0	3.666758	1.994575	-0.979500
20	8	0	1.715116	5.689359	1.041357
21	6	0	3.479038	2.887418	-0.152272
22	6	0	4.137692	3.103419	1.168500
23	6	0	5.059871	2.318056	1.839706
24	1	0	5.407415	1.371491	1.442209
25	6	0	5.478468	2.766011	3.105557
26	1	0	6.196932	2.176820	3.662044
27	6	0	4.966258	3.940267	3.669108
28	1	0	5.306530	4.255312	4.648267
29	6	0	3.995100	4.699922	2.994631
30	1	0	3.565163	5.592052	3.433801
31	6	0	3.597370	4.258779	1.744187
32	6	0	2.519718	4.776717	0.848000
33	7	0	-4.574473	1.310750	-0.435226
34	8	0	-3.399094	3.227836	-1.112659
35	8	0	-5.863448	-0.200593	0.820063
36	6	0	-4.224316	2.680360	-0.386354
37	6	0	-5.061646	3.254061	0.711920
38	6	0	-5.153756	4.554742	1.171919
39	1	0	-4.574892	5.347271	0.713867
40	6	0	-6.015191	4.802127	2.252795
41	1	0	-6.115727	5.809586	2.638644

42	6	0	-6.746570	3.763328	2.843138
43	1	0	-7.401992	3.980835	3.677963
44	6	0	-6.641669	2.446637	2.366240
45	1	0	-7.201882	1.635108	2.814476
46	6	0	-5.795616	2.219495	1.295454
47	6	0	-5.464905	0.944481	0.587226
48	7	0	-1.706305	-4.147216	-0.021866
49	8	0	-3.231104	-2.565337	-0.834834
50	8	0	-0.457253	-5.513950	1.421959
51	6	0	-2.841396	-3.315719	0.063660
52	6	0	-3.401292	-3.534270	1.425018
53	6	0	-4.495105	-2.943263	2.035024
54	1	0	-5.081450	-2.183156	1.528835
55	6	0	-4.779015	-3.337923	3.353685
56	1	0	-5.626082	-2.900936	3.868971
57	6	0	-3.983060	-4.280618	4.016029
58	1	0	-4.228469	-4.564646	5.032544
59	6	0	-2.863059	-4.850668	3.388695
60	1	0	-2.228070	-5.562930	3.901026
61	6	0	-2.591378	-4.459877	2.090363
62	6	0	-1.449263	-4.819650	1.194390
63	8	0	2.046361	-0.394447	-0.170494
64	8	0	2.144299	-0.433443	-2.457469
65	8	0	0.612406	2.079392	-0.242685
66	8	0	0.616132	2.038769	-2.534650
67	8	0	-1.949835	0.492119	-0.245622
68	8	0	-1.879690	0.369897	-2.534488
69	8	0	-0.372742	-1.877329	-0.136500
70	8	0	-0.259284	-1.996083	-2.420320
71	6	0	2.658986	-0.612689	-1.291961
72	6	0	4.105569	-1.093028	-1.110596
73	1	0	4.643188	-0.206743	-0.753239
74	6	0	4.853384	-1.621818	-2.368053
75	6	0	6.237455	-2.141242	-1.906495
76	1	0	6.846879	-2.380472	-2.784751
77	1	0	6.129254	-3.047106	-1.301414
78	1	0	6.758875	-1.384740	-1.308092
79	6	0	4.093456	-2.749744	-3.101194
80	1	0	3.121726	-2.387539	-3.441559
81	1	0	3.931660	-3.610107	-2.448231
82	1	0	4.681379	-3.069826	-3.969566
83	6	0	5.065516	-0.423856	-3.329326
84	1	0	4.102523	-0.039406	-3.669186
85	1	0	5.649018	-0.753608	-4.196223

86	1	0	5.610180	0.384233	-2.826633
87	6	0	0.862537	2.600878	-1.401733
88	6	0	1.490410	4.008845	-1.323798
89	1	0	0.729848	4.658623	-0.869315
90	6	0	1.930489	4.674365	-2.659930
91	6	0	2.910135	3.808041	-3.483359
92	1	0	3.810586	3.573244	-2.911049
93	1	0	3.200251	4.361157	-4.384388
94	1	0	2.432272	2.872028	-3.775515
95	6	0	2.604173	6.025778	-2.314750
96	1	0	3.567055	5.862060	-1.819978
97	1	0	1.969490	6.624802	-1.651132
98	1	0	2.781005	6.587829	-3.238166
99	6	0	0.649693	4.952267	-3.487553
100	1	0	-0.032020	5.611930	-2.936350
101	1	0	0.136085	4.016183	-3.715443
102	1	0	0.924038	5.447008	-4.425836
103	6	0	-2.512877	0.443764	-1.411464
104	6	0	-4.045295	0.347228	-1.407896
105	1	0	-4.238889	-0.636432	-0.961242
106	6	0	-4.771344	0.375875	-2.792215
107	6	0	-4.399447	-0.921504	-3.556944
108	1	0	-4.628711	-1.805649	-2.953152
109	1	0	-3.334390	-0.929219	-3.791107
110	1	0	-4.974071	-0.966970	-4.488948
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112	1	0	-6.569973	-0.461278	-1.852189
113	1	0	-6.826446	0.225679	-3.476811
114	1	0	-6.629120	1.302622	-2.080512
115	6	0	-4.415270	1.609929	-3.652332
116	1	0	-3.344367	1.624931	-3.859613
117	1	0	-4.685608	2.541766	-3.149898
118	1	0	-4.964201	1.552017	-4.599946
119	6	0	-0.433617	-2.524653	-1.261419
120	6	0	-0.686567	-4.028944	-1.080842
121	1	0	0.238157	-4.396837	-0.618814
122	6	0	-0.949509	-4.880360	-2.353274
123	6	0	0.352466	-4.884751	-3.195443
124	1	0	0.579465	-3.876848	-3.546614
125	1	0	0.222446	-5.546670	-4.058932
126	1	0	1.197936	-5.244770	-2.598027
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129	1	0	-0.469073	-6.692085	-1.213018

130	1	0	-1.292635	-6.986115	-2.767461
131	6	0	-2.125283	-4.355092	-3.206040
132	1	0	-1.924618	-3.335107	-3.538264
133	1	0	-3.059435	-4.358700	-2.638691
134	1	0	-2.245400	-5.000932	-4.083810
135	6	0	-2.652282	2.606893	2.989684
136	6	0	-1.849245	3.751662	3.036495
137	6	0	-0.457778	3.669967	2.906741
138	6	0	0.105605	2.412012	2.743915
139	6	0	-0.706866	1.259261	2.640119
140	6	0	-2.086432	1.346329	2.764280
141	7	0	1.450970	2.040886	2.674203
142	6	0	1.636058	0.668872	2.524114
143	6	0	0.215842	0.147022	2.382167
144	8	0	2.704534	0.058165	2.546863
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146	1	0	-2.311935	4.722041	3.171677
147	1	0	0.157902	4.561067	2.897625
148	1	0	-2.707159	0.463273	2.670510
149	1	0	2.234567	2.682030	2.696765
150	7	0	-0.038340	-1.136072	2.571971
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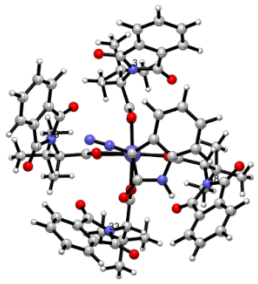
C8:



E= -4334.4444109 a.u. (E_{rel}=0.8 kcal/mol)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
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4	8	0	2.767962	-3.973853	-0.937893
5	8	0	5.789933	-0.879237	0.761052
6	6	0	3.652428	-3.507260	-0.224849
7	6	0	4.344220	-4.113158	0.955841

8	6	0	4.203931	-5.369075	1.520027
9	1	0	3.508919	-6.088846	1.104358
10	6	0	4.996876	-5.671094	2.639117
11	1	0	4.916546	-6.645660	3.105633
12	6	0	5.894435	-4.730567	3.160109
13	1	0	6.494121	-4.988983	4.024592
14	6	0	6.029355	-3.461731	2.575214
15	1	0	6.723869	-2.728434	2.966456
16	6	0	5.244501	-3.178326	1.471491
17	6	0	5.174203	-1.940579	0.634306
18	7	0	2.611648	3.663425	-0.092602
19	8	0	3.751084	1.771303	-0.862705
20	8	0	1.771519	5.369817	1.284969
21	6	0	3.589655	2.654324	-0.015834
22	6	0	4.317259	2.897011	1.260291
23	6	0	5.352194	2.181518	1.836598
24	1	0	5.730946	1.276260	1.374591
25	6	0	5.841366	2.648135	3.069055
26	1	0	6.652682	2.118897	3.554589
27	6	0	5.292575	3.778905	3.685431
28	1	0	5.691358	4.114470	4.635462
29	6	0	4.221308	4.473825	3.099443
30	1	0	3.773339	5.334427	3.580936
31	6	0	3.750682	4.012959	1.884352
32	6	0	2.598822	4.485149	1.055574
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35	8	0	-5.189041	2.053986	1.515095
36	6	0	-2.322335	3.636836	0.242795
37	6	0	-2.379272	4.215060	1.611927
38	6	0	-1.482977	5.050532	2.255826
39	1	0	-0.556442	5.361879	1.784893
40	6	0	-1.797693	5.432500	3.570889
41	1	0	-1.123434	6.086570	4.110882
42	6	0	-2.962187	4.974640	4.198352
43	1	0	-3.178132	5.286540	5.213478
44	6	0	-3.843073	4.101658	3.539397
45	1	0	-4.730169	3.718159	4.028121
46	6	0	-3.528883	3.735196	2.245068
47	6	0	-4.210650	2.778924	1.322530
48	7	0	-3.443931	-3.310902	-0.313172
49	8	0	-3.999825	-1.105065	-0.885830
50	8	0	-3.263727	-5.355923	0.830616
51	6	0	-4.061022	-2.062142	-0.112395

52	6	0	-4.783908	-2.172925	1.189626
53	6	0	-5.483473	-1.210668	1.903096
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55	6	0	-6.052091	-1.611433	3.125570
56	1	0	-6.600274	-0.887478	3.716272
57	6	0	-5.918283	-2.925100	3.594426
58	1	0	-6.374812	-3.203795	4.536634
59	6	0	-5.187498	-3.879232	2.867581
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61	6	0	-4.621525	-3.474253	1.671197
62	6	0	-3.720259	-4.218969	0.737622
63	8	0	1.804727	-1.012860	-0.240258
64	8	0	1.739060	-0.871648	-2.528264
65	8	0	0.831813	1.661097	-0.129496
66	8	0	0.711684	1.801019	-2.412455
67	8	0	-1.874409	0.771945	-0.112440
68	8	0	-1.987085	0.868415	-2.397891
69	8	0	-1.090786	-1.960001	-0.233719
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74	6	0	4.570744	-1.505870	-2.797879
75	6	0	6.068622	-1.803371	-2.535542
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78	1	0	6.514030	-1.034353	-1.894057
79	6	0	3.946105	-2.669855	-3.601107
80	1	0	2.901567	-2.448106	-3.826419
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82	1	0	4.497652	-2.790441	-4.541171
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85	1	0	5.021205	-0.313188	-4.559704
86	1	0	4.908482	0.644041	-3.058775
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88	6	0	1.552808	3.710572	-1.113129
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90	6	0	1.940099	4.468982	-2.416869
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92	1	0	3.892488	3.523034	-2.737351
93	1	0	3.192711	4.297633	-4.176173
94	1	0	2.550155	2.740899	-3.593623
95	6	0	2.537777	5.837785	-2.005335

96	1	0	3.514029	5.706406	-1.527011
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109	1	0	-4.013773	0.858728	-3.559046
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113	1	0	-6.236752	3.681929	-2.625366
114	1	0	-5.364398	4.207933	-1.168466
115	6	0	-3.481316	3.515396	-3.031226
116	1	0	-2.588201	2.982330	-3.361671
117	1	0	-3.171309	4.362045	-2.413864
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122	6	0	-3.021918	-4.085231	-2.709644
123	6	0	-1.852956	-4.649017	-3.557541
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125	1	0	-2.244025	-5.026554	-4.508770
126	1	0	-1.360938	-5.478892	-3.034717
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128	1	0	-4.916682	-4.850645	-1.922552
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131	6	0	-3.751195	-2.967223	-3.488286
132	1	0	-3.056887	-2.163312	-3.733231
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137	6	0	-1.297884	-3.582878	3.094499
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139	6	0	0.156454	-1.708348	2.556141

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142	6	0	-1.491559	0.061730	2.615596
143	6	0	-0.038305	-0.272395	2.310751
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145	1	0	1.957560	-4.553777	2.747541
146	1	0	-0.290770	-5.472015	3.251196
147	1	0	-2.276316	-3.989827	3.309490
148	1	0	2.239530	-2.135066	2.242470
149	1	0	-3.065859	-1.299830	2.949772
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151	7	0	1.639933	1.511085	2.577303

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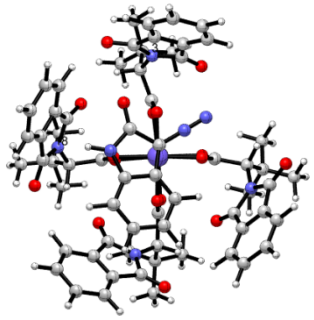

E= -4334.4430481 a.u. (E_{rel}=1.7 kcal/mol)

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6	6	0	3.891094	-3.140423	0.497037
7	6	0	4.415925	-3.229382	1.893204
8	6	0	4.204090	-4.198276	2.857933
9	1	0	3.577210	-5.057477	2.653034
10	6	0	4.828236	-4.022054	4.102904
11	1	0	4.686451	-4.760468	4.883054
12	6	0	5.633483	-2.903460	4.350992
13	1	0	6.104661	-2.791181	5.320286
14	6	0	5.836008	-1.926911	3.363017
15	1	0	6.453115	-1.055954	3.545839
16	6	0	5.213625	-2.111509	2.141961
17	6	0	5.229719	-1.260363	0.914918

18	7	0	2.197589	3.641627	-0.739654
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20	8	0	1.000671	5.355637	0.329654
21	6	0	3.272802	2.769100	-0.434768
22	6	0	3.787185	3.225812	0.887240
23	6	0	4.797787	2.697569	1.671965
24	1	0	5.337690	1.810723	1.360885
25	6	0	5.044444	3.328838	2.903113
26	1	0	5.829385	2.949920	3.546485
27	6	0	4.280778	4.423963	3.326330
28	1	0	4.492930	4.884351	4.284064
29	6	0	3.233361	4.923194	2.533540
30	1	0	2.624745	5.759380	2.856334
31	6	0	3.008645	4.307017	1.313530
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37	6	0	-2.989898	4.125758	0.657062
38	6	0	-2.265621	5.230398	1.069975
39	1	0	-1.317394	5.485529	0.608780
40	6	0	-2.782876	5.965097	2.150611
41	1	0	-2.251697	6.841799	2.501980
42	6	0	-3.974123	5.583823	2.781481
43	1	0	-4.354821	6.177558	3.604363
44	6	0	-4.673915	4.436089	2.372521
45	1	0	-5.582397	4.119324	2.870554
46	6	0	-4.157769	3.719264	1.308347
47	6	0	-4.621395	2.437913	0.688254
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51	6	0	-3.715289	-2.671084	0.301156
52	6	0	-4.377395	-2.583873	1.634196
53	6	0	-5.219115	-1.608229	2.145454
54	1	0	-5.467392	-0.711658	1.586344
55	6	0	-5.699953	-1.801367	3.452055
56	1	0	-6.365177	-1.064784	3.886992
57	6	0	-5.332355	-2.925242	4.202938
58	1	0	-5.720299	-3.044868	5.207482
59	6	0	-4.459255	-3.890973	3.677283
60	1	0	-4.153824	-4.754604	4.255225
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66	8	0	0.562099	1.219335	-2.759382
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68	8	0	-1.990167	-0.017429	-2.456692
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72	6	0	4.069561	-1.349614	-1.314232
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74	6	0	4.809636	-1.915333	-2.566336
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76	1	0	6.877404	-2.304865	-3.105857
77	1	0	6.447277	-2.890802	-1.484535
78	1	0	6.696921	-1.151213	-1.757549
79	6	0	4.235878	-3.270439	-3.039097
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82	1	0	4.834410	-3.642838	-3.878724
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84	1	0	3.643171	-0.715287	-3.966802
85	1	0	5.234016	-1.227221	-4.586510
86	1	0	5.122519	0.089734	-3.392707
87	6	0	0.844786	1.899650	-1.702373
88	6	0	1.218385	3.383805	-1.806546
89	1	0	0.308365	3.905023	-1.481795
90	6	0	1.603068	3.937620	-3.209662
91	6	0	2.721601	3.125176	-3.899040
92	1	0	3.630293	3.106529	-3.292890
93	1	0	2.951797	3.583839	-4.867915
94	1	0	2.393488	2.096589	-4.061533
95	6	0	2.064307	5.404591	-3.022655
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97	1	0	1.324119	5.976616	-2.450727
98	1	0	2.191929	5.872082	-4.005004
99	6	0	0.326722	3.930147	-4.090480
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103	6	0	-2.452054	0.424402	-1.336475
104	6	0	-3.853305	1.047421	-1.276549
105	1	0	-4.446893	0.324062	-0.709162

106	6	0	-4.586090	1.298268	-2.629221
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113	1	0	-6.538358	2.038405	-3.229897
114	1	0	-5.782933	3.001469	-1.943861
115	6	0	-3.777211	2.189642	-3.598309
116	1	0	-2.811401	1.731202	-3.814470
117	1	0	-3.605871	3.183290	-3.175111
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134	1	0	-3.726795	-4.782981	-3.664519
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136	6	0	-2.311737	2.212982	3.802922
137	6	0	-1.002316	2.603489	3.493800
138	6	0	-0.123504	1.639287	3.022818
139	6	0	-0.551396	0.301331	2.845420
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146	1	0	-3.007401	2.957193	4.167439
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149	1	0	1.769457	2.601520	2.668049

150	7	0	0.794824	-1.731163	2.402543
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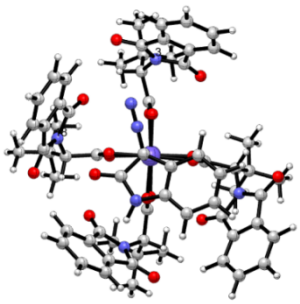
C10:



E= -4334.4424423 a.u. (E_{rel}=2.1 kcal/mol)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
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2	45	0	0.006546	-0.307805	-2.555965
3	7	0	4.011276	-2.767369	-0.089113
4	8	0	2.227193	-4.258228	-0.447582
5	8	0	5.746783	-1.549230	0.917261
6	6	0	3.146193	-3.833411	0.249518
7	6	0	3.598888	-4.287755	1.599944
8	6	0	3.121763	-5.312594	2.397410
9	1	0	2.296158	-5.932862	2.070103
10	6	0	3.747807	-5.515972	3.637609
11	1	0	3.401630	-6.309778	4.288670
12	6	0	4.815736	-4.707205	4.045748
13	1	0	5.281884	-4.886004	5.007300
14	6	0	5.288837	-3.669949	3.226571
15	1	0	6.113585	-3.037862	3.532093
16	6	0	4.663093	-3.480555	2.007551
17	6	0	4.925529	-2.468603	0.939508
18	7	0	3.047257	3.263571	-0.300181
19	8	0	4.077727	1.248382	-0.917174
20	8	0	2.190833	5.041637	0.968212
21	6	0	3.886622	2.148661	-0.094453
22	6	0	4.435205	2.311125	1.280852
23	6	0	5.309584	1.499392	1.984383
24	1	0	5.683571	0.574685	1.558638
25	6	0	5.648085	1.903398	3.286911
26	1	0	6.330301	1.297809	3.871745

27	6	0	5.114340	3.071281	3.845061
28	1	0	5.394362	3.356694	4.852304
29	6	0	4.211200	3.869354	3.124246
30	1	0	3.775749	4.762635	3.554520
31	6	0	3.885220	3.467010	1.842611
32	6	0	2.935487	4.067286	0.858625
33	7	0	-3.133433	3.081920	-0.234775
34	8	0	-0.998511	3.796987	-0.905358
35	8	0	-4.999601	2.538666	1.083888
36	6	0	-1.896399	3.750345	-0.063814
37	6	0	-1.945219	4.333965	1.304918
38	6	0	-0.967841	5.021397	2.004104
39	1	0	0.013735	5.198323	1.579605
40	6	0	-1.285985	5.421887	3.313931
41	1	0	-0.549896	5.963042	3.895701
42	6	0	-2.523718	5.111445	3.889901
43	1	0	-2.734793	5.429675	4.903933
44	6	0	-3.487295	4.372913	3.180131
45	1	0	-4.438656	4.105413	3.624099
46	6	0	-3.173479	3.997014	1.884726
47	6	0	-3.930630	3.134226	0.924327
48	7	0	-3.639116	-3.064093	-0.225089
49	8	0	-3.911517	-0.875346	-1.021190
50	8	0	-3.777937	-5.006454	1.089547
51	6	0	-4.193876	-1.772188	-0.223187
52	6	0	-5.176112	-1.755823	0.899266
53	6	0	-5.959046	-0.718734	1.378277
54	1	0	-5.872700	0.288442	0.985103
55	6	0	-6.820727	-1.010140	2.449133
56	1	0	-7.452676	-0.227163	2.851265
57	6	0	-6.874908	-2.293536	3.008680
58	1	0	-7.558189	-2.490063	3.826605
59	6	0	-6.043977	-3.322039	2.535226
60	1	0	-6.056080	-4.310859	2.977784
61	6	0	-5.198719	-3.024270	1.481825
62	6	0	-4.158078	-3.868649	0.820892
63	8	0	1.800230	-1.296500	-0.205521
64	8	0	1.831014	-1.262101	-2.493649
65	8	0	1.176447	1.462873	-0.329657
66	8	0	1.001196	1.500073	-2.611357
67	8	0	-1.625674	0.935895	-0.226980
68	8	0	-1.747863	0.751567	-2.511538
69	8	0	-1.132229	-1.900310	-0.095455
70	8	0	-1.059844	-2.059014	-2.380805

71	6	0	2.380225	-1.488823	-1.351143
72	6	0	3.854881	-1.903826	-1.268446
73	1	0	4.372242	-0.971088	-0.997362
74	6	0	4.518136	-2.446864	-2.571714
75	6	0	5.934211	-2.957775	-2.206740
76	1	0	6.481121	-3.190116	-3.126941
77	1	0	5.876153	-3.867859	-1.600696
78	1	0	6.490501	-2.198824	-1.644803
79	6	0	3.707401	-3.585858	-3.230508
80	1	0	2.729791	-3.214448	-3.544515
81	1	0	3.554407	-4.417194	-2.538037
82	1	0	4.250232	-3.950821	-4.110269
83	6	0	4.664684	-1.261851	-3.561413
84	1	0	3.681503	-0.885350	-3.847184
85	1	0	5.195105	-1.602130	-4.458045
86	1	0	5.233931	-0.444840	-3.102987
87	6	0	1.380656	2.006037	-1.489368
88	6	0	2.078204	3.368703	-1.403486
89	1	0	1.298941	4.040938	-1.019462
90	6	0	2.629249	3.984216	-2.719947
91	6	0	3.567945	3.028648	-3.489934
92	1	0	4.424919	2.735923	-2.878883
93	1	0	3.931344	3.533797	-4.392620
94	1	0	3.027581	2.125481	-3.781160
95	6	0	3.392957	5.279496	-2.348596
96	1	0	4.313025	5.044246	-1.803884
97	1	0	2.774033	5.930092	-1.719446
98	1	0	3.659701	5.819166	-3.263840
99	6	0	1.416872	4.360076	-3.610231
100	1	0	0.744819	5.043297	-3.077752
101	1	0	0.858314	3.463950	-3.885830
102	1	0	1.774098	4.855461	-4.520004
103	6	0	-2.161518	1.201614	-1.379334
104	6	0	-3.398111	2.108515	-1.308603
105	1	0	-4.183659	1.457880	-0.908193
106	6	0	-3.928193	2.717821	-2.639413
107	6	0	-4.491982	1.559883	-3.503215
108	1	0	-5.254357	0.999054	-2.949687
109	1	0	-3.691347	0.874428	-3.783763
110	1	0	-4.949276	1.973804	-4.409001
111	6	0	-5.088370	3.679340	-2.281672
112	1	0	-5.827743	3.180180	-1.643940
113	1	0	-5.581491	4.010950	-3.201721
114	1	0	-4.711739	4.560411	-1.752331

115	6	0	-2.846489	3.484081	-3.433007
116	1	0	-2.026798	2.812636	-3.693994
117	1	0	-2.440786	4.314826	-2.851316
118	1	0	-3.291917	3.880576	-4.353037
119	6	0	-1.511302	-2.409359	-1.222828
120	6	0	-2.562098	-3.537332	-1.116578
121	1	0	-2.089852	-4.351871	-0.551048
122	6	0	-3.076618	-4.140322	-2.461436
123	6	0	-1.884542	-4.850688	-3.151600
124	1	0	-1.094458	-4.133053	-3.376903
125	1	0	-2.227781	-5.310864	-4.084800
126	1	0	-1.481321	-5.641393	-2.506585
127	6	0	-4.157479	-5.202579	-2.136549
128	1	0	-5.067397	-4.725662	-1.756949
129	1	0	-3.802108	-5.916720	-1.386296
130	1	0	-4.412875	-5.744166	-3.053829
131	6	0	-3.686542	-3.079152	-3.405911
132	1	0	-2.935081	-2.339692	-3.681727
133	1	0	-4.525986	-2.563856	-2.930817
134	1	0	-4.053374	-3.578650	-4.310382
135	6	0	-2.126227	-2.579012	3.480070
136	6	0	-3.145746	-1.670687	3.783478
137	6	0	-2.969227	-0.292842	3.606229
138	6	0	-1.745059	0.155637	3.132961
139	6	0	-0.714392	-0.761742	2.822092
140	6	0	-0.895924	-2.127557	2.987007
141	7	0	-1.291974	1.460211	2.913150
142	6	0	0.034095	1.512618	2.482037
143	6	0	0.404402	0.050797	2.329210
144	8	0	0.719905	2.522400	2.314485
145	1	0	-2.297556	-3.642047	3.599455
146	1	0	-4.099951	-2.035372	4.139928
147	1	0	-3.770079	0.400496	3.829791
148	1	0	-0.113612	-2.826625	2.715145
149	1	0	-1.855484	2.298369	3.001565
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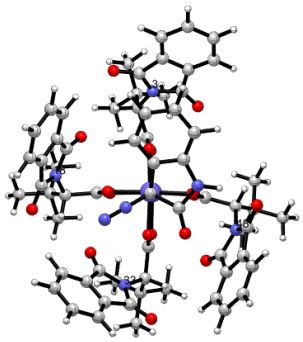
151	7	0	2.774989	-0.608747	2.317954

C11:



E= -4334.4409739 a.u. (E_{rel}=3.0 kcal/mol)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
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3	7	0	4.680218	-1.020063	-0.542988
4	8	0	3.640125	-3.059200	-1.066352
5	8	0	5.908309	0.646127	0.573387
6	6	0	4.466962	-2.412716	-0.427667
7	6	0	5.448423	-2.870424	0.603937
8	6	0	5.706714	-4.141186	1.083609
9	1	0	5.159337	-4.997615	0.709381
10	6	0	6.699362	-4.275562	2.067950
11	1	0	6.932807	-5.256856	2.463707
12	6	0	7.396461	-3.157536	2.544126
13	1	0	8.161211	-3.288820	3.300475
14	6	0	7.119073	-1.872094	2.051147
15	1	0	7.650910	-0.999993	2.412017
16	6	0	6.140761	-1.756255	1.080515
17	6	0	5.613318	-0.538566	0.390482
18	7	0	1.362781	4.189065	-0.169463
19	8	0	3.022589	2.751888	-0.992174
20	8	0	-0.006373	5.413110	1.295805
21	6	0	2.573080	3.467738	-0.094268
22	6	0	3.122951	3.741012	1.260816
23	6	0	4.280599	3.264435	1.853906
24	1	0	4.934782	2.571302	1.334033
25	6	0	4.536456	3.679026	3.172425
26	1	0	5.430939	3.332027	3.675892
27	6	0	3.651591	4.526904	3.850774
28	1	0	3.876564	4.827433	4.867203
29	6	0	2.470943	4.980395	3.239703
30	1	0	1.771098	5.619343	3.764202

31	6	0	2.227595	4.572644	1.940427
32	6	0	1.048144	4.823654	1.053671
33	7	0	-4.306060	1.676713	0.026938
34	8	0	-2.565505	3.103836	-0.629537
35	8	0	-5.963934	0.582038	1.279083
36	6	0	-3.417937	2.757445	0.192728
37	6	0	-3.743753	3.342121	1.522847
38	6	0	-3.149821	4.399963	2.190085
39	1	0	-2.289852	4.915897	1.776018
40	6	0	-3.670522	4.731061	3.451998
41	1	0	-3.234789	5.551821	4.009064
42	6	0	-4.735204	4.011291	4.007940
43	1	0	-5.114195	4.290164	4.984048
44	6	0	-5.307524	2.923776	3.327694
45	1	0	-6.116088	2.347079	3.759685
46	6	0	-4.793126	2.607438	2.083634
47	6	0	-5.145209	1.493625	1.149251
48	7	0	-2.458488	-4.011053	0.009240
49	8	0	-3.789669	-2.364292	-1.016541
50	8	0	-1.339398	-5.149942	1.730730
51	6	0	-3.550958	-3.109397	-0.063708
52	6	0	-4.283148	-3.261622	1.225230
53	6	0	-5.413250	-2.612466	1.687836
54	1	0	-5.894123	-1.825428	1.121059
55	6	0	-5.866008	-2.948212	2.975054
56	1	0	-6.747260	-2.457916	3.370706
57	6	0	-5.186232	-3.884512	3.761288
58	1	0	-5.558773	-4.122292	4.750608
59	6	0	-4.010031	-4.494832	3.297102
60	1	0	-3.450490	-5.187644	3.913686
61	6	0	-3.581235	-4.164990	2.026145
62	6	0	-2.336481	-4.550553	1.309601
63	8	0	1.976150	-0.452029	-0.278224
64	8	0	1.824674	-0.441080	-2.565070
65	8	0	0.245404	1.817481	-0.167815
66	8	0	0.066505	1.831238	-2.453246
67	8	0	-2.085986	0.188272	-0.078478
68	8	0	-2.222090	0.130277	-2.363916
69	8	0	-0.453850	-2.186291	-0.105701
70	8	0	-0.620535	-2.252212	-2.388202
71	6	0	2.497367	-0.404285	-1.463632
72	6	0	4.010974	-0.150967	-1.518003
73	1	0	4.116504	0.863503	-1.111859
74	6	0	4.683585	-0.156743	-2.930295

75	6	0	6.210158	0.028849	-2.733543
76	1	0	6.680400	0.182010	-3.710814
77	1	0	6.658287	-0.859062	-2.274713
78	1	0	6.422322	0.895852	-2.098004
79	6	0	4.426990	-1.455039	-3.729192
80	1	0	3.357299	-1.584217	-3.899092
81	1	0	4.804713	-2.334001	-3.200713
82	1	0	4.938929	-1.383661	-4.696435
83	6	0	4.150274	1.063702	-3.725308
84	1	0	3.084442	0.948313	-3.924674
85	1	0	4.688523	1.136138	-4.677193
86	1	0	4.300428	1.988835	-3.159407
87	6	0	0.219241	2.418814	-1.319578
88	6	0	0.338621	3.945984	-1.203046
89	1	0	-0.605800	4.246072	-0.731993
90	6	0	0.497310	4.769076	-2.509997
91	6	0	1.696352	4.319865	-3.373115
92	1	0	2.638717	4.433130	-2.831653
93	1	0	1.735406	4.936617	-4.278760
94	1	0	1.584275	3.272494	-3.658371
95	6	0	0.672862	6.254686	-2.108592
96	1	0	1.635232	6.410160	-1.610147
97	1	0	-0.126572	6.572308	-1.428588
98	1	0	0.642141	6.879946	-3.007489
99	6	0	-0.818697	4.624747	-3.317752
100	1	0	-1.679240	4.929099	-2.710888
101	1	0	-0.961574	3.587842	-3.626165
102	1	0	-0.770555	5.261937	-4.207861
103	6	0	-2.731151	0.316368	-1.196775
104	6	0	-4.214920	0.686144	-1.057014
105	1	0	-4.687722	-0.217773	-0.657845
106	6	0	-4.982037	1.076012	-2.357314
107	6	0	-5.069913	-0.178322	-3.264861
108	1	0	-5.499520	-1.024397	-2.717426
109	1	0	-4.076309	-0.462718	-3.612190
110	1	0	-5.706029	0.045884	-4.128682
111	6	0	-6.418172	1.488782	-1.947151
112	1	0	-6.883074	0.722431	-1.316839
113	1	0	-7.025786	1.625650	-2.848205
114	1	0	-6.406514	2.432685	-1.392217
115	6	0	-4.317072	2.238251	-3.128097
116	1	0	-3.302927	1.964482	-3.422961
117	1	0	-4.269524	3.143734	-2.517816
118	1	0	-4.906298	2.453245	-4.027519

119	6	0	-0.776889	-2.765214	-1.217794
120	6	0	-1.373896	-4.165225	-0.986155
121	1	0	-0.608005	-4.714916	-0.422503
122	6	0	-1.729424	-5.013336	-2.238764
123	6	0	-0.401514	-5.285029	-2.992430
124	1	0	0.042808	-4.344727	-3.326303
125	1	0	-0.601568	-5.913879	-3.866859
126	1	0	0.312754	-5.809943	-2.345861
127	6	0	-2.314173	-6.361810	-1.754276
128	1	0	-3.272496	-6.211132	-1.247210
129	1	0	-1.625768	-6.862745	-1.062393
130	1	0	-2.477260	-7.016683	-2.617047
131	6	0	-2.733487	-4.328634	-3.194789
132	1	0	-2.332395	-3.375145	-3.540258
133	1	0	-3.691081	-4.143111	-2.704461
134	1	0	-2.900672	-4.984413	-4.057397
135	6	0	3.701496	-0.632979	3.204749
136	6	0	3.680165	-2.018888	3.391038
137	6	0	2.495449	-2.751674	3.246017
138	6	0	1.333128	-2.065485	2.922090
139	6	0	1.359985	-0.665908	2.719385
140	6	0	2.534297	0.057228	2.856204
141	7	0	0.024357	-2.536561	2.784998
142	6	0	-0.888814	-1.517034	2.521287
143	6	0	-0.015849	-0.282309	2.380848
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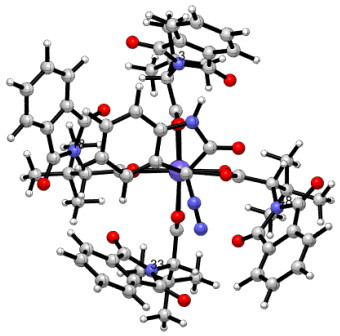
146	1	0	4.596430	-2.539371	3.639618
147	1	0	2.484314	-3.824025	3.395860
148	1	0	2.557964	1.124913	2.673920
149	1	0	-0.246262	-3.514832	2.692590
150	7	0	-0.502873	0.938424	2.538148
151	7	0	-0.915449	1.999293	2.609247

C12:



E= -4334.4397362 a.u. (E_{rel}=3.8 kcal/mol)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.295355	-0.285676	-0.111835
2	45	0	-0.576491	-0.299843	-2.517689
3	7	0	3.438985	-3.124807	-0.445060
4	8	0	1.503081	-4.460724	-0.301913
5	8	0	5.467617	-2.055124	0.056910
6	6	0	2.554244	-4.041373	0.171995
7	6	0	3.193482	-4.370690	1.485597
8	6	0	2.751447	-5.198674	2.504673
9	1	0	1.812427	-5.732179	2.417494
10	6	0	3.561314	-5.308297	3.647964
11	1	0	3.246840	-5.943729	4.467027
12	6	0	4.770889	-4.608152	3.744297
13	1	0	5.377458	-4.714277	4.635615
14	6	0	5.205061	-3.771354	2.702926
15	1	0	6.138827	-3.225542	2.765111
16	6	0	4.394583	-3.665905	1.585806
17	6	0	4.560583	-2.837199	0.351117
18	7	0	3.179679	2.864195	-0.732667
19	8	0	3.740459	0.725171	-1.503934
20	8	0	2.978906	4.764932	0.633997
21	6	0	3.955828	1.686452	-0.763186
22	6	0	5.029493	1.896120	0.250262
23	6	0	6.062223	1.057748	0.631015
24	1	0	6.143500	0.055691	0.226110
25	6	0	6.950951	1.540021	1.606984
26	1	0	7.779658	0.919105	1.926594
27	6	0	6.782300	2.807903	2.177884
28	1	0	7.488831	3.156316	2.922254
29	6	0	5.703423	3.628376	1.807594
30	1	0	5.550336	4.600713	2.260269

31	6	0	4.840048	3.149119	0.839824
32	6	0	3.583955	3.746333	0.287520
33	7	0	-2.992003	3.373062	0.164902
34	8	0	-0.926255	3.840381	-0.852838
35	8	0	-4.645732	2.999235	1.790933
36	6	0	-1.672785	3.876044	0.127997
37	6	0	-1.403713	4.408465	1.492497
38	6	0	-0.252462	4.985629	2.005664
39	1	0	0.647851	5.097767	1.408612
40	6	0	-0.282798	5.375161	3.355942
41	1	0	0.595428	5.830351	3.797880
42	6	0	-1.424226	5.177045	4.142981
43	1	0	-1.414963	5.486908	5.181168
44	6	0	-2.572775	4.568436	3.611470
45	1	0	-3.452577	4.391106	4.217788
46	6	0	-2.537731	4.191609	2.280883
47	6	0	-3.556283	3.467747	1.457425
48	7	0	-4.180499	-2.698605	0.235599
49	8	0	-4.408018	-0.451717	-0.401865
50	8	0	-4.189478	-4.694515	1.471234
51	6	0	-4.542202	-1.355257	0.429415
52	6	0	-5.109507	-1.285928	1.807282
53	6	0	-5.586485	-0.194357	2.515035
54	1	0	-5.543672	0.809913	2.108016
55	6	0	-6.070237	-0.434899	3.811805
56	1	0	-6.450671	0.392461	4.398842
57	6	0	-6.059262	-1.722105	4.362687
58	1	0	-6.439070	-1.875673	5.365874
59	6	0	-5.548833	-2.812643	3.640284
60	1	0	-5.515147	-3.808898	4.063768
61	6	0	-5.078250	-2.567563	2.363444
62	6	0	-4.449596	-3.498172	1.379213
63	8	0	1.335770	-1.515754	-0.353135
64	8	0	1.095595	-1.487415	-2.633159
65	8	0	0.979095	1.311288	-0.345350
66	8	0	0.631087	1.352023	-2.613404
67	8	0	-1.838843	1.035610	-0.024495
68	8	0	-2.191273	0.969153	-2.286873
69	8	0	-1.674603	-1.793621	-0.031564
70	8	0	-1.853138	-1.910356	-2.309974
71	6	0	1.742576	-1.776684	-1.553726
72	6	0	3.150557	-2.377315	-1.677806
73	1	0	3.814165	-1.501289	-1.625658
74	6	0	3.479468	-3.144204	-3.000105

75	6	0	4.838201	-3.863368	-2.811701
76	1	0	5.166680	-4.268703	-3.774830
77	1	0	4.747905	-4.692236	-2.102173
78	1	0	5.599549	-3.166519	-2.442419
79	6	0	2.390933	-4.173961	-3.380694
80	1	0	1.447513	-3.661297	-3.581440
81	1	0	2.225413	-4.894191	-2.576177
82	1	0	2.702849	-4.711038	-4.284070
83	6	0	3.635615	-2.100228	-4.135790
84	1	0	2.699689	-1.559480	-4.279385
85	1	0	3.904316	-2.613914	-5.065793
86	1	0	4.427275	-1.382138	-3.890767
87	6	0	1.148953	1.814772	-1.527407
88	6	0	1.989922	3.097035	-1.563086
89	1	0	1.389125	3.828349	-1.011096
90	6	0	2.305172	3.709445	-2.962912
91	6	0	3.013254	2.718695	-3.914513
92	1	0	3.967685	2.381402	-3.500931
93	1	0	3.207777	3.220518	-4.869802
94	1	0	2.379941	1.848195	-4.088696
95	6	0	3.214059	4.945573	-2.746126
96	1	0	4.207277	4.641592	-2.398742
97	1	0	2.780377	5.629428	-2.007583
98	1	0	3.331164	5.478319	-3.696093
99	6	0	0.970552	4.185341	-3.591494
100	1	0	0.449963	4.875025	-2.918588
101	1	0	0.318331	3.332494	-3.782041
102	1	0	1.180279	4.699605	-4.536125
103	6	0	-2.446951	1.412742	-1.110253
104	6	0	-3.547249	2.451125	-0.847806
105	1	0	-4.319826	1.887231	-0.312273
106	6	0	-4.218953	3.128110	-2.072260
107	6	0	-4.996949	2.033778	-2.848477
108	1	0	-5.709152	1.523822	-2.189540
109	1	0	-4.305757	1.292764	-3.253036
110	1	0	-5.549426	2.498705	-3.672614
111	6	0	-5.230473	4.170456	-1.535039
112	1	0	-5.910266	3.714123	-0.805782
113	1	0	-5.820330	4.567001	-2.368425
114	1	0	-4.710033	5.003399	-1.051358
115	6	0	-3.211221	3.821451	-3.015993
116	1	0	-2.494494	3.094448	-3.402279
117	1	0	-2.659336	4.610245	-2.499279
118	1	0	-3.757624	4.266291	-3.855941

119	6	0	-2.225903	-2.230822	-1.117982
120	6	0	-3.388816	-3.217495	-0.894085
121	1	0	-2.942975	-4.139199	-0.493999
122	6	0	-4.226335	-3.617563	-2.146859
123	6	0	-3.316542	-4.461114	-3.076121
124	1	0	-2.460699	-3.869863	-3.406720
125	1	0	-3.890232	-4.780385	-3.953378
126	1	0	-2.957514	-5.357373	-2.554897
127	6	0	-5.401994	-4.505481	-1.666992
128	1	0	-6.133578	-3.908855	-1.112317
129	1	0	-5.046950	-5.311550	-1.015335
130	1	0	-5.902298	-4.942793	-2.537819
131	6	0	-4.787925	-2.402065	-2.919704
132	1	0	-3.972931	-1.786893	-3.303261
133	1	0	-5.416932	-1.781019	-2.277425
134	1	0	-5.391808	-2.764235	-3.760096
135	6	0	2.611934	2.045005	3.131674
136	6	0	3.589379	1.070267	3.355489
137	6	0	3.293565	-0.293865	3.240685
138	6	0	1.996275	-0.658897	2.906945
139	6	0	1.013147	0.328031	2.669242
140	6	0	1.309011	1.678057	2.774530
141	7	0	1.420344	-1.926483	2.793202
142	6	0	0.049203	-1.886157	2.523497
143	6	0	-0.219130	-0.399623	2.331192
144	8	0	-0.721956	-2.840747	2.494169
145	1	0	2.865603	3.094968	3.206020
146	1	0	4.598905	1.373311	3.602252
147	1	0	4.052449	-1.045509	3.417037
148	1	0	0.559246	2.431080	2.567519
149	1	0	1.920750	-2.806149	2.849270
150	7	0	-1.429962	0.097733	2.555481
151	7	0	-2.470638	0.545471	2.668062
