Supporting Information:

Theoretical study on NHC-catalysed enantioselective cycloaddition of ketenes and 3-aroylcoumarins: Mechanism and enantioselectivity.

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Table S1. B3LYP/6-31G* total energies (*E*, au), thermal correction to *H* (au, 298.15 K) and *S* (Cal/Mol-Kelvin, 298.15 K) of all species involved in the reaction of ketene **2** and chromenone **3** catalysed with the NHC **1**,in gas phase. Mechanism A and Mechanism B.

	Gas phase[a]		
species	*E*	Thermal correction to *H*	*S*
1	-1166.617606	0.422919	159.3
2	-422.969910	0.153264	93.3
3	-841.403004	0.233622	122.3
4-*SS*	-1264.393454	0.391135	159.8
TS1-*E*	-1589.577026	0.577045	209.9
IN1-*E*	-1589.622161	0.579279	203.4
TS1-*Z*	-1589.581265	0.577289	209.7
IN1-*Z*	-1589.624082	0.579731	199.8
TS3-*SS*-a1	-2430.998353	0.813989	269.4
IN2-*SS*-a1	-2431.005380	0.815878	269.8
TS5-*SS*-a1	-2430.986043	0.814516	263.5
TS3-*SS*-a2	-2430.992827	0.814597	270.5
IN3-*SS*-a2	-2431.002036	0.816632	263.8
TS5-*SS*-a2	-2430.993319	0.815013	268.1
TS6-*R*	-2008.010884	0.657561	230.1
IN4-*R*	-2008.020740	0.657651	228.7
TS7-*RZ*	-2430.981774	0.813116	271.1
IN5-*RZ*	-2430.990549	0.815136	270.2
TS8-*RZ*	-2430.984936	0.814622	262.4
IN6-*RZ*	-2431.011111	0.816950	264.0
TS9-*RZ*	-2430.972047	0.815218	259.7
TS6-*S*	-2008.010325	0.657450	228.8
IN4-*S*	-2008.020712	0.658387	227.0
TS7-*SZ*	-2430.987184	0.812861	271.6
IN5-*SZ*	-2431.011779	0.815222	266.1
TS8-*SZ*	-2430.978679	0.813338	262.4
IN6-*SZ*	-2430.989860	0.815786	264.1
TS9-*SZ*	-2430.984245	0.814667	264.5
1-4-*SS*[b]	-2431.019811	0.816453	280.3
TS10-*SS*	-2430.987449	0.814878	260.8
IN7-*SS*	-2430.988294	0.815699	265.3
TS11-*SS*	-2430.987443	0.814831	261.9

[a] Structures fully optimized.
[b] Molecular complex between **1** and **4-*SS***

Table S2. B3LYP/6-31G* total energies (*E* and *H*, au), *S* (Cal/Mol-Kelvin, 298.15 K) and relative energies (Δ*G*, kcal/mol) of species involved in the reaction of **2** and **3** catalysed with the NHC **1**, in gas phase. Mechanism A

	Gas phase			
species	*E*	*H*[a]	*S*	Δ*G*[b]
TS1-*E*	-1589.577026	-1588.999981	209.9	19.8[c]
TS1-*Z*	-1589.624082	-1589.003976	209.7	17.4[c]
1-2-3[d]	-2430.991332	-2430.180714	318.3	0.0
TS1-*Z* + 3[e]	-2430.984421	-2430.176469	272.7	16.2
IN1-*Z* + 3[e]	-2431.025150	-2430.213112	281.0	-9.3
TS3-*SS*-a1	-2430.998353	-2430.184364	269.4	12.2
IN2-*SS*-a1	-2431.005380	-2430.189502	269.8	8.9
TS5-*SS*-a1	-2430.986043	-2430.171527	263.5	22.0
TS3-*SS*-a2	-2430.992827	-2430.178230	270.5	15.7
IN3-*SS*-a2	-2431.002036	-2430.185404	263.8	13.2
TS5-*SS*-a2	-2430.993319	-2430.178306	268.1	16.4
TS10-*SS*	-2430.987449	-2430.172571	260.8	22.2
IN7-*SS*	-2430.988294	-2430.172595	265.3	20.8
TS11-*SS*	-2430.987443	-2430.172612	261.9	21.8
1-4-*SS*	-2431.019811	-2430.203358	280.3	-3.0

[a] *H*=*E* + thermal correction to *H*.
[b] from **1-2-3**, Δ*G*=Δ*H* - TΔ*S*
[c] from **1**+**2**
[d] Reading made by placing **1**, **2** and **3** in the same matrix at a distance of about 10 Å
[e] Reading made by placing **TS1-*Z*** or **IN1-*Z*** and **3** in the same matrix at a distance of about 10 Å

Table S3. B3LYP/6-31G* total energies (*E* and *H*, au), *S* (Cal/Mol-Kelvin, 298.15 K) and relative energies (Δ*G*, kcal/mol) of species involved in the reaction of ketene **2** and chromenone **3** catalysed with the NHC **1**, in gas phase. Mechanism B

	Gas phase			
species	*E*	*H*[a]	*S*	Δ*G*[b]
1-2-3[c]	-2430.991332	-2430.180714	318.3	0.0
TS6-*R* + 2[d]	-2430.980827	-2430.172885	266.3	20.3
IN4-*R* + 2[d]	-2430.990527	-2430.181419	278.0	11.5
TS7-*RZ*	-2430.981774	-2430.168658	271.1	21.5
IN5-*RZ*	-2430.990549	-2430.175413	270.2	17.6
TS8-*RZ*	-2430.984936	-2430.170314	262.4	23.1
IN6-*RZ*	-2431.011111	-2430.194161	264.0	7.7
TS9-*RZ*	-2430.972047	-2430.156829	259.7	32.4
TS6-*S* + 2[d]	-2430.980364	-2430.171589	274.8	18.6
IN4-*S* + 2[d]	-2430.990627	-2430.180003	286.2	9.9
TS7-*SZ*	-2430.987184	-2430.174323	271.6	17.8
IN5-*SZ*	-2431.011779	-2430.196557	266.1	5.5
TS8-*SZ*	-2430.978679	-2430.165341	262.4	26.2
IN6-*SZ*	-2430.989860	-2430.174074	264.1	20.2
TS9-*SZ*	-2430.984245	-2430.169578	264.5	22.9
1-4-*SS*	-2431.019811	-2430.203358	280.3	-3.0

[a] *H*=*E* + thermal correction to *H*.
[b] from **1-2-3**, Δ*G*=Δ*H* - TΔ*S*
[c] Reading made by placing **1**, **2** and **3** in the same matrix at a distance of about 10 Å
[d] Reading made by placing **TS6-*R*** , **IN4-*R*** , **TS6-*S*** , **IN4-*S*** and **2** in the same matrix at a distance of about 10 Å

Table S4. MPWB1K/6-311G** in toluene//B3LYP/6-31G* in gas phase. Total energies (*E* and *H*, au), *S* (Cal/Mol-Kelvin, 298.15 K) and relative energies (Δ*G*, kcal/mol) of species involved in the reaction of ketene **2** and chromenone **3** catalysed with the NHC **1**. Mechanism A (channel A2) and Mechanism B (channel B2).

	MPWB1K/6-311G** in toluene//B3LYP/6-31G* in gas phase			
species	*E*	*H*[a]	*S*	Δ*G*[b]
1-2-3[c]	-2430.399228	-2429.580070	269.7	0.0
TS1-*Z* + 3[d]	-2430.369267	-2429.550819	266.3	19.4
IN1-*Z* + 3[d]	-2430.414700	-2429.595350	248.8	-3.3
TS3-*SS*-a2	-2430.400206	-2429.579915	240.4	8.8
IN3-*SS*-a2	-2430.419474	-2429.597559	234.6	-0.5
TS5-*SS*-a2	-2430.404178	-2429.582999	233.3	9.0
TS6-*S* + 2[e]	-2430.372148	-2429.554252	247.2	22.9
IN4-*S* + 2[e]	-2430.388874	-2429.569830	261.0	9.0
TS7-*SZ*	-2430.387311	-2429.569348	242.4	14.9
IN5-*SZ*	-2430.421156	-2429.600290	238.3	-3.3
TS8-*SZ*	-2430.396944	-2429.578900	234.2	11.3
IN6-*SZ*	-2430.415497	-2429.594212	236.3	1.1
TS9-*SZ*	-2430.402052	-2429.581764	237.7	8.5
1-4-*SS*	-2430.428364	-2429.606114	244.2	-8.7
TS8-enant	-2430.403942	-2429.584491	232.9	8.2

[a] *H*=*E* + thermal correction to *H*.
[b] from **1-2-3**, Δ*G*=Δ*H* - TΔ*S*
[c] Reading made by placing **1**, **2** and **3** in the same matrix at a distance of about 10 Å
[d] Reading made by placing **TS1-*Z*** or **IN1-*Z*** and **3** in the same matrix at a distance of about 10 Å
[e] Reading made by placing **TS6-*S*** or **IN4-*S*** and **2** in the same matrix at a distance of about 10 Å

Table S5. MPWB1K/6-311G** total energies (*E*, au), thermal correction to *H* (au, 298.15 K) and *S* (Cal/Mol-Kelvin, 298.15 K) of species involved in the reaction of ketene **2** and chromenone **3** catalysed with the NHC **1**,in toluene. Mechanism A2-*SS* and mechanism A2-*RR* (enantiomer).

	MPWB1K/6-311G** [a]		
species	*E*	Thermal correction to *H*	*S*
1	-1166.334752	0.429196	146.6
2	-422.855746	0.154754	90.4
3	-841.208412	0.236754	116.2
4	-1264.106597	0.396602	148.2
TS1-*Z*	-1589.184339	0.585615	190.6
IN1-*Z*	-1589.232971	0.588082	185.0
TS3-*SS*-a2	-2430.425300	0.826445	242.3
IN3-*SS*-a2	-2430.445984	0.828297	237.2
TS5-*SS*-a2	-2430.430617	0.827006	239.2
1-4-*SS*[b]	-2430.452815	0.827719	244.3
TS3-*RR*-a2	-2430.421948	0.826477	240.0
IN3-*RR*-a2	-2430.448822	0.828265	236.6
TS5-*RR*-a2	-2430.435854	0.827162	238.4
1-4-*RR*[b]	-2430.453025	0.826204	240.5

[a] Structures fully optimized.
[b] Molecular complex between **1** and **4**

Table S6. MPWB1K/6-311G** total energies (*E* and *H*, au), *S* (Cal/Mol-Kelvin, 298.15 K) and relative energies (Δ*G*, kcal/mol) of species involved in the reaction of ketene **2** and chromenone **3** catalysed with the NHC **1**, in toluene. Mechanism A2-*SS* and mechanism A2-*RR* (enantiomer).

	MPWB1K/6-311G**			
species	*E*	*H*[a]	*S*	Δ*G*[b]
1-2-3[c]	-2430.399228	-2429.580070	269.7	0.0
TS1-*Z* + 3[d]	-2430.392773	-2429.572130	234.9	15.4
IN1-*Z* + 3[d]	-2430.440524	-2429.615455	242.9	-14.2
TS3-*SS*-a2	-2430.425300	-2429.598855	242.3	-3.6
IN3-*SS*-a2	-2430.445984	-2429.617687	237.2	-13.9
TS5-*SS*-a2	-2430.430617	-2429.603611	239.2	-5.7
1-4-*SS*	-2430.452815	-2429.625096	244.3	-20.7
TS3-*RR*-a2	-2430.421948	-2429.595471	240.0	-0.8
IN3-*RR*-a2	-2430.448822	-2429.620557	236.6	-15.5
TS5-*RR*-a2	-2430.435854	-2429.608692	238.4	-8.6
1-4-*RR*	-2430.453025	-2429.626821	240.5	-20.6

[a] *H*=*E* + thermal correction to *H*.
[b] from **1-2-3**, Δ*G*=Δ*H* - TΔ*S*
[c] Reading made by placing **1**, **2** and **3** in the same matrix at a distance of about 10 Å
[d] Reading made by placing **TS1-*Z*** or **IN1-*Z*** and **3** in the same matrix at a distance of about 10 Å

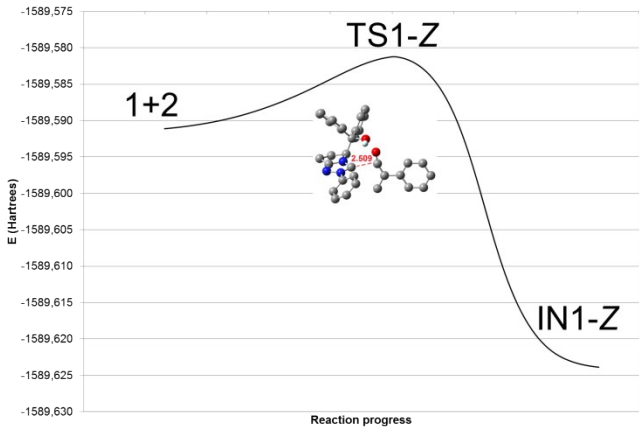


Figure S1. Energy profile (IRC, *E*) corresponding to the transition structure **TS1-*Z*** in **gas-phase**

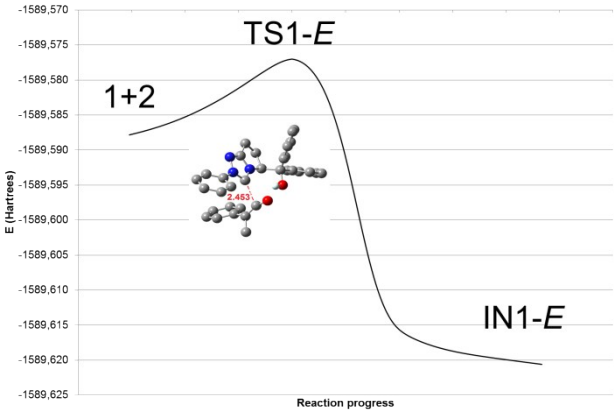


Figure S2. Energy profile (IRC, *E*) corresponding to the transition structure **TS1-*E*** in **gas-phase**

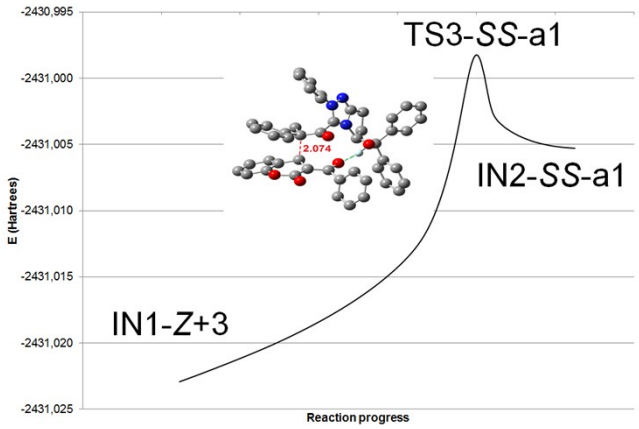


Figure S3. Energy profile (IRC, *E*) corresponding to the transition structure **TS3-*SS*-a1** in **gas-phase**

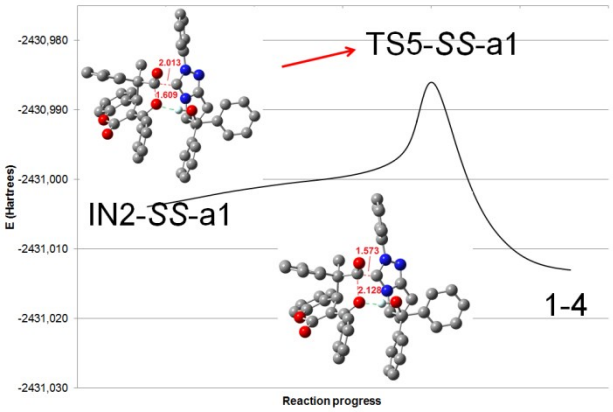


Figure S4. Energy profile (IRC, *E*) corresponding to the transition structure **TS5-*SS*-a1** in **gas-phase**

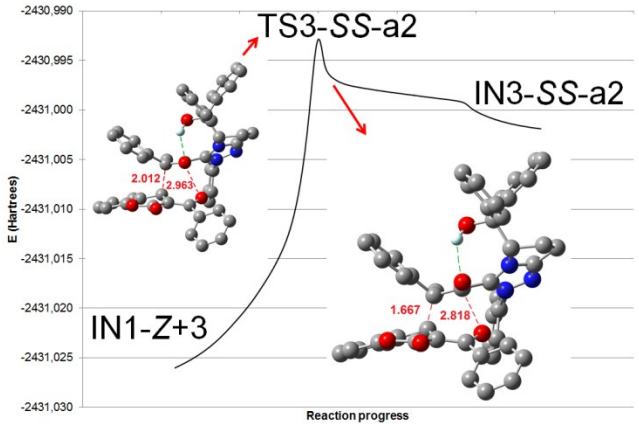


Figure S5. Energy profile (IRC, *E*) corresponding to the transition structure **TS3-*SS*-a2** in **gas-phase**

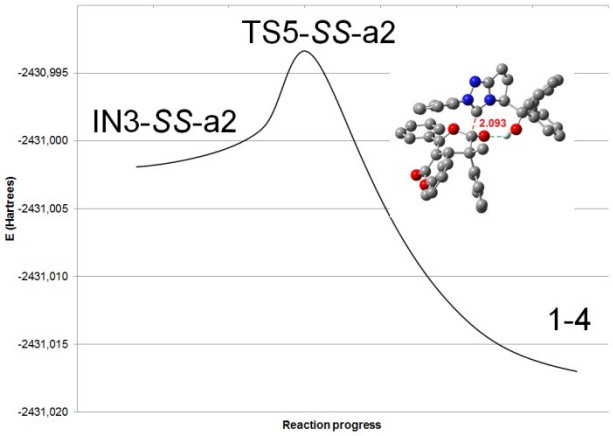


Figure S6. Energy profile (IRC, *E*) corresponding to the transition structure **TS5-*SS*-a2** in **gas-phase**

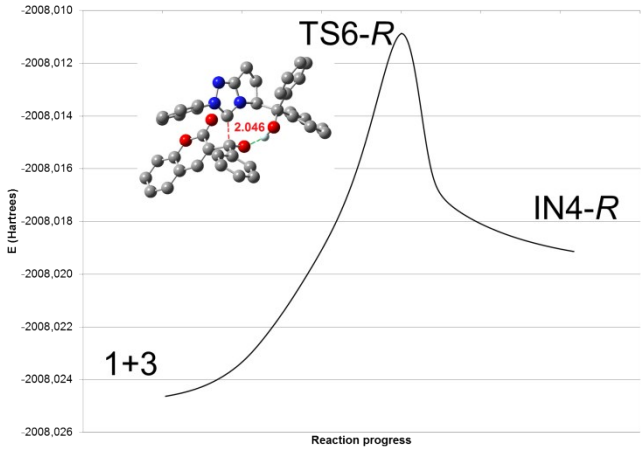


Figure S7. Energy profile (IRC, *E*) corresponding to the transition structure **TS6-*R*** in **gas-phase**

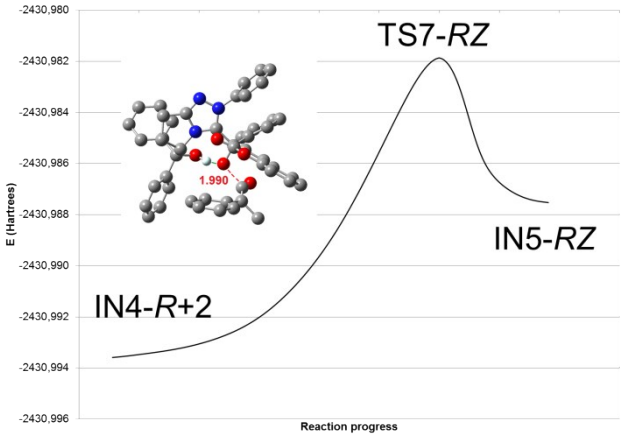


Figure S8. Energy profile (IRC, *E*) corresponding to the transition structure **TS7-*RZ*** in **gas-phase**

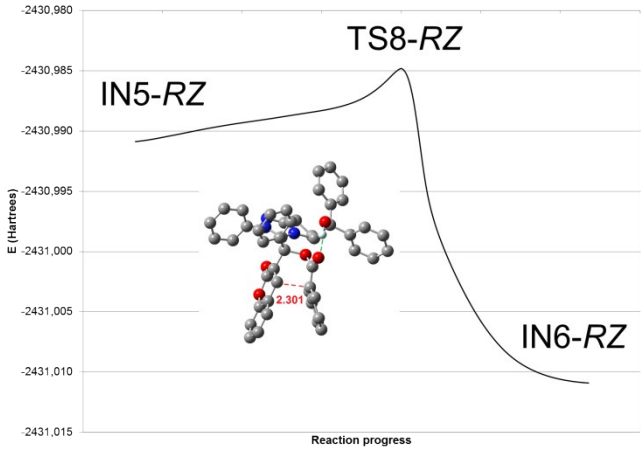


Figure S9. Energy profile (IRC, *E*) corresponding to the transition structure **TS8-*RZ*** in **gas-phase**

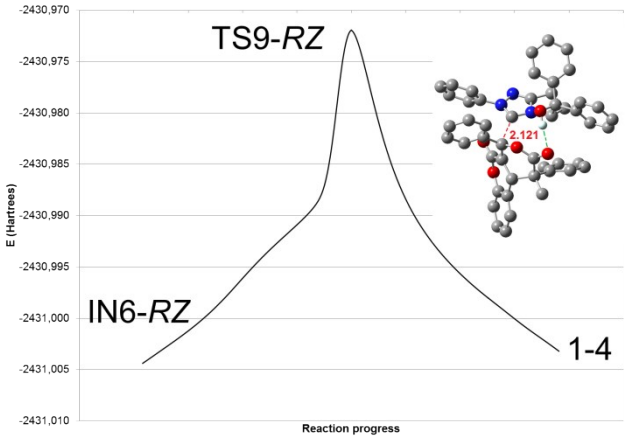


Figure S10. Energy profile (IRC, *E*) corresponding to the transition structure **TS9-*RZ*** in **gas-phase**

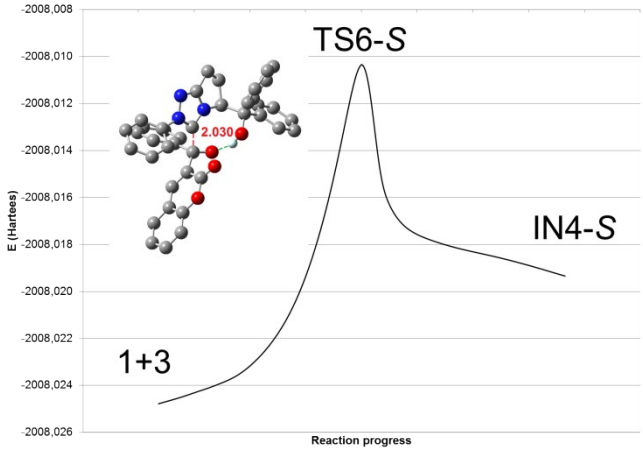


Figure S11. Energy profile (IRC, *E*) corresponding to the transition structure **TS6-*S*** in **gas-phase**

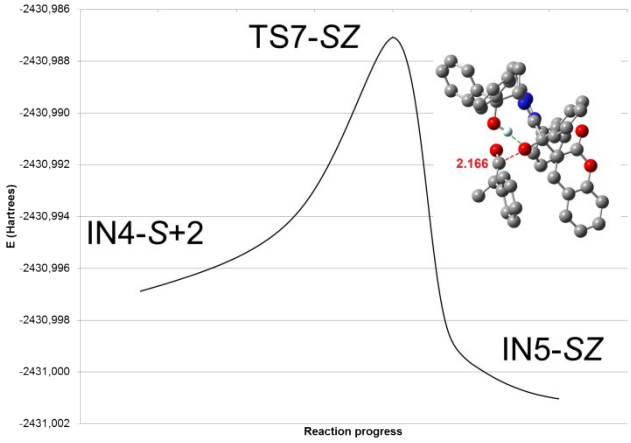


Figure S12. Energy profile (IRC, *E*) corresponding to the transition structure **TS7-*SZ*** in **gas-phase**

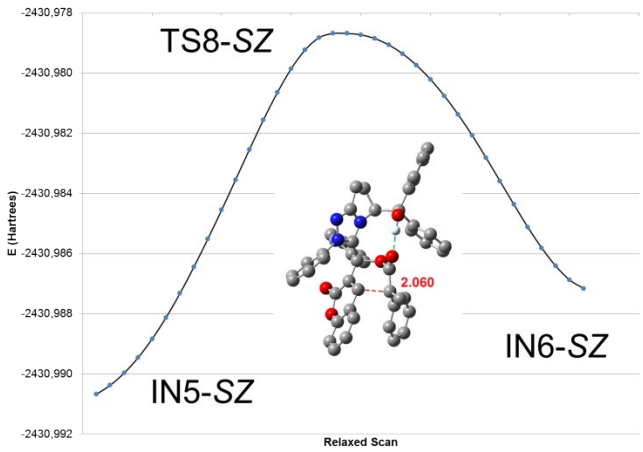


Figure S13. Energy profile (Relaxed Scan, *E*) corresponding to the **TS8-*SZ*** in **gas-phase**

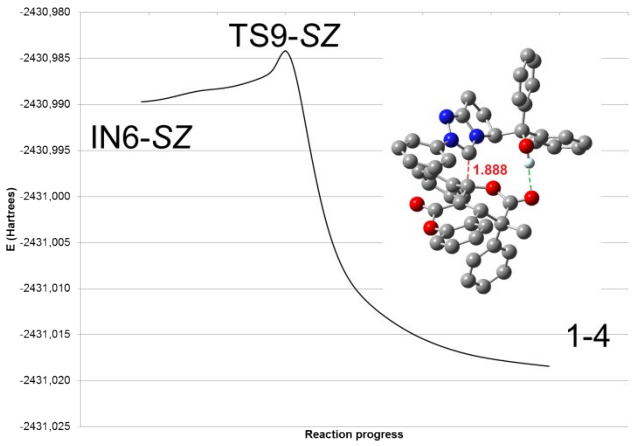


Figure S14. Energy profile (IRC, *E*) corresponding to the transition structure **TS9-*SZ*** in **gas-phase**

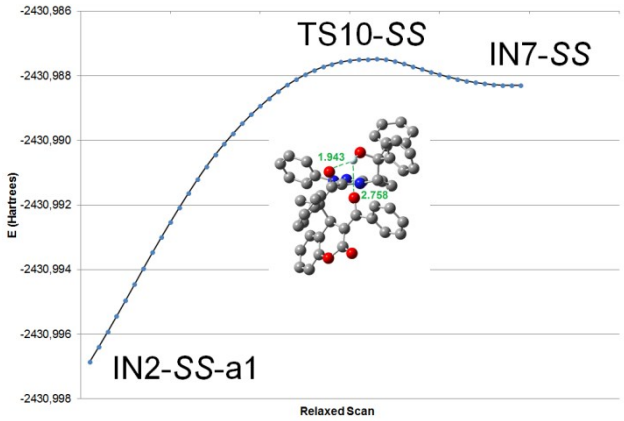


Figure S15. Energy profile (Relaxed Scan, *E*) corresponding to the **TS10-*SS*** in **gas-phase**

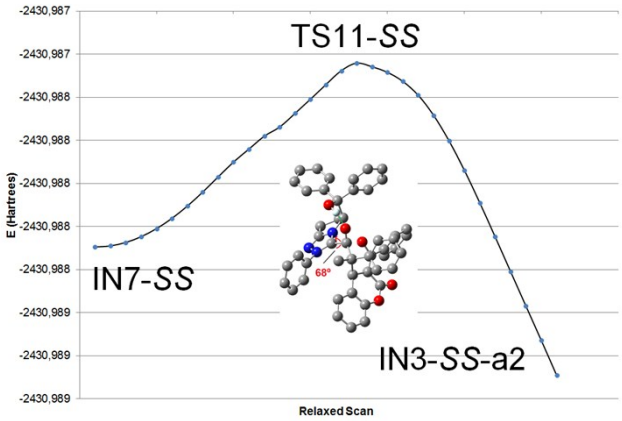


Figure S16. Energy profile (Relaxed Scan, *E*) corresponding to the **TS11-*SS*** in **gas-phase**

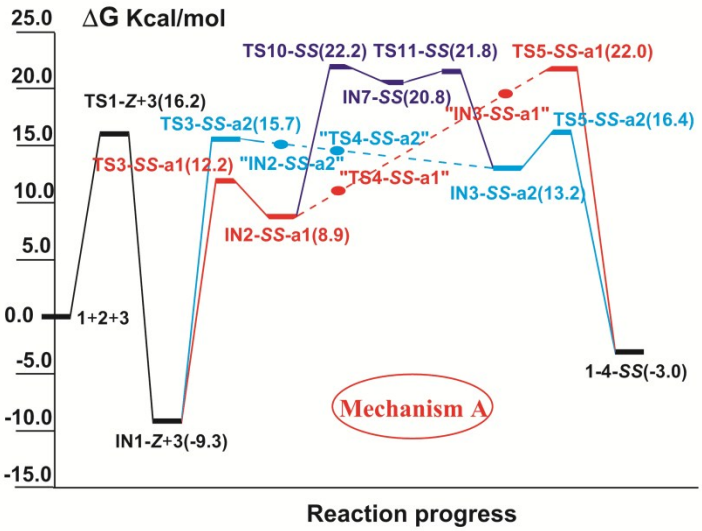
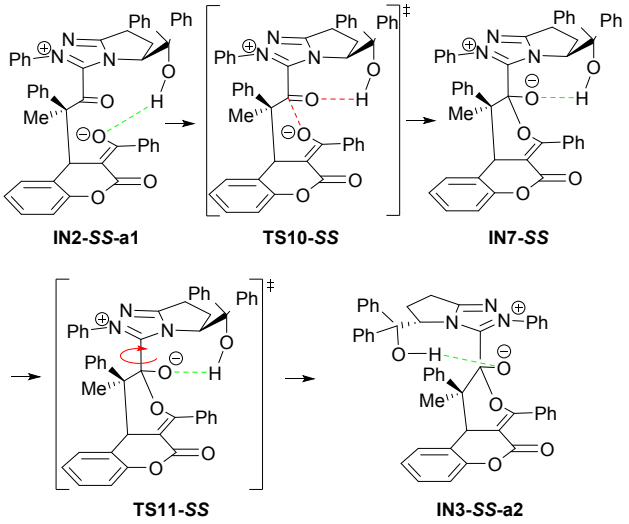


Figure S17. Free energy profile (ΔG in kcal mol^{-1}) at B3LYP/6-31G* level of species involved in the reaction of ketene **2** and chromenone **3** catalysed with the NHC **1**, in gas phase. Mechanism A: channel A1 (in red), channel A2 (in blue), channel A3 (in deep blue).

Channel A3

This channel corresponds to the conversion of intermediate **IN2-*SS*-a1** to intermediate **IN3-*SS*-a2**.



Scheme S1. Conversion of intermediate **IN2-*SS*-a1** to intermediate **IN3-*SS*-a2**.

As it was shown in Scheme S1 and Figure S17, the conversion proceeds through **TS10-*SS***, **IN7-*SS*** and **TS11-*SS***. **TS10-*SS*** corresponds to the exchange of the hydrogen bond between the hydroxyl group of NHC and the O3 to the oxygen of carbonyl C2=O to give **IN7-*SS***. Simultaneously, the closure of the O3-C2 bond occurs. In the **TS11-*SS***, the dihedral angle C2-NHC is turned to finally give the intermediate **IN3-*SS*-a2**.

The Gibbs free energy barriers via **TS10-*SS*** and **TS11-*SS*** from **1**+**2**+**3** are 22.2 and 21.8 kcal mol^{-1}, respectively (Table S1 and Table S2). The energy of both TSs is similar to the energy of the **TS5-*SS*-a1.**

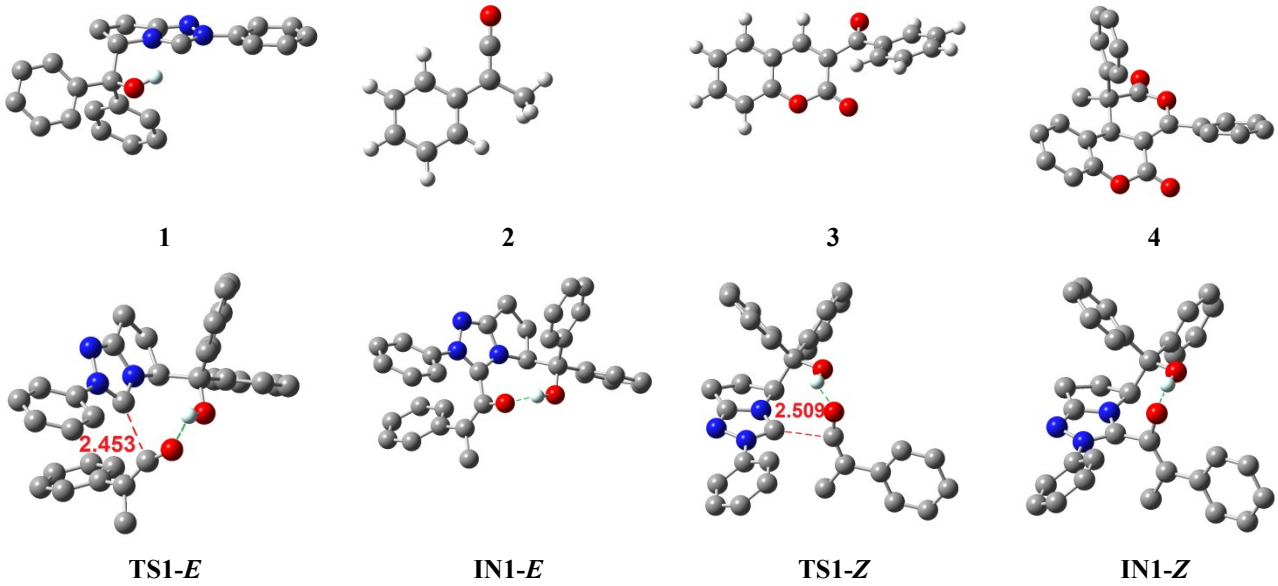
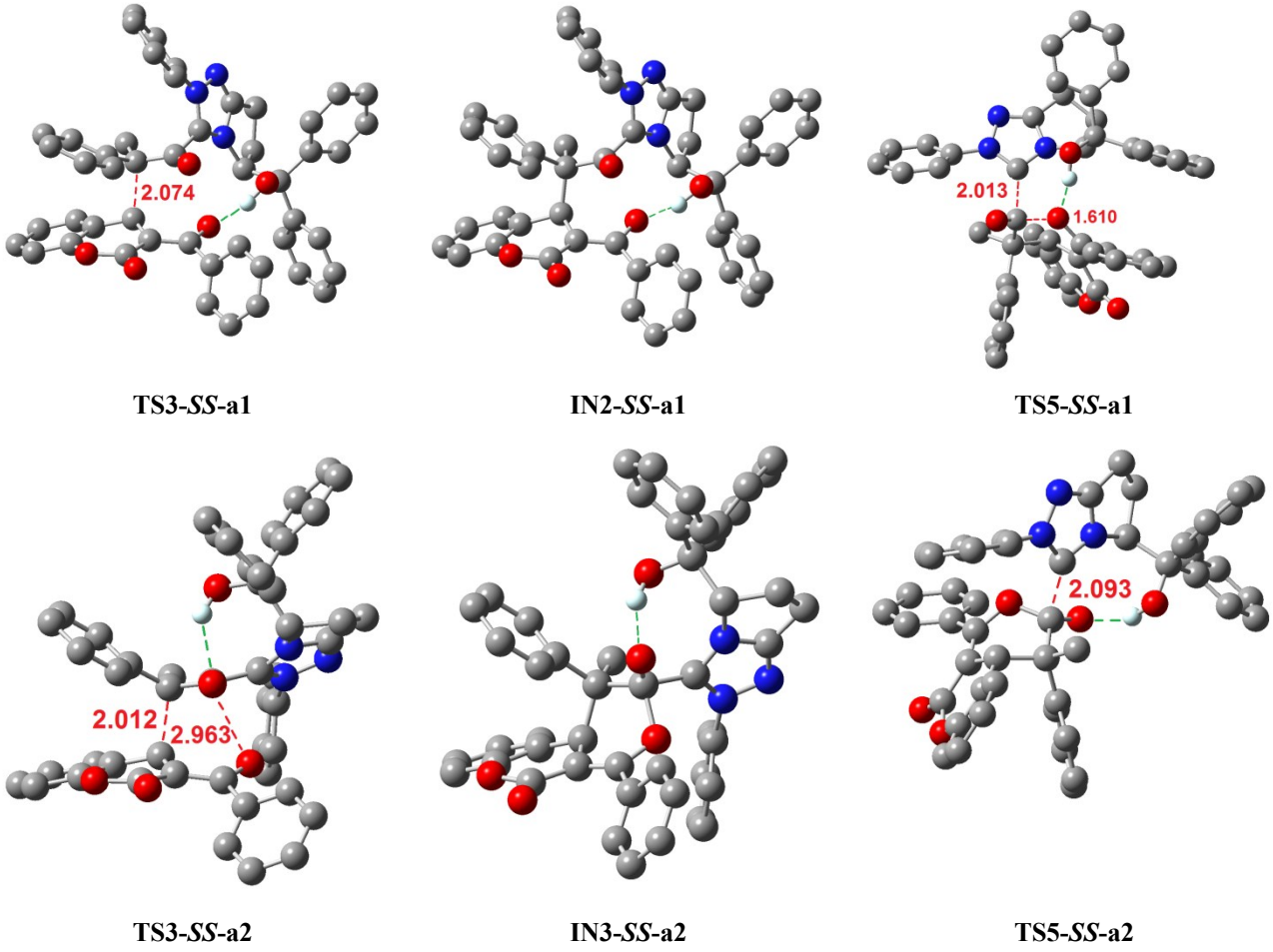


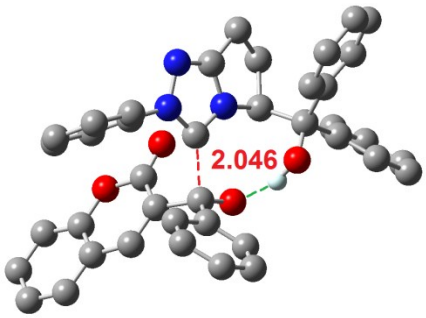
Figure S18. Geometries at B3LYP/6-31G* level of species involved in the reaction of ketene **2** and chromenone **3** catalysed with the NHC **1**, in gas phase. Mechanism A: Initial stage.



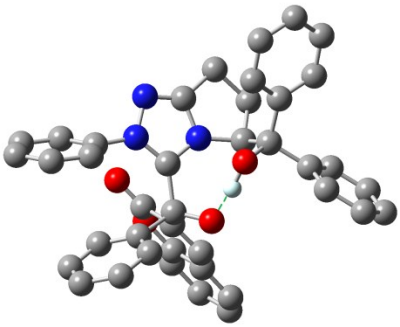
TS3-*SS*-a1 **IN2-*SS*-a1** **TS5-*SS*-a1**

TS3-*SS*-a2 **IN3-*SS*-a2** **TS5-*SS*-a2**

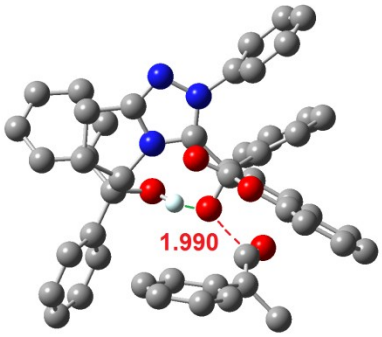
Figure S19. Geometries at B3LYP/6-31G* level of species involved in the reaction of ketene **2** and chromenone **3** catalysed with the NHC **1**, in gas phase. Mechanism A: channel A1 and channel A2.



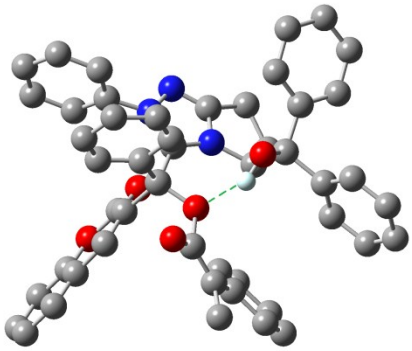
TS6-*R*



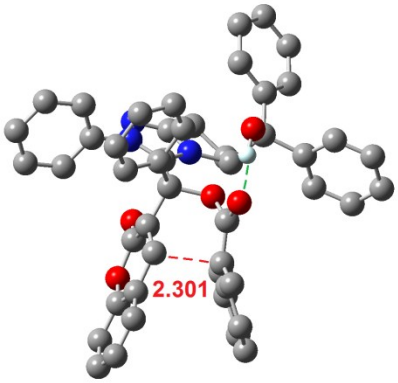
IN4-*R*



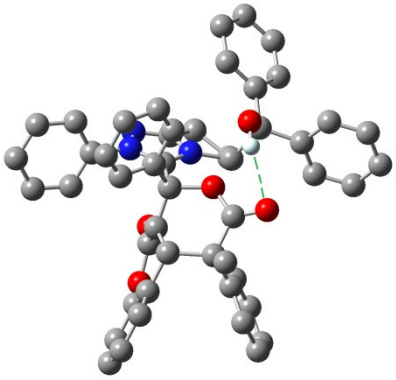
TS7-*RZ*



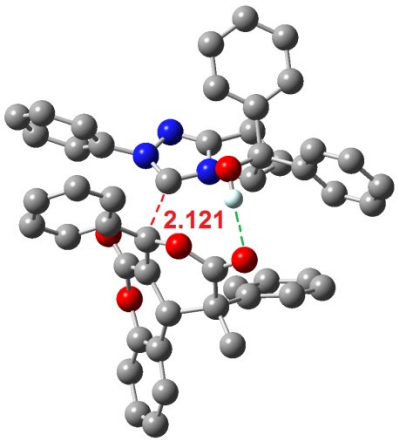
IN5-*RZ*



TS8-*RZ*



IN6-*RZ*



TS9-*RZ*

Figure S20. Geometries at B3LYP/6-31G* level of species involved in the reaction of ketene **2** and chromenone **3** catalysed with the NHC **1**, in gas phase. Mechanism B: channel B1.

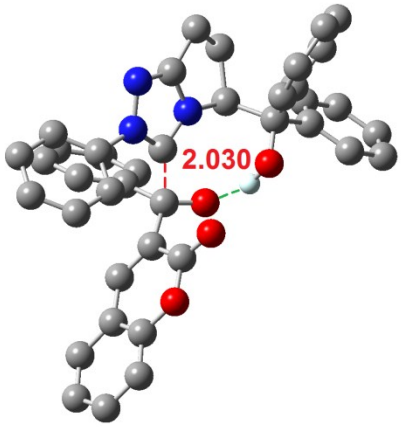
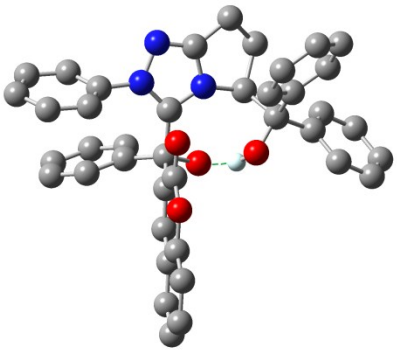
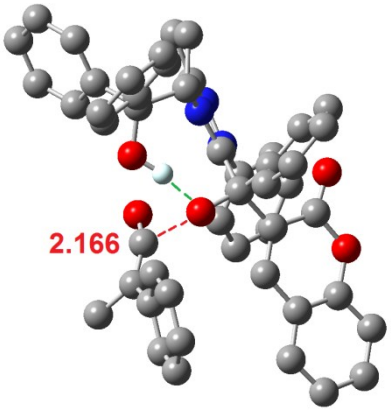
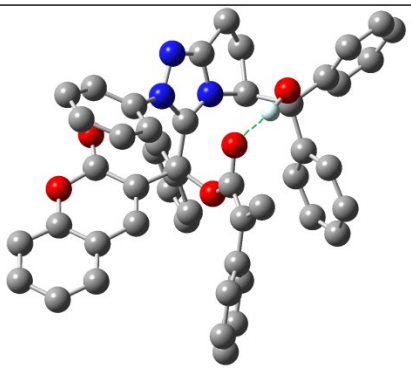
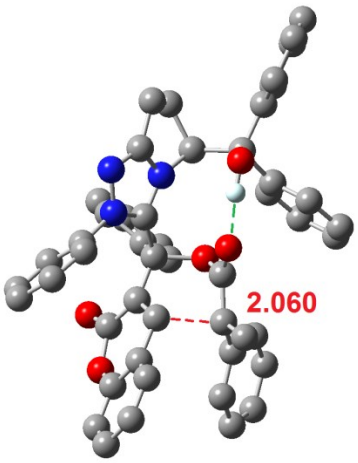
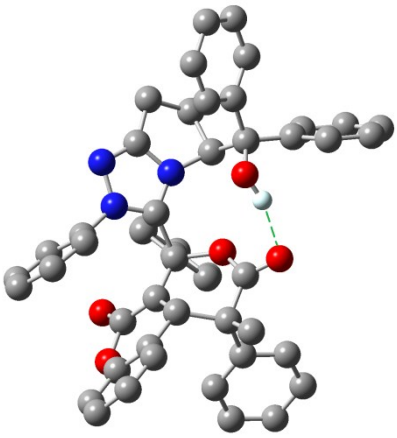
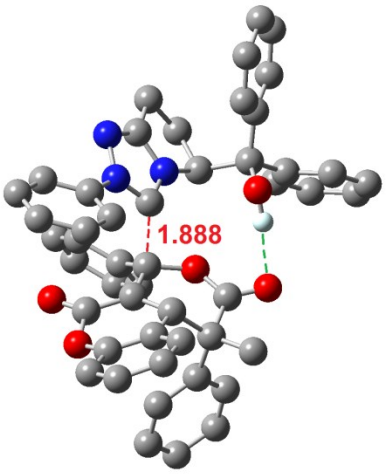
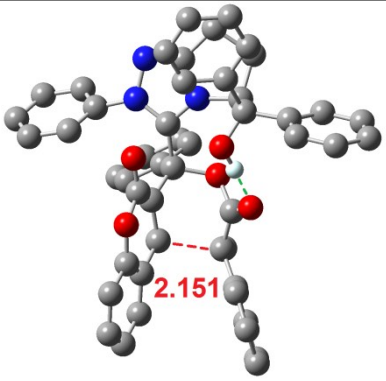
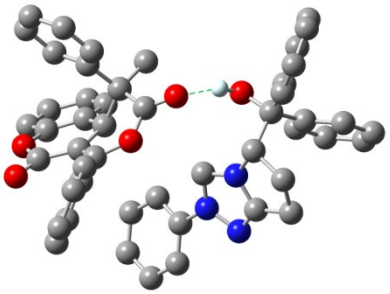
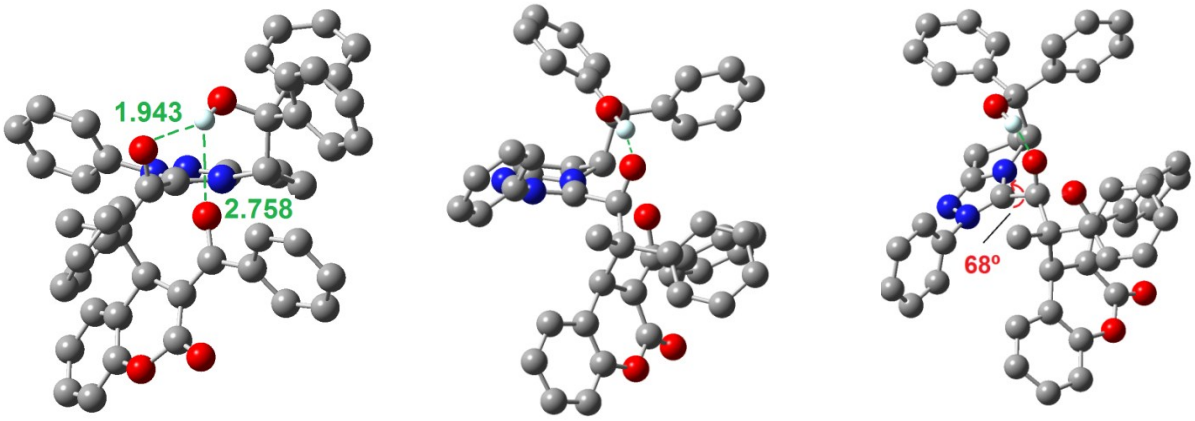
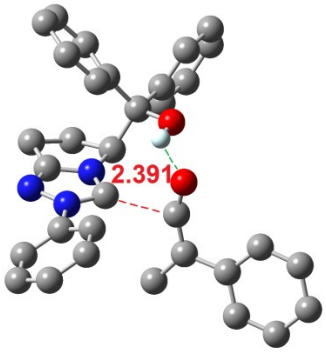
		
TS6-*S*	**IN4-*S***	**TS7-*SZ***
		
IN5-*SZ*	**TS8-*SZ***	**IN6-*SZ***
		
TS9-*SZ*	**TS8-enant**	**1-4-*SS***

Figure S21. Geometries at B3LYP/6-31G* level of species involved in the reaction of ketene **2** and chromenone **3** catalysed with the NHC **1**, in gas phase. Mechanism B: channel B2.

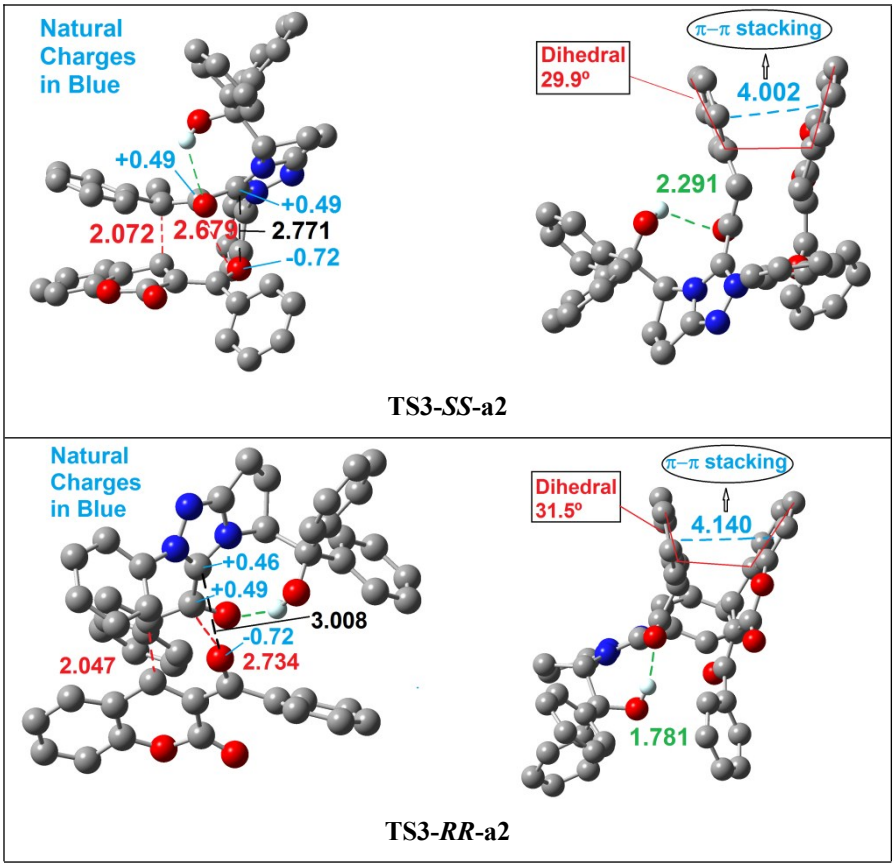


TS10-*SS* **IN7-*SS*** **TS11-*SS***

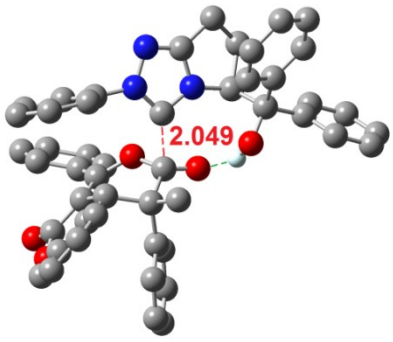
Figure S22. Geometries at B3LYP/6-31G* level of species involved in the reaction of ketene **2** and chromenone **3** catalysed with the NHC **1**, in gas phase. Mechanism A: channel A3.



TS1-*Z*

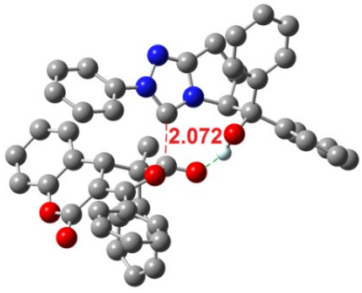


TS3-*SS*-a2



TS5-*SS*-a2

TS3-*RR*-a2



TS5-*RR*-a2

Figure S23. Geometries at MPWB1K/6-311G** level of species involved in the reaction of ketene **2** and chromenone **3** catalysed with the NHC **1**, in toluene. Mechanism A2-*SS* isomer and mechanism A2-*RR* isomer .

XYZ matrices B3LYP/6-31G*

1

HF=-1166.6176057

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.000000	0.000000
2	7	0	0.000000	0.000000	1.361695
3	7	0	1.340600	0.000000	-0.234036
4	6	0	1.960299	-0.016665	-1.518295
5	6	0	3.353199	0.018536	-1.624597
6	6	0	1.160701	-0.065781	-2.665611
7	6	0	3.942691	0.005274	-2.888876
8	1	0	3.955595	0.055812	-0.725500
9	6	0	1.764998	-0.076974	-3.920391
10	1	0	0.082914	-0.095545	-2.557162
11	6	0	3.156425	-0.042064	-4.040519
12	1	0	5.026100	0.032398	-2.968650
13	1	0	1.141039	-0.115452	-4.809187
14	1	0	3.621887	-0.052210	-5.022075
15	6	0	1.273623	0.030189	1.865656
16	7	0	2.152411	0.017005	0.908776
17	6	0	-1.065992	0.073677	2.362823
18	6	0	1.262376	0.129246	3.355587
19	6	0	-0.250558	-0.073944	3.691397
20	1	0	1.900480	-0.619162	3.834250
21	1	0	1.615795	1.116974	3.670392
22	1	0	-0.407454	-1.081774	4.087786
23	1	0	-0.582706	0.630014	4.453688
24	1	0	-1.736408	-0.777047	2.214564
25	6	0	-1.936787	1.358128	2.126664
26	6	0	-3.184161	1.387974	3.023036
27	6	0	-4.107422	2.422585	2.802776
28	6	0	-3.477934	0.435054	4.003447
29	6	0	-5.281818	2.504445	3.544802
30	1	0	-3.897911	3.158750	2.033269
31	6	0	-4.655834	0.517905	4.754131
32	1	0	-2.803964	-0.392903	4.197042
33	6	0	-5.560335	1.552153	4.529064
34	1	0	-5.983848	3.311820	3.353360
35	1	0	-4.861692	-0.234774	5.510770
36	1	0	-6.476297	1.615959	5.110432
37	6	0	-1.091338	2.635187	2.319924
38	6	0	-0.494860	3.263153	1.219212
39	6	0	-0.880810	3.187903	3.593312
40	6	0	0.312038	4.390122	1.387015
41	1	0	-0.677652	2.878118	0.222531
42	6	0	-0.073380	4.313272	3.763687
43	1	0	-1.378542	2.757493	4.457588
44	6	0	0.532099	4.916412	2.659906
45	1	0	0.764008	4.859067	0.516905
46	1	0	0.069736	4.726064	4.759098
47	1	0	1.157718	5.795430	2.790068
48	8	0	-2.450938	1.274991	0.798428
49	1	0	-1.759050	0.907666	0.196675

2

HF=-422.9699098

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.000000	0.000000
2	6	0	0.000000	0.000000	1.521218
3	6	0	1.240858	0.000000	2.317340
4	6	0	-1.183968	-0.082909	2.111612
5	8	0	-2.240606	-0.142878	2.617786
6	6	0	1.225698	-0.233179	3.706735
7	6	0	2.484179	0.196676	1.693905
8	6	0	2.403417	-0.236615	4.443118
9	1	0	0.281372	-0.418243	4.214417
10	6	0	3.664725	0.201794	2.439126

11	1	0	2.531991	0.369615	0.623381
12	6	0	3.635040	-0.014635	3.815159
13	1	0	2.362878	-0.426795	5.512625
14	1	0	4.611330	0.377114	1.934134
15	1	0	4.554150	-0.021883	4.393726
16	1	0	0.550432	-0.866535	-0.386640
17	1	0	0.473628	0.906829	-0.396020
18	1	0	-1.016484	-0.041664	-0.401405

3

HF=-841.4030037

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.000000	0.000000
2	6	0	0.000000	0.000000	1.390827
3	6	0	1.223264	0.000000	2.063933
4	6	0	2.444117	0.004748	1.362544
5	6	0	2.414579	0.003132	-0.046460
6	6	0	1.204494	0.000193	-0.723014
7	1	0	-0.947373	-0.001557	-0.531494
8	1	0	-0.920108	-0.003213	1.965385
9	6	0	3.647641	0.017573	2.140387
10	1	0	3.355196	0.004315	-0.590849
11	1	0	1.186049	-0.001756	-1.808402
12	6	0	3.627997	0.059950	3.501260
13	6	0	2.349350	-0.007008	4.220308
14	1	0	4.610238	-0.002853	1.635555
15	8	0	1.197356	-0.009398	3.425211
16	8	0	2.189430	-0.083287	5.414307
17	6	0	4.954925	0.034160	4.222645
18	8	0	5.866506	-0.611059	3.716053
19	6	0	5.185879	0.821575	5.468475
20	6	0	4.395177	1.919551	5.837482
21	6	0	6.305776	0.489435	6.248184
22	6	0	4.717907	2.668812	6.967062
23	1	0	3.533540	2.198900	5.241791
24	6	0	6.614772	1.225771	7.387176
25	1	0	6.919204	-0.351006	5.940869
26	6	0	5.821623	2.319109	7.747475
27	1	0	4.104099	3.522131	7.241345
28	1	0	7.474818	0.952982	7.992558
29	1	0	6.064409	2.898161	8.634629

4-SS

HF=-1264.3934539

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.000000	0.000000
2	6	0	0.000000	0.000000	1.535438
3	8	0	0.973222	0.000000	-0.702857
4	6	0	-0.129025	-1.436773	2.072981
5	6	0	-0.167687	-2.551584	1.224496
6	6	0	-0.167938	-1.659661	3.458821
7	6	0	-0.261318	-3.845784	1.739810
8	1	0	-0.111706	-2.425481	0.146983
9	6	0	-0.265686	-2.951498	3.974305
10	1	0	-0.122441	-0.820636	4.144758
11	6	0	-0.315230	-4.051487	3.116993
12	1	0	-0.291366	-4.691497	1.058297
13	1	0	-0.301124	-3.095724	5.050753
14	1	0	-0.391167	-5.057839	3.519232
15	6	0	1.349115	0.601160	1.977184
16	1	0	1.471265	1.622610	1.600181
17	1	0	2.166105	-0.001653	1.575428
18	1	0	1.427595	0.615053	3.065881
19	6	0	-0.739536	2.732414	5.232457
20	6	0	-0.561286	2.318590	3.914289
21	6	0	-1.408329	1.369333	3.321919
22	6	0	-2.482709	0.904170	4.083390

23	6	0	-2.678473	1.306494	5.406559
24	6	0	-1.796436	2.213129	5.985240
25	1	0	-1.085549	1.826048	1.294184
26	1	0	-0.063285	3.463365	5.665630
27	1	0	0.246421	2.745135	3.327692
28	6	0	-1.242984	0.913320	1.891094
29	1	0	-3.528675	0.906742	5.949473
30	1	0	-1.945684	2.528669	7.013861
31	6	0	-3.569593	-0.235590	2.236799
32	6	0	-2.489203	0.229467	1.347702
33	8	0	-3.426334	0.033809	3.583446
34	8	0	-4.543357	-0.878492	1.921264
35	6	0	-2.435110	-0.129882	0.035540
36	8	0	-1.235578	0.045964	-0.636463
37	6	0	-3.455556	-0.656643	-0.887390
38	6	0	-4.790721	-0.223018	-0.837214
39	6	0	-3.067737	-1.550277	-1.901757
40	6	0	-5.716427	-0.690723	-1.764290
41	1	0	-5.099347	0.480356	-0.074522
42	6	0	-4.001083	-2.027674	-2.818063
43	1	0	-2.032910	-1.867792	-1.967922
44	6	0	-5.327938	-1.599212	-2.751980
45	1	0	-6.744590	-0.343720	-1.716145
46	1	0	-3.689882	-2.728298	-3.587746
47	1	0	-6.055473	-1.965779	-3.471188

TS1-E

HF=-1589.5770257; 1 imaginary frequencies=-129.7929

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.591427	0.640392	2.073348
2	6	0	2.382865	1.678397	1.800773
3	6	0	1.018883	-0.270581	-0.131489
4	8	0	1.040147	-0.176563	2.745496
5	7	0	-0.087049	-0.315911	-0.931068
6	7	0	1.811324	-1.182542	-0.752667
7	6	0	2.437662	2.428297	0.527824
8	6	0	1.267432	2.925598	-0.074111
9	6	0	3.670274	2.735983	-0.071613
10	6	0	1.327084	3.676268	-1.247709
11	1	0	0.313443	2.731545	0.407889
12	6	0	3.730621	3.491862	-1.242677
13	1	0	4.589018	2.366298	0.375580
14	6	0	2.559668	3.962708	-1.839316
15	1	0	0.409651	4.058154	-1.690198
16	1	0	4.696306	3.709949	-1.692176
17	1	0	2.607815	4.555636	-2.748989
18	6	0	3.235275	2.149553	2.977803
19	1	0	3.049219	1.548815	3.873031
20	1	0	3.020108	3.197841	3.220812
21	1	0	4.306063	2.074624	2.747090
22	6	0	3.132753	-1.578886	-0.379249
23	6	0	4.092296	-1.763058	-1.378045
24	6	0	3.445747	-1.805346	0.962670
25	6	0	5.379731	-2.163846	-1.025485
26	1	0	3.820969	-1.595723	-2.414219
27	6	0	4.741292	-2.195489	1.302914
28	1	0	2.681935	-1.691324	1.722968
29	6	0	5.710281	-2.375903	0.314689
30	1	0	6.126579	-2.306127	-1.801686
31	1	0	4.986440	-2.371397	2.346671
32	1	0	6.715583	-2.686131	0.586105
33	6	0	0.096593	-1.206866	-1.962163
34	7	0	1.264863	-1.767199	-1.902764
35	6	0	-1.374856	0.394732	-0.980326
36	6	0	-1.101415	-1.278829	-2.846109
37	6	0	-1.901165	-0.022466	-2.394870
38	1	0	-0.843281	-1.257115	-3.908244
39	1	0	-1.659745	-2.201541	-2.653825
40	1	0	-1.711490	0.800022	-3.091947
41	1	0	-2.974813	-0.207669	-2.393417
42	1	0	-1.166825	1.465265	-0.937142
43	6	0	-2.279562	0.073162	0.260359

44	6	0	-3.578647	0.898104	0.252603
45	6	0	-4.461014	0.714766	1.329250
46	6	0	-3.899669	1.862409	-0.708325
47	6	0	-5.633726	1.457256	1.431074
48	1	0	-4.212649	-0.013518	2.094523
49	6	0	-5.079576	2.607652	-0.610761
50	1	0	-3.238935	2.059630	-1.545401
51	6	0	-5.951564	2.406690	0.455793
52	1	0	-6.299727	1.297423	2.274857
53	1	0	-5.307616	3.349184	-1.371900
54	1	0	-6.867652	2.986231	0.532061
55	6	0	-2.576024	-1.439136	0.341444
56	6	0	-1.762897	-2.293267	1.099476
57	6	0	-3.645808	-2.005426	-0.370355
58	6	0	-1.997271	-3.669621	1.125445
59	1	0	-0.945808	-1.897751	1.693901
60	6	0	-3.880006	-3.380736	-0.347153
61	1	0	-4.322596	-1.362803	-0.925385
62	6	0	-3.051766	-4.220922	0.398442
63	1	0	-1.352467	-4.308838	1.722438
64	1	0	-4.719235	-3.791675	-0.902420
65	1	0	-3.234120	-5.291861	0.421823
66	8	0	-1.603303	0.546004	1.423844
67	1	0	-0.754402	0.086189	1.543061

IN1-E

HF=-1589.6221608

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.186124	-0.436918	1.334713
2	6	0	-2.095672	-1.434364	1.561056
3	6	0	-0.952383	0.136292	-0.027245
4	8	0	-0.491084	0.248060	2.198117
5	7	0	0.178412	0.083984	-0.771048
6	7	0	-1.724530	1.045264	-0.657281
7	6	0	-2.862347	-2.099489	0.492578
8	6	0	-2.293569	-2.464483	-0.745831
9	6	0	-4.220410	-2.431003	0.691257
10	6	0	-3.048783	-3.073160	-1.747588
11	1	0	-1.230594	-2.312757	-0.907075
12	6	0	-4.971823	-3.051920	-0.302812
13	1	0	-4.692735	-2.181566	1.636220
14	6	0	-4.395471	-3.369446	-1.535295
15	1	0	-2.573787	-3.343556	-2.687506
16	1	0	-6.016937	-3.285412	-0.116072
17	1	0	-4.981657	-3.856044	-2.309516
18	6	0	-2.371825	-1.795399	3.001829
19	1	0	-1.553735	-1.437028	3.630547
20	1	0	-2.479009	-2.878027	3.132398
21	1	0	-3.295477	-1.329303	3.375670
22	6	0	-2.994070	1.564025	-0.240606
23	6	0	-3.987229	1.753650	-1.201080
24	6	0	-3.190841	1.908176	1.098978
25	6	0	-5.211008	2.291995	-0.807384
26	1	0	-3.795641	1.484233	-2.233272
27	6	0	-4.425793	2.434193	1.476085
28	1	0	-2.390838	1.769795	1.819376
29	6	0	-5.433703	2.627995	0.529293
30	1	0	-5.991660	2.442779	-1.546630
31	1	0	-4.592842	2.703755	2.514377
32	1	0	-6.390080	3.044069	0.831805
33	6	0	0.010490	0.922753	-1.843210
34	7	0	-1.138895	1.532595	-1.814326
35	6	0	1.456306	-0.673185	-0.789138
36	6	0	1.182476	0.873218	-2.760685
37	6	0	1.907570	-0.409358	-2.264912
38	1	0	0.883694	0.817819	-3.809971
39	1	0	1.803283	1.764442	-2.627286
40	1	0	1.605501	-1.261096	-2.882206
41	1	0	2.989135	-0.314554	-2.340523
42	1	0	1.221416	-1.724325	-0.609627

43	6	0	2.460457	-0.240026	0.349496
44	6	0	3.764663	-1.063691	0.258398
45	6	0	4.776515	-0.747311	1.179407
46	6	0	3.968048	-2.156653	-0.590600
47	6	0	5.959973	-1.477345	1.228116
48	1	0	4.619850	0.075537	1.868595
49	6	0	5.156886	-2.893102	-0.544575
50	1	0	3.206646	-2.469615	-1.296759
51	6	0	6.159148	-2.553823	0.359429
52	1	0	6.726638	-1.209877	1.949923
53	1	0	5.288534	-3.736751	-1.216356
54	1	0	7.082453	-3.124956	0.395032
55	6	0	2.741133	1.277602	0.244176
56	6	0	1.923770	2.191894	0.925912
57	6	0	3.783169	1.781360	-0.550904
58	6	0	2.137196	3.566322	0.802090
59	1	0	1.113005	1.834155	1.553290
60	6	0	3.994738	3.155825	-0.674470
61	1	0	4.456621	1.095579	-1.055659
62	6	0	3.169235	4.055464	0.001101
63	1	0	1.492967	4.255922	1.340531
64	1	0	4.814192	3.520176	-1.288212
65	1	0	3.335047	5.125316	-0.088848
66	8	0	1.941562	-0.615730	1.599770
67	1	0	1.072941	-0.180768	1.837766

TS1-Z

HF=-1589.581265; 1 imaginary frequencies=-97.0334

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.943517	0.835166	0.492323
2	6	0	2.727755	1.377068	-0.445143
3	6	0	0.674893	-1.041965	-0.585244
4	8	0	1.461323	0.689097	1.571842
5	7	0	-0.617010	-1.093393	-1.023255
6	7	0	1.004629	-2.359641	-0.623351
7	6	0	3.527167	2.554597	-0.003559
8	6	0	3.418009	3.126370	1.281666
9	6	0	4.443003	3.144579	-0.897090
10	6	0	4.186532	4.226348	1.648546
11	1	0	2.721664	2.709353	2.001833
12	6	0	5.210837	4.248189	-0.523545
13	1	0	4.563104	2.740250	-1.895951
14	6	0	5.091230	4.799039	0.750657
15	1	0	4.073770	4.641393	2.647209
16	1	0	5.907452	4.675945	-1.240733
17	1	0	5.689040	5.658711	1.040826
18	6	0	2.853780	0.880488	-1.861640
19	1	0	2.172304	0.048584	-2.034460
20	1	0	3.874187	0.536563	-2.076304
21	1	0	2.618930	1.677008	-2.579844
22	6	0	2.265093	-2.935481	-0.275322
23	6	0	2.726347	-4.047406	-0.985313
24	6	0	3.015295	-2.393846	0.771332
25	6	0	3.957031	-4.609535	-0.650687
26	1	0	2.119406	-4.459955	-1.782917
27	6	0	4.250775	-2.959158	1.086593
28	1	0	2.627775	-1.556496	1.338793
29	6	0	4.726111	-4.064836	0.379733
30	1	0	4.316746	-5.473323	-1.202866
31	1	0	4.835986	-2.536353	1.898230
32	1	0	5.686850	-4.503492	0.634235
33	6	0	-0.974616	-2.389037	-1.319018
34	7	0	0.000180	-3.214441	-1.091071
35	6	0	-1.679590	-0.109046	-1.301142
36	6	0	-2.366108	-2.469347	-1.847124
37	6	0	-2.667190	-0.973523	-2.153385
38	1	0	-2.439537	-3.105177	-2.733567
39	1	0	-3.044189	-2.871155	-1.087070
40	1	0	-2.479004	-0.773857	-3.213446
41	1	0	-3.707927	-0.720514	-1.953857
42	1	0	-1.242751	0.703669	-1.884950
43	6	0	-2.255871	0.551096	0.003735

44	6	0	-3.316560	1.619956	-0.323535
45	6	0	-3.917465	2.277499	0.761809
46	6	0	-3.654673	2.035058	-1.615761
47	6	0	-4.840566	3.299617	0.561650
48	1	0	-3.645363	1.984830	1.770749
49	6	0	-4.584727	3.059861	-1.820467
50	1	0	-3.198069	1.580046	-2.487994
51	6	0	-5.183469	3.693091	-0.734780
52	1	0	-5.290339	3.793271	1.419010
53	1	0	-4.831515	3.362140	-2.834797
54	1	0	-5.905128	4.489792	-0.893949
55	6	0	-2.819998	-0.525205	0.956297
56	6	0	-2.017428	-1.086243	1.959294
57	6	0	-4.137749	-0.993047	0.827499
58	6	0	-2.506887	-2.096263	2.789989
59	1	0	-1.003892	-0.732956	2.118354
60	6	0	-4.628513	-2.003492	1.655390
61	1	0	-4.798291	-0.544002	0.092042
62	6	0	-3.811858	-2.563807	2.638867
63	1	0	-1.863287	-2.512422	3.560253
64	1	0	-5.654830	-2.341880	1.538552
65	1	0	-4.192939	-3.347594	3.287773
66	8	0	-1.220340	1.310772	0.613894
67	1	0	-0.477263	0.750281	0.896950

IN1-Z

HF=-1589.6240816

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.476771	0.542795	0.045967
2	6	0	2.299609	1.390591	-0.650338
3	6	0	0.922546	-0.689807	-0.605676
4	8	0	1.041881	0.553534	1.275111
5	7	0	-0.347782	-0.893165	-1.025504
6	7	0	1.493679	-1.911758	-0.669824
7	6	0	2.894679	2.595195	-0.042374
8	6	0	2.648516	2.975371	1.298373
9	6	0	3.752809	3.426878	-0.796107
10	6	0	3.229510	4.119012	1.839624
11	1	0	1.995550	2.357264	1.900159
12	6	0	4.332115	4.569558	-0.247357
13	1	0	3.976897	3.182406	-1.829047
14	6	0	4.075399	4.926467	1.076352
15	1	0	3.015879	4.382015	2.873207
16	1	0	4.987612	5.182967	-0.861358
17	1	0	4.525639	5.818148	1.505101
18	6	0	2.630970	1.097413	-2.098346
19	1	0	2.128649	0.196885	-2.466545
20	1	0	3.708275	0.946353	-2.252067
21	1	0	2.330704	1.921942	-2.759186
22	6	0	2.821610	-2.284529	-0.278927
23	6	0	3.513539	-3.209064	-1.063112
24	6	0	3.378439	-1.743374	0.882636
25	6	0	4.798162	-3.590339	-0.680370
26	1	0	3.044591	-3.620890	-1.949702
27	6	0	4.669962	-2.128134	1.242034
28	1	0	2.806776	-1.048683	1.489719
29	6	0	5.380019	-3.046995	0.467057
30	1	0	5.345004	-4.308909	-1.283810
31	1	0	5.115800	-1.710610	2.139787
32	1	0	6.383616	-3.342904	0.758886
33	6	0	-0.471514	-2.216659	-1.363733
34	7	0	0.631193	-2.878383	-1.161927
35	6	0	-1.575524	-0.091491	-1.259161
36	6	0	-1.828416	-2.515032	-1.902121
37	6	0	-2.375376	-1.082893	-2.167857
38	1	0	-1.788295	-3.130642	-2.804414
39	1	0	-2.425749	-3.044507	-1.153320
40	1	0	-2.204034	-0.816206	-3.215973
41	1	0	-3.446585	-1.018849	-1.982662
42	1	0	-1.280873	0.816021	-1.789191
43	6	0	-2.279762	0.376790	0.075217
44	6	0	-3.546608	1.200669	-0.246741

45	6	0	-4.310466	1.640430	0.846474
46	6	0	-3.922165	1.627426	-1.524796
47	6	0	-5.424967	2.453716	0.665276
48	1	0	-4.012966	1.345455	1.847300
49	6	0	-5.042654	2.444484	-1.711099
50	1	0	-3.348740	1.347107	-2.402125
51	6	0	-5.801087	2.856510	-0.619201
52	1	0	-5.998166	2.779632	1.529133
53	1	0	-5.312036	2.760330	-2.715482
54	1	0	-6.671185	3.491239	-0.763235
55	6	0	-2.612878	-0.855972	0.947694
56	6	0	-1.679134	-1.333074	1.880104
57	6	0	-3.827389	-1.547539	0.809872
58	6	0	-1.949907	-2.474964	2.637487
59	1	0	-0.733023	-0.818430	2.018585
60	6	0	-4.096276	-2.689514	1.566375
61	1	0	-4.584408	-1.176040	0.125881
62	6	0	-3.155206	-3.159908	2.483467
63	1	0	-1.212408	-2.825177	3.354873
64	1	0	-5.047899	-3.201242	1.447333
65	1	0	-3.363988	-4.045203	3.078095
66	8	0	-1.460281	1.310291	0.736191
67	1	0	-0.579007	0.948953	1.030285

TS3-SS-a1

HF=-2430.9983529; 1 imaginary frequencies=-306.2609

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.766377	0.831473	-0.330560
2	6	0	1.960855	0.729671	0.517825
3	6	0	-0.352235	1.774992	0.186032
4	8	0	0.613988	0.386900	-1.466859
5	7	0	-1.457352	1.610750	0.944621
6	7	0	-0.258518	3.113592	0.018208
7	6	0	3.267336	0.839751	-0.225032
8	6	0	3.459742	0.284192	-1.507049
9	6	0	4.361026	1.511625	0.356152
10	6	0	4.682226	0.403432	-2.166906
11	1	0	2.650129	-0.245764	-1.987672
12	6	0	5.580957	1.630904	-0.308975
13	1	0	4.272035	1.957851	1.339638
14	6	0	5.751205	1.077817	-1.577182
15	1	0	4.796313	-0.049108	-3.148504
16	1	0	6.400271	2.158092	0.173940
17	1	0	6.703475	1.164190	-2.094100
18	6	0	1.882142	1.528501	1.816023
19	1	0	0.936568	1.353638	2.341832
20	1	0	1.987541	2.610024	1.655431
21	1	0	2.677344	1.232772	2.501577
22	6	0	0.728298	3.867217	-0.706155
23	6	0	1.234695	5.027517	-0.114150
24	6	0	1.129140	3.462615	-1.980379
25	6	0	2.174357	5.784665	-0.809293
26	1	0	0.887493	5.326689	0.868343
27	6	0	2.081177	4.226039	-2.655875
28	1	0	0.716909	2.565970	-2.427371
29	6	0	2.603032	5.382849	-2.076743
30	1	0	2.575383	6.686310	-0.355980
31	1	0	2.408654	3.911418	-3.641793
32	1	0	3.341973	5.972101	-2.611801
33	6	0	-1.939020	2.858635	1.257967
34	7	0	-1.239376	3.804742	0.701306
35	6	0	-2.322044	0.522409	1.470157
36	6	0	-3.087784	2.784487	2.206316
37	6	0	-3.039791	1.284667	2.622632
38	1	0	-2.952849	3.464385	3.052104
39	1	0	-4.025020	3.043340	1.706731
40	1	0	-2.455813	1.176509	3.543078
41	1	0	-4.037369	0.888770	2.808695
42	1	0	-1.680621	-0.288855	1.811339
43	6	0	-3.251270	-0.055881	0.318000
44	6	0	-3.871578	-1.400151	0.754117
45	6	0	-4.455727	-2.179575	-0.256652

46	6	0	-3.885927	-1.892078	2.063896
47	6	0	-5.042293	-3.407295	0.035190
48	1	0	-4.424194	-1.818159	-1.279134
49	6	0	-4.475748	-3.125703	2.359146
50	1	0	-3.427796	-1.338466	2.877320
51	6	0	-5.057778	-3.885779	1.348171
52	1	0	-5.480983	-3.996649	-0.765449
53	1	0	-4.468778	-3.490162	3.383037
54	1	0	-5.511947	-4.846057	1.576912
55	6	0	-4.345636	0.947917	-0.084255
56	6	0	-4.096088	1.866672	-1.113856
57	6	0	-5.591101	0.986019	0.559779
58	6	0	-5.052609	2.821570	-1.463904
59	1	0	-3.157604	1.808479	-1.653158
60	6	0	-6.546081	1.942823	0.212427
61	1	0	-5.826942	0.248976	1.321671
62	6	0	-6.277207	2.870376	-0.796273
63	1	0	-4.840967	3.523550	-2.266207
64	1	0	-7.506314	1.952831	0.721588
65	1	0	-7.022460	3.612182	-1.070586
66	8	0	-2.446521	-0.243020	-0.821529
67	1	0	-1.761665	-0.924192	-0.573970
68	6	0	4.626549	-1.249627	3.903834
69	6	0	3.410477	-1.030562	3.263573
70	6	0	3.208625	-1.414515	1.926095
71	6	0	4.253606	-2.088764	1.271138
72	6	0	5.483497	-2.304079	1.900120
73	6	0	5.669944	-1.873561	3.209630
74	1	0	1.073206	-1.074773	1.826597
75	1	0	4.760163	-0.946351	4.938271
76	1	0	2.587684	-0.575634	3.808830
77	6	0	1.946167	-1.228555	1.200290
78	1	0	6.263223	-2.822403	1.351637
79	1	0	6.624721	-2.044938	3.699555
80	6	0	2.844361	-2.723020	-0.606067
81	6	0	1.723736	-2.121788	0.096494
82	8	0	4.107404	-2.590898	0.015004
83	8	0	2.847558	-3.327510	-1.654976
84	6	0	0.367846	-2.287109	-0.316564
85	8	0	-0.543279	-1.646906	0.289191
86	6	0	-0.061181	-3.210190	-1.421000
87	6	0	0.135180	-4.593137	-1.323324
88	6	0	-0.767423	-2.694300	-2.515124
89	6	0	-0.374756	-5.447653	-2.298663
90	1	0	0.688899	-4.998534	-0.481672
91	6	0	-1.258663	-3.549849	-3.501597
92	1	0	-0.908372	-1.621306	-2.602309
93	6	0	-1.070256	-4.928389	-3.392967
94	1	0	-0.221551	-6.520071	-2.208708
95	1	0	-1.790356	-3.137213	-4.355449
96	1	0	-1.459001	-5.595187	-4.158625

IN2-SS-a1

HF=-2431.0053797

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.812443	0.716707	-0.324959
2	6	0	1.928767	0.406388	0.707394
3	6	0	-0.292423	1.703066	0.131338
4	8	0	0.887930	0.499814	-1.518048
5	7	0	-1.375783	1.583867	0.925627
6	7	0	-0.153797	3.036861	-0.053250
7	6	0	3.265237	0.877002	0.092326
8	6	0	3.701201	0.392346	-1.153797
9	6	0	4.102239	1.779510	0.767616
10	6	0	4.926036	0.787385	-1.689782
11	1	0	3.078998	-0.290513	-1.715179
12	6	0	5.327446	2.176733	0.228868
13	1	0	3.817144	2.184144	1.731610
14	6	0	5.747902	1.681339	-1.003404
15	1	0	5.237641	0.382645	-2.648912
16	1	0	5.952456	2.872843	0.782771
17	1	0	6.704139	1.984426	-1.422038

18	6	0	1.630282	1.120059	2.040854
19	1	0	0.697113	0.749087	2.476829
20	1	0	1.558018	2.208234	1.938337
21	1	0	2.422585	0.917924	2.761478
22	6	0	0.835801	3.763907	-0.804100
23	6	0	1.456178	4.852490	-0.186056
24	6	0	1.116247	3.415744	-2.125944
25	6	0	2.391916	5.592523	-0.903991
26	1	0	1.199880	5.111627	0.835191
27	6	0	2.063749	4.161820	-2.826502
28	1	0	0.618259	2.571521	-2.586032
29	6	0	2.700241	5.245849	-2.221506
30	1	0	2.883020	6.437529	-0.430819
31	1	0	2.297208	3.892375	-3.851841
32	1	0	3.435056	5.822127	-2.776053
33	6	0	-1.805319	2.848105	1.240881
34	7	0	-1.088835	3.765407	0.656135
35	6	0	-2.269092	0.529725	1.469740
36	6	0	-2.928278	2.817725	2.222755
37	6	0	-2.918989	1.318123	2.644118
38	1	0	-2.743619	3.495797	3.060634
39	1	0	-3.870698	3.107984	1.751409
40	1	0	-2.305920	1.192143	3.543212
41	1	0	-3.923065	0.960410	2.867307
42	1	0	-1.651624	-0.308465	1.788254
43	6	0	-3.255148	-0.003475	0.334978
44	6	0	-3.841398	-1.369224	0.753215
45	6	0	-4.384165	-2.164756	-0.267293
46	6	0	-3.877916	-1.855185	2.065469
47	6	0	-4.950206	-3.404266	0.017275
48	1	0	-4.334594	-1.807250	-1.290054
49	6	0	-4.446927	-3.100107	2.352857
50	1	0	-3.454002	-1.286255	2.887208
51	6	0	-4.986852	-3.877517	1.331377
52	1	0	-5.355944	-4.006818	-0.790829
53	1	0	-4.457335	-3.459592	3.378502
54	1	0	-5.424733	-4.846836	1.553619
55	6	0	-4.379881	1.004717	0.036877
56	6	0	-4.203433	1.957223	-0.977224
57	6	0	-5.580979	1.014470	0.761430
58	6	0	-5.184987	2.916647	-1.232807
59	1	0	-3.301697	1.923230	-1.577399
60	6	0	-6.560637	1.975963	0.508907
61	1	0	-5.764662	0.251766	1.512357
62	6	0	-6.363093	2.936849	-0.484825
63	1	0	-5.029894	3.644650	-2.024860
64	1	0	-7.485312	1.963273	1.080028
65	1	0	-7.127943	3.682204	-0.685764
66	8	0	-2.514441	-0.134542	-0.851937
67	1	0	-1.771145	-0.779978	-0.652212
68	6	0	4.644831	-1.820245	3.757521
69	6	0	3.466396	-1.414562	3.133023
70	6	0	3.247590	-1.618948	1.762793
71	6	0	4.227967	-2.323330	1.051021
72	6	0	5.419437	-2.729897	1.659752
73	6	0	5.632718	-2.464589	3.008728
74	1	0	1.137610	-1.319388	1.738774
75	1	0	4.787213	-1.642877	4.819819
76	1	0	2.685779	-0.949328	3.728959
77	6	0	1.980165	-1.208268	1.049216
78	1	0	6.148552	-3.265752	1.060423
79	1	0	6.557927	-2.784397	3.480859
80	6	0	2.787229	-2.743390	-0.852632
81	6	0	1.713603	-2.106158	-0.121067
82	8	0	4.067786	-2.672254	-0.261745
83	8	0	2.748842	-3.300256	-1.929388
84	6	0	0.375061	-2.157543	-0.514119
85	8	0	-0.464270	-1.377523	0.083078
86	6	0	-0.171917	-3.058424	-1.578068
87	6	0	-0.031198	-4.449290	-1.491325
88	6	0	-0.911925	-2.513681	-2.635865
89	6	0	-0.623734	-5.280050	-2.439855
90	1	0	0.545257	-4.876378	-0.676366
91	6	0	-1.489560	-3.344978	-3.595770
92	1	0	-1.013805	-1.435714	-2.717729
93	6	0	-1.352611	-4.730418	-3.497133
94	1	0	-0.511138	-6.358131	-2.357696

95	1	0	-2.046745	-2.908888	-4.421314
96	1	0	-1.807950	-5.378919	-4.241574

TS5-SS-a1

HF=-2430.9860428; 1 imaginary frequencies=-179.1765

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.000007	0.733928	-1.164780
2	6	0	2.302873	0.666655	-0.295262
3	6	0	-0.325719	1.838046	-0.126888
4	8	0	0.967277	1.085765	-2.322692
5	7	0	-1.267317	1.464307	0.781865
6	7	0	-0.392346	3.192529	-0.055774
7	6	0	3.453964	-0.011140	-1.087179
8	6	0	3.311099	-0.601967	-2.351560
9	6	0	4.728699	-0.056259	-0.493857
10	6	0	4.392299	-1.213273	-2.989502
11	1	0	2.357970	-0.567750	-2.860742
12	6	0	5.807936	-0.669950	-1.128676
13	1	0	4.890598	0.382052	0.484707
14	6	0	5.646426	-1.253274	-2.384480
15	1	0	4.243807	-1.661533	-3.968527
16	1	0	6.775843	-0.690093	-0.634497
17	1	0	6.485330	-1.732097	-2.882461
18	6	0	2.739578	2.108211	0.025043
19	1	0	2.021305	2.626800	0.662975
20	1	0	2.843978	2.671782	-0.905856
21	1	0	3.701664	2.119727	0.538495
22	6	0	0.287550	4.180002	-0.843520
23	6	0	0.751013	5.336817	-0.210908
24	6	0	0.428590	4.002807	-2.220222
25	6	0	1.382532	6.320173	-0.969041
26	1	0	0.606968	5.459221	0.856618
27	6	0	1.074388	4.991532	-2.963744
28	1	0	0.065431	3.097778	-2.690629
29	6	0	1.549947	6.148505	-2.345280
30	1	0	1.746457	7.220046	-0.481474
31	1	0	1.195621	4.854303	-4.034217
32	1	0	2.045986	6.915908	-2.932858
33	6	0	-1.789373	2.578184	1.393631
34	7	0	-1.284113	3.670433	0.906109
35	6	0	-1.956173	0.225787	1.186962
36	6	0	-2.752319	2.212122	2.474585
37	6	0	-2.538781	0.671396	2.562541
38	1	0	-2.520922	2.722304	3.413989
39	1	0	-3.776822	2.469646	2.193079
40	1	0	-1.804327	0.446416	3.343503
41	1	0	-3.463035	0.150464	2.809365
42	1	0	-1.219960	-0.570062	1.295076
43	6	0	-3.013805	-0.230068	0.086134
44	6	0	-3.357460	-1.723348	0.265887
45	6	0	-3.939128	-2.382227	-0.828352
46	6	0	-3.156443	-2.448406	1.446979
47	6	0	-4.311276	-3.720768	-0.742243
48	1	0	-4.082124	-1.831699	-1.752020
49	6	0	-3.532222	-3.792834	1.535605
50	1	0	-2.702022	-1.986602	2.317992
51	6	0	-4.112851	-4.432774	0.443545
52	1	0	-4.754282	-4.211209	-1.604842
53	1	0	-3.363560	-4.335163	2.462274
54	1	0	-4.403524	-5.477596	0.511564
55	6	0	-4.290586	0.630679	0.137800
56	6	0	-4.371890	1.795170	-0.639455
57	6	0	-5.377979	0.297106	0.958240
58	6	0	-5.496780	2.619173	-0.572419
59	1	0	-3.555365	2.039918	-1.308108
60	6	0	-6.500735	1.123254	1.028555
61	1	0	-5.359131	-0.624375	1.532270
62	6	0	-6.562264	2.291913	0.267434
63	1	0	-5.539854	3.517012	-1.183377
64	1	0	-7.332786	0.844336	1.669841
65	1	0	-7.438231	2.933110	0.317921

66	8	0	-2.467662	-0.008908	-1.199873
67	1	0	-1.580763	-0.428038	-1.252641
68	6	0	3.758473	1.036545	4.129763
69	6	0	2.916253	1.000886	3.020145
70	6	0	2.848648	-0.121635	2.181311
71	6	0	3.615604	-1.234846	2.536079
72	6	0	4.466341	-1.218854	3.645030
73	6	0	4.545662	-0.077034	4.435637
74	1	0	0.971566	0.229995	1.317278
75	1	0	3.794809	1.924280	4.754657
76	1	0	2.292534	1.862000	2.798174
77	6	0	1.928606	-0.191679	0.984282
78	1	0	5.041669	-2.111507	3.868405
79	1	0	5.206726	-0.062945	5.297754
80	6	0	2.580559	-2.714738	0.911195
81	6	0	1.676140	-1.624769	0.534096
82	8	0	3.579185	-2.412594	1.831053
83	8	0	2.581203	-3.852609	0.499164
84	6	0	0.739139	-1.751910	-0.458745
85	8	0	0.163108	-0.620566	-0.927183
86	6	0	0.212156	-2.954817	-1.146104
87	6	0	-0.059855	-4.156694	-0.474952
88	6	0	-0.088224	-2.858158	-2.516557
89	6	0	-0.595754	-5.240505	-1.164487
90	1	0	0.150610	-4.241285	0.583219
91	6	0	-0.606798	-3.951354	-3.206976
92	1	0	0.093086	-1.921585	-3.033374
93	6	0	-0.861853	-5.146209	-2.532512
94	1	0	-0.804391	-6.163635	-0.631000
95	1	0	-0.815668	-3.866903	-4.270062
96	1	0	-1.270947	-5.999002	-3.068281

TS3-SS-a2

HF=-2430.99282671; 1 imaginary frequencies=-320.9688

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.289564	0.307612	-0.173489
2	6	0	1.268155	0.500622	-1.242777
3	6	0	-0.565642	1.390804	0.479307
4	8	0	-0.014428	-0.826911	0.236196
5	7	0	-1.797153	1.031458	0.940658
6	7	0	-0.491741	2.718483	0.777470
7	6	0	1.207456	-0.590042	-2.299662
8	6	0	1.153957	-1.965141	-1.987669
9	6	0	1.190962	-0.249366	-3.667136
10	6	0	1.089039	-2.934374	-2.989231
11	1	0	1.162978	-2.286694	-0.957773
12	6	0	1.120747	-1.219954	-4.665987
13	1	0	1.215251	0.788278	-3.976467
14	6	0	1.070354	-2.572712	-4.335089
15	1	0	1.061882	-3.982546	-2.703200
16	1	0	1.103364	-0.909034	-5.707743
17	1	0	1.021045	-3.330978	-5.112239
18	6	0	1.417551	1.901538	-1.817373
19	1	0	1.700807	2.625002	-1.057118
20	1	0	0.497057	2.257361	-2.299410
21	1	0	2.204748	1.918010	-2.572767
22	6	0	0.545270	3.717509	0.655352
23	6	0	1.710754	3.636775	1.416526
24	6	0	0.275686	4.820619	-0.157867
25	6	0	2.643632	4.672105	1.314138
26	1	0	1.876541	2.774529	2.051434
27	6	0	1.213994	5.846134	-0.244348
28	1	0	-0.654970	4.865045	-0.713923
29	6	0	2.402155	5.769850	0.487536
30	1	0	3.559595	4.618181	1.895308
31	1	0	1.016569	6.703129	-0.881607
32	1	0	3.133768	6.569994	0.418468
33	6	0	-2.384827	2.123655	1.508671
34	7	0	-1.628335	3.177214	1.427968
35	6	0	-2.638390	-0.189096	1.025736
36	6	0	-3.702229	1.791492	2.124291
37	6	0	-3.637008	0.237813	2.144848

38	1	0	-3.806017	2.227485	3.121090
39	1	0	-4.524071	2.159026	1.502416
40	1	0	-3.244449	-0.098421	3.110128
41	1	0	-4.620407	-0.210632	2.007768
42	1	0	-1.987535	-1.002615	1.334675
43	6	0	-3.277036	-0.568692	-0.369672
44	6	0	-3.822896	-2.009538	-0.342351
45	6	0	-4.190445	-2.570911	-1.576519
46	6	0	-3.954057	-2.792875	0.810014
47	6	0	-4.680406	-3.871032	-1.653361
48	1	0	-4.072429	-1.977865	-2.477713
49	6	0	-4.446358	-4.100151	0.733775
50	1	0	-3.667866	-2.411138	1.784442
51	6	0	-4.812759	-4.642471	-0.495081
52	1	0	-4.954600	-4.285987	-2.619550
53	1	0	-4.532784	-4.691789	1.641033
54	1	0	-5.191612	-5.659120	-0.553777
55	6	0	-4.365392	0.437799	-0.776317
56	6	0	-4.016832	1.585625	-1.503002
57	6	0	-5.707922	0.258133	-0.412788
58	6	0	-4.980550	2.540892	-1.830563
59	1	0	-2.991379	1.712655	-1.829725
60	6	0	-6.670380	1.216068	-0.735482
61	1	0	-6.009923	-0.645656	0.107723
62	6	0	-6.308997	2.365272	-1.440805
63	1	0	-4.691691	3.421299	-2.398702
64	1	0	-7.705479	1.055580	-0.445866
65	1	0	-7.058722	3.108761	-1.697502
66	8	0	-2.275775	-0.471515	-1.375519
67	1	0	-1.541012	-1.068872	-1.136470
68	6	0	5.664293	0.737489	-2.873912
69	6	0	4.649654	1.015149	-1.962331
70	6	0	4.042570	-0.006810	-1.213366
71	6	0	4.529126	-1.312928	-1.372277
72	6	0	5.541165	-1.606902	-2.289724
73	6	0	6.099301	-0.581398	-3.046202
74	1	0	2.959075	1.233899	0.187513
75	1	0	6.120281	1.543428	-3.441886
76	1	0	4.329645	2.041536	-1.806809
77	6	0	2.978261	0.226256	-0.218788
78	1	0	5.878977	-2.634198	-2.380177
79	1	0	6.888293	-0.807686	-3.758359
80	6	0	3.252782	-2.159146	0.515846
81	6	0	2.845001	-0.792351	0.795829
82	8	0	4.055167	-2.351610	-0.624597
83	8	0	2.980528	-3.170106	1.128473
84	6	0	2.174494	-0.387802	2.004325
85	8	0	1.611096	0.740064	2.026711
86	6	0	2.131502	-1.182640	3.277437
87	6	0	1.001700	-1.040537	4.096134
88	6	0	3.207734	-1.949615	3.743376
89	6	0	0.929654	-1.677531	5.332972
90	1	0	0.186636	-0.415614	3.745399
91	6	0	3.146638	-2.569537	4.990353
92	1	0	4.096258	-2.061127	3.133497
93	6	0	2.005680	-2.444088	5.785496
94	1	0	0.039935	-1.569341	5.948848
95	1	0	3.992244	-3.156019	5.340042
96	1	0	1.957654	-2.936772	6.753454

IN3-SS-a2

HF=-2431.002036

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.277047	-0.023044	0.395657
2	6	0	1.033648	-0.013200	-1.034971
3	6	0	-0.575259	1.292127	0.750134
4	8	0	-0.430997	-1.047518	0.675616
5	7	0	-1.877872	1.198162	1.105962
6	7	0	-0.270042	2.590013	0.992267
7	6	0	0.864782	-1.381007	-1.734418
8	6	0	1.120037	-2.596042	-1.067800
9	6	0	0.485702	-1.470673	-3.084016

10	6	0	1.027068	-3.822191	-1.723769
11	1	0	1.375160	-2.596175	-0.018876
12	6	0	0.385049	-2.698472	-3.742795
13	1	0	0.256842	-0.579640	-3.654799
14	6	0	0.661081	-3.884047	-3.068036
15	1	0	1.238945	-4.733723	-1.171138
16	1	0	0.090489	-2.717220	-4.789245
17	1	0	0.587753	-4.841335	-3.577956
18	6	0	0.434403	1.111980	-1.900126
19	1	0	0.611060	2.091639	-1.452160
20	1	0	-0.642187	0.964684	-2.029528
21	1	0	0.893105	1.138672	-2.889173
22	6	0	0.961214	3.330195	0.854080
23	6	0	2.021985	3.110298	1.732326
24	6	0	1.010220	4.343587	-0.105353
25	6	0	3.168887	3.896050	1.611047
26	1	0	1.949291	2.329355	2.477703
27	6	0	2.161202	5.122743	-0.214590
28	1	0	0.153951	4.517630	-0.748824
29	6	0	3.242755	4.895526	0.639226
30	1	0	4.003617	3.726360	2.284460
31	1	0	2.209150	5.907958	-0.963210
32	1	0	4.139841	5.501605	0.551223
33	6	0	-2.299588	2.426290	1.537516
34	7	0	-1.348804	3.313121	1.480576
35	6	0	-2.909445	0.138453	1.268173
36	6	0	-3.703139	2.385595	2.039434
37	6	0	-3.904654	0.855775	2.231047
38	1	0	-3.821689	2.952857	2.965884
39	1	0	-4.392241	2.796838	1.294847
40	1	0	-3.656484	0.581953	3.262078
41	1	0	-4.936781	0.561708	2.044070
42	1	0	-2.405467	-0.706720	1.731399
43	6	0	-3.490567	-0.350540	-0.116844
44	6	0	-4.205758	-1.707418	0.058368
45	6	0	-4.451790	-2.447936	-1.108702
46	6	0	-4.610396	-2.247621	1.284663
47	6	0	-5.089354	-3.683824	-1.051139
48	1	0	-4.115478	-2.048997	-2.059839
49	6	0	-5.250291	-3.490400	1.344289
50	1	0	-4.427007	-1.722864	2.216846
51	6	0	-5.494463	-4.211088	0.178271
52	1	0	-5.263843	-4.241459	-1.967516
53	1	0	-5.549142	-3.892124	2.308944
54	1	0	-5.988437	-5.177870	0.224825
55	6	0	-4.432779	0.702736	-0.726790
56	6	0	-3.907897	1.723958	-1.531966
57	6	0	-5.811975	0.698257	-0.471830
58	6	0	-4.733954	2.726006	-2.043861
59	1	0	-2.851564	1.716290	-1.772253
60	6	0	-6.638256	1.702227	-0.980040
61	1	0	-6.249179	-0.107992	0.109380
62	6	0	-6.101407	2.724397	-1.764137
63	1	0	-4.307418	3.505408	-2.670214
64	1	0	-7.704747	1.675814	-0.772167
65	1	0	-6.744526	3.503174	-2.165228
66	8	0	-2.417111	-0.505383	-1.023555
67	1	0	-1.690851	-0.992188	-0.549706
68	6	0	4.337467	1.401244	-3.980433
69	6	0	3.493516	1.396736	-2.870977
70	6	0	3.474012	0.326867	-1.963320
71	6	0	4.395392	-0.703672	-2.171898
72	6	0	5.245632	-0.720446	-3.280195
73	6	0	5.204678	0.327206	-4.194451
74	1	0	2.567540	1.300608	-0.320482
75	1	0	4.321962	2.240426	-4.670331
76	1	0	2.845514	2.249645	-2.692678
77	6	0	2.569764	0.291694	-0.751744
78	1	0	5.933649	-1.552222	-3.392038
79	1	0	5.864885	0.316391	-5.057440
80	6	0	4.073886	-1.698763	0.012393
81	6	0	3.111007	-0.638763	0.318677
82	8	0	4.551383	-1.748097	-1.288982
83	8	0	4.463764	-2.574109	0.754120
84	6	0	2.450349	-0.554177	1.515551
85	8	0	1.352814	0.230316	1.542951
86	6	0	2.748686	-1.160973	2.829962

87	6	0	4.056472	-1.284556	3.324444
88	6	0	1.670308	-1.551887	3.641850
89	6	0	4.278830	-1.794919	4.600169
90	1	0	4.893940	-0.983546	2.706452
91	6	0	1.898467	-2.080268	4.910860
92	1	0	0.663571	-1.451182	3.249714
93	6	0	3.202490	-2.197896	5.395628
94	1	0	5.295300	-1.882269	4.974440
95	1	0	1.058182	-2.397457	5.523204
96	1	0	3.381124	-2.601529	6.389100

TS5-SS-a2

HF=-2430.9933185; 1 imaginary frequencies=-126.2199

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.512832	0.403148	-0.345045
2	6	0	1.785787	0.520795	-1.064564
3	6	0	-0.315455	1.499136	0.308007
4	8	0	-0.000320	-0.721561	-0.182507
5	7	0	-1.612250	1.228873	0.636976
6	7	0	-0.163180	2.806297	0.668398
7	6	0	1.872112	-0.463171	-2.231177
8	6	0	1.657390	-1.847804	-2.088771
9	6	0	2.159498	0.004718	-3.527744
10	6	0	1.737735	-2.711701	-3.180555
11	1	0	1.419607	-2.258658	-1.120454
12	6	0	2.231126	-0.858538	-4.621500
13	1	0	2.316401	1.060732	-3.710769
14	6	0	2.024326	-2.226128	-4.455554
15	1	0	1.577439	-3.775052	-3.023083
16	1	0	2.448321	-0.451550	-5.605965
17	1	0	2.085444	-2.901903	-5.304580
18	6	0	2.286910	1.912160	-1.430040
19	1	0	2.520893	2.506838	-0.552111
20	1	0	1.560249	2.470967	-2.032979
21	1	0	3.204803	1.835435	-2.014021
22	6	0	0.979110	3.681452	0.783770
23	6	0	1.949272	3.437092	1.755932
24	6	0	1.006188	4.829189	-0.008303
25	6	0	2.995514	4.351720	1.896300
26	1	0	1.882605	2.538937	2.359291
27	6	0	2.054827	5.733920	0.146386
28	1	0	0.217966	5.002937	-0.733633
29	6	0	3.052536	5.493199	1.094593
30	1	0	3.763708	4.170352	2.642421
31	1	0	2.090993	6.626087	-0.471859
32	1	0	3.869270	6.199761	1.212684
33	6	0	-2.150435	2.340754	1.218173
34	7	0	-1.308809	3.329447	1.250397
35	6	0	-2.544008	0.069571	0.651363
36	6	0	-3.520628	2.088752	1.750021
37	6	0	-3.551713	0.535088	1.745244
38	1	0	-3.648366	2.515280	2.748012
39	1	0	-4.281530	2.518483	1.092119
40	1	0	-3.206558	0.159915	2.714009
41	1	0	-4.555168	0.148644	1.569526
42	1	0	-1.969334	-0.796126	0.967494
43	6	0	-3.160614	-0.227419	-0.775037
44	6	0	-3.769904	-1.643735	-0.806467
45	6	0	-4.118886	-2.155753	-2.067138
46	6	0	-3.977901	-2.449784	0.319160
47	6	0	-4.664080	-3.429587	-2.196629
48	1	0	-3.942225	-1.545519	-2.947013
49	6	0	-4.526286	-3.730489	0.189612
50	1	0	-3.707576	-2.110202	1.313649
51	6	0	-4.872681	-4.223889	-1.065399
52	1	0	-4.922464	-3.806194	-3.182782
53	1	0	-4.673192	-4.340018	1.077152
54	1	0	-5.295451	-5.219886	-1.165144
55	6	0	-4.195535	0.837779	-1.173119
56	6	0	-3.774582	1.996812	-1.841230
57	6	0	-5.555923	0.701754	-0.861559

58	6	0	-4.685562	3.004522	-2.162152
59	1	0	-2.733181	2.091251	-2.125802
60	6	0	-6.466145	1.711549	-1.178123
61	1	0	-5.912375	-0.207065	-0.386128
62	6	0	-6.033208	2.870455	-1.824709
63	1	0	-4.340668	3.893635	-2.683622
64	1	0	-7.516455	1.584672	-0.929376
65	1	0	-6.742178	3.654682	-2.076144
66	8	0	-2.135686	-0.139622	-1.756334
67	1	0	-1.407056	-0.729131	-1.479142
68	6	0	6.432149	0.220200	-1.344972
69	6	0	5.222883	0.570891	-0.752072
70	6	0	4.317953	-0.406643	-0.304624
71	6	0	4.703437	-1.749542	-0.414359
72	6	0	5.910052	-2.117711	-1.016132
73	6	0	6.766683	-1.130832	-1.491599
74	1	0	3.014477	0.863033	0.852297
75	1	0	7.115238	0.993680	-1.684276
76	1	0	4.975865	1.619174	-0.613447
77	6	0	3.021719	-0.092749	0.335095
78	1	0	6.158170	-3.172130	-1.081064
79	1	0	7.706918	-1.413780	-1.957115
80	6	0	2.872772	-2.532558	0.980117
81	6	0	2.445939	-1.153857	1.144327
82	8	0	3.940003	-2.760435	0.094455
83	8	0	2.429997	-3.530585	1.510211
84	6	0	1.474215	-0.726713	2.115051
85	8	0	1.231931	0.508715	2.217251
86	6	0	0.673384	-1.612573	3.032250
87	6	0	-0.059478	-2.722475	2.589539
88	6	0	0.533282	-1.197585	4.365026
89	6	0	-0.904923	-3.403203	3.466497
90	1	0	0.035843	-3.051584	1.563227
91	6	0	-0.287838	-1.896424	5.248869
92	1	0	1.074047	-0.317237	4.699008
93	6	0	-1.014672	-3.000948	4.799711
94	1	0	-1.469516	-4.260286	3.107661
95	1	0	-0.366531	-1.574376	6.284361
96	1	0	-1.661194	-3.545302	5.483800

TS6-R

HF=-2008.0108844; 1 imaginary frequencies= -152.1398

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.172666	0.748565	-0.463469
2	7	0	0.998767	0.490918	-1.096323
3	7	0	-0.592219	1.870154	-1.096618
4	6	0	-1.805209	2.609538	-0.907616
5	6	0	-3.016163	2.082387	-1.357203
6	6	0	-1.746530	3.875242	-0.322611
7	6	0	-4.188708	2.820081	-1.185434
8	1	0	-3.031970	1.113463	-1.844114
9	6	0	-2.920904	4.609433	-0.162761
10	1	0	-0.789426	4.267482	0.004840
11	6	0	-4.142574	4.080558	-0.587083
12	1	0	-5.134792	2.412064	-1.529286
13	1	0	-2.881716	5.593521	0.295427
14	1	0	-5.056271	4.654107	-0.458373
15	6	0	1.202144	1.419802	-2.086219
16	7	0	0.252853	2.306650	-2.122899
17	6	0	1.995451	-0.600724	-1.114050
18	6	0	2.393517	1.083632	-2.918524
19	6	0	2.601497	-0.410945	-2.538258
20	1	0	2.199088	1.227788	-3.984336
21	1	0	3.255023	1.698408	-2.640119
22	1	0	2.043693	-1.042304	-3.237580
23	1	0	3.652000	-0.698287	-2.583049
24	1	0	1.442437	-1.534096	-1.019887
25	6	0	3.007580	-0.505230	0.093027
26	6	0	3.791097	-1.827594	0.251230
27	6	0	4.524381	-1.989562	1.438265
28	6	0	3.800330	-2.873635	-0.678293

29	6	0	5.249532	-3.151800	1.682317
30	1	0	4.503282	-1.193171	2.175170
31	6	0	4.527113	-4.044602	-0.434366
32	1	0	3.235107	-2.805050	-1.601712
33	6	0	5.255788	-4.187696	0.743206
34	1	0	5.807970	-3.253395	2.609508
35	1	0	4.513244	-4.844681	-1.170075
36	1	0	5.819208	-5.097553	0.932924
37	6	0	3.964199	0.688778	-0.070849
38	6	0	3.590230	1.941827	0.435396
39	6	0	5.193308	0.577012	-0.736652
40	6	0	4.409865	3.057055	0.254883
41	1	0	2.661284	2.023633	0.987366
42	6	0	6.011991	1.692801	-0.920320
43	1	0	5.524725	-0.392009	-1.097866
44	6	0	5.620711	2.939780	-0.429797
45	1	0	4.102823	4.019504	0.656626
46	1	0	6.962036	1.582696	-1.437117
47	1	0	6.259718	3.808075	-0.568164
48	8	0	2.273894	-0.263092	1.276312
49	1	0	1.481994	-0.870548	1.271459
50	6	0	-0.871583	-0.637294	0.869481
51	8	0	0.013892	-1.547081	0.884208
52	6	0	-1.044770	0.208031	2.133833
53	6	0	-1.930447	1.290411	2.235554
54	6	0	-0.309408	-0.162065	3.266213
55	6	0	-2.057958	1.998135	3.430328
56	1	0	-2.526062	1.585553	1.379375
57	6	0	-0.432592	0.547121	4.461842
58	1	0	0.355650	-1.015411	3.199804
59	6	0	-1.305034	1.631911	4.548551
60	1	0	-2.746305	2.837791	3.485426
61	1	0	0.152724	0.246721	5.327052
62	1	0	-1.403023	2.184730	5.479358
63	6	0	-2.161880	-1.069432	0.170178
64	6	0	-3.328098	-1.228642	0.848341
65	6	0	-2.064911	-1.545274	-1.219649
66	6	0	-4.488743	-1.834990	0.251961
67	1	0	-3.397733	-0.899675	1.881169
68	6	0	-4.380245	-2.272792	-1.078401
69	8	0	-1.108316	-1.462705	-1.956684
70	8	0	-3.215660	-2.111536	-1.769807
71	6	0	-5.714240	-2.020162	0.920150
72	1	0	-5.805489	-1.687133	1.950859
73	6	0	-5.450476	-2.878250	-1.739173
74	1	0	-5.322406	-3.203181	-2.766394
75	6	0	-6.785873	-2.619816	0.273502
76	6	0	-6.650722	-3.048106	-1.056570
77	1	0	-7.727494	-2.759831	0.795774
78	1	0	-7.489618	-3.518900	-1.561175

IN4-R

HF=-2008.0207403

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.533806	-0.883348	-0.319093
2	7	0	-0.615725	-0.603706	-0.971588
3	7	0	0.979392	-2.004907	-0.919881
4	6	0	2.122109	-2.832871	-0.643844
5	6	0	3.144568	-2.903630	-1.588760
6	6	0	2.134295	-3.614561	0.509803
7	6	0	4.213172	-3.768200	-1.356402
8	1	0	3.101934	-2.274412	-2.469514
9	6	0	3.213438	-4.467880	0.734665
10	1	0	1.318118	-3.544077	1.220635
11	6	0	4.249843	-4.547194	-0.197485
12	1	0	5.019740	-3.829499	-2.081349
13	1	0	3.239664	-5.072134	1.636410
14	1	0	5.086995	-5.216955	-0.020925
15	6	0	-0.771168	-1.504139	-1.986370
16	7	0	0.179684	-2.394284	-1.987344
17	6	0	-1.773293	0.295419	-0.813659
18	6	0	-1.962841	-1.166842	-2.825303

19	6	0	-2.332659	0.242460	-2.265975
20	1	0	-1.713401	-1.146194	-3.889749
21	1	0	-2.766902	-1.891929	-2.675973
22	1	0	-1.832791	1.012818	-2.863648
23	1	0	-3.406180	0.423238	-2.306865
24	1	0	-1.407417	1.280487	-0.533100
25	6	0	-2.735528	-0.230344	0.368207
26	6	0	-3.443291	0.989953	0.999708
27	6	0	-3.794507	0.912210	2.354165
28	6	0	-3.776338	2.153767	0.293356
29	6	0	-4.457441	1.964251	2.983005
30	1	0	-3.522551	0.019284	2.905858
31	6	0	-4.440826	3.210790	0.922258
32	1	0	-3.520281	2.258898	-0.757903
33	6	0	-4.784634	3.119943	2.269856
34	1	0	-4.715338	1.883336	4.036002
35	1	0	-4.684321	4.105297	0.354302
36	1	0	-5.299056	3.941833	2.760942
37	6	0	-3.777667	-1.248744	-0.147781
38	6	0	-3.498176	-2.619367	-0.044329
39	6	0	-5.000143	-0.862180	-0.715953
40	6	0	-4.398184	-3.571941	-0.525024
41	1	0	-2.575946	-2.925332	0.434683
42	6	0	-5.900201	-1.813680	-1.199491
43	1	0	-5.266786	0.189457	-0.761176
44	6	0	-5.600567	-3.173916	-1.112031
45	1	0	-4.160393	-4.628814	-0.433026
46	1	0	-6.842817	-1.488779	-1.632743
47	1	0	-6.303062	-3.915481	-1.483397
48	8	0	-1.969696	-0.907286	1.320941
49	1	0	-1.138733	-0.328222	1.533840
50	6	0	1.097261	0.116629	0.755824
51	8	0	0.077484	0.511203	1.540651
52	6	0	2.273388	-0.484155	1.585142
53	6	0	3.596605	-0.583697	1.135149
54	6	0	1.977286	-0.872869	2.896359
55	6	0	4.595979	-1.075854	1.976621
56	1	0	3.856528	-0.299200	0.122040
57	6	0	2.973799	-1.374941	3.734053
58	1	0	0.958713	-0.743391	3.244541
59	6	0	4.289050	-1.477155	3.277602
60	1	0	5.617497	-1.144707	1.610881
61	1	0	2.724215	-1.673209	4.749675
62	1	0	5.069488	-1.858040	3.931871
63	6	0	1.619008	1.364889	-0.057545
64	6	0	1.326125	2.587846	0.453781
65	6	0	2.360900	1.265532	-1.309595
66	6	0	1.778998	3.801338	-0.168935
67	1	0	0.725720	2.613515	1.359575
68	6	0	2.511057	3.683797	-1.363480
69	8	0	2.644303	0.242773	-1.906892
70	8	0	2.763568	2.456364	-1.905696
71	6	0	1.533823	5.091575	0.340243
72	1	0	0.968004	5.190693	1.262745
73	6	0	2.994486	4.804248	-2.041087
74	1	0	3.555856	4.667561	-2.959483
75	6	0	2.010047	6.213182	-0.323744
76	6	0	2.740526	6.066301	-1.513895
77	1	0	1.819084	7.204486	0.076237
78	1	0	3.113051	6.945592	-2.031812

TS7-RZ

HF=-2430.981774; 1 imaginary frequencies= -125.7192

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.145302	1.344060	-0.530413
2	7	0	1.300032	0.913231	-1.081511
3	7	0	-0.075938	2.541368	-1.118122
4	6	0	-1.179110	3.462877	-1.015130
5	6	0	-2.307381	3.261338	-1.809641
6	6	0	-1.042291	4.595318	-0.214555
7	6	0	-3.337116	4.202301	-1.767425

8	1	0	-2.357982	2.395387	-2.459868
9	6	0	-2.073184	5.532834	-0.187711
10	1	0	-0.148486	4.725676	0.385931
11	6	0	-3.221485	5.334174	-0.957946
12	1	0	-4.222688	4.055285	-2.378748
13	1	0	-1.979715	6.415526	0.437754
14	1	0	-4.023426	6.066756	-0.933423
15	6	0	1.673742	1.822650	-2.037054
16	7	0	0.867494	2.840287	-2.085345
17	6	0	2.158656	-0.301527	-1.080540
18	6	0	2.827850	1.338134	-2.844913
19	6	0	2.812644	-0.174761	-2.490366
20	1	0	2.675547	1.526812	-3.910439
21	1	0	3.758930	1.823062	-2.537638
22	1	0	2.187527	-0.711474	-3.211063
23	1	0	3.815087	-0.599215	-2.519308
24	1	0	1.495196	-1.161047	-1.006781
25	6	0	3.153227	-0.321212	0.154290
26	6	0	3.711662	-1.747354	0.372692
27	6	0	4.174726	-2.055740	1.661234
28	6	0	3.802996	-2.735052	-0.616491
29	6	0	4.715449	-3.306384	1.948899
30	1	0	4.085452	-1.304104	2.437651
31	6	0	4.342669	-3.993267	-0.328213
32	1	0	3.444816	-2.551773	-1.623943
33	6	0	4.803422	-4.282994	0.953677
34	1	0	5.062625	-3.521914	2.956046
35	1	0	4.393409	-4.745228	-1.111309
36	1	0	5.219983	-5.261089	1.178583
37	6	0	4.303101	0.690115	-0.028838
38	6	0	4.140935	2.007798	0.423595
39	6	0	5.508742	0.344892	-0.656591
40	6	0	5.142293	2.959549	0.224062
41	1	0	3.231834	2.273411	0.950192
42	6	0	6.509308	1.297036	-0.859268
43	1	0	5.679231	-0.679828	-0.972388
44	6	0	6.327777	2.611136	-0.425203
45	1	0	4.997006	3.974854	0.584347
46	1	0	7.436545	1.005743	-1.345972
47	1	0	7.108269	3.351801	-0.578001
48	8	0	2.447350	0.083117	1.303242
49	1	0	1.514409	-0.295067	1.267537
50	6	0	-0.720924	0.601110	0.534538
51	8	0	-0.027441	-0.546288	0.895565
52	6	0	-0.932434	1.622751	1.703143
53	6	0	-2.106115	2.369338	1.870051
54	6	0	0.116772	1.831429	2.611475
55	6	0	-2.242373	3.273609	2.926741
56	1	0	-2.925587	2.263864	1.168742
57	6	0	-0.012839	2.744297	3.656288
58	1	0	1.036552	1.270184	2.517090
59	6	0	-1.196445	3.465543	3.825923
60	1	0	-3.169826	3.830003	3.035712
61	1	0	0.812718	2.879086	4.350236
62	1	0	-1.300509	4.166678	4.650019
63	6	0	-2.051640	0.131102	-0.101239
64	6	0	-3.081678	-0.268559	0.696500
65	6	0	-2.096600	-0.172335	-1.527474
66	6	0	-4.252207	-0.905155	0.160518
67	1	0	-3.040548	-0.090711	1.765754
68	6	0	-4.294329	-1.130160	-1.225327
69	8	0	-1.229841	0.080387	-2.348129
70	8	0	-3.253810	-0.751142	-2.021243
71	6	0	-5.352472	-1.315167	0.939138
72	1	0	-5.326208	-1.148402	2.012680
73	6	0	-5.391864	-1.737688	-1.836576
74	1	0	-5.380506	-1.893955	-2.910108
75	6	0	-6.448880	-1.922425	0.343269
76	6	0	-6.465940	-2.131648	-1.045232
77	1	0	-7.292816	-2.236986	0.949722
78	1	0	-7.324587	-2.608141	-1.509703
79	6	0	-0.886260	-1.644373	2.315986
80	8	0	-0.779959	-1.007954	3.318268
81	6	0	-1.409605	-2.755386	1.737453
82	6	0	-1.180922	-3.292013	0.388797
83	6	0	-2.239125	-3.897209	-0.320114
84	6	0	0.096255	-3.337482	-0.205513

85	6	0	-2.041044	-4.477970	-1.573470
86	1	0	-3.234764	-3.907630	0.113583
87	6	0	0.293773	-3.917524	-1.456312
88	1	0	0.941794	-2.947436	0.349404
89	6	0	-0.774136	-4.486764	-2.155919
90	1	0	-2.884498	-4.925089	-2.094753
91	1	0	1.297335	-3.954015	-1.873917
92	1	0	-0.616199	-4.943881	-3.129302
93	6	0	-2.299657	-3.558739	2.684645
94	1	0	-2.018829	-4.619972	2.682579
95	1	0	-2.215581	-3.188233	3.709883
96	1	0	-3.362481	-3.505130	2.403788

IN5-RZ

HF=-2430.990549

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.326079	-1.238714	-0.475995
2	7	0	-0.876898	-1.028551	-1.055179
3	7	0	0.783517	-2.374873	-1.045070
4	6	0	2.020708	-3.099873	-0.875560
5	6	0	3.071121	-2.848490	-1.758306
6	6	0	2.087244	-4.117820	0.073815
7	6	0	4.227202	-3.623305	-1.654889
8	1	0	2.962295	-2.071908	-2.507480
9	6	0	3.242242	-4.891353	0.167484
10	1	0	1.254200	-4.289543	0.742334
11	6	0	4.312760	-4.636673	-0.698514
12	1	0	5.056983	-3.439464	-2.331287
13	1	0	3.299660	-5.679586	0.911767
14	1	0	5.213866	-5.239599	-0.627113
15	6	0	-1.037297	-1.984426	-2.026388
16	7	0	-0.051630	-2.832249	-2.041053
17	6	0	-2.021253	-0.071664	-1.031490
18	6	0	-2.240020	-1.734159	-2.868055
19	6	0	-2.586443	-0.274965	-2.457322
20	1	0	-2.002562	-1.829175	-3.930926
21	1	0	-3.044833	-2.436112	-2.632011
22	1	0	-2.083582	0.425204	-3.131779
23	1	0	-3.657375	-0.077958	-2.501078
24	1	0	-1.613472	0.926903	-0.896838
25	6	0	-3.030999	-0.372186	0.147850
26	6	0	-3.991546	0.817413	0.356984
27	6	0	-4.845757	0.746076	1.470926
28	6	0	-4.038570	1.963199	-0.443630
29	6	0	-5.728972	1.779627	1.764054
30	1	0	-4.799390	-0.127062	2.114735
31	6	0	-4.925274	3.004386	-0.147092
32	1	0	-3.376705	2.092968	-1.292866
33	6	0	-5.775444	2.915376	0.950734
34	1	0	-6.377509	1.703308	2.632970
35	1	0	-4.926151	3.890535	-0.774761
36	1	0	-6.460727	3.726716	1.181450
37	6	0	-3.802183	-1.681721	-0.084766
38	6	0	-3.260145	-2.897558	0.354982
39	6	0	-5.032567	-1.707423	-0.758773
40	6	0	-3.913573	-4.105037	0.102566
41	1	0	-2.333646	-2.886551	0.910937
42	6	0	-5.680911	-2.916409	-1.012871
43	1	0	-5.500838	-0.772191	-1.067291
44	6	0	-5.116461	-4.118310	-0.583877
45	1	0	-3.476734	-5.034787	0.455532
46	1	0	-6.634917	-2.914439	-1.534445
47	1	0	-5.626274	-5.057234	-0.779456
48	8	0	-2.288604	-0.578718	1.339983
49	1	0	-1.600536	0.118068	1.399136
50	6	0	1.061607	-0.343913	0.544402
51	8	0	0.085606	0.658682	0.869683
52	6	0	1.461389	-1.249171	1.743830
53	6	0	2.783928	-1.606964	2.019635
54	6	0	0.445851	-1.799976	2.540784
55	6	0	3.098078	-2.459081	3.080986

56	1	0	3.590280	-1.238913	1.400211
57	6	0	0.753718	-2.659618	3.592755
58	1	0	-0.589058	-1.543436	2.354394
59	6	0	2.084246	-2.993689	3.877972
60	1	0	4.140663	-2.707013	3.275311
61	1	0	-0.050904	-3.059454	4.204520
62	1	0	2.324938	-3.656027	4.706486
63	6	0	2.258353	0.384928	-0.105362
64	6	0	3.087424	1.141143	0.677605
65	6	0	2.366887	0.491849	-1.556542
66	6	0	4.156150	1.915880	0.117479
67	6	0	4.317213	1.898820	-1.277968
68	8	0	1.602502	0.019413	-2.383071
69	8	0	3.449968	1.190097	-2.060302
70	6	0	5.059839	2.678627	0.884851
71	1	0	4.925271	2.701324	1.968410
72	6	0	5.343810	2.594827	-1.909986
73	1	0	5.432500	2.547838	-2.987521
74	6	0	6.082874	3.380543	0.270513
75	6	0	6.226161	3.334273	-1.129126
76	1	0	6.771507	3.964904	0.873200
77	1	0	7.027783	3.884367	-1.613467
78	6	0	0.478693	1.680216	1.911108
79	8	0	1.052119	1.218739	2.903875
80	6	0	0.050372	2.969310	1.613202
81	6	0	0.153379	3.933584	2.782598
82	1	0	0.793357	3.506937	3.556064
83	1	0	0.576577	4.899864	2.474648
84	1	0	-0.821513	4.148324	3.248841
85	6	0	-0.501600	3.485505	0.362574
86	6	0	-0.251160	2.942478	-0.926125
87	6	0	-1.285167	4.670083	0.373467
88	6	0	-0.752411	3.521660	-2.090257
89	1	0	0.372623	2.064045	-1.018549
90	6	0	-1.799490	5.236811	-0.789499
91	1	0	-1.512031	5.145176	1.321509
92	6	0	-1.536460	4.678577	-2.040278
93	1	0	-0.500544	3.073905	-3.050387
94	1	0	-2.396494	6.143708	-0.715177
95	1	0	-1.919082	5.134341	-2.949605
96	1	0	2.942975	1.149872	1.754426

TS8-RZ

HF=-2430.9849364; 1 imaginary frequencies=-168.3423

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.269744	1.312578	-0.527636
2	7	0	1.374292	0.751140	-1.068004
3	7	0	0.196192	2.533853	-1.093666
4	6	0	-0.793809	3.576026	-0.963216
5	6	0	-1.931245	3.535532	-1.768728
6	6	0	-0.530996	4.648431	-0.113050
7	6	0	-2.840731	4.590956	-1.691422
8	1	0	-2.078478	2.697086	-2.440096
9	6	0	-1.445947	5.698071	-0.049853
10	1	0	0.365386	4.647583	0.497846
11	6	0	-2.600439	5.667874	-0.835430
12	1	0	-3.733937	4.572722	-2.308991
13	1	0	-1.256566	6.536143	0.614143
14	1	0	-3.311437	6.487879	-0.783932
15	6	0	1.839895	1.612904	-2.031163
16	7	0	1.158209	2.718050	-2.066555
17	6	0	2.149346	-0.517313	-1.027602
18	6	0	2.922066	0.995538	-2.851780
19	6	0	2.770185	-0.500163	-2.454584
20	1	0	2.753673	1.167668	-3.917785
21	1	0	3.904661	1.396484	-2.588645
22	1	0	2.071103	-0.987795	-3.141524
23	1	0	3.719893	-1.032508	-2.495279
24	1	0	1.447263	-1.335083	-0.896794
25	6	0	3.182336	-0.560053	0.176167
26	6	0	3.582876	-2.021036	0.472805

27	6	0	4.210622	-2.268158	1.704431
28	6	0	3.360557	-3.101803	-0.388775
29	6	0	4.605132	-3.554285	2.060666
30	1	0	4.368454	-1.439626	2.386784
31	6	0	3.756104	-4.395137	-0.031007
32	1	0	2.866610	-2.967490	-1.345614
33	6	0	4.380308	-4.625836	1.191869
34	1	0	5.083312	-3.722594	3.021937
35	1	0	3.563181	-5.219339	-0.712189
36	1	0	4.683262	-5.631233	1.471261
37	6	0	4.422411	0.308844	-0.098720
38	6	0	4.422816	1.660546	0.274701
39	6	0	5.558968	-0.208622	-0.736490
40	6	0	5.518467	2.477980	-0.008226
41	1	0	3.566860	2.063921	0.802578
42	6	0	6.652520	0.609544	-1.023964
43	1	0	5.599898	-1.262538	-0.994323
44	6	0	6.634811	1.958534	-0.665339
45	1	0	5.499715	3.522497	0.291663
46	1	0	7.523662	0.186935	-1.517568
47	1	0	7.488138	2.594805	-0.884001
48	8	0	2.576830	-0.001183	1.328968
49	1	0	1.695146	-0.415188	1.453742
50	6	0	-0.707953	0.721163	0.494813
51	8	0	-0.032443	-0.545595	0.917876
52	6	0	-0.821722	1.713301	1.681178
53	6	0	-2.003920	2.425090	1.917577
54	6	0	0.286929	1.963263	2.503830
55	6	0	-2.088796	3.342019	2.966898
56	1	0	-2.857182	2.278692	1.265882
57	6	0	0.203552	2.885256	3.545329
58	1	0	1.217119	1.433412	2.344092
59	6	0	-0.986654	3.574578	3.787163
60	1	0	-3.019543	3.877762	3.132810
61	1	0	1.071301	3.054718	4.177166
62	1	0	-1.051478	4.286522	4.605833
63	6	0	-2.028273	0.313869	-0.109502
64	6	0	-2.934891	-0.329330	0.768100
65	6	0	-2.139966	0.141688	-1.521366
66	6	0	-4.182430	-0.820249	0.207092
67	1	0	-2.966970	-0.031387	1.810550
68	6	0	-4.323437	-0.833700	-1.190923
69	8	0	-1.310793	0.458212	-2.379683
70	8	0	-3.332934	-0.378091	-2.016478
71	6	0	-5.273779	-1.249094	0.984860
72	1	0	-5.188526	-1.216185	2.067316
73	6	0	-5.496405	-1.281943	-1.800902
74	1	0	-5.557762	-1.275193	-2.884333
75	6	0	-6.447320	-1.696008	0.388321
76	6	0	-6.553755	-1.718050	-1.008239
77	1	0	-7.279558	-2.023324	1.004715
78	1	0	-7.467860	-2.068406	-1.479650
79	6	0	-0.734691	-1.294242	1.928004
80	8	0	-0.449505	-1.034085	3.086366
81	6	0	-1.778241	-2.187577	1.478174
82	6	0	-2.574501	-2.735338	2.648653
83	1	0	-2.625314	-1.994590	3.449792
84	1	0	-3.593915	-2.998684	2.347788
85	1	0	-2.114703	-3.635635	3.080900
86	6	0	-1.714028	-3.027483	0.263392
87	6	0	-1.000361	-2.692660	-0.910398
88	6	0	-2.424644	-4.252409	0.222200
89	6	0	-1.002980	-3.512415	-2.037576
90	1	0	-0.455953	-1.764496	-0.950243
91	6	0	-2.415770	-5.076833	-0.900063
92	1	0	-2.986303	-4.580535	1.088172
93	6	0	-1.705471	-4.716646	-2.045663
94	1	0	-0.454532	-3.194685	-2.921656
95	1	0	-2.973475	-6.010235	-0.874880
96	1	0	-1.704178	-5.356661	-2.923930

IN6-RZ

HF=-2431.011111

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.326745	1.353627	-0.461275
2	7	0	1.462458	0.821574	-0.965690
3	7	0	0.244978	2.578599	-1.016989
4	6	0	-0.790980	3.578316	-0.928870
5	6	0	-1.929805	3.441740	-1.721641
6	6	0	-0.577357	4.698759	-0.128828
7	6	0	-2.891602	4.451789	-1.682052
8	1	0	-2.030854	2.568357	-2.356783
9	6	0	-1.545045	5.702043	-0.102952
10	1	0	0.324338	4.772026	0.470205
11	6	0	-2.701953	5.576394	-0.875564
12	1	0	-3.787309	4.360023	-2.289338
13	1	0	-1.394898	6.578338	0.520707
14	1	0	-3.454577	6.359873	-0.853399
15	6	0	1.918137	1.688936	-1.931034
16	7	0	1.217905	2.780636	-1.977068
17	6	0	2.209869	-0.461342	-0.964235
18	6	0	2.979381	1.070361	-2.776535
19	6	0	2.800630	-0.429519	-2.406692
20	1	0	2.792885	1.265080	-3.835512
21	1	0	3.974552	1.446590	-2.526263
22	1	0	2.071026	-0.881076	-3.086080
23	1	0	3.735273	-0.984448	-2.480397
24	1	0	1.490388	-1.266495	-0.834387
25	6	0	3.288575	-0.562470	0.196437
26	6	0	3.737956	-2.028692	0.373619
27	6	0	4.483171	-2.325344	1.526753
28	6	0	3.446317	-3.072005	-0.512789
29	6	0	4.925420	-3.619695	1.781385
30	1	0	4.697649	-1.528035	2.230780
31	6	0	3.889249	-4.374111	-0.257176
32	1	0	2.862727	-2.901880	-1.411500
33	6	0	4.630867	-4.652717	0.887296
34	1	0	5.496219	-3.824766	2.683151
35	1	0	3.642267	-5.168094	-0.956646
36	1	0	4.971427	-5.665031	1.086860
37	6	0	4.490944	0.360801	-0.068402
38	6	0	4.449581	1.695369	0.361210
39	6	0	5.630670	-0.086609	-0.751103
40	6	0	5.507358	2.564387	0.089485
41	1	0	3.591040	2.045510	0.922090
42	6	0	6.686844	0.783393	-1.026773
43	1	0	5.702835	-1.126024	-1.055886
44	6	0	6.627115	2.114801	-0.612105
45	1	0	5.456390	3.594709	0.431676
46	1	0	7.561340	0.414676	-1.556317
47	1	0	7.450723	2.791704	-0.822537
48	8	0	2.731074	-0.103671	1.419030
49	1	0	1.941640	-0.644305	1.616520
50	6	0	-0.670481	0.750724	0.530395
51	8	0	0.086114	-0.435281	1.088798
52	6	0	-0.843473	1.715790	1.727994
53	6	0	-2.039288	2.419739	1.905783
54	6	0	0.210582	1.924624	2.630140
55	6	0	-2.192241	3.296070	2.981014
56	1	0	-2.839188	2.285341	1.184731
57	6	0	0.059056	2.809689	3.697973
58	1	0	1.148816	1.395330	2.500257
59	6	0	-1.144803	3.493395	3.881208
60	1	0	-3.130847	3.828720	3.108167
61	1	0	0.883172	2.959333	4.390597
62	1	0	-1.263309	4.176844	4.717995
63	6	0	-1.916716	0.285881	-0.112273
64	6	0	-2.786648	-0.515974	0.818978
65	6	0	-1.958383	0.092432	-1.495924
66	6	0	-4.123161	-0.773206	0.161095
67	1	0	-2.974170	0.052120	1.739712
68	6	0	-4.207529	-0.741450	-1.238621
69	8	0	-1.104964	0.404557	-2.348643
70	8	0	-3.128082	-0.471262	-2.037607

71	6	0	-5.302225	-0.998950	0.882827
72	1	0	-5.265723	-0.977546	1.969368
73	6	0	-5.418469	-0.980514	-1.895180
74	1	0	-5.433011	-0.951119	-2.980241
75	6	0	-6.517378	-1.236224	0.241102
76	6	0	-6.569112	-1.237139	-1.155125
77	1	0	-7.415965	-1.413551	0.825461
78	1	0	-7.508884	-1.422121	-1.668882
79	6	0	-0.524025	-1.569396	1.539890
80	8	0	0.200883	-2.361445	2.102309
81	6	0	-2.030991	-1.835020	1.324415
82	6	0	-2.567167	-2.231236	2.719331
83	1	0	-2.378165	-1.424151	3.435769
84	1	0	-3.646691	-2.397711	2.688764
85	1	0	-2.076723	-3.134950	3.087077
86	6	0	-2.134459	-2.992185	0.314089
87	6	0	-1.355890	-3.000314	-0.854295
88	6	0	-3.024607	-4.057864	0.508404
89	6	0	-1.464859	-4.026906	-1.791473
90	1	0	-0.667471	-2.186055	-1.054466
91	6	0	-3.133918	-5.088614	-0.425887
92	1	0	-3.646928	-4.096017	1.394868
93	6	0	-2.354278	-5.079904	-1.581470
94	1	0	-0.853488	-3.997550	-2.689615
95	1	0	-3.834249	-5.900106	-0.245233
96	1	0	-2.439593	-5.882351	-2.309434

TS9-RZ

HF=-2430.9720464; 1 imaginary frequencies=-205.3411

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.165259	1.254432	-0.367600
2	7	0	1.055008	0.441447	-1.018054
3	7	0	0.039551	2.284794	-1.238769
4	6	0	-0.565875	3.576293	-1.060002
5	6	0	-1.475812	4.046336	-2.007389
6	6	0	-0.126981	4.393219	-0.019976
7	6	0	-1.966558	5.344182	-1.890190
8	1	0	-1.804764	3.387581	-2.800103
9	6	0	-0.635417	5.687313	0.097502
10	1	0	0.603238	4.017717	0.687227
11	6	0	-1.552349	6.165682	-0.838062
12	1	0	-2.681637	5.712273	-2.620513
13	1	0	-0.302645	6.320502	0.914865
14	1	0	-1.941999	7.176481	-0.751145
15	6	0	1.368499	0.998942	-2.236002
16	7	0	0.770690	2.134997	-2.416461
17	6	0	1.890808	-0.741155	-0.714285
18	6	0	2.329995	0.165548	-3.010762
19	6	0	2.398645	-1.119789	-2.141736
20	1	0	1.973203	-0.032881	-4.025605
21	1	0	3.299730	0.666553	-3.086947
22	1	0	1.730515	-1.881332	-2.553485
23	1	0	3.404768	-1.537804	-2.116493
24	1	0	1.261733	-1.532515	-0.312597
25	6	0	3.004470	-0.420331	0.359527
26	6	0	3.770580	-1.689709	0.785731
27	6	0	4.713825	-1.541389	1.817077
28	6	0	3.557417	-2.970453	0.264310
29	6	0	5.430793	-2.632430	2.298342
30	1	0	4.872961	-0.556544	2.245093
31	6	0	4.279021	-4.068275	0.746174
32	1	0	2.820432	-3.144414	-0.511306
33	6	0	5.218999	-3.904970	1.759973
34	1	0	6.154814	-2.490777	3.096458
35	1	0	4.096035	-5.053373	0.324597
36	1	0	5.778250	-4.758803	2.133010
37	6	0	3.967648	0.662085	-0.150356
38	6	0	3.696905	2.014268	0.099941
39	6	0	5.115213	0.336474	-0.888717
40	6	0	4.536912	3.013309	-0.394399
41	1	0	2.831524	2.276366	0.696806
42	6	0	5.953959	1.335117	-1.385764

43	1	0	5.370960	-0.705140	-1.057843
44	6	0	5.665126	2.679283	-1.144029
45	1	0	4.307033	4.055764	-0.190747
46	1	0	6.840052	1.059434	-1.951694
47	1	0	6.318965	3.457761	-1.527917
48	8	0	2.366455	0.122999	1.513080
49	1	0	1.846347	-0.593829	1.931228
50	6	0	-1.319150	0.623535	1.009040
51	8	0	-0.550234	-0.240154	1.828159
52	6	0	-1.489676	1.902616	1.779204
53	6	0	-2.694036	2.612888	1.730486
54	6	0	-0.478262	2.328926	2.656035
55	6	0	-2.883848	3.732548	2.541248
56	1	0	-3.478939	2.294546	1.056278
57	6	0	-0.679569	3.434942	3.477839
58	1	0	0.461830	1.788291	2.687495
59	6	0	-1.883847	4.142571	3.422599
60	1	0	-3.821884	4.278128	2.486847
61	1	0	0.105300	3.745299	4.162920
62	1	0	-2.040169	5.006188	4.063907
63	6	0	-2.369138	-0.057089	0.325643
64	6	0	-2.777331	-1.392144	0.935146
65	6	0	-3.020277	0.523735	-0.789921
66	6	0	-4.082509	-1.901095	0.344978
67	1	0	-2.995001	-1.201844	2.000409
68	6	0	-4.628877	-1.289869	-0.789864
69	8	0	-2.772198	1.592959	-1.329946
70	8	0	-4.019961	-0.240446	-1.430079
71	6	0	-4.845841	-2.908493	0.956730
72	1	0	-4.495814	-3.351406	1.882462
73	6	0	-5.839428	-1.717549	-1.344653
74	1	0	-6.206134	-1.209784	-2.231066
75	6	0	-6.055056	-3.344469	0.419587
76	6	0	-6.546997	-2.754013	-0.746967
77	1	0	-6.614500	-4.131706	0.916703
78	1	0	-7.488744	-3.084076	-1.176926
79	6	0	-0.427694	-1.583759	1.664246
80	8	0	0.583723	-2.089961	2.112111
81	6	0	-1.570062	-2.392644	1.021334
82	6	0	-1.870667	-3.542296	2.022461
83	1	0	-2.343668	-3.148244	2.929033
84	1	0	-2.538611	-4.273649	1.563377
85	1	0	-0.953119	-4.048051	2.324741
86	6	0	-1.063211	-3.000299	-0.308048
87	6	0	-1.542478	-2.601132	-1.564131
88	6	0	-0.100360	-4.026655	-0.274299
89	6	0	-1.100654	-3.222433	-2.735955
90	1	0	-2.266689	-1.806090	-1.653242
91	6	0	0.342236	-4.645360	-1.443591
92	1	0	0.321465	-4.341297	0.672918
93	6	0	-0.162073	-4.251344	-2.684546
94	1	0	-1.505342	-2.896333	-3.690351
95	1	0	1.076602	-5.444487	-1.379649
96	1	0	0.171227	-4.740946	-3.595814

TS6-S

HF=-2008.0103248; 1 imaginary frequencies= -154.5940

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.112236	0.914094	0.338859
2	7	0	-1.202318	1.042094	0.652406
3	7	0	0.522425	2.206185	0.328086
4	6	0	1.820439	2.720439	0.021202
5	6	0	2.411903	3.632413	0.899934
6	6	0	2.456863	2.347109	-1.163301
7	6	0	3.667470	4.155518	0.596044
8	1	0	1.883633	3.923945	1.801193
9	6	0	3.719510	2.868719	-1.449885
10	1	0	1.953631	1.679163	-1.852504
11	6	0	4.326816	3.769796	-0.574067
12	1	0	4.131599	4.864389	1.275985
13	1	0	4.218653	2.579495	-2.370237
14	1	0	5.306489	4.178272	-0.805783

15	6	0	-1.504965	2.365823	0.855166
16	7	0	-0.472032	3.131237	0.664845
17	6	0	-2.342786	0.136867	0.896618
18	6	0	-2.916737	2.539324	1.306473
19	6	0	-3.284401	1.080287	1.707719
20	1	0	-2.998605	3.241984	2.139993
21	1	0	-3.544640	2.906157	0.488628
22	1	0	-3.087863	0.937661	2.776037
23	1	0	-4.337753	0.868267	1.527414
24	1	0	-1.978449	-0.698578	1.492351
25	6	0	-2.921328	-0.466268	-0.449252
26	6	0	-3.780622	-1.714240	-0.146089
27	6	0	-4.040505	-2.581571	-1.218977
28	6	0	-4.309067	-2.038863	1.108988
29	6	0	-4.808081	-3.729561	-1.044044
30	1	0	-3.613004	-2.348520	-2.188439
31	6	0	-5.078945	-3.193475	1.287869
32	1	0	-4.126323	-1.407140	1.972583
33	6	0	-5.333718	-4.041450	0.213129
34	1	0	-4.992423	-4.386910	-1.889987
35	1	0	-5.473472	-3.426037	2.273862
36	1	0	-5.930629	-4.939061	0.351871
37	6	0	-3.731471	0.589327	-1.225430
38	6	0	-3.070762	1.410814	-2.150888
39	6	0	-5.106100	0.777765	-1.023551
40	6	0	-3.763025	2.414463	-2.830607
41	1	0	-2.019031	1.235566	-2.345590
42	6	0	-5.797327	1.783647	-1.701720
43	1	0	-5.647998	0.120649	-0.349512
44	6	0	-5.126495	2.610992	-2.603827
45	1	0	-3.234444	3.039836	-3.545668
46	1	0	-6.863772	1.910373	-1.532882
47	1	0	-5.664707	3.391169	-3.135974
48	8	0	-1.853641	-0.820305	-1.294629
49	1	0	-1.166866	-1.318461	-0.780555
50	6	0	0.867165	-0.931804	0.718614
51	8	0	-0.066413	-1.746593	0.452447
52	6	0	2.099528	-1.053813	-0.174285
53	6	0	3.287714	-1.501326	0.309594
54	6	0	1.919545	-0.914852	-1.626952
55	6	0	4.389930	-1.843256	-0.549552
56	1	0	3.422418	-1.623722	1.380603
57	6	0	4.196475	-1.710847	-1.934744
58	6	0	1.148468	-0.674206	2.205608
59	6	0	0.461381	-1.463567	3.135729
60	6	0	2.061509	0.281842	2.674914
61	6	0	0.668220	-1.292191	4.505796
62	1	0	-0.223311	-2.216096	2.758775
63	6	0	1.571293	-0.332380	4.964478
64	6	0	2.269980	0.452586	4.043068
65	1	0	2.609109	0.900171	1.969973
66	1	0	2.978159	1.200726	4.390379
67	1	0	1.734688	-0.198510	6.030693
68	1	0	0.128483	-1.915033	5.214825
69	8	0	0.944251	-0.491043	-2.201348
70	8	0	3.011254	-1.257209	-2.430161
71	6	0	5.203526	-2.032640	-2.846719
72	1	0	5.010810	-1.919719	-3.908473
73	6	0	5.635298	-2.310095	-0.087712
74	1	0	5.791541	-2.417189	0.982742
75	6	0	6.644990	-2.629637	-0.984598
76	6	0	6.425365	-2.490167	-2.364177
77	1	0	7.602841	-2.989216	-0.620891
78	1	0	7.215358	-2.742741	-3.065778

IN4-S

HF=-2008.0207122

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.539429	-1.230046	0.117671
2	7	0	0.737238	-1.678151	0.148160
3	7	0	-1.203390	-2.189425	-0.567359
4	6	0	-2.598804	-2.317357	-0.902504

5	6	0	-3.354416	-3.262671	-0.207778
6	6	0	-3.142356	-1.582650	-1.955161
7	6	0	-4.689496	-3.454445	-0.555178
8	1	0	-2.899923	-3.825292	0.600692
9	6	0	-4.483602	-1.780462	-2.289806
10	1	0	-2.517635	-0.882951	-2.497014
11	6	0	-5.256425	-2.710489	-1.592881
12	1	0	-5.286616	-4.181913	-0.013270
13	1	0	-4.918788	-1.212242	-3.107003
14	1	0	-6.298314	-2.861468	-1.861837
15	6	0	0.788648	-2.868501	-0.526231
16	7	0	-0.377696	-3.223962	-0.979822
17	6	0	2.014063	-1.341324	0.837783
18	6	0	2.151051	-3.470658	-0.477379
19	6	0	2.774700	-2.698821	0.718312
20	1	0	2.119358	-4.552114	-0.323947
21	1	0	2.689883	-3.270687	-1.409361
22	1	0	2.624862	-3.271728	1.640080
23	1	0	3.845978	-2.553772	0.583212
24	1	0	1.740677	-1.096968	1.862118
25	6	0	2.722220	-0.070012	0.226701
26	6	0	3.799577	0.453349	1.205999
27	6	0	4.288849	1.747793	0.966937
28	6	0	4.297815	-0.245901	2.310871
29	6	0	5.251020	2.316668	1.795732
30	1	0	3.885757	2.307063	0.129162
31	6	0	5.262522	0.325163	3.149001
32	1	0	3.939459	-1.242073	2.549706
33	6	0	5.745406	1.605517	2.893550
34	1	0	5.612655	3.320995	1.589802
35	1	0	5.628630	-0.237462	4.004148
36	1	0	6.494249	2.049794	3.544044
37	6	0	3.334567	-0.391632	-1.149382
38	6	0	2.540577	-0.279283	-2.300139
39	6	0	4.659013	-0.832797	-1.289569
40	6	0	3.055151	-0.622394	-3.552128
41	1	0	1.524377	0.086855	-2.213112
42	6	0	5.171152	-1.177926	-2.541905
43	1	0	5.305241	-0.887038	-0.418220
44	6	0	4.368607	-1.077974	-3.679438
45	1	0	2.423452	-0.526553	-4.431694
46	1	0	6.201877	-1.513216	-2.626932
47	1	0	4.766964	-1.341309	-4.656026
48	8	0	1.751092	0.931273	0.043315
49	1	0	1.109916	0.875716	0.838881
50	6	0	-1.017410	0.009490	0.979146
51	8	0	-0.008374	0.338747	1.808949
52	6	0	-1.374755	1.242809	0.092635
53	6	0	-1.759438	2.370672	0.747470
54	6	0	-1.118508	1.308785	-1.340897
55	6	0	-1.968590	3.619049	0.072093
56	1	0	-1.890738	2.330188	1.825537
57	6	0	-1.724527	3.652609	-1.311579
58	6	0	-2.262534	-0.468118	1.792984
59	6	0	-2.011005	-1.106107	3.014240
60	6	0	-3.590254	-0.260563	1.404265
61	6	0	-3.061256	-1.546455	3.818109
62	1	0	-0.978892	-1.211120	3.330932
63	6	0	-4.384996	-1.337192	3.421580
64	6	0	-4.645207	-0.687571	2.215373
65	1	0	-3.810927	0.239722	0.466730
66	1	0	-5.670233	-0.509864	1.899908
67	1	0	-5.205357	-1.668436	4.053377
68	1	0	-2.847601	-2.038298	4.764115
69	8	0	-0.758231	0.392004	-2.060163
70	8	0	-1.315314	2.530166	-1.968726
71	6	0	-1.890165	4.820184	-2.058121
72	1	0	-1.687321	4.801108	-3.123754
73	6	0	-2.390124	4.804789	0.705875
74	1	0	-2.577165	4.789087	1.776365
75	6	0	-2.560111	5.970983	-0.025619
76	6	0	-2.309023	5.975937	-1.407659
77	1	0	-2.884665	6.881330	0.469387
78	1	0	-2.440653	6.891219	-1.977726

TS7-SZ

HF=-2430.9871839; 1 imaginary frequencies= -103.7749

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.011849	-1.477882	0.324229
2	7	0	1.321664	-1.686867	0.474630
3	7	0	-0.479264	-2.662406	-0.127018
4	6	0	-1.796582	-3.097727	-0.521076
5	6	0	-2.331774	-4.215005	0.123386
6	6	0	-2.466099	-2.471300	-1.569258
7	6	0	-3.573670	-4.697177	-0.278515
8	1	0	-1.785073	-4.679323	0.935293
9	6	0	-3.716660	-2.960418	-1.954972
10	1	0	-1.996108	-1.645863	-2.087345
11	6	0	-4.270728	-4.067807	-1.314044
12	1	0	-4.001219	-5.559493	0.224342
13	1	0	-4.246940	-2.478087	-2.770918
14	1	0	-5.241923	-4.445206	-1.621897
15	6	0	1.580143	-3.001269	0.194030
16	7	0	0.510443	-3.631503	-0.191431
17	6	0	2.522195	-0.957396	0.971280
18	6	0	2.980798	-3.373559	0.550629
19	6	0	3.378345	-2.167876	1.450553
20	1	0	3.018734	-4.329460	1.079332
21	1	0	3.611703	-3.446108	-0.339208
22	1	0	3.115558	-2.388651	2.491077
23	1	0	4.446306	-1.960728	1.403139
24	1	0	2.200255	-0.333004	1.802011
25	6	0	3.200699	-0.018031	-0.112815
26	6	0	4.065898	1.042518	0.614020
27	6	0	4.414224	2.184819	-0.124278
28	6	0	4.526107	0.942934	1.932629
29	6	0	5.196551	3.190678	0.436209
30	1	0	4.050137	2.276813	-1.141814
31	6	0	5.310472	1.954220	2.498852
32	1	0	4.279371	0.085429	2.550956
33	6	0	5.650081	3.080234	1.753845
34	1	0	5.450418	4.066226	-0.155911
35	1	0	5.648696	1.855308	3.527145
36	1	0	6.258324	3.866277	2.193475
37	6	0	4.061566	-0.832156	-1.105951
38	6	0	3.459618	-1.337973	-2.268329
39	6	0	5.420268	-1.097637	-0.883624
40	6	0	4.193518	-2.117638	-3.164258
41	1	0	2.420644	-1.101349	-2.470127
42	6	0	6.152656	-1.878258	-1.780419
43	1	0	5.919489	-0.676354	-0.015842
44	6	0	5.540079	-2.396918	-2.922193
45	1	0	3.710265	-2.500632	-4.059525
46	1	0	7.206054	-2.068583	-1.590928
47	1	0	6.110510	-3.000360	-3.623552
48	8	0	2.233201	0.631586	-0.893429
49	1	0	1.339249	0.756570	-0.447905
50	6	0	-0.684689	-0.115910	0.672036
51	8	0	-0.249931	0.817062	-0.229388
52	6	0	-2.232572	-0.165330	0.736736
53	6	0	-2.936756	0.814001	0.113591
54	6	0	-2.925708	-1.123034	1.598218
55	6	0	-4.363092	0.920707	0.250234
56	1	0	-2.398881	1.536162	-0.490521
57	6	0	-5.012792	-0.017699	1.070199
58	8	0	-2.415464	-2.034906	2.218865
59	8	0	-4.302747	-0.991538	1.710224
60	6	0	-5.139065	1.914912	-0.377420
61	1	0	-4.637208	2.650289	-1.000539
62	6	0	-6.394392	0.013504	1.266347
63	1	0	-6.855587	-0.728990	1.909125
64	6	0	-6.513466	1.954829	-0.190783
65	6	0	-7.138171	1.002027	0.630309
66	1	0	-7.106694	2.724120	-0.676059
67	1	0	-8.214283	1.036110	0.775736
68	6	0	-0.437380	0.566835	-2.372986
69	8	0	-0.147160	-0.580046	-2.523005
70	6	0	-0.851183	1.755441	-2.833770

71	6	0	-1.223671	1.709445	-4.317954
72	1	0	-0.716188	2.513028	-4.866051
73	1	0	-0.935916	0.756775	-4.771286
74	1	0	-2.304116	1.832822	-4.476210
75	6	0	-0.949393	3.048170	-2.127680
76	6	0	0.053567	3.516502	-1.256623
77	6	0	-2.036382	3.905019	-2.390024
78	6	0	-0.051367	4.765813	-0.648628
79	1	0	0.924511	2.898245	-1.075420
80	6	0	-2.136470	5.159326	-1.784940
81	1	0	-2.814995	3.585649	-3.077909
82	6	0	-1.146965	5.595478	-0.904379
83	1	0	0.741224	5.102117	0.015846
84	1	0	-2.990110	5.795724	-2.006545
85	1	0	-1.219986	6.572469	-0.433806
86	6	0	-0.217056	0.295416	2.117052
87	6	0	-0.058343	-0.600130	3.184737
88	6	0	0.029329	1.656801	2.333663
89	6	0	0.350854	-0.139554	4.438517
90	1	0	-0.273998	-1.653320	3.050399
91	6	0	0.428522	2.114337	3.589937
92	1	0	-0.087491	2.343724	1.503411
93	6	0	0.594982	1.218500	4.647215
94	1	0	0.470081	-0.848055	5.254523
95	1	0	0.616210	3.174599	3.738463
96	1	0	0.910692	1.574605	5.624440

IN5-SZ

HF=-2431.0117794

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.245599	-1.491344	-0.096354
2	7	0	1.559101	-1.783218	0.094667
3	7	0	-0.243422	-2.560635	-0.769446
4	6	0	-1.512401	-2.776355	-1.417492
5	6	0	-2.205774	-3.951879	-1.124156
6	6	0	-1.959221	-1.886725	-2.395676
7	6	0	-3.392681	-4.222979	-1.801575
8	1	0	-1.825268	-4.622878	-0.363393
9	6	0	-3.154932	-2.168836	-3.057920
10	1	0	-1.362406	-1.012177	-2.628095
11	6	0	-3.871756	-3.330259	-2.763699
12	1	0	-3.944532	-5.130017	-1.573032
13	1	0	-3.516040	-1.482189	-3.818196
14	1	0	-4.799959	-3.543668	-3.286780
15	6	0	1.802901	-2.991705	-0.515959
16	7	0	0.736785	-3.499428	-1.047731
17	6	0	2.823856	-1.173697	0.610792
18	6	0	3.220620	-3.415743	-0.343947
19	6	0	3.642186	-2.480559	0.813889
20	1	0	3.313390	-4.477529	-0.103435
21	1	0	3.790235	-3.209236	-1.255691
22	1	0	3.332034	-2.922586	1.767799
23	1	0	4.714706	-2.304438	0.852838
24	1	0	2.617762	-0.697094	1.565304
25	6	0	3.448747	-0.136451	-0.436651
26	6	0	3.070945	1.333970	-0.146181
27	6	0	2.999182	2.219678	-1.230912
28	6	0	2.926794	1.857845	1.145187
29	6	0	2.783830	3.581966	-1.032650
30	1	0	3.116057	1.830010	-2.235801
31	6	0	2.718947	3.223900	1.345964
32	1	0	2.972571	1.217608	2.020683
33	6	0	2.648264	4.093437	0.258206
34	1	0	2.720462	4.244528	-1.891425
35	1	0	2.607903	3.603231	2.358578
36	1	0	2.480469	5.155560	0.413620
37	6	0	4.992824	-0.207593	-0.399229
38	6	0	5.700666	-0.612066	-1.536565
39	6	0	5.717627	0.152758	0.746813
40	6	0	7.097118	-0.662329	-1.525709
41	1	0	5.148066	-0.874862	-2.430282

42	6	0	7.110385	0.095355	0.759908
43	1	0	5.197449	0.494359	1.636757
44	6	0	7.808567	-0.312663	-0.379163
45	1	0	7.627137	-0.973987	-2.422241
46	1	0	7.650016	0.379101	1.659765
47	1	0	8.894598	-0.350618	-0.372365
48	8	0	3.052600	-0.526746	-1.729736
49	1	0	2.099272	-0.263924	-1.858267
50	6	0	-0.531766	-0.383884	0.656235
51	8	0	-0.258795	0.889134	0.083269
52	6	0	-2.058975	-0.617562	0.711275
53	6	0	-2.925327	0.346741	0.306533
54	6	0	-2.573952	-1.829804	1.353049
55	6	0	-4.344362	0.210332	0.481723
56	1	0	-2.551248	1.248443	-0.162396
57	6	0	-4.817268	-0.942690	1.130887
58	8	0	-1.916830	-2.775197	1.737501
59	8	0	-3.950650	-1.909449	1.553395
60	6	0	-5.274780	1.182105	0.064171
61	1	0	-4.909644	2.077660	-0.431616
62	6	0	-6.177397	-1.141035	1.370604
63	1	0	-6.501474	-2.044139	1.876702
64	6	0	-6.630217	0.993859	0.293906
65	6	0	-7.077844	-0.168246	0.947792
66	1	0	-7.345115	1.744714	-0.028752
67	1	0	-8.139597	-0.312493	1.127587
68	6	0	-0.182292	0.983142	-1.338153
69	8	0	0.418250	-0.004638	-1.896343
70	6	0	-0.749826	2.071036	-1.954659
71	6	0	-0.657547	2.110249	-3.468304
72	1	0	-1.598915	1.822451	-3.962946
73	1	0	-0.409014	3.116948	-3.829653
74	1	0	0.111378	1.418178	-3.818074
75	6	0	-1.474234	3.161686	-1.283097
76	6	0	-1.130506	3.663492	-0.006382
77	6	0	-2.562241	3.791005	-1.934204
78	6	0	-1.854993	4.691620	0.593990
79	1	0	-0.260400	3.261635	0.497086
80	6	0	-3.283235	4.822456	-1.332908
81	1	0	-2.850829	3.460386	-2.927639
82	6	0	-2.942356	5.278096	-0.057592
83	1	0	-1.552675	5.052041	1.575186
84	1	0	-4.115480	5.274441	-1.868620
85	1	0	-3.501673	6.083392	0.411241
86	6	0	-0.048814	-0.285299	2.132404
87	6	0	0.351080	-1.395549	2.888121
88	6	0	-0.106250	0.968808	2.757235
89	6	0	0.718729	-1.246594	4.227319
90	1	0	0.354603	-2.384588	2.448952
91	6	0	0.255391	1.111651	4.096665
92	1	0	-0.434854	1.830658	2.191259
93	6	0	0.676303	0.006437	4.836945
94	1	0	1.025992	-2.121477	4.794001
95	1	0	0.205255	2.092998	4.560946
96	1	0	0.958225	0.119031	5.880408

TS8-SZ

HF=-2430.9786788; 1 imaginary frequencies=-254.6757

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.224024	-1.541594	0.267030
2	7	0	1.567943	-1.723845	0.229680
3	7	0	-0.291362	-2.738261	-0.090252
4	6	0	-1.649887	-3.222364	-0.152613
5	6	0	-2.432977	-3.285935	1.000185
6	6	0	-2.105270	-3.712896	-1.374880
7	6	0	-3.710793	-3.834925	0.911448
8	1	0	-2.069233	-2.891227	1.942450
9	6	0	-3.384827	-4.264926	-1.447788
10	1	0	-1.462054	-3.665500	-2.247257
11	6	0	-4.187127	-4.323342	-0.308155
12	1	0	-4.333617	-3.875929	1.799601
13	1	0	-3.750802	-4.645877	-2.396470

14	1	0	-5.184660	-4.748773	-0.368294
15	6	0	1.797599	-3.019395	-0.154255
16	7	0	0.693123	-3.670880	-0.370003
17	6	0	2.846806	-1.017951	0.570460
18	6	0	3.241109	-3.371951	-0.049777
19	6	0	3.696587	-2.269675	0.940443
20	1	0	3.391825	-4.388097	0.321226
21	1	0	3.739074	-3.269674	-1.018962
22	1	0	3.436883	-2.571754	1.961679
23	1	0	4.765788	-2.076878	0.901596
24	1	0	2.660994	-0.389179	1.437258
25	6	0	3.414341	-0.171847	-0.672558
26	6	0	3.159024	1.347579	-0.553884
27	6	0	3.066741	2.087926	-1.741029
28	6	0	3.143591	2.041653	0.662322
29	6	0	2.951443	3.476703	-1.713331
30	1	0	3.084186	1.563258	-2.689660
31	6	0	3.034067	3.433688	0.692101
32	1	0	3.204591	1.515988	1.610387
33	6	0	2.938098	4.158884	-0.495224
34	1	0	2.874917	4.026510	-2.647643
35	1	0	3.020183	3.947373	1.649848
36	1	0	2.852009	5.241824	-0.472181
37	6	0	4.950019	-0.344014	-0.787030
38	6	0	5.499020	-1.013171	-1.887182
39	6	0	5.822033	0.172678	0.183418
40	6	0	6.882177	-1.174506	-2.006081
41	1	0	4.835185	-1.389169	-2.656143
42	6	0	7.201161	0.004689	0.068621
43	1	0	5.428290	0.724873	1.031594
44	6	0	7.739219	-0.672201	-1.028375
45	1	0	7.286986	-1.691724	-2.872330
46	1	0	7.856273	0.414092	0.833177
47	1	0	8.814647	-0.796631	-1.122183
48	8	0	2.861154	-0.706098	-1.851612
49	1	0	1.925143	-0.379979	-1.947335
50	6	0	-0.493187	-0.300215	0.800034
51	8	0	0.170326	0.829438	-0.008360
52	6	0	-1.956778	-0.234551	0.565863
53	6	0	-2.388586	-0.112402	-0.802530
54	6	0	-2.863065	-0.065910	1.662874
55	6	0	-3.840687	-0.057356	-1.028217
56	1	0	-1.879626	-0.738115	-1.540453
57	6	0	-4.685848	0.159222	0.070940
58	8	0	-2.652437	-0.201476	2.856280
59	8	0	-4.206762	0.232426	1.340159
60	6	0	-4.433455	-0.231409	-2.291316
61	1	0	-3.794945	-0.441873	-3.144052
62	6	0	-6.072184	0.264761	-0.089385
63	1	0	-6.684133	0.438700	0.789958
64	6	0	-5.810775	-0.135877	-2.462109
65	6	0	-6.629240	0.127906	-1.356225
66	1	0	-6.247395	-0.268108	-3.447915
67	1	0	-7.705831	0.208722	-1.481030
68	6	0	-0.233307	0.891026	-1.319660
69	8	0	0.345608	0.179521	-2.164213
70	6	0	-1.482500	1.569941	-1.573348
71	6	0	-1.852607	1.649278	-3.045684
72	1	0	-1.654707	0.702140	-3.554873
73	1	0	-2.903309	1.917856	-3.180447
74	1	0	-1.249326	2.418111	-3.546387
75	6	0	-1.885149	2.767044	-0.766877
76	6	0	-0.946984	3.557687	-0.078037
77	6	0	-3.224953	3.196401	-0.759060
78	6	0	-1.337049	4.706182	0.611247
79	1	0	0.101266	3.283085	-0.096731
80	6	0	-3.615829	4.340776	-0.064620
81	1	0	-3.976300	2.628164	-1.296214
82	6	0	-2.674752	5.102093	0.628726
83	1	0	-0.585179	5.298943	1.126930
84	1	0	-4.661826	4.636716	-0.068702
85	1	0	-2.978350	5.996190	1.166987
86	6	0	0.000873	-0.067704	2.237121
87	6	0	0.324113	-1.132302	3.087178
88	6	0	0.145140	1.241737	2.707830
89	6	0	0.777843	-0.896682	4.384935
90	1	0	0.203075	-2.160644	2.755494

91	6	0	0.597954	1.475720	4.005634
92	1	0	-0.111849	2.070791	2.060782
93	6	0	0.918937	0.410947	4.848998
94	1	0	1.011819	-1.737066	5.033080
95	1	0	0.693915	2.498679	4.360047
96	1	0	1.270437	0.598071	5.860080

IN6-SZ

HF=-2430.9898601

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.334982	-1.121970	0.631994
2	7	0	1.672860	-1.142385	0.840486
3	7	0	-0.040102	-2.409759	0.762650
4	6	0	-1.320807	-3.041221	0.524805
5	6	0	-2.151622	-3.347339	1.600609
6	6	0	-1.617066	-3.451242	-0.775670
7	6	0	-3.330818	-4.047766	1.351238
8	1	0	-1.914197	-2.991257	2.595156
9	6	0	-2.797948	-4.152528	-1.008941
10	1	0	-0.934069	-3.217812	-1.586702
11	6	0	-3.653813	-4.450268	0.053994
12	1	0	-4.003131	-4.265647	2.175142
13	1	0	-3.050559	-4.460021	-2.019027
14	1	0	-4.576886	-4.991906	-0.130896
15	6	0	2.029640	-2.418409	1.182749
16	7	0	1.014668	-3.235313	1.119122
17	6	0	2.805822	-0.195109	0.880449
18	6	0	3.435532	-2.468615	1.690712
19	6	0	3.726711	-0.947886	1.887023
20	1	0	3.495151	-3.031933	2.625846
21	1	0	4.112472	-2.931623	0.968916
22	1	0	3.441608	-0.652353	2.902385
23	1	0	4.780628	-0.712919	1.744086
24	1	0	2.435234	0.750888	1.273021
25	6	0	3.422874	0.060881	-0.571937
26	6	0	4.192728	1.395282	-0.586139
27	6	0	4.473161	1.960657	-1.840408
28	6	0	4.640400	2.064197	0.559859
29	6	0	5.173349	3.159490	-1.943941
30	1	0	4.125480	1.453061	-2.734210
31	6	0	5.346475	3.266795	0.456403
32	1	0	4.445166	1.669404	1.551923
33	6	0	5.614805	3.818826	-0.793964
34	1	0	5.372315	3.581553	-2.925299
35	1	0	5.678918	3.770548	1.360053
36	1	0	6.159676	4.755473	-0.873722
37	6	0	4.340078	-1.099016	-1.011568
38	6	0	3.803145	-2.160567	-1.754601
39	6	0	5.703989	-1.132144	-0.689123
40	6	0	4.601310	-3.241888	-2.131758
41	1	0	2.761644	-2.123858	-2.050949
42	6	0	6.502029	-2.214240	-1.064286
43	1	0	6.154947	-0.297918	-0.160010
44	6	0	5.951944	-3.278019	-1.781290
45	1	0	4.165814	-4.054399	-2.707439
46	1	0	7.557726	-2.217265	-0.806083
47	1	0	6.573345	-4.118823	-2.077374
48	8	0	2.382456	0.088639	-1.525626
49	1	0	1.930496	0.961443	-1.528533
50	6	0	-0.599086	0.130833	0.767163
51	8	0	0.128562	1.102057	-0.097603
52	6	0	-2.001064	-0.050647	0.356184
53	6	0	-2.254534	0.117567	-1.119007
54	6	0	-2.993257	-0.325188	1.307236
55	6	0	-3.642488	-0.357830	-1.506503
56	1	0	-1.555470	-0.530168	-1.688744
57	6	0	-4.596313	-0.598848	-0.506971
58	8	0	-2.898894	-0.539029	2.512785
59	8	0	-4.340664	-0.404164	0.816960
60	6	0	-3.994582	-0.676315	-2.827087
61	1	0	-3.253017	-0.563393	-3.611867

62	6	0	-5.881314	-1.057115	-0.827614
63	1	0	-6.585603	-1.214088	-0.016524
64	6	0	-5.266253	-1.139690	-3.158708
65	6	0	-6.218661	-1.316192	-2.150917
66	1	0	-5.509301	-1.365038	-4.193399
67	1	0	-7.216593	-1.672216	-2.394006
68	6	0	-0.319264	1.609784	-1.266608
69	8	0	0.533068	2.088388	-1.999256
70	6	0	-1.811855	1.575109	-1.592707
71	6	0	-1.965551	1.768281	-3.116947
72	1	0	-1.485265	0.953023	-3.670166
73	1	0	-3.025378	1.799253	-3.379805
74	1	0	-1.500386	2.701755	-3.438138
75	6	0	-2.460875	2.788072	-0.884727
76	6	0	-1.850833	4.047598	-1.031444
77	6	0	-3.655752	2.721464	-0.157496
78	6	0	-2.412496	5.195642	-0.472956
79	1	0	-0.922190	4.133723	-1.588609
80	6	0	-4.221074	3.872166	0.397005
81	1	0	-4.155063	1.778248	0.002111
82	6	0	-3.605977	5.113710	0.244595
83	1	0	-1.914219	6.153145	-0.602734
84	1	0	-5.147786	3.786251	0.958148
85	1	0	-4.048642	6.005162	0.681315
86	6	0	-0.371999	0.676228	2.199960
87	6	0	-0.506537	2.054404	2.401498
88	6	0	-0.026869	-0.133240	3.287856
89	6	0	-0.295225	2.609050	3.663995
90	1	0	-0.785181	2.694648	1.572679
91	6	0	0.188219	0.422115	4.548654
92	1	0	0.041248	-1.210782	3.176020
93	6	0	0.058374	1.797752	4.741829
94	1	0	-0.410169	3.680992	3.800307
95	1	0	0.440610	-0.226608	5.383388
96	1	0	0.222631	2.230864	5.724896

TS9-SZ

HF=-2430.9842446; 1 imaginary frequencies=-238.2910

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.440635	-1.274463	0.355059
2	7	0	1.750049	-1.156733	0.709528
3	7	0	0.193756	-2.584868	0.597202
4	6	0	-1.005981	-3.314528	0.340978
5	6	0	-1.408695	-4.304922	1.240806
6	6	0	-1.738740	-3.050014	-0.815343
7	6	0	-2.572080	-5.023062	0.978964
8	1	0	-0.813804	-4.500919	2.125397
9	6	0	-2.910054	-3.767943	-1.060217
10	1	0	-1.376293	-2.314022	-1.523549
11	6	0	-3.327493	-4.752825	-0.165571
12	1	0	-2.895303	-5.788890	1.677846
13	1	0	-3.489852	-3.553860	-1.952606
14	1	0	-4.238954	-5.310990	-0.358963
15	6	0	2.195668	-2.354884	1.202081
16	7	0	1.276898	-3.274553	1.139464
17	6	0	2.765207	-0.090090	0.760110
18	6	0	3.582339	-2.241669	1.742178
19	6	0	3.745980	-0.693942	1.814204
20	1	0	3.677070	-2.722003	2.719640
21	1	0	4.308280	-2.700544	1.064387
22	1	0	3.443325	-0.344100	2.806748
23	1	0	4.777718	-0.386247	1.645713
24	1	0	2.282829	0.816354	1.124190
25	6	0	3.380642	0.222331	-0.666992
26	6	0	4.154350	1.554785	-0.646876
27	6	0	4.550852	2.077927	-1.889186
28	6	0	4.464478	2.282628	0.507931
29	6	0	5.237982	3.285206	-1.972428
30	1	0	4.301283	1.529268	-2.791734
31	6	0	5.155837	3.496180	0.425682

32	1	0	4.170023	1.927822	1.489983
33	6	0	5.545942	4.000871	-0.811959
34	1	0	5.530908	3.671046	-2.945225
35	1	0	5.381674	4.044701	1.336284
36	1	0	6.080993	4.944505	-0.875308
37	6	0	4.275195	-0.934706	-1.143701
38	6	0	3.707968	-1.996334	-1.863199
39	6	0	5.647344	-0.976652	-0.858991
40	6	0	4.488091	-3.082689	-2.262626
41	1	0	2.656575	-1.955772	-2.122573
42	6	0	6.427284	-2.064160	-1.256177
43	1	0	6.116800	-0.145467	-0.341410
44	6	0	5.848998	-3.125011	-1.955254
45	1	0	4.029785	-3.895432	-2.819960
46	1	0	7.490001	-2.074404	-1.028424
47	1	0	6.455963	-3.970243	-2.268477
48	8	0	2.329816	0.307790	-1.615864
49	1	0	1.857085	1.161353	-1.515003
50	6	0	-0.757588	0.136710	0.726418
51	8	0	-0.004124	1.119608	-0.016872
52	6	0	-2.097478	-0.039224	0.280210
53	6	0	-2.347262	0.352432	-1.160293
54	6	0	-3.115570	-0.555707	1.135061
55	6	0	-3.705550	-0.101269	-1.657574
56	1	0	-1.608597	-0.178528	-1.795043
57	6	0	-4.665169	-0.545364	-0.739247
58	8	0	-3.033477	-0.971617	2.277220
59	8	0	-4.434598	-0.572954	0.606441
60	6	0	-4.020169	-0.205835	-3.021721
61	1	0	-3.272687	0.067851	-3.759616
62	6	0	-5.923215	-0.995052	-1.158158
63	1	0	-6.631343	-1.317786	-0.401533
64	6	0	-5.264856	-0.659169	-3.454805
65	6	0	-6.226060	-1.041251	-2.514186
66	1	0	-5.480175	-0.717853	-4.517867
67	1	0	-7.202119	-1.393033	-2.837666
68	6	0	-0.439786	1.836126	-1.076796
69	8	0	0.416990	2.408891	-1.726788
70	6	0	-1.935815	1.871400	-1.377451
71	6	0	-2.116750	2.340497	-2.835104
72	1	0	-1.627391	1.656930	-3.537673
73	1	0	-3.180463	2.399332	-3.076547
74	1	0	-1.673572	3.328374	-2.975061
75	6	0	-2.580162	2.917878	-0.442500
76	6	0	-1.933053	4.154043	-0.269117
77	6	0	-3.819053	2.732423	0.182684
78	6	0	-2.499037	5.164040	0.508817
79	1	0	-0.976063	4.334456	-0.751444
80	6	0	-4.388109	3.745027	0.957722
81	1	0	-4.353094	1.798548	0.083672
82	6	0	-3.733118	4.963871	1.127490
83	1	0	-1.972755	6.107886	0.626656
84	1	0	-5.348640	3.569479	1.434698
85	1	0	-4.177940	5.747525	1.734972
86	6	0	-0.427258	0.375901	2.199949
87	6	0	-0.120047	1.681956	2.609403
88	6	0	-0.406431	-0.647620	3.157280
89	6	0	0.203568	1.955352	3.940043
90	1	0	-0.148634	2.493179	1.891716
91	6	0	-0.072343	-0.374271	4.481808
92	1	0	-0.677935	-1.656536	2.877919
93	6	0	0.237445	0.927595	4.880738
94	1	0	0.426448	2.977322	4.235129
95	1	0	-0.068550	-1.183342	5.207285
96	1	0	0.492321	1.138222	5.916111

1-4-SS

HF=-2431.0198109

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.638612	-1.556891	-0.133389
2	6	0	1.497301	-1.156110	-1.336717

3	6	0	-1.168684	1.458087	0.527003
4	8	0	-0.470299	-2.039961	-0.188523
5	7	0	-2.312395	0.948825	1.085453
6	7	0	-1.198462	2.714424	1.063506
7	6	0	2.525332	-2.274225	-1.611250
8	6	0	2.311896	-3.584322	-1.157041
9	6	0	3.658441	-2.026015	-2.400216
10	6	0	3.214417	-4.606559	-1.456512
11	1	0	1.426522	-3.825518	-0.575401
12	6	0	4.560497	-3.046910	-2.699434
13	1	0	3.839677	-1.032679	-2.794363
14	6	0	4.346559	-4.341376	-2.224928
15	1	0	3.025457	-5.611390	-1.088304
16	1	0	5.433967	-2.825212	-3.306698
17	1	0	5.051720	-5.134743	-2.456723
18	6	0	0.564481	-1.020255	-2.555666
19	1	0	-0.190452	-0.244055	-2.394747
20	1	0	0.047025	-1.966785	-2.729937
21	1	0	1.145821	-0.783016	-3.449173
22	6	0	-0.230493	3.737895	0.857369
23	6	0	0.523710	3.754888	-0.318849
24	6	0	-0.042312	4.725347	1.829574
25	6	0	1.488862	4.742578	-0.507510
26	1	0	0.341579	3.001103	-1.074362
27	6	0	0.915427	5.717465	1.622882
28	1	0	-0.645836	4.707048	2.729122
29	6	0	1.689193	5.728461	0.460747
30	1	0	2.076471	4.740780	-1.421337
31	1	0	1.059820	6.482579	2.381056
32	1	0	2.437843	6.501043	0.308912
33	6	0	-2.921002	1.872180	1.904392
34	7	0	-2.266980	2.991001	1.929417
35	6	0	-2.993463	-0.354010	1.070511
36	6	0	-4.143583	1.315926	2.551886
37	6	0	-3.968542	-0.207029	2.284303
38	1	0	-4.199086	1.554304	3.617606
39	1	0	-5.046616	1.707513	2.071623
40	1	0	-3.514824	-0.682952	3.160064
41	1	0	-4.925806	-0.695847	2.102293
42	1	0	-2.244683	-1.128337	1.250060
43	6	0	-3.660996	-0.673479	-0.317001
44	6	0	-4.202408	-2.116896	-0.372634
45	6	0	-4.708225	-2.559027	-1.607174
46	6	0	-4.164309	-3.028455	0.688262
47	6	0	-5.176223	-3.859228	-1.769157
48	1	0	-4.720052	-1.868675	-2.444794
49	6	0	-4.633505	-4.337071	0.528007
50	1	0	-3.761918	-2.743817	1.654214
51	6	0	-5.143759	-4.756637	-0.697371
52	1	0	-5.564176	-4.175561	-2.734010
53	1	0	-4.591911	-5.025672	1.367952
54	1	0	-5.508182	-5.772960	-0.821234
55	6	0	-4.748274	0.356653	-0.650204
56	6	0	-4.396812	1.554973	-1.288086
57	6	0	-6.089834	0.155597	-0.294649
58	6	0	-5.359700	2.531089	-1.547844
59	1	0	-3.366202	1.710264	-1.583883
60	6	0	-7.052169	1.134044	-0.551057
61	1	0	-6.391925	-0.780236	0.165904
62	6	0	-6.689636	2.327856	-1.176448
63	1	0	-5.067365	3.453417	-2.043027
64	1	0	-8.087142	0.955867	-0.270613
65	1	0	-7.438455	3.088773	-1.380161
66	8	0	-2.663924	-0.542844	-1.329799
67	1	0	-1.936583	-1.153260	-1.102201
68	6	0	2.754272	2.580344	-3.816659
69	6	0	2.113866	1.726018	-2.920979
70	6	0	2.806085	1.102762	-1.870133
71	6	0	4.158942	1.422344	-1.724910
72	6	0	4.819667	2.275730	-2.611841
73	6	0	4.117417	2.849108	-3.666528
74	1	0	1.246218	0.779592	-0.487304
75	1	0	2.188441	3.037239	-4.623178
76	1	0	1.051190	1.543498	-3.034067
77	6	0	2.120321	0.213781	-0.854148
78	1	0	5.872882	2.477969	-2.446494
79	1	0	4.628382	3.512364	-4.358580

80	6	0	4.428268	0.275346	0.399390
81	6	0	2.997110	-0.083851	0.355416
82	8	0	4.940362	0.922750	-0.704441
83	8	0	5.211425	0.019563	1.283412
84	6	0	2.442628	-0.852830	1.326199
85	8	0	1.169646	-1.374715	1.114709
86	6	0	2.926040	-1.264167	2.657895
87	6	0	3.489166	-0.339693	3.550422
88	6	0	2.731290	-2.590370	3.077445
89	6	0	3.862616	-0.739309	4.830139
90	1	0	3.629757	0.688469	3.239047
91	6	0	3.122620	-2.990480	4.352951
92	1	0	2.282408	-3.306386	2.396689
93	6	0	3.686274	-2.065204	5.233225
94	1	0	4.292941	-0.013587	5.514330
95	1	0	2.981951	-4.022918	4.660658
96	1	0	3.984043	-2.374766	6.231489

TS10-SS

HF=-2430.9874494; 1 imaginary frequencies=-15.2318

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.610367	0.646361	1.035241
2	6	0	-2.144430	0.388447	0.899994
3	6	0	0.136791	1.502537	-0.070518
4	8	0	-0.016433	0.680183	2.117420
5	7	0	1.142383	1.133169	-0.900064
6	7	0	-0.031699	2.822566	-0.337282
7	6	0	-2.630314	-0.741713	1.846303
8	6	0	-1.817885	-1.463936	2.731841
9	6	0	-4.001729	-1.052902	1.828090
10	6	0	-2.356193	-2.455275	3.556635
11	1	0	-0.760631	-1.252706	2.789566
12	6	0	-4.537630	-2.047031	2.644137
13	1	0	-4.670147	-0.524668	1.156070
14	6	0	-3.715516	-2.755719	3.519699
15	1	0	-1.696900	-2.995135	4.232040
16	1	0	-5.600404	-2.267405	2.588199
17	1	0	-4.128771	-3.530931	4.159535
18	6	0	-2.883409	1.668365	1.364392
19	1	0	-2.700439	2.531898	0.727514
20	1	0	-2.572646	1.917932	2.383163
21	1	0	-3.960586	1.496919	1.370667
22	6	0	-0.687450	3.851239	0.422816
23	6	0	-1.439310	4.811506	-0.256004
24	6	0	-0.473304	3.924845	1.800052
25	6	0	-2.017953	5.849979	0.471061
26	1	0	-1.556573	4.743427	-1.332094
27	6	0	-1.064736	4.967298	2.513337
28	1	0	0.127913	3.171309	2.297343
29	6	0	-1.836443	5.926102	1.854464
30	1	0	-2.610305	6.599736	-0.044756
31	1	0	-0.912435	5.031044	3.586551
32	1	0	-2.291424	6.736300	2.416760
33	6	0	1.457281	2.203983	-1.695582
34	7	0	0.766432	3.261041	-1.384171
35	6	0	2.161428	0.058143	-1.012749
36	6	0	2.504644	1.854519	-2.703085
37	6	0	2.667289	0.325063	-2.455088
38	1	0	2.174843	2.084498	-3.720354
39	1	0	3.426420	2.409360	-2.510834
40	1	0	2.032217	-0.230695	-3.152852
41	1	0	3.696219	-0.001829	-2.600168
42	1	0	1.657772	-0.894208	-0.902232
43	6	0	3.226824	0.202677	0.182397
44	6	0	3.772416	-1.184473	0.567032
45	6	0	4.301283	-1.342139	1.856980
46	6	0	3.815849	-2.274282	-0.310548
47	6	0	4.853232	-2.556616	2.257759
48	1	0	4.267975	-0.502691	2.543334
49	6	0	4.372178	-3.492278	0.090066
50	1	0	3.406948	-2.202131	-1.314005

51	6	0	4.893439	-3.637735	1.373890
52	1	0	5.252055	-2.659068	3.263614
53	1	0	4.378714	-4.328328	-0.603128
54	1	0	5.322300	-4.585996	1.686490
55	6	0	4.390323	1.147311	-0.187244
56	6	0	4.341410	2.499498	0.182415
57	6	0	5.511260	0.691526	-0.896499
58	6	0	5.369028	3.374727	-0.175020
59	1	0	3.502653	2.858807	0.765975
60	6	0	6.535590	1.567174	-1.258623
61	1	0	5.598542	-0.360770	-1.149400
62	6	0	6.466558	2.915471	-0.904094
63	1	0	5.311472	4.417911	0.124785
64	1	0	7.394687	1.189386	-1.806668
65	1	0	7.266653	3.596917	-1.180295
66	8	0	2.606309	0.818701	1.295608
67	1	0	1.826037	0.321135	1.617458
68	6	0	-5.244382	2.128652	-2.148285
69	6	0	-4.034196	1.763750	-1.563016
70	6	0	-3.733513	0.430104	-1.245884
71	6	0	-4.670395	-0.541990	-1.616412
72	6	0	-5.894492	-0.193177	-2.199877
73	6	0	-6.186181	1.142065	-2.453890
74	1	0	-1.653158	0.585233	-1.188702
75	1	0	-5.447744	3.172342	-2.371038
76	1	0	-3.297908	2.534163	-1.351481
77	6	0	-2.411472	0.010159	-0.634371
78	1	0	-6.585484	-0.989264	-2.458157
79	1	0	-7.135922	1.410239	-2.908859
80	6	0	-3.161471	-2.407157	-1.234679
81	6	0	-2.121016	-1.462364	-0.878337
82	8	0	-4.450528	-1.879406	-1.447973
83	8	0	-3.088824	-3.612220	-1.344205
84	6	0	-0.870078	-1.885521	-0.454884
85	8	0	-0.067585	-1.063613	0.167823
86	6	0	-0.275728	-3.243359	-0.657000
87	6	0	-0.281053	-3.867735	-1.912656
88	6	0	0.402860	-3.857611	0.404285
89	6	0	0.365569	-5.087358	-2.097646
90	1	0	-0.805485	-3.399066	-2.738428
91	6	0	1.028019	-5.091460	0.225351
92	1	0	0.425894	-3.365410	1.370703
93	6	0	1.014785	-5.707972	-1.026819
94	1	0	0.352057	-5.561166	-3.075870
95	1	0	1.532452	-5.565975	1.062929
96	1	0	1.505345	-6.667913	-1.168708

IN7-SS

HF=-2430.9882943

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.542096	0.429343	0.913790
2	6	0	-2.114340	0.266697	0.987624
3	6	0	0.091078	1.403311	-0.189485
4	8	0	0.116604	0.587609	1.994197
5	7	0	1.140860	1.070744	-0.981394
6	7	0	-0.141786	2.702379	-0.498535
7	6	0	-2.492535	-0.967466	1.856278
8	6	0	-1.612094	-1.613413	2.738359
9	6	0	-3.823685	-1.417542	1.826142
10	6	0	-2.042914	-2.683161	3.527939
11	1	0	-0.589674	-1.270704	2.817025
12	6	0	-4.252514	-2.487012	2.611413
13	1	0	-4.547145	-0.927745	1.183774
14	6	0	-3.360633	-3.132205	3.467312
15	1	0	-1.334791	-3.161528	4.200598
16	1	0	-5.287772	-2.812619	2.549585
17	1	0	-3.690134	-3.966307	4.081437
18	6	0	-2.743362	1.469523	1.716377
19	1	0	-2.669621	2.404477	1.165221
20	1	0	-2.236700	1.598300	2.676895
21	1	0	-3.801416	1.279288	1.910342

22	6	0	-0.861469	3.714688	0.221848
23	6	0	-1.748886	4.539844	-0.468653
24	6	0	-0.565629	3.915960	1.571071
25	6	0	-2.380460	5.573677	0.222050
26	1	0	-1.930648	4.373993	-1.525215
27	6	0	-1.207900	4.951943	2.248219
28	1	0	0.127646	3.249562	2.074200
29	6	0	-2.113495	5.777600	1.578378
30	1	0	-3.078151	6.220805	-0.301117
31	1	0	-0.995260	5.114242	3.300604
32	1	0	-2.608570	6.584012	2.111721
33	6	0	1.435677	2.142333	-1.783288
34	7	0	0.678019	3.165927	-1.523281
35	6	0	2.237777	0.070241	-0.996597
36	6	0	2.553407	1.830345	-2.726111
37	6	0	2.790078	0.320299	-2.425774
38	1	0	2.269402	2.016107	-3.765987
39	1	0	3.430746	2.441031	-2.498500
40	1	0	2.212783	-0.290480	-3.128231
41	1	0	3.839666	0.045563	-2.520957
42	1	0	1.811890	-0.919196	-0.886659
43	6	0	3.232330	0.344295	0.257353
44	6	0	3.690139	-1.003380	0.847837
45	6	0	4.005854	-1.053003	2.212761
46	6	0	3.865489	-2.161584	0.079720
47	6	0	4.477399	-2.228828	2.793488
48	1	0	3.871238	-0.159347	2.812134
49	6	0	4.342574	-3.339579	0.659987
50	1	0	3.627376	-2.168807	-0.980457
51	6	0	4.650200	-3.377914	2.018882
52	1	0	4.710245	-2.246866	3.855053
53	1	0	4.459336	-4.227466	0.045082
54	1	0	5.017518	-4.294986	2.471792
55	6	0	4.467542	1.179966	-0.156932
56	6	0	4.477233	2.563961	0.071346
57	6	0	5.596337	0.598587	-0.752562
58	6	0	5.570677	3.344289	-0.309915
59	1	0	3.628056	3.020696	0.564671
60	6	0	6.687949	1.378616	-1.137408
61	1	0	5.638452	-0.476540	-0.897505
62	6	0	6.678823	2.757268	-0.921924
63	1	0	5.556538	4.414358	-0.118786
64	1	0	7.551627	0.902466	-1.594254
65	1	0	7.531099	3.364423	-1.215150
66	8	0	2.578899	1.123289	1.229087
67	1	0	1.748139	0.698343	1.590911
68	6	0	-5.885889	1.914591	-1.222150
69	6	0	-4.574383	1.656151	-0.830308
70	6	0	-4.013007	0.371317	-0.910657
71	6	0	-4.806595	-0.629245	-1.481823
72	6	0	-6.126731	-0.390294	-1.877086
73	6	0	-6.672357	0.880127	-1.735075
74	1	0	-1.996192	0.834492	-1.079559
75	1	0	-6.287551	2.920098	-1.134320
76	1	0	-3.968392	2.475769	-0.460717
77	6	0	-2.572399	0.080308	-0.523370
78	1	0	-6.691421	-1.212701	-2.304314
79	1	0	-7.697612	1.066241	-2.042779
80	6	0	-3.005655	-2.251316	-1.641281
81	6	0	-2.103589	-1.290887	-1.004018
82	8	0	-4.350415	-1.901696	-1.716448
83	8	0	-2.732801	-3.347084	-2.078120
84	6	0	-0.855474	-1.694357	-0.606921
85	8	0	-0.086101	-0.962506	0.209170
86	6	0	-0.147176	-2.955740	-0.971446
87	6	0	0.142901	-3.265114	-2.308023
88	6	0	0.336102	-3.789486	0.045684
89	6	0	0.895018	-4.395004	-2.621388
90	1	0	-0.242038	-2.628843	-3.098601
91	6	0	1.065520	-4.935064	-0.272292
92	1	0	0.122613	-3.543081	1.080543
93	6	0	1.351566	-5.237877	-1.604446
94	1	0	1.110445	-4.627608	-3.660982
95	1	0	1.416642	-5.586105	0.523626
96	1	0	1.924060	-6.128436	-1.851291

TS11-SS

HF=-2430.9874431; 1 imaginary frequencies=-11.4985

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.408496	0.276087	0.919199
2	6	0	-1.947930	0.091129	1.189326
3	6	0	0.159132	1.353509	-0.139956
4	8	0	0.364537	0.255615	1.921934
5	7	0	1.324735	1.112293	-0.789589
6	7	0	-0.206736	2.574400	-0.603315
7	6	0	-2.212666	-1.260904	1.916463
8	6	0	-1.215394	-2.096991	2.443675
9	6	0	-3.549640	-1.642929	2.123663
10	6	0	-1.546689	-3.276487	3.115246
11	1	0	-0.175460	-1.820560	2.345923
12	6	0	-3.880081	-2.821753	2.791903
13	1	0	-4.355337	-1.015172	1.760778
14	6	0	-2.877235	-3.651985	3.289750
15	1	0	-0.748252	-3.900084	3.510480
16	1	0	-4.926695	-3.085681	2.920985
17	1	0	-3.129224	-4.571592	3.811548
18	6	0	-2.381852	1.182561	2.190544
19	1	0	-2.304696	2.192477	1.789158
20	1	0	-1.729120	1.113527	3.065006
21	1	0	-3.410861	1.024353	2.518712
22	6	0	-1.199494	3.515548	-0.158488
23	6	0	-2.224286	3.887947	-1.026725
24	6	0	-1.023341	4.142622	1.076012
25	6	0	-3.111730	4.889613	-0.632834
26	1	0	-2.317247	3.404883	-1.993560
27	6	0	-1.919816	5.138704	1.461377
28	1	0	-0.199566	3.845701	1.717708
29	6	0	-2.962517	5.510865	0.609120
30	1	0	-3.918718	5.181816	-1.297681
31	1	0	-1.797295	5.627842	2.422937
32	1	0	-3.655402	6.291111	0.910606
33	6	0	1.561246	2.132767	-1.666468
34	7	0	0.654570	3.061816	-1.582670
35	6	0	2.443345	0.135944	-0.754647
36	6	0	2.752885	1.850754	-2.524288
37	6	0	3.011030	0.352929	-2.183778
38	1	0	2.535832	2.018130	-3.582671
39	1	0	3.595595	2.487460	-2.241845
40	1	0	2.449719	-0.283315	-2.876871
41	1	0	4.066148	0.093241	-2.258855
42	1	0	2.011434	-0.849841	-0.625167
43	6	0	3.422485	0.440930	0.493627
44	6	0	3.882065	-0.901539	1.100952
45	6	0	4.181301	-0.938613	2.469542
46	6	0	4.056679	-2.070658	0.347969
47	6	0	4.634682	-2.112122	3.069506
48	1	0	4.042267	-0.037795	3.057058
49	6	0	4.514051	-3.246890	0.947870
50	1	0	3.833721	-2.087243	-0.715436
51	6	0	4.803879	-3.272487	2.311140
52	1	0	4.853660	-2.120396	4.134135
53	1	0	4.634972	-4.142838	0.344687
54	1	0	5.154828	-4.188173	2.779488
55	6	0	4.653013	1.284651	0.089091
56	6	0	4.639758	2.671258	0.300130
57	6	0	5.800106	0.711101	-0.478140
58	6	0	5.729762	3.461737	-0.069631
59	1	0	3.774687	3.119892	0.773279
60	6	0	6.888552	1.501144	-0.851789
61	1	0	5.858483	-0.365152	-0.609216
62	6	0	6.857107	2.881953	-0.653161
63	1	0	5.698573	4.533796	0.108196
64	1	0	7.767020	1.031457	-1.286608
65	1	0	7.706893	3.496873	-0.937338
66	8	0	2.739671	1.213152	1.449269
67	1	0	1.896690	0.747140	1.726785
68	6	0	-6.116916	1.793133	0.097656
69	6	0	-4.746348	1.558401	0.185180
70	6	0	-4.159170	0.374639	-0.293042

71	6	0	-5.010428	-0.532848	-0.933296
72	6	0	-6.389364	-0.316295	-1.026915
73	6	0	-6.946971	0.842244	-0.500433
74	1	0	-2.219903	0.978946	-0.749381
75	1	0	-6.531482	2.717087	0.491033
76	1	0	-4.118337	2.317792	0.632578
77	6	0	-2.659559	0.115909	-0.230853
78	1	0	-6.991997	-1.067170	-1.527682
79	1	0	-8.018141	1.009453	-0.572451
80	6	0	-3.222670	-1.976987	-1.716502
81	6	0	-2.252696	-1.137276	-1.014163
82	8	0	-4.568087	-1.681590	-1.536501
83	8	0	-2.998785	-2.941615	-2.414702
84	6	0	-0.956637	-1.574049	-0.897704
85	8	0	-0.077192	-1.008486	-0.070833
86	6	0	-0.291817	-2.701751	-1.618848
87	6	0	-0.208448	-2.725026	-3.018056
88	6	0	0.393705	-3.673947	-0.877112
89	6	0	0.540081	-3.707626	-3.662465
90	1	0	-0.745292	-1.981077	-3.597076
91	6	0	1.123297	-4.670965	-1.525573
92	1	0	0.340498	-3.650211	0.206457
93	6	0	1.203872	-4.686961	-2.918799
94	1	0	0.595172	-3.716577	-4.747909
95	1	0	1.631317	-5.432379	-0.939537
96	1	0	1.777321	-5.459828	-3.424219

XYZ matrices MPWB1K/6-311G**

TS3-SS-a2

HF=-2430.4253002 1 imaginary frequencies=-368.7250

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.000000	0.000000
2	6	0	0.000000	0.000000	1.424498
3	6	0	1.247943	0.000000	-0.870011
4	8	0	-1.012346	-0.062853	-0.684245
5	7	0	1.164619	-0.688084	-2.016261
6	7	0	2.484114	0.511647	-0.899235
7	6	0	-1.142421	-0.687609	2.086803
8	6	0	-2.424519	-0.778468	1.539985
9	6	0	-0.956614	-1.249377	3.351886
10	6	0	-3.450503	-1.402141	2.223329
11	1	0	-2.630454	-0.341727	0.583305
12	6	0	-1.983199	-1.873349	4.028037
13	1	0	0.004816	-1.212739	3.830508
14	6	0	-3.242372	-1.954867	3.468693
15	1	0	-4.428094	-1.437914	1.770739
16	1	0	-1.792826	-2.294569	5.002102
17	1	0	-4.048228	-2.436501	3.998182
18	6	0	1.312880	-0.163466	2.127213
19	1	0	1.616310	-1.209315	2.152594
20	1	0	1.246502	0.176337	3.153313
21	1	0	2.101389	0.411428	1.670028
22	6	0	3.218404	1.344312	0.000274
23	6	0	2.811169	2.627753	0.284943
24	6	0	4.392753	0.823282	0.510195
25	6	0	3.580010	3.385418	1.150547
26	1	0	1.913193	3.008627	-0.167906
27	6	0	5.152366	1.593036	1.362637
28	1	0	4.695049	-0.174468	0.240216
29	6	0	4.740402	2.871971	1.692360
30	1	0	3.269977	4.389512	1.387019
31	1	0	6.065214	1.193837	1.771603
32	1	0	5.333611	3.471594	2.362622
33	6	0	2.330583	-0.561938	-2.678623
34	7	0	3.161032	0.166573	-2.024904
35	6	0	0.220327	-1.578976	-2.681790
36	6	0	2.310262	-1.279302	-3.966794
37	6	0	0.816993	-1.613836	-4.098176
38	1	0	2.676880	-0.661049	-4.776815
39	1	0	2.930429	-2.169785	-3.904730
40	1	0	0.325055	-0.857966	-4.701809
41	1	0	0.660726	-2.575701	-4.569609
42	1	0	-0.757526	-1.122094	-2.646393
43	6	0	0.166561	-2.949442	-1.958663
44	6	0	-0.987836	-3.784649	-2.477379
45	6	0	-1.259875	-4.965990	-1.799908
46	6	0	-1.789650	-3.430494	-3.547562
47	6	0	-2.304627	-5.775174	-2.187172
48	1	0	-0.644979	-5.233239	-0.955724
49	6	0	-2.837593	-4.245688	-3.939752
50	1	0	-1.629719	-2.514907	-4.091819
51	6	0	-3.096815	-5.417768	-3.264039
52	1	0	-2.504939	-6.685672	-1.646702
53	1	0	-3.455194	-3.952195	-4.772461
54	1	0	-3.915931	-6.048637	-3.567562
55	6	0	1.495754	-3.654181	-2.126541
56	6	0	2.541481	-3.341686	-1.271262
57	6	0	1.720148	-4.543324	-3.165325
58	6	0	3.797752	-3.876760	-1.476691
59	1	0	2.358855	-2.682271	-0.438659
60	6	0	2.977184	-5.077090	-3.371719
61	1	0	0.905817	-4.823824	-3.814399
62	6	0	4.022322	-4.736603	-2.534369
63	1	0	4.602695	-3.624027	-0.805957
64	1	0	3.138050	-5.765644	-4.184903
65	1	0	5.003076	-5.152799	-2.695722
66	8	0	0.017561	-2.737359	-0.579450
67	1	0	-0.834152	-2.330547	-0.412647

68	6	0	-0.283624	2.260907	5.376915
69	6	0	0.098870	2.201519	4.055879
70	6	0	-0.845445	2.088138	3.043117
71	6	0	-2.188224	2.102521	3.386978
72	6	0	-2.584701	2.154449	4.709519
73	6	0	-1.630228	2.218650	5.700160
74	1	0	0.485331	2.325821	1.372408
75	1	0	0.458547	2.347830	6.152656
76	1	0	1.141959	2.260767	3.787500
77	6	0	-0.506355	1.997982	1.635299
78	1	0	-3.637577	2.152733	4.934379
79	1	0	-1.939088	2.258441	6.731828
80	6	0	-2.907378	2.232555	1.105023
81	6	0	-1.527499	2.339958	0.717435
82	8	0	-3.156323	2.088721	2.452505
83	8	0	-3.879950	2.248180	0.407286
84	6	0	-1.097443	2.654905	-0.610447
85	8	0	0.091149	2.517208	-0.913586
86	6	0	-1.994035	3.188054	-1.669407
87	6	0	-1.816529	2.713812	-2.958085
88	6	0	-2.890509	4.217642	-1.442817
89	6	0	-2.548334	3.236939	-4.003707
90	1	0	-1.095743	1.929227	-3.120074
91	6	0	-3.602693	4.761385	-2.491647
92	1	0	-3.025405	4.594921	-0.443307
93	6	0	-3.440774	4.266408	-3.771962
94	1	0	-2.418393	2.849382	-5.001400
95	1	0	-4.291646	5.569769	-2.308609
96	1	0	-4.007572	4.684790	-4.588017

IN3-SS-a2

HF=-2430.4459835

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.000000	0.000000
2	6	0	0.000000	0.000000	1.582426
3	6	0	1.419462	0.000000	-0.674167
4	8	0	-0.688731	-0.906777	-0.572515
5	7	0	1.765182	-0.913042	-1.583272
6	7	0	2.416188	0.883582	-0.712144
7	6	0	-1.180271	-0.772407	2.158759
8	6	0	-2.434741	-0.811041	1.553958
9	6	0	-1.065563	-1.362131	3.411918
10	6	0	-3.510472	-1.412695	2.174319
11	1	0	-2.572585	-0.383637	0.579343
12	6	0	-2.141460	-1.964859	4.035026
13	1	0	-0.128940	-1.346561	3.939230
14	6	0	-3.372919	-1.993976	3.419027
15	1	0	-4.466129	-1.419362	1.675925
16	1	0	-2.008927	-2.405566	5.009925
17	1	0	-4.216717	-2.460167	3.901413
18	6	0	1.318507	-0.593076	2.057638
19	1	0	2.158901	-0.006196	1.699521
20	1	0	1.420218	-1.613714	1.706026
21	1	0	1.394163	-0.594397	3.136031
22	6	0	2.576011	2.116297	-0.012866
23	6	0	1.854723	3.223738	-0.407661
24	6	0	3.504130	2.182422	1.005064
25	6	0	2.028039	4.408144	0.278135
26	1	0	1.151162	3.140589	-1.216101
27	6	0	3.672180	3.373963	1.681112
28	1	0	4.082952	1.310626	1.261193
29	6	0	2.925625	4.480877	1.326376
30	1	0	1.458432	5.275756	-0.008721
31	1	0	4.386054	3.435731	2.485091
32	1	0	3.050637	5.406417	1.863043
33	6	0	2.951994	-0.544524	-2.119168
34	7	0	3.381570	0.552359	-1.605482
35	6	0	1.216227	-2.123485	-2.201129
36	6	0	3.378609	-1.462471	-3.191131
37	6	0	2.069034	-2.209162	-3.475568
38	1	0	3.756488	-0.925328	-4.051935

39	1	0	4.159267	-2.124781	-2.826437
40	1	0	1.539420	-1.718943	-4.286459
41	1	0	2.248146	-3.237241	-3.763183
42	1	0	0.169089	-1.940712	-2.395065
43	6	0	1.337806	-3.332997	-1.246444
44	6	0	0.557976	-4.523388	-1.780281
45	6	0	0.465083	-5.619329	-0.932968
46	6	0	-0.078126	-4.576651	-3.006441
47	6	0	-0.233547	-6.744511	-1.306354
48	1	0	0.940194	-5.565772	0.033018
49	6	0	-0.783495	-5.708362	-3.383786
50	1	0	-0.050718	-3.742374	-3.687948
51	6	0	-0.859899	-6.794017	-2.539805
52	1	0	-0.297101	-7.583977	-0.633424
53	1	0	-1.277682	-5.730959	-4.341279
54	1	0	-1.410538	-7.672271	-2.834448
55	6	0	2.804999	-3.672554	-1.064003
56	6	0	3.555970	-2.951603	-0.147981
57	6	0	3.441648	-4.619831	-1.850188
58	6	0	4.919394	-3.145347	-0.047123
59	1	0	3.059752	-2.236959	0.486588
60	6	0	4.806084	-4.813698	-1.751228
61	1	0	2.864566	-5.213330	-2.541334
62	6	0	5.551051	-4.069626	-0.856131
63	1	0	5.489587	-2.574865	0.667869
64	1	0	5.286512	-5.553327	-2.370634
65	1	0	6.615114	-4.221597	-0.778760
66	8	0	0.836562	-2.971507	0.001729
67	1	0	0.062553	-2.385791	-0.128684
68	6	0	1.182855	1.919238	5.570038
69	6	0	1.146223	1.732523	4.204353
70	6	0	-0.053441	1.705931	3.510611
71	6	0	-1.212344	1.943857	4.220542
72	6	0	-1.198202	2.131081	5.588979
73	6	0	0.001276	2.103907	6.264963
74	1	0	0.706562	2.011312	1.586307
75	1	0	2.126668	1.928785	6.089321
76	1	0	2.064206	1.613179	3.650987
77	6	0	-0.127711	1.483231	2.041038
78	1	0	-2.132774	2.303773	6.094990
79	1	0	0.014928	2.248173	7.332702
80	6	0	-2.568593	2.257537	2.281828
81	6	0	-1.388895	2.038433	1.462337
82	8	0	-2.427166	2.028644	3.615284
83	8	0	-3.660143	2.560664	1.907771
84	6	0	-1.432435	1.976744	0.114676
85	8	0	-0.407143	1.381541	-0.494405
86	6	0	-2.442913	2.475155	-0.816335
87	6	0	-3.060169	3.703256	-0.635973
88	6	0	-2.737710	1.713343	-1.938230
89	6	0	-3.971981	4.159337	-1.561345
90	1	0	-2.822202	4.290632	0.233656
91	6	0	-3.669655	2.162838	-2.851358
92	1	0	-2.234870	0.767023	-2.062475
93	6	0	-4.283585	3.387100	-2.666009
94	1	0	-4.446296	5.116525	-1.420442
95	1	0	-3.914129	1.560187	-3.710740
96	1	0	-5.004690	3.742090	-3.384419

TS5-SS-a2

HF=-2430.4306166; 1 imaginary frequencies= -188.3539

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.000000	0.000000
2	6	0	0.000000	0.000000	1.532810
3	6	0	1.930500	0.000000	-0.687777
4	8	0	-0.486438	-0.926945	-0.624486
5	7	0	2.136374	-0.747278	-1.790942
6	7	0	2.996160	0.809044	-0.716198
7	6	0	-1.430254	-0.141639	2.043533
8	6	0	-2.556007	0.021161	1.249213

9	6	0	-1.620193	-0.380984	3.398728
10	6	0	-3.824287	-0.056641	1.791298
11	1	0	-2.453691	0.191143	0.191214
12	6	0	-2.886918	-0.457116	3.941646
13	1	0	-0.769748	-0.502862	4.048231
14	6	0	-3.997324	-0.295609	3.138972
15	1	0	-4.680976	0.074202	1.150553
16	1	0	-3.001775	-0.642395	4.997205
17	1	0	-4.987856	-0.354269	3.559411
18	6	0	0.833678	-1.177111	2.001526
19	1	0	1.838458	-1.124420	1.590276
20	1	0	0.380619	-2.106712	1.679104
21	1	0	0.900667	-1.201262	3.081625
22	6	0	3.296738	1.892985	0.151568
23	6	0	2.709226	3.120162	-0.076707
24	6	0	4.183735	1.701057	1.189857
25	6	0	2.986537	4.164351	0.782929
26	1	0	2.031178	3.239478	-0.906182
27	6	0	4.459049	2.752148	2.040427
28	1	0	4.637999	0.734090	1.328668
29	6	0	3.854055	3.978674	1.842128
30	1	0	2.522689	5.123554	0.624591
31	1	0	5.139170	2.611544	2.863605
32	1	0	4.061962	4.794038	2.514676
33	6	0	3.285916	-0.355642	-2.396636
34	7	0	3.847131	0.606704	-1.763395
35	6	0	1.453134	-1.804367	-2.530441
36	6	0	3.542835	-1.112955	-3.634664
37	6	0	2.161182	-1.724009	-3.891693
38	1	0	3.881327	-0.474184	-4.440776
39	1	0	4.298525	-1.873692	-3.454481
40	1	0	1.590619	-1.070961	-4.545026
41	1	0	2.226010	-2.696503	-4.363264
42	1	0	0.404044	-1.548802	-2.591434
43	6	0	1.573167	-3.170882	-1.817636
44	6	0	0.658753	-4.195464	-2.470872
45	6	0	0.551645	-5.429420	-1.843659
46	6	0	-0.085374	-3.967759	-3.614393
47	6	0	-0.267607	-6.412398	-2.352108
48	1	0	1.116870	-5.600918	-0.941842
49	6	0	-0.909265	-4.955372	-4.128409
50	1	0	-0.049268	-3.019900	-4.124585
51	6	0	-1.000482	-6.178951	-3.503218
52	1	0	-0.339086	-7.363197	-1.849512
53	1	0	-1.483226	-4.757952	-5.019019
54	1	0	-1.642682	-6.946627	-3.902760
55	6	0	3.017655	-3.626313	-1.830591
56	6	0	3.882313	-3.144280	-0.859864
57	6	0	3.521239	-4.441161	-2.832135
58	6	0	5.231043	-3.434892	-0.915512
59	1	0	3.479947	-2.544675	-0.060304
60	6	0	4.870339	-4.733211	-2.887302
61	1	0	2.853981	-4.853144	-3.572584
62	6	0	5.731224	-4.221297	-1.935386
63	1	0	5.893517	-3.048374	-0.158175
64	1	0	5.248208	-5.366566	-3.673255
65	1	0	6.783988	-4.447596	-1.979478
66	8	0	1.215274	-3.007842	-0.478269
67	1	0	0.435613	-2.435275	-0.442174
68	6	0	2.160077	1.117460	5.401698
69	6	0	1.917890	0.939772	4.056552
70	6	0	0.843960	1.551750	3.425338
71	6	0	0.064126	2.404604	4.178004
72	6	0	0.290346	2.598121	5.527007
73	6	0	1.331989	1.941895	6.142185
74	1	0	1.510438	1.461213	1.461088
75	1	0	2.994458	0.621817	5.869056
76	1	0	2.574887	0.317207	3.471896
77	6	0	0.558509	1.368820	1.974000
78	1	0	-0.357011	3.269329	6.065201
79	1	0	1.508834	2.088579	7.194836
80	6	0	-1.122989	3.304906	2.310555
81	6	0	-0.354358	2.431224	1.436792
82	8	0	-0.964944	3.114649	3.644725
83	8	0	-1.922736	4.127703	1.985591
84	6	0	-0.641044	2.343624	0.122896
85	8	0	-0.238720	1.279935	-0.588208

86	6	0	-1.340034	3.292618	-0.746694
87	6	0	-1.103199	4.655595	-0.655482
88	6	0	-2.173635	2.808686	-1.744289
89	6	0	-1.707141	5.523533	-1.537880
90	1	0	-0.446202	5.025534	0.112648
91	6	0	-2.794186	3.681274	-2.613471
92	1	0	-2.327554	1.746156	-1.832360
93	6	0	-2.559992	5.038969	-2.512778
94	1	0	-1.515628	6.581204	-1.464446
95	1	0	-3.455144	3.300805	-3.374607
96	1	0	-3.037644	5.720641	-3.197535

TS3-RR-a2

HF=-2430.4219478; 1 imaginary frequencies=-383.1652

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.000000	0.000000
2	6	0	0.000000	0.000000	1.429823
3	6	0	1.268735	0.000000	-0.828339
4	8	0	-1.019187	0.168343	-0.664785
5	7	0	1.302616	0.842703	-1.871537
6	7	0	2.545524	-0.388117	-0.698995
7	6	0	-1.048171	0.867276	2.051623
8	6	0	-2.362519	0.935436	1.589376
9	6	0	-0.727548	1.652526	3.157826
10	6	0	-3.300197	1.733276	2.213027
11	1	0	-2.655782	0.361620	0.733523
12	6	0	-1.664567	2.457057	3.773815
13	1	0	0.273898	1.664739	3.547889
14	6	0	-2.962317	2.500034	3.308934
15	1	0	-4.308917	1.745558	1.833363
16	1	0	-1.371248	3.051702	4.623984
17	1	0	-3.698393	3.121006	3.792868
18	6	0	1.313364	-0.022286	2.156233
19	1	0	1.874214	-0.921826	1.949585
20	1	0	1.939397	0.836340	1.914930
21	1	0	1.149154	-0.012718	3.224449
22	6	0	3.158343	-1.387809	0.108125
23	6	0	4.349468	-1.071521	0.732289
24	6	0	2.587250	-2.635876	0.216731
25	6	0	4.962752	-2.025196	1.514005
26	1	0	4.776836	-0.092117	0.604152
27	6	0	3.211281	-3.578240	1.013979
28	1	0	1.667353	-2.852721	-0.299139
29	6	0	4.390263	-3.276553	1.663944
30	1	0	5.888273	-1.789363	2.011804
31	1	0	2.771384	-4.556373	1.113493
32	1	0	4.871801	-4.017282	2.280364
33	6	0	2.582319	0.986322	-2.267602
34	7	0	3.367554	0.236608	-1.579640
35	6	0	0.370334	1.620156	-2.676638
36	6	0	2.716349	2.041102	-3.295022
37	6	0	1.324854	2.692500	-3.220965
38	1	0	2.926835	1.613423	-4.270569
39	1	0	3.513254	2.730242	-3.042800
40	1	0	1.004841	3.072242	-4.181577
41	1	0	1.349466	3.520477	-2.519012
42	6	0	-0.371495	-2.124890	5.447137
43	6	0	-0.036725	-2.105032	4.112611
44	6	0	-1.009149	-1.938793	3.132701
45	6	0	-2.332930	-1.869020	3.530098
46	6	0	-2.682721	-1.872198	4.867440
47	6	0	-1.698782	-1.987108	5.822046
48	1	0	0.217231	-2.331691	1.410343
49	1	0	0.392864	-2.255594	6.194643
50	1	0	0.989099	-2.235426	3.807750
51	6	0	-0.723245	-1.894839	1.707609
52	1	0	-3.724866	-1.805323	5.128975
53	1	0	-1.968993	-1.995112	6.865199
54	6	0	-3.158906	-2.108258	1.298243

55	6	0	-1.802052	-2.149365	0.826362
56	8	0	-3.336868	-1.843384	2.636323
57	8	0	-4.168771	-2.278001	0.678600
58	6	0	-1.426070	-2.515802	-0.509408
59	8	0	-0.226361	-2.609889	-0.782719
60	6	0	-2.370324	-2.821619	-1.619580
61	6	0	-3.417843	-1.999672	-1.998286
62	6	0	-2.066175	-3.932942	-2.389492
63	6	0	-4.158233	-2.301055	-3.123814
64	1	0	-3.649860	-1.125637	-1.414952
65	6	0	-2.824784	-4.251408	-3.495415
66	1	0	-1.222839	-4.541162	-2.108114
67	6	0	-3.873245	-3.431599	-3.866306
68	1	0	-4.961912	-1.647260	-3.421790
69	1	0	-2.592412	-5.130595	-4.074228
70	1	0	-4.464980	-3.669723	-4.735718
71	6	0	-0.302509	0.699402	-3.749987
72	1	0	-0.399353	2.023410	-2.032884
73	6	0	0.667332	0.435961	-4.885564
74	6	0	0.754809	1.283394	-5.978529
75	6	0	1.538627	-0.638649	-4.793745
76	6	0	1.735055	1.097949	-6.932612
77	1	0	0.050474	2.093061	-6.087194
78	6	0	2.516745	-0.826222	-5.751794
79	1	0	1.437013	-1.321053	-3.966959
80	6	0	2.628005	0.049486	-6.814531
81	1	0	1.795784	1.767735	-7.774800
82	1	0	3.192853	-1.661187	-5.666691
83	1	0	3.393549	-0.096005	-7.559035
84	6	0	-1.578463	1.348130	-4.258687
85	6	0	-1.877665	2.693075	-4.129568
86	6	0	-2.482544	0.520607	-4.908350
87	6	0	-3.058374	3.202984	-4.641839
88	1	0	-1.207719	3.367868	-3.621797
89	6	0	-3.658639	1.027248	-5.416231
90	1	0	-2.255606	-0.529282	-4.988247
91	6	0	-3.950368	2.373461	-5.286927
92	1	0	-3.279011	4.251675	-4.527462
93	1	0	-4.353473	0.368642	-5.911655
94	1	0	-4.871381	2.770172	-5.681533
95	8	0	-0.574045	-0.545147	-3.197838
96	1	0	-1.007500	-0.425151	-2.344095

IN3-RR-a2

HF=-2430.4488217

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.000000	0.000000
2	6	0	0.000000	0.000000	1.566613
3	6	0	1.471828	0.000000	-0.548394
4	8	0	-0.627230	0.983845	-0.519901
5	7	0	2.025507	1.140530	-0.958011
6	7	0	2.484066	-0.870739	-0.566535
7	6	0	-1.358838	0.398604	2.125995
8	6	0	-2.537688	0.315801	1.394115
9	6	0	-1.460841	0.743828	3.467994
10	6	0	-3.759556	0.580071	1.977294
11	1	0	-2.500555	0.071957	0.349450
12	6	0	-2.684326	1.006633	4.054616
13	1	0	-0.581204	0.788980	4.087897
14	6	0	-3.841998	0.928704	3.310288
15	1	0	-4.654242	0.506660	1.380743
16	1	0	-2.725692	1.266157	5.100048
17	1	0	-4.798308	1.131749	3.764133
18	6	0	1.063954	0.996608	1.999538
19	1	0	2.065558	0.652970	1.746140
20	1	0	0.883000	1.947091	1.503764
21	1	0	1.052015	1.166670	3.067644
22	6	0	2.520328	-2.277141	-0.326753
23	6	0	3.443780	-2.748362	0.586640
24	6	0	1.711415	-3.132203	-1.043249
25	6	0	3.527389	-4.104299	0.814992
26	1	0	4.081544	-2.053771	1.106331

27	6	0	1.798919	-4.488648	-0.797019
28	1	0	1.017843	-2.740574	-1.765613
29	6	0	2.699242	-4.974015	0.130031
30	1	0	4.236636	-4.480991	1.532319
31	1	0	1.160453	-5.164212	-1.341033
32	1	0	2.761021	-6.033232	0.315869
33	6	0	3.347707	0.935604	-1.136524
34	7	0	3.664120	-0.290184	-0.909266
35	6	0	1.601371	2.476892	-1.358120
36	6	0	4.048246	2.189475	-1.481570
37	6	0	2.936516	3.224762	-1.236773
38	1	0	4.384819	2.170303	-2.513803
39	1	0	4.910936	2.345019	-0.844632
40	1	0	2.999811	4.055374	-1.927174
41	1	0	3.022553	3.617490	-0.227965
42	6	0	2.021150	-1.412470	5.395250
43	6	0	1.785517	-1.244010	4.047601
44	6	0	0.592127	-1.643675	3.463056
45	6	0	-0.333040	-2.276749	4.267733
46	6	0	-0.116029	-2.454584	5.620836
47	6	0	1.057238	-2.010138	6.186769
48	1	0	1.201089	-1.750022	1.476158
49	1	0	2.953700	-1.086728	5.824857
50	1	0	2.544286	-0.793358	3.428530
51	6	0	0.304458	-1.450401	2.013584
52	1	0	-0.876837	-2.947425	6.201806
53	1	0	1.226705	-2.146948	7.241974
54	6	0	-1.742115	-2.957377	2.460422
55	6	0	-0.818555	-2.323557	1.537072
56	8	0	-1.503206	-2.767989	3.787045
57	8	0	-2.721553	-3.582607	2.190282
58	6	0	-1.109865	-2.216202	0.220877
59	8	0	-0.485470	-1.309950	-0.522519
60	6	0	-2.035042	-3.006406	-0.597220
61	6	0	-2.736521	-2.368097	-1.609699
62	6	0	-2.149726	-4.380077	-0.446164
63	6	0	-3.577466	-3.088675	-2.432399
64	1	0	-2.614448	-1.306238	-1.744711
65	6	0	-2.972991	-5.100502	-1.283409
66	1	0	-1.593379	-4.872749	0.332205
67	6	0	-3.695162	-4.455385	-2.271324
68	1	0	-4.134037	-2.583766	-3.204570
69	1	0	-3.056840	-6.168016	-1.163124
70	1	0	-4.345258	-5.020854	-2.919079
71	6	0	0.980861	2.419143	-2.792228
72	1	0	0.841709	2.822032	-0.670336
73	6	0	2.084594	2.229108	-3.817295
74	6	0	2.740804	3.302345	-4.399559
75	6	0	2.498219	0.942704	-4.125809
76	6	0	3.824473	3.095763	-5.230164
77	1	0	2.398283	4.306511	-4.205384
78	6	0	3.581202	0.734941	-4.957946
79	1	0	1.954998	0.111306	-3.709013
80	6	0	4.256259	1.810911	-5.501648
81	1	0	4.327654	3.939802	-5.673027
82	1	0	3.896975	-0.270692	-5.183093
83	1	0	5.102320	1.649447	-6.149424
84	6	0	0.204359	3.697650	-3.068802
85	6	0	0.278177	4.850609	-2.308692
86	6	0	-0.630551	3.683393	-4.177274
87	6	0	-0.465198	5.968613	-2.650737
88	1	0	0.902081	4.903120	-1.431415
89	6	0	-1.368628	4.793987	-4.519671
90	1	0	-0.701159	2.777672	-4.756415
91	6	0	-1.287069	5.945203	-3.755968
92	1	0	-0.400759	6.855894	-2.042233
93	1	0	-2.014969	4.762366	-5.381719
94	1	0	-1.867090	6.814439	-4.019434
95	8	0	0.148547	1.316905	-2.895045
96	1	0	-0.325560	1.197274	-2.028811

TS5-RR-a2

HF=-2430.4358537; 1 imaginary frequencies=-192.1034

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.000000	0.000000
2	6	0	0.000000	0.000000	1.533301
3	6	0	2.019161	0.000000	-0.463408
4	8	0	-0.399867	0.974121	-0.614014
5	7	0	2.511456	1.194182	-0.832549
6	7	0	3.143919	-0.695127	-0.252248
7	6	0	-1.420735	0.219877	2.045562
8	6	0	-2.548816	0.170314	1.239759
9	6	0	-1.605106	0.411641	3.409452
10	6	0	-3.813236	0.307359	1.779285
11	1	0	-2.451406	0.043072	0.175953
12	6	0	-2.867970	0.545096	3.949844
13	1	0	-0.755060	0.446739	4.070193
14	6	0	-3.980624	0.494246	3.135571
15	1	0	-4.671359	0.263360	1.128799
16	1	0	-2.978093	0.687604	5.012481
17	1	0	-4.968295	0.597637	3.554019
18	6	0	0.897708	1.133047	1.998294
19	1	0	1.942532	0.916164	1.800131
20	1	0	0.621300	2.041271	1.470855
21	1	0	0.793268	1.308575	3.061360
22	6	0	3.241763	-2.074682	0.046787
23	6	0	4.181863	-2.507436	0.960775
24	6	0	2.395324	-2.961307	-0.588277
25	6	0	4.256142	-3.852159	1.257050
26	1	0	4.839525	-1.792733	1.424756
27	6	0	2.470505	-4.302870	-0.271474
28	1	0	1.691218	-2.596133	-1.317154
29	6	0	3.397300	-4.749441	0.649834
30	1	0	4.982949	-4.198920	1.972385
31	1	0	1.808479	-4.998394	-0.759809
32	1	0	3.455878	-5.797660	0.891053
33	6	0	3.865287	1.168317	-0.785497
34	7	0	4.298083	0.015000	-0.424479
35	6	0	1.992148	2.426765	-1.397845
36	6	0	4.447679	2.472518	-1.157494
37	6	0	3.194645	3.363045	-1.203221
38	1	0	4.941257	2.400696	-2.122873
39	1	0	5.174588	2.812378	-0.429294
40	1	0	3.255607	4.102567	-1.991497
41	1	0	3.082933	3.885629	-0.258191
42	6	0	2.180747	-1.276758	5.343121
43	6	0	1.921339	-1.075925	4.004353
44	6	0	0.795949	-1.613379	3.396481
45	6	0	-0.022679	-2.417293	4.161590
46	6	0	0.220396	-2.632307	5.504345
47	6	0	1.316617	-2.048826	6.098283
48	1	0	1.418465	-1.554545	1.414926
49	1	0	3.057677	-0.842534	5.793244
50	1	0	2.609352	-0.497591	3.409928
51	6	0	0.488376	-1.401774	1.954721
52	1	0	-0.456876	-3.262835	6.054759
53	1	0	1.507422	-2.213799	7.145745
54	6	0	-1.323638	-3.206407	2.315534
55	6	0	-0.500165	-2.399059	1.428249
56	8	0	-1.109681	-3.050589	3.647803
57	8	0	-2.207982	-3.944294	2.007227
58	6	0	-0.785800	-2.288084	0.114804
59	8	0	-0.316707	-1.245426	-0.590400
60	6	0	-1.537330	-3.192098	-0.757000
61	6	0	-2.283570	-2.666111	-1.802262
62	6	0	-1.433589	-4.568604	-0.618009
63	6	0	-2.947474	-3.505637	-2.672192
64	1	0	-2.336469	-1.598232	-1.928985
65	6	0	-2.082714	-5.404456	-1.498762
66	1	0	-0.843167	-4.975721	0.184029
67	6	0	-2.846629	-4.874829	-2.523090
68	1	0	-3.536686	-3.089671	-3.472517
69	1	0	-1.994784	-6.472356	-1.386446
70	1	0	-3.357930	-5.531072	-3.208405

71	6	0	1.571478	2.193910	-2.877385
72	1	0	1.119119	2.738485	-0.839543
73	6	0	2.809874	1.959806	-3.720952
74	6	0	3.462998	2.996133	-4.369863
75	6	0	3.351201	0.684880	-3.779159
76	6	0	4.658735	2.771345	-5.023971
77	1	0	3.032693	3.985077	-4.366447
78	6	0	4.547128	0.459875	-4.431872
79	1	0	2.823065	-0.126050	-3.305496
80	6	0	5.210445	1.504413	-5.046559
81	1	0	5.157044	3.587110	-5.521943
82	1	0	4.961417	-0.534639	-4.458998
83	1	0	6.144579	1.329642	-5.554912
84	6	0	0.765423	3.370155	-3.402457
85	6	0	0.579591	4.567818	-2.737570
86	6	0	0.167979	3.197486	-4.643987
87	6	0	-0.183556	5.575913	-3.304989
88	1	0	1.013096	4.738938	-1.765885
89	6	0	-0.589338	4.197651	-5.209806
90	1	0	0.300197	2.255387	-5.150590
91	6	0	-0.766302	5.396089	-4.540361
92	1	0	-0.322605	6.501435	-2.770490
93	1	0	-1.047240	4.043840	-6.173377
94	1	0	-1.360670	6.180830	-4.978885
95	8	0	0.813292	1.026932	-2.966843
96	1	0	0.166074	1.016721	-2.243844