Supporting Information for

Palladium catalysed Alkyne Alkoxycarbonylation with P,N Chelating Ligands Revisited: A Density Functional Theory Study

Shahbaz Ahmad,[a] Ashley Lockett,[a] Timothy A. Shuttleworth[b] Alexandra Miles-Hobbs, [b] Paul G. Pringle[b] and Michael Bühl*[b]

Contents

Methoxycarbonylation of Phenylacetylene

In experimental studies, we have used phenylacetylene as a substrate (instead of propyne). To compare our theoretical results with experimental observations, and particularly the substituents effects, we have tested whether the *in-situ* base mechanism (pathway **D**) would be followed for phenylacetylene or if the steric imposition could trigger the alternative catalytic cycles. The calculated energy barrier for the terminating methanolysis step of methoxycarbonylation of phenylacetylene (22.5 kcal mol^{-1}) is very close to the methanolysis barrier observed in the methoxycarbonylation of propyne (22.9 kcal mol^{-1}). When using phenylacetylene as a substrate, we observed the selectivity towards branched and linear products comparable to original pathway **D** of methoxycarbonylation of propyne (Table S1, Figures S1 – S2).

Table S1. Reaction energies in the gas phase (ΔE)[a]; DFT-D3BJ corrections (δ_{D3}), Solvation (δE_{solv})[a,b] and thermochemistry (δE_G and δE_H)[c]; Final free energies (ΔG) and enthalpies (ΔH) in kcal/mol. δE_{solv} = (ΔE_{PCM} - ΔE); ΔG_1 = relative free energies and ΔH_1 = relative enthalpies [d].

Step	ΔE	δ_{D3}	δE_{Solv}	δE_G	δE_H	ΔG	ΔH	ΔG_1	ΔH_1
***Pathway D** with phenylacetylene substrate*									
1(PhAcet) → TS1-2(PhAcet)	6.6	-1.6	4.0	-4.2	-3.9	***4.9***	5.2	***4.9***	5.2
1(PhAcet) → 2(PhAcet)	-23.0	-1.6	4.5	-0.4	0.3	***-20.5***	-19.8	***-20.5***	-19.8
2(PhAcet) + CO → 3(PhAcet)	-3.3	-11.7	-0.6	11.9	1.1	***-3.6***	-14.5	***-24.2***	-34.3
3(PhAcet) → TS3-4a(PhAcet)	6.3	4.0	-0.1	-0.4	-0.7	***9.8***	9.5	***-14.4***	-24.8
3(PhAcet) → 4a(PhAcet)	-11.1	9.5	-1.0	1.1	1.1	***-1.4***	-1.4	***-25.6***	-35.8
4a(PhAcet) + MeOH → 5a(PhAcet)	-4.0	-13.5	3.8	14.3	1.5	***0.5***	-12.3	***-25.1***	-48.1
5a(PhAcet) → TS5a-7a(PhAcet)	21.5	4.8	-3.6	-1.8	-1.5	***20.8***	21.2	***-4.2***	-26.9
5a(PhAcet) → 7a(PhAcet)	-15.4	18.1	0.6	-2.0	1.5	***1.3***	4.7	***-23.8***	-43.3
7a(PhAcet)+ phenylacetylene → 1(PhAcet) + product	-0.1	-8.6	-5.0	3.3	-0.5	***-10.4***	-14.2	***-34.1***	-57.5

[a] B3PW91/ECP2 energies; [b] model solvent MeOH, [c] B3PW91/ECP1 energies; [d] free energies and enthalpies of the respective products relative to that of **1** set to 0 kcal mol^{-1}.

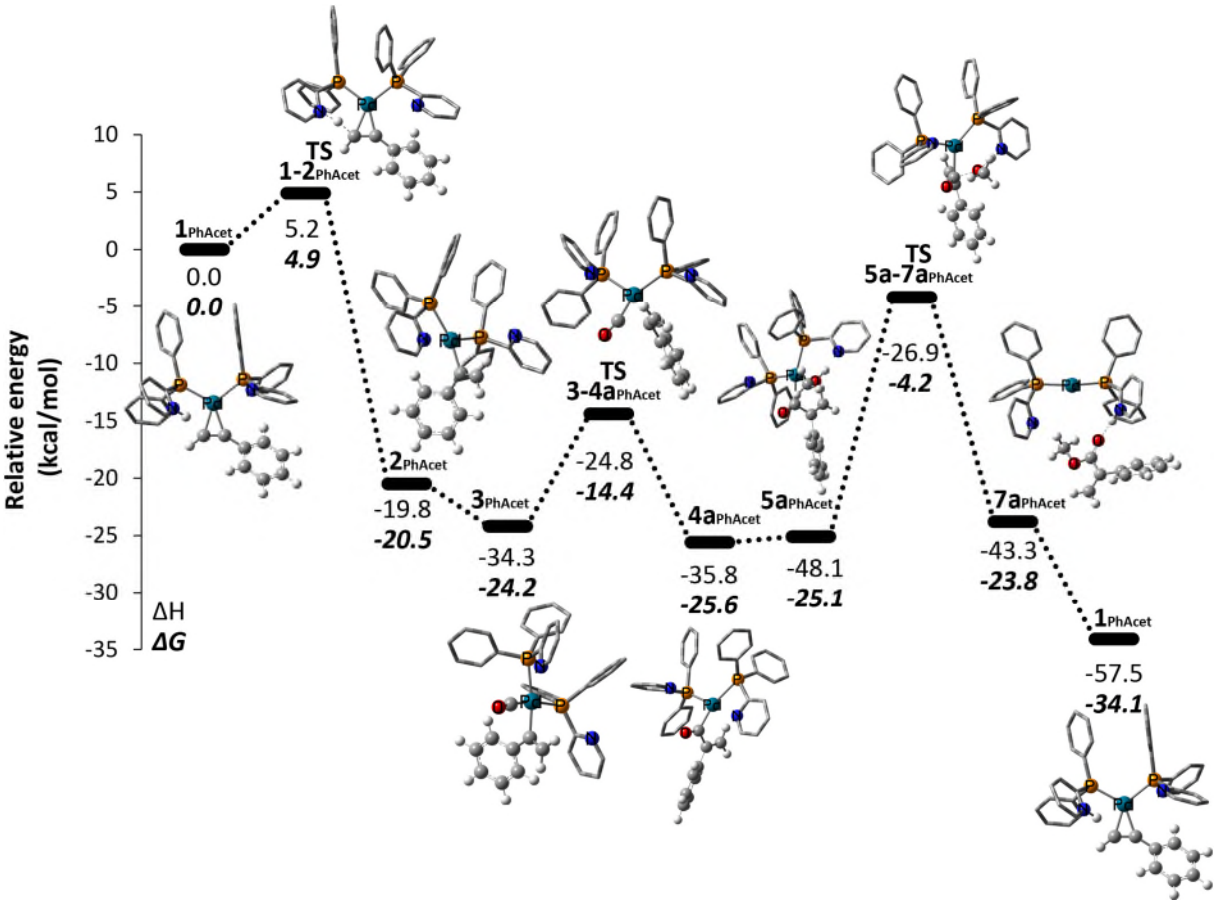

Figure S1. Reaction pathway ***D*** with phenylacetylene as substrate : free-energy profile [all energies in kcal mol^{-1} relative to **1**$_{\text{PhAcet}}$], with calculations carried at the B3PW91-D3/ECP2/PCM // B3PW91/ECP1 level of theory using methanol as the model solvent. Reaction energies for every individual step are given in **Table S1**.

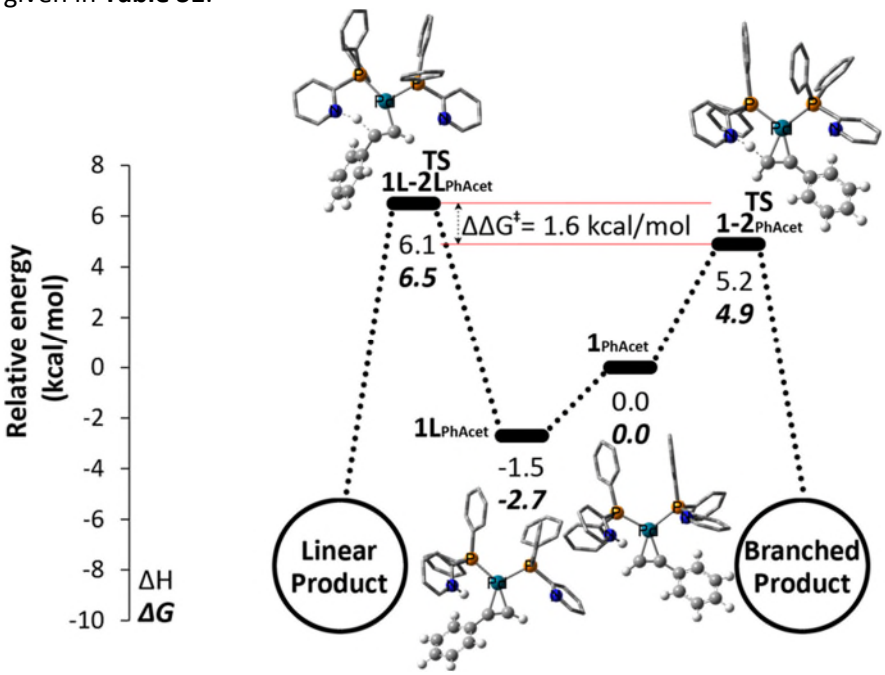

Figure S2. Pathways for formation of branched (right) and linear (left) products; energies are in kcal mol^{-1} relative to **1**.

Table S2. Reaction energies in the gas phase (ΔE)[a]; DFT-D3BJ corrections (δ_{D3}), Solvation (δE_{solv})[a,b] and thermochemistry (δE_G and δE_H)[c]; Final free energies (ΔG) and enthalpies (ΔH) in kcal/mol. δE_{solv} = (ΔE_{PCM} - ΔE); ΔG_1 = relative free energies and ΔH_1 = relative enthalpies [d].

Step	ΔE	δ_{D3}	δE_{Solv}	δE_G	δE_H	ΔG	ΔH	ΔG_1	ΔH_1
***Pathway E** (Monocationic)*									
1a → TS1a-1	12.6	4.2	-2.4	-0.1	-0.3	***14.4***	14.2	***14.4***	14.2
1a → 1	8.6	1.0	-1.5	-0.3	0.0	***7.8***	8.1	***7.8***	8.1
1 → TS1-2i	5.1	-0.1	3.5	-2.7	-3.5	***5.7***	4.9	***13.5***	13.0
1 → 2i	-6.6	-1.6	3.6	-0.7	-0.4	***-5.4***	-5.1	***2.4***	3.0
2i → TS2i-2	0.1	-0.4	-0.2	1.3	-0.4	***0.8***	-0.9	***3.2***	2.2
2i → 2	-12.8	1.3	0.8	1.2	1.0	***-9.5***	-9.7	***-7.1***	-6.7
2 + CO → TS2-3	6.3	-9.1	0.3	11.1	0.2	***8.6***	-2.3	***1.5***	-8.9
2 + CO → 3	-5.4	-9.6	-0.5	12.1	1.1	***-3.4***	-14.4	***-10.5***	-17.2
3 → TS3-4	8.0	3.1	-0.5	-0.9	-0.5	***9.7***	10.1	***-0.8***	-7.0
3 → 4	-8.6	4.1	-1.4	0.6	0.7	***-5.4***	-5.2	***-15.9***	-22.4
4 + MeOH → 5	-8.3	-7.7	4.9	12.7	1.7	***1.5***	-9.5	***-14.4***	-31.9
5 → TS5-6	2.5	-0.5	0.8	0.7	-0.5	***3.6***	2.3	***-10.8***	-29.6
5 → 6	2.5	-0.3	0.8	-0.1	0.1	***2.9***	3.1	***-11.5***	-28.8
5 → TS6-7	1.1	-0.2	0.2	1.6	-0.7	***2.7***	0.4	***-8.8***	-28.4
6 → 7	-27.6	1.9	-2.5	4.2	0.7	***-24.1***	-27.6	***-35.5***	-56.3
7 → TS7-8	17.1	6.4	-1.9	-3.1	-0.1	***18.6***	21.6	***-17.0***	-34.7
7 → 8 + MMA	15.8	20.8	-4.0	-16.9	-0.9	***15.7***	31.7	***-19.8***	-24.6
8 + Propyne → 1a	-17.6	-16.2	2.6	14.7	1.0	***-16.5***	-30.2	***-36.3***	-54.8

[a] B3PW91/ECP2 energies; [b] model solvent MeOH, [c] B3PW91/ECP1 energies; [d] free energies and enthalpies of the respective products relative to that of **1** set to 0 kcal mol^{-1}.

Revised *In Situ* Base Mechanism with diprotonated, dicationic intermediates (E)

Briefly, this pathway has been discussed within the paper. For full energy profile see Figure S6.

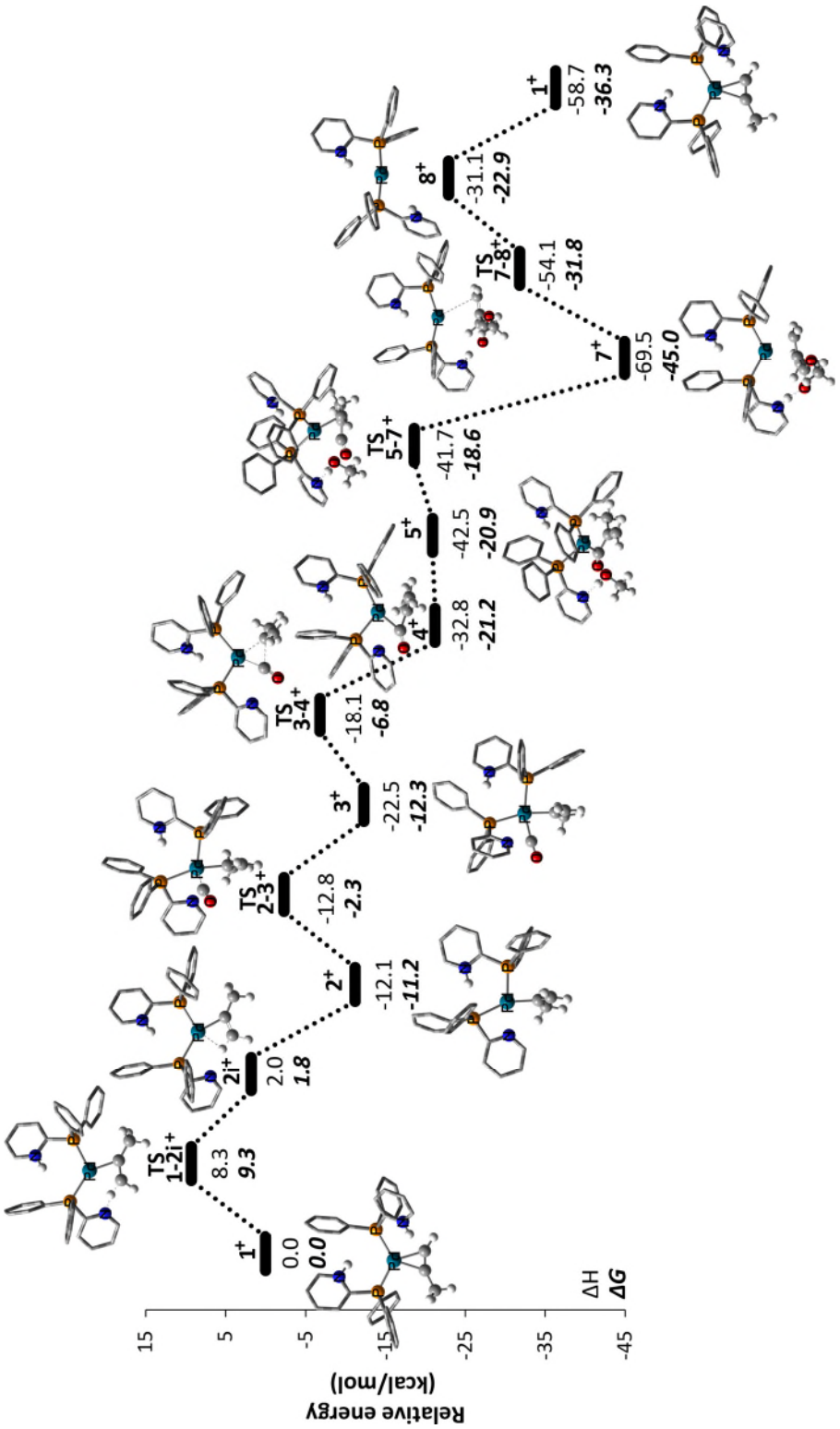

Figure S3. Full reaction profile for *in situ* base mechanism involving diprotonated, dicationic intermediates. Energies are in kcal mol^{-1} relative to **1**. Reaction energies and enthalpies for every individual step are given in **Table S3**.

Table S3. Reaction energies in the gas phase (ΔE)[a]; DFT-D3BJ corrections (δ_{D3}), Solvation (δE_{solv})[a,b] and thermochemistry (δE_G and δE_H)[c]; Final free energies (ΔG) and enthalpies (ΔH) in kcal/mol. δE_{solv} = (ΔE_{PCM} - ΔE); ΔG_1 = relative free energies and ΔH_1 = relative enthalpies [d].

Step	ΔE	δ_{D3}	δE_{Solv}	δE_G	δE_H	ΔG	ΔH	ΔG_1	ΔH_1
Pathway E *(Dicationic) reaction energies and enthalpies for every individual step*									
1^+ → TS1-$2i^+$	11.8	-0.7	1.4	-3.3	-4.3	***9.3***	8.3	***9.3***	8.3
1^+ → $2i^+$	6.4	-2.1	-0.9	-1.6	-1.4	***1.8***	2.0	***1.8***	2.0
$2i^+$ → 2^+	-16.0	0.6	0.0	2.5	1.3	***-13.0***	-14.1	***-11.2***	-12.1
2^+ + CO → TS2-3^+	6.2	-9.2	2.0	9.8	0.3	***8.9***	-0.7	***-2.3***	-12.8
2^+ + CO → 3^+	-3.6	-8.6	0.7	10.4	1.1	***-1.1***	-10.4	***-12.3***	-22.5
3^+ → TS3-4^+	6.8	0.3	-2.1	0.6	-0.5	***5.5***	4.4	***-6.8***	-18.1
3^+ → 4^+	-13.1	2.0	-0.2	2.4	1.0	***-8.9***	-10.3	***-21.2***	-32.8
4^+ + MeOH → 5^+	-5.8	-9.5	4.2	11.5	1.4	***0.3***	-9.7	***-20.9***	-42.5
5^+ → TS5-7^+	0.8	-0.2	0.9	0.9	-0.6	***2.3***	0.8	***-18.6***	-41.7
5^+ → 7^+	-35.7	4.4	2.9	4.3	1.4	***-24.1***	-27.0	***-45.0***	-69.5
7^+ → TS7-8^+	9.8	4.5	1.7	-2.8	-0.6	***13.2***	15.5	***-31.8***	-54.1
7^+ → 8^+ + MMA	21.5	25.5	-7.6	-17.3	-1.0	***22.1***	38.4	***-22.9***	-31.1
8^+ + Propyne → 1^+	-13.9	-18.6	3.7	15.4	1.3	***-13.4***	-27.6	***-36.3***	-58.7

[a] B3PW91/ECP2 energies; [b] model solvent MeOH, [c] B3PW91/ECP1 energies; [d] free energies and enthalpies of the respective products relative to that of **1** set to 0 kcal mol^{-1}.

Table S4. The **MARI**, **HETS** and high energy **TOF** determining intermediate (**TDI**) and their degree of TOF control (X_{TOF}) for dicationic pathway **E**.

Ligand	MARI	X_{TOF} (%)	HETS	X_{TOF} (%)	High energy TDI	X_{TOF} (%)	Energy Span
2-$PyPPh_2$	**7^+**	100	**TS1-$2i^+$**	87	**8^+**	13	16.8
2-(6-Me)$PyPPh_2$	**7^+**	100	**TS1-$2i^+$**	100		0	18.2
2-(4-NMe_2)$PyPPh_2$	**7^+**	100	**TS1-$2i^+$**	100		0	19.6
2-(6-Cl)$PyPPh_2$	**7^+**	100	**TS1-$2i^+$**	1	**8^+**	99	16.4
2-(4-Cl)$PyPPh_2$	**7^+**	100	**TS1-$2i^+$**	78	**8^+**	22	16.7

Tables S5a – S5p. BSSE corrections calculated at the B3PW91/ECP2 level of theory of each ligand, product (MMA) and substrate (Propyne) separately.

Table S5a **7 → TS7-8** $\delta E'_{BSSE} = E_{intra\text{-}BSSE}$ (**TS7-8**) – $E_{intra\text{-}BSSE}$ (**7**)			
$E_{intra\text{-}BSSE}$ **7**		$E_{intra\text{-}BSSE}$ **TS7-8**	
2-$PyPPh_2$	2.9	2-$PyPPh_2$	2.8
2-$PyHPPh_2^+$	3.4	2-$PyHPPh_2^+$	2.3
MMA	2.8	MMA	2.2
Total	9.1	**Total**	7.3

Table S5b	**7 → 8 + MMA**		
$\delta E'_{BSSE} = E_{intra\text{-}BSSE}$ (**8**) – $E_{intra\text{-}BSSE}$ (**7**)			
$E_{intra\text{-}BSSE}$ **7**		$E_{intra\text{-}BSSE}$ **8**	
2-$PyPPh_2$	2.9	2-$PyPPh_2$	2.2
2-$PyHPPh_2^+$	3.4	2-$PyHPPh_2^+$	2.2
MMA	2.8		
Total	9.1	**Total**	4.4

Table S5c	**7 → TS7-8 (6Me)**		
$\delta E'_{BSSE} = E_{intra\text{-}BSSE}$ (**TS7-8**) – $E_{intra\text{-}BSSE}$ (**7**)			
$E_{intra\text{-}BSSE}$ **7**		$E_{intra\text{-}BSSE}$ **TS7-8**	
2-(6-Me)$PyPPh_2$	3.0	2-(6-Me)$PyPPh_2$	2.4
2-(6-Me)$PyHPPh_2^+$	3.7	2-(6-Me)$PyHPPh_2^+$	3.0
MMA	2.8	MMA	2.3
Total	9.6	**Total**	7.7

Table S5d	**7 → TS7-8 (4NMe_2)**		
$\delta E'_{BSSE} = E_{intra\text{-}BSSE}$ (**TS7-8**) – $E_{intra\text{-}BSSE}$ (**7**)			
$E_{intra\text{-}BSSE}$ **7**		$E_{intra\text{-}BSSE}$ **TS7-8**	
2-(4-NMe_2)$PyPPh_2$	2.9	2-(4-NMe_2)$PyPPh_2$	2.3
2-(4-NMe_2)$PyHPPh_2^+$	3.5	2-(4-NMe_2)$PyHPPh_2^+$	2.8
MMA	2.7	MMA	2.1
Total	9.1	**Total**	7.3

Table S5e	**7 → TS7-8 (6Cl)**		
$\delta E'_{BSSE} = E_{intra\text{-}BSSE}$ (**TS7-8**) – $E_{intra\text{-}BSSE}$ (**7**)			
$E_{intra\text{-}BSSE}$ **7**		$E_{intra\text{-}BSSE}$ **TS7-8**	
2-(6-Cl)$PyPPh_2$	3.5	2-(6-Cl)$PyPPh_2$	2.8
2-(6-Cl)$PyHPPh_2^+$	4.4	2-(6-Cl)$PyHPPh_2^+$	3.6
MMA	3.2	MMA	2.6
Total	11.1	**Total**	8.9

Table S5f	**7 → TS7-8 (4Cl)**		
$\delta E'_{BSSE} = E_{intra\text{-}BSSE}$ (**TS7-8**) – $E_{intra\text{-}BSSE}$ (**7**)			
$E_{intra\text{-}BSSE}$ **7**		$E_{intra\text{-}BSSE}$ **TS7-8**	
2-(4-Cl)$PyPPh_2$	3.1	2-(4-Cl)$PyPPh_2$	2.4
2-(4-Cl)$PyHPPh_2^+$	3.8	2-(4-Cl)$PyHPPh_2^+$	3.0
MMA	2.9	MMA	2.2
Total	9.8	**Total**	7.6

Table S5g **7^+ + Propyne → TS1-2i$^+$ + MMA** $\delta E'_{BSSE} = E_{intra\text{-}BSSE}$ (**TS1-2i$^+$**) – $E_{intra\text{-}BSSE}$ (**7^+**)			
$E_{intra\text{-}BSSE}$ **7^+**		$E_{intra\text{-}BSSE}$ **TS1-2i$^+$**	
2-PyHPPh$_2^+$**–1**	3.2	2-PyHPPh$_2^+$**–1**	2.8
2-PyHPPh$_2^+$**–2**	2.7	2-PyHPPh$_2^+$**–2**	1.8
MMA	2.7	MMA	2.8
Total	8.6	**Total**	7.5

Table S5h **7^+ → 8^+ + MMA** $\delta E'_{BSSE} = E_{intra\text{-}BSSE}$ (**8^+**) – $E_{intra\text{-}BSSE}$ (**7^+**)			
$E_{intra\text{-}BSSE}$ **7^+**		$E_{intra\text{-}BSSE}$ **8^+**	
2-PyHPPh$_2^+$**–1**	3.2	2-PyHPPh$_2^+$**–1**	1.6
2-PyHPPh$_2^+$**–2**	2.7	2-PyHPPh$_2^+$**–2**	1.7
MMA	2.7		
Total	8.6	**Total**	3.3

Table S5i **7^+ + Propyne → TS1-2i$^+$ + MMA (6Me)** $\delta E'_{BSSE} = E_{intra\text{-}BSSE}$ (**TS1-2i$^+$**) – $E_{intra\text{-}BSSE}$ (**7^+**)			
$E_{intra\text{-}BSSE}$ **7^+**		$E_{intra\text{-}BSSE}$ **TS1-2i$^+$**	
2-(6-Me)PyHPPh$_2^+$**–1**	3.5	2-(6-Me)PyHPPh$_2^+$**–1**	2.9
2-(6-Me)PyHPPh$_2^+$**–2**	2.8	2-(6-Me)PyHPPh$_2^+$**–2**	2.9
MMA	2.9	MMA	1.8
Total	9.2	**Total**	7.6

Table S5j **7^+ → 8^+ + MMA (6Me)** $\delta E'_{BSSE} = E_{intra\text{-}BSSE}$ (**8^+**) – $E_{intra\text{-}BSSE}$ (**7^+**)			
$E_{intra\text{-}BSSE}$ **7^+**		$E_{intra\text{-}BSSE}$ **8^+**	
2-(6-Me)PyHPPh$_2^+$**–1**	3.5	2-(6-Me)PyHPPh$_2^+$**–1**	1.8
2-(6-Me)PyHPPh$_2^+$**–2**	2.8	2-(6-Me)PyHPPh$_2^+$**–2**	1.6
MMA	2.9		
Total	9.2	**Total**	3.4

Table S5k **7^+ + Propyne → TS1-2i$^+$ + MMA (4NMe$_2$)** $\delta E'_{BSSE} = E_{intra\text{-}BSSE}$ (**TS1-2i$^+$**) – $E_{intra\text{-}BSSE}$ (**7^+**)			
$E_{intra\text{-}BSSE}$ **7^+**		$E_{intra\text{-}BSSE}$ **TS1-2i$^+$**	
2-(4-NMe$_2$)PyHPPh$_2^+$**–1**	3.2	2-(4-NMe$_2$)PyHPPh$_2^+$**–1**	2.7
2-(4-NMe$_2$)PyHPPh$_2^+$**–2**	2.7	2-(4-NMe$_2$)PyHPPh$_2^+$**–2**	2.7
MMA	2.7	MMA	1.7
Total	8.7	**Total**	7.2

Table S5l	**7^+ → 8^+ + MMA ($4NMe_2$)**		
$\delta E'_{BSSE} = E_{intra\text{-}BSSE}$ (**8^+**) – $E_{intra\text{-}BSSE}$ (**7^+**)			
$E_{intra\text{-}BSSE}$ **7^+**		$E_{intra\text{-}BSSE}$ **8^+**	
2-(4-NMe_2)PyHPPh_2^+**–1**	3.2	2-(4-NMe_2)PyHPPh_2^+**–1**	1.5
2-(4-NMe_2)PyHPPh_2^+**–2**	2.7	2-(4-NMe_2)PyHPPh_2^+**–2**	1.4
MMA	2.7		
Total	8.7	**Total**	2.9

Table S5m	**7^+ + Propyne → TS1-2i$^+$ + MMA (6Cl)**		
$\delta E'_{BSSE} = E_{intra\text{-}BSSE}$ (**TS1-2i$^+$**) – $E_{intra\text{-}BSSE}$ (**7^+**)			
$E_{intra\text{-}BSSE}$ **7^+**		$E_{intra\text{-}BSSE}$ **TS1-2i$^+$**	
2-(6-Cl)PyHPPh_2^+**–1**	4.1	2-(6-Cl)PyHPPh_2^+**–1**	3.5
2-(6-Cl)PyHPPh_2^+**–2**	3.2	2-(6-Cl)PyHPPh_2^+**–2**	3.4
MMA	3.2	MMA	1.9
Total	10.4	**Total**	8.7

Table S5n	**7^+ → 8^+ + MMA (6Cl)**		
$\delta E'_{BSSE} = E_{intra\text{-}BSSE}$ (**8^+**) – $E_{intra\text{-}BSSE}$ (**7^+**)			
$E_{intra\text{-}BSSE}$ **7^+**		$E_{intra\text{-}BSSE}$ **8^+**	
2-(6-Cl)PyHPPh_2^+**–1**	4.1	2-(6-Cl)PyHPPh_2^+**–1**	2.0
2-(6-Cl)PyHPPh_2^+**–2**	3.2	2-(6-Cl)PyHPPh_2^+**–2**	2.1
MMA	3.2		
Total	10.4	**Total**	4.1

Table S5o	**7^+ + Propyne → TS1-2i$^+$ + MMA (4Cl)**		
$\delta E'_{BSSE} = E_{intra\text{-}BSSE}$ (**TS1-2i$^+$**) – $E_{intra\text{-}BSSE}$ (**7^+**)			
$E_{intra\text{-}BSSE}$ **7^+**		$E_{intra\text{-}BSSE}$ **TS1-2i$^+$**	
2-(4-Cl)PyHPPh_2^+**–1**	3.7	2-(4-Cl)PyHPPh_2^+**–1**	2.9
2-(4-Cl)PyHPPh_2^+**–2**	3.2	2-(4-Cl)PyHPPh_2^+**–2**	2.9
MMA	2.8	MMA	1.8
Total	9.7	**Total**	7.6

Table S5p $7^+ \rightarrow 8^+ + MMA$ (4Cl) $\delta E'_{BSSE} = E_{intra\text{-}BSSE}(8^+) - E_{intra\text{-}BSSE}(7^+)$			
$E_{intra\text{-}BSSE}$ **7**$^+$		$E_{intra\text{-}BSSE}$ **8**$^+$	
2-(4-Cl)PyHPPh$_2^+$**–1**	3.7	2-(4-Cl)PyHPPh$_2^+$**–1**	1.7
2-(4-Cl)PyHPPh$_2^+$**–2**	3.2	2-(4-Cl)PyHPPh$_2^+$**–2**	1.7
MMA	2.8		
Total	9.7	**Total**	3.5

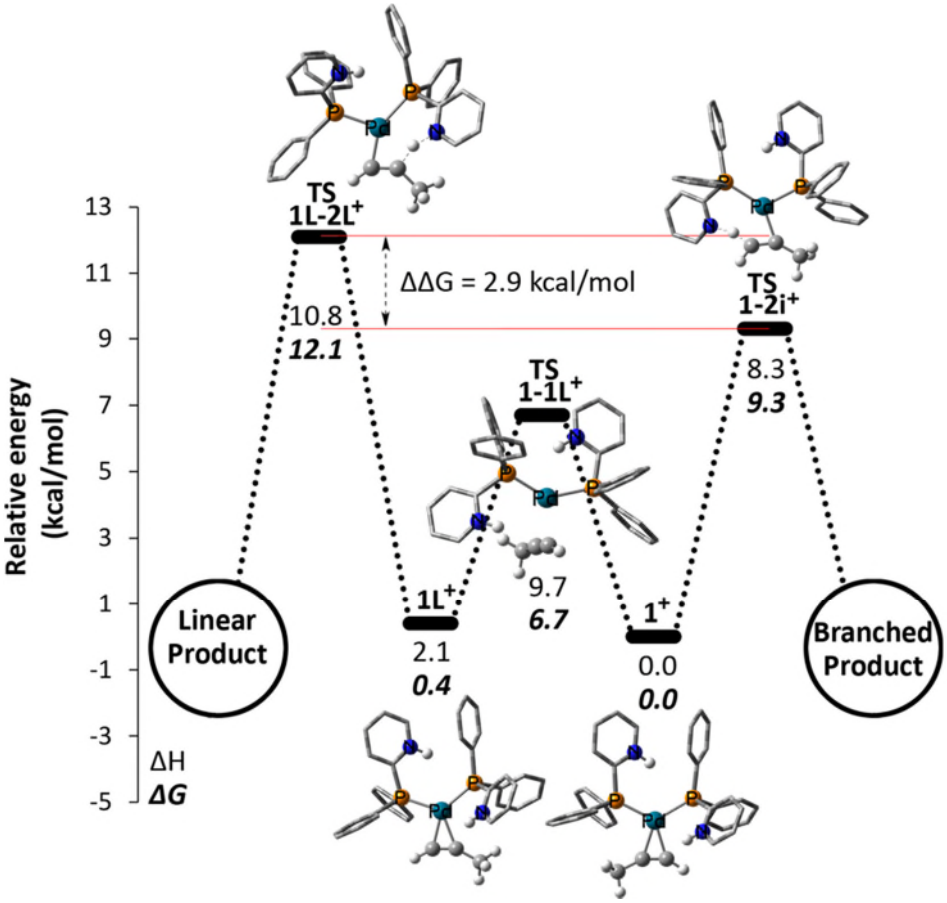

Figure S4: Profile for formation of branched (right) and linear (left) products on the dicationic pathway; energies are in kcal mol^{-1} relative to **1**$^+$. Note that **1**$^+$ and **1L**$^+$ can now interconvert directly

Tables S6. Mechanism ***E***, branched to linear products selectivities.

Step	ΔE	δ_{D3}	δE_{Solv}	δE_G	δE_H	$\Delta\Delta G^{\ddagger}$
$\Delta G^{\ddagger}_{1L\rightarrow 2L} - \Delta G^{\ddagger}_{1\rightarrow 1a}$ **(2-PyPPh$_2$)**	5.2	-2.6	4.3	-3.2	-3.0	***3.7***
$\Delta G^{\ddagger}_{1\rightarrow 2i} - \Delta G^{\ddagger}_{1\rightarrow 1a}$ **(2-PyPPh$_2$)**	1.0	-3.3	4.4	-3.0	-3.2	***-0.9***
$\Delta G^{\ddagger}_{1L\rightarrow 2L} - \Delta G^{\ddagger}_{1\rightarrow 2i}$ **(2-(6-Me)PyPPh$_2$)**	6.2	1.2	-0.3	-0.7	0.1	***6.3***
$\Delta G^{\ddagger}_{1\rightarrow 2i} - \Delta G^{\ddagger}_{1\rightarrow 1a}$ **(2-(6-Me)PyPPh$_2$)**	10.3	-3.0	3.9	-3.5	-3.2	***7.8***
$\Delta G^{\ddagger}_{1L\rightarrow 2L} - \Delta G^{\ddagger}_{1\rightarrow 2i}$ **(2-(4-NMe$_2$)PyPPh$_2$)**	3.8	0.8	0.0	-0.1	0.3	***4.4***
$\Delta G^{\ddagger}_{1\rightarrow 2i} - \Delta G^{\ddagger}_{1\rightarrow 1a}$ **(2-(4-NMe$_2$)PyPPh$_2$)**	5.7	-3.4	4.8	-2.6	-3.5	***4.5***
$\Delta G^{\ddagger}_{1L\rightarrow 2L} - \Delta G^{\ddagger}_{1\rightarrow 2i}$ **(2-(6-Cl)PyPPh$_2$)**	6.1	0.6	-0.2	-0.7	0.0	***5.9***
$\Delta G^{\ddagger}_{1\rightarrow 2i} - \Delta G^{\ddagger}_{1\rightarrow 1a}$ **(2-(6-Cl)PyPPh$_2$)**	7.1	-3.2	2.9	-3.8	-3.3	***3.1***
$\Delta G^{\ddagger}_{1L\rightarrow 2L} - \Delta G^{\ddagger}_{1\rightarrow 2i}$ **(2-(4-Cl)PyPPh$_2$)**	4.3	0.7	-0.1	-0.1	0.2	***4.8***
$\Delta G^{\ddagger}_{1\rightarrow 2i} - \Delta G^{\ddagger}_{1\rightarrow 1a}$ **(2-(4-Cl)PyPPh$_2$)**	5.2	-2.9	4.0	-2.9	-3.0	***3.4***

Gaussian 09 full reference

Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, J. A., Jr.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, J. M.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, Ö.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J., Gaussian 09, Revision D.01, Gaussian, Inc., Wallingford CT, **2009**.

Typical spectra obtained in the experimental phenyl acetylene methoxycarbonylation catalysis

The catalysis was carried out as described in the manuscript. The conversion and selectivity were determined from ^{1}H NMR spectra of samples of the product. Below are typical spectra obtained.

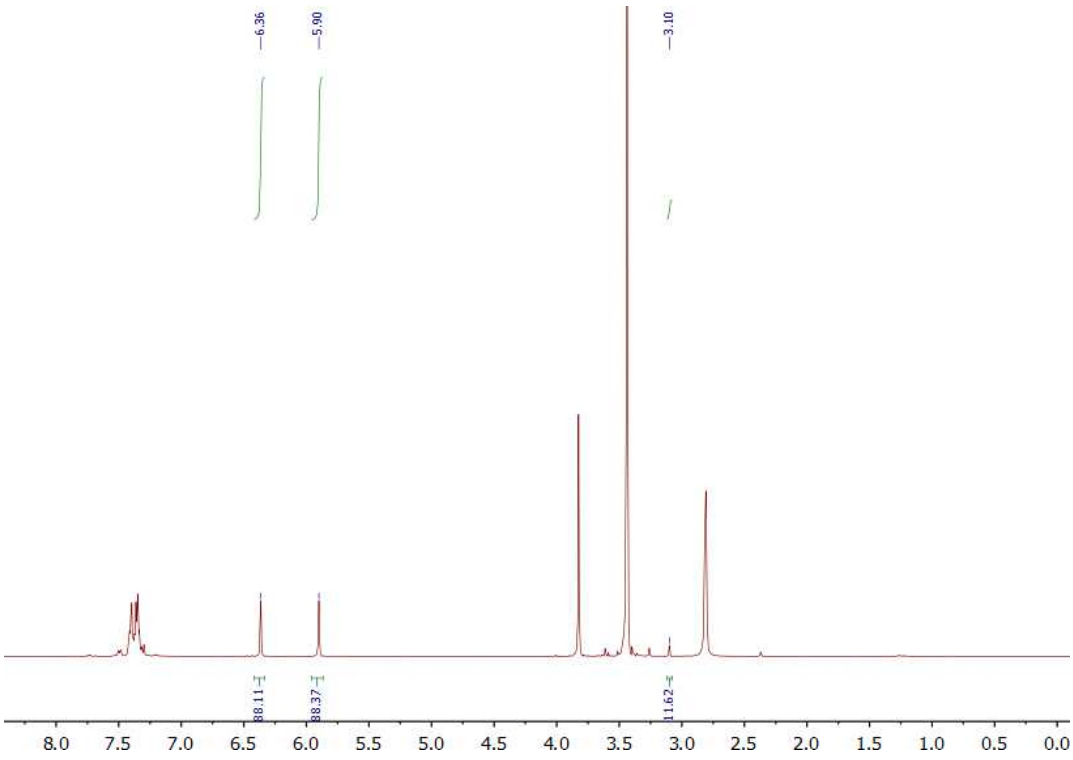

Figure S5: Example ^{1}H NMR spectrum of $PyPPh_2$ catalysis run using Method B. Conversion determined by integration of the phenyacetylene alkynyl proton (δ_H 3.10 ppm) and the methyl atropate (δ_H 6.36 and 5.90 ppm) alkenyl protons.

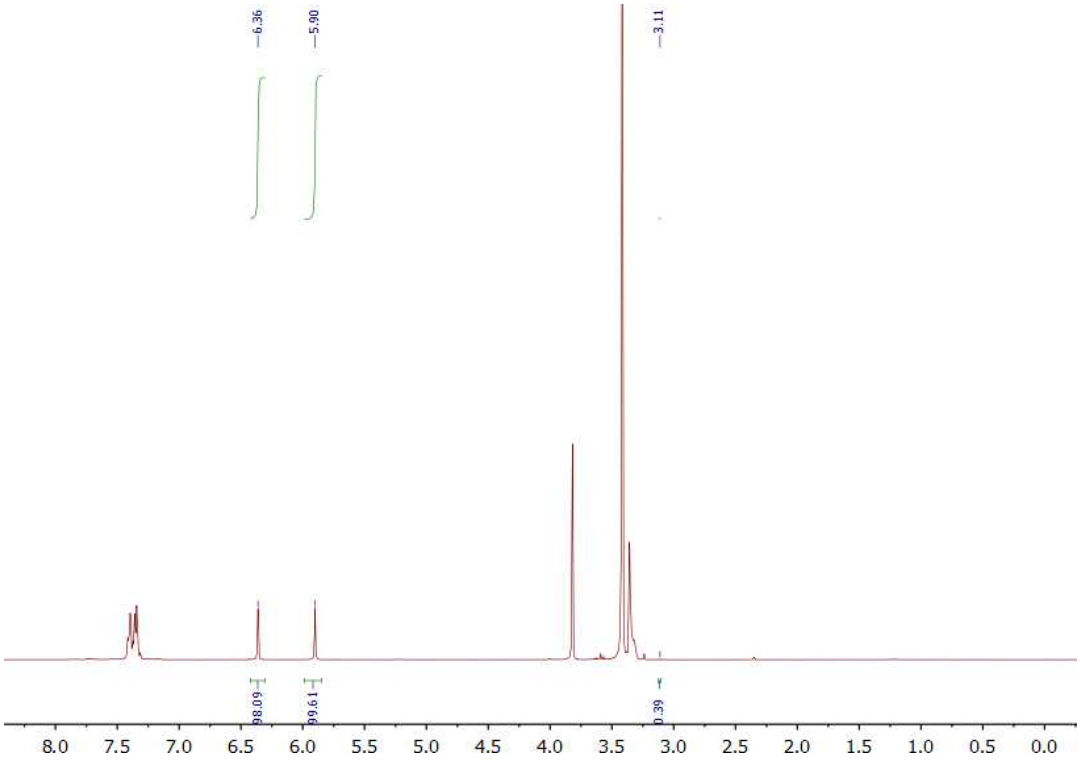

Figure S6: Example ^{1}H NMR spectrum of 2-(6-Cl)PyPPh$_2$ catalysis run using Method B. Conversion determined by integration of the phenyacetylene alkynyl proton (δ_H 3.11 ppm) and the methyl atropate (δ_H 6.36 and 5.90 ppm) alkenyl protons.

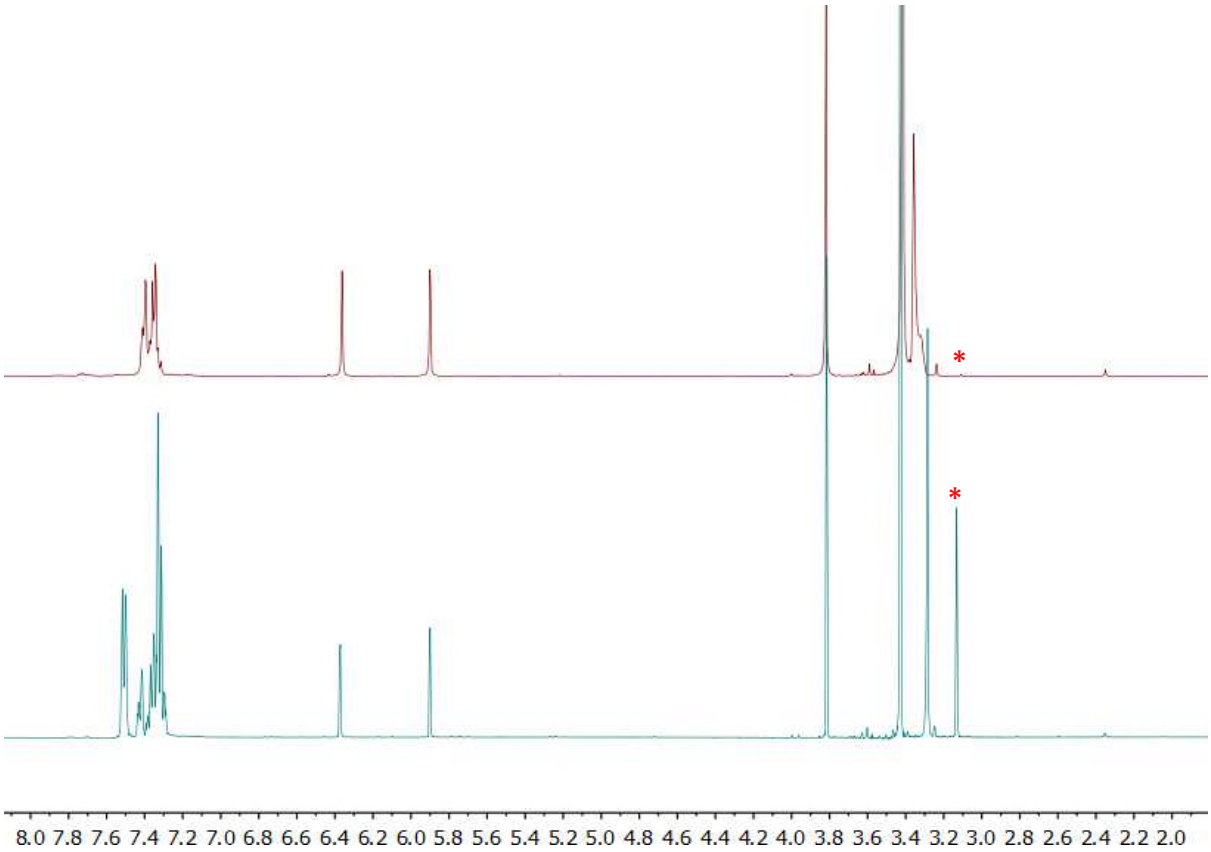

Figure S7: Top spectrum: ^{1}H NMR at end of catalysis when using 2-(6-Cl)PyPPh$_2$, Method B. Bottom spectrum: an aliquot of phenylacetylene has been added to the NMR sample to confirm the identity of its alkynyl proton peak (*) – can see this peak increase upon addition.

Atomic coordinates (in Å) of all intermediate and transition states, optimised at the B3PW91/ECP1 level, and corresponding SCF energies (in a.u.).

Complex 1

SCF done: -2349.135055

Pd	0.017544	-1.400554	0.178972
P	-1.893841	-0.080878	0.031166
C	-3.321924	-1.216755	-0.415965
N	-3.006306	-2.524573	-0.397866
C	-4.609378	-0.861606	-0.813133
C	-3.853522	-3.511188	-0.730430
C	-5.522028	-1.855614	-1.161083
H	-6.527494	-1.584743	-1.469569
C	-5.143601	-3.200096	-1.120176
H	-5.831577	-3.991677	-1.393953
H	-4.879330	0.187685	-0.858185
H	-3.465272	-4.522354	-0.683018
C	-2.451270	0.645057	1.620318
C	-3.605054	0.257137	2.312511
C	-1.596182	1.605824	2.185015
C	-3.905520	0.828513	3.548825
H	-4.276777	-0.492442	1.904727
C	-1.910625	2.178354	3.414403
H	-0.690961	1.900320	1.656499
C	-3.062268	1.790714	4.099735
H	-4.801069	0.518745	4.079676
H	-1.246514	2.923713	3.842444
H	-3.299375	2.233949	5.062451
C	-2.217665	1.216736	-1.226736
C	-3.039831	2.323597	-0.979499
C	-1.644574	1.049773	-2.494460
C	-3.293206	3.244099	-1.995632
H	-3.468685	2.472212	0.007701
C	-1.905832	1.968738	-3.508008
H	-0.984234	0.205666	-2.679549
C	-2.731705	3.065239	-3.259825
H	-3.928604	4.102927	-1.798389
H	-1.458530	1.833692	-4.488501
H	-2.932327	3.783841	-4.049243
H	-1.997338	-2.720610	-0.110663
P	1.882934	0.008656	-0.051942
C	2.645158	0.442884	1.560591
C	3.794811	1.021766	4.049383
C	3.527529	1.524457	1.701091
C	2.333341	-0.332723	2.684629
C	2.909338	-0.046453	3.921565
C	4.100206	1.808681	2.938512
H	3.763120	2.151464	0.845532
H	1.625542	-1.152370	2.588168
H	2.658728	-0.654247	4.786325
H	4.782455	2.648362	3.036169
H	4.241112	1.247126	5.013715
C	1.693844	1.682462	-0.826007
C	1.276913	4.210614	-1.782269
N	0.796770	2.462055	-0.205925
C	2.415373	2.104505	-1.945476
C	2.197084	3.393942	-2.429993
C	0.603424	3.695570	-0.674636
H	3.136556	1.446345	-2.417320
H	2.746089	3.753621	-3.295825
H	-0.129143	4.300009	-0.143659
H	1.080647	5.222626	-2.121440
C	3.229269	-0.746829	-1.051651
C	5.174023	-1.930976	-2.689423
C	4.587304	-0.645315	-0.726215
C	2.856842	-1.459581	-2.201762
C	3.822952	-2.039911	-3.020414
C	5.552080	-1.238604	-1.540414
H	4.895323	-0.112863	0.168225
H	1.801955	-1.571701	-2.443404
H	3.521064	-2.587307	-3.908948
H	6.602027	-1.159432	-1.273215
H	5.928376	-2.391450	-3.320826
C	2.312150	-3.722673	0.711580
H	2.896329	-3.138238	1.428837
H	2.827677	-3.652530	-0.251039
H	2.312041	-4.770546	1.031317
C	0.932620	-3.209226	0.602174
H	-1.008935	-4.203315	0.985262
C	-0.328334	-3.421116	0.672071

Complex 1L

SCF done: -2349.130687

Pd	-0.032508	-1.411263	0.014397
P	-1.805621	0.070505	0.004172
C	-3.369613	-0.888978	-0.404259
N	-3.179534	-2.217987	-0.492825
C	-4.640260	-0.389964	-0.683091
C	-4.138841	-3.096564	-0.830733
C	-5.664533	-1.266975	-1.031623
H	-6.657141	-0.883803	-1.249441
C	-5.413841	-2.639856	-1.107907
H	-6.190492	-3.343742	-1.384050
H	-4.810790	0.679910	-0.638034
H	-3.851685	-4.140134	-0.871837
C	-2.245276	0.841985	1.609046
C	-3.353983	0.468844	2.379096
C	-1.347368	1.798556	2.109914
C	-3.571669	1.054556	3.625675
H	-4.054603	-0.280854	2.023440
C	-1.577914	2.383992	3.352047
H	-0.471773	2.075469	1.525104
C	-2.687777	2.014921	4.112197
H	-4.434176	0.757324	4.215195
H	-0.880489	3.125711	3.730468
H	-2.859988	2.470093	5.083102
C	-2.020563	1.396721	-1.246894
C	-2.727447	2.578504	-0.990941
C	-1.484504	1.172783	-2.521888
C	-2.904796	3.517730	-2.005978
H	-3.121868	2.772725	0.002713
C	-1.669586	2.111542	-3.534165
H	-0.909352	0.269120	-2.711094
C	-2.381284	3.283429	-3.277542
H	-3.450307	4.434847	-1.802025
H	-1.250892	1.932554	-4.520265
H	-2.521955	4.017182	-4.065987
H	-2.177629	-2.511080	-0.295526
P	1.940282	-0.112860	-0.043663
C	2.566409	0.260435	1.640657
C	3.521305	0.714286	4.235770
C	3.397573	1.357486	1.909396
C	2.212904	-0.600267	2.688578
C	2.692682	-0.376269	3.977662
C	3.870869	1.581123	3.200578
H	3.676225	2.041748	1.113225
H	1.554932	-1.442457	2.490013
H	2.412432	-1.051249	4.781306
H	4.513869	2.434320	3.397525
H	3.891644	0.891473	5.241449
C	1.940856	1.561822	-0.838647
C	1.777957	4.091896	-1.868185
N	1.041211	2.409836	-0.318661
C	2.789317	1.915786	-1.891010
C	2.700790	3.205893	-2.412725
C	0.972112	3.643070	-0.821929

H	3.507654	1.204907	-2.283899
H	3.350528	3.511948	-3.227923
H	0.232316	4.302268	-0.372448
H	1.679320	5.106620	-2.240134
C	3.333454	-0.961223	-0.892886
C	5.382534	-2.253679	-2.303475
C	4.655439	-0.903471	-0.433636
C	3.048682	-1.684494	-2.060885
C	4.068431	-2.318594	-2.766913
C	5.672175	-1.550752	-1.135139
H	4.892251	-0.359739	0.475782
H	2.020129	-1.760966	-2.406064
H	3.835276	-2.874125	-3.670899
H	6.692598	-1.505467	-0.765432
H	6.176982	-2.756830	-2.847112
C	-1.258402	-4.679283	0.529787
H	-1.679676	-5.044710	-0.416090
H	-2.086840	-4.427145	1.200980
H	-0.716216	-5.518059	0.978678
C	-0.338451	-3.531834	0.298849
H	1.928826	-3.513756	0.210221
C	0.893385	-3.213767	0.209464

TS1-2i

SCF done: -2349.127651

Pd	0.060652	-1.357955	0.128165
P	-1.908634	-0.057438	0.000758
C	-3.218826	-1.330333	-0.397879
N	-2.825831	-2.606147	-0.274956
C	-4.510775	-1.036325	-0.834137
C	-3.650741	-3.621610	-0.550055
C	-5.384936	-2.082521	-1.124786
H	-6.393761	-1.870709	-1.466535
C	-4.952696	-3.399550	-0.979555
H	-5.603206	-4.237921	-1.203256
H	-4.818319	-0.002958	-0.953419
H	-3.243318	-4.621465	-0.431292
C	-2.463017	0.647337	1.598589
C	-3.633589	0.261125	2.263828
C	-1.612660	1.596261	2.189550
C	-3.953434	0.822636	3.499732
H	-4.301188	-0.478255	1.832353
C	-1.946258	2.159185	3.418333
H	-0.697650	1.890335	1.679110
C	-3.113881	1.772856	4.076837
H	-4.861576	0.514668	4.009773
H	-1.285766	2.895658	3.866971
H	-3.366582	2.208230	5.039237
C	-2.289459	1.214028	-1.260825
C	-3.134677	2.300767	-1.004043
C	-1.732415	1.056758	-2.537149
C	-3.426138	3.211468	-2.019118
H	-3.556288	2.439358	-0.012440
C	-2.032048	1.965111	-3.549038
H	-1.057995	0.226433	-2.733199
C	-2.879880	3.042740	-3.290907
H	-4.081573	4.053388	-1.814957
H	-1.599306	1.836035	-4.536865
H	-3.111024	3.752992	-4.079524
H	-1.536514	-2.777829	0.069235
P	1.893638	0.032883	-0.038664
C	2.597293	0.469981	1.594569
C	3.674381	1.062191	4.109872
C	3.454345	1.568670	1.757522
C	2.274296	-0.317365	2.707088
C	2.814278	-0.023594	3.958117
C	3.991042	1.859239	3.009358
H	3.698475	2.202467	0.909468
H	1.586445	-1.151212	2.591550
H	2.555481	-0.639106	4.814805
H	4.653825	2.711800	3.126253
H	4.092432	1.293183	5.085379
C	1.660927	1.694241	-0.822532
C	1.188773	4.203671	-1.793197
N	0.737675	2.450547	-0.214673
C	2.386863	2.129074	-1.933609
C	2.139683	3.410887	-2.425518
C	0.515500	3.676004	-0.691013
H	3.130925	1.488965	-2.394403
H	2.689404	3.782116	-3.285845
H	-0.239878	4.261807	-0.171704
H	0.968582	5.208080	-2.140025
C	3.267733	-0.699716	-1.012101
C	5.274873	-1.837350	-2.603036
C	4.610685	-0.611187	-0.626862
C	2.939853	-1.374503	-2.198338
C	3.938303	-1.931781	-2.993327
C	5.607013	-1.181981	-1.418935
H	4.882202	-0.106609	0.295050
H	1.896508	-1.474636	-2.489612
H	3.672666	-2.449608	-3.910550
H	6.645127	-1.114008	-1.106675
H	6.053536	-2.280377	-3.217049
C	2.309180	-3.700502	0.613573
H	2.873550	-3.161835	1.380871
H	2.870202	-3.603986	-0.321232
H	2.267684	-4.761081	0.885402
C	0.949700	-3.143841	0.459632
H	-0.814409	-4.376858	0.764645
C	-0.312064	-3.454334	0.479169

TS1L-2iL

SCF done: -2349.121046

Pd	0.019028	-1.338637	0.011713
P	-1.818885	0.110400	-0.008740
C	-3.226390	-1.046807	-0.423060
N	-2.924482	-2.354787	-0.402377
C	-4.502407	-0.622485	-0.794081
C	-3.839137	-3.275056	-0.737449
C	-5.463971	-1.568971	-1.139877
H	-6.461233	-1.254541	-1.432991
C	-5.127637	-2.920439	-1.113731
H	-5.842908	-3.688922	-1.385776
H	-4.728432	0.438105	-0.823675
H	-3.519397	-4.310276	-0.707506
C	-2.293907	0.819086	1.611894
C	-3.449948	0.456568	2.314522
C	-1.396211	1.736013	2.182975
C	-3.709537	1.010872	3.567630
H	-4.152891	-0.258093	1.897928
C	-1.669559	2.291978	3.429606
H	-0.490148	2.008983	1.645865
C	-2.823674	1.930256	4.124955
H	-4.607325	0.721962	4.106353
H	-0.972640	3.003546	3.862923
H	-3.029725	2.360613	5.100622
C	-2.119137	1.433667	-1.238763
C	-2.858913	2.584846	-0.942136
C	-1.611836	1.250245	-2.532326
C	-3.096799	3.534849	-1.935066
H	-3.239562	2.743191	0.062901
C	-1.857602	2.198854	-3.521514
H	-1.017655	0.368041	-2.759644
C	-2.600949	3.341505	-3.223835
H	-3.670888	4.426671	-1.700102
H	-1.463814	2.049883	-4.522752
H	-2.789972	4.082624	-3.995081
H	-1.626268	-2.621046	-0.095638
P	1.958174	-0.085145	-0.039839
C	2.581219	0.286583	1.641599
C	3.552596	0.751468	4.226172
C	3.399338	1.395543	1.901962

C	2.247944	-0.580137	2.690909
C	2.735768	-0.349717	3.975599
C	3.881764	1.623698	3.188772
H	3.659377	2.085169	1.104139
H	1.598844	-1.430427	2.498916
H	2.470844	-1.027758	4.781684
H	4.514487	2.485475	3.380856
H	3.929139	0.933257	5.228628
C	1.890765	1.586820	-0.831497
C	1.651973	4.112621	-1.844550
N	0.991507	2.413325	-0.280375
C	2.703214	1.956420	-1.905586
C	2.575656	3.247012	-2.419070
C	0.883836	3.646283	-0.777145
H	3.421987	1.259225	-2.321530
H	3.195179	3.568251	-3.251608
H	0.144772	4.289684	-0.304757
H	1.523301	5.126295	-2.209997
C	3.342493	-0.914710	-0.914216
C	5.392512	-2.162753	-2.358003
C	4.671600	-0.817162	-0.482899
C	3.050086	-1.652718	-2.070741
C	4.071089	-2.265917	-2.792943
C	5.689342	-1.442972	-1.201775
H	4.913322	-0.261661	0.418030
H	2.017273	-1.756748	-2.395149
H	3.833605	-2.834209	-3.687675
H	6.715837	-1.368535	-0.854612
H	6.187944	-2.649477	-2.914860
C	-1.121414	-4.764202	0.555093
H	-1.487727	-5.228378	-0.368286
H	-1.975764	-4.604576	1.220502
H	-0.447258	-5.478582	1.034708
C	-0.390492	-3.484968	0.262841
H	1.858855	-3.532853	0.264583
C	0.855837	-3.135537	0.207758

Complex 2

SCF done: -2349.167479

Pd	0.118581	-1.293933	0.033360
P	-1.960659	-0.018949	-0.051170
C	-2.658851	-1.725586	-0.200424
N	-1.617924	-2.562401	0.023266
C	-3.925574	-2.207281	-0.510059
C	-1.802152	-3.886274	0.012491
C	-4.121285	-3.589083	-0.532815
H	-5.099793	-3.998818	-0.765821
C	-3.052791	-4.437800	-0.252731
H	-3.176680	-5.515486	-0.254496
H	-4.733478	-1.519822	-0.738677
H	-0.923988	-4.490577	0.218220
C	-2.622124	0.614978	1.529836
C	-3.913916	0.309423	1.983218
C	-1.785149	1.414645	2.320947
C	-4.361435	0.801499	3.206691
H	-4.572152	-0.318251	1.390683
C	-2.240669	1.906648	3.542694
H	-0.786636	1.653481	1.969009
C	-3.525607	1.600529	3.987045
H	-5.361697	0.557388	3.552254
H	-1.586152	2.524261	4.150718
H	-3.875916	1.979727	4.942642
C	-2.756436	0.916328	-1.403179
C	-3.720436	1.904398	-1.170575
C	-2.371638	0.621719	-2.719645
C	-4.299431	2.579840	-2.245013
H	-4.020916	2.146206	-0.155385
C	-2.959102	1.293223	-3.787780
H	-1.611655	-0.133122	-2.908594
C	-3.923489	2.274058	-3.551558
H	-5.048849	3.343565	-2.057856
H	-2.661269	1.055157	-4.804819
H	-4.378700	2.800053	-4.385607
H	1.045986	-3.037314	2.341558
P	1.833685	0.225332	-0.027594
C	2.442406	0.722902	1.626753
C	3.428133	1.407794	4.155161
C	2.715299	2.062059	1.939998
C	2.669829	-0.269794	2.590612
C	3.164977	0.073857	3.846497
C	3.203413	2.398908	3.200893
H	2.551907	2.844723	1.206413
H	2.470527	-1.308979	2.349551
H	3.341999	-0.702807	4.584800
H	3.410888	3.438988	3.435151
H	3.809228	1.674649	5.136601
C	1.311515	1.844323	-0.778211
C	0.453978	4.277911	-1.685879
N	0.140581	2.317467	-0.334898
C	2.114050	2.544688	-1.683100
C	1.668570	3.782997	-2.145943
C	-0.270659	3.507251	-0.776977
H	3.064174	2.139882	-2.011642
H	2.269188	4.350317	-2.851060
H	-1.226064	3.855776	-0.391843
H	0.070885	5.237208	-2.018389
C	3.323897	-0.210093	-0.996432
C	5.553529	-0.850277	-2.563144
C	4.603926	-0.213687	-0.432148
C	3.168506	-0.538591	-2.352960
C	4.279121	-0.847529	-3.133074
C	5.712220	-0.537782	-1.215131
H	4.739459	0.036790	0.615100
H	2.176879	-0.551250	-2.799679
H	4.149636	-1.094634	-4.182759
H	6.701675	-0.540950	-0.767530
H	6.419225	-1.098246	-3.170173
C	1.910322	-3.499657	-1.020627
H	2.648832	-2.854564	-1.504484
H	1.116913	-3.680053	-1.756880
H	2.393743	-4.460750	-0.801726
C	1.362591	-2.882487	0.232332
H	1.995282	-4.412146	1.550192
C	1.470929	-3.460841	1.434379

Complex 2i

SCF done: -2349.146234

Pd	0.115052	-1.386491	-0.042851
P	-1.936814	-0.098546	-0.035255
C	-3.223422	-1.233785	-0.738609
N	-3.016239	-2.526820	-0.450888
C	-4.313575	-0.792499	-1.492612
C	-3.901177	-3.422858	-0.893917
C	-5.225859	-1.739313	-1.957482
H	-6.083380	-1.429615	-2.547918
C	-5.020642	-3.080556	-1.651800
H	-5.705214	-3.849567	-1.994576
H	-4.446075	0.261976	-1.709127
H	-3.702049	-4.461091	-0.637452
C	-2.541287	0.239039	1.661032
C	-3.847835	-0.064344	2.067014
C	-1.646120	0.808399	2.579734
C	-4.251938	0.198667	3.374773
H	-4.551327	-0.508587	1.369754
C	-2.060333	1.074075	3.882835
H	-0.637491	1.061179	2.262540
C	-3.360300	0.766152	4.283491
H	-5.265096	-0.042907	3.682751
H	-1.362993	1.517079	4.588197
H	-3.678035	0.966415	5.302686
C	-2.203217	1.442113	-0.987314
C	-3.005743	2.483660	-0.505214

C	-1.640293	1.542916	-2.267162
C	-3.245597	3.605796	-1.297432
H	-3.445334	2.415958	0.485547
C	-1.887302	2.662832	-3.057273
H	-1.013429	0.740503	-2.649059
C	-2.690393	3.695816	-2.573081
H	-3.872111	4.407963	-0.917829
H	-1.453265	2.729462	-4.050796
H	-2.883608	4.568647	-3.190073
H	-0.890084	-3.264687	0.164108
P	1.883401	0.017135	-0.025208
C	2.726428	0.069781	1.596235
C	4.020830	0.143363	4.075970
C	3.631018	1.101709	1.893076
C	2.461556	-0.909451	2.561378
C	3.109814	-0.872750	3.794888
C	4.277777	1.131734	3.125447
H	3.824667	1.888033	1.168710
H	1.735641	-1.690498	2.351817
H	2.894866	-1.635119	4.537798
H	4.977333	1.932531	3.346263
H	4.523375	0.172348	5.038299
C	1.512294	1.801094	-0.327705
C	0.933338	4.457781	-0.507459
N	0.686315	2.332372	0.580239
C	2.082719	2.534869	-1.368965
C	1.782015	3.894918	-1.453252
C	0.407374	3.632209	0.487988
H	2.749745	2.064958	-2.083036
H	2.211992	4.501744	-2.244922
H	-0.268022	4.031752	1.241036
H	0.677844	5.512018	-0.534764
C	3.128458	-0.395343	-1.302245
C	4.937408	-0.995951	-3.351716
C	4.506992	-0.323051	-1.069008
C	2.663736	-0.782651	-2.568451
C	3.564414	-1.074368	-3.589333
C	5.405104	-0.625170	-2.092331
H	4.883354	-0.045268	-0.089762
H	1.594663	-0.874627	-2.746110
H	3.195246	-1.374872	-4.565525
H	6.472877	-0.574377	-1.900676
H	5.640478	-1.232598	-4.144857
C	2.655722	-3.468577	-0.062116
H	3.262312	-2.986124	0.710405
H	3.087961	-3.196000	-1.029124
H	2.741996	-4.554091	0.061889
C	1.233750	-3.055395	0.021634
H	0.043797	-4.845943	0.168281
C	0.117226	-3.758480	0.130339

TS2-3

SCF done: -2462.420797

Pd	0.093137	-1.148038	0.507940
P	-1.969796	0.017869	-0.087876
C	-2.674086	-1.675204	-0.308139
N	-1.736732	-2.561172	0.091855
C	-3.901385	-2.079489	-0.826851
C	-2.014634	-3.867345	0.054606
C	-4.185396	-3.444348	-0.873918
H	-5.135787	-3.794302	-1.266137
C	-3.235786	-4.351199	-0.410940
H	-3.426101	-5.419289	-0.420920
H	-4.608788	-1.344821	-1.198090
H	-1.236960	-4.539148	0.406317
C	-2.950978	0.835852	1.219644
C	-4.283963	0.510113	1.504828
C	-2.305753	1.826234	1.976424
C	-4.961438	1.169895	2.528567
H	-4.796655	-0.263998	0.943092
C	-2.992354	2.487819	2.992400
H	-1.269912	2.070642	1.755613
C	-4.318806	2.160165	3.270555
H	-5.992392	0.907364	2.747115
H	-2.487164	3.254103	3.573364
H	-4.850169	2.671252	4.068061
C	-2.388749	0.847394	-1.662692
C	-3.278648	1.924726	-1.729789
C	-1.794671	0.367366	-2.839347
C	-3.573067	2.510305	-2.961270
H	-3.745016	2.303598	-0.825285
C	-2.097839	0.950686	-4.065930
H	-1.102278	-0.470669	-2.795487
C	-2.986739	2.025047	-4.128206
H	-4.267453	3.344385	-3.006421
H	-1.641588	0.567708	-4.974313
H	-3.221515	2.481123	-5.085474
H	2.225131	-2.067134	2.700995
P	1.836239	0.222358	-0.019209
C	2.903791	0.808228	1.352869
C	4.428640	1.871686	3.446940
C	4.136950	1.423860	1.090387
C	2.437090	0.750731	2.669641
C	3.196449	1.279074	3.712409
C	4.895756	1.945151	2.134394
H	4.509740	1.496171	0.073215
H	1.476473	0.296374	2.881215
H	2.823797	1.223586	4.730989
H	5.852509	2.412849	1.921235
H	5.023382	2.279582	4.258925
C	1.319243	1.865648	-0.730007
C	0.566700	4.383617	-1.488664
N	0.228633	2.401454	-0.174978
C	2.091276	2.541266	-1.680574
C	1.700003	3.821718	-2.066284
C	-0.132350	3.631967	-0.546674
H	2.975566	2.082966	-2.108788
H	2.278136	4.370396	-2.804246
H	-1.025245	4.031242	-0.070248
H	0.228204	5.378839	-1.757691
C	2.955490	-0.473985	-1.288674
C	4.524105	-1.715752	-3.252098
C	4.170495	-1.080747	-0.945253
C	2.524245	-0.516209	-2.624128
C	3.308069	-1.127041	-3.599752
C	4.949884	-1.693807	-1.925325
H	4.504683	-1.084362	0.086947
H	1.575871	-0.066058	-2.905640
H	2.968081	-1.144691	-4.631166
H	5.891964	-2.157198	-1.647380
H	5.134854	-2.193201	-4.012599
C	1.602825	-3.497641	-0.439111
H	1.983317	-2.976635	-1.323716
H	0.625211	-3.906813	-0.712283
H	2.275967	-4.338527	-0.228804
C	1.527306	-2.576649	0.745840
H	2.895853	-3.619844	1.962466
C	2.243750	-2.750613	1.858552
C	-0.633648	-1.337168	2.764434
O	-0.349582	-1.246154	3.864355

Complex 3

SCF done: -2462.438975

Pd	0.053242	-1.366915	0.336022
P	-1.907746	0.031671	-0.041459
C	-3.253766	-1.117415	-0.612022
N	-3.277992	-2.290661	0.027205
C	-4.184937	-0.783101	-1.599814
C	-4.234072	-3.170220	-0.273962
C	-5.177230	-1.711159	-1.916371
H	-5.914834	-1.482275	-2.680169
C	-5.208723	-2.926938	-1.241336

H	-5.963120	-3.675701	-1.459614
H	-4.138327	0.174242	-2.106990
H	-4.212937	-4.108854	0.275742
C	-2.657217	0.846214	1.416131
C	-4.044509	1.016879	1.533180
C	-1.820471	1.282985	2.452824
C	-4.582391	1.623265	2.666073
H	-4.709393	0.670878	0.747388
C	-2.365246	1.888245	3.583608
H	-0.745350	1.172675	2.354927
C	-3.744712	2.058076	3.692510
H	-5.657939	1.749095	2.748975
H	-1.710016	2.223214	4.382597
H	-4.167627	2.524260	4.577650
C	-1.881879	1.252958	-1.404442
C	-2.482301	2.512073	-1.304391
C	-1.294466	0.865102	-2.617746
C	-2.494362	3.370349	-2.403978
H	-2.943537	2.820094	-0.370926
C	-1.313920	1.722435	-3.715068
H	-0.837808	-0.118362	-2.710191
C	-1.913193	2.978257	-3.608439
H	-2.964674	4.345802	-2.318831
H	-0.867844	1.409251	-4.654786
H	-1.930045	3.647017	-4.464010
H	2.299471	-2.752918	2.246544
P	1.882048	0.087232	-0.008745
C	2.863155	0.236845	1.530750
C	4.251899	0.642687	3.925662
C	4.138916	0.817660	1.518149
C	2.283216	-0.119033	2.754378
C	2.975536	0.083728	3.946804
C	4.831022	1.010113	2.711071
H	4.595020	1.121957	0.580571
H	1.287384	-0.555871	2.772653
H	2.518233	-0.198873	4.890511
H	5.822517	1.452836	2.691494
H	4.794035	0.796014	4.854083
C	1.545814	1.886669	-0.307432
C	1.067817	4.573122	-0.313592
N	0.559963	2.359100	0.459903
C	2.337006	2.701935	-1.120221
C	2.083908	4.072988	-1.120922
C	0.332310	3.673393	0.456575
H	3.132640	2.284182	-1.726901
H	2.680773	4.738252	-1.738262
H	-0.474881	4.019600	1.098548
H	0.845697	5.634730	-0.278147
C	3.011724	-0.412458	-1.354595
C	4.597601	-1.303991	-3.484416
C	4.179969	-1.144775	-1.107500
C	2.635801	-0.147003	-2.681458
C	3.429013	-0.586282	-3.738841
C	4.968330	-1.582964	-2.170290
H	4.470404	-1.379021	-0.088891
H	1.727651	0.413081	-2.890286
H	3.133950	-0.368236	-4.761104
H	5.874823	-2.145790	-1.967879
H	5.215631	-1.646860	-4.308912
C	1.458228	-3.511639	-1.075158
H	1.649259	-2.809352	-1.894021
H	0.478527	-3.968573	-1.260007
H	2.213192	-4.305736	-1.132138
C	1.506935	-2.839232	0.267624
H	2.985558	-4.058474	1.133192
C	2.294838	-3.224755	1.270200
C	-0.967055	-2.814716	1.189383
O	-1.319926	-3.666069	1.860743

TS3-4
SCF done: -2462.426139

Pd	-0.059627	-1.338224	0.034229
P	-1.978223	0.058732	-0.068677
C	-3.491397	-0.960996	-0.381837
N	-3.625383	-1.993918	0.458334
C	-4.406257	-0.680292	-1.399225
C	-4.690504	-2.785350	0.318859
C	-5.509236	-1.522593	-1.540611
H	-6.239954	-1.338420	-2.322867
C	-5.659220	-2.593757	-0.666791
H	-6.502873	-3.271871	-0.744391
H	-4.266586	0.168888	-2.058514
H	-4.766782	-3.613150	1.020358
C	-2.354387	0.949840	1.490183
C	-3.492135	0.660136	2.255324
C	-1.459016	1.937914	1.929150
C	-3.732057	1.355452	3.439352
H	-4.187168	-0.109093	1.941229
C	-1.711607	2.630123	3.111143
H	-0.578232	2.171435	1.335161
C	-2.845583	2.340331	3.869567
H	-4.617593	1.124337	4.024178
H	-1.016199	3.396904	3.440759
H	-3.037559	2.880060	4.792475
C	-2.021355	1.296260	-1.409987
C	-2.735601	2.495271	-1.290443
C	-1.386647	0.987963	-2.620214
C	-2.808411	3.372908	-2.370927
H	-3.231989	2.741649	-0.356411
C	-1.466507	1.865216	-3.699039
H	-0.831958	0.056976	-2.716341
C	-2.175825	3.059820	-3.574110
H	-3.365166	4.300601	-2.273638
H	-0.975501	1.618059	-4.635855
H	-2.237843	3.744993	-4.414613
H	0.786973	-3.020289	2.424537
P	1.874547	0.144105	-0.004289
C	2.458577	0.516038	1.688882
C	3.285769	1.106798	4.294972
C	3.632171	1.253288	1.908526
C	1.698589	0.093267	2.785559
C	2.112068	0.387050	4.084421
C	4.043684	1.541834	3.206179
H	4.223459	1.604818	1.067393
H	0.773001	-0.452363	2.622089
H	1.513454	0.057814	4.928595
H	4.954401	2.110796	3.368611
H	3.608979	1.335746	5.306275
C	1.870527	1.831049	-0.777027
C	1.718029	4.409756	-1.671490
N	0.852218	2.593025	-0.364706
C	2.863387	2.299847	-1.641235
C	2.777964	3.616081	-2.094546
C	0.782032	3.850692	-0.802005
H	3.685248	1.662791	-1.946856
H	3.535692	4.012326	-2.764505
H	-0.063262	4.434150	-0.444295
H	1.615734	5.438873	-2.000093
C	3.258322	-0.703668	-0.857437
C	5.263022	-2.092949	-2.242583
C	4.339330	-1.262318	-0.166196
C	3.183122	-0.865766	-2.251510
C	4.184731	-1.546086	-2.939626
C	5.334283	-1.953648	-0.858282
H	4.409700	-1.157800	0.911733
H	2.342713	-0.452772	-2.804877
H	4.120055	-1.654158	-4.018478
H	6.169981	-2.379582	-0.310594
H	6.042632	-2.626611	-2.778011
C	1.760009	-3.853535	-0.847225
H	2.116339	-3.127136	-1.581135
H	1.068346	-4.532168	-1.359108

H	2.618315	-4.442161	-0.506210
C	1.089215	-3.196223	0.319806
H	2.175450	-4.116840	1.882013
C	1.360102	-3.447010	1.607031
C	-0.822858	-3.071932	0.013476
O	-1.451206	-4.021213	-0.185569

Complex 4

SCF done: -2462.453125

Pd	0.014354	-1.295514	0.392184
P	-1.854123	0.100027	-0.017641
C	-2.830818	0.082802	1.548335
N	-2.072585	0.356822	2.621408
C	-4.190766	-0.212428	1.628924
C	-2.662539	0.355657	3.818747
C	-4.790890	-0.216558	2.887727
H	-5.846899	-0.449131	2.989842
C	-4.016484	0.074436	4.005008
H	-4.443548	0.077880	5.002626
H	-4.763632	-0.443206	0.737876
H	-2.022553	0.583248	4.668703
C	-1.700338	1.885079	-0.408675
C	-2.298702	2.878899	0.374829
C	-1.016522	2.245689	-1.577959
C	-2.215845	4.216218	-0.011614
H	-2.830370	2.618209	1.283625
C	-0.938929	3.582221	-1.957797
H	-0.544974	1.478122	-2.185105
C	-1.539166	4.569885	-1.176619
H	-2.686342	4.980927	0.599722
H	-0.409519	3.853587	-2.866689
H	-1.479682	5.612247	-1.476121
C	-2.970081	-0.496043	-1.342190
C	-4.072105	0.270886	-1.752087
C	-2.720402	-1.720589	-1.971249
C	-4.922704	-0.201221	-2.747838
H	-4.258399	1.241234	-1.300178
C	-3.569420	-2.188230	-2.973204
H	-1.842986	-2.295247	-1.687961
C	-4.674742	-1.432175	-3.357062
H	-5.775732	0.396620	-3.055308
H	-3.364168	-3.138625	-3.457384
H	-5.337371	-1.794889	-4.137400
H	1.227674	-2.522129	2.264219
P	1.980016	0.053768	-0.026222
C	1.938291	1.771207	0.603381
C	1.954460	4.312072	1.770560
C	2.782825	2.772567	0.104187
C	1.094362	2.055333	1.684798
C	1.110902	3.321912	2.268407
C	2.785434	4.037785	0.683662
H	3.438242	2.571747	-0.737403
H	0.412438	1.297601	2.066100
H	0.454778	3.534047	3.107273
H	3.439569	4.809581	0.288557
H	1.962936	5.298926	2.224279
C	2.326126	0.140322	-1.842479
C	2.652079	0.211169	-4.556629
N	1.263533	-0.112998	-2.620156
C	3.593319	0.426799	-2.362083
C	3.753120	0.467717	-3.745754
C	1.432084	-0.075100	-3.945291
H	4.437296	0.595429	-1.701213
H	4.723592	0.690690	-4.179646
H	0.548921	-0.287395	-4.544120
H	2.732434	0.225445	-5.638827
C	3.557511	-0.600863	0.666049
C	5.879318	-1.707052	1.787476
C	4.093619	-0.076914	1.848585
C	4.196896	-1.690818	0.053311
C	5.352581	-2.234782	0.607718
C	5.247109	-0.630783	2.404897
H	3.618480	0.770398	2.333413
H	3.801649	-2.109145	-0.869453
H	5.844270	-3.069536	0.116253
H	5.653833	-0.211450	3.320545
H	6.780226	-2.132231	2.219698
C	-0.039284	-4.479150	-0.391485
H	-0.936860	-4.358423	-1.000952
H	-0.060123	-5.492217	0.026851
H	0.839854	-4.385976	-1.033786
C	0.015007	-3.501964	0.755213
H	2.146674	-3.271891	0.852854
C	1.194815	-2.951821	1.264009
C	-1.187273	-2.838269	1.169745
O	-2.245262	-2.954730	1.685559

Complex 5

SCF done: -2578.151009

Pd	0.022694	-0.923502	0.874430
P	1.835217	0.297284	0.013053
C	3.311429	-0.809232	-0.167476
N	3.066045	-1.974915	-0.789120
C	4.576749	-0.467818	0.308854
C	4.080940	-2.827207	-0.962605
C	5.625065	-1.368973	0.129550
H	6.619202	-1.130900	0.496413
C	5.377238	-2.571544	-0.521360
H	6.162724	-3.302735	-0.680743
H	4.739628	0.477757	0.812963
H	3.843890	-3.758530	-1.471458
C	1.699330	1.068015	-1.647081
C	2.378042	0.569675	-2.766142
C	0.889957	2.205168	-1.782601
C	2.253402	1.207582	-3.999576
H	3.003740	-0.311769	-2.685335
C	0.775154	2.839188	-3.016045
H	0.355859	2.587733	-0.917926
C	1.456449	2.342742	-4.127098
H	2.788409	0.816616	-4.860234
H	0.150176	3.722501	-3.109402
H	1.366812	2.839950	-5.088583
C	2.413543	1.652485	1.097515
C	3.223374	2.686302	0.604911
C	2.074478	1.634831	2.455662
C	3.695685	3.675147	1.465392
H	3.480224	2.720898	-0.449769
C	2.550431	2.623841	3.314008
H	1.424795	0.850292	2.834029
C	3.362819	3.643583	2.819911
H	4.323243	4.471786	1.076479
H	2.282806	2.601187	4.366442
H	3.732776	4.415913	3.488076
H	-0.775969	-3.260352	0.658945
P	-1.997395	0.130269	-0.025602
C	-2.122100	0.269470	-1.845171
C	-2.362775	0.311783	-4.629246
C	-2.897616	1.254797	-2.471214
C	-1.461082	-0.692303	-2.622241
C	-1.590668	-0.669548	-4.010641
C	-3.012934	1.275719	-3.858473
H	-3.409380	2.009175	-1.881108
H	-0.849685	-1.459479	-2.148921
H	-1.080595	-1.418845	-4.608977
H	-3.613612	2.043559	-4.337583
H	-2.457569	0.328016	-5.711260
C	-2.267905	1.839297	0.636067
C	-2.475764	4.373849	1.643499
N	-1.143470	2.500806	0.941213
C	-3.541275	2.392336	0.811961
C	-3.641365	3.685536	1.322112
C	-1.252824	3.738259	1.432214

H	-4.430580	1.822277	0.564650
H	-4.615627	4.143358	1.467558
H	-0.317311	4.239141	1.671508
H	-2.507856	5.379335	2.050713
C	-3.554701	-0.727679	0.456576
C	-5.835689	-2.136418	1.283228
C	-4.311338	-1.455960	-0.468029
C	-3.953042	-0.714608	1.803767
C	-5.088735	-1.408515	2.211735
C	-5.443989	-2.158426	-0.052764
H	-4.022226	-1.473883	-1.514205
H	-3.381260	-0.149209	2.536388
H	-5.393093	-1.380120	3.254279
H	-6.022921	-2.718656	-0.781280
H	-6.720032	-2.680109	1.602092
C	-0.429609	-2.046864	3.966320
H	0.071680	-1.119246	4.253591
H	-0.065336	-2.835941	4.634269
H	-1.504630	-1.927769	4.118498
C	-0.128886	-2.441992	2.544988
H	-2.122379	-2.844774	1.885003
C	-1.074601	-2.802670	1.603975
C	1.197757	-2.172208	2.006190
O	2.336181	-2.461854	2.176940
H	-0.332458	-4.811701	-2.162340
C	0.654435	-4.365905	-2.013758
H	1.084281	-4.160400	-3.003935
H	1.286468	-5.107814	-1.505400
O	0.486618	-3.187201	-1.246824
H	1.357871	-2.748657	-1.136038

TS5-6

SCF done: -2578.145878

Pd	0.070972	-0.970215	-0.776697
P	-1.767947	0.375465	-0.032887
C	-3.276272	-0.680231	0.209302
N	-3.078446	-1.768685	0.975769
C	-4.522706	-0.381663	-0.346324
C	-4.121788	-2.564941	1.234786
C	-5.598164	-1.227375	-0.080498
H	-6.577169	-1.014906	-0.500404
C	-5.400788	-2.336335	0.734946
H	-6.211238	-3.016835	0.973978
H	-4.649924	0.497875	-0.966910
H	-3.920272	-3.429220	1.863239
C	-1.702626	1.314238	1.548602
C	-2.429589	0.941364	2.685444
C	-0.884077	2.451807	1.602126
C	-2.344602	1.700049	3.852423
H	-3.062667	0.061552	2.672034
C	-0.808758	3.207841	2.768253
H	-0.311477	2.740584	0.725831
C	-1.538772	2.834893	3.896454
H	-2.917463	1.402885	4.726247
H	-0.176129	4.090444	2.795657
H	-1.479585	3.426918	4.805176
C	-2.316805	1.623337	-1.258297
C	-3.145184	2.700480	-0.910819
C	-1.914669	1.473537	-2.591170
C	-3.574058	3.598339	-1.886546
H	-3.449639	2.841808	0.122304
C	-2.347857	2.370338	-3.566040
H	-1.242351	0.661199	-2.855593
C	-3.179859	3.432656	-3.214754
H	-4.215809	4.429395	-1.608272
H	-2.029191	2.245481	-4.597077
H	-3.515839	4.134474	-3.972706
H	1.273917	-3.240668	-0.776033
P	2.011980	0.075705	-0.015447
C	2.059205	0.353230	1.791954
C	2.191890	0.618633	4.570518
C	2.806237	1.390655	2.366028
C	1.374729	-0.549765	2.617239
C	1.449457	-0.415216	4.003059
C	2.867885	1.522147	3.750690
H	3.338268	2.099188	1.738264
H	0.789462	-1.357553	2.179877
H	0.920086	-1.118405	4.639459
H	3.446262	2.330178	4.189417
H	2.243468	0.722493	5.650559
C	2.305892	1.735819	-0.785474
C	2.550441	4.208808	-1.928315
N	1.192006	2.397495	-1.123020
C	3.587437	2.259390	-0.990075
C	3.705541	3.521546	-1.570143
C	1.318420	3.604064	-1.680925
H	4.468938	1.692794	-0.710129
H	4.686480	3.956088	-1.740112
H	0.389544	4.105007	-1.944942
H	2.597163	5.190080	-2.389626
C	3.585884	-0.813603	-0.361500
C	5.923983	-2.245716	-0.956901
C	4.290953	-1.472941	0.651838
C	4.062812	-0.887017	-1.680921
C	5.227194	-1.591291	-1.974103
C	5.452199	-2.186553	0.351792
H	3.940735	-1.425804	1.678121
H	3.531431	-0.377464	-2.481895
H	5.591201	-1.629339	-2.996927
H	5.990849	-2.690855	1.148837
H	6.830890	-2.797406	-1.186045
C	-0.365090	-2.229277	-3.749053
H	-1.386774	-1.911813	-3.968723
H	-0.121274	-3.078657	-4.395455
H	0.309237	-1.403571	-3.987305
C	-0.179010	-2.626368	-2.291730
H	1.952880	-2.380111	-2.245845
C	1.091314	-2.568550	-1.611741
C	-1.276847	-3.104689	-1.640260
O	-2.246460	-3.626901	-1.274663
H	0.244032	-4.835920	1.959050
C	-0.717931	-4.317086	1.961663
H	-1.020696	-4.173130	3.007990
H	-1.456045	-4.967533	1.471024
O	-0.548420	-3.086944	1.279928
H	-1.398539	-2.595165	1.289467

Complex 6

SCF done: -2578.145890

Pd	0.072971	-0.969962	-0.761563
P	-1.762584	0.396071	-0.039515
C	-3.284075	-0.647985	0.174056
N	-3.101981	-1.756976	0.914703
C	-4.525854	-0.320072	-0.375815
C	-4.155722	-2.546727	1.151430
C	-5.612352	-1.158413	-0.133001
H	-6.587844	-0.923127	-0.548935
C	-5.430460	-2.290194	0.654398
H	-6.249782	-2.966443	0.874499
H	-4.640637	0.576104	-0.974668
H	-3.966393	-3.428673	1.758674
C	-1.709834	1.317892	1.552094
C	-2.450188	0.934793	2.676883
C	-0.883073	2.448164	1.629254
C	-2.369748	1.675795	3.855480
H	-3.090469	0.060564	2.644958
C	-0.812594	3.186895	2.806758
H	-0.300022	2.744088	0.762291
C	-1.555410	2.803428	3.923018
H	-2.952840	1.370801	4.719796
H	-0.173363	4.063954	2.852596
H	-1.499677	3.381750	4.840737

C	-2.288138	1.654917	-1.263693
C	-3.089095	2.752882	-0.918045
C	-1.895575	1.488790	-2.597583
C	-3.499592	3.656543	-1.896614
H	-3.386389	2.905880	0.115461
C	-2.311062	2.390683	-3.575168
H	-1.245247	0.658184	-2.860525
C	-3.115135	3.474991	-3.225526
H	-4.119980	4.504204	-1.619901
H	-2.000212	2.252868	-4.606923
H	-3.437136	4.181183	-3.985486
H	1.274279	-3.247444	-0.731440
P	2.014955	0.073858	-0.021362
C	2.069284	0.344920	1.786802
C	2.208019	0.605081	4.565355
C	2.831545	1.371029	2.361371
C	1.372741	-0.549283	2.611505
C	1.450427	-0.417435	3.997411
C	2.896298	1.499926	3.746123
H	3.373157	2.072323	1.733599
H	0.774808	-1.347122	2.172956
H	0.911456	-1.113449	4.633626
H	3.486571	2.298972	4.185441
H	2.261891	0.706964	5.645479
C	2.308781	1.737575	-0.783988
C	2.551385	4.218255	-1.910449
N	1.194179	2.411905	-1.092564
C	3.590375	2.251964	-1.010100
C	3.707444	3.518063	-1.581883
C	1.319439	3.622078	-1.642567
H	4.472528	1.676090	-0.752203
H	4.688455	3.945745	-1.768071
H	0.389703	4.133331	-1.882747
H	2.597232	5.203046	-2.364289
C	3.584095	-0.817899	-0.379448
C	5.914181	-2.254356	-0.994521
C	4.301397	-1.470944	0.629377
C	4.044459	-0.899919	-1.704241
C	5.205018	-1.606296	-2.007271
C	5.458735	-2.186730	0.319559
H	3.963602	-1.417274	1.659509
H	3.502995	-0.395317	-2.501588
H	5.556279	-1.651187	-3.034259
H	6.007129	-2.686159	1.113021
H	6.818017	-2.807842	-1.231372
C	-0.414591	-2.292136	-3.694559
H	-1.444031	-1.997184	-3.909851
H	-0.155000	-3.139117	-4.337829
H	0.239732	-1.453106	-3.941652
C	-0.209848	-2.668844	-2.232512
H	1.921956	-2.405212	-2.223642
C	1.072799	-2.583710	-1.569565
C	-1.276737	-3.224317	-1.596217
O	-2.224235	-3.773820	-1.218783
H	0.211003	-4.787638	2.061155
C	-0.753281	-4.274132	2.029345
H	-1.064822	-4.075829	3.064005
H	-1.484699	-4.953714	1.568984
O	-0.584598	-3.081204	1.283978
H	-1.433515	-2.586843	1.272386

TS6-7

SCF done: -2578.145279

Pd	0.071128	-1.011304	-0.627590
P	-1.739235	0.455565	-0.077778
C	-3.301404	-0.513143	0.204658
N	-3.160297	-1.602919	0.983252
C	-4.540866	-0.134962	-0.317455
C	-4.251801	-2.315945	1.287609
C	-5.666315	-0.895334	-0.006632
H	-6.639294	-0.619040	-0.402643
C	-5.525520	-2.001828	0.823719
H	-6.375192	-2.617304	1.099696
H	-4.623030	0.741933	-0.949289
H	-4.095766	-3.183493	1.924192
C	-1.684215	1.495474	1.441073
C	-2.474254	1.235591	2.567617
C	-0.802273	2.586400	1.461917
C	-2.387285	2.056617	3.691604
H	-3.160762	0.396494	2.580656
C	-0.726994	3.406846	2.583787
H	-0.179365	2.787838	0.595148
C	-1.518015	3.144427	3.702096
H	-3.008914	1.846049	4.557257
H	-0.045103	4.252417	2.584894
H	-1.457433	3.785906	4.576529
C	-2.212955	1.629506	-1.403533
C	-2.956136	2.791624	-1.153458
C	-1.835316	1.328397	-2.718183
C	-3.325893	3.626810	-2.206490
H	-3.239835	3.046878	-0.136500
C	-2.210318	2.162069	-3.769790
H	-1.229680	0.445598	-2.908730
C	-2.957722	3.311402	-3.514778
H	-3.901900	4.525350	-2.004264
H	-1.912289	1.919733	-4.785920
H	-3.248247	3.964095	-4.333034
H	1.206449	-3.303706	-0.248390
P	2.043726	0.045038	-0.011137
C	2.124731	0.457723	1.770422
C	2.278130	0.939168	4.519570
C	2.973687	1.456878	2.264955
C	1.351910	-0.296911	2.662693
C	1.434601	-0.058052	4.033399
C	3.045469	1.696929	3.634605
H	3.578413	2.049069	1.584468
H	0.688299	-1.069456	2.280460
H	0.834195	-0.647077	4.720444
H	3.703137	2.474969	4.011404
H	2.337624	1.127893	5.587593
C	2.376800	1.639931	-0.897305
C	2.672882	4.024979	-2.203671
N	1.278345	2.334275	-1.218957
C	3.668175	2.087420	-1.197442
C	3.812490	3.304944	-1.861060
C	1.429483	3.497853	-1.855953
H	4.537175	1.498236	-0.925462
H	4.801861	3.680099	-2.106816
H	0.511627	4.027443	-2.102074
H	2.739956	4.972939	-2.727820
C	3.586996	-0.911657	-0.309372
C	5.868317	-2.459409	-0.830817
C	4.315134	-1.478489	0.742956
C	4.011619	-1.136818	-1.629508
C	5.147918	-1.898523	-1.886808
C	5.448326	-2.249670	0.480017
H	4.004509	-1.315215	1.770113
H	3.460316	-0.702920	-2.460956
H	5.471332	-2.054958	-2.912006
H	6.005375	-2.681232	1.306602
H	6.753109	-3.056179	-1.031791
C	-0.465649	-2.768780	-3.308948
H	-1.478677	-2.459302	-3.575629
H	-0.247174	-3.714972	-3.814577
H	0.229618	-2.010104	-3.675539
C	-0.279963	-2.919221	-1.799273
H	1.851822	-2.705792	-1.854869
C	1.007785	-2.770265	-1.173551
C	-1.399202	-3.393602	-1.166067
O	-2.458794	-3.842142	-1.006928
H	-0.280189	-5.044160	1.841235
C	-1.162569	-4.400717	1.859455

H	-1.410031	-4.184224	2.905547
H	-2.000184	-4.942750	1.399669
O	-0.848837	-3.211351	1.147226
H	-1.605035	-2.577659	1.228471

Complex 7

SCF done: -2578.195080

Pd	-0.001857	-0.887485	-0.670969
P	-1.708790	0.563067	-0.011065
C	-3.355653	0.362505	-0.891799
N	-3.846214	-0.890187	-1.041056
C	-4.103299	1.410626	-1.433675
C	-5.009479	-1.165676	-1.652864
C	-5.313429	1.155491	-2.075647
H	-5.889633	1.979570	-2.486264
C	-5.785539	-0.152244	-2.184032
H	-6.723513	-0.384336	-2.674697
H	-3.732619	2.423978	-1.337735
H	-5.271965	-2.216931	-1.702614
C	-2.260536	0.333967	1.726285
C	-3.566960	0.591657	2.168034
C	-1.303789	-0.119847	2.645709
C	-3.909129	0.395598	3.504364
H	-4.324225	0.949368	1.475636
C	-1.649271	-0.305929	3.982741
H	-0.288757	-0.314487	2.312418
C	-2.950924	-0.052977	4.412869
H	-4.924064	0.595389	3.835753
H	-0.898240	-0.651975	4.686873
H	-3.219823	-0.204576	5.454235
C	-1.499991	2.371657	-0.244699
C	-2.011837	3.325885	0.643121
C	-0.816509	2.795268	-1.392617
C	-1.851761	4.684941	0.375767
H	-2.526960	3.009407	1.545179
C	-0.667582	4.153915	-1.661607
H	-0.394914	2.055424	-2.069153
C	-1.186134	5.100039	-0.777497
H	-2.248059	5.420310	1.070300
H	-0.138816	4.473610	-2.554831
H	-1.065584	6.159666	-0.983563
H	1.154292	-3.333046	-0.758108
P	2.112163	-0.025473	-0.091891
C	2.850446	-0.814890	1.395370
C	3.958423	-2.077246	3.641128
C	3.921151	-0.228254	2.086354
C	2.334029	-2.033814	1.853507
C	2.887929	-2.662460	2.968263
C	4.472251	-0.857865	3.199595
H	4.323938	0.725866	1.758514
H	1.490971	-2.485261	1.337917
H	2.480428	-3.609096	3.311901
H	5.302070	-0.393749	3.724947
H	4.389100	-2.566118	4.510263
C	2.314346	1.764490	0.338917
C	2.482870	4.346811	1.212246
N	1.512478	2.152159	1.340287
C	3.219180	2.624845	-0.288004
C	3.299183	3.942718	0.161551
C	1.606009	3.412335	1.765153
H	3.852010	2.269989	-1.094248
H	3.996717	4.637162	-0.298685
H	0.946128	3.691072	2.584084
H	2.518834	5.360518	1.598334
C	3.342655	-0.272138	-1.436758
C	5.110516	-0.590859	-3.591991
C	4.648306	-0.729329	-1.221482
C	2.930171	0.010081	-2.748559
C	3.810187	-0.137844	-3.817465
C	5.523859	-0.890527	-2.295627
H	4.982955	-0.969282	-0.217124
H	1.908280	0.337148	-2.930253
H	3.478681	0.088577	-4.827028
H	6.531956	-1.253084	-2.115845
H	5.795379	-0.717332	-4.425453
C	-1.427333	-2.497217	-2.956763
H	-2.341897	-1.905250	-2.888722
H	-1.692981	-3.459485	-3.413079
H	-0.750647	-1.981661	-3.641854
C	-0.744247	-2.712812	-1.620166
H	1.258071	-2.564047	-2.417397
C	0.667309	-2.734089	-1.520746
C	-1.558787	-3.318557	-0.555708
O	-2.791250	-3.176500	-0.442332
H	-2.476435	-5.220732	1.036622
C	-1.642617	-4.620210	1.404564
H	-0.939862	-5.241836	1.957760
H	-2.025199	-3.816814	2.038615
O	-0.889458	-4.078814	0.309232
H	-3.303086	-1.767127	-0.730589

TS7-8

SCF done: -2578.166543

Pd	0.049630	-0.237832	-0.399255
P	-2.006994	0.574138	-0.031509
C	-3.434708	0.127233	-1.154622
N	-3.705316	-1.189965	-1.332167
C	-4.188331	1.035289	-1.905092
C	-4.658082	-1.657991	-2.157773
C	-5.179533	0.583018	-2.770190
H	-5.765562	1.298696	-3.339516
C	-5.429481	-0.786199	-2.899728
H	-6.196829	-1.167879	-3.562717
H	-3.993260	2.094839	-1.789422
H	-4.759744	-2.736754	-2.194903
C	-2.725604	0.120533	1.600501
C	-4.100295	0.017152	1.857232
C	-1.816627	-0.101476	2.646179
C	-4.556040	-0.312998	3.132679
H	-4.826067	0.199224	1.068939
C	-2.277498	-0.417030	3.922833
H	-0.750032	-0.017981	2.449883
C	-3.646217	-0.529483	4.166597
H	-5.623114	-0.393706	3.319341
H	-1.564748	-0.576704	4.726847
H	-4.003967	-0.781403	5.160714
C	-2.124192	2.405992	-0.113233
C	-3.031696	3.148607	0.654178
C	-1.257074	3.072029	-0.989915
C	-3.078714	4.536160	0.531917
H	-3.691888	2.648592	1.356838
C	-1.316893	4.458123	-1.118881
H	-0.524366	2.495121	-1.549501
C	-2.227378	5.191053	-0.358209
H	-3.778622	5.106253	1.136145
H	-0.641299	4.966098	-1.800951
H	-2.266641	6.272720	-0.450085
H	1.514563	-3.553713	-0.339058
P	2.325340	0.162864	-0.052195
C	3.045724	-0.508009	1.497946
C	4.104218	-1.622162	3.842386
C	4.188075	0.044105	2.094263
C	2.433519	-1.615101	2.098899
C	2.963566	-2.173144	3.261222
C	4.712976	-0.511020	3.259206
H	4.666511	0.913513	1.652118
H	1.531241	-2.029721	1.655508
H	2.481888	-3.033443	3.717731
H	5.597259	-0.073352	3.713653
H	4.514945	-2.052523	4.751240
C	2.734380	1.964872	0.093241
C	3.161164	4.634686	0.486244

N	2.051163	2.582870	1.066761
C	3.650986	2.624514	-0.729855
C	3.861623	3.988257	-0.526228
C	2.270243	3.884099	1.255743
H	4.190471	2.086389	-1.501832
H	4.569018	4.531544	-1.146782
H	1.703928	4.351714	2.058906
H	3.297824	5.693640	0.681406
C	3.454206	-0.424383	-1.384916
C	5.048992	-1.291023	-3.525950
C	4.704060	-1.009872	-1.147906
C	3.009008	-0.289334	-2.710049
C	3.804914	-0.709243	-3.773374
C	5.492930	-1.443534	-2.213714
H	5.061976	-1.134441	-0.130537
H	2.029667	0.145486	-2.902221
H	3.451529	-0.590500	-4.794007
H	6.458476	-1.900414	-2.015608
H	5.667228	-1.627851	-4.353117
C	-0.934488	-2.924858	-2.758103
H	-1.433837	-1.950968	-2.734993
H	-1.684052	-3.682026	-3.011269
H	-0.193343	-2.896029	-3.559156
C	-0.269177	-3.237842	-1.446137
H	1.732411	-3.099261	-2.122017
C	1.063530	-3.300690	-1.291271
C	-1.168242	-3.510670	-0.296303
O	-2.379281	-3.275787	-0.298927
H	-2.238263	-4.995656	1.599223
C	-1.404226	-4.352389	1.886062
H	-0.755489	-4.861090	2.597339
H	-1.787940	-3.422011	2.309561
O	-0.573228	-4.075938	0.745893
H	-3.126591	-1.921306	-0.849564

Complex 8

SCF done: -2232.506257

Pd	-0.022246	-0.024922	-1.148995
P	-2.164698	0.068820	-0.468587
C	-2.140685	-0.929944	1.109789
N	-1.063073	-0.773148	1.916649
C	-3.096757	-1.873022	1.487416
C	-0.871747	-1.476812	3.042741
C	-2.925695	-2.618717	2.652331
C	-1.796231	-2.422934	3.447425
H	-1.628638	-2.993510	4.353295
H	-3.965628	-2.017660	0.855181
H	0.046293	-1.263593	3.578803
C	-2.747058	1.692980	0.156206
C	-3.630678	1.838329	1.235907
C	-2.278181	2.837166	-0.504263
C	-4.040777	3.106613	1.642072
H	-4.004996	0.963627	1.761810
C	-2.699420	4.102871	-0.102321
H	-1.577566	2.728570	-1.328362
C	-3.578484	4.238879	0.971230
H	-4.724679	3.210362	2.479623
H	-2.335481	4.982938	-0.624317
H	-3.902118	5.226252	1.287370
C	-3.601871	-0.678868	-1.330936
C	-4.914040	-0.196632	-1.231771
C	-3.332910	-1.775710	-2.164703
C	-5.940739	-0.815175	-1.943807
H	-5.133660	0.669161	-0.614361
C	-4.364141	-2.397761	-2.863678
H	-2.309538	-2.129134	-2.272751
C	-5.669049	-1.917067	-2.754130
H	-6.953820	-0.430547	-1.869556
H	-4.146507	-3.245535	-3.506695
H	-6.471667	-2.392880	-3.310045
P	2.142194	-0.052163	-0.395520
C	2.696754	-1.637432	0.349058
C	3.519304	-4.121283	1.352697
C	3.496466	-1.708644	1.498366
C	2.306883	-2.825459	-0.285627
C	2.723002	-4.059418	0.209312
C	3.902366	-2.945724	1.997605
H	3.808387	-0.799127	2.004687
H	1.674656	-2.776482	-1.169020
H	2.422609	-4.972815	-0.296115
H	4.524664	-2.990224	2.887108
H	3.841256	-5.083511	1.740438
C	2.194909	1.105964	1.057614
C	2.043987	2.816982	3.206282
N	1.170537	0.978361	1.926618
C	3.179351	2.081363	1.224761
C	3.100372	2.949853	2.312375
C	1.108278	1.813053	2.969495
H	3.990528	2.158113	0.509117
H	0.261460	1.682444	3.640905
H	1.937175	3.473379	4.063310
C	3.551898	0.497451	-1.434501
C	5.598816	1.424189	-3.104499
C	4.872851	0.072469	-1.236208
C	3.266114	1.379245	-2.487154
C	4.286332	1.846409	-3.312643
C	5.889393	0.535250	-2.069566
H	5.107376	-0.629071	-0.440939
H	2.237750	1.688587	-2.661761
H	4.054342	2.528281	-4.125615
H	6.909491	0.196079	-1.913638
H	6.393431	1.778912	-3.754506
H	-0.279948	-0.098376	1.663790
H	3.854644	3.718352	2.455262
H	-3.672875	-3.353360	2.938244

Complex 1a

SCF done: -2349.148609

Pd	-0.031970	-1.413188	-0.467521
P	-1.975618	-0.185788	-0.212335
C	-2.069243	0.592817	1.478584
N	-1.073941	1.447646	1.810639
C	-3.008731	0.278160	2.463110
C	-0.942655	1.988749	3.031541
C	-2.899615	0.830853	3.736254
C	-1.847621	1.698161	4.035401
H	-1.729840	2.136685	5.019329
H	-3.818595	-0.399345	2.219536
H	-0.088684	2.643323	3.168562
C	-2.246795	1.275809	-1.289375
C	-3.051112	2.368963	-0.932925
C	-1.625351	1.263981	-2.545377
C	-3.224705	3.431367	-1.817888
H	-3.555088	2.389987	0.030294
C	-1.812525	2.321728	-3.433418
H	-0.994616	0.421315	-2.818415
C	-2.608080	3.407114	-3.069468
H	-3.850974	4.272895	-1.535056
H	-1.334248	2.298761	-4.408314
H	-2.751855	4.232584	-3.760685
C	-3.575188	-1.092741	-0.247601
C	-4.716115	-0.617453	-0.906298
C	-3.624797	-2.342884	0.390942
C	-5.887345	-1.374635	-0.914868
H	-4.692212	0.337103	-1.422230
C	-4.803251	-3.085621	0.396970
H	-2.732297	-2.735993	0.872239
C	-5.936031	-2.603453	-0.259520
H	-6.763393	-1.000690	-1.436888
H	-4.831239	-4.048532	0.898971
H	-6.850492	-3.189314	-0.268558
P	1.857445	-0.116634	-0.011077

C	2.326229	-0.040069	1.766083
C	2.994084	-0.067896	4.489091
C	3.102332	0.990243	2.318207
C	1.883555	-1.079212	2.597064
C	2.221219	-1.095252	3.949567
C	3.431634	0.975824	3.672742
H	3.457705	1.803186	1.690234
H	1.270383	-1.871543	2.172782
H	1.880086	-1.910703	4.581153
H	4.037927	1.775548	4.089138
H	3.257941	-0.080387	5.542794
C	1.808426	1.696493	-0.441151
C	1.500729	4.373379	-1.035586
N	0.790246	2.389109	0.105134
C	2.713275	2.316406	-1.306502
C	2.556466	3.668647	-1.604988
C	0.642682	3.686525	-0.184285
H	3.529213	1.745886	-1.734782
H	-0.205213	4.188355	0.276533
H	1.339559	5.425503	-1.243945
C	3.391009	-0.635697	-0.884931
C	5.641211	-1.420639	-2.361109
C	4.654591	-0.672282	-0.283302
C	3.264675	-1.011485	-2.231485
C	4.385056	-1.388779	-2.968188
C	5.771540	-1.069400	-1.018758
H	4.770888	-0.400057	0.761320
H	2.280079	-1.022877	-2.694509
H	4.274950	-1.672932	-4.010902
H	6.745608	-1.103454	-0.539139
H	6.513467	-1.727434	-2.930944
H	-0.318540	1.733699	1.072768
H	3.254635	4.163800	-2.273868
H	-3.636574	0.585371	4.495428
C	-0.644852	-3.320663	-1.036894
H	-1.613127	-3.737620	-1.250080
C	0.611479	-3.403457	-0.933556
C	1.899760	-4.118395	-0.977978
H	2.364554	-4.145966	0.012702
H	2.606529	-3.623404	-1.649374
H	1.756925	-5.149319	-1.320007

TS1a-1

SCF done: -2349.128446

Pd	-0.070772	-1.175868	-0.113363
P	-2.113185	-0.025723	-0.166354
C	-2.405721	0.356678	1.637446
N	-1.649837	-0.380948	2.481496
C	-3.238147	1.323361	2.196021
C	-1.660567	-0.257711	3.818181
C	-3.282735	1.481263	3.580371
C	-2.489987	0.679588	4.405966
H	-2.502425	0.787821	5.484198
H	-3.833959	1.946766	1.538155
H	-0.992090	-0.906154	4.372311
C	-2.589411	1.582504	-0.916135
C	-3.776305	1.764102	-1.638961
C	-1.689734	2.650198	-0.782320
C	-4.059490	3.002844	-2.213320
H	-4.475294	0.942837	-1.760482
C	-1.986399	3.887378	-1.347490
H	-0.758143	2.510053	-0.239210
C	-3.169198	4.064996	-2.065993
H	-4.977754	3.135073	-2.778165
H	-1.284665	4.709242	-1.239152
H	-3.393042	5.027587	-2.516716
C	-3.543191	-1.114780	-0.559324
C	-3.377599	-1.996388	-1.637517
C	-4.769230	-1.090554	0.118987
C	-4.423203	-2.825835	-2.036923
H	-2.422962	-2.038627	-2.155334
C	-5.806490	-1.936587	-0.270568
H	-4.927794	-0.413608	0.953405
C	-5.636880	-2.801326	-1.350842
H	-4.284568	-3.498751	-2.877997
H	-6.749285	-1.915818	0.268385
H	-6.447657	-3.456739	-1.654837
P	1.967955	0.047018	-0.157398
C	2.885337	-0.036962	1.438983
C	4.259002	-0.266049	3.877765
C	3.930385	0.843315	1.754835
C	2.534529	-1.025176	2.367730
C	3.218930	-1.143370	3.576767
C	4.611269	0.727863	2.965088
H	4.212088	1.627170	1.058000
H	1.719655	-1.704710	2.128246
H	2.942118	-1.922274	4.282399
H	5.418727	1.417030	3.195564
H	4.793122	-0.354556	4.819438
C	2.130177	1.859274	-0.532370
C	2.320116	4.571320	-0.857795
N	1.530658	2.656075	0.366075
C	2.823190	2.358413	-1.639157
C	2.911814	3.739968	-1.803281
C	1.639905	3.977413	0.205343
H	3.292483	1.684082	-2.346909
H	1.156930	4.592154	0.963256
H	2.379273	5.652132	-0.937744
C	3.101482	-0.710670	-1.395062
C	4.701786	-1.870251	-3.385356
C	4.477455	-0.875721	-1.192044
C	2.535754	-1.142943	-2.604468
C	3.332230	-1.711081	-3.596625
C	5.270329	-1.456007	-2.181696
H	4.932774	-0.562728	-0.257290
H	1.463747	-1.042075	-2.761476
H	2.881740	-2.038587	-4.529335
H	6.335115	-1.585430	-2.009556
H	5.322515	-2.321814	-4.153853
H	-0.985837	-1.026088	1.997583
H	3.446400	4.156912	-2.652188
H	-3.934302	2.231465	4.018789
C	-0.698931	-3.140975	0.150942
H	-1.658859	-3.626219	0.197761
C	0.566375	-3.197539	0.101868
C	1.854339	-3.914188	0.070658
H	2.535543	-3.552212	0.846516
H	2.355303	-3.758225	-0.889549
H	1.702200	-4.989267	0.215541

TS1a-1L

SCF done: -2349.146894

Pd	-0.002778	-1.437332	-0.452864
P	-1.953774	-0.197472	-0.190143
C	-2.027814	0.684543	1.449952
N	-1.031160	1.562010	1.697968
C	-2.971154	0.422314	2.445856
C	-0.923291	2.175972	2.883304
C	-2.868827	1.058529	3.680851
C	-1.824392	1.950613	3.912970
H	-1.707183	2.458345	4.863633
H	-3.775858	-0.275897	2.247203
H	-0.080012	2.852122	2.993680
C	-2.261701	1.189983	-1.354329
C	-3.065001	2.298510	-1.046472
C	-1.669289	1.106526	-2.621827
C	-3.268246	3.303630	-1.990497
H	-3.543995	2.374645	-0.073495
C	-1.883378	2.107848	-3.567715
H	-1.039454	0.251660	-2.857275
C	-2.679758	3.207922	-3.252324
H	-3.896047	4.155887	-1.745373

H	-1.427996	2.028248	-4.550692
H	-2.846819	3.988269	-3.989314
C	-3.534944	-1.136686	-0.155760
C	-4.702421	-0.708121	-0.799538
C	-3.544539	-2.360396	0.533417
C	-5.859680	-1.484725	-0.745354
H	-4.710551	0.225537	-1.352777
C	-4.708264	-3.122884	0.601283
H	-2.632693	-2.717914	1.006009
C	-5.867477	-2.687297	-0.041417
H	-6.756630	-1.146757	-1.256344
H	-4.704766	-4.065074	1.141939
H	-6.770856	-3.288889	-0.001190
P	1.860218	-0.139318	0.018035
C	2.295409	0.021585	1.796241
C	2.910459	0.110809	4.528349
C	3.048450	1.083379	2.320150
C	1.848680	-0.989701	2.658436
C	2.160889	-0.947268	4.016221
C	3.351287	1.127232	3.680042
H	3.407755	1.875159	1.667451
H	1.251713	-1.804587	2.254693
H	1.816485	-1.740263	4.673865
H	3.938899	1.950844	4.076012
H	3.153119	0.144041	5.586624
C	1.769821	1.656426	-0.483730
C	1.358940	4.297423	-1.239143
N	0.725276	2.361717	0.000293
C	2.653989	2.271264	-1.373312
C	2.448754	3.596666	-1.750152
C	0.516682	3.634819	-0.359697
H	3.495665	1.709886	-1.761426
H	-0.360154	4.112485	0.068035
H	1.161736	5.327377	-1.514022
C	3.424219	-0.628032	-0.818573
C	5.717013	-1.390099	-2.238061
C	4.679288	-0.606640	-0.198508
C	3.327535	-1.051103	-2.153706
C	4.469465	-1.416544	-2.862802
C	5.817919	-0.992808	-0.905905
H	4.771410	-0.299566	0.838675
H	2.349762	-1.108633	-2.627789
H	4.383154	-1.737952	-3.896866
H	6.785572	-0.982759	-0.412485
H	6.606161	-1.688497	-2.785798
H	-0.137587	1.872932	0.814945
H	3.137725	4.077756	-2.438412
H	-3.602523	0.857884	4.456261
C	-0.629370	-3.341895	-1.014283
H	-1.601931	-3.752097	-1.220986
C	0.626481	-3.431098	-0.906664
C	1.907792	-4.159963	-0.937256
H	2.349812	-4.208523	0.063165
H	2.635528	-3.663138	-1.584481
H	1.761725	-5.183920	-1.298239

Complex 1aL

SCF done: -2349.148561

Pd	-0.018119	-1.457459	0.281159
P	-1.888478	-0.150179	-0.044584
C	-1.808614	1.571138	0.676851
N	-0.768569	2.345420	0.292555
C	-2.674284	2.082520	1.645914
C	-0.530531	3.564985	0.798926
C	-2.455139	3.348496	2.182742
C	-1.364521	4.108210	1.758583
H	-1.161329	5.093006	2.162511
H	-3.515654	1.481256	1.969281
H	0.350302	4.070550	0.418668
C	-2.316475	0.244220	-1.786843
C	-3.099659	1.344787	-2.166801
C	-1.829758	-0.623252	-2.774366
C	-3.392105	1.568548	-3.510781
H	-3.491271	2.026428	-1.415665
C	-2.133142	-0.402152	-4.116595
H	-1.207757	-1.465291	-2.479603
C	-2.911926	0.693593	-4.485894
H	-4.001322	2.421557	-3.796216
H	-1.757027	-1.084052	-4.873760
H	-3.145869	0.866933	-5.532349
C	-3.456585	-0.724589	0.726383
C	-4.707245	-0.647564	0.101623
C	-3.364560	-1.285720	2.010025
C	-5.847060	-1.115022	0.756077
H	-4.794436	-0.235221	-0.898642
C	-4.508218	-1.732167	2.668240
H	-2.388854	-1.385508	2.481418
C	-5.751595	-1.649206	2.039918
H	-6.811384	-1.061416	0.259014
H	-4.426299	-2.160823	3.662973
H	-6.641915	-2.010671	2.546149
P	1.954525	-0.204066	0.131756
C	2.270103	1.039786	1.449444
C	2.715996	2.828686	3.561642
C	3.054482	2.186574	1.255787
C	1.711529	0.801735	2.713057
C	1.939440	1.688455	3.764628
C	3.271836	3.077505	2.305985
H	3.508399	2.379146	0.287232
H	1.101265	-0.085705	2.865356
H	1.511865	1.487120	4.742825
H	3.886851	3.959177	2.147482
H	2.894425	3.519097	4.381149
C	2.078919	0.843960	-1.403247
C	1.985873	2.377735	-3.694860
N	1.084181	1.738553	-1.568132
C	3.071432	0.689212	-2.373548
C	3.022231	1.464205	-3.530638
C	1.040951	2.481128	-2.679876
H	3.869328	-0.028058	-2.219987
H	0.208777	3.177057	-2.760515
H	1.906037	2.995577	-4.582695
C	3.516709	-1.173866	0.049273
C	5.822941	-2.757839	-0.145036
C	4.658018	-0.859110	0.796923
C	3.540258	-2.300819	-0.788530
C	4.690529	-3.079017	-0.894298
C	5.801550	-1.652129	0.702380
H	4.657746	-0.000115	1.460248
H	2.649932	-2.570756	-1.351383
H	4.697316	-3.944478	-1.550839
H	6.677593	-1.402208	1.294030
H	6.715467	-3.372579	-0.216523
H	-0.050613	1.989907	-0.453128
H	3.788018	1.354130	-4.293170
H	-3.136286	3.742367	2.931514
C	-0.626804	-3.498043	0.516222
C	0.628949	-3.410354	0.617720
H	1.611256	-3.824430	0.760301
C	-1.901568	-4.238360	0.478622
H	-2.345387	-4.194285	-0.521294
H	-2.632986	-3.815142	1.172465
H	-1.744397	-5.291179	0.737354

TS1aL-1L

SCF done: -2349.126004

Pd	-0.084509	-1.191783	-0.031930
P	-2.023970	0.104248	-0.112582
C	-2.347159	0.480850	1.689720
N	-1.592428	-0.254143	2.535657
C	-3.185034	1.445000	2.243150
C	-1.608010	-0.130920	3.872002

C	-3.238089	1.601100	3.627899
C	-2.445405	0.802472	4.456084
H	-2.462628	0.910981	5.534306
H	-3.774627	2.071408	1.582482
H	-0.937682	-0.775262	4.429002
C	-2.322209	1.770178	-0.830831
C	-3.454094	2.076826	-1.597921
C	-1.345706	2.753427	-0.616074
C	-3.605687	3.353958	-2.137158
H	-4.212815	1.323232	-1.783085
C	-1.510815	4.029851	-1.146579
H	-0.455737	2.518222	-0.037919
C	-2.638622	4.331530	-1.910439
H	-4.482166	3.582158	-2.736736
H	-0.748995	4.784485	-0.974469
H	-2.760219	5.324385	-2.333810
C	-3.527329	-0.828655	-0.614104
C	-3.404125	-1.601744	-1.778474
C	-4.759363	-0.789821	0.050738
C	-4.498168	-2.305750	-2.276513
H	-2.444797	-1.659759	-2.287429
C	-5.845900	-1.515033	-0.437451
H	-4.885918	-0.198294	0.952558
C	-5.719328	-2.268027	-1.603375
H	-4.392446	-2.893473	-3.183688
H	-6.793729	-1.485728	0.092185
H	-6.568695	-2.827088	-1.984536
P	2.039559	-0.099025	-0.150609
C	3.104613	-0.373210	1.328895
C	4.706596	-0.860274	3.583944
C	4.273150	0.371869	1.550068
C	2.749609	-1.357929	2.258808
C	3.546430	-1.603063	3.376541
C	5.067173	0.128123	2.668273
H	4.566019	1.148571	0.849535
H	1.845865	-1.938312	2.094692
H	3.260885	-2.376574	4.084427
H	5.969191	0.712907	2.824746
H	5.328005	-1.048549	4.454749
C	2.315324	1.720771	-0.395780
C	2.706118	4.428391	-0.499020
N	1.834017	2.476091	0.604127
C	2.982960	2.263348	-1.497688
C	3.174643	3.643356	-1.547756
C	2.040383	3.794438	0.550277
H	3.355037	1.620923	-2.288124
H	1.651893	4.373419	1.386562
H	2.849120	5.504297	-0.489216
C	2.969362	-0.841469	-1.554204
C	4.247450	-1.965007	-3.783605
C	4.303933	-1.256787	-1.471533
C	2.278951	-1.007711	-2.765211
C	2.916864	-1.555796	-3.875081
C	4.935775	-1.819052	-2.580822
H	4.851488	-1.150852	-0.540138
H	1.234031	-0.712163	-2.832656
H	2.371937	-1.674640	-4.807309
H	5.969518	-2.143575	-2.502133
H	4.743055	-2.402621	-4.645366
H	-0.925981	-0.899243	2.045122
H	3.693966	4.093636	-2.389129
H	-3.893426	2.349425	4.063883
C	-0.672921	-3.220625	0.270603
C	0.589644	-3.142203	0.200286
H	1.566736	-3.592514	0.180842
C	-1.915838	-4.004949	0.412898
H	-1.689548	-5.073876	0.489128
H	-2.580838	-3.849943	-0.440847
H	-2.475110	-3.710306	1.307134

Complex 1+

SCF done: -2349.457038

Pd	0.011578	-1.139543	-0.009037
P	-2.041357	-0.015227	0.029740
C	-3.083909	-0.751551	-1.348257
N	-2.680251	-1.966334	-1.780076
C	-4.220428	-0.205835	-1.938668
C	-3.315830	-2.691652	-2.717242
C	-4.909420	-0.924461	-2.916401
H	-5.800474	-0.501184	-3.370873
C	-4.457977	-2.185695	-3.310581
H	-4.975085	-2.764017	-4.067710
H	-4.557667	0.779562	-1.638283
H	-2.881239	-3.653489	-2.965546
C	-3.070929	-0.390350	1.497925
C	-4.428020	-0.041431	1.593436
C	-2.456575	-1.064106	2.562980
C	-5.153321	-0.364897	2.735865
H	-4.922866	0.491451	0.786588
C	-3.186471	-1.379802	3.708162
H	-1.409406	-1.344828	2.484440
C	-4.533342	-1.033876	3.793604
H	-6.202833	-0.094705	2.803120
H	-2.703194	-1.898823	4.530332
H	-5.103328	-1.284270	4.683265
C	-2.323865	1.775070	-0.304444
C	-2.737771	2.653688	0.708436
C	-2.037269	2.292567	-1.580151
C	-2.894213	4.015970	0.438314
H	-2.966279	2.275409	1.700460
C	-2.208008	3.648735	-1.848125
H	-1.694010	1.633613	-2.374842
C	-2.642300	4.513501	-0.840186
H	-3.238448	4.681213	1.225122
H	-2.011348	4.030130	-2.846018
H	-2.791127	5.567932	-1.053799
H	-1.813293	-2.329610	-1.331766
P	2.059271	-0.014093	0.005281
C	2.853531	-0.023401	1.659237
C	4.010245	-0.166570	4.205730
C	3.911310	0.832140	2.007865
C	2.376843	-0.943081	2.605311
C	2.957819	-1.016225	3.869968
C	4.484334	0.758645	3.274817
H	4.297829	1.555591	1.295389
H	1.550955	-1.600419	2.344839
H	2.586319	-1.735849	4.593338
H	5.302872	1.422922	3.535222
H	4.460752	-0.222127	5.192088
C	2.075276	1.824091	-0.322995
C	1.849627	4.597632	-0.572367
N	1.025308	2.520645	0.170120
C	3.052486	2.542792	-1.007269
C	2.943193	3.928014	-1.127296
C	0.880630	3.856044	0.075350
H	3.895005	2.008096	-1.432060
H	3.713706	4.487576	-1.649862
H	-0.020825	4.275611	0.506264
H	1.742500	5.673340	-0.650173
C	3.314713	-0.568055	-1.205244
C	5.123528	-1.448595	-3.149684
C	4.649654	-0.820045	-0.862451
C	2.889024	-0.776895	-2.527422
C	3.793001	-1.205516	-3.495659
C	5.547274	-1.261313	-1.835075
H	4.989515	-0.687780	0.160071
H	1.846821	-0.614580	-2.794200
H	3.458735	-1.361117	-4.517142
H	6.578756	-1.462044	-1.561413
H	5.825986	-1.792715	-3.902781
C	2.039409	-3.794233	-0.123630
H	2.705025	-3.467312	0.680993

H	2.519304	-3.525943	-1.069346
H	1.942654	-4.883641	-0.075970
C	0.717108	-3.157585	-0.006330
H	-1.414242	-3.756680	0.385116
C	-0.543991	-3.173756	0.126722
H	0.280013	1.977507	0.609746

Complex 1L+

SCF done: -2349.453509

Pd	-0.004843	-1.140219	-0.072597
P	-1.962395	0.120569	0.008418
C	-3.043464	-0.472631	-1.408881
N	-2.656277	-1.652323	-1.940740
C	-4.174667	0.133831	-1.947848
C	-3.299082	-2.288707	-2.936072
C	-4.874358	-0.493309	-2.979314
H	-5.761558	-0.023933	-3.394352
C	-4.436455	-1.721387	-3.480534
H	-4.960764	-2.226967	-4.283465
H	-4.497909	1.096099	-1.568112
H	-2.874952	-3.229182	-3.269230
C	-3.027298	-0.220295	1.459990
C	-4.333858	0.277321	1.592899
C	-2.490145	-1.023889	2.475657
C	-5.087047	-0.031835	2.721083
H	-4.765430	0.917845	0.829325
C	-3.246998	-1.325385	3.607358
H	-1.478283	-1.408393	2.370692
C	-4.544830	-0.833346	3.728332
H	-6.097183	0.354549	2.817773
H	-2.822632	-1.944091	4.392266
H	-5.136263	-1.070514	4.607559
C	-2.098665	1.941726	-0.245229
C	-2.347361	2.799767	0.837376
C	-1.864754	2.498037	-1.514869
C	-2.396326	4.182675	0.644048
H	-2.534951	2.391384	1.826244
C	-1.929087	3.876813	-1.705610
H	-1.646865	1.855776	-2.365283
C	-2.201325	4.722599	-0.627472
H	-2.614962	4.833301	1.486058
H	-1.776826	4.290924	-2.698234
H	-2.270264	5.795692	-0.780557
H	-1.792035	-2.050666	-1.520716
P	2.121969	-0.140106	-0.002493
C	2.833237	-0.141416	1.688509
C	3.876962	-0.278943	4.283785
C	3.891657	0.697377	2.073906
C	2.301448	-1.045182	2.620699
C	2.827035	-1.115557	3.909340
C	4.406937	0.628316	3.365784
H	4.325413	1.402622	1.370327
H	1.481748	-1.697303	2.331076
H	2.414584	-1.824159	4.621285
H	5.225891	1.280243	3.654630
H	4.283313	-0.332480	5.289248
C	2.310004	1.670500	-0.408531
C	2.347008	4.439022	-0.793526
N	1.344070	2.490338	0.069911
C	3.335174	2.257775	-1.146678
C	3.356751	3.639297	-1.335060
C	1.328469	3.827771	-0.088579
H	4.115117	1.624803	-1.555486
H	4.165981	4.094744	-1.898617
H	0.484803	4.353872	0.342144
H	2.342975	5.515121	-0.922477
C	3.380840	-0.861248	-1.115481
C	5.204044	-1.982458	-2.915916
C	4.681769	-1.172024	-0.697519
C	2.995188	-1.132909	-2.438397
C	3.907480	-1.680604	-3.335833
C	5.586421	-1.733914	-1.598658
H	4.988426	-0.990696	0.328060
H	1.976457	-0.926112	-2.759443
H	3.604846	-1.884921	-4.358552
H	6.590398	-1.980947	-1.266880
H	5.911919	-2.420844	-3.612886
C	-1.708332	-4.102382	0.301056
H	-2.189811	-4.426709	-0.628895
H	-2.460282	-3.596498	0.911815
H	-1.391112	-5.009192	0.826047
C	-0.530166	-3.245191	0.035075
H	1.711852	-3.485156	-0.255215
C	0.714045	-3.098812	-0.137462
H	0.561445	2.050408	0.555689

TS1-2i+

SCF done: -2349.438839

Pd	0.066426	-1.171441	-0.046174
P	-2.049257	-0.027297	0.006915
C	-3.085776	-1.029787	-1.177219
N	-2.641354	-2.273581	-1.402036
C	-4.256714	-0.572554	-1.781472
C	-3.315914	-3.113682	-2.192231
C	-4.969429	-1.439569	-2.611380
H	-5.885724	-1.105248	-3.088804
C	-4.496782	-2.732293	-2.820869
H	-5.023249	-3.431024	-3.461904
H	-4.603779	0.441190	-1.613253
H	-2.887544	-4.103392	-2.324707
C	-2.895076	-0.208181	1.615108
C	-4.288697	-0.107926	1.750109
C	-2.108657	-0.461860	2.747961
C	-4.880120	-0.258611	3.000760
H	-4.916828	0.083404	0.885188
C	-2.706171	-0.606234	3.999089
H	-1.030112	-0.554089	2.645821
C	-4.090255	-0.506709	4.125174
H	-5.958968	-0.185366	3.098795
H	-2.091991	-0.802469	4.872660
H	-4.556895	-0.625903	5.098326
C	-2.401500	1.691761	-0.544868
C	-2.872484	2.666927	0.347278
C	-2.155315	2.048681	-1.883087
C	-3.117214	3.968662	-0.099250
H	-3.078826	2.406737	1.381425
C	-2.411530	3.344438	-2.324795
H	-1.786667	1.307210	-2.588519
C	-2.897118	4.306492	-1.434597
H	-3.505083	4.708840	0.594752
H	-2.245491	3.601368	-3.367021
H	-3.112750	5.311747	-1.784707
H	-1.407059	-2.621582	-0.743230
P	2.035968	0.014666	0.004555
C	2.738412	0.146582	1.688398
C	3.787694	0.209349	4.282258
C	3.728451	1.082504	2.029754
C	2.274295	-0.749762	2.663442
C	2.802630	-0.719980	3.952450
C	4.247496	1.110971	3.321478
H	4.103056	1.790564	1.296066
H	1.501031	-1.470311	2.408742
H	2.443420	-1.422026	4.698834
H	5.013013	1.836952	3.578009
H	4.196779	0.234107	5.287695
C	1.953896	1.816440	-0.477489
C	1.612936	4.539181	-0.990644
N	0.822915	2.483642	-0.155389
C	2.960697	2.533344	-1.116885
C	2.793174	3.896138	-1.368095
C	0.618365	3.794438	-0.384477
H	3.868704	2.018130	-1.410409

H	3.584564	4.456061	-1.857990
H	-0.347792	4.189136	-0.090545
H	1.457291	5.595861	-1.175267
C	3.352602	-0.564077	-1.119882
C	5.271273	-1.478643	-2.934267
C	4.677374	-0.751794	-0.704613
C	2.990853	-0.851728	-2.446667
C	3.950478	-1.298413	-3.350389
C	5.630722	-1.210767	-1.614357
H	4.966464	-0.556481	0.323399
H	1.957623	-0.738421	-2.768419
H	3.667186	-1.517200	-4.375555
H	6.654760	-1.362531	-1.286807
H	6.017039	-1.836889	-3.637437
C	2.175054	-3.684509	0.021084
H	2.768690	-3.284074	0.847185
H	2.734861	-3.499722	-0.902601
H	2.071931	-4.768357	0.140771
C	0.848164	-3.052941	-0.062909
H	-0.971383	-4.189546	0.165112
C	-0.429035	-3.295833	-0.142955
H	0.055873	1.938275	0.242675

TS1-2L+

SCF done: -2349.433045

Pd	-0.031976	1.307939	-0.006650
P	1.879870	-0.096230	0.028058
C	3.151094	0.938213	-0.862144
N	2.775567	2.197603	-1.132354
C	4.424652	0.483714	-1.202705
C	3.611140	3.037396	-1.757382
C	5.305453	1.352313	-1.845619
H	6.303222	1.018737	-2.114613
C	4.890720	2.649494	-2.137184
H	5.543628	3.353053	-2.642288
H	4.725182	-0.531716	-0.968461
H	3.238802	4.037515	-1.953215
C	2.658627	-0.396692	1.653409
C	3.635918	-1.381723	1.859210
C	2.306125	0.460295	2.707072
C	4.245482	-1.506153	3.105120
H	3.917419	-2.059492	1.058475
C	2.924236	0.333530	3.949574
H	1.552528	1.229979	2.552136
C	3.892318	-0.649949	4.148999
H	4.999094	-2.272248	3.260880
H	2.648998	1.001379	4.760320
H	4.372398	-0.750516	5.117731
C	1.930568	-1.704048	-0.860216
C	1.533092	-2.870210	-0.180540
C	2.260809	-1.791501	-2.223804
C	1.501974	-4.096704	-0.842355
H	1.270115	-2.824974	0.872682
C	2.235601	-3.025321	-2.877945
H	2.566550	-0.906875	-2.775226
C	1.862616	-4.179964	-2.188276
H	1.213267	-4.991549	-0.299056
H	2.530380	-3.083772	-3.922146
H	1.863484	-5.141211	-2.693674
H	1.494859	2.568624	-0.595491
P	-2.016487	0.136268	0.109224
C	-2.115132	-1.201141	1.348739
C	-2.250238	-3.169524	3.328384
C	-3.109880	-2.191337	1.293657
C	-1.192645	-1.204506	2.404027
C	-1.265404	-2.185239	3.392493
C	-3.171310	-3.172196	2.278928
H	-3.845438	-2.196026	0.493997
H	-0.425197	-0.437525	2.454975
H	-0.554109	-2.176212	4.212731
H	-3.942313	-3.935329	2.232669
H	-2.305605	-3.933200	4.098360
C	-2.350344	-0.817859	-1.462043
C	-2.590673	-2.358764	-3.781856
N	-1.304403	-1.483372	-2.008227
C	-3.578245	-0.915793	-2.109847
C	-3.699579	-1.685049	-3.268237
C	-1.383122	-2.239045	-3.120150
H	-4.431330	-0.385183	-1.702595
H	-4.661441	-1.760364	-3.767184
H	-0.463569	-2.717720	-3.436027
H	-2.656184	-2.962775	-4.679547
C	-3.553393	1.110094	0.266911
C	-5.836104	2.709137	0.503819
C	-4.404987	0.961237	1.369203
C	-3.845642	2.078411	-0.710095
C	-4.989501	2.863154	-0.596211
C	-5.539779	1.764919	1.484149
H	-4.188829	0.226704	2.138302
H	-3.182432	2.220478	-1.560867
H	-5.215275	3.601904	-1.359432
H	-6.192902	1.647695	2.343450
H	-6.722207	3.329546	0.597080
C	1.329737	4.687263	0.166120
H	0.799375	5.380087	0.823079
H	1.517768	5.204667	-0.780929
H	2.293362	4.443491	0.620692
C	0.491727	3.458529	-0.060167
H	-1.753133	3.581474	0.166700
C	-0.765365	3.165588	0.031548
H	-0.391711	-1.407449	-1.550267

Complex 2+

SCF done: -2349.473608

Pd	-0.055010	0.960920	-0.649232
P	2.144513	-0.030493	-0.001169
C	2.726955	1.319238	-1.105868
N	1.631670	2.049580	-1.419102
C	4.000486	1.675461	-1.528301
C	1.763541	3.177442	-2.127127
C	4.138289	2.841196	-2.284522
H	5.118118	3.154696	-2.632152
C	3.010315	3.605009	-2.576676
H	3.088705	4.523879	-3.147931
H	4.860391	1.066115	-1.271465
H	0.853806	3.735492	-2.321306
C	2.817150	0.349050	1.644558
C	4.177326	0.178827	1.951916
C	1.953054	0.905229	2.598716
C	4.656784	0.555126	3.202774
H	4.859908	-0.251205	1.224380
C	2.442413	1.284521	3.847403
H	0.903711	1.056845	2.356812
C	3.791443	1.107745	4.149387
H	5.708109	0.421570	3.438902
H	1.772488	1.721245	4.581745
H	4.172717	1.403069	5.122218
C	2.912976	-1.581305	-0.589217
C	3.337231	-2.569416	0.314593
C	2.983046	-1.834012	-1.969595
C	3.839992	-3.781645	-0.161204
H	3.307776	-2.383612	1.384862
C	3.487299	-3.046020	-2.435059
H	2.661544	-1.080637	-2.684588
C	3.916130	-4.021094	-1.533315
H	4.192228	-4.530084	0.542938
H	3.554180	-3.225629	-3.503857
H	4.318314	-4.960649	-1.899865
H	-1.500164	3.374897	0.440263
P	-1.940442	-0.085818	0.107500
C	-2.785879	0.716512	1.505948
C	-3.960442	2.078245	3.648621

C	-2.335562	0.496182	2.817959
C	-3.813069	1.644338	1.274176
C	-4.399269	2.313812	2.346526
C	-2.925843	1.172345	3.882466
H	-1.528442	-0.203500	3.019644
H	-4.154340	1.848522	0.264846
H	-5.200262	3.022676	2.160591
H	-2.579249	0.989620	4.895075
H	-4.421878	2.601648	4.480393
C	-1.592689	-1.792467	0.803350
C	-0.974248	-4.429182	1.471566
N	-0.416497	-2.367925	0.476876
C	-2.510626	-2.560921	1.514167
C	-2.200346	-3.876964	1.852682
C	-0.080833	-3.640236	0.773810
H	-3.463094	-2.125661	1.793920
H	-2.916721	-4.475327	2.407973
H	0.899738	-3.967365	0.446460
H	-0.713424	-5.453069	1.714141
C	-3.178225	-0.611678	-1.128216
C	-4.946035	-1.626787	-3.039464
C	-4.537594	-0.764801	-0.817098
C	-2.709067	-0.985977	-2.397170
C	-3.592006	-1.494168	-3.346959
C	-5.415585	-1.262000	-1.777537
H	-4.918299	-0.488675	0.161214
H	-1.655820	-0.871680	-2.644301
H	-3.224970	-1.776823	-4.328907
H	-6.469785	-1.363631	-1.538372
H	-5.635950	-2.013203	-3.783465
C	-1.607100	2.254170	-2.890924
H	-2.303562	1.446088	-3.132731
H	-0.693628	2.073340	-3.469014
H	-2.053451	3.191689	-3.245195
C	-1.339520	2.336280	-1.418202
H	-2.227338	4.210761	-1.039419
C	-1.702576	3.347006	-0.626797
H	0.264328	-1.775019	-0.012719

Complex 2i+

SCF done: -2349.446603

Pd	0.095895	-1.262385	-0.120860
P	-2.053204	-0.086543	-0.056176
C	-3.213277	-1.012391	-1.163422
N	-2.880564	-2.295750	-1.348605
C	-4.357299	-0.436181	-1.720196
C	-3.687807	-3.059685	-2.089800
C	-5.191164	-1.242234	-2.496221
H	-6.090834	-0.829074	-2.942565
C	-4.853581	-2.578068	-2.685014
H	-5.473813	-3.237511	-3.282994
H	-4.595909	0.608847	-1.553981
H	-3.386341	-4.096388	-2.217681
C	-2.750363	-0.254024	1.624598
C	-4.121238	-0.449063	1.848039
C	-1.878592	-0.173617	2.721565
C	-4.607110	-0.556735	3.148873
H	-4.810082	-0.527222	1.012560
C	-2.371860	-0.272145	4.020939
H	-0.810228	-0.046089	2.560183
C	-3.735844	-0.466115	4.234786
H	-5.668456	-0.714781	3.314460
H	-1.691625	-0.208231	4.864919
H	-4.119866	-0.553344	5.246641
C	-2.347298	1.666710	-0.530524
C	-2.852249	2.607708	0.379045
C	-2.086091	2.061968	-1.854772
C	-3.108083	3.918424	-0.035575
H	-3.079721	2.311735	1.399140
C	-2.351745	3.366082	-2.264643
H	-1.704811	1.340825	-2.574516
C	-2.866462	4.296293	-1.356451
H	-3.523729	4.632519	0.669666
H	-2.174992	3.653852	-3.297034
H	-3.091508	5.307472	-1.682971
H	-1.016774	-2.949310	-0.514447
P	1.992681	-0.018014	-0.036668
C	2.661318	0.148437	1.654080
C	3.675874	0.296296	4.256351
C	3.631114	1.111449	1.981902
C	2.196955	-0.729276	2.645910
C	2.708477	-0.656241	3.940043
C	4.133716	1.180587	3.278272
H	4.001892	1.807418	1.234549
H	1.437467	-1.468078	2.402292
H	2.350280	-1.343777	4.700195
H	4.884773	1.924739	3.525156
H	4.072552	0.353138	5.265452
C	1.834887	1.778849	-0.519247
C	1.482441	4.508430	-0.989943
N	0.751831	2.460468	-0.080596
C	2.781793	2.484622	-1.253937
C	2.609084	3.851627	-1.484242
C	0.543320	3.773580	-0.289291
H	3.651126	1.960442	-1.634512
H	3.356261	4.401524	-2.049159
H	-0.385517	4.178605	0.096459
H	1.322486	5.567759	-1.154881
C	3.321218	-0.546803	-1.165849
C	5.271189	-1.369386	-2.986857
C	4.659216	-0.645148	-0.761360
C	2.961701	-0.874166	-2.484025
C	3.937593	-1.276384	-3.391120
C	5.628682	-1.058703	-1.675540
H	4.946676	-0.418583	0.260521
H	1.920541	-0.830005	-2.795973
H	3.656993	-1.529668	-4.408932
H	6.663448	-1.143402	-1.357882
H	6.029646	-1.693719	-3.692893
C	2.461212	-3.527425	0.159233
H	2.943503	-3.079820	1.032510
H	3.084272	-3.311836	-0.714279
H	2.435116	-4.614847	0.292333
C	1.087550	-3.024689	-0.043203
H	-0.376564	-4.606216	-0.080581
C	-0.102766	-3.559120	-0.211937
H	0.014434	1.937298	0.392062

TS2-3+

SCF done: -2462.726057

Pd	0.065988	1.055083	0.422070
P	-2.119713	-0.092829	0.029957
C	-2.745145	0.909329	1.436751
N	-1.773439	1.766091	1.813246
C	-3.982111	0.852515	2.071915
C	-2.027331	2.642739	2.790087
C	-4.238080	1.761594	3.100055
H	-5.194546	1.753483	3.614103
C	-3.253699	2.680269	3.452829
H	-3.422416	3.411836	4.236076
H	-4.721487	0.112776	1.782139
H	-1.229270	3.333706	3.045764
C	-3.043424	0.363353	-1.471779
C	-4.398042	0.726661	-1.451590
C	-2.354869	0.328787	-2.694269
C	-5.048429	1.052645	-2.639158
H	-4.947588	0.768252	-0.516855
C	-3.014855	0.642837	-3.880352
H	-1.301634	0.058837	-2.717633
C	-4.360239	1.008229	-3.852118
H	-6.094421	1.342759	-2.617073
H	-2.478663	0.610981	-4.823990

H	-4.872554	1.263320	-4.774781
C	-2.629724	-1.807437	0.447586
C	-3.339067	-2.609257	-0.457163
C	-2.260744	-2.336450	1.698138
C	-3.684406	-3.916788	-0.109816
H	-3.638494	-2.210348	-1.421747
C	-2.609270	-3.642889	2.038193
H	-1.727589	-1.720507	2.420596
C	-3.322068	-4.434983	1.133901
H	-4.250431	-4.525127	-0.809192
H	-2.339970	-4.036904	3.013845
H	-3.604579	-5.447936	1.404758
H	2.127731	3.304706	-0.411331
P	1.976198	-0.109659	-0.116568
C	2.857789	0.542741	-1.579386
C	4.090843	1.477453	-3.912610
C	4.226989	0.316244	-1.795199
C	2.115084	1.235390	-2.546659
C	2.729469	1.699200	-3.707318
C	4.835856	0.786076	-2.957558
H	4.823497	-0.210213	-1.056665
H	1.056278	1.418421	-2.386272
H	2.147660	2.240483	-4.447265
H	5.897120	0.616377	-3.112328
H	4.571996	1.846623	-4.813179
C	1.635224	-1.861412	-0.707860
C	0.977933	-4.491226	-1.380267
N	0.503751	-2.462480	-0.282264
C	2.483635	-2.602165	-1.525244
C	2.156322	-3.915866	-1.860984
C	0.148458	-3.728785	-0.580648
H	3.392313	-2.145038	-1.899226
H	2.822024	-4.491194	-2.497756
H	-0.793329	-4.073837	-0.168094
H	0.702119	-5.510491	-1.625623
C	3.238010	-0.482485	1.160090
C	5.086498	-0.983512	3.204401
C	4.285316	0.419334	1.404375
C	3.118755	-1.628491	1.961402
C	4.040370	-1.876337	2.976147
C	5.204739	0.162358	2.418882
H	4.380842	1.323264	0.812685
H	2.310963	-2.338266	1.807050
H	3.941559	-2.769037	3.586136
H	6.015355	0.862951	2.595007
H	5.806028	-1.179384	3.993405
C	1.542654	1.968888	2.792417
H	1.923938	0.965936	3.010372
H	0.563823	2.049080	3.271943
H	2.214355	2.693408	3.268700
C	1.480286	2.227859	1.317918
H	2.792263	3.866874	1.218150
C	2.160878	3.170146	0.665015
C	-0.674815	2.845589	-0.767561
O	-0.911799	3.885351	-1.155945
H	-0.146148	-1.903312	0.277491

Complex 3+

SCF done: -2462.741285

Pd	0.079885	-1.323081	-0.098348
P	-1.995566	0.039184	-0.107362
C	-2.873174	-0.435504	1.447948
N	-2.477425	-1.613377	1.947317
C	-3.882736	0.336093	2.028457
C	-3.090767	-2.079370	3.038322
C	-4.512993	-0.157073	3.171769
H	-5.306430	0.411746	3.647437
C	-4.113831	-1.386372	3.686379
H	-4.580571	-1.804665	4.572119
H	-4.173347	1.291467	1.604206
H	-2.748175	-3.042694	3.408310
C	-2.171874	1.872484	-0.140197
C	-2.827608	2.530663	-1.193601
C	-1.664764	2.631155	0.932763
C	-2.987336	3.918186	-1.163396
H	-3.239689	1.958454	-2.019357
C	-1.826036	4.014907	0.954541
H	-1.165444	2.138771	1.764019
C	-2.491696	4.660130	-0.090566
H	-3.519669	4.413850	-1.970227
H	-1.447713	4.588039	1.795831
H	-2.633114	5.736545	-0.062045
C	-3.027971	-0.560614	-1.487851
C	-2.386319	-0.963023	-2.669566
C	-4.426427	-0.626030	-1.403398
C	-3.133420	-1.414635	-3.755539
H	-1.300068	-0.934081	-2.736408
C	-5.167066	-1.086404	-2.489422
H	-4.938682	-0.331884	-0.492214
C	-4.523447	-1.478120	-3.664093
H	-2.631587	-1.727272	-4.666234
H	-6.248793	-1.144257	-2.416478
H	-5.106041	-1.840246	-4.505716
H	1.520159	-2.745476	2.201096
P	1.998491	0.082545	-0.009047
C	2.159782	0.789276	1.666921
C	2.367312	1.817098	4.257181
C	3.164013	1.720212	1.978508
C	1.260800	0.379409	2.662827
C	1.369400	0.891938	3.954897
C	3.262957	2.230915	3.269029
H	3.878738	2.037576	1.224677
H	0.485527	-0.348093	2.431460
H	0.679264	0.562569	4.725724
H	4.043400	2.947322	3.506576
H	2.452710	2.213412	5.264499
C	1.988916	1.637694	-1.058671
C	1.762643	4.020694	-2.507889
N	0.805321	2.257753	-1.266720
C	3.122421	2.234687	-1.605048
C	3.010437	3.423964	-2.327777
C	0.655420	3.406787	-1.953185
H	4.087341	1.760630	-1.469783
H	3.900207	3.883300	-2.748601
H	-0.357464	3.786543	-2.026651
H	1.646262	4.942586	-3.066189
C	3.626066	-0.592486	-0.482780
C	6.073642	-1.712525	-1.236171
C	4.583167	-0.908013	0.489948
C	3.896869	-0.856440	-1.836001
C	5.120313	-1.406919	-2.208549
C	5.802499	-1.465640	0.108575
H	4.381298	-0.726920	1.540387
H	3.161630	-0.629150	-2.605116
H	5.326550	-1.602711	-3.256428
H	6.540925	-1.706978	0.866974
H	7.025748	-2.145203	-1.527850
C	1.834841	-3.550589	-1.208903
H	2.156028	-2.849061	-1.983896
H	0.987299	-4.115109	-1.614622
H	2.654677	-4.257439	-1.035726
C	1.467968	-2.865704	0.069757
H	2.573884	-4.044789	1.413580
C	1.865273	-3.224687	1.289618
C	-1.079626	-2.906669	-0.019559
O	-1.665228	-3.880205	-0.053739
H	-0.042780	1.853150	-0.859142

TS3-4+

SCF done: -2462.730967

Pd	-0.042259	-1.329204	-0.111707
P	-1.985024	0.058742	-0.030343

C	-3.455279	-0.997233	0.332799
N	-3.213445	-1.924767	1.267695
C	-4.691458	-0.831680	-0.290474
C	-4.221467	-2.723732	1.629456
C	-5.730787	-1.683389	0.087207
H	-6.707617	-1.593907	-0.378547
C	-5.495496	-2.643835	1.064943
H	-6.277153	-3.325234	1.384239
H	-4.846017	-0.070268	-1.047056
H	-3.997136	-3.463464	2.394033
C	-2.013820	1.342407	1.277984
C	-2.525153	1.031177	2.546601
C	-1.467897	2.616118	1.054288
C	-2.504286	1.985659	3.562736
H	-2.941333	0.048531	2.742390
C	-1.454262	3.565613	2.073272
H	-1.086671	2.886853	0.073913
C	-1.972661	3.252689	3.329708
H	-2.917718	1.738451	4.536004
H	-1.051208	4.556045	1.883165
H	-1.969443	3.996862	4.120289
C	-2.359827	0.899743	-1.613943
C	-3.145358	2.060286	-1.694890
C	-1.891060	0.305540	-2.800057
C	-3.445610	2.616952	-2.938063
H	-3.527075	2.525311	-0.790781
C	-2.194307	0.866829	-4.041988
H	-1.321413	-0.622222	-2.752069
C	-2.970533	2.025309	-4.110448
H	-4.062286	3.509403	-2.991522
H	-1.844430	0.388756	-4.952450
H	-3.218452	2.456897	-5.075739
H	0.725228	-3.363136	2.003616
P	1.899717	0.083881	0.084146
C	2.342381	0.535915	1.789939
C	2.918611	1.233369	4.432496
C	3.650233	0.901954	2.153279
C	1.330759	0.513275	2.761573
C	1.622484	0.862769	4.078307
C	3.930699	1.251970	3.470838
H	4.453160	0.885290	1.421690
H	0.318304	0.226371	2.491838
H	0.836873	0.839709	4.826820
H	4.942919	1.528248	3.750139
H	3.145303	1.499516	5.460530
C	1.808807	1.736505	-0.787563
C	1.527487	4.076098	-2.289421
N	0.869989	1.877267	-1.751841
C	2.645197	2.821801	-0.547270
C	2.507191	3.990067	-1.296896
C	0.701254	2.988498	-2.497794
H	3.396751	2.748113	0.230209
H	3.165203	4.833439	-1.108541
H	-0.100358	2.957439	-3.227595
H	1.401115	4.971586	-2.887386
C	3.412287	-0.601045	-0.686591
C	5.624944	-1.835022	-1.876474
C	4.198968	-1.501063	0.048257
C	3.736846	-0.335276	-2.025300
C	4.840911	-0.948626	-2.613928
C	5.301910	-2.109048	-0.547837
H	3.960646	-1.722505	1.083903
H	3.142044	0.350928	-2.622230
H	5.090234	-0.730001	-3.647795
H	5.912487	-2.795443	0.031092
H	6.486955	-2.309024	-2.335657
C	1.742639	-3.659313	-1.358195
H	2.190685	-2.826833	-1.908263
H	1.030048	-4.154937	-2.026493
H	2.534565	-4.379073	-1.125584
C	1.075020	-3.208716	-0.096160
H	2.093214	-4.405346	1.315565
C	1.306488	-3.671269	1.138952
C	-0.868375	-3.025976	-0.367707
O	-1.555609	-3.898800	-0.669423
H	0.210240	1.108658	-1.905670

Complex 4

SCF done: -2462.764047

Pd	0.115216	-1.263398	-0.292553
P	1.964889	0.142813	0.123426
C	2.915305	0.132396	-1.463196
N	2.136519	0.415093	-2.519425
C	4.266848	-0.187821	-1.570586
C	2.705248	0.418881	-3.728684
C	4.842327	-0.188781	-2.841870
H	5.892007	-0.437716	-2.965623
C	4.052392	0.125889	-3.941308
H	4.461573	0.135098	-4.946120
H	4.854979	-0.446976	-0.698449
H	2.054358	0.658968	-4.566264
C	1.661025	1.937508	0.419873
C	1.108634	2.720695	-0.610852
C	1.976678	2.544724	1.642929
C	0.911541	4.090958	-0.424868
H	0.883625	2.264388	-1.570281
C	1.790601	3.918001	1.817154
H	2.397290	1.959348	2.454020
C	1.266319	4.696012	0.785140
H	0.515780	4.691206	-1.239437
H	2.076207	4.380335	2.757873
H	1.152752	5.769184	0.911692
C	3.077475	-0.387784	1.461844
C	4.289560	0.276477	1.721741
C	2.716944	-1.486296	2.253626
C	5.125272	-0.168653	2.742195
H	4.580610	1.142605	1.133483
C	3.554619	-1.925641	3.277188
H	1.773213	-1.994040	2.068021
C	4.760370	-1.270279	3.518299
H	6.062667	0.345177	2.932585
H	3.267649	-2.778515	3.884800
H	5.416195	-1.614413	4.312264
H	-0.800278	-2.501755	-2.335913
P	-1.984999	-0.050707	0.007163
C	-2.439450	0.990044	-1.418366
C	-3.111918	2.494844	-3.676367
C	-3.572709	1.823248	-1.402387
C	-1.638911	0.931048	-2.569363
C	-1.981703	1.679738	-3.694850
C	-3.903408	2.571156	-2.528170
H	-4.203911	1.882307	-0.519115
H	-0.737143	0.321791	-2.580825
H	-1.363603	1.627315	-4.585844
H	-4.782040	3.208966	-2.513352
H	-3.377165	3.075060	-4.555054
C	-2.212249	1.168817	1.403840
C	-2.449697	3.141668	3.375795
N	-1.576179	2.364415	1.322193
C	-2.996265	0.942696	2.532053
C	-3.115332	1.924235	3.516516
C	-1.674554	3.337254	2.248934
H	-3.529102	0.003862	2.624775
H	-3.738886	1.740667	4.386634
H	-1.115423	4.242125	2.045589
H	-2.530497	3.927171	4.118293
C	-3.360389	-1.213686	0.336426
C	-5.357416	-3.098975	0.875722
C	-4.544338	-1.217055	-0.410484
C	-3.174704	-2.176892	1.344570
C	-4.176489	-3.103844	1.621474
C	-5.534443	-2.163171	-0.141113

H	-4.695135	-0.499588	-1.210159
H	-2.245318	-2.206000	1.910701
H	-4.033197	-3.836081	2.410694
H	-6.446421	-2.165117	-0.730314
H	-6.133255	-3.829460	1.083632
C	0.031179	-4.492495	0.464210
H	0.701669	-4.255747	1.293163
H	0.328069	-5.473582	0.074826
H	-0.992880	-4.561397	0.836300
C	0.129035	-3.498022	-0.660792
H	-1.949934	-3.319727	-1.136359
C	-0.945836	-2.978025	-1.367010
C	1.383558	-2.822218	-0.895050
O	2.506768	-2.956376	-1.226127
H	-0.969999	2.553799	0.516710

Complex 5+

SCF done: -2578.457049

Pd	-0.036069	-0.901267	-0.889615
P	-1.867635	0.279106	0.036858
C	-3.418455	-0.722964	-0.030349
N	-3.281609	-1.980293	0.421661
C	-4.626115	-0.215449	-0.503181
C	-4.359047	-2.771751	0.422349
C	-5.742084	-1.053634	-0.503561
H	-6.698190	-0.690872	-0.868700
C	-5.609300	-2.354017	-0.031999
H	-6.450616	-3.038720	-0.017262
H	-4.700975	0.804295	-0.863522
H	-4.214176	-3.782219	0.796001
C	-1.754253	0.792077	1.793270
C	-2.485940	0.142585	2.796023
C	-0.915259	1.860131	2.147231
C	-2.384794	0.562868	4.121822
H	-3.138744	-0.687328	2.551879
C	-0.822961	2.280524	3.469963
H	-0.347695	2.390729	1.387769
C	-1.558565	1.631117	4.461614
H	-2.965511	0.057484	4.887629
H	-0.180955	3.117449	3.727232
H	-1.491993	1.962392	5.493449
C	-2.254115	1.823722	-0.877849
C	-2.896458	2.914023	-0.268063
C	-1.957084	1.886122	-2.250335
C	-3.228745	4.040497	-1.018939
H	-3.140296	2.881420	0.789317
C	-2.295833	3.014020	-2.999066
H	-1.483931	1.035228	-2.736235
C	-2.931196	4.092926	-2.382283
H	-3.731332	4.875499	-0.539807
H	-2.080098	3.042761	-4.063297
H	-3.204156	4.968269	-2.964389
H	0.642266	-3.279007	-0.936184
P	2.027773	-0.002806	0.073652
C	2.125585	0.062324	1.891111
C	2.288081	-0.098214	4.672745
C	3.006764	0.898413	2.593987
C	1.322835	-0.853532	2.588112
C	1.416493	-0.933280	3.977051
C	3.079854	0.820617	3.981048
H	3.643071	1.607525	2.073648
H	0.635039	-1.507417	2.053105
H	0.802189	-1.648588	4.514890
H	3.761409	1.470097	4.522078
H	2.355499	-0.162448	5.754691
C	2.289861	1.760668	-0.482915
C	2.404221	4.404996	-1.383401
N	1.202509	2.427614	-0.937224
C	3.507021	2.436894	-0.506819
C	3.563896	3.760202	-0.946309
C	1.215022	3.700733	-1.378688
H	4.405844	1.915653	-0.196128
H	4.513890	4.286747	-0.953838
H	0.266646	4.098208	-1.722981
H	2.422535	5.429789	-1.736597
C	3.611434	-0.732139	-0.489309
C	5.957117	-1.939895	-1.418399
C	4.451664	-1.411918	0.400645
C	3.950935	-0.667121	-1.851733
C	5.123117	-1.260678	-2.309933
C	5.618952	-2.016089	-0.069387
H	4.201931	-1.472025	1.455151
H	3.305175	-0.148801	-2.558089
H	5.386768	-1.197281	-3.361567
H	6.265188	-2.543537	0.625596
H	6.868106	-2.408401	-1.778024
C	0.475417	-1.730433	-4.114830
H	0.012599	-0.767328	-4.343046
H	0.105779	-2.450663	-4.853987
H	1.558153	-1.642876	-4.227680
C	0.115957	-2.233771	-2.742541
H	2.053573	-2.843298	-2.079313
C	1.002241	-2.754263	-1.822144
C	-1.217207	-1.964132	-2.228852
O	-2.359751	-2.146159	-2.467257
H	0.342847	-4.620803	1.775942
C	-0.696823	-4.313805	1.639981
H	-1.153770	-4.207079	2.631751
H	-1.219843	-5.109006	1.094008
O	-0.697943	-3.084913	0.920598
H	-1.622724	-2.769010	0.813495
H	0.315494	1.913998	-0.976550

TS5-7+

SCF done: -2578.455113

Pd	0.045516	-1.009719	-0.739381
P	-1.824322	0.308616	0.024999
C	-3.360360	-0.710879	0.193875
N	-3.207146	-1.825280	0.930363
C	-4.580226	-0.349448	-0.376873
C	-4.277801	-2.599311	1.141334
C	-5.686550	-1.171579	-0.159502
H	-6.650166	-0.916055	-0.590130
C	-5.537734	-2.313168	0.619717
H	-6.373416	-2.975960	0.817614
H	-4.671555	0.552741	-0.970859
H	-4.116952	-3.487900	1.746523
C	-1.730527	1.188669	1.636495
C	-2.433502	0.750114	2.765384
C	-0.928610	2.335461	1.739717
C	-2.341647	1.452593	3.966908
H	-3.056740	-0.135130	2.716854
C	-0.844285	3.036686	2.938450
H	-0.388771	2.708424	0.873777
C	-1.552173	2.595920	4.056787
H	-2.900471	1.106530	4.831270
H	-0.232095	3.931554	2.999172
H	-1.492081	3.145900	4.990988
C	-2.282937	1.626001	-1.172952
C	-2.993704	2.776324	-0.793678
C	-1.943885	1.450478	-2.525245
C	-3.353673	3.725280	-1.749006
H	-3.265784	2.929924	0.246172
C	-2.309268	2.401069	-3.480359
H	-1.407805	0.552752	-2.829442
C	-3.013811	3.540821	-3.090871
H	-3.908495	4.608324	-1.445927
H	-2.057163	2.245941	-4.525653
H	-3.305736	4.279496	-3.831570
H	1.128513	-3.316285	-0.811618
P	2.038417	-0.025336	0.051678
C	2.089279	0.290755	1.845828

C	2.208188	0.507610	4.625265
C	2.928432	1.244681	2.441356
C	1.307883	-0.554226	2.648332
C	1.379998	-0.445362	4.036674
C	2.979116	1.354981	3.827109
H	3.547193	1.902081	1.839015
H	0.657357	-1.300306	2.193720
H	0.783056	-1.106082	4.657758
H	3.626809	2.096270	4.285337
H	2.258139	0.591026	5.706828
C	2.279307	1.646815	-0.745414
C	2.342105	4.133946	-2.017933
N	1.196574	2.187234	-1.350322
C	3.468916	2.368275	-0.804090
C	3.498563	3.614930	-1.431106
C	1.183054	3.381589	-1.972393
H	4.368771	1.941763	-0.375020
H	4.426115	4.178941	-1.467705
H	0.240675	3.678730	-2.419362
H	2.341189	5.096735	-2.516265
C	3.655546	-0.786677	-0.352680
C	6.069864	-2.041357	-1.004646
C	4.428651	-1.388025	0.648232
C	4.097053	-0.826620	-1.686458
C	5.302846	-1.443203	-2.006902
C	5.630354	-2.015398	0.316726
H	4.102419	-1.365317	1.683167
H	3.506995	-0.369965	-2.479084
H	5.643832	-1.460654	-3.037787
H	6.224473	-2.479247	1.098183
H	7.007734	-2.526708	-1.256675
C	-0.152253	-2.060593	-3.864886
H	-1.114133	-1.620390	-4.135664
H	0.012655	-2.927867	-4.512945
H	0.636648	-1.329169	-4.054810
C	-0.105067	-2.520953	-2.420187
H	2.021404	-2.458059	-2.173982
C	1.084708	-2.628143	-1.652443
C	-1.311455	-2.758208	-1.786215
O	-2.365708	-3.187957	-1.550397
H	0.486434	-4.562845	1.649111
C	-0.552258	-4.228952	1.707862
H	-0.849390	-4.230145	2.763575
H	-1.177877	-4.947495	1.163412
O	-0.624944	-2.923207	1.143687
H	-1.548394	-2.585567	1.206878
H	0.337874	1.622182	-1.353369

Complex 7+

SCF done: -2578.518299

Pd	0.045027	-0.749126	-0.588174
P	-1.844880	0.539937	-0.029381
C	-3.422137	0.346428	-1.029281
N	-3.873550	-0.911214	-1.246057
C	-4.166220	1.398956	-1.559232
C	-5.000163	-1.188339	-1.922764
C	-5.338983	1.141941	-2.271904
H	-5.915608	1.968525	-2.676721
C	-5.771130	-0.169750	-2.455496
H	-6.678667	-0.402621	-3.000522
H	-3.832530	2.417972	-1.406657
H	-5.243940	-2.240913	-2.020157
C	-2.490036	0.207167	1.654150
C	-3.799575	0.522324	2.050667
C	-1.614315	-0.373619	2.583201
C	-4.219453	0.261108	3.352678
H	-4.496421	0.974018	1.349969
C	-2.036260	-0.623917	3.887850
H	-0.604090	-0.635542	2.277456
C	-3.338814	-0.309693	4.272433
H	-5.235168	0.504019	3.650117
H	-1.349988	-1.070857	4.600974
H	-3.670695	-0.511750	5.286381
C	-1.667299	2.372310	-0.133916
C	-2.069747	3.243012	0.889482
C	-1.102886	2.907717	-1.305806
C	-1.926498	4.624587	0.733336
H	-2.509340	2.847835	1.800365
C	-0.978230	4.286274	-1.463954
H	-0.772125	2.241759	-2.100317
C	-1.391900	5.147624	-0.444455
H	-2.255639	5.290889	1.525887
H	-0.563777	4.689537	-2.383487
H	-1.303277	6.222697	-0.571459
H	1.197255	-3.221612	-0.575640
P	2.216104	-0.044179	-0.084887
C	2.857003	-0.694967	1.507565
C	3.770433	-1.807937	3.911229
C	4.008632	-0.190497	2.132400
C	2.167423	-1.761072	2.104682
C	2.627265	-2.316735	3.297463
C	4.459073	-0.743840	3.328205
H	4.567000	0.629317	1.689819
H	1.275898	-2.159345	1.626762
H	2.093328	-3.149069	3.746210
H	5.351422	-0.347060	3.802884
H	4.126945	-2.239972	4.841407
C	2.585740	1.772022	0.156956
C	2.877710	4.492316	0.728605
N	1.619060	2.501758	0.759691
C	3.750010	2.441461	-0.214747
C	3.899236	3.796930	0.076209
C	1.721339	3.811720	1.055885
H	4.532691	1.889065	-0.723165
H	4.814464	4.311701	-0.201677
H	0.858643	4.268439	1.525662
H	2.969031	5.545740	0.966674
C	3.466637	-0.441907	-1.361188
C	5.260941	-1.059209	-3.415796
C	4.632654	-1.164836	-1.082076
C	3.197907	-0.042363	-2.681153
C	4.097577	-0.341054	-3.700215
C	5.523179	-1.473252	-2.111546
H	4.844774	-1.496048	-0.070516
H	2.280186	0.494942	-2.912183
H	3.887428	-0.024719	-4.717612
H	6.422296	-2.040484	-1.890399
H	5.957232	-1.301701	-4.212853
C	-1.236634	-2.403632	-2.937927
H	-2.154025	-1.813542	-2.920636
H	-1.475766	-3.365646	-3.407504
H	-0.521437	-1.889407	-3.583283
C	-0.632520	-2.630149	-1.566083
H	1.405864	-2.471183	-2.241721
C	0.757174	-2.653164	-1.389011
C	-1.511032	-3.281576	-0.563162
O	-2.741369	-3.134528	-0.519817
H	-2.456429	-5.363033	0.783808
C	-1.706091	-4.742269	1.275842
H	-1.017792	-5.359301	1.850567
H	-2.200435	-4.008752	1.915924
O	-0.888171	-4.078673	0.291293
H	-3.326470	-1.773630	-0.911533
H	0.737265	2.024215	0.955197

TS7-8+

SCF done: -2578.501886

Pd	0.107274	-0.244887	-0.329200
P	-2.025484	0.527002	-0.003476
C	-3.444030	0.113885	-1.160374
N	-3.669855	-1.194459	-1.429099
C	-4.281259	1.047405	-1.769268

C	-4.660455	-1.632483	-2.225114
C	-5.315230	0.625235	-2.605809
H	-5.967759	1.359491	-3.069199
C	-5.515915	-0.734949	-2.837795
H	-6.312596	-1.094704	-3.478629
H	-4.126113	2.102431	-1.577924
H	-4.728227	-2.708013	-2.346143
C	-2.776608	0.061972	1.601183
C	-4.141357	0.227446	1.885704
C	-1.928526	-0.466934	2.585192
C	-4.644237	-0.130176	3.134207
H	-4.816707	0.638906	1.140253
C	-2.435535	-0.815283	3.835895
H	-0.872201	-0.600842	2.360877
C	-3.792460	-0.649899	4.109943
H	-5.701296	-0.001408	3.346755
H	-1.771804	-1.217510	4.595576
H	-4.188490	-0.925819	5.082652
C	-2.088658	2.365607	-0.087294
C	-2.649079	3.157297	0.923922
C	-1.519921	2.989151	-1.212417
C	-2.651153	4.549110	0.803759
H	-3.086995	2.694050	1.802820
C	-1.546345	4.376358	-1.338565
H	-1.059211	2.382935	-1.990045
C	-2.111889	5.159379	-0.328489
H	-3.090753	5.153994	1.591555
H	-1.126386	4.846670	-2.223190
H	-2.134872	6.240826	-0.426685
H	1.548791	-3.590558	-0.443647
P	2.381790	0.070944	-0.046406
C	3.073139	-0.556604	1.530780
C	4.030375	-1.652376	3.923476
C	4.239041	-0.051434	2.126045
C	2.389230	-1.611780	2.152836
C	2.871407	-2.160726	3.339481
C	4.711390	-0.596236	3.317393
H	4.788584	0.765410	1.667949
H	1.479476	-1.999714	1.700846
H	2.340928	-2.983149	3.810054
H	5.613454	-0.197767	3.771811
H	4.403393	-2.076467	4.850830
C	2.651371	1.909277	0.145782
C	2.675360	4.657490	0.604422
N	1.554011	2.590565	0.541371
C	3.819522	2.633541	-0.070341
C	3.832008	4.009008	0.163813
C	1.522350	3.913293	0.778414
H	4.703866	2.118249	-0.429536
H	4.743272	4.577374	0.001664
H	0.568120	4.331052	1.078023
H	2.661424	5.725020	0.791803
C	3.600599	-0.320455	-1.353846
C	5.344250	-0.918565	-3.456603
C	4.796063	-1.005553	-1.102369
C	3.276429	0.048959	-2.670301
C	4.151130	-0.240160	-3.713577
C	5.661548	-1.303819	-2.155355
H	5.050284	-1.313959	-0.093184
H	2.336744	0.557831	-2.876841
H	3.899666	0.054513	-4.728151
H	6.584911	-1.839181	-1.955522
H	6.021940	-1.152005	-4.272241
C	-0.768722	-2.640674	-2.888753
H	-1.322681	-1.704709	-2.764547
H	-1.457397	-3.384133	-3.303593
H	0.019308	-2.463070	-3.622960
C	-0.173712	-3.121264	-1.593006
H	1.859826	-2.873390	-2.126098
C	1.149450	-3.190992	-1.369095
C	-1.128843	-3.588575	-0.551223
O	-2.329556	-3.304511	-0.545787
H	-2.288985	-5.447258	0.927801
C	-1.478646	-4.879483	1.387978
H	-0.860377	-5.527541	2.006229
H	-1.893634	-4.058419	1.975931
O	-0.593153	-4.368829	0.370895
H	-3.049109	-1.949773	-1.030058
H	0.692472	2.014275	0.595651

Complex 8+

SCF done: -2232.820029

Pd	-0.005579	0.118617	-0.229377
P	2.263381	0.008165	0.026391
C	3.050355	-0.295159	-1.636623
N	3.272345	0.777598	-2.436418
C	3.322599	-1.552740	-2.173984
C	3.719793	0.705011	-3.708533
C	3.792474	-1.669153	-3.479208
H	4.011885	-2.651338	-3.887426
C	3.987295	-0.527775	-4.265232
H	4.349174	-0.592201	-5.284769
H	3.171661	-2.431068	-1.556354
H	3.856140	1.645849	-4.229511
C	3.151238	1.523493	0.534641
C	4.539860	1.691628	0.375251
C	2.398646	2.554103	1.119208
C	5.155784	2.865558	0.801495
H	5.144756	0.907492	-0.074150
C	3.022094	3.724156	1.548738
H	1.323829	2.429747	1.229031
C	4.398323	3.879728	1.390868
H	6.227814	2.987621	0.678981
H	2.433442	4.515733	2.002393
H	4.883318	4.792434	1.723703
C	2.884797	-1.402267	1.011067
C	4.041058	-1.346407	1.800134
C	2.129055	-2.586391	0.970200
C	4.444620	-2.469343	2.520552
H	4.619042	-0.430969	1.871695
C	2.550484	-3.710394	1.677401
H	1.207633	-2.617595	0.391001
C	3.708658	-3.652010	2.453036
H	5.337975	-2.418647	3.135679
H	1.969052	-4.626636	1.633086
H	4.032002	-4.524439	3.012859
H	3.116651	1.699133	-2.031195
P	-2.321546	0.073202	-0.155177
C	-3.242221	1.623990	-0.442242
C	-4.543900	4.072509	-0.782442
C	-4.632808	1.662125	-0.633002
C	-2.510997	2.820604	-0.431126
C	-3.162523	4.040730	-0.598571
C	-5.276719	2.884199	-0.802648
H	-5.209832	0.742701	-0.677008
H	-1.431762	2.786208	-0.298326
H	-2.592293	4.964741	-0.593453
H	-6.351184	2.910162	-0.957172
H	-5.051445	5.022783	-0.918423
C	-2.777561	-0.300749	1.620938
C	-3.056252	-0.710873	4.362200
N	-1.721024	-0.325744	2.462938
C	-4.043154	-0.499773	2.162240
C	-4.182709	-0.704854	3.534786
C	-1.811712	-0.517508	3.791610
H	-4.909320	-0.493411	1.510769
H	-5.169397	-0.858223	3.961976
H	-0.883815	-0.512201	4.352017
H	-3.140335	-0.865312	5.431948
C	-3.207906	-1.238607	-1.068713
C	-4.369391	-3.282234	-2.586338
C	-3.684973	-0.974308	-2.361010

C	-3.297535	-2.539898	-0.552873
C	-3.883387	-3.553218	-1.307550
C	-4.265418	-1.994943	-3.111498
H	-3.616056	0.025514	-2.780098
H	-2.915489	-2.772587	0.438013
H	-3.961140	-4.554928	-0.895570
H	-4.641124	-1.780183	-4.107350
H	-4.827597	-4.073113	-3.172256
H	-0.801528	-0.182484	1.990766

TS1-2i (6Me)

SCF done: -2427.747063

Pd	-0.014241	-1.310113	0.295761
P	-1.831471	0.154000	0.028603
C	-3.249563	-1.003859	-0.350183
N	-3.015897	-2.305491	-0.117206
C	-4.465129	-0.583269	-0.883696
C	-3.938560	-3.250463	-0.377846
C	-5.441094	-1.538200	-1.161304
H	-6.397404	-1.238427	-1.579999
C	-5.176579	-2.878547	-0.907247
H	-5.914711	-3.643196	-1.125203
H	-4.633265	0.468032	-1.089653
C	-2.340165	0.993163	1.575019
C	-3.613064	0.882209	2.148660
C	-1.355309	1.759425	2.219617
C	-3.898290	1.532555	3.348908
H	-4.386255	0.288169	1.671271
C	-1.652446	2.414097	3.412303
H	-0.365006	1.847610	1.778115
C	-2.921272	2.299239	3.980619
H	-4.886597	1.437558	3.789366
H	-0.886499	3.007366	3.903365
H	-3.146956	2.803104	4.915947
C	-2.044308	1.390666	-1.304844
C	-2.770668	2.574964	-1.127204
C	-1.483245	1.105629	-2.557149
C	-2.941413	3.455706	-2.195030
H	-3.198146	2.811377	-0.156703
C	-1.661840	1.985192	-3.621622
H	-0.901589	0.197058	-2.693838
C	-2.391407	3.160753	-3.441667
H	-3.505601	4.372767	-2.051148
H	-1.226660	1.756611	-4.590152
H	-2.527775	3.847712	-4.271878
H	-1.750876	-2.577285	0.330919
P	1.957056	-0.168909	-0.049348
C	2.808823	0.261597	1.514270
C	4.105525	0.857923	3.923692
C	3.822105	1.231390	1.553393
C	2.440153	-0.389678	2.697915
C	3.089144	-0.094804	3.896116
C	4.468332	1.522899	2.751952
H	4.101694	1.766030	0.649813
H	1.631076	-1.115310	2.679654
H	2.793525	-0.604433	4.808644
H	5.252773	2.273977	2.771954
H	4.609502	1.089479	4.857582
C	1.890016	1.467797	-0.913516
C	1.709697	3.962667	-1.981208
N	1.187645	2.394938	-0.251367
C	2.526120	1.711195	-2.130780
C	2.422318	2.992222	-2.671943
C	1.103319	3.631128	-0.761075
H	3.091119	0.933314	-2.631534
H	2.902314	3.228635	-3.617608
H	1.620477	4.971097	-2.373234
C	3.159630	-1.133870	-1.048339
C	4.895108	-2.617991	-2.674590
C	4.534743	-1.152268	-0.784827
C	2.662303	-1.878242	-2.129239
C	3.525908	-2.607937	-2.942755
C	5.395134	-1.894729	-1.593360
H	4.936980	-0.598192	0.057380
H	1.591802	-1.896301	-2.322593
H	3.129010	-3.178029	-3.777946
H	6.458961	-1.907795	-1.374476
H	5.568314	-3.194890	-3.301987
C	1.958892	-3.836119	1.003763
H	2.608683	-3.291576	1.695480
H	2.495688	-3.903816	0.051663
H	1.803846	-4.850735	1.387174
C	0.671779	-3.137373	0.814025
H	-1.210354	-4.081729	1.346834
C	-0.618840	-3.289639	0.894220
H	-4.356275	-5.349290	-0.497448
C	-3.594861	-4.681489	-0.091132
H	-2.628472	-4.949554	-0.526990
H	-3.537051	-4.857896	0.988617
H	0.126963	5.543897	-0.542185
C	0.356391	4.653111	0.046890
H	-0.574819	4.231426	0.432250
H	0.956333	4.963620	0.909883

TS1L-2L (6Me)

SCF done: -2427.736852

Pd	-0.063832	-1.234508	0.386047
P	-1.761994	0.339711	0.050553
C	-3.186703	-0.759279	-0.465290
N	-2.974800	-2.082202	-0.345039
C	-4.349709	-0.275755	-1.056533
C	-3.847009	-2.984545	-0.830014
C	-5.294324	-1.187748	-1.525768
H	-6.212584	-0.836858	-1.987584
C	-5.033940	-2.547650	-1.427097
H	-5.731653	-3.279649	-1.820918
H	-4.498529	0.792524	-1.169137
C	-2.315188	1.176996	1.578989
C	-3.617160	1.102374	2.089182
C	-1.335363	1.897694	2.281460
C	-3.936724	1.745208	3.284824
H	-4.385308	0.541419	1.565402
C	-1.666239	2.545326	3.468781
H	-0.320282	1.950920	1.893652
C	-2.964601	2.467788	3.973670
H	-4.947575	1.679412	3.676765
H	-0.904919	3.103282	4.006146
H	-3.217042	2.966179	4.905039
C	-1.850590	1.606830	-1.268825
C	-2.520467	2.825429	-1.101026
C	-1.255699	1.308740	-2.502149
C	-2.599397	3.729190	-2.160558
H	-2.976080	3.069486	-0.145331
C	-1.343822	2.210979	-3.558639
H	-0.718629	0.371879	-2.629634
C	-2.015424	3.422186	-3.388684
H	-3.119439	4.673232	-2.024943
H	-0.882143	1.972724	-4.512407
H	-2.080394	4.127450	-4.212160
H	-1.781976	-2.372514	0.323570
P	2.018056	-0.328335	-0.036780
C	2.958753	0.012467	1.500566
C	4.402899	0.458749	3.859624
C	4.007547	0.944048	1.525707
C	2.634414	-0.680838	2.673296
C	3.355781	-0.460386	3.845347
C	4.725789	1.161747	2.698975
H	4.260526	1.507716	0.632304
H	1.807134	-1.384533	2.668741
H	3.093336	-1.002765	4.749142
H	5.536141	1.885042	2.707223
H	4.962749	0.632820	4.773968

C	2.096886	1.305125	-0.900832
C	2.157171	3.812185	-1.953094
N	1.486575	2.291022	-0.232722
C	2.749668	1.492496	-2.119652
C	2.770557	2.780983	-2.652029
C	1.519647	3.532249	-0.736130
H	3.237918	0.666659	-2.624845
H	3.272333	2.976507	-3.595753
H	2.169042	4.827584	-2.336851
C	3.084372	-1.426651	-1.049058
C	4.621830	-3.095325	-2.692567
C	4.476103	-1.482368	-0.897125
C	2.471361	-2.225251	-2.025162
C	3.236700	-3.048608	-2.847878
C	5.237927	-2.316179	-1.714294
H	4.966050	-0.886527	-0.133133
H	1.388338	-2.210586	-2.125706
H	2.751023	-3.662468	-3.601067
H	6.315251	-2.358705	-1.582530
H	5.218942	-3.744477	-3.326444
C	-1.779549	-3.892760	2.069047
H	-1.691087	-4.966036	1.873204
H	-2.823089	-3.598482	1.934099
H	-1.524290	-3.724405	3.119916
C	-0.838143	-3.105461	1.199815
H	1.352717	-3.630794	1.196322
C	0.448459	-3.065683	1.021098
H	-2.428508	-4.596203	-0.698345
C	-3.508336	-4.442167	-0.736784
H	-3.949901	-4.890409	0.159974
H	-3.908590	-4.978946	-1.600200
H	-0.224166	4.405228	0.151949
C	0.847880	4.608234	0.067629
H	1.256484	4.634035	1.082353
H	0.978976	5.593051	-0.386113

Complex 7 (6Me)

SCF done: -2656.816940

Pd	-0.051080	-1.027653	-0.533739
P	-1.563765	0.698158	-0.112457
C	-3.273011	0.531149	-0.873594
N	-3.950301	-0.633292	-0.697698
C	-3.879521	1.519604	-1.643882
C	-5.183111	-0.884267	-1.194796
C	-5.144387	1.300440	-2.187980
H	-5.615591	2.074220	-2.787258
C	-5.805097	0.100230	-1.957100
H	-6.791729	-0.089018	-2.364651
H	-3.362007	2.456727	-1.805614
C	-2.015894	0.894467	1.657393
C	-3.284167	1.295926	2.101765
C	-1.010238	0.632975	2.600241
C	-3.543309	1.426294	3.465002
H	-4.076010	1.514741	1.390531
C	-1.273071	0.773970	3.961434
H	-0.020135	0.339405	2.263540
C	-2.539061	1.164588	4.396125
H	-4.529636	1.735804	3.798643
H	-0.485423	0.573744	4.682012
H	-2.743308	1.266740	5.458018
C	-1.163444	2.387619	-0.708138
C	-1.581514	3.551597	-0.050163
C	-0.430418	2.494479	-1.897332
C	-1.280192	4.803023	-0.585427
H	-2.137687	3.481430	0.880194
C	-0.139684	3.746623	-2.434595
H	-0.082117	1.591391	-2.393008
C	-0.565045	4.901740	-1.779025
H	-1.604509	5.701905	-0.068797
H	0.426964	3.820629	-3.358160
H	-0.333869	5.878445	-2.194275
H	0.859159	-3.554825	-0.198208
P	2.175274	-0.326304	-0.204430
C	2.906806	-0.948242	1.363780
C	3.998423	-1.957148	3.742008
C	4.089548	-0.407295	1.890436
C	2.271168	-1.988143	2.053443
C	2.816747	-2.492025	3.233801
C	4.631809	-0.911468	3.069891
H	4.586465	0.413448	1.380690
H	1.341611	-2.396831	1.667612
H	2.316045	-3.301643	3.757328
H	5.549299	-0.485524	3.466010
H	4.423507	-2.348777	4.661736
C	2.607373	1.471431	-0.089323
C	3.114870	4.113705	0.324052
N	1.974067	2.094783	0.912944
C	3.506355	2.112432	-0.942230
C	3.755675	3.467382	-0.724200
C	2.226402	3.390562	1.133524
H	4.001871	1.570393	-1.739978
H	4.450168	4.006993	-1.362544
H	3.295906	5.165742	0.522843
C	3.283834	-0.942014	-1.537384
C	4.864919	-1.837744	-3.675965
C	4.536143	-1.521069	-1.300230
C	2.828665	-0.830198	-2.860566
C	3.617017	-1.264673	-3.923033
C	5.318297	-1.968920	-2.365125
H	4.901245	-1.632995	-0.284211
H	1.844405	-0.408915	-3.054955
H	3.253221	-1.167446	-4.942157
H	6.285002	-2.422845	-2.166392
H	5.477059	-2.187280	-4.502297
C	-1.825790	-2.901188	-2.330949
H	-2.688224	-2.232198	-2.314137
H	-2.195939	-3.908595	-2.562184
H	-1.181037	-2.589573	-3.155877
C	-1.042677	-2.907994	-1.033554
H	0.880394	-3.151853	-1.985267
C	0.363009	-3.070154	-1.032350
C	-1.804855	-3.166053	0.198273
O	-2.999660	-2.862083	0.368696
H	-2.729412	-4.554880	2.253471
C	-1.814193	-3.980280	2.407702
H	-1.119931	-4.533279	3.039073
H	-2.061523	-3.017828	2.861887
O	-1.125139	-3.786408	1.164536
H	-3.488139	-1.456636	-0.206395
H	-5.073978	-3.006140	-0.877257
C	-5.813282	-2.202990	-0.880454
H	-6.263756	-2.174379	0.118492
H	-6.601421	-2.428594	-1.600308
C	1.540348	4.028399	2.307919
H	2.106418	3.835180	3.226844
H	0.544076	3.602393	2.441737
H	1.458970	5.111841	2.189646

TS7-8 (6Me)

SCF done: -2656.788746

Pd	0.057616	-0.352293	-0.368619
P	-1.868654	0.757035	-0.083991
C	-3.400244	0.338499	-1.072454
N	-3.895625	-0.925657	-0.978354
C	-4.016409	1.199665	-1.978199
C	-4.959375	-1.393140	-1.671694
C	-5.103958	0.758438	-2.727904
H	-5.584527	1.433511	-3.430271
C	-5.585442	-0.538528	-2.571524
H	-6.436330	-0.897317	-3.139457
H	-3.642266	2.211021	-2.079587
C	-2.541472	0.681698	1.627717

C	-3.899553	0.799920	1.955704
C	-1.600900	0.531833	2.658279
C	-4.308774	0.758790	3.287951
H	-4.647318	0.932247	1.178194
C	-2.012914	0.506774	3.989151
H	-0.546834	0.441025	2.404654
C	-3.367221	0.613857	4.305791
H	-5.363895	0.848532	3.530423
H	-1.274101	0.401199	4.778489
H	-3.688436	0.588334	5.343065
C	-1.751897	2.553959	-0.457543
C	-2.550464	3.518131	0.172752
C	-0.814243	2.958383	-1.417194
C	-2.420670	4.863868	-0.165145
H	-3.264309	3.223306	0.936271
C	-0.696361	4.303779	-1.761476
H	-0.166408	2.212442	-1.871647
C	-1.499066	5.257355	-1.136134
H	-3.037592	5.606087	0.333399
H	0.033816	4.607596	-2.505899
H	-1.400441	6.307292	-1.396804
H	1.153992	-3.782432	0.291863
P	2.385581	-0.196361	-0.182588
C	3.102076	-0.668764	1.440677
C	4.135259	-1.476489	3.918905
C	4.338726	-0.182092	1.887943
C	2.385321	-1.552741	2.256877
C	2.901657	-1.959354	3.486221
C	4.850723	-0.585154	3.119374
H	4.900686	0.518699	1.276827
H	1.413507	-1.912099	1.927219
H	2.337794	-2.647551	4.109951
H	5.809047	-0.200160	3.456331
H	4.536619	-1.788018	4.879034
C	3.024421	1.531310	-0.389382
C	3.800033	4.139289	-0.495658
N	2.508237	2.388276	0.498652
C	3.940149	1.908468	-1.373938
C	4.326889	3.247155	-1.421440
C	2.887775	3.671515	0.460739
H	4.343914	1.182082	-2.070393
H	5.040183	3.585371	-2.168338
H	4.088530	5.186023	-0.505284
C	3.351258	-1.161609	-1.419848
C	4.700913	-2.596817	-3.419506
C	4.544936	-1.833839	-1.128902
C	2.837024	-1.228037	-2.724839
C	3.511866	-1.931268	-3.720123
C	5.211471	-2.549826	-2.123430
H	4.954256	-1.805138	-0.123641
H	1.899500	-0.724781	-2.954688
H	3.106762	-1.966288	-4.727790
H	6.134037	-3.070702	-1.882890
H	5.224284	-3.153377	-4.191675
C	-1.329656	-3.272094	-2.117852
H	-1.742411	-2.267219	-2.251113
H	-2.152116	-3.989408	-2.211588
H	-0.626478	-3.452501	-2.933196
C	-0.634607	-3.413928	-0.792174
H	1.314417	-3.731226	-1.553343
C	0.681384	-3.656142	-0.674926
C	-1.489517	-3.312685	0.418227
O	-2.671925	-2.963965	0.396960
H	-2.596579	-4.181498	2.631788
C	-1.680504	-3.598684	2.744948
H	-1.053637	-4.019503	3.529620
H	-1.931527	-2.559600	2.968238
O	-0.890113	-3.673749	1.547083
H	-3.400568	-1.616460	-0.374441
C	2.275689	4.584963	1.484484
H	2.746225	5.571052	1.482042
H	2.369344	4.149769	2.483367
H	1.206201	4.711076	1.285353
C	-5.414459	-2.792120	-1.405381
H	-4.594129	-3.420118	-1.054114
H	-5.851056	-3.228833	-2.305687
H	-6.187560	-2.789713	-0.628016

TS1-2i+ (6Me)

SCF done: -2428.064197

Pd	-0.011328	-1.153811	0.421655
P	-1.942513	0.202519	0.059215
C	-3.120468	-0.993601	-0.754940
N	-2.874738	-2.292910	-0.525088
C	-4.194794	-0.589713	-1.542383
C	-3.667314	-3.256777	-1.025273
C	-5.030234	-1.571107	-2.078367
H	-5.877178	-1.289365	-2.697122
C	-4.767730	-2.909110	-1.817350
H	-5.398826	-3.690484	-2.227674
H	-4.371590	0.461882	-1.739794
C	-2.780685	0.664337	1.617086
C	-4.163383	0.890945	1.699024
C	-1.996812	0.781349	2.774251
C	-4.744032	1.238140	2.916159
H	-4.793052	0.790009	0.819988
C	-2.581693	1.133806	3.989106
H	-0.929793	0.576528	2.725076
C	-3.954721	1.362471	4.060417
H	-5.815141	1.407071	2.972746
H	-1.968448	1.218698	4.881283
H	-4.412726	1.629310	5.008060
C	-2.060195	1.662844	-1.043361
C	-2.641314	2.871348	-0.637097
C	-1.552043	1.549374	-2.348082
C	-2.726199	3.943173	-1.529052
H	-3.047498	2.971929	0.364876
C	-1.646075	2.618183	-3.235613
H	-1.104402	0.614268	-2.678330
C	-2.234303	3.817685	-2.827554
H	-3.199235	4.868539	-1.212412
H	-1.275177	2.511779	-4.251069
H	-2.320984	4.645994	-3.524693
H	-1.656647	-2.561797	0.255732
P	2.040344	-0.223157	0.008898
C	2.911993	0.297519	1.531175
C	4.216453	1.000516	3.906034
C	4.030897	1.149041	1.501505
C	2.449491	-0.186251	2.764593
C	3.103566	0.162261	3.945255
C	4.677579	1.495557	2.684713
H	4.406443	1.537244	0.557870
H	1.577051	-0.834631	2.794091
H	2.742868	-0.220863	4.895067
H	5.544608	2.148583	2.654097
H	4.725481	1.270766	4.826275
C	2.080927	1.387351	-0.931443
C	2.024253	3.913067	-2.105519
N	1.545075	2.474555	-0.317766
C	2.603846	1.564400	-2.203449
C	2.576731	2.833741	-2.787212
C	1.489744	3.724348	-0.834712
H	3.047158	0.719427	-2.717335
H	3.002836	2.980616	-3.775573
H	2.006819	4.904463	-2.543737
C	3.167820	-1.253083	-0.993099
C	4.782030	-2.872574	-2.601419
C	4.541038	-1.354928	-0.733580
C	2.605112	-1.982407	-2.054026
C	3.413699	-2.779459	-2.860751
C	5.340848	-2.167232	-1.536358
H	4.987197	-0.821626	0.099478

H	1.533835	-1.936112	-2.238532
H	2.974603	-3.338791	-3.681421
H	6.402464	-2.251306	-1.324696
H	5.409943	-3.503933	-3.222791
C	1.806331	-3.738785	1.302260
H	2.500133	-3.153205	1.911541
H	2.316251	-3.964829	0.358678
H	1.593518	-4.688481	1.804817
C	0.559049	-3.005608	1.027341
H	-1.366078	-3.756680	1.659983
C	-0.743058	-3.102235	1.051738
H	1.170636	2.340271	0.619136
C	0.847048	4.796013	-0.020495
H	1.203613	5.779215	-0.331166
H	1.052873	4.676574	1.047303
H	-0.239282	4.767766	-0.166873
C	-3.337975	-4.683376	-0.703277
H	-2.262166	-4.866453	-0.763685
H	-3.846229	-5.364841	-1.387595
H	-3.665178	-4.931506	0.313058

TS1L-2L+ (6Me)

SCF done: -2428.053858

Pd	-0.017737	1.222569	0.156954
P	1.813381	-0.288704	0.219795
C	3.208525	0.749175	-0.453108
N	2.868869	1.971995	-0.900844
C	4.521339	0.296432	-0.514897
C	3.772167	2.773120	-1.495348
C	5.488468	1.129381	-1.081247
H	6.525391	0.810412	-1.130901
C	5.107038	2.360432	-1.595223
H	5.832182	3.015138	-2.068231
H	4.785195	-0.681119	-0.126256
C	2.417179	-0.789321	1.870828
C	3.187210	-1.941611	2.080923
C	2.128822	0.059060	2.951056
C	3.664598	-2.234760	3.357056
H	3.407055	-2.615957	1.258252
C	2.613303	-0.237896	4.222809
H	1.526175	0.951746	2.795354
C	3.380718	-1.384971	4.426203
H	4.259535	-3.129214	3.515826
H	2.389434	0.423519	5.054479
H	3.755881	-1.617970	5.418190
C	1.873512	-1.815816	-0.801611
C	1.096186	-2.908560	-0.375064
C	2.619525	-1.933571	-1.983072
C	1.092118	-4.097284	-1.101441
H	0.517105	-2.842766	0.542687
C	2.613847	-3.129286	-2.704637
H	3.225934	-1.107113	-2.339234
C	1.856706	-4.213956	-2.264091
H	0.505362	-4.940056	-0.747884
H	3.216091	-3.214143	-3.604643
H	1.868715	-5.148332	-2.817359
H	1.598433	2.417518	-0.362375
P	-2.083730	0.200995	0.151554
C	-2.231985	-1.298150	1.186893
C	-2.437397	-3.483189	2.918941
C	-3.217485	-2.274672	0.976404
C	-1.354644	-1.423468	2.273338
C	-1.462524	-2.511093	3.138677
C	-3.312479	-3.364614	1.837840
H	-3.917407	-2.190118	0.150344
H	-0.591021	-0.669955	2.443697
H	-0.784199	-2.596338	3.982017
H	-4.075185	-4.118870	1.669280
H	-2.520020	-4.331895	3.591233
C	-2.570976	-0.424136	-1.536664
C	-3.032176	-1.414650	-4.093782
N	-1.572172	-0.876280	-2.337055
C	-3.864312	-0.455539	-2.036617
C	-4.093781	-0.958681	-3.319949
C	-1.735537	-1.367010	-3.588689
H	-4.678894	-0.083445	-1.425998
H	-5.105260	-0.992851	-3.714481
H	-3.193801	-1.801490	-5.093696
C	-3.529748	1.238656	0.566572
C	-5.673770	2.910547	1.220926
C	-4.310915	0.970527	1.697577
C	-3.823211	2.359097	-0.230370
C	-4.898251	3.182421	0.091532
C	-5.376709	1.810386	2.021758
H	-4.094128	0.112996	2.326205
H	-3.217237	2.585771	-1.105177
H	-5.127251	4.040289	-0.533714
H	-5.976290	1.598783	2.901791
H	-6.506140	3.559486	1.475576
C	1.640709	4.354661	0.862641
H	1.284076	4.695792	1.837839
H	1.658737	5.220066	0.193545
H	2.662074	3.986399	0.978553
C	0.709559	3.297013	0.329311
H	-1.520853	3.646383	0.450662
C	-0.577909	3.137166	0.311690
H	-0.623942	-0.826007	-1.956123
H	-0.806322	-2.409660	-5.199004
C	-0.523783	-1.785738	-4.350067
H	-0.000094	-0.905703	-4.742349
H	0.175536	-2.345203	-3.721976
H	3.700800	4.216194	-3.069459
C	3.319019	4.089013	-2.052175
H	3.710081	4.922211	-1.458881
H	2.230785	4.158268	-2.082172

Complex 7+ (6Me)

SCF done: -2657.146590

Pd	-0.043323	-0.953566	-0.466400
P	-1.633667	0.744373	-0.090019
C	-3.272662	0.680271	-0.998247
N	-3.998430	-0.466920	-0.917266
C	-3.788655	1.722034	-1.756723
C	-5.200035	-0.654897	-1.506802
C	-5.023122	1.569755	-2.395533
H	-5.427658	2.385265	-2.988033
C	-5.733482	0.385455	-2.267597
H	-6.694588	0.249236	-2.751054
H	-3.235209	2.648583	-1.843478
C	-2.227103	0.781956	1.645029
C	-3.425775	1.397718	2.037245
C	-1.425622	0.165120	2.616507
C	-3.806384	1.402539	3.377480
H	-4.066736	1.875431	1.300982
C	-1.806007	0.178381	3.957586
H	-0.511473	-0.338484	2.307977
C	-2.996482	0.796561	4.338551
H	-4.736600	1.879112	3.672159
H	-1.179493	-0.302072	4.703561
H	-3.297621	0.801185	5.381850
C	-1.139526	2.470270	-0.490151
C	-1.450492	3.571938	0.318700
C	-0.442956	2.677168	-1.691545
C	-1.082191	4.858847	-0.077076
H	-1.988155	3.430899	1.251455
C	-0.093709	3.965535	-2.091936
H	-0.188350	1.825691	-2.319308
C	-0.413242	5.058544	-1.284616
H	-1.337369	5.707981	0.550720
H	0.421645	4.117480	-3.036018
H	-0.147910	6.063648	-1.599391
H	0.710452	-3.522092	0.053128

P	2.221953	-0.442726	-0.218060
C	2.939643	-0.956327	1.391990
C	3.972389	-1.834293	3.846181
C	4.210420	-0.534319	1.823383
C	2.194141	-1.817231	2.211330
C	2.711275	-2.255908	3.429436
C	4.720198	-0.971488	3.043186
H	4.811966	0.126521	1.204014
H	1.210599	-2.147274	1.887593
H	2.130040	-2.930020	4.051450
H	5.705242	-0.645627	3.363886
H	4.375512	-2.177785	4.794124
C	2.811549	1.327265	-0.226967
C	3.488123	4.028681	-0.018176
N	2.498086	2.090610	0.852635
C	3.494644	1.951815	-1.264845
C	3.836796	3.298515	-1.153838
C	2.798273	3.403110	1.011084
H	3.774485	1.372067	-2.136744
H	4.391717	3.780327	-1.953812
H	3.754079	5.074703	0.081011
C	3.268787	-1.150030	-1.544337
C	4.740489	-2.216588	-3.671584
C	4.492163	-1.787493	-1.303699
C	2.778633	-1.068640	-2.858520
C	3.519007	-1.588155	-3.917801
C	5.219748	-2.321405	-2.366926
H	4.873165	-1.886664	-0.292547
H	1.810311	-0.609347	-3.047945
H	3.136467	-1.517299	-4.931725
H	6.162637	-2.823525	-2.172333
H	5.311777	-2.634112	-4.495139
C	-1.766545	-2.815070	-2.301160
H	-2.580253	-2.090851	-2.362925
H	-2.187690	-3.802326	-2.528240
H	-1.045154	-2.575947	-3.085321
C	-1.082502	-2.839219	-0.949209
H	0.884211	-3.206317	-1.749012
C	0.298040	-3.071290	-0.843714
C	-1.962594	-3.065830	0.223353
O	-3.140538	-2.689301	0.289519
H	-3.113594	-4.549671	2.092286
C	-2.224551	-3.984359	2.376397
H	-1.602988	-4.568282	3.053105
H	-2.523777	-3.040742	2.837396
O	-1.400799	-3.738594	1.220781
H	-3.603670	-1.304586	-0.402077
H	2.022801	1.624628	1.622642
C	2.359598	4.070361	2.272513
H	2.628395	3.478480	3.153541
H	1.272206	4.207081	2.271602
H	2.824090	5.052306	2.368210
C	-5.899789	-1.958385	-1.297250
H	-5.210008	-2.745689	-0.990633
H	-6.417837	-2.261822	-2.209777
H	-6.656940	-1.848870	-0.511812

Complex 8+ (6Me)

SCF done: -2311.450587

Pd	0.062601	-0.212770	0.022480
P	-2.181252	0.224069	0.012066
C	-3.058394	-1.085258	-0.982550
N	-3.295501	-2.277325	-0.375180
C	-3.391286	-0.978800	-2.327579
C	-3.818200	-3.379011	-0.970964
C	-3.938207	-2.076956	-2.989622
H	-4.208936	-1.993478	-4.038182
C	-4.146333	-3.280479	-2.316361
H	-4.569427	-4.140423	-2.822745
H	-3.229259	-0.038169	-2.841236
C	-3.097245	0.106068	1.590390
C	-4.496113	-0.030922	1.658001
C	-2.355793	0.168601	2.780171
C	-5.133675	-0.094278	2.894333
H	-5.090963	-0.082227	0.749077
C	-3.000171	0.109635	4.014567
H	-1.273362	0.259471	2.726415
C	-4.386825	-0.020986	4.071881
H	-6.213923	-0.195465	2.940179
H	-2.420065	0.160979	4.930999
H	-4.888407	-0.068883	5.033767
C	-2.687410	1.760679	-0.843283
C	-3.799795	2.525921	-0.469819
C	-1.889216	2.177785	-1.921977
C	-4.117521	3.682435	-1.180404
H	-4.410269	2.236034	0.379148
C	-2.224512	3.324407	-2.639119
H	-1.004948	1.602070	-2.190386
C	-3.339011	4.077426	-2.268032
H	-4.977563	4.274920	-0.883093
H	-1.611567	3.635115	-3.480216
H	-3.595977	4.976094	-2.820793
H	-3.083983	-2.336428	0.619457
P	2.372478	-0.341531	-0.020789
C	3.222705	-1.295872	1.285462
C	4.430655	-2.674752	3.394046
C	4.576739	-1.657359	1.206776
C	2.479219	-1.637844	2.424131
C	3.084357	-2.322754	3.475874
C	5.173979	-2.345290	2.259125
H	5.158582	-1.427751	0.318486
H	1.426009	-1.369759	2.474271
H	2.504443	-2.588176	4.354721
H	6.219783	-2.629711	2.192206
H	4.901424	-3.213271	4.211070
C	3.030945	1.379440	0.293863
C	3.618460	4.018959	0.920577
N	2.075553	2.286599	0.606353
C	4.351558	1.801860	0.284521
C	4.642695	3.130714	0.599536
C	2.296847	3.582048	0.924109
H	5.139165	1.102099	0.031279
H	5.672785	3.475122	0.594707
H	3.833925	5.052614	1.167630
C	3.180035	-0.791507	-1.598555
C	4.205040	-1.565837	-4.084739
C	3.460401	-2.141399	-1.858144
C	3.397794	0.162875	-2.602477
C	3.914779	-0.224716	-3.836529
C	3.973798	-2.521591	-3.096271
H	3.291231	-2.895163	-1.094243
H	3.170040	1.211681	-2.430452
H	4.092608	0.522623	-4.604060
H	4.198417	-3.567020	-3.285220
H	4.610663	-1.865022	-5.046366
H	1.109012	1.903087	0.581059
C	-3.996854	-4.604074	-0.136135
H	-4.557543	-4.384412	0.778646
H	-4.539701	-5.369231	-0.691694
H	-3.025767	-5.021614	0.153740
C	1.121612	4.435476	1.271803
H	0.274016	4.240694	0.608290
H	0.798956	4.237696	2.300765
H	1.381863	5.492481	1.201678

TS1-2i (4NMe$_2$)

SCF done: -2617.002141

Pd	-0.082435	-1.513376	-0.571114
P	-1.681911	-0.025863	0.343683
C	-3.243715	-0.482025	-0.574066
N	-3.178759	-1.640957	-1.251361
C	-4.376998	0.310430	-0.585993

C	-4.249163	-2.045416	-1.950150
C	-5.524697	-0.093060	-1.320293
C	-5.423094	-1.326326	-2.014705
H	-6.242675	-1.713118	-2.606351
H	-4.367153	1.245046	-0.039539
H	-4.145454	-2.984742	-2.486920
C	-2.093573	-0.349212	2.101166
C	-3.341030	-0.820254	2.529781
C	-1.066715	-0.158638	3.040610
C	-3.560886	-1.091651	3.879968
H	-4.144778	-0.980717	1.818209
C	-1.300086	-0.421047	4.388145
H	-0.094251	0.200301	2.708028
C	-2.543973	-0.890524	4.810629
H	-4.530251	-1.461403	4.202063
H	-0.502289	-0.266867	5.109200
H	-2.718665	-1.102852	5.861507
C	-1.697935	1.796928	0.158338
C	-2.217995	2.651002	1.138012
C	-1.203101	2.337551	-1.035813
C	-2.251915	4.028076	0.917725
H	-2.588359	2.241827	2.073699
C	-1.244475	3.711850	-1.254051
H	-0.781923	1.678767	-1.791571
C	-1.770211	4.559024	-0.277784
H	-2.654686	4.685674	1.683166
H	-0.860854	4.122965	-2.183532
H	-1.798838	5.631736	-0.446905
H	-1.938352	-2.275900	-1.262745
P	2.022792	-0.724210	-0.094202
C	2.769852	-1.545274	1.363785
C	3.898475	-2.854660	3.566099
C	3.850869	-0.973573	2.050551
C	2.249815	-2.769177	1.803257
C	2.815335	-3.421953	2.897617
C	4.413023	-1.628724	3.143381
H	4.248229	-0.012190	1.736961
H	1.389594	-3.198013	1.295218
H	2.402289	-4.369206	3.232221
H	5.250069	-1.178526	3.669397
H	4.336458	-3.361677	4.421091
C	2.215945	1.066097	0.331783
C	2.421333	3.642938	1.168016
N	1.446822	1.444388	1.361520
C	3.100046	1.900980	-0.338552
C	3.226108	3.251503	0.074408
C	1.572182	2.717043	1.752489
H	3.691660	1.509654	-1.155716
H	0.947279	3.021219	2.589982
H	2.451074	4.651697	1.560817
C	3.209468	-0.968965	-1.476369
C	4.928239	-1.278710	-3.670004
C	4.531992	-1.387916	-1.286364
C	2.755404	-0.715288	-2.779703
C	3.611407	-0.861456	-3.868661
C	5.383758	-1.544512	-2.380042
H	4.897075	-1.603817	-0.287009
H	1.720912	-0.419570	-2.939458
H	3.247071	-0.663058	-4.872724
H	6.404783	-1.879744	-2.221183
H	5.593466	-1.404937	-4.519369
C	1.517909	-4.065381	-1.878719
H	2.162569	-4.263497	-1.016966
H	2.126012	-3.530515	-2.615070
H	1.208456	-5.022334	-2.313813
C	0.342569	-3.256905	-1.492611
H	-1.658527	-4.038337	-1.808964
C	-0.959385	-3.255872	-1.517461
N	4.080500	4.114104	-0.544272
N	-6.649622	0.660834	-1.355627
C	-6.706516	1.924481	-0.637419
H	-5.950259	2.630073	-1.001634
H	-6.561460	1.780958	0.439969
H	-7.687017	2.375309	-0.785906
C	-7.801005	0.219776	-2.127684
H	-8.600490	0.952980	-2.027931
H	-8.181148	-0.743691	-1.767661
H	-7.559514	0.126161	-3.193366
C	4.904380	3.658317	-1.648453
H	5.495268	4.493917	-2.023282
H	4.294027	3.280822	-2.478164
H	5.597922	2.864149	-1.342510
C	4.212518	5.475290	-0.058594
H	4.564452	5.504979	0.980676
H	3.261071	6.018665	-0.116889
H	4.938441	6.007045	-0.673427

TS1L-2L (4NMe$_2$)

SCF done: -2616.996196

Pd	-0.097342	-1.434810	-0.603721
P	-1.611229	0.091230	0.337264
C	-3.207141	-0.348588	-0.525681
N	-3.188282	-1.506596	-1.213271
C	-4.321735	0.468465	-0.489298
C	-4.300095	-1.873092	-1.873949
C	-5.505707	0.103789	-1.183453
C	-5.456639	-1.124780	-1.889731
H	-6.304918	-1.489538	-2.454395
H	-4.267840	1.396864	0.065097
H	-4.249886	-2.808874	-2.419745
C	-1.979892	-0.170342	2.113854
C	-3.215546	-0.626347	2.590004
C	-0.928111	0.048996	3.018595
C	-3.399587	-0.853239	3.953722
H	-4.037501	-0.809889	1.905330
C	-1.125778	-0.168936	4.379614
H	0.036064	0.392820	2.647702
C	-2.358332	-0.622529	4.849981
H	-4.360011	-1.211520	4.313387
H	-0.308852	0.006892	5.073722
H	-2.505172	-0.800001	5.911529
C	-1.578750	1.907140	0.097336
C	-2.046751	2.805979	1.063002
C	-1.097037	2.395544	-1.124487
C	-2.042358	4.176355	0.801825
H	-2.404705	2.437154	2.020027
C	-1.100870	3.763344	-1.383404
H	-0.713902	1.701491	-1.868936
C	-1.574732	4.655628	-0.420863
H	-2.403921	4.869216	1.556672
H	-0.727343	4.134052	-2.333737
H	-1.573278	5.723244	-0.621641
H	-1.950214	-2.147204	-1.264003
P	2.048944	-0.793325	-0.075916
C	2.651817	-1.606936	1.450876
C	3.576773	-2.938936	3.733523
C	3.640364	-1.025755	2.257842
C	2.124660	-2.855875	1.805554
C	2.589685	-3.519617	2.938919
C	4.098941	-1.691484	3.392683
H	4.049564	-0.051940	2.005094
H	1.342045	-3.300593	1.196370
H	2.173493	-4.487005	3.204941
H	4.864127	-1.233011	4.012687
H	3.935172	-3.454195	4.620082
C	2.369738	0.997900	0.253237
C	2.730552	3.612394	0.899392
N	1.597914	1.506299	1.224485
C	3.331738	1.715921	-0.444010
C	3.539855	3.082966	-0.131020
C	1.801663	2.794055	1.522356
H	3.919316	1.222968	-1.207310

H	1.175063	3.204559	2.311806
H	2.817878	4.644942	1.214132
C	3.272283	-1.231244	-1.375178
C	5.081695	-1.828834	-3.429744
C	4.559876	-1.691743	-1.072566
C	2.898475	-1.080949	-2.718700
C	3.801085	-1.370026	-3.739477
C	5.456874	-1.992552	-2.097314
H	4.860418	-1.826089	-0.037914
H	1.890771	-0.751913	-2.961281
H	3.499758	-1.250941	-4.776394
H	6.449466	-2.359279	-1.851670
H	5.781752	-2.066965	-4.225471
C	-1.915759	-4.249511	-2.102592
H	-2.374960	-3.944842	-3.050101
H	-2.717544	-4.430069	-1.379347
H	-1.391947	-5.193086	-2.275682
C	-0.954363	-3.204513	-1.609957
H	1.230974	-3.684328	-1.803092
C	0.340163	-3.133619	-1.536299
N	-6.611200	0.885099	-1.172535
N	4.471421	3.833414	-0.782982
C	-7.801015	0.477312	-1.903893
H	-8.189635	-0.479943	-1.536660
H	-7.601555	0.387156	-2.978442
H	-8.578777	1.227869	-1.768461
C	-6.609392	2.145799	-0.446285
H	-6.441767	1.991695	0.626375
H	-7.578085	2.628856	-0.568202
H	-5.840277	2.828187	-0.826864
C	5.286343	3.238756	-1.826407
H	5.903834	2.416145	-1.443528
H	5.954301	3.996851	-2.235055
H	4.671893	2.853096	-2.649590
C	4.667896	5.223625	-0.416259
H	4.980759	5.327933	0.630587
H	3.754490	5.813761	-0.563907
H	5.448667	5.653505	-1.043532

Complex 7 ($4NMe_2$)

SCF done: -2846.073720

Pd	-0.086014	-1.197252	-0.731167
P	-1.591707	0.212067	0.367899
C	-3.349933	0.232360	-0.286476
N	-3.912868	-0.967684	-0.586437
C	-4.083366	1.380260	-0.503047
C	-5.165701	-1.061127	-1.073329
C	-5.407885	1.333613	-1.023996
C	-5.941526	0.044322	-1.299632
H	-6.939066	-0.090593	-1.694776
H	-3.624154	2.327109	-0.256044
H	-5.507854	-2.068955	-1.281546
C	-1.890997	-0.214735	2.132272
C	-3.162645	-0.334622	2.708207
C	-0.753007	-0.435269	2.924279
C	-3.295401	-0.682385	4.052195
H	-4.057661	-0.154534	2.120380
C	-0.894376	-0.769697	4.268920
H	0.237380	-0.308628	2.493014
C	-2.162831	-0.902096	4.833651
H	-4.286194	-0.777496	4.487521
H	-0.007321	-0.931903	4.874578
H	-2.268776	-1.172360	5.880435
C	-1.269712	2.021009	0.377423
C	-1.648818	2.853048	1.438643
C	-0.639378	2.578667	-0.742123
C	-1.410802	4.225251	1.371277
H	-2.121517	2.426321	2.318888
C	-0.410293	3.951236	-0.810207
H	-0.317674	1.928514	-1.552297
C	-0.796911	4.775868	0.246152
H	-1.700800	4.863921	2.201144
H	0.080386	4.375040	-1.681776
H	-0.611167	5.845175	0.197309
H	0.909384	-3.623729	-1.393258
P	2.144074	-0.607082	-0.239309
C	2.900175	-1.701226	1.030861
C	4.017838	-3.419760	2.944171
C	4.077986	-1.345915	1.705363
C	2.283338	-2.920205	1.338696
C	2.842201	-3.776037	2.287205
C	4.633023	-2.201753	2.653575
H	4.558926	-0.394835	1.494251
H	1.356858	-3.191721	0.840680
H	2.354769	-4.719533	2.516177
H	5.545410	-1.915366	3.169179
H	4.451946	-4.085089	3.685137
C	2.574967	1.059538	0.443548
C	3.088279	3.434867	1.662565
N	1.904383	1.333984	1.572538
C	3.502978	1.909503	-0.144118
C	3.785141	3.157214	0.465487
C	2.183039	2.505492	2.152152
H	4.010386	1.601952	-1.049463
H	1.644003	2.721503	3.072980
C	3.240509	-0.758136	-1.711379
C	4.798735	-0.928029	-4.040555
C	4.463352	-1.439297	-1.699784
C	2.803547	-0.172563	-2.910309
C	3.580669	-0.247289	-4.063356
C	5.233898	-1.525967	-2.859979
H	4.813371	-1.910708	-0.786888
H	1.842381	0.336517	-2.939139
H	3.230146	0.213273	-4.982986
H	6.176643	-2.065519	-2.838456
H	5.400576	-0.998808	-4.942074
C	-1.859297	-2.320309	-3.074151
H	-2.748539	-1.758856	-2.782300
H	-2.195131	-3.174188	-3.677057
H	-1.253626	-1.677559	-3.717239
C	-1.038115	-2.795567	-1.891856
H	0.865617	-2.563653	-2.886749
C	0.372063	-2.878002	-1.970165
C	-1.759301	-3.567454	-0.866398
O	-2.964465	-3.430261	-0.601296
H	-2.556559	-5.705589	0.473419
C	-1.676793	-5.177438	0.846178
H	-0.938965	-5.884949	1.222788
H	-1.979065	-4.483876	1.634834
O	-1.021869	-4.473808	-0.217158
H	-3.393017	-1.884002	-0.522217
N	-6.121475	2.457717	-1.237153
C	-7.482056	2.376305	-1.753055
H	-8.127619	1.795980	-1.084312
H	-7.505763	1.923441	-2.751000
H	-7.895437	3.380835	-1.828743
C	-5.536968	3.764740	-0.963636
H	-5.292759	3.880276	0.098342
H	-6.255105	4.538107	-1.232025
H	-4.627941	3.925384	-1.553457
H	3.244971	4.356478	2.209619
N	4.685443	4.031320	-0.071315
C	5.421791	3.673291	-1.268802
H	6.059231	4.508114	-1.560458
H	4.746237	3.459971	-2.106085
H	6.062367	2.794871	-1.113262
C	5.002121	5.262846	0.626345
H	5.434498	5.074835	1.618179
H	4.112874	5.892835	0.752726
H	5.729558	5.828688	0.044165

TS7-8 ($4NMe_2$)

SCF done: -2846.044537

Pd	0.016172	-0.562433	-0.313832
P	-1.878155	0.291659	0.537572
C	-3.483910	0.313341	-0.423580
N	-3.917466	-0.882827	-0.907739
C	-4.200138	1.449993	-0.737284
C	-5.028391	-0.986709	-1.664035
C	-5.373786	1.395083	-1.540197
C	-5.779370	0.107961	-1.996963
H	-6.660058	-0.031141	-2.608875
H	-3.844136	2.391389	-0.341796
H	-5.279250	-1.988768	-1.993308
C	-2.441474	-0.530683	2.085866
C	-3.778464	-0.606305	2.500591
C	-1.442179	-1.091277	2.895931
C	-4.109749	-1.237630	3.698956
H	-4.569030	-0.170585	1.895139
C	-1.776606	-1.708613	4.099372
H	-0.404577	-1.033515	2.574391
C	-3.110314	-1.787669	4.500182
H	-5.149617	-1.294869	4.008372
H	-0.992991	-2.130834	4.722057
H	-3.370708	-2.275387	5.435219
C	-1.759510	2.074411	0.978316
C	-2.478468	2.649410	2.035209
C	-0.899516	2.876625	0.216582
C	-2.349881	4.009693	2.311678
H	-3.125428	2.033269	2.653170
C	-0.783492	4.238499	0.487609
H	-0.305000	2.415816	-0.569059
C	-1.508192	4.806300	1.534946
H	-2.901105	4.445371	3.140437
H	-0.110992	4.851029	-0.106073
H	-1.406515	5.865102	1.756331
H	1.060485	-3.781380	-1.429697
P	2.342067	-0.496249	-0.152868
C	3.100164	-1.695673	1.015984
C	4.197056	-3.596448	2.762357
C	4.337705	-1.464302	1.632563
C	2.413956	-2.883522	1.298183
C	2.961983	-3.831461	2.160977
C	4.881434	-2.409905	2.499472
H	4.873850	-0.538754	1.442024
H	1.439275	-3.054690	0.847556
H	2.420935	-4.750237	2.370220
H	5.839740	-2.217618	2.973840
H	4.622585	-4.331374	3.439799
C	2.993113	1.114756	0.492025
C	3.817948	3.446488	1.619648
N	2.456222	1.452331	1.673341
C	3.935945	1.874410	-0.190127
C	4.378627	3.097248	0.371337
C	2.886526	2.600155	2.204738
H	4.329050	1.519522	-1.133862
H	2.455517	2.868192	3.168056
H	4.100189	4.357974	2.132191
C	3.273407	-0.743234	-1.726077
C	4.558725	-1.049405	-4.204278
C	4.463416	-1.475070	-1.824507
C	2.731584	-0.174120	-2.890007
C	3.374268	-0.316637	-4.117817
C	5.097776	-1.629863	-3.057519
H	4.893813	-1.931443	-0.938210
H	1.795527	0.377800	-2.826058
H	2.945865	0.134695	-5.008782
H	6.016575	-2.206479	-3.120083
H	5.055516	-1.171897	-5.162600
C	-1.591671	-2.371566	-3.224802
H	-2.006931	-1.428718	-2.855614
H	-2.425074	-2.986387	-3.580553
H	-0.947106	-2.140716	-4.075361
C	-0.808344	-3.085663	-2.158329
H	1.108571	-2.833003	-3.020119
C	0.524799	-3.241700	-2.201415
C	-1.591083	-3.638466	-1.023520
O	-2.763194	-3.342072	-0.790008
H	-2.567626	-5.533954	0.518945
C	-1.641250	-5.058564	0.847227
H	-0.968922	-5.793519	1.287334
H	-1.871232	-4.267925	1.564759
O	-0.930308	-4.519350	-0.278594
H	-3.377126	-1.757189	-0.754932
N	5.300474	3.884202	-0.258123
C	5.764682	5.102707	0.375919
H	6.491385	5.591269	-0.273391
H	6.252599	4.903603	1.339330
H	4.941495	5.808008	0.547782
C	5.871101	3.465008	-1.523442
H	6.564925	4.229069	-1.874610
H	5.098230	3.335201	-2.291546
H	6.424991	2.521060	-1.432933
N	-6.073143	2.506767	-1.844266
C	-5.619179	3.811707	-1.378587
H	-4.618234	4.043480	-1.758817
H	-5.600223	3.861079	-0.284264
H	-6.304829	4.576350	-1.740503
C	-7.281452	2.416645	-2.653913
H	-8.035945	1.782886	-2.174454
H	-7.065930	2.019227	-3.652422
H	-7.706508	3.412117	-2.772616

TS1-2i+ (4NMe$_2$)

SCF done: -2617.339645

Pd	-0.078753	-1.387421	-0.493931
P	-1.887743	-0.125729	0.487157
C	-3.226369	-0.231676	-0.802137
N	-3.073424	-1.242804	-1.671028
C	-4.300197	0.640394	-0.848568
C	-4.013164	-1.420154	-2.613009
C	-5.305725	0.474018	-1.843752
C	-5.120802	-0.610603	-2.741194
H	-5.829415	-0.816220	-3.532994
H	-4.363445	1.446500	-0.128887
H	-3.854601	-2.248839	-3.298270
C	-2.560627	-0.993561	1.949228
C	-3.911934	-0.915687	2.317350
C	-1.678297	-1.758334	2.726020
C	-4.367673	-1.590921	3.446259
H	-4.610990	-0.339523	1.718828
C	-2.138268	-2.425786	3.859851
H	-0.633699	-1.839263	2.434766
C	-3.482222	-2.343694	4.219170
H	-5.416365	-1.533167	3.721987
H	-1.449586	-3.016175	4.456704
H	-3.842861	-2.870358	5.097616
C	-1.903745	1.658112	0.935668
C	-2.078668	2.084343	2.259954
C	-1.699394	2.617911	-0.071626
C	-2.069619	3.447848	2.567197
H	-2.249316	1.356827	3.048036
C	-1.703068	3.975404	0.238134
H	-1.560361	2.303792	-1.103507
C	-1.891469	4.393864	1.558397
H	-2.225957	3.766744	3.593771
H	-1.568784	4.708786	-0.551917
H	-1.908011	5.453503	1.796570
H	-1.836948	-2.082536	-1.511860
P	2.080903	-0.683096	-0.183680
C	2.882311	-1.487714	1.252515
C	4.068410	-2.831554	3.402551
C	4.025887	-0.961482	1.872863
C	2.334931	-2.689609	1.726732

C	2.930750	-3.359230	2.793874
C	4.612925	-1.632096	2.942912
H	4.461983	-0.029091	1.526196
H	1.441881	-3.096679	1.258503
H	2.503976	-4.291815	3.150642
H	5.496881	-1.218160	3.418710
H	4.529669	-3.352027	4.236409
C	2.357912	1.115975	0.213099
C	2.614279	3.753029	1.055991
N	1.451522	1.691259	1.046582
C	3.418615	1.860940	-0.240620
C	3.597438	3.221053	0.167316
C	1.566876	2.974581	1.459618
H	4.124450	1.384706	-0.908518
H	0.777275	3.340246	2.105670
H	2.664048	4.772968	1.411962
C	3.186994	-0.892527	-1.624439
C	4.771477	-1.200809	-3.906936
C	4.470454	-1.443403	-1.519016
C	2.697253	-0.506821	-2.882846
C	3.491371	-0.653101	-4.016727
C	5.256534	-1.597507	-2.661927
H	4.852332	-1.766758	-0.555459
H	1.688934	-0.109065	-2.975752
H	3.107227	-0.354728	-4.987682
H	6.246336	-2.036188	-2.577274
H	5.384839	-1.328115	-4.793958
C	1.463149	-3.892457	-1.945658
H	2.164238	-4.057298	-1.122945
H	2.009682	-3.373472	-2.740765
H	1.135355	-4.860862	-2.339059
C	0.298275	-3.092504	-1.527661
H	-1.688664	-3.917906	-1.674554
C	-1.006282	-3.078411	-1.541986
H	0.623700	1.162476	1.307200
N	-6.371074	1.300547	-1.927278
N	4.635700	3.953256	-0.257769
C	5.609104	3.392540	-1.193252
H	6.331289	4.162614	-1.457483
H	5.122076	3.055683	-2.113814
H	6.153513	2.554559	-0.744638
C	4.812493	5.327875	0.209290
H	5.746396	5.721144	-0.187661
H	4.868486	5.367207	1.301741
H	3.996905	5.972441	-0.135949
C	-6.527709	2.397418	-0.983978
H	-5.677639	3.088090	-1.028214
H	-6.635321	2.033170	0.044991
H	-7.426213	2.959169	-1.234714
C	-7.388365	1.083735	-2.949201
H	-7.863304	0.102172	-2.839454
H	-6.965070	1.163266	-3.956899
H	-8.161832	1.843711	-2.849684

TS1L-2L+ ($4NMe_2$)

SCF done: -2617.335484

Pd	-0.036588	-1.012647	-1.016899
P	-1.784376	-0.134670	0.334843
C	-3.123221	0.229529	-0.907835
N	-2.847788	-0.168964	-2.162466
C	-4.317412	0.831587	-0.556766
C	-3.773695	0.057392	-3.111906
C	-5.317343	1.063885	-1.542991
C	-4.986828	0.659298	-2.864064
H	-5.674870	0.801414	-3.687327
H	-4.485586	1.114912	0.474452
H	-3.519902	-0.263485	-4.117435
C	-2.585939	-1.297761	1.497115
C	-3.379466	-0.878118	2.573766
C	-2.445628	-2.668850	1.235916
C	-4.018807	-1.820090	3.376773
H	-3.491756	0.178962	2.796839
C	-3.093405	-3.606083	2.038247
H	-1.832923	-3.001198	0.400193
C	-3.878484	-3.182254	3.109827
H	-4.627821	-1.489660	4.213049
H	-2.982789	-4.665687	1.827765
H	-4.379937	-3.912450	3.737931
C	-1.574936	1.435815	1.264135
C	-1.002285	1.394681	2.548485
C	-1.865133	2.684560	0.689666
C	-0.763204	2.573514	3.252545
H	-0.759075	0.439709	3.006044
C	-1.623777	3.861567	1.401447
H	-2.303478	2.742190	-0.302148
C	-1.079735	3.808769	2.685177
H	-0.340641	2.524651	4.251742
H	-1.881413	4.818813	0.956516
H	-0.910693	4.724371	3.244291
H	-1.619034	-0.978826	-2.323268
P	2.026770	-0.720883	-0.043625
C	2.129371	-1.074203	1.747122
C	2.265751	-1.758050	4.454918
C	3.141001	-0.540127	2.560041
C	1.189461	-1.953437	2.301794
C	1.262270	-2.296629	3.651098
C	3.202949	-0.879208	3.908956
H	3.883592	0.134939	2.144184
H	0.404199	-2.370308	1.677926
H	0.534771	-2.984445	4.071207
H	3.986889	-0.462296	4.534120
H	2.321432	-2.024318	5.506218
C	2.589531	1.054123	-0.119018
C	3.196534	3.770707	-0.130986
N	1.652647	1.997486	0.175971
C	3.864292	1.454526	-0.435115
C	4.226395	2.838862	-0.461596
C	1.945046	3.318774	0.177656
H	4.592416	0.689044	-0.666983
H	1.128449	3.982984	0.434187
H	3.375794	4.837178	-0.123811
C	3.438218	-1.596264	-0.811055
C	5.503512	-3.000776	-2.073439
C	4.188137	-2.538845	-0.096811
C	3.724661	-1.369183	-2.168648
C	4.760099	-2.060943	-2.790924
C	5.214341	-3.239245	-0.732016
H	3.974155	-2.732445	0.949321
H	3.137893	-0.652794	-2.739318
H	4.978383	-1.877616	-3.838994
H	5.786940	-3.973190	-0.173101
H	6.301850	-3.549880	-2.563522
C	-1.737135	-2.627628	-3.826419
H	-1.305306	-3.563480	-4.187489
H	-1.939983	-1.992369	-4.695288
H	-2.690240	-2.843489	-3.336511
C	-0.779900	-1.945026	-2.887514
H	1.402404	-2.502176	-2.989588
C	0.489603	-2.043185	-2.638252
H	0.702803	1.707411	0.402445
N	5.466851	3.235235	-0.774148
N	-6.502768	1.634290	-1.241670
C	-6.814681	2.001675	0.132540
H	-7.818491	2.421754	0.170688
H	-6.119382	2.759296	0.512908
H	-6.789696	1.129595	0.796413
C	-7.500975	1.845650	-2.283892
H	-8.371863	2.334446	-1.850000
H	-7.829034	0.896782	-2.723720
H	-7.114677	2.492346	-3.079408
C	5.815271	4.655828	-0.761176
H	5.638362	5.095513	0.225639

H	5.244247	5.210210	-1.513551
H	6.873368	4.764392	-0.991393
C	6.494434	2.257410	-1.128645
H	6.175775	1.641052	-1.974990
H	6.735561	1.608285	-0.279795
H	7.400525	2.785114	-1.420116

Complex 7+ ($4NMe_2$)

SCF done: -2846.424099

Pd	-0.059874	-1.006811	-0.695930
P	-1.769653	0.237844	0.346927
C	-3.494146	0.251482	-0.388057
N	-4.024910	-0.958023	-0.705948
C	-4.241195	1.388992	-0.602098
C	-5.271544	-1.070577	-1.210965
C	-5.560368	1.321955	-1.147932
C	-6.062289	0.021828	-1.440006
H	-7.051992	-0.129734	-1.848532
H	-3.810291	2.343698	-0.335331
H	-5.597460	-2.081613	-1.429416
C	-2.149856	-0.316843	2.054256
C	-3.367060	-0.043657	2.697812
C	-1.160244	-1.035410	2.740319
C	-3.583011	-0.477550	4.003688
H	-4.150301	0.505965	2.182972
C	-1.377155	-1.459190	4.050248
H	-0.223363	-1.271543	2.241495
C	-2.588201	-1.182442	4.682331
H	-4.529709	-0.266324	4.492052
H	-0.602625	-2.013670	4.571804
H	-2.761101	-1.519774	5.699948
C	-1.488908	2.056026	0.481890
C	-1.696177	2.782236	1.663456
C	-1.039954	2.732094	-0.666146
C	-1.473501	4.161752	1.689615
H	-2.042473	2.275484	2.559551
C	-0.835089	4.109656	-0.640410
H	-0.854138	2.173905	-1.581411
C	-1.053163	4.827589	0.538151
H	-1.646935	4.715984	2.607950
H	-0.504228	4.623543	-1.538496
H	-0.897256	5.902457	0.557218
H	0.975813	-3.434493	-1.387446
P	2.191080	-0.553472	-0.227234
C	2.787297	-1.502038	1.231044
C	3.630702	-3.079207	3.390281
C	3.888911	-1.113665	2.007715
C	2.111904	-2.689864	1.551808
C	2.537702	-3.475582	2.621161
C	4.303159	-1.896676	3.083332
H	4.431856	-0.202262	1.775819
H	1.255421	-3.000876	0.959148
H	2.014896	-4.398671	2.853437
H	5.155833	-1.584859	3.679265
H	3.959714	-3.689967	4.225671
C	2.768784	1.163597	0.223932
C	3.390785	3.739491	1.078923
N	1.913842	1.890879	0.992419
C	3.964152	1.726255	-0.154646
C	4.330072	3.045524	0.256551
C	2.208868	3.141870	1.413945
H	4.628698	1.132184	-0.768004
H	1.451369	3.636479	2.009764
H	3.581865	4.741625	1.437681
C	3.369829	-0.933699	-1.580351
C	5.060965	-1.501885	-3.737560
C	4.486392	-1.759404	-1.401924
C	3.101369	-0.402225	-2.852513
C	3.949057	-0.677265	-3.921795
C	5.324643	-2.043564	-2.481442
H	4.699364	-2.190544	-0.428565
H	2.221272	0.218850	-3.007327
H	3.735280	-0.261852	-4.902332
H	6.182420	-2.693941	-2.337713
H	5.713506	-1.728692	-4.575406
C	-1.779069	-2.131090	-3.085410
H	-2.661153	-1.561491	-2.790744
H	-2.122999	-2.974799	-3.696440
H	-1.161891	-1.491792	-3.720624
C	-0.968247	-2.636227	-1.908766
H	0.938850	-2.346377	-2.865731
C	0.430703	-2.700795	-1.972793
C	-1.697701	-3.480288	-0.928596
O	-2.899607	-3.359836	-0.668619
H	-2.465720	-5.784206	0.125549
C	-1.631797	-5.266895	0.602908
H	-0.880459	-5.981588	0.934861
H	-2.004280	-4.675807	1.442419
O	-0.958974	-4.422216	-0.348526
H	-3.479729	-1.855192	-0.628617
H	0.997330	1.499810	1.194769
N	-6.292276	2.427943	-1.365090
N	5.496822	3.597972	-0.105690
C	5.860703	4.934659	0.360702
H	6.860898	5.175234	0.005392
H	5.871996	4.981111	1.454502
H	5.170644	5.691993	-0.026925
C	6.424409	2.871851	-0.971058
H	7.276182	3.511596	-1.194182
H	5.948409	2.599267	-1.918317
H	6.797695	1.965503	-0.482103
C	-5.746045	3.748793	-1.073890
H	-4.815639	3.921890	-1.624909
H	-5.556877	3.876654	-0.001973
H	-6.464133	4.506337	-1.382897
C	-7.650954	2.320357	-1.892153
H	-8.285672	1.721148	-1.230879
H	-7.654520	1.876492	-2.893646
H	-8.085634	3.315840	-1.961964

Complex 8+ ($4NMe_2$)

SCF done: -2500.730750

Pd	-0.023959	0.147917	-0.271893
P	-2.141541	-0.722983	-0.217669
C	-3.411490	0.632174	-0.361728
N	-3.088959	1.627784	-1.234357
C	-4.598949	0.701481	0.322772
C	-3.911890	2.677360	-1.464356
C	-5.505565	1.790613	0.126167
C	-5.108943	2.788956	-0.816409
H	-5.730471	3.648181	-1.027839
H	-4.828642	-0.095485	1.018037
H	-3.565595	3.416999	-2.177033
C	-2.622149	-1.809771	-1.609809
C	-3.956417	-2.059316	-1.966157
C	-1.590345	-2.420473	-2.337223
C	-4.248851	-2.912214	-3.027375
H	-4.769431	-1.588245	-1.420650
C	-1.888506	-3.279066	-3.393368
H	-0.556611	-2.210500	-2.072109
C	-3.216307	-3.524523	-3.739130
H	-5.283118	-3.099331	-3.300356
H	-1.084569	-3.750308	-3.950882
H	-3.448691	-4.188480	-4.566342
C	-2.656711	-1.560135	1.326001
C	-3.364043	-2.769033	1.338364
C	-2.281651	-0.963589	2.541444
C	-3.700328	-3.366456	2.553743
H	-3.642703	-3.250934	0.406288
C	-2.634549	-1.557214	3.749972
H	-1.708206	-0.038841	2.536067
C	-3.342155	-2.761124	3.756977

H	-4.241821	-4.307842	2.557226
H	-2.347057	-1.088198	4.686502
H	-3.606260	-3.230049	4.700275
H	-2.177308	1.585115	-1.683682
P	2.177669	0.836181	-0.168898
C	3.063148	1.315317	-1.694534
C	4.373546	1.918134	-4.088453
C	4.191937	2.148344	-1.688831
C	2.589814	0.797941	-2.908951
C	3.248410	1.094317	-4.100189
C	4.841496	2.446799	-2.884812
H	4.548345	2.582665	-0.758751
H	1.701993	0.169229	-2.913914
H	2.877821	0.691663	-5.038190
H	5.708887	3.100382	-2.878386
H	4.880571	2.157359	-5.018513
C	3.183561	-0.614795	0.434836
C	4.355590	-2.945992	1.380628
N	2.435333	-1.653028	0.895233
C	4.551418	-0.718225	0.429248
C	5.203541	-1.899398	0.903489
C	2.997316	-2.791925	1.357916
H	5.124549	0.115425	0.045082
H	2.318048	-3.564479	1.699576
H	4.761017	-3.875309	1.757090
C	2.563675	2.142993	1.056656
C	2.928672	4.207718	2.913112
C	2.247536	3.467676	0.716049
C	3.051071	1.862754	2.339017
C	3.231974	2.893148	3.260904
C	2.437270	4.492586	1.638837
H	1.866631	3.702787	-0.274599
H	3.296338	0.845409	2.629544
H	3.614887	2.666162	4.251510
H	2.202282	5.515831	1.361191
H	3.075224	5.008562	3.631448
H	1.414331	-1.537367	0.824244
N	-6.668725	1.867175	0.786528
N	6.538819	-2.018321	0.900762
C	7.175337	-3.237723	1.395943
H	6.878808	-4.108693	0.801827
H	6.926247	-3.414453	2.447565
H	8.255739	-3.130555	1.320438
C	7.377937	-0.934709	0.393395
H	7.244460	-0.021732	0.983474
H	7.155966	-0.722203	-0.657682
H	8.422597	-1.231640	0.464061
C	-7.037911	0.841592	1.760304
H	-7.991272	1.108222	2.212473
H	-6.292453	0.769047	2.558794
H	-7.150365	-0.137298	1.281814
C	-7.586520	2.980261	0.545796
H	-7.881239	3.026720	-0.507494
H	-7.137096	3.934855	0.839534
H	-8.486757	2.833032	1.139333

TS1-2i (6Cl)

SCF done: -3268.199998

Pd	-0.165975	-1.288365	0.336014
P	-1.700907	0.458919	0.041082
C	-3.297961	-0.445330	-0.331653
N	-3.277245	-1.771233	-0.097142
C	-4.434519	0.154965	-0.864125
C	-4.342121	-2.530434	-0.361476
C	-5.553159	-0.631632	-1.140198
H	-6.450414	-0.183086	-1.556310
C	-5.515872	-1.997652	-0.888137
H	-6.358397	-2.646188	-1.097106
H	-4.434497	1.219508	-1.070114
C	-2.084102	1.403210	1.561539
C	-3.343697	1.430591	2.173857
C	-1.012738	2.094217	2.150778
C	-3.530164	2.142055	3.358317
H	-4.184927	0.898851	1.740161
C	-1.211916	2.812241	3.326882
H	-0.030948	2.078324	1.683577
C	-2.467168	2.834220	3.934685
H	-4.508980	2.153886	3.828851
H	-0.380113	3.350513	3.771492
H	-2.615957	3.387873	4.857095
C	-1.710732	1.675264	-1.327155
C	-2.206607	2.975943	-1.175596
C	-1.235611	1.255333	-2.577763
C	-2.239254	3.839986	-2.269736
H	-2.555358	3.315582	-0.204780
C	-1.277029	2.120086	-3.668008
H	-0.830391	0.252639	-2.693650
C	-1.780996	3.412413	-3.514936
H	-2.620124	4.849499	-2.146045
H	-0.911972	1.788068	-4.635636
H	-1.810101	4.087965	-4.364963
H	-2.126590	-2.216978	0.343275
P	1.980203	-0.517278	-0.036676
C	2.902926	-0.198232	1.512910
C	4.280959	0.224372	3.913165
C	4.071817	0.577771	1.532306
C	2.423286	-0.742508	2.711075
C	3.112651	-0.534799	3.904710
C	4.757259	0.783210	2.726831
H	4.444689	1.030849	0.617786
H	1.498989	-1.314623	2.706970
H	2.730623	-0.959609	4.828441
H	5.660924	1.385732	2.732323
H	4.816217	0.389301	4.843731
C	2.195301	1.088051	-0.935412
C	2.439027	3.576682	-2.056854
N	1.652457	2.138234	-0.298309
C	2.865924	1.210622	-2.150994
C	2.980815	2.482976	-2.716258
C	1.787393	3.330402	-0.844430
H	3.297544	0.342963	-2.636455
H	3.500956	2.619031	-3.660121
H	2.513060	4.583537	-2.450418
C	2.996234	-1.683490	-1.026015
C	4.441099	-3.465917	-2.634948
C	4.357052	-1.910233	-0.785137
C	2.364309	-2.369692	-2.074295
C	3.084737	-3.248950	-2.879459
C	5.072472	-2.800366	-1.585493
H	4.858408	-1.404890	0.034278
H	1.299803	-2.224744	-2.245317
H	2.584924	-3.773975	-3.688465
H	6.125484	-2.975159	-1.384634
H	5.001692	-4.158928	-3.255489
C	1.358973	-4.099396	1.103027
H	2.081568	-3.665511	1.801002
H	1.886016	-4.261313	0.157319
H	1.034579	-5.071824	1.489357
C	0.203113	-3.203350	0.899470
H	-1.843014	-3.763536	1.410862
C	-1.088668	-3.116207	0.972787
Cl	1.109046	4.678935	0.027681
Cl	-4.228631	-4.221353	-0.048691

TS1L-2L (6Cl)

SCF done: -3268.189830

Pd	-0.234699	-1.223856	0.441744
P	-1.593326	0.637020	0.078895
C	-3.222282	-0.180426	-0.358836
N	-3.248763	-1.519123	-0.209360
C	-4.304997	0.487441	-0.922207
C	-4.291182	-2.231361	-0.642215

C	-5.419961	-0.246104	-1.327642
H	-6.279865	0.255537	-1.761512
C	-5.415854	-1.629951	-1.202738
H	-6.244292	-2.241573	-1.540157
H	-4.262783	1.562278	-1.059262
C	-1.945709	1.649806	1.557721
C	-3.215679	1.794512	2.130027
C	-0.838406	2.270973	2.158201
C	-3.376776	2.555146	3.287460
H	-4.083185	1.316297	1.685300
C	-1.011307	3.038586	3.306606
H	0.151207	2.159537	1.721254
C	-2.277665	3.178632	3.874816
H	-4.363832	2.659766	3.728375
H	-0.151920	3.522296	3.761302
H	-2.407143	3.770995	4.775829
C	-1.478229	1.811256	-1.321934
C	-1.851515	3.155947	-1.211745
C	-1.036944	1.312284	-2.555909
C	-1.796996	3.986713	-2.330719
H	-2.172162	3.556071	-0.254465
C	-0.992140	2.144257	-3.670942
H	-0.725607	0.273444	-2.639263
C	-1.373857	3.482116	-3.559187
H	-2.082546	5.030514	-2.239082
H	-0.654210	1.751271	-4.625487
H	-1.335160	4.132081	-4.428556
H	-2.142437	-1.989633	0.406464
P	1.978737	-0.718453	-0.019777
C	2.964189	-0.452827	1.503187
C	4.457850	-0.128110	3.849846
C	4.160344	0.280153	1.487406
C	2.519336	-1.008337	2.709499
C	3.265489	-0.848669	3.875718
C	4.902627	0.437803	2.655102
H	4.511459	0.736095	0.566054
H	1.582275	-1.556951	2.734455
H	2.909974	-1.282439	4.805866
H	5.826885	1.007822	2.632389
H	5.037276	-0.000898	4.759643
C	2.335834	0.832644	-0.966034
C	2.802795	3.252114	-2.163249
N	1.889474	1.946933	-0.361986
C	3.012006	0.855401	-2.184253
C	3.241162	2.093899	-2.788698
C	2.132828	3.103995	-0.944657
H	3.362436	-0.063630	-2.639862
H	3.769660	2.153293	-3.735865
H	2.968565	4.235463	-2.587140
C	2.850383	-2.021792	-0.973376
C	4.091338	-4.001365	-2.518461
C	4.215384	-2.294303	-0.810856
C	2.112039	-2.760950	-1.909083
C	2.731462	-3.739682	-2.683021
C	4.829277	-3.281822	-1.579347
H	4.797940	-1.748210	-0.075227
H	1.045233	-2.577843	-2.015761
H	2.149816	-4.306635	-3.404210
H	5.885695	-3.491915	-1.439560
H	4.572863	-4.771635	-3.113863
C	-2.366132	-3.419130	2.258745
H	-2.504979	-4.493379	2.107048
H	-3.331114	-2.926077	2.121784
H	-2.059799	-3.260980	3.297714
C	-1.296482	-2.886320	1.351038
H	0.760712	-3.812821	1.283886
C	-0.039014	-3.103274	1.132390
Cl	-4.197921	-3.948050	-0.539042
Cl	1.583790	4.535729	-0.114581

Complex 7 (6Cl)

SCF done: -3497.264853

Pd	-0.107191	-1.135493	-0.404140
P	-1.390407	0.802331	-0.183923
C	-3.136278	0.758627	-0.886005
N	-3.939742	-0.291839	-0.566883
C	-3.643645	1.732188	-1.744041
C	-5.197233	-0.403583	-1.028871
C	-4.943325	1.626128	-2.237475
H	-5.336267	2.391809	-2.900034
C	-5.744646	0.550231	-1.876080
H	-6.760931	0.435560	-2.232390
H	-3.019821	2.575513	-2.011726
C	-1.753518	1.274701	1.551095
C	-2.918366	1.948013	1.947922
C	-0.789192	0.945385	2.514601
C	-3.117461	2.277378	3.286816
H	-3.674268	2.224526	1.218095
C	-0.989142	1.286656	3.850559
H	0.122840	0.438931	2.212391
C	-2.153908	1.946657	4.239161
H	-4.024116	2.795832	3.584964
H	-0.231183	1.035573	4.586620
H	-2.310622	2.206433	5.282045
C	-0.802075	2.327798	-1.015513
C	-0.928040	3.604914	-0.456293
C	-0.217374	2.183563	-2.282345
C	-0.487060	4.722646	-1.164183
H	-1.357396	3.727002	0.533130
C	0.209075	3.303737	-2.991472
H	-0.095555	1.189987	-2.708202
C	0.073553	4.575002	-2.432246
H	-0.579381	5.709588	-0.720523
H	0.655183	3.184058	-3.974555
H	0.411886	5.448944	-2.981425
H	0.462392	-3.686712	0.303315
P	2.199253	-0.682790	-0.239650
C	2.929558	-1.159526	1.377739
C	3.998064	-1.946514	3.848374
C	4.185107	-0.689925	1.793123
C	2.211906	-2.014060	2.223987
C	2.745613	-2.408492	3.450118
C	4.715201	-1.084027	3.019044
H	4.749530	-0.008808	1.162284
H	1.228124	-2.362168	1.923512
H	2.180043	-3.074398	4.095745
H	5.688077	-0.713390	3.328858
H	4.413343	-2.251399	4.804591
C	2.838358	1.050106	-0.391997
C	3.667298	3.662969	-0.361276
N	2.344967	1.873390	0.547930
C	3.743738	1.475642	-1.362982
C	4.157207	2.809573	-1.340030
C	2.760004	3.122984	0.555622
H	4.126397	0.783852	-2.104713
H	4.867633	3.176707	-2.075415
H	3.969038	4.701718	-0.297029
C	3.167932	-1.590355	-1.512000
C	4.539778	-2.920208	-3.565640
C	4.402220	-2.201805	-1.259782
C	2.622972	-1.667457	-2.803066
C	3.308345	-2.318555	-3.825769
C	5.080178	-2.865343	-2.282231
H	4.832466	-2.172835	-0.263520
H	1.648532	-1.224502	-2.999369
H	2.876405	-2.367561	-4.821418
H	6.033123	-3.342506	-2.072095
H	5.071238	-3.438051	-4.358774
C	-2.187342	-2.992405	-1.859766
H	-2.946936	-2.213174	-1.941636
H	-2.704281	-3.958959	-1.913071
H	-1.538977	-2.915358	-2.735425

C	-1.359784	-2.904727	-0.592717
H	0.469366	-3.574715	-1.525111
C	0.006753	-3.271077	-0.589296
C	-2.093163	-2.846715	0.681160
O	-3.199962	-2.293754	0.842161
H	-3.168349	-3.758230	2.928837
C	-2.157447	-3.350335	2.981097
H	-1.544850	-3.935119	3.665758
H	-2.201433	-2.306143	3.298691
O	-1.506260	-3.458917	1.704657
H	-3.566533	-1.139218	0.040189
Cl	-6.101902	-1.772931	-0.540842
Cl	2.125632	4.155787	1.812224

TS7-8 (6Cl)

SCF done: -3497.236938

Pd	0.051542	-0.471078	-0.380588
P	-1.686188	0.927563	-0.119203
C	-3.340576	0.634034	-0.951531
N	-3.981251	-0.545006	-0.713792
C	-3.918516	1.503281	-1.878085
C	-5.143942	-0.882334	-1.303877
C	-5.114944	1.168433	-2.504944
H	-5.565487	1.855321	-3.215516
C	-5.752053	-0.037035	-2.216574
H	-6.688057	-0.325028	-2.678642
H	-3.427808	2.445660	-2.087204
C	-2.221156	1.142194	1.626939
C	-3.528640	1.458106	2.021846
C	-1.222363	1.016180	2.604634
C	-3.833611	1.632379	3.371010
H	-4.317509	1.577698	1.283952
C	-1.529268	1.206615	3.950346
H	-0.205545	0.777932	2.300828
C	-2.835375	1.508214	4.336175
H	-4.850809	1.873242	3.666333
H	-0.745282	1.118358	4.696957
H	-3.074388	1.651081	5.386002
C	-1.357923	2.630735	-0.723922
C	-1.905361	3.771038	-0.121094
C	-0.520813	2.774679	-1.838942
C	-1.627426	5.035284	-0.637478
H	-2.535867	3.675202	0.758020
C	-0.257611	4.039579	-2.360187
H	-0.066105	1.889922	-2.278899
C	-0.809890	5.170538	-1.759433
H	-2.045919	5.915915	-0.158846
H	0.391336	4.142857	-3.225037
H	-0.594244	6.157851	-2.157498
H	0.666078	-3.957181	0.502385
P	2.378873	-0.599479	-0.252192
C	3.083102	-1.044801	1.382995
C	4.089040	-1.813617	3.883322
C	4.378120	-0.674039	1.772344
C	2.295026	-1.792779	2.266988
C	2.798240	-2.180873	3.507515
C	4.876190	-1.056748	3.015725
H	4.998270	-0.079325	1.107606
H	1.280429	-2.059916	1.981756
H	2.180161	-2.763698	4.184759
H	5.879472	-0.760707	3.308409
H	4.479753	-2.109950	4.852525
C	3.217374	1.018966	-0.589141
C	4.299851	3.518489	-0.901959
N	2.853411	1.991591	0.262696
C	4.121723	1.230943	-1.629445
C	4.664232	2.509073	-1.781944
C	3.387280	3.184427	0.104492
H	4.402405	0.422491	-2.294921
H	5.374261	2.712164	-2.578764
H	4.698685	4.523185	-0.978164
C	3.186150	-1.745384	-1.446392
C	4.293694	-3.455779	-3.374899
C	4.315755	-2.516775	-1.145535
C	2.612032	-1.850661	-2.723468
C	3.168172	-2.691675	-3.684830
C	4.861600	-3.369562	-2.104826
H	4.767200	-2.458983	-0.159814
H	1.722024	-1.269175	-2.957704
H	2.718772	-2.757646	-4.671887
H	5.734744	-3.966812	-1.857676
H	4.723252	-4.119654	-4.119620
C	-1.894186	-3.149478	-1.742245
H	-2.050178	-2.090167	-1.971495
H	-2.874072	-3.633502	-1.678217
H	-1.349159	-3.590102	-2.579350
C	-1.116110	-3.324966	-0.466858
H	0.656065	-4.076876	-1.346346
C	0.135708	-3.812137	-0.431269
C	-1.818294	-2.979074	0.795927
O	-2.902012	-2.391047	0.849030
H	-2.868863	-3.508183	3.154933
C	-1.858782	-3.094527	3.144532
H	-1.243880	-3.566270	3.909239
H	-1.902992	-2.013972	3.293892
O	-1.210126	-3.398948	1.896923
H	-3.529968	-1.268784	-0.078760
Cl	2.907026	4.419224	1.240660
Cl	-5.834361	-2.390189	-0.878346

TS1-2i+ (6Cl)

SCF done: -3268.501046

Pd	-0.216231	-1.143144	0.493247
P	-1.773307	0.607740	0.054840
C	-3.264890	-0.334599	-0.563638
N	-3.299004	-1.635457	-0.222076
C	-4.297609	0.232018	-1.303327
C	-4.334243	-2.401184	-0.565980
C	-5.384813	-0.566952	-1.666240
H	-6.205736	-0.146730	-2.239729
C	-5.415352	-1.904248	-1.293526
H	-6.238408	-2.557782	-1.558419
H	-4.251863	1.273610	-1.600334
C	-2.395992	1.446216	1.555026
C	-3.569957	2.216133	1.561695
C	-1.675926	1.281236	2.746875
C	-4.007592	2.812879	2.740231
H	-4.146957	2.353459	0.652053
C	-2.117110	1.882994	3.924423
H	-0.778152	0.667489	2.752580
C	-3.281776	2.647831	3.921484
H	-4.918118	3.404386	2.738835
H	-1.556605	1.747547	4.844517
H	-3.629335	3.111975	4.839516
C	-1.596356	1.901954	-1.231801
C	-1.595411	3.267943	-0.919586
C	-1.420737	1.503433	-2.567873
C	-1.443747	4.218183	-1.931043
H	-1.737883	3.594321	0.106178
C	-1.282694	2.456063	-3.574004
H	-1.418157	0.447070	-2.827824
C	-1.296102	3.816231	-3.257327
H	-1.465934	5.274939	-1.680774
H	-1.180488	2.137821	-4.607685
H	-1.205670	4.558914	-4.044698
H	-2.167486	-2.101633	0.463421
P	1.974946	-0.692374	-0.007823
C	3.020731	-0.368179	1.457224
C	4.569463	0.033880	3.755866
C	4.308845	0.192210	1.358735
C	2.517900	-0.711360	2.722245
C	3.292370	-0.513842	3.864205

C	5.075240	0.390041	2.504073
H	4.721447	0.468622	0.391255
H	1.519351	-1.133063	2.806134
H	2.897104	-0.787124	4.837813
H	6.069975	0.817194	2.419854
H	5.172287	0.186686	4.645920
C	2.271586	0.884099	-0.957375
C	2.540174	3.391806	-2.175720
N	2.254321	2.046224	-0.252695
C	2.434091	0.972864	-2.333469
C	2.571013	2.223983	-2.936041
C	2.379345	3.273839	-0.805229
H	2.470016	0.062170	-2.920148
H	2.713438	2.293142	-4.010506
H	2.649566	4.373232	-2.620929
C	2.792643	-1.924897	-1.078922
C	3.904856	-3.835240	-2.790095
C	4.141687	-2.282252	-0.950618
C	1.998921	-2.547455	-2.057157
C	2.558771	-3.490241	-2.916403
C	4.689962	-3.237775	-1.804409
H	4.761448	-1.840164	-0.177744
H	0.940244	-2.306917	-2.131067
H	1.941199	-3.967763	-3.671176
H	5.732727	-3.519448	-1.694183
H	4.338222	-4.579998	-3.450753
C	1.030167	-4.038347	1.429510
H	1.863131	-3.613316	1.996289
H	1.432956	-4.389498	0.472770
H	0.634337	-4.906952	1.966461
C	-0.036923	-3.051714	1.189020
H	-2.077291	-3.304259	1.887458
C	-1.316523	-2.833814	1.267580
H	2.186182	1.984770	0.763313
Cl	2.351695	4.606603	0.251900
Cl	-4.293741	-4.056387	-0.094845

TS1L-2L+ (6Cl)

SCF done: -3268.492203

Pd	-0.247806	-1.070075	0.510390
P	-1.705211	0.747506	0.062744
C	-3.127653	-0.154731	-0.746774
N	-3.167676	-1.481670	-0.517742
C	-4.074159	0.457023	-1.561777
C	-4.110153	-2.235024	-1.085707
C	-5.081886	-0.325067	-2.131180
H	-5.838613	0.130420	-2.763048
C	-5.104716	-1.693771	-1.900923
H	-5.854506	-2.339672	-2.342914
H	-4.019665	1.521408	-1.760420
C	-2.431831	1.488473	1.565571
C	-3.657221	2.173510	1.560081
C	-1.728849	1.346284	2.770773
C	-4.163756	2.707635	2.741435
H	-4.221871	2.292146	0.640054
C	-2.238032	1.887581	3.949911
H	-0.788371	0.800390	2.785036
C	-3.454948	2.566496	3.935871
H	-5.114218	3.232448	2.731128
H	-1.688752	1.773042	4.879563
H	-3.855503	2.982737	4.855262
C	-1.422049	2.120927	-1.115799
C	-1.531783	3.465028	-0.736506
C	-1.059073	1.805096	-2.436176
C	-1.301000	4.476656	-1.670544
H	-1.814091	3.725472	0.278983
C	-0.843522	2.818402	-3.366185
H	-0.969677	0.765623	-2.744912
C	-0.965442	4.156783	-2.984648
H	-1.402650	5.515666	-1.371233
H	-0.594749	2.565325	-4.392975
H	-0.809700	4.946586	-3.713734
H	-2.123945	-1.942505	0.349454
P	1.996086	-0.810717	0.075459
C	2.995073	-0.463751	1.567661
C	4.478054	-0.049680	3.906424
C	4.295364	0.070579	1.500175
C	2.448253	-0.781267	2.820767
C	3.190604	-0.578132	3.982553
C	5.028532	0.276469	2.665727
H	4.746120	0.318207	0.542025
H	1.444314	-1.192666	2.881013
H	2.762185	-0.832851	4.947116
H	6.032837	0.684863	2.605687
H	5.054945	0.108626	4.812537
C	2.469259	0.656099	-0.972299
C	3.052601	3.016480	-2.363087
N	2.411722	1.882794	-0.389223
C	2.829169	0.600887	-2.312458
C	3.123496	1.779189	-3.000700
C	2.687764	3.042718	-1.026580
H	2.898167	-0.365077	-2.799578
H	3.423637	1.734850	-4.043724
H	3.284643	3.943174	-2.873897
C	2.765641	-2.183502	-0.847740
C	3.826318	-4.305553	-2.323609
C	4.098425	-2.574428	-0.657122
C	1.963112	-2.873564	-1.770947
C	2.497719	-3.924132	-2.513035
C	4.620985	-3.635794	-1.393211
H	4.722403	-2.075050	0.076783
H	0.917340	-2.599506	-1.891680
H	1.873241	-4.455630	-3.224704
H	5.649550	-3.944424	-1.233220
H	4.238745	-5.133962	-2.891598
C	-2.588925	-3.186291	2.205782
H	-3.541943	-2.725606	1.940672
H	-2.370468	-2.941343	3.249405
H	-2.691639	-4.271722	2.124208
C	-1.455469	-2.708949	1.338701
H	0.579816	-3.686292	1.431633
C	-0.185885	-2.950968	1.232240
H	2.184577	1.928716	0.603631
Cl	2.587593	4.473602	-0.112842
Cl	-4.049277	-3.933951	-0.819438

Complex 7+ (6Cl)

SCF done: -3497.577100

Pd	-0.121030	-1.044327	-0.331715
P	-1.472150	0.877844	-0.140482
C	-3.158701	0.889652	-0.967036
N	-4.001600	-0.146155	-0.706971
C	-3.592889	1.886587	-1.832764
C	-5.236804	-0.228215	-1.235705
C	-4.869307	1.815571	-2.397518
H	-5.209552	2.599211	-3.068195
C	-5.711597	0.753585	-2.097896
H	-6.709242	0.669393	-2.511914
H	-2.940065	2.720894	-2.056149
C	-1.958089	1.235840	1.589913
C	-3.054292	2.043560	1.930034
C	-1.175409	0.679320	2.611958
C	-3.354732	2.291879	3.267518
H	-3.676997	2.484640	1.156258
C	-1.474325	0.936941	3.948753
H	-0.339330	0.033659	2.351059
C	-2.564606	1.741758	4.277200
H	-4.206622	2.915364	3.521775
H	-0.862185	0.503344	4.734248
H	-2.802590	1.937005	5.318508
C	-0.801118	2.451042	-0.813487
C	-0.894927	3.679062	-0.145161

C	-0.185189	2.400497	-2.074793
C	-0.395061	4.839028	-0.738541
H	-1.361061	3.735276	0.833761
C	0.292887	3.564853	-2.672414
H	-0.096722	1.447814	-2.593177
C	0.187637	4.786418	-2.004339
H	-0.476717	5.787501	-0.215618
H	0.740884	3.520888	-3.661122
H	0.554195	5.695712	-2.471877
H	0.321337	-3.586229	0.556081
P	2.199971	-0.807328	-0.256589
C	2.952143	-1.183407	1.373737
C	4.025123	-1.856889	3.874792
C	4.295711	-0.893061	1.675918
C	2.155396	-1.806870	2.346109
C	2.692180	-2.144606	3.587475
C	4.825164	-1.228054	2.919304
H	4.937959	-0.416682	0.939100
H	1.116248	-2.032887	2.122236
H	2.069653	-2.635730	4.329299
H	5.864780	-1.005414	3.140210
H	4.442968	-2.122129	4.841236
C	2.986753	0.858185	-0.548937
C	3.973196	3.476914	-0.789637
N	2.909995	1.771259	0.456893
C	3.582494	1.276322	-1.735933
C	4.078523	2.573244	-1.848570
C	3.371835	3.040013	0.376518
H	3.675546	0.569839	-2.552636
H	4.565786	2.886849	-2.767346
H	4.355260	4.488475	-0.852498
C	3.064302	-1.806043	-1.525385
C	4.249051	-3.318822	-3.558905
C	4.233150	-2.534098	-1.270528
C	2.481224	-1.859032	-2.802787
C	3.080074	-2.601890	-3.817569
C	4.817377	-3.289897	-2.286351
H	4.680176	-2.532546	-0.281960
H	1.549617	-1.330253	-2.995409
H	2.626316	-2.635526	-4.803650
H	5.717535	-3.860715	-2.079351
H	4.708611	-3.909545	-4.345522
C	-2.163014	-2.911594	-1.798932
H	-2.888928	-2.110776	-1.947248
H	-2.710527	-3.860596	-1.851932
H	-1.461640	-2.887554	-2.635520
C	-1.414900	-2.818273	-0.483855
H	0.440270	-3.573468	-1.277570
C	-0.074294	-3.222695	-0.386916
C	-2.250748	-2.741321	0.740397
O	-3.337919	-2.148918	0.806283
H	-3.543944	-3.761085	2.812476
C	-2.549791	-3.351673	2.997618
H	-2.007399	-3.972024	3.708844
H	-2.637997	-2.325936	3.361075
O	-1.765082	-3.388703	1.788205
H	-3.683999	-0.975146	-0.079920
H	2.516315	1.467936	1.346252
Cl	3.192055	4.017026	1.760405
Cl	-6.188478	-1.579731	-0.814165

Complex 8+ (6Cl)

SCF done: -3151.880647

Pd	0.118779	-0.185437	-0.082183
P	-2.077104	0.456084	-0.075339
C	-3.063469	-0.866923	-0.945225
N	-3.382797	-1.977415	-0.227717
C	-3.401243	-0.861466	-2.294167
C	-3.987940	-3.072546	-0.743979
C	-4.032583	-1.970257	-2.856629
H	-4.304589	-1.961081	-3.908155
C	-4.326567	-3.095950	-2.085924
H	-4.813948	-3.969310	-2.502351
H	-3.175473	0.015021	-2.890616
C	-2.949443	0.508688	1.529669
C	-4.351983	0.467326	1.641262
C	-2.171511	0.613102	2.693191
C	-4.956221	0.535265	2.893862
H	-4.976263	0.389801	0.754198
C	-2.782871	0.687687	3.943271
H	-1.087758	0.633812	2.608421
C	-4.172592	0.648750	4.043909
H	-6.038770	0.505354	2.972997
H	-2.174500	0.772452	4.838572
H	-4.648181	0.704385	5.018445
C	-2.513734	1.950711	-1.032199
C	-3.559278	2.811964	-0.675050
C	-1.734162	2.235788	-2.165987
C	-3.832859	3.932463	-1.457147
H	-4.149142	2.625647	0.216257
C	-2.026396	3.347908	-2.952634
H	-0.896169	1.589500	-2.421009
C	-3.075777	4.196374	-2.598216
H	-4.639900	4.600857	-1.172747
H	-1.427537	3.559523	-3.833556
H	-3.296435	5.069139	-3.205402
H	-3.178516	-1.972496	0.771551
P	2.402773	-0.570931	-0.059803
C	3.098534	-1.498099	1.351270
C	4.061340	-2.836242	3.607115
C	4.430718	-1.939925	1.393425
C	2.253900	-1.738491	2.444791
C	2.736625	-2.404602	3.569394
C	4.905639	-2.606500	2.518823
H	5.089757	-1.791346	0.542767
H	1.218483	-1.407012	2.402039
H	2.078167	-2.592695	4.412026
H	5.934290	-2.953117	2.545670
H	4.436986	-3.359335	4.481397
C	3.218147	1.101395	0.164293
C	4.035708	3.716998	0.684163
N	2.338028	2.094739	0.436743
C	4.568617	1.416335	0.132573
C	4.973649	2.727560	0.393950
C	2.692365	3.368366	0.697542
H	5.294396	0.644789	-0.095181
H	6.028939	2.984139	0.374825
H	4.326679	4.739746	0.893288
C	3.225446	-1.204263	-1.562753
C	4.270928	-2.236523	-3.943523
C	3.483548	-2.577578	-1.683351
C	3.473101	-0.356692	-2.653075
C	4.002095	-0.872132	-3.833455
C	4.006558	-3.086371	-2.870708
H	3.287308	-3.249950	-0.853245
H	3.256693	0.706977	-2.590257
H	4.203773	-0.207667	-4.668292
H	4.211938	-4.149377	-2.953240
H	4.684150	-2.635998	-4.864619
H	1.335813	1.797096	0.421545
Cl	1.444720	4.481018	1.025333
Cl	-4.303861	-4.358079	0.325147

TS1-2i (4Cl)

SCF done: -3268.199994

Pd	-0.038118	-1.405685	-0.590439
P	-1.728073	-0.000071	0.272289
C	-3.238973	-0.545691	-0.690144
N	-3.091890	-1.683577	-1.383601
C	-4.433949	0.166781	-0.745217
C	-4.086264	-2.170585	-2.133778
C	-5.477582	-0.335394	-1.525130

C	-5.309673	-1.526709	-2.234280
H	-6.103265	-1.930555	-2.851928
H	-4.546425	1.098534	-0.202271
C	-2.185650	-0.332372	2.014981
C	-3.435065	-0.820529	2.418455
C	-1.185168	-0.114968	2.976918
C	-3.682726	-1.082431	3.765544
H	-4.222151	-1.004170	1.694042
C	-1.445915	-0.368915	4.320841
H	-0.211418	0.259745	2.668234
C	-2.691594	-0.855404	4.717754
H	-4.653673	-1.463807	4.067872
H	-0.668622	-0.194003	5.059116
H	-2.888158	-1.060181	5.766070
C	-1.851279	1.814308	0.060124
C	-2.462303	2.643268	1.009353
C	-1.336856	2.372414	-1.118379
C	-2.565671	4.013871	0.773116
H	-2.849085	2.221002	1.932586
C	-1.448060	3.740586	-1.351655
H	-0.845873	1.734370	-1.849610
C	-2.063137	4.562207	-0.406204
H	-3.041068	4.652687	1.511979
H	-1.050230	4.166897	-2.267960
H	-2.147176	5.629752	-0.587695
H	-1.870384	-2.229251	-1.330956
P	2.019183	-0.500082	-0.079577
C	2.770498	-1.242381	1.415721
C	3.905105	-2.445846	3.673575
C	3.818954	-0.612403	2.102731
C	2.286592	-2.471732	1.881363
C	2.855346	-3.071448	3.003944
C	4.383931	-1.214890	3.223816
H	4.192175	0.351425	1.767783
H	1.453482	-2.948570	1.370917
H	2.471802	-4.023744	3.358484
H	5.196087	-0.720776	3.749120
H	4.346146	-2.912124	4.549792
C	2.084162	1.310456	0.313478
C	2.060634	3.937048	1.075667
N	1.318097	1.665269	1.352450
C	2.866121	2.214880	-0.406239
C	2.841606	3.551638	-0.008259
C	1.318749	2.947175	1.718465
H	3.479768	1.895685	-1.240230
H	2.027780	4.968268	1.408036
C	3.252810	-0.676967	-1.426688
C	5.046040	-0.879911	-3.570257
C	4.591355	-1.019081	-1.198817
C	2.819344	-0.448815	-2.742211
C	3.713188	-0.540682	-3.806256
C	5.480324	-1.122886	-2.268569
H	4.941540	-1.214802	-0.190136
H	1.774892	-0.211344	-2.932267
H	3.367327	-0.358297	-4.819644
H	6.514810	-1.395800	-2.081439
H	5.741796	-0.961014	-4.400213
C	1.739889	-3.875442	-1.821432
H	2.371796	-4.023202	-0.940500
H	2.331609	-3.310461	-2.548293
H	1.502378	-4.854010	-2.253016
C	0.506034	-3.140474	-1.477216
H	-1.459024	-4.016010	-1.789482
C	-0.791085	-3.199631	-1.521068
Cl	-6.969779	0.517274	-1.615707
Cl	3.789937	4.722517	-0.861309
H	0.689069	3.206755	2.566418
H	-3.883640	-3.091738	-2.672244

TS1L-2L (4Cl)
SCF done: -3268.193278

Pd	-0.068364	-1.370107	-0.577156
P	-1.646174	0.115730	0.303763
C	-3.201364	-0.389593	-0.604309
N	-3.117399	-1.534116	-1.301645
C	-4.364414	0.375207	-0.624286
C	-4.157572	-1.963354	-2.029893
C	-5.450803	-0.071087	-1.377682
C	-5.351107	-1.262219	-2.097983
H	-6.174865	-1.627283	-2.700162
H	-4.418466	1.309505	-0.076537
C	-2.066032	-0.134167	2.068308
C	-3.313325	-0.582400	2.521274
C	-1.036632	0.100612	2.994906
C	-3.530714	-0.786892	3.883466
H	-4.121650	-0.779263	1.824133
C	-1.267073	-0.096117	4.353803
H	-0.063712	0.441377	2.646506
C	-2.511097	-0.542163	4.800562
H	-4.500294	-1.137276	4.225126
H	-0.467756	0.091484	5.064878
H	-2.684212	-0.701933	5.860764
C	-1.686696	1.924674	0.028071
C	-2.229581	2.816547	0.961310
C	-1.179353	2.412897	-1.184159
C	-2.271799	4.181246	0.676808
H	-2.610378	2.447824	1.909508
C	-1.229866	3.775557	-1.465447
H	-0.740271	1.724895	-1.903076
C	-1.776454	4.660575	-0.535183
H	-2.693872	4.869527	1.403534
H	-0.837487	4.147983	-2.407229
H	-1.812821	5.723787	-0.754137
H	-1.894140	-2.117192	-1.261201
P	2.051342	-0.594719	-0.084117
C	2.717904	-1.307464	1.464273
C	3.739520	-2.484462	3.788739
C	3.738514	-0.674242	2.188723
C	2.207271	-2.529173	1.922235
C	2.720246	-3.115403	3.077851
C	4.246093	-1.263006	3.344317
H	4.136775	0.280037	1.855917
H	1.402093	-3.013442	1.375908
H	2.317697	-4.062433	3.425323
H	5.036767	-0.766088	3.898966
H	4.136256	-2.940510	4.691145
C	2.244265	1.225772	0.196175
C	2.393908	3.894253	0.772417
N	1.500938	1.701821	1.203461
C	3.085487	2.023356	-0.580753
C	3.148609	3.383608	-0.278038
C	1.587465	3.003302	1.479127
H	3.677744	1.604993	-1.385977
H	2.428996	4.946168	1.031658
C	3.287069	-0.962461	-1.389115
C	5.109669	-1.443520	-3.460158
C	4.609873	-1.319322	-1.097678
C	2.884134	-0.859210	-2.729167
C	3.793688	-1.089714	-3.758404
C	5.513549	-1.562272	-2.131394
H	4.934192	-1.418092	-0.066372
H	1.851659	-0.610444	-2.963407
H	3.472099	-1.004681	-4.792370
H	6.534917	-1.846507	-1.895541
H	5.816717	-1.633453	-4.262389
C	-1.759086	-4.314683	-1.910602
H	-2.166236	-4.135653	-2.912844
H	-2.596311	-4.414645	-1.212577
H	-1.226958	-5.268990	-1.940104
C	-0.819567	-3.215143	-1.506480
H	1.394199	-3.586379	-1.674282
C	0.467021	-3.083155	-1.442203

Cl	-6.904240	0.848046	-1.423714
Cl	4.171734	4.427261	-1.206060
H	-4.021630	-2.889254	-2.576882
H	0.975532	3.363232	2.303034

Complex 7 (6Cl)

SCF done: -3497.267810

Pd	-0.043529	-1.059437	-0.764562
P	-1.596959	0.318047	0.305999
C	-3.332198	0.320681	-0.415951
N	-3.898006	-0.873051	-0.713630
C	-4.062022	1.473447	-0.699226
C	-5.126301	-0.992538	-1.243111
C	-5.339326	1.370984	-1.254176
C	-5.894742	0.117671	-1.527827
H	-6.884166	0.015118	-1.956326
H	-3.637646	2.445086	-0.478414
C	-1.977815	-0.183788	2.030203
C	-3.228986	-0.005092	2.639272
C	-0.936229	-0.771582	2.762731
C	-3.434080	-0.412582	3.955846
H	-4.049679	0.454760	2.095392
C	-1.144614	-1.168269	4.081767
H	0.038105	-0.901049	2.301373
C	-2.392804	-0.994661	4.678118
H	-4.407224	-0.272666	4.417549
H	-0.328877	-1.616803	4.641178
H	-2.555193	-1.310960	5.704410
C	-1.321501	2.131346	0.352741
C	-1.719587	2.939846	1.425056
C	-0.707000	2.718207	-0.762084
C	-1.516914	4.318322	1.372396
H	-2.179876	2.494437	2.302184
C	-0.513930	4.096940	-0.814330
H	-0.373588	2.089052	-1.584211
C	-0.920113	4.898111	0.252858
H	-1.826272	4.939938	2.207858
H	-0.039472	4.544333	-1.682809
H	-0.766159	5.972588	0.214447
H	0.975132	-3.489955	-1.383918
P	2.157794	-0.412818	-0.228321
C	2.935560	-1.478193	1.050775
C	4.093366	-3.164568	2.968651
C	4.081574	-1.075956	1.753537
C	2.371678	-2.729406	1.331261
C	2.950442	-3.569011	2.282266
C	4.656100	-1.915644	2.704457
H	4.526728	-0.103639	1.562117
H	1.472639	-3.040920	0.807076
H	2.505924	-4.538632	2.488101
H	5.543718	-1.593043	3.241069
H	4.543661	-3.817496	3.710770
C	2.483223	1.267086	0.483214
C	2.828345	3.672956	1.736560
N	1.792524	1.503763	1.606836
C	3.361500	2.190287	-0.087627
C	3.522851	3.414317	0.560107
C	1.976187	2.676568	2.212474
H	3.909214	1.964320	-0.995085
H	2.942559	4.613679	2.262941
C	3.287857	-0.484245	-1.676545
C	4.902500	-0.532999	-3.969491
C	4.555230	-1.077883	-1.638442
C	2.834305	0.073469	-2.882614
C	3.639948	0.059046	-4.018203
C	5.354240	-1.104016	-2.781731
H	4.919073	-1.528186	-0.720277
H	1.840505	0.513795	-2.931697
H	3.279062	0.499626	-4.943297
H	6.333112	-1.573080	-2.740956
H	5.528331	-0.554184	-4.856878
C	-1.769764	-2.210154	-3.122549
H	-2.647450	-1.617940	-2.857291
H	-2.120228	-3.072666	-3.703867
H	-1.145185	-1.600263	-3.779007
C	-0.965844	-2.670126	-1.922184
H	0.951929	-2.449378	-2.891852
C	0.445050	-2.753904	-1.979417
C	-1.696983	-3.420964	-0.889001
O	-2.899508	-3.250766	-0.610188
H	-2.542161	-5.548803	0.448292
C	-1.649648	-5.041289	0.818575
H	-0.923755	-5.765712	1.185255
H	-1.930214	-4.343440	1.610942
O	-0.986303	-4.347047	-0.248900
H	-3.371407	-1.810017	-0.610958
Cl	-6.238298	2.794687	-1.593115
Cl	4.597283	4.605177	-0.098534
H	1.410146	2.840290	3.126846
H	-5.456708	-2.007176	-1.438124

TS7-8 (4Cl)

SCF done: -3497.239427

Pd	0.038664	-0.442202	-0.378066
P	-1.876617	0.416226	0.407673
C	-3.468356	0.322565	-0.573924
N	-3.864112	-0.900861	-1.006888
C	-4.227728	1.422624	-0.973157
C	-4.949859	-1.103926	-1.773524
C	-5.355345	1.236907	-1.771886
C	-5.735986	-0.048295	-2.180688
H	-6.609341	-0.211494	-2.799761
H	-3.939668	2.414652	-0.646475
H	-5.150105	-2.133713	-2.047400
C	-2.437804	-0.334800	1.990250
C	-3.775059	-0.385509	2.409912
C	-1.438549	-0.858398	2.824836
C	-4.106350	-0.956376	3.637773
H	-4.566842	0.023521	1.787693
C	-1.773675	-1.415313	4.057300
H	-0.400866	-0.819259	2.501220
C	-3.106884	-1.469808	4.463205
H	-5.145572	-0.993263	3.951760
H	-0.990641	-1.808490	4.699275
H	-3.367262	-1.909005	5.421860
C	-1.822893	2.225745	0.716082
C	-2.528572	2.845673	1.756185
C	-1.031068	3.004369	-0.139761
C	-2.453192	4.227414	1.924331
H	-3.124571	2.252114	2.443320
C	-0.969711	4.386494	0.024139
H	-0.450450	2.514944	-0.918562
C	-1.680653	4.998791	1.056054
H	-2.996551	4.700893	2.737013
H	-0.355454	4.982698	-0.644368
H	-1.625218	6.075262	1.190214
H	1.185456	-3.743516	-1.326162
P	2.355353	-0.317817	-0.126873
C	3.097918	-1.428494	1.131930
C	4.173163	-3.208793	3.011605
C	4.297506	-1.126176	1.791758
C	2.438831	-2.626604	1.435642
C	2.977001	-3.514867	2.365304
C	4.830161	-2.012145	2.725717
H	4.815181	-0.194178	1.583312
H	1.494656	-2.854509	0.946869
H	2.458966	-4.442843	2.590902
H	5.758829	-1.765911	3.232556
H	4.590642	-3.897227	3.740721
C	2.904089	1.350166	0.470096
C	3.536657	3.799341	1.511568
N	2.362411	1.700846	1.644212

C	3.775438	2.170577	-0.249738
C	4.083332	3.418070	0.291458
C	2.684329	2.893356	2.143818
H	4.205982	1.852537	-1.192012
H	2.237236	3.150086	3.102023
H	3.763814	4.762139	1.954881
C	3.362353	-0.580491	-1.645277
C	4.779061	-0.905814	-4.044468
C	4.597357	-1.241101	-1.655742
C	2.840425	-0.095673	-2.855416
C	3.548982	-0.247344	-4.045273
C	5.297486	-1.405048	-2.850779
H	5.011531	-1.634501	-0.732518
H	1.872030	0.401507	-2.858118
H	3.138643	0.141263	-4.973207
H	6.252463	-1.922808	-2.846874
H	5.329343	-1.032727	-4.972287
C	-1.452869	-2.394170	-3.188250
H	-1.865598	-1.433429	-2.864403
H	-2.284876	-3.022031	-3.524139
H	-0.803148	-2.201992	-4.044264
C	-0.677291	-3.064191	-2.087416
H	1.242563	-2.867563	-2.957398
C	0.654639	-3.234501	-2.121951
C	-1.465053	-3.566833	-0.933050
O	-2.637950	-3.253898	-0.711946
H	-2.457203	-5.413700	0.665744
C	-1.534505	-4.925547	0.984865
H	-0.863388	-5.644000	1.452649
H	-1.769843	-4.110909	1.672969
O	-0.816542	-4.423235	-0.155657
H	-3.290666	-1.756046	-0.798177
Cl	5.155306	4.486378	-0.556483
Cl	-6.298586	2.590832	-2.247721

TS1-2i+ (4Cl)

SCF done: -3268.506294

Pd	0.049412	-1.297288	0.422376
P	1.924346	-0.047308	-0.410493
C	3.173044	-0.230738	0.967659
N	2.967148	-1.275061	1.781841
C	4.267875	0.610535	1.140890
C	3.824069	-1.545969	2.771872
C	5.165494	0.333540	2.178091
C	4.946379	-0.765174	3.010788
H	5.625015	-0.999359	3.823014
H	4.427450	1.467125	0.496236
C	2.735763	-0.846699	-1.838282
C	4.050334	-0.536799	-2.222710
C	2.017838	-1.815472	-2.553677
C	4.631106	-1.187147	-3.306835
H	4.624912	0.209114	-1.681398
C	2.603966	-2.461444	-3.641213
H	1.004252	-2.068255	-2.252591
C	3.908892	-2.149103	-4.016340
H	5.649170	-0.946398	-3.597411
H	2.043466	-3.211197	-4.191248
H	4.367352	-2.656081	-4.860012
C	1.992861	1.758948	-0.746831
C	2.194886	2.256487	-2.043523
C	1.790952	2.664955	0.310107
C	2.223657	3.635519	-2.270927
H	2.363922	1.573692	-2.871120
C	1.831163	4.037887	0.079168
H	1.628245	2.299998	1.321720
C	2.052952	4.526571	-1.211346
H	2.407881	4.008800	-3.274286
H	1.705070	4.727585	0.908736
H	2.104119	5.597257	-1.386387
H	1.789754	-2.053072	1.512573
P	-2.090900	-0.513999	0.120319
C	-2.906984	-1.216354	-1.358061
C	-4.107502	-2.413742	-3.583756
C	-4.046795	-0.640977	-1.942951
C	-2.372358	-2.393090	-1.904564
C	-2.975606	-2.990111	-3.009507
C	-4.640692	-1.239260	-3.051127
H	-4.480386	0.269729	-1.539440
H	-1.486234	-2.839706	-1.460363
H	-2.560153	-3.904274	-3.422591
H	-5.521797	-0.789157	-3.498261
H	-4.574785	-2.877573	-4.447095
C	-2.285624	1.312402	-0.221423
C	-2.399970	4.004880	-0.954105
N	-1.345277	1.894323	-1.002418
C	-3.324938	2.104158	0.243247
C	-3.388725	3.454826	-0.126633
C	-1.371061	3.189356	-1.373249
H	-4.083764	1.670899	0.885205
H	-2.429207	5.046868	-1.249972
C	-3.220054	-0.704500	1.541628
C	-4.847852	-0.971325	3.796666
C	-4.526518	-1.193294	1.409457
C	-2.728115	-0.363250	2.812734
C	-3.544472	-0.488591	3.933142
C	-5.334062	-1.326728	2.539481
H	-4.910657	-1.483513	0.436594
H	-1.704250	-0.013081	2.926335
H	-3.161968	-0.221176	4.913557
H	-6.343226	-1.713468	2.434845
H	-5.480473	-1.078397	4.672619
C	-1.589398	-3.808065	1.753845
H	-2.290638	-3.905653	0.920803
H	-2.118043	-3.296187	2.566038
H	-1.307898	-4.804458	2.111120
C	-0.389510	-3.042913	1.378397
H	1.585645	-3.908065	1.433516
C	0.913360	-3.051167	1.392051
H	-0.543894	1.327271	-1.280818
Cl	-4.674108	4.428163	0.428306
Cl	6.529798	1.345667	2.419616
H	-0.543326	3.534122	-1.982871
H	3.593852	-2.407425	3.392632

TS1L-2L+ (4Cl)

SCF done: -3268.499989

Pd	0.075490	-1.217586	0.496016
P	1.842493	0.110984	-0.397835
C	3.199045	-0.184993	0.848901
N	3.038854	-1.277667	1.610528
C	4.308851	0.640758	0.995524
C	3.958748	-1.599696	2.528654
C	5.273278	0.304864	1.951711
C	5.098451	-0.836307	2.735995
H	5.824179	-1.116974	3.490777
H	4.426015	1.535434	0.394885
C	2.517142	-0.529905	-1.967961
C	3.816581	-0.230420	-2.407318
C	1.695703	-1.354707	-2.749592
C	4.282056	-0.751664	-3.610438
H	4.469401	0.405708	-1.817185
C	2.166332	-1.869187	-3.956752
H	0.691484	-1.595332	-2.410195
C	3.457906	-1.570398	-4.385476
H	5.289391	-0.521224	-3.943597
H	1.525768	-2.506315	-4.558819
H	3.826530	-1.976230	-5.322722
C	1.867190	1.943654	-0.553832
C	1.964381	2.570239	-1.805698
C	1.740088	2.735998	0.602375
C	1.962553	3.965282	-1.894552
H	2.072366	1.974731	-2.707539

C	1.752852	4.125458	0.508292
H	1.657139	2.269197	1.581299
C	1.869162	4.743214	-0.740424
H	2.062368	4.439859	-2.866474
H	1.685638	4.727199	1.410012
H	1.897438	5.826698	-0.810508
H	1.811468	-1.977814	1.391881
P	-2.110168	-0.588520	0.129352
C	-2.736455	-1.174176	-1.485850
C	-3.680115	-2.238921	-3.894495
C	-3.743826	-0.512868	-2.204622
C	-2.204909	-2.373510	-1.986225
C	-2.683109	-2.904419	-3.181878
C	-4.207310	-1.043392	-3.406541
H	-4.179156	0.410683	-1.834389
H	-1.426670	-2.893785	-1.433625
H	-2.276325	-3.838789	-3.556773
H	-4.985413	-0.525144	-3.958667
H	-4.048000	-2.651918	-4.828812
C	-2.444290	1.244957	0.016393
C	-2.738877	4.001791	-0.318066
N	-1.490683	2.013679	-0.559882
C	-3.595527	1.869694	0.471889
C	-3.748754	3.253125	0.302714
C	-1.602427	3.344667	-0.737902
H	-4.370128	1.281643	0.951466
H	-2.836933	5.071950	-0.457262
C	-3.329827	-1.074691	1.395846
C	-5.139721	-1.771858	3.404724
C	-4.590609	-1.585643	1.056897
C	-2.975384	-0.926876	2.746848
C	-3.883316	-1.267103	3.745506
C	-5.489265	-1.934877	2.064959
H	-4.868420	-1.723715	0.016353
H	-1.987410	-0.559607	3.015589
H	-3.607194	-1.150706	4.789103
H	-6.461565	-2.339223	1.800419
H	-5.842589	-2.047232	4.185178
C	1.840078	-4.193641	1.707329
H	2.740578	-4.107557	1.094057
H	1.353401	-5.145217	1.482723
H	2.140136	-4.214340	2.760813
C	0.884486	-3.057729	1.455701
H	-1.332670	-3.405310	1.693178
C	-0.402157	-2.923028	1.432295
H	-0.614288	1.564664	-0.829752
H	3.769036	-2.489679	3.119729
H	-0.757131	3.841709	-1.201032
Cl	6.656409	1.296912	2.158084
Cl	-5.168002	4.023934	0.848168

Complex 7+ (4Cl)

SCF done: -3497.585718

Pd	0.083778	-1.044210	-0.714037
P	-1.626307	0.205568	0.325875
C	-3.345316	0.215071	-0.431214
N	-3.864540	-0.970997	-0.827853
C	-4.115725	1.358583	-0.606979
C	-5.092573	-1.090935	-1.361237
C	-5.395953	1.258827	-1.165788
C	-5.901537	0.012076	-1.546304
H	-6.889708	-0.091673	-1.978519
H	-3.728372	2.324362	-0.306259
C	-2.031358	-0.385235	2.013498
C	-3.198280	-0.023041	2.704882
C	-1.116513	-1.254371	2.626052
C	-3.432475	-0.510249	3.988808
H	-3.931196	0.636203	2.247514
C	-1.352364	-1.736430	3.912430
H	-0.229477	-1.563140	2.076005
C	-2.509727	-1.363888	4.594739
H	-4.338789	-0.226647	4.515407
H	-0.640743	-2.412877	4.377089
H	-2.699177	-1.744799	5.593800
C	-1.355003	2.018520	0.447871
C	-1.613430	2.768571	1.602747
C	-0.891723	2.672035	-0.706059
C	-1.427617	4.152027	1.595090
H	-1.967387	2.278869	2.504908
C	-0.725182	4.055093	-0.714357
H	-0.675320	2.095057	-1.602851
C	-0.994922	4.797359	0.437039
H	-1.639889	4.727302	2.491765
H	-0.390861	4.554626	-1.619069
H	-0.872583	5.876457	0.428977
H	1.158375	-3.461532	-1.404557
P	2.271516	-0.395063	-0.224149
C	3.159782	-1.473295	0.964917
C	4.464970	-3.216755	2.730639
C	4.389275	-1.111528	1.547671
C	2.593585	-2.716388	1.287118
C	3.246469	-3.583298	2.162230
C	5.034286	-1.979340	2.425077
H	4.853585	-0.157471	1.309972
H	1.644177	-3.003396	0.843362
H	2.804489	-4.546749	2.397660
H	5.985658	-1.693868	2.863975
H	4.973586	-3.893556	3.410546
C	2.557830	1.244545	0.614919
C	2.748576	3.644499	2.051431
N	2.371117	1.315692	1.958420
C	2.858682	2.428427	-0.050975
C	2.959978	3.623385	0.662417
C	2.455201	2.456507	2.676676
H	3.034494	2.406635	-1.120400
H	2.827091	4.562320	2.621233
C	3.315252	-0.200615	-1.715451
C	4.767670	0.141803	-4.082231
C	4.659128	-0.590746	-1.779027
C	2.698656	0.341798	-2.855549
C	3.427013	0.524209	-4.028893
C	5.377097	-0.421474	-2.961962
H	5.145338	-1.044490	-0.921853
H	1.642568	0.603384	-2.825577
H	2.945079	0.947438	-4.905207
H	6.415495	-0.735457	-3.007722
H	5.332769	0.270476	-5.000364
C	-1.506946	-2.091947	-3.195093
H	-2.402372	-1.529444	-2.926030
H	-1.822507	-2.917340	-3.845208
H	-0.862121	-1.436209	-3.783920
C	-0.751816	-2.632702	-1.996940
H	1.200628	-2.344371	-2.862077
C	0.650300	-2.708330	-1.998163
C	-1.534732	-3.486883	-1.068121
O	-2.737552	-3.320189	-0.819675
H	-2.427677	-5.802878	-0.135783
C	-1.580009	-5.346925	0.377982
H	-0.864556	-6.108414	0.683148
H	-1.937344	-4.779523	1.239884
O	-0.856472	-4.486579	-0.524358
H	-3.302878	-1.881945	-0.779223
H	2.205757	0.442453	2.453508
Cl	3.360832	5.071147	-0.152225
Cl	-6.344299	2.667503	-1.373802
H	2.296000	2.372744	3.745610
H	-5.392271	-2.095966	-1.638520

Complex 8+ (4Cl)

SCF done: -3151.887175

Pd	-0.097971	-0.046222	-0.367750
P	-2.249390	-0.644692	0.117218

C	-3.409281	0.641877	-0.577707
N	-3.694691	0.579175	-1.903941
C	-3.909563	1.723058	0.136990
C	-4.418629	1.507915	-2.565818
C	-4.666643	2.700220	-0.516145
C	-4.920904	2.597635	-1.894064
H	-5.503484	3.345809	-2.418096
H	-3.714269	1.796470	1.200899
H	-4.579386	1.338314	-3.624478
C	-2.923713	-2.146525	-0.676195
C	-4.302986	-2.408581	-0.776960
C	-2.008684	-3.078311	-1.190468
C	-4.749042	-3.583790	-1.375799
H	-5.031356	-1.703456	-0.383371
C	-2.461763	-4.255547	-1.782913
H	-0.943487	-2.870022	-1.122749
C	-3.829475	-4.508103	-1.875731
H	-5.814256	-3.781919	-1.447924
H	-1.747782	-4.973386	-2.175127
H	-4.182213	-5.424296	-2.339610
C	-2.705818	-0.658798	1.887575
C	-3.624978	-1.561214	2.438447
C	-2.070169	0.280060	2.718163
C	-3.917866	-1.508378	3.800226
H	-4.100842	-2.313412	1.817953
C	-2.384372	0.339575	4.074148
H	-1.325745	0.954347	2.298236
C	-3.308062	-0.555379	4.615446
H	-4.626289	-2.213812	4.223887
H	-1.900556	1.075342	4.709805
H	-3.545545	-0.515969	5.674282
H	-3.363978	-0.235277	-2.416901
P	2.165314	0.405866	-0.572364
C	3.056136	-0.305163	-1.999355
C	4.334452	-1.534852	-4.158050
C	4.383615	0.026771	-2.314577
C	2.375046	-1.251615	-2.778438
C	3.015064	-1.864970	-3.853497
C	5.015973	-0.587547	-3.391183
H	4.916688	0.780239	-1.741717
H	1.342167	-1.495432	-2.538899
H	2.482877	-2.594148	-4.456857
H	6.040397	-0.323995	-3.636230
H	4.832524	-2.009420	-4.998182
C	3.007812	-0.468648	0.854300
C	3.925648	-2.036034	2.967924
N	2.198734	-1.310785	1.536332
C	4.336728	-0.378894	1.238349
C	4.800928	-1.165535	2.299963
C	2.610281	-2.084706	2.558640
H	5.007856	0.297524	0.722420
H	1.866874	-2.721173	3.024991
H	4.268455	-2.653557	3.789879
C	2.760834	2.122162	-0.378116
C	3.449848	4.819939	-0.108633
C	3.012274	2.903069	-1.515499
C	2.834419	2.710226	0.893760
C	3.186561	4.050882	1.025072
C	3.357346	4.246190	-1.375554
H	2.948879	2.467037	-2.508194
H	2.619089	2.129254	1.787289
H	3.254909	4.495484	2.013399
H	3.559180	4.842220	-2.260405
H	3.725070	5.864932	-0.003847
H	1.208980	-1.306923	1.214495
Cl	-5.291351	4.021973	0.363266
Cl	6.434802	-1.068022	2.782979

TS1-1a (6Me)
SCF done: -2427.752351

Pd	-0.113958	-1.228970	-0.217544
P	-2.096326	0.016884	-0.319436
C	-2.511792	0.293328	1.478925
N	-1.911117	-0.579760	2.321875
C	-3.298302	1.293218	2.036634
C	-2.019584	-0.574272	3.667211
C	-3.455065	1.342968	3.421859
C	-2.821872	0.407998	4.238696
H	-2.931031	0.441431	5.316734
H	-3.772340	2.019594	1.386094
C	-2.446364	1.685499	-1.002556
C	-3.581680	1.973523	-1.772119
C	-1.493560	2.689754	-0.775852
C	-3.763902	3.252823	-2.296334
H	-4.319222	1.202850	-1.971484
C	-1.688312	3.967604	-1.293213
H	-0.596297	2.467509	-0.203127
C	-2.821920	4.251115	-2.055415
H	-4.643476	3.465867	-2.896971
H	-0.942977	4.737441	-1.116486
H	-2.965866	5.245227	-2.468738
C	-3.537322	-0.985903	-0.872386
C	-3.321522	-1.864582	-1.943617
C	-4.818041	-0.899827	-0.308791
C	-4.369712	-2.630688	-2.449294
H	-2.326180	-1.956043	-2.370272
C	-5.859911	-1.681935	-0.804793
H	-5.014406	-0.222100	0.517256
C	-5.638386	-2.544695	-1.877470
H	-4.191059	-3.302736	-3.283505
H	-6.846225	-1.613144	-0.355010
H	-6.452381	-3.150673	-2.264298
P	1.975339	-0.100226	-0.252663
C	2.923697	-0.286781	1.317250
C	4.343990	-0.671168	3.710801
C	4.030014	0.517072	1.628660
C	2.534020	-1.274801	2.230069
C	3.241658	-1.470962	3.415703
C	4.734206	0.324315	2.815544
H	4.341639	1.302919	0.946860
H	1.668607	-1.891017	1.998262
H	2.934936	-2.251209	4.107534
H	5.589879	0.954435	3.041269
H	4.896572	-0.820530	4.633955
C	2.204640	1.718394	-0.554648
C	2.502047	4.423152	-0.753870
N	1.712310	2.492740	0.421506
C	2.840799	2.235497	-1.685560
C	2.981199	3.618521	-1.781266
C	1.867398	3.822353	0.340762
H	3.225953	1.578735	-2.457227
H	2.616010	5.502231	-0.792809
C	3.046753	-0.853815	-1.547865
C	4.548823	-1.991311	-3.626268
C	4.426359	-1.047766	-1.402715
C	2.428043	-1.246624	-2.744539
C	3.175412	-1.803883	-3.780276
C	5.170242	-1.616717	-2.435708
H	4.922698	-0.766012	-0.479160
H	1.352840	-1.122680	-2.856341
H	2.683639	-2.100537	-4.702431
H	6.238346	-1.768461	-2.308015
H	5.131576	-2.434072	-4.428897
H	-1.276970	-1.253601	1.844859
H	3.472652	4.060945	-2.643436
H	-4.074286	2.115463	3.868760
C	-0.848540	-3.158781	0.029728
H	-1.824378	-3.614598	0.050350
C	0.414265	-3.276963	-0.026086
C	1.658922	-4.066173	-0.077367
H	2.347723	-3.782823	0.724198

H	2.183378	-3.890356	-1.021457
H	1.444606	-5.136808	0.011344
C	-1.244636	-1.594740	4.434358
H	-1.527642	-1.580518	5.487423
H	-1.416346	-2.600986	4.039872
H	-0.171221	-1.385108	4.362885
C	1.325605	4.632943	1.485507
H	1.773155	4.302129	2.427672
H	1.527480	5.699045	1.359033
H	0.243127	4.493950	1.577968

TS1-1a (4NMe$_2$)

SCF done: 2617.010199

Pd	-0.069582	-1.658492	-0.222336
P	-1.928108	-0.384877	-0.852919
C	-2.727407	0.068882	0.768437
N	-2.375661	-0.747497	1.796032
C	-3.563420	1.132253	1.014160
C	-2.821207	-0.556133	3.053033
C	-4.065850	1.384625	2.324069
C	-3.663384	0.481226	3.351238
H	-3.990085	0.603014	4.374805
H	-3.819027	1.775071	0.181813
H	-2.468417	-1.254373	3.803046
C	-2.041338	1.217544	-1.749853
C	-2.959090	1.450321	-2.783188
C	-1.130184	2.223743	-1.397074
C	-2.966652	2.676403	-3.448368
H	-3.662193	0.676781	-3.075267
C	-1.152099	3.449626	-2.057138
H	-0.407007	2.046043	-0.604855
C	-2.067115	3.677217	-3.085827
H	-3.675676	2.845494	-4.253927
H	-0.440117	4.220298	-1.775794
H	-2.073309	4.629050	-3.609594
C	-3.245991	-1.392588	-1.654790
C	-2.834625	-2.273879	-2.665516
C	-4.607888	-1.311865	-1.336743
C	-3.768742	-3.046211	-3.352158
H	-1.777666	-2.362163	-2.903144
C	-5.538312	-2.101169	-2.011962
H	-4.951472	-0.633849	-0.560793
C	-5.121518	-2.965433	-3.022982
H	-3.437113	-3.720044	-4.136813
H	-6.590514	-2.037226	-1.749345
H	-5.847921	-3.577222	-3.549875
P	1.928063	-0.539265	0.400842
C	2.321889	-0.727397	2.193029
C	2.896721	-1.109145	4.915634
C	3.250031	0.094470	2.848550
C	1.678319	-1.732381	2.926108
C	1.966633	-1.926567	4.276503
C	3.535198	-0.097226	4.198976
H	3.747861	0.892446	2.305252
H	0.947406	-2.362026	2.423927
H	1.465179	-2.717036	4.828786
H	4.256915	0.547320	4.693048
H	3.122330	-1.257064	5.967959
C	2.257999	1.276001	0.188801
C	2.630714	3.971902	0.067537
N	1.405387	2.052287	0.879838
C	3.297090	1.762241	-0.593783
C	3.507274	3.160463	-0.688643
C	1.626062	3.370493	0.810368
H	3.944412	1.066798	-1.111729
H	0.948108	3.996796	1.389245
H	2.726886	5.050686	0.082732
C	3.357793	-1.312607	-0.469398
C	5.439950	-2.496613	-1.931922
C	4.592149	-1.575892	0.137871
C	3.178029	-1.658416	-1.817580
C	4.214490	-2.238158	-2.546480
C	5.624228	-2.168333	-0.589659
H	4.746633	-1.329902	1.183965
H	2.214368	-1.480806	-2.290331
H	4.060708	-2.499936	-3.589699
H	6.573558	-2.376284	-0.103777
H	6.245091	-2.960014	-2.495099
H	-1.671874	-1.468010	1.568288
C	-0.844019	-3.585393	-0.235664
H	-1.796130	-4.016142	-0.495087
C	0.373123	-3.715064	0.096112
C	1.569174	-4.513075	0.424372
H	1.991941	-4.224137	1.391412
H	2.351673	-4.353938	-0.323872
H	1.327756	-5.581266	0.456630
N	-4.882991	2.424196	2.578083
N	4.505325	3.685663	-1.453702
C	5.400956	2.808389	-2.185236
H	6.104317	3.412310	-2.758448
H	5.979213	2.160230	-1.514023
H	4.852768	2.171466	-2.890115
C	4.714626	5.120655	-1.487145
H	4.969971	5.521418	-0.497288
H	5.538753	5.347623	-2.163339
H	3.825380	5.648657	-1.853954
C	-5.242174	3.355617	1.514562
H	-5.853292	4.153700	1.933084
H	-4.351371	3.809313	1.067530
H	-5.821473	2.860163	0.727112
C	-5.406560	2.640036	3.921776
H	-6.096865	3.481894	3.903910
H	-5.956835	1.762276	4.277455
H	-4.605079	2.871443	4.632848

TS1-1a (6Cl)

SCF done: -3268.200353

Pd	-0.142285	-1.346342	-0.300803
P	-2.062526	-0.030843	-0.500599
C	-2.475383	0.422143	1.264400
N	-1.954616	-0.431165	2.181550
C	-3.186724	1.519521	1.734242
C	-2.106743	-0.296742	3.511114
C	-3.358870	1.692371	3.108075
C	-2.824556	0.777606	4.014268
H	-2.942843	0.890194	5.084991
H	-3.586978	2.231825	1.021949
C	-2.325785	1.591459	-1.318649
C	-3.322851	1.792951	-2.282061
C	-1.453674	2.642130	-0.997084
C	-3.449876	3.033931	-2.905257
H	-3.998508	0.986926	-2.548775
C	-1.600240	3.884472	-1.607940
H	-0.658027	2.484304	-0.273361
C	-2.596297	4.081423	-2.565268
H	-4.222086	3.180460	-3.654842
H	-0.929610	4.695851	-1.341444
H	-2.702971	5.048252	-3.048528
C	-3.560390	-0.989976	-0.978027
C	-3.387761	-2.012379	-1.921519
C	-4.845935	-0.724958	-0.484851
C	-4.482771	-2.750133	-2.368105
H	-2.391835	-2.234473	-2.295477
C	-5.934771	-1.478489	-0.917981
H	-5.008662	0.072327	0.234887
C	-5.755093	-2.489547	-1.861906
H	-4.338226	-3.534982	-3.104733
H	-6.924871	-1.271723	-0.522219
H	-6.605930	-3.073107	-2.200963
P	1.976504	-0.270459	-0.323486
C	2.904895	-0.418457	1.259263
C	4.286218	-0.734700	3.682114

C	4.040855	0.355910	1.539498
C	2.465378	-1.341059	2.216537
C	3.154115	-1.502547	3.417976
C	4.726076	0.196646	2.741682
H	4.391660	1.091972	0.821623
H	1.575477	-1.930994	2.011495
H	2.804471	-2.226642	4.148676
H	5.603597	0.803673	2.945123
H	4.822499	-0.856783	4.618729
C	2.245048	1.534109	-0.672449
C	2.593786	4.247868	-0.928082
N	1.706277	2.348464	0.252260
C	2.951952	2.021411	-1.772054
C	3.121607	3.401870	-1.894688
C	1.890890	3.646174	0.118530
H	3.372464	1.341793	-2.504156
H	2.713073	5.323989	-0.973379
C	3.044988	-1.069039	-1.592283
C	4.541923	-2.283460	-3.629221
C	4.408486	-1.332349	-1.409387
C	2.438178	-1.432746	-2.804502
C	3.183927	-2.028193	-3.819677
C	5.149813	-1.939180	-2.422724
H	4.892428	-1.075974	-0.472043
H	1.373576	-1.257186	-2.944679
H	2.702433	-2.302174	-4.754117
H	6.204988	-2.144864	-2.266604
H	5.122662	-2.756193	-4.416018
H	-1.350467	-1.179753	1.784387
H	3.673430	3.813930	-2.734748
H	-3.916250	2.546419	3.481624
C	-0.894245	-3.274998	-0.050539
H	-1.877512	-3.713089	-0.031271
C	0.366956	-3.399386	-0.061175
C	1.616522	-4.181471	-0.053654
H	2.272041	-3.881112	0.769292
H	2.174832	-4.021228	-0.980932
H	1.401802	-5.250905	0.046612
Cl	-1.382639	-1.476821	4.507773
Cl	1.177301	4.668372	1.346859

TS1-1a (4Cl)

SCF done: -3268.200446

Pd	-0.086662	-1.490128	-0.218664
P	-1.994862	-0.210206	-0.672224
C	-2.652585	0.143685	1.038130
N	-2.203324	-0.709483	1.987948
C	-3.476556	1.188740	1.435805
C	-2.517284	-0.618251	3.290616
C	-3.824944	1.310925	2.783735
C	-3.345017	0.393995	3.729352
H	-3.601004	0.480982	4.778211
H	-3.831547	1.900559	0.698825
H	-2.081971	-1.358030	3.952323
C	-2.205412	1.435671	-1.457894
C	-3.194743	1.698792	-2.415233
C	-1.298197	2.445850	-1.105417
C	-3.277252	2.960376	-3.003403
H	-3.895087	0.923121	-2.707670
C	-1.396064	3.706896	-1.686875
H	-0.517798	2.241147	-0.377446
C	-2.383082	3.965180	-2.638721
H	-4.042286	3.155332	-3.749273
H	-0.690879	4.483970	-1.406979
H	-2.450200	4.945871	-3.100659
C	-3.364299	-1.204826	-1.393837
C	-3.017069	-2.097716	-2.418276
C	-4.707857	-1.096983	-1.008900
C	-3.997601	-2.857433	-3.052627
H	-1.975372	-2.204432	-2.709409
C	-5.683062	-1.874417	-1.631792
H	-5.006835	-0.406457	-0.225303
C	-5.330227	-2.751720	-2.656352
H	-3.717258	-3.539755	-3.849671
H	-6.719761	-1.789638	-1.319188
H	-6.092244	-3.353309	-3.142927
P	1.975277	-0.395448	0.217090
C	2.586894	-0.654379	1.935245
C	3.485668	-1.135843	4.551044
C	3.629251	0.107738	2.483416
C	1.994957	-1.650053	2.722291
C	2.444010	-1.893656	4.019790
C	4.075206	-0.133466	3.780986
H	4.093888	0.897271	1.899762
H	1.178340	-2.233818	2.303799
H	1.981215	-2.676080	4.615317
H	4.884086	0.464060	4.191614
H	3.836447	-1.322651	5.561912
C	2.252850	1.436830	0.067202
C	2.572204	4.158517	0.063696
N	1.510154	2.168343	0.911979
C	3.163482	1.999029	-0.830740
C	3.310847	3.385415	-0.827085
C	1.686268	3.491583	0.908312
H	3.749073	1.381212	-1.501147
H	1.084969	4.059222	1.616222
H	2.680798	5.236639	0.098854
C	3.284528	-1.083585	-0.877748
C	5.168339	-2.109646	-2.684245
C	4.595567	-1.347934	-0.461041
C	2.925915	-1.352656	-2.208023
C	3.864276	-1.853803	-3.107533
C	5.529228	-1.861110	-1.360742
H	4.889644	-1.164646	0.567929
H	1.903022	-1.175683	-2.534176
H	3.574508	-2.053023	-4.135314
H	6.541459	-2.067067	-1.024608
H	5.899177	-2.507822	-3.382102
H	-1.518059	-1.412865	1.639637
C	-0.864905	-3.420159	-0.164401
H	-1.838569	-3.848773	-0.330630
C	0.381794	-3.554812	0.020232
C	1.616273	-4.342558	0.188175
H	2.140229	-4.077330	1.111317
H	2.307470	-4.149174	-0.637730
H	1.390344	-5.414107	0.213017
Cl	-4.849205	2.589859	3.288612
Cl	4.424983	4.139473	-1.917510