

Supporting Information for

Palladium–catalysed methoxycarbonylation of ethene with bidentate diphosphine ligands: a density functional theory study

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Table S1. (Carbomethoxy Pathway – A) 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. $\delta E_{solv} = (\Delta E_{PCM} - \Delta E)$; ΔG_1 = relative free energies and ΔH_1 = relative enthalpies ^d. For the overall barriers, please see Table S5.

Step	ΔE	δ_{D3}	δE_{solv}	δE_G	δE_H	ΔG	ΔH	ΔG_1	ΔH_1
<i>Carbomethoxy Pathway – A reaction energies and enthalpies for every individual step</i>									
1 + CO → 2	-11.7	-4.5	2.7	13.3	1.9	-0.3	-11.7	-0.3	-11.7
2 → TS2–3	1.8	-0.4	-0.4	-0.6	-1.0	0.4	0.0	0.1	-11.6
2 → 3	-11.9	2.2	-1.1	-1.4	0.3	-12.1	-10.5	-12.4	-22.1
3 + Ethylene → 4	-3.6	-11.0	3.1	15.8	2.4	4.2	-9.2	-8.2	-31.3
4 → TS4–5	14.5	1.7	-0.1	1.1	-0.3	17.2	15.8	9.0	-15.5
4 → 5	-23.1	4.2	-0.7	0.3	0.2	-19.3	-19.4	-27.5	-50.8
5 + MeOH → 6	-6.2	-9.8	5.7	15.8	2.6	5.4	-7.7	-22.0	-58.5
6 → TS6–1	35.5	1.2	-3.9	-5.4	-4.2	27.5	28.7	5.5	-29.8
6 → 1 + MeP	-5.5	-13.8	8.5	17.5	2.3	6.7	-8.5	-15.4	-66.9

^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 S2. (Ketene Pathway – B) 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. $\delta E_{solv} = (\Delta E_{PCM} - \Delta E)$; ΔG_1 = relative free energies and ΔH_1 = relative enthalpies ^d. For the overall barriers, please see Table S5.

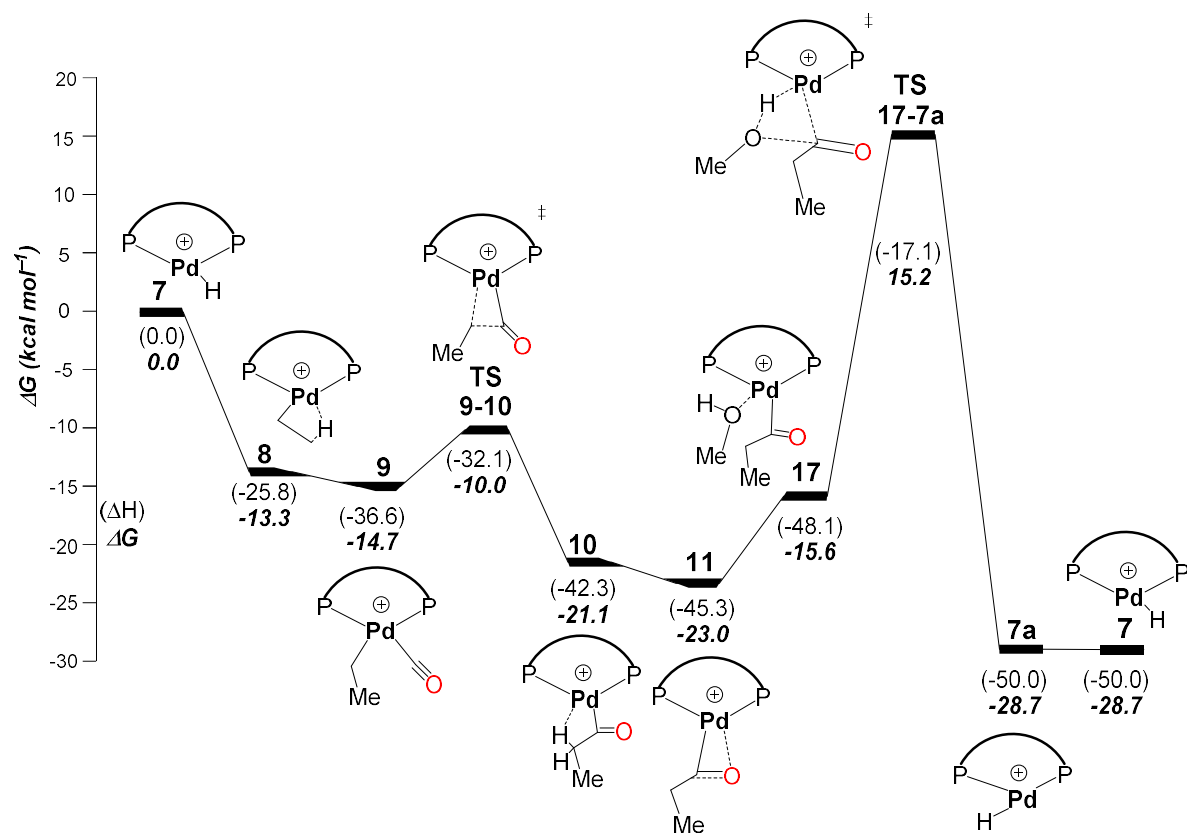
Step	ΔE	δ_{D3}	δE_{solv}	δE_G	δE_H	ΔG	ΔH	ΔG_1	ΔH_1
<i>Ketene Pathway – B reaction energies and enthalpies for every individual step</i>									
7 + Ethylene → 8	-25.2	-9.2	5.3	15.8	3.3	-13.3	-25.8	-13.3	-25.8
8 + CO → 9	-8.1	-5.6	0.3	12.0	2.6	-1.4	-10.8	-14.7	-36.6
9 → TS9–10	4.9	0.5	-0.1	-0.6	-0.8	4.7	4.5	-10.0	-32.1
9 → 10	-6.3	2.3	-1.9	-0.6	0.1	-6.4	-5.7	-21.1	-42.3
10 → TS10–12	28.0	-0.5	1.0	-2.0	-3.0	26.5	25.5	5.4	-16.8
10 → 12	23.0	-1.0	1.7	-3.2	-2.1	20.6	21.6	-0.5	-20.7
12 → TS12–13	3.9	3.8	-1.9	-3.4	-1.3	2.3	4.4	1.8	-16.3
12 → 13	-3.0	5.3	1.7	-1.8	-0.3	2.2	3.7	1.7	-17.0
13 → 7a + Ketene	7.8	6.3	-7.7	-10.8	-1.5	-4.4	4.9	-2.8	-12.1
7a → 7	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-2.8	-12.1

^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 **7** set to 0 kcal mol⁻¹.

Table S3. (*Hydride-hydroxyalkylpalladium pathway – C*) 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. $\delta E_{solv} = (\Delta E_{PCM} - \Delta E)$; ΔG_1 = relative free energies and ΔH_1 = relative enthalpies^d. For the overall barriers, please see Table S5.

Step	ΔE	δ_{D3}	δE_{solv}	δE_G	δE_H	ΔG	ΔH	ΔG_1	ΔH_1
<i>Hydride-hydroxyalkylpalladium pathway – C reaction energies and enthalpies for every individual step</i>									
7.2MeOH + Ethylene → 8.2MeOH	-12.6	-5.4	1.6	11.5	2.7	-4.9	-13.7	-4.9	-13.7
8.2MeOH + CO → 9.2MeOH	-6.6	-4.8	0.1	12.1	2.8	0.8	-8.5	-4.1	-22.2
9.2MeOH → TS9–10.2MeOH	5.3	-1.0	-0.3	0.6	-0.7	4.6	3.3	0.5	-18.8
9.2MeOH → 10.2MeOH	-7.6	-0.6	-1.3	1.2	-0.2	-8.3	-9.8	-12.5	-32.0
10.2MeOH → 11.2MeOH	-5.7	0.9	1.4	1.3	0.5	-2.1	-2.9	-14.6	-34.8
11.2MeOH → TS11–14.MeOH	17.3	-3.4	-0.8	3.3	-2.9	16.3	10.2	1.8	-24.6
11.2MeOH → 14.MeOH	4.9	-3.3	0.3	4.5	0.1	6.4	2.0	-8.1	-32.8
14.MeOH → TS14–7a.MeOH	17.5	2.8	-2.8	-2.0	-1.3	15.6	16.2	7.4	-16.6
14.MeOH → 7a.MeOH + MeP	6.3	17.4	-8.4	-22.4	-4.0	-7.2	11.2	-15.4	-21.6
7a.MeOH + MeOH → 14.MeOH	-29.6	-9.3	7.5	18.1	3.0	-13.3	-28.4	-28.7	-50.0

^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 **7.2MeOH** set to 0 kcal mol⁻¹.



Scheme S1 . Hydride (unsolvated) pathway – C': free-energy profile [kcal mol⁻¹] relative to **7**, at the B3PW91-D3/ECP2/PCM // B3PW91/ECP1 level of theory using methanol as the model solvent.

Table S4. (*Hydride (unsolvated) pathway – C'*) 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. $\delta E_{\text{solv}} = (\Delta E_{\text{PCM}} - \Delta E)$; ΔG_1 = relative free energies and ΔH_1 = relative enthalpies^d. For the overall barriers, please see Table S5.

Step	ΔE	δ_{D3}	δE_{solv}	δE_G	δE_H	ΔG	ΔH	ΔG_1	ΔH_1
<i>Hydride (unsolvated) pathway – C' reaction energies and enthalpies for every individual step</i>									
7 + Ethylene → 8	-25.2	-9.2	5.3	15.8	3.3	-13.3	-25.8	-13.3	-25.8
8 + CO → 9	-8.1	-5.6	0.3	12.0	2.6	-1.4	-10.8	-14.7	-36.6
9 → TS9–10	4.9	0.5	-0.1	-0.6	-0.8	4.7	4.5	-10.0	-32.1
9 → 10	-6.3	2.3	-1.9	-0.6	0.1	-6.4	-5.7	-21.1	-42.3
10 → 11	-6.6	1.1	2.1	1.5	0.4	-1.9	-3.0	-23.0	-45.3
11 + MeOH → 17	3.0	-9.8	2.3	11.9	1.7	7.4	-2.8	-15.6	-48.1
17 → TS17–7a	28.9	3.7	1.0	-2.8	-2.5	30.8	31.0	15.2	-17.1
17 → 7a + MeP	-7.8	16.0	-6.8	-14.4	-3.2	-13.1	-1.8	-28.7	-50.0
7a → 7	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-28.7	-50.0

^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 **7** set to 0 kcal mol⁻¹.

Table S5. (overall barriers) 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. $\delta E_{\text{solv}} = (\Delta E_{\text{PCM}} - \Delta E)$.

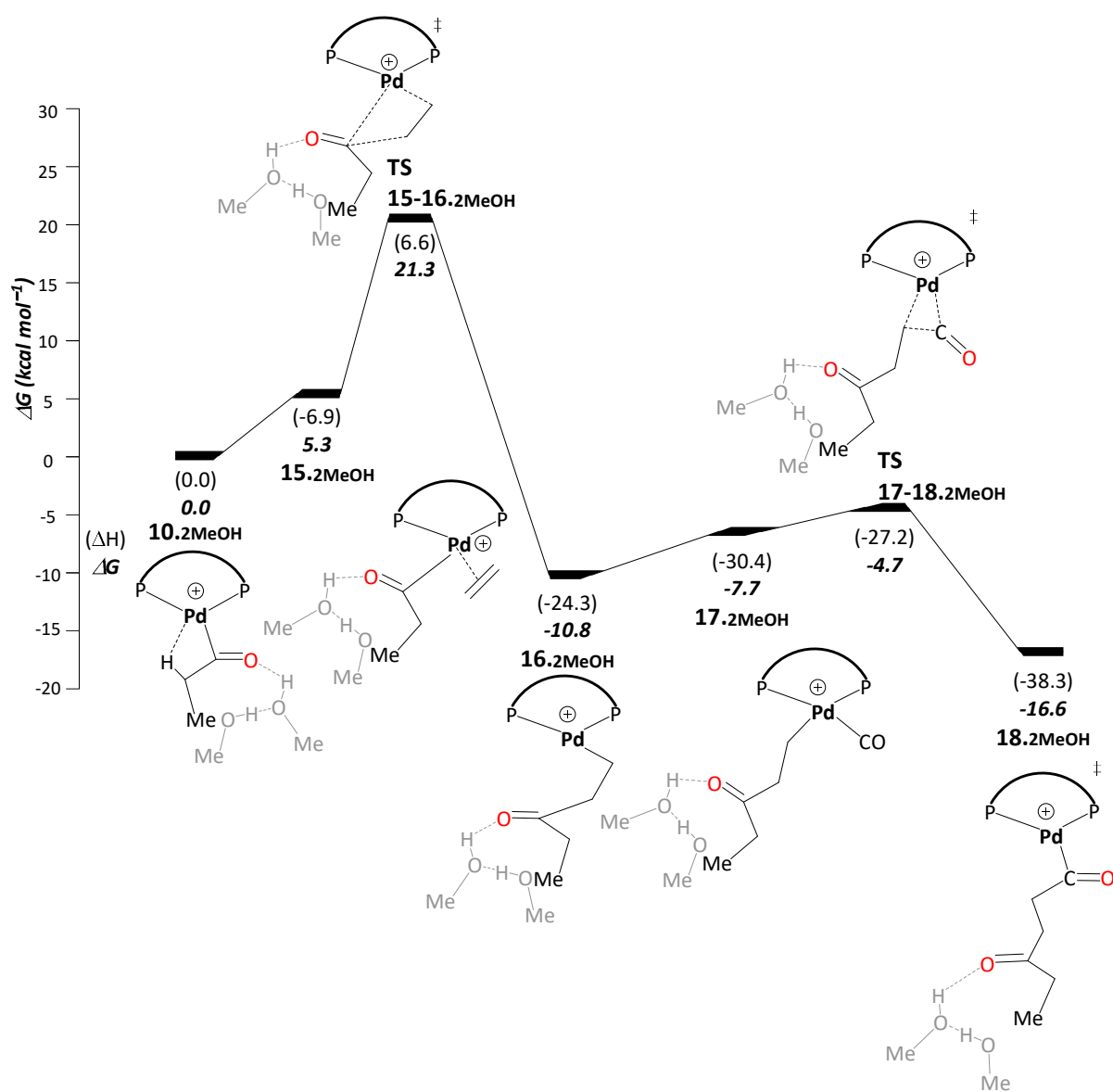
Step	ΔE	δ_{D3}	δE_{solv}	δE_G	δE_H	ΔG	ΔH
<i>Carbomethoxy Pathway – A (DTBPX)</i>							
5 + MeOH → TS6–1	29.4	-8.6	1.8	10.4	-1.5	32.9	21.0
<i>Ketene Pathway – B (DTBPX)</i>							
11 → TS10–12	34.6	-1.6	-1.1	-3.5	-3.4	28.4	28.5
<i>Hydride-hydroxyalkylpalladium pathway – C (DTBPX)</i>							
11'.MeOH → TS14–7a.MeOH	20.3	5.3	-2.1	-0.5	-1.4	23.0	22.0
<i>Hydride-hydroxyalkylpalladium pathway – C (DMBPX)</i>							
11'.MeOH → TS14–7a.MeOH	28.1	2.9	-0.2	-0.8	-1.7	30.1	29.1
<i>Hydride-hydroxyalkylpalladium pathway – C (DTBPX – 3 explicit solvent molecules)</i>							
11'.2MeOH → TS14–7a.2MeOH	17.9	1.3	-1.2	-0.2	-2.3	17.8	15.7
<i>Hydride-hydroxyalkylpalladium pathway – C (DMBPX – 3 explicit solvent molecules)</i>							
11'.2MeOH → TS14–7a.2MeOH	23.1	2.0	-0.6	0.0	-2.0	24.5	23.1
<i>Hydride (unsolvated) pathway – C' (DTBPX)</i>							
11 + MeOH → TS17–7a	31.9	-6.1	3.2	9.1	-0.9	38.1	28.2

^a B3PW91/ECP2 energies; ^b model solvent MeOH, ^c B3PW91/ECP1 energies.

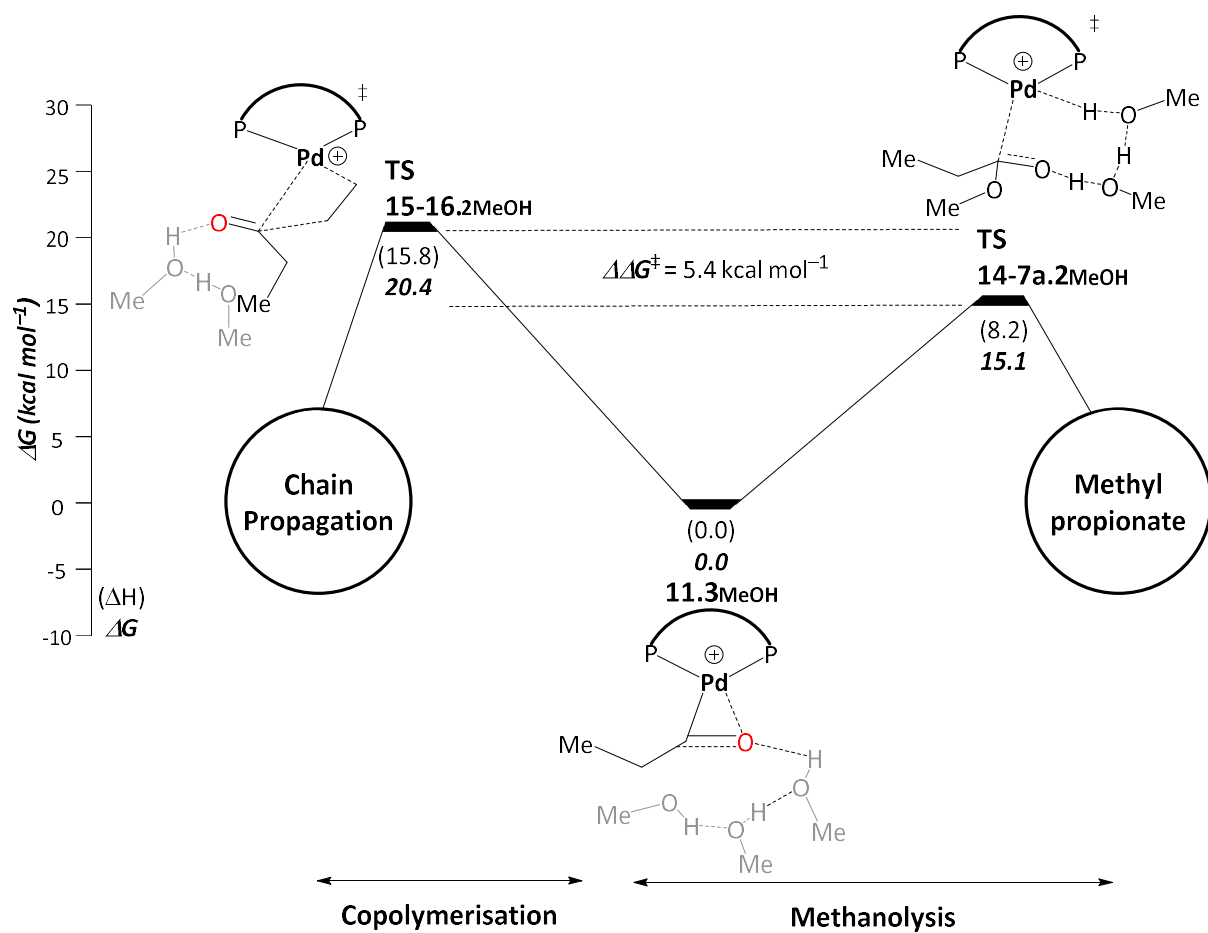
Table S6. (*selectivities*) Reaction energies in the gas phase (ΔE)^a; DFT-D3BJ corrections (δ_{D3}), Solvation (δE_{solv})^{a,b} and thermochemistry (δE_G and δE_H)^c; Final free energies (ΔG) and enthalpies (ΔH) in kcal/mol. $\delta E_{solv} = (\Delta E_{PCM} - \Delta E)$.

Step	ΔE	δ_{D3}	δE_{solv}	δE_G	δE_H	ΔG	ΔH	Selectivity (%) MePro
<i>1,2-bis(di-tert-butylphosphinomethyl)benzene (DTBPX)</i>								
TS14–7a.MeOH ^d + Ethylene → TS15–16.2MeOH	-3.6	-8.2	0.2	13.0	2.7	1.4	-8.8	88.0
TS14–7a.2MeOH ^e + Ethylene → TS15–16.2MeOH	9.6	0.8	-4.8	-0.2	2.0	5.4	7.6	99.9
<i>1,2-bis((dimethylphosphaneyl)methyl)benzene (DMBPX)</i>								
TS14–7a.MeOH ^d + Ethene → TS15–16.2MeOH	-18.2	-6.6	1.3	13.7	2.9	-9.9	-20.6	0.0
TS14–7a.2MeOH ^e + Ethene → TS15–16.2MeOH	-1.9	-0.9	-3.0	0.9	1.6	-4.8	-4.1	0.2

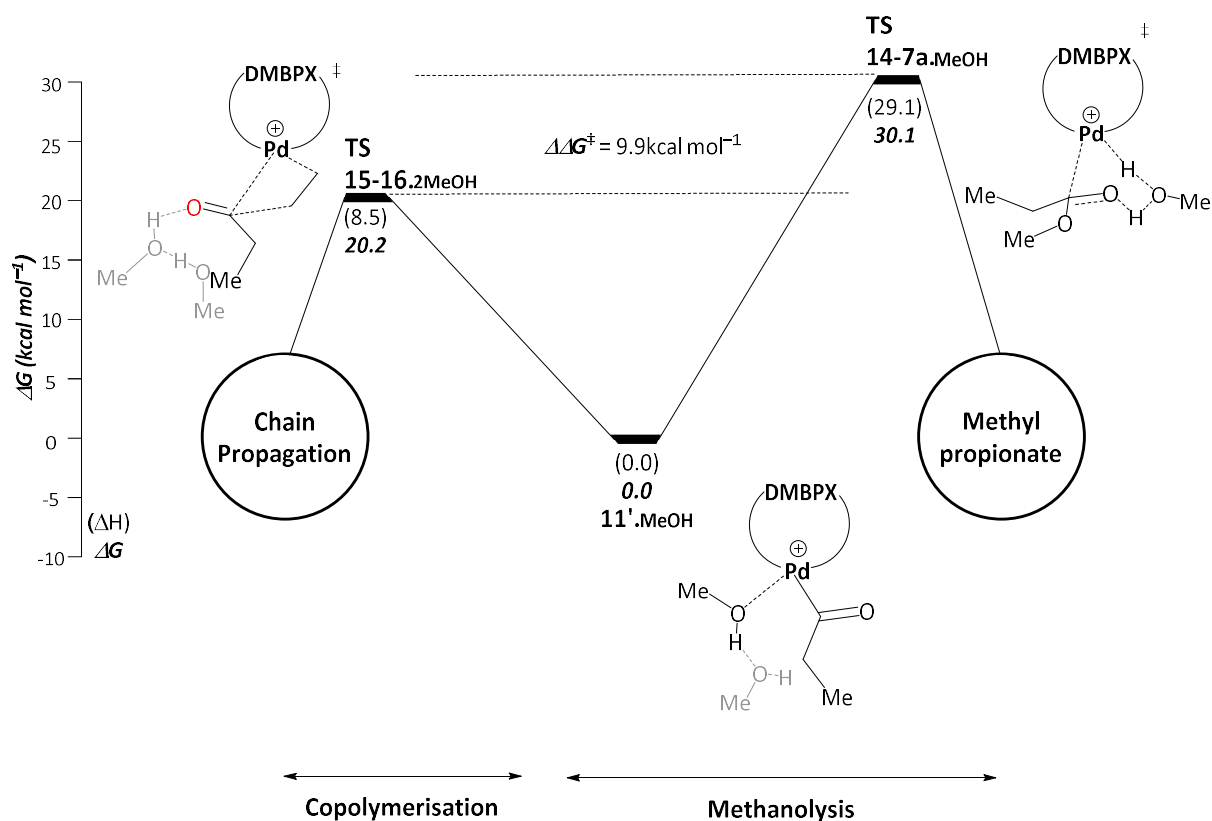
^a B3PW91/ECP2 energies; ^b model solvent MeOH, ^c B3PW91/ECP1 energies ^d transition state obtained by using two explicit solvent molecules in the prior steps ^e transition state obtained by using three explicit solvent molecules in the prior steps.



Scheme S2 . Co-polymerisation (using **DTBPX** ligand): Free energy profile using methanol as the model solvent at the B3PW91-D3/ECP2/PCM level. Energies are in kcal mol^{-1} relative to **10.2MeOH**. Explicit solvent molecules are shown in light grey colour.

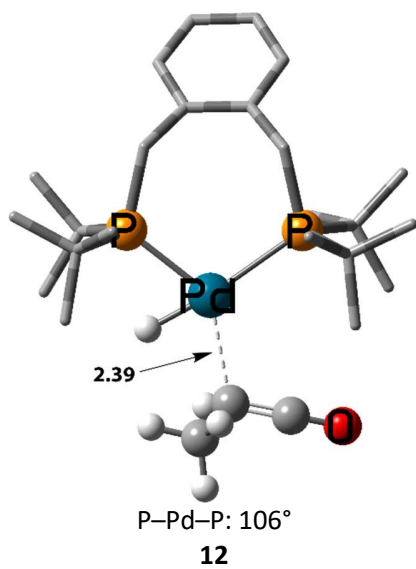


Scheme S3 . Methanolysis/copolymerisation selectivity: right – pathway C using **three explicit solvent molecules**, leading to the production of MePro, left – copolymerisation leading to the formation of oligo-/polymers. All energies are in kcal mol^{-1} relative to 11.3 MeOH . Explicit solvent molecules are shown in light grey colour.

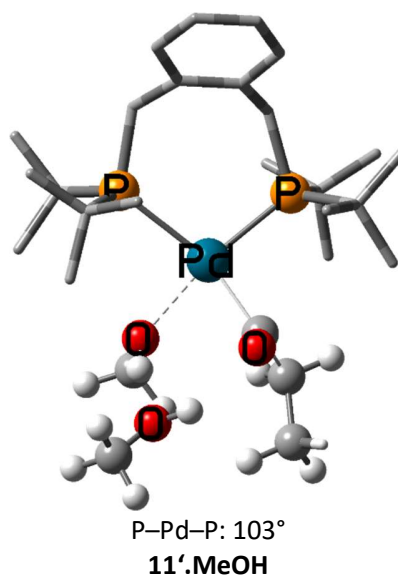


Scheme S4 . Methanolysis/copolymerisation selectivity: right – pathway C using **DMBPX** ligand, leading to the production of MePro, left – copolymerisation leading to the formation of oligo-/polymers. All energies are in kcal mol⁻¹ relative to **11'.MeOH**. Explicit solvent molecules are shown in light grey colour. Energies for **TS14-7a.2MeOH** with **DMBPX** are given in Table S5.

a)



b)



c)

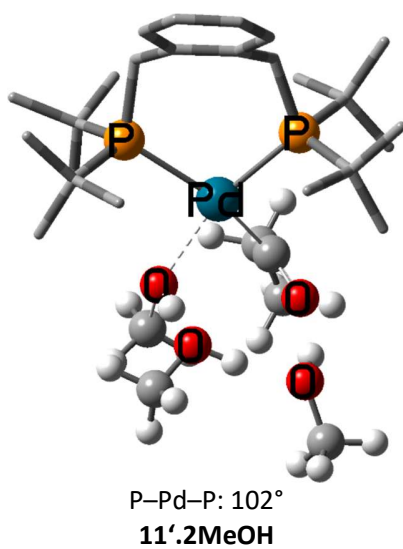


Figure S1. 3D representations of selected intermediates. Distances are given in Å.

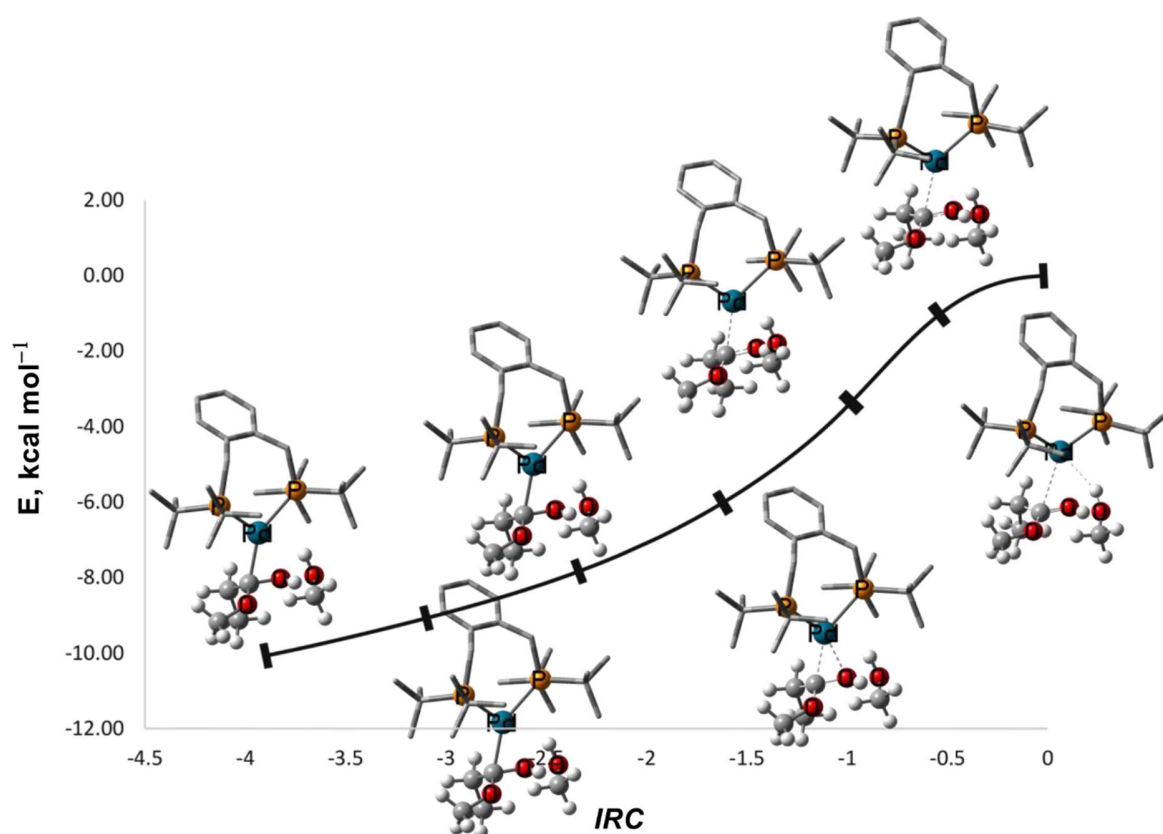


Figure S2. Gas phase intrinsic reaction coordinate calculation (reverse direction) starting from **TS14-7a.MeOH**.

Table S7. The relative TOFs

Ligand	MARI	HETS	Energy Span ^a	TOF (h ⁻¹)	TOF (relative) ^b
<i>Pathway C</i>					
DTBPX	11'.MeOH ^c	TS14–7a.MeOH ^c	23.0	155	1
DTBPX	11'.2MeOH ^d	TS14–7a.2MeOH ^c	17.8	256,000	1.65 × 10 ³
DMBPX	11'.MeOH ^c	TS14–7a.MeOH ^c	30.1	0.01	4.03 × 10 ⁻⁵
DMBPX	11'.2MeOH ^d	TS14–7a.2MeOH ^d	24.5	18.30	1.18 × 10 ⁻¹

^aIn kcal/mol, from computed free energies according to Shaik's model (refs 38-40 in the main paper);

^bRelative to the TOF computed for the **DTBPX** ligand with one additional MeOH;

^cMARI and HETS for the pathways using two explicit methanol molecules

^dMARI and HETS for the pathways using three explicit methanol molecules

Table S8. (overall barriers) 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. $\delta E_{solv} = (\Delta E_{PCM} - \Delta E)$; thermochemistry on geometries optimised using PCM optimised geometries (δE_{G-PCM} and δE_{H-PCM}); ^d Reaction energies in the solution phase (ΔE_{PCM})^e

Carbomethoxy Pathway – A (DTBPX)

	ΔE	δ_{D3}	δE_{solv}	δE_G	δE_H	ΔG	ΔH
5 + MeOH → TS6–1	29.4	-8.6	1.8	10.4	-1.5	32.9	21.0
	ΔE_{PCM}	δ_{D3}		δE_{G-PCM}	δE_{H-PCM}	ΔG	ΔH
5 + MeOH → TS6–1	31.0	-9.0		10.4	-1.3	32.4	20.7

Ketene Pathway – B (DTBPX)

	ΔE	δ_{D3}	δE_{solv}	δE_G	δE_H	ΔG	ΔH
11 → TS10–12	34.6	-1.6	-1.1	-3.5	-3.4	28.4	28.5
	ΔE_{PCM}	δ_{D3}		δE_{G-PCM}	δE_{H-PCM}	ΔG	ΔH
11 → TS10–12	33.5	-1.8		-2.9	-3.4	28.8	28.4

Hydride-hydroxyalkylpalladium pathway – C (DTBPX)

	ΔE	δ_{D3}	δE_{solv}	δE_G	δE_H	ΔG	ΔH
11'.MeOH → TS14–7a.MeOH	20.3	5.3	-2.1	-0.5	-1.4	23.0	22.0
	ΔE_{PCM}	δ_{D3}		δE_{G-PCM}	δE_{H-PCM}	ΔG	ΔH
11'.MeOH → TS14–7a.MeOH	15.4	8.4		0.3	-1.7	24.1	22.1

Hydride-hydroxyalkylpalladium pathway – C (DTBPX – 3 explicit solvent molecules)

	ΔE	δ_{D3}	δE_{solv}	δE_G	δE_H	ΔG	ΔH
11'.2MeOH → TS14–7a.2MeOH	17.9	1.3	-1.2	-0.2	-2.3	17.8	15.7
	ΔE_{PCM}	δ_{D3}		δE_{G-PCM}	δE_{H-PCM}	ΔG	ΔH
11'.2MeOH → TS14–7a.2MeOH	16.3	2.9		0.9	-1.9	20.2	17.3

Hydride (unsolvated) pathway – C' (DTBPX)

	ΔE	δ_{D3}	δE_{solv}	δE_G	δE_H	ΔG	ΔH
11 + MeOH → TS17–7a	31.9	-6.1	3.2	9.1	-0.9	38.1	28.2
	ΔE_{PCM}	δ_{D3}		δE_{G-PCM}	δE_{H-PCM}	ΔG	ΔH
11 + MeOH → TS17–7a	35.2	-5.8		9.5	-0.7	38.8	28.7

^a B3PW91/ECP2 energies; ^b model solvent MeOH, ^c B3PW91/ECP1 energies, ^d B3PW91/ECP1/PCM energies

^e B3PW91/ECP2/PCM energies

Possible reductive elimination process for MePro formation

Previous calculations have suggested that reductive elimination from neutral Pd(II) DTBPX complexes can be very rapid.²⁵ In context of the present system this could become conceivable if coordinated MeOH ligands can be deprotonated, affording methoxide species. Reductive elimination with the acyl fragment would then produce MePro directly, and the resulting Pd(0) fragment could be re-protonated to regenerate the hydride catalyst. Entry into such a pathway could, for instance, occur at the stage of complex **17** in Scheme S1. The structures of **17** and its possible deprotonation product, **17-H⁺**, are depicted in Figure S3. Indeed, upon deprotonation of the coordinated methanol, the resulting methoxide ligand comes closer to the carbonyl carbon of the neighbouring acyl moiety [see the (Me)O...C(=O) and (Me)O...Pd distances in Figure S3]. **17-H⁺** would thus seem poised for facile reductive elimination, in agreement with previous studies.²⁵

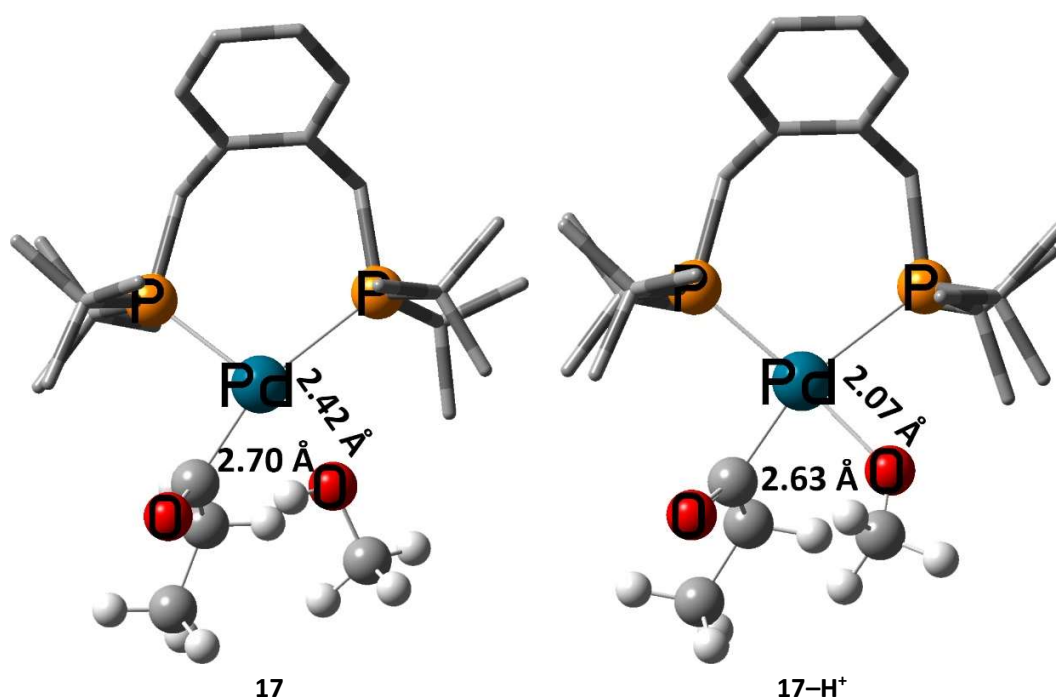
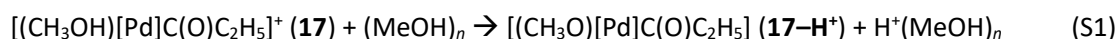


Figure S3. Optimised structures of **17** and **17-H⁺** (H atoms on the ligand omitted for clarity), including (Me)O...C(=O) and (Me)O...Pd distances [in Å].

The problem is to evaluate the driving force for this deprotonation step. There are no bases of notable strength present that could promote this step. In fact, the reaction is conducted under strongly acidic conditions. We have attempted to model this step using MeOH as proton acceptor according to:



For a single MeOH molecule ($n = 1$ in eq. S1) this step is predicted to be uphill by $\Delta G = 47.9 \text{ kcal mol}^{-1}$ (second entry in Table S9). Taking into account that production of **17** itself is endergonic by $\Delta G = 7.9 \text{ kcal mol}^{-1}$ (through MeOH addition to **11**, see Scheme S1), formation of **17-H⁺** would further be disfavoured

under turnover conditions (to more than 55 kcal mol⁻¹, see ΔG_1 value in Table S9). The reliability of this value, however, may be doubted because of possible shortcomings of the simple continuum model involved. The resulting protonated methanol is likely to be stabilised by H-bonding interactions, which are not properly described by this model. In order to account for these interactions, we have added additional explicit MeOH molecules to form neutral and protonated MeOH clusters. Fife *et al.*³⁵ have shown that the properties of methanol clusters begin to converge and represent that of bulk methanol when the cluster size reaches nine units. Using the preferential geometries given in ref 35, we have re-evaluated the energetics of eq. S1 for $n = 9$ (third entry in Table S9). Using such cluster models for MeOH (in conjunction with the continuum model), the driving force for deprotonation is indeed reduced, but is still substantial. Relative to **11**, **17-H⁺** is computed to be less stable by 29.1 kcal mol⁻¹ (ΔG_1 value in Table S9). Taking into account that any barrier for reductive elimination would come on top of that value, and that under strongly acidic conditions of the experiment the equilibrium of eq. S1 would be further shifted to the left, we are confident that entry into such a reductive elimination pathway can be excluded.

We have tested the same process for the Pd catalyst with the less bulky ligand, DMBPX. Unlike the DTBPX ligand system, the MeOH uptake is not uphill ($\Delta G_{11.DMBPX \rightarrow 17.DMBPX} = -0.1$ kcal mol⁻¹). On going from DTBPX to DMBPX, the thermodynamic cost according to eq. S1 decreases slightly (from $\Delta G = 21.7$ kcal mol⁻¹ to 20.5 kcal mol⁻¹, Table S9), and much more so when taken relative to **11** (from $\Delta G_1 = 29.1$ kcal mol⁻¹ to 20.4 kcal mol⁻¹, Table S9). This result is again in disagreement with the experimental observations based on ligand bulk (where increased bulk is instrumental to promote the reaction) and can be taken as further evidence against a deprotonation/reductive-elimination mechanism.

Table S9. (Possible reductive elimination process for MePro formation) 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. $\delta E_{solv} = (\Delta E_{PCM} - \Delta E)$; $\Delta G_1 =$ relative free energies and $\Delta H_1 =$ relative enthalpies ^d. For the overall barriers, please see Table S5.

Step	ΔE	δ_{D3}	δE_{solv}	δE_G	δE_H	ΔG	ΔH	ΔG_1	ΔH_1
<i>Possible reductive elimination process for MePro formation (DTBPX)</i>									
11 + MeOH → 17	3.0	-9.8	2.3	11.9	1.7	7.4	-2.8	7.4	-2.8
17 + MeOH → 17-H⁺ + MeOH₂⁺	81.1	0.7	-35.1	1.1	-0.4	47.9	46.3	55.3	43.5
17 + (MeOH)₉ → 17-H⁺ + H⁺(MeOH)₉	23.5	2.6	-0.6	-3.8	-3.2	21.7	22.2	29.1	19.4
<i>Possible reductive elimination process for MePro formation (DMBPX)</i>									
11.DMBPX + MeOH → 17.DMBPX	-7.1	-8.9	3.1	12.8	1.7	-0.1	-11.2	-0.1	-11.2
17.DMBPX + MeOH → 17-H⁺.DMBPX + MeOH₂⁺	77.3	0.4	-32.0	0.9	-0.8	46.6	44.9	46.5	33.7
17.DMBPX + (MeOH)₉ → 17-H⁺.DMBPX + H⁺(MeOH)₉	19.7	2.2	2.5	-3.9	-3.6	20.5	20.8	20.4	9.6

^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 **11** set to 0 kcal mol⁻¹.

References

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- [3S] Fifen, J. J.; Nsangou, M.; Dhaouadi, Z.; Motapon, O.; Jaidane, N.-E. *J. Chem. Theory Comput.* 2013, **9**, 1173-1181.

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: -1866.281302

Pd	0.213330	-1.190986	-0.583737
P	-1.788221	-0.424279	0.260551
P	1.705506	0.260961	0.333364
C	-2.506707	-1.817893	1.357624
C	-1.913403	-1.684270	2.768864
H	-2.306361	-0.822352	3.315001
H	-0.822267	-1.625813	2.750734
H	-2.179886	-2.577369	3.344784
C	-4.037006	-1.780964	1.476772
H	-4.404863	-0.823076	1.857064
H	-4.345686	-2.549910	2.194617
H	-4.542282	-2.001600	0.534434
C	-2.055731	-3.171665	0.779584
H	-0.963126	-3.264631	0.779053
H	-2.414092	-3.345559	-0.236563
H	-2.452227	-3.977276	1.408489
C	-2.854980	-0.128024	-1.294378
C	-3.095238	-1.459824	-2.026372
H	-2.162052	-1.986493	-2.256801
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H	-3.753933	-2.136687	-1.477558
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H	-4.074198	1.546699	-0.575499
C	-2.052858	0.789250	-2.235124
H	-1.138596	0.304087	-2.587631
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C	-1.916031	1.093741	1.326748
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C	-1.357240	2.388791	0.789704
C	-2.250161	3.397119	0.404173
H	-3.318378	3.213570	0.478800
C	-1.809901	4.640964	-0.036367
H	-2.529312	5.400036	-0.327523
C	-0.445402	4.909157	-0.064719
H	-0.079147	5.881803	-0.378229
C	0.451358	3.930676	0.351954
H	1.508135	4.176353	0.392300
C	0.027591	2.660076	0.764424
C	1.047103	1.696787	1.327365
H	0.650248	1.234836	2.235770
H	1.935325	2.256979	1.640792
C	2.699040	0.980425	-1.128573
C	3.547047	2.196083	-0.717894
H	4.298593	1.967902	0.038087
H	2.938992	3.030426	-0.366857
H	4.080643	2.544240	-1.609282
C	1.679724	1.419718	-2.194869
H	1.157496	0.558225	-2.618911
H	2.225451	1.909379	-3.009775
H	0.944695	2.132412	-1.812367
C	3.601141	-0.096814	-1.746198
H	3.024558	-0.984888	-2.020522
H	4.433221	-0.378372	-1.095787
H	4.036736	0.313830	-2.664288
C	2.819669	-0.642121	1.602646
C	2.056888	-0.792865	2.928433
H	1.933981	0.152241	3.463829
H	2.633743	-1.456066	3.582094
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C	4.125707	0.119256	1.880869
H	3.958634	1.146860	2.217312
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H	4.654560	-0.399209	2.688911
C	3.140538	-2.050616	1.083622

H	3.653697	-2.044687	0.121498
H	2.233414	-2.653154	0.982310
H	3.795693	-2.548747	1.807389
O	1.189187	-2.279951	-1.886834
C	1.852643	-3.505203	-1.758083
H	1.571250	-4.074345	-0.860016
H	2.946071	-3.379859	-1.766781
H	1.597796	-4.118224	-2.634884

Complex 2

scf done: -1979.562617

Pd	0.057560	-1.263840	-0.411134
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P	1.849488	0.177927	0.316798
C	-2.858751	-1.048935	1.640944
C	-2.105036	-0.933459	2.977369
H	-2.173066	0.062405	3.422354
H	-1.050986	-1.208528	2.880074
H	-2.556476	-1.632084	3.690361
C	-4.287537	-0.518420	1.838095
H	-4.320794	0.552126	2.059250
H	-4.730157	-1.034253	2.697873
H	-4.931315	-0.718156	0.978797
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H	-1.932400	-3.004854	1.312667
H	-3.374994	-2.733943	0.305609
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C	-1.691868	3.813654	0.085713
H	-2.771197	3.784117	0.198853
C	-1.110416	4.966834	-0.429560
H	-1.736417	5.791206	-0.756716
C	0.275417	5.066469	-0.470167
H	0.755916	5.970685	-0.830798
C	1.047462	4.013432	0.008471
H	2.123399	4.143609	0.061179
C	0.479405	2.822404	0.482646
C	1.376973	1.795943	1.133683
H	0.924599	1.484089	2.079411
H	2.320051	2.280556	1.402789
C	2.971580	0.639186	-1.172816
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H	4.341831	1.916973	0.002755
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H	4.445295	2.082647	-1.745611
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H	1.551466	-0.093965	-2.659462
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C	3.990466	-0.457152	-1.522958
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H	4.600525	-0.340174	2.931572
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H	2.293649	-2.709011	1.290716
H	3.790675	-2.507483	2.211429
O	1.620340	-2.228699	-1.267781
C	1.797065	-3.623948	-1.271283
H	1.614566	-4.102441	-0.297348
H	2.847793	-3.821279	-1.528878
H	1.178384	-4.135844	-2.023354
C	-0.970514	-2.754701	-1.127522
O	-1.366964	-3.712309	-1.599024

TS2-3

scf done: -1979.560554

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C	-1.869492	-1.048523	3.004258
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H	-0.817550	-1.299254	2.840826
H	-2.264733	-1.769702	3.728047
C	-4.128000	-0.700172	1.999092
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H	-4.503849	-1.269316	2.856987
H	-4.807338	-0.892453	1.166340
C	-2.701489	-2.642318	1.299676
H	-1.687523	-3.048660	1.242801
H	-3.205001	-2.829027	0.349656
H	-3.236955	-3.210374	2.068703
C	-2.991348	0.214174	-1.135758
C	-3.662041	-1.074086	-1.633514
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H	-4.389004	-1.476369	-0.924068
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H	-4.762557	0.914956	-0.011725
H	-4.723558	1.334753	-1.719583
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H	-1.343143	0.061607	-2.578372
H	-1.610944	1.709594	-1.974938
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C	-1.633049	1.541308	1.227909
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H	-1.068162	1.296921	2.132617
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C	-1.292586	4.917985	-0.498449
H	-1.959544	5.708949	-0.827120
C	0.085626	5.055178	-0.618860
H	0.517829	5.953310	-1.049064
C	0.913568	4.050334	-0.129845
H	1.987437	4.208806	-0.143856
C	0.404763	2.871998	0.433072
C	1.362091	1.914319	1.100057
H	0.965809	1.649136	2.084414
H	2.307029	2.433041	1.291156
C	2.857390	0.687172	-1.222246
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H	4.439250	1.849934	-0.205535
H	3.158918	2.842238	-0.928982
H	4.343196	2.046497	-1.951583
C	1.842918	0.957913	-2.347901
H	1.275234	0.056834	-2.598400
H	2.390078	1.262621	-3.247803
H	1.146441	1.763638	-2.097280
C	3.738044	-0.504110	-1.628426
H	3.145477	-1.413465	-1.748457
H	4.551742	-0.681537	-0.920841
H	4.199990	-0.267511	-2.594204
C	2.901092	-0.479101	1.730620
C	2.146737	-0.363487	3.066916
H	2.123147	0.656987	3.458478
H	2.668274	-0.976094	3.810550

H	1.122657	-0.741305	3.001321
C	4.258696	0.223519	1.887253
H	4.162734	1.296441	2.079542
H	4.910386	0.079376	1.023822
H	4.770547	-0.210137	2.754256
C	3.116489	-1.971092	1.446334
H	3.592142	-2.158077	0.483602
H	2.168638	-2.516187	1.470434
H	3.761004	-2.390265	2.227554
O	1.360742	-2.500513	-1.437628
C	1.781416	-3.797576	-1.068169
H	1.636466	-4.031929	-0.005791
H	2.855077	-3.886117	-1.281644
H	1.256384	-4.561823	-1.659366
C	-0.743357	-2.711389	-1.322693
O	-1.145474	-3.627177	-1.881163

Complex 3

scf done: -1979.583385

Pd	-0.227080	-1.130479	-0.236502
P	-1.756600	0.468665	0.357365
P	1.950729	-0.225245	0.353004
C	-2.841913	-0.117046	1.824083
C	-1.967135	-0.210904	3.086286
H	-1.657801	0.763475	3.473407
H	-1.080642	-0.831352	2.921728
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H	-4.740060	0.863663	1.295134
C	-3.397641	-1.521081	1.546180
H	-2.594434	-2.260931	1.506932
H	-3.962796	-1.594091	0.617845
H	-4.064433	-1.795145	2.371505
C	-2.798671	1.069983	-1.127070
C	-3.923067	0.080539	-1.467702
H	-3.574157	-0.942203	-1.604846
H	-4.378025	0.409792	-2.409115
H	-4.715325	0.083031	-0.714859
C	-3.433196	2.448607	-0.878923
H	-4.039873	2.492428	0.026672
H	-4.098236	2.663450	-1.722897
H	-2.691760	3.243570	-0.849362
C	-1.833677	1.175037	-2.320341
H	-1.434730	0.196166	-2.603422
H	-0.996744	1.850436	-2.119948
H	-2.383081	1.572875	-3.181361
C	-0.899025	1.960884	1.120243
H	-1.718178	2.575263	1.512623
H	-0.400687	1.528158	1.991805
C	0.069482	2.863621	0.384413
C	-0.402109	4.077622	-0.136811
H	-1.449955	4.331438	-0.018339
C	0.435639	5.003460	-0.748978
H	0.024950	5.928849	-1.140831
C	1.800694	4.747918	-0.815449
H	2.478317	5.464033	-1.269988
C	2.298531	3.583451	-0.241767
H	3.373195	3.424670	-0.224618
C	1.463648	2.630098	0.357625
C	2.116207	1.475817	1.078248
H	1.698669	1.393740	2.086717
H	3.182398	1.684703	1.209981
C	2.964104	-0.223907	-1.261465
C	4.309561	0.507680	-1.157810
H	4.981611	0.071758	-0.416730
H	4.184173	1.568474	-0.930208
H	4.814263	0.448541	-2.129215
C	2.094405	0.478882	-2.320871
H	1.154843	-0.057173	-2.492033
H	2.642434	0.500705	-3.270360
H	1.855883	1.510057	-2.050412
C	3.197583	-1.670372	-1.725449
H	2.264641	-2.241796	-1.786969
H	3.897721	-2.212953	-1.085732
H	3.630556	-1.648525	-2.732279

C	2.725594	-1.351454	1.686688
C	2.135857	-0.947843	3.049705
H	2.540844	-0.003109	3.422730
H	2.393585	-1.718249	3.784988
H	1.043809	-0.877165	3.024580
C	4.254816	-1.270253	1.776256
H	4.610346	-0.248080	1.939481
H	4.750463	-1.673247	0.890266
H	4.590843	-1.867548	2.632159
C	2.288289	-2.799480	1.401911
H	2.651571	-3.178522	0.444978
H	1.195855	-2.899031	1.417379
H	2.685090	-3.455844	2.185300
O	-0.381967	-3.275186	-1.268149
C	-0.614492	-4.549926	-1.919155
H	-1.269839	-5.160286	-1.295430
H	0.364908	-5.011915	-2.027022
H	-1.078301	-4.379969	-2.892348
C	-1.469973	-2.494939	-1.011314
O	-2.597006	-2.807615	-1.281599

Complex 4

scf done: -2058.152772

Pd	-0.265688	-1.247465	-0.157656
P	-1.690386	0.581939	0.604699
P	2.077925	-0.293147	0.241148
C	-2.449904	-0.046959	2.257304
C	-1.279386	-0.389893	3.197996
H	-0.769941	0.494738	3.590392
H	-0.540347	-1.032162	2.707329
H	-1.674220	-0.936983	4.061321
C	-3.358512	0.977119	2.953402
H	-2.887111	1.952477	3.101770
H	-3.610736	0.590965	3.948130
H	-4.302050	1.118308	2.421764
C	-3.252866	-1.334918	2.023347
H	-2.654763	-2.120839	1.562745
H	-4.129534	-1.181503	1.393959
H	-3.607680	-1.700735	2.993967
C	-3.026304	1.301729	-0.567665
C	-4.184195	0.320036	-0.806763
H	-3.870172	-0.692085	-1.059740
H	-4.782678	0.699894	-1.643036
H	-4.850264	0.260109	0.057769
C	-3.652904	2.604410	-0.041703
H	-4.174621	2.475247	0.907018
H	-4.395239	2.939176	-0.775419
H	-2.935722	3.415483	0.070470
C	-2.312231	1.592731	-1.900838
H	-1.927698	0.682104	-2.363857
H	-1.486088	2.298623	-1.783399
H	-3.033755	2.044239	-2.592284
C	-0.751937	2.084377	1.223906
H	-1.508588	2.747386	1.654443
H	-0.182088	1.696189	2.071803
C	0.167512	2.909438	0.353009
C	-0.311561	4.100890	-0.211557
H	-1.356202	4.364370	-0.089488
C	0.516003	4.992933	-0.883920
H	0.102108	5.903273	-1.306598
C	1.879406	4.730697	-0.957807
H	2.555643	5.434401	-1.433364
C	2.377298	3.570963	-0.375842
H	3.451464	3.410196	-0.369642
C	1.546301	2.628850	0.249428
C	2.194906	1.450479	0.931019
H	1.798756	1.355775	1.947273
H	3.261021	1.664808	1.044819
C	2.764083	-0.190611	-1.549186
C	3.930301	0.790785	-1.730028
H	4.791607	0.561908	-1.100879
H	3.626195	1.820303	-1.551790
H	4.267639	0.734659	-2.771992
C	1.580625	0.284470	-2.412867
H	0.751504	-0.435133	-2.402781
H	1.913002	0.381926	-3.453843
H	1.197895	1.257856	-2.095061

C	3.216646	-1.564785	-2.063806
H	2.429648	-2.319328	-2.009353
H	4.105452	-1.934695	-1.547104
H	3.483470	-1.462010	-3.122046
C	3.340199	-1.141273	1.429861
C	2.869351	-0.868979	2.871973
H	3.025230	0.167233	3.182020
H	3.453207	-1.495607	3.555646
H	1.814238	-1.122440	3.020977
C	4.779329	-0.625267	1.270464
H	4.868730	0.461828	1.342040
H	5.230851	-0.949343	0.329621
H	5.388606	-1.045577	2.079393
C	3.371740	-2.665710	1.240887
H	3.651812	-2.968431	0.230336
H	2.422907	-3.136202	1.502888
H	4.126217	-3.083114	1.917726
O	-1.668655	-1.651522	-2.428681
C	-2.539758	-2.283736	-3.398568
H	-2.428978	-3.368792	-3.354323
H	-2.219030	-1.900243	-4.365669
H	-3.579715	-2.016338	-3.202090
C	-1.846249	-2.023746	-1.147050
O	-2.689155	-2.810595	-0.791702
C	0.514289	-3.425874	-0.462374
C	-0.141530	-3.328413	0.738833
H	0.404288	-3.180033	1.666270
H	1.593567	-3.387351	-0.509794
H	0.003845	-3.800100	-1.345002
H	-1.184559	-3.614432	0.825476

TS4-5

scf done: -2058.129790

Pd	-0.074817	-1.250505	-0.117752
P	-1.705246	0.478934	0.631840
P	2.088773	-0.148560	0.256680
C	-2.438502	-0.129130	2.301407
C	-1.274394	-0.293835	3.291440
H	-0.808268	0.652621	3.579161
H	-0.508537	-0.962760	2.885536
H	-1.656683	-0.752785	4.210395
C	-3.476744	0.825325	2.907311
H	-3.098535	1.841845	3.050064
H	-3.757887	0.448985	3.898062
H	-4.392216	0.872317	2.313933
C	-3.070742	-1.518001	2.126558
H	-2.342504	-2.249818	1.769525
H	-3.910840	-1.529255	1.433678
H	-3.436741	-1.856909	3.102930
C	-3.112044	1.054059	-0.556960
C	-4.278738	0.058295	-0.653220
H	-3.978744	-0.963201	-0.873341
H	-4.937484	0.396707	-1.462240
H	-4.882360	0.051210	0.258479
C	-3.735562	2.400866	-0.153306
H	-4.121544	2.411058	0.867021
H	-4.584832	2.589882	-0.819881
H	-3.050986	3.234278	-0.278438
C	-2.446757	1.214692	-1.935405
H	-2.031566	0.273967	-2.304317
H	-1.640995	1.953994	-1.916175
H	-3.195991	1.563423	-2.656379
C	-0.910434	2.096929	1.173271
H	-1.711560	2.701425	1.607022
H	-0.264864	1.808054	2.007820
C	-0.128172	2.949133	0.199816
C	-0.713191	4.117079	-0.311298
H	-1.715381	4.387426	0.001079
C	-0.034553	4.984847	-1.159703
H	-0.530610	5.875397	-1.533323
C	1.292043	4.722606	-1.479182
H	1.856148	5.399042	-2.113907
C	1.913979	3.614141	-0.916247
H	2.979683	3.486726	-1.074665
C	1.232257	2.707982	-0.091055
C	2.035527	1.678404	0.664596
H	1.711378	1.696807	1.707865

H	3.080293	2.002211	0.674846
C	3.084822	-0.250333	-1.385140
C	4.117692	0.875316	-1.554445
H	4.841497	0.931877	-0.739665
H	3.644141	1.847107	-1.677157
H	4.682728	0.681077	-2.473342
C	2.046642	-0.113178	-2.514170
H	1.319655	-0.930780	-2.516807
H	2.565730	-0.120769	-3.480223
H	1.495077	0.829819	-2.444137
C	3.843581	-1.579833	-1.533190
H	3.226606	-2.462391	-1.378974
H	4.703155	-1.644041	-0.861671
H	4.235579	-1.636239	-2.555376
C	3.187588	-0.717006	1.750085
C	2.539742	-0.231215	3.060060
H	2.665311	0.841418	3.226797
H	3.033065	-0.737305	3.897511
H	1.476462	-0.475341	3.114784
C	4.614571	-0.147332	1.686880
H	4.638618	0.944112	1.629288
H	5.199139	-0.553814	0.859331
H	5.133981	-0.424709	2.611813
C	3.276591	-2.247335	1.841539
H	3.670603	-2.714008	0.936507
H	2.306974	-2.689750	2.088374
H	3.959695	-2.506679	2.658345
O	-1.327418	-2.161489	-2.390546
C	-2.364003	-2.374753	-3.378307
H	-2.769807	-3.384166	-3.278482
H	-1.872863	-2.247307	-4.341402
H	-3.166245	-1.645484	-3.257003
C	-1.691232	-2.364618	-1.109341
O	-2.797269	-2.668240	-0.745663
C	0.989133	-3.074098	-0.504919
C	-0.336744	-3.544606	-0.345354
H	-0.701327	-3.816971	0.642121
H	1.694018	-3.221375	0.299881
H	1.397956	-3.102847	-1.510335
H	-0.736089	-4.175062	-1.136780

Complex 5

scf done: -2058.189010

Pd	-0.598312	-0.694499	0.278150
P	-0.686728	1.701825	0.616069
P	1.641524	-1.283167	0.302035
C	-1.554719	2.156399	2.263216
C	-0.555613	1.930953	3.411133
H	0.227955	2.692609	3.443163
H	-0.085912	0.944169	3.360352
H	-1.095410	1.986233	4.363218
C	-2.047767	3.608523	2.333683
H	-1.250106	4.331688	2.139490
H	-2.419036	3.805823	3.346321
H	-2.872437	3.808448	1.645870
C	-2.735611	1.196605	2.482664
H	-2.391248	0.161850	2.584513
H	-3.477020	1.239410	1.681475
H	-3.247476	1.463229	3.414729
C	-1.592352	2.472099	-0.881127
C	-3.088965	2.130592	-0.841998
H	-3.269081	1.053103	-0.802517
H	-3.547787	2.487451	-1.771123
H	-3.615034	2.613754	-0.015484
C	-1.437869	3.996428	-0.986284
H	-1.849075	4.532577	-0.129792
H	-1.981643	4.337664	-1.874938
H	-0.398442	4.296655	-1.118135
C	-0.987944	1.818212	-2.138730
H	-1.170677	0.739192	-2.161707
H	0.086354	1.996625	-2.226102
H	-1.469561	2.249342	-3.024682
C	0.936420	2.614107	0.766796
H	0.710374	3.672621	0.932744
H	1.367730	2.244754	1.702458
C	1.951126	2.491202	-0.344946
C	2.160846	3.604031	-1.172282

H	1.576437	4.503270	-1.001557
C	3.122273	3.614774	-2.176203
H	3.251268	4.496243	-2.796703
C	3.938405	2.501801	-2.342573
H	4.720386	2.494045	-3.095633
C	3.777031	1.409532	-1.497634
H	4.481109	0.588561	-1.580676
C	2.783295	1.360530	-0.508857
C	2.783119	0.199681	0.462591
H	2.558553	0.577208	1.463382
H	3.797723	-0.209612	0.516119
C	2.184997	-2.217331	-1.273023
C	3.706012	-2.216114	-1.492383
H	4.262194	-2.665263	-0.668588
H	4.098759	-1.217805	-1.674413
H	3.920056	-2.808536	-2.389246
C	1.512549	-1.489358	-2.451065
H	0.421276	-1.525462	-2.386838
H	1.811512	-1.976222	-3.386777
H	1.816058	-0.440407	-2.511317
C	1.722704	-3.682233	-1.246162
H	0.660146	-3.795922	-1.033762
H	2.287375	-4.282150	-0.527865
H	1.903864	-4.115549	-2.236542
C	2.099259	-2.255352	1.895823
C	1.981734	-1.302056	3.097527
H	2.779590	-0.555993	3.133794
H	2.056129	-1.891777	4.018045
H	1.013662	-0.792554	3.114116
C	3.525234	-2.827591	1.859835
H	4.287185	-2.068985	1.658598
H	3.633796	-3.633773	1.131044
H	3.752011	-3.252825	2.844436
C	1.101330	-3.399006	2.130509
H	1.056924	-4.109165	1.303289
H	0.095608	-3.012834	2.316373
H	1.412036	-3.955398	3.022299
O	-4.742026	-2.345815	-0.873147
C	-5.660416	-2.371022	-1.983097
H	-5.864122	-1.355225	-2.327839
H	-6.565827	-2.837740	-1.599259
H	-5.242056	-2.955440	-2.804953
C	-3.548323	-1.814032	-1.123830
O	-3.193535	-1.345686	-2.182544
C	-1.354419	-2.567660	-0.146043
C	-2.654622	-1.878967	0.103960
H	-2.485645	-0.742231	0.331325
H	-1.111682	-3.370355	0.543911
H	-1.179271	-2.825244	-1.189300
H	-3.178929	-2.229460	0.994757

Complex 6

scf done: -2173.886086

Pd	0.729784	0.084754	-0.358461
P	-0.661703	-1.836380	0.427560
P	-0.566936	1.917714	0.198638
C	0.393375	-2.670061	1.795453
C	0.426782	-1.723745	3.009799
H	-0.520041	-1.701477	3.556566
H	0.693415	-0.700550	2.724875
H	1.189926	-2.079185	3.711922
C	-0.137601	-4.034076	2.257961
H	-1.177603	-3.991487	2.594844
H	0.461067	-4.373977	3.111682
H	-0.054981	-4.799605	1.483322
C	1.840393	-2.829095	1.301741
H	2.295403	-1.856543	1.089821
H	1.926629	-3.443104	0.404851
H	2.434185	-3.304863	2.091430
C	-1.183898	-3.110527	-0.899997
C	0.028462	-3.912577	-1.399770
H	0.876414	-3.276188	-1.654470
H	-0.270340	-4.466637	-2.297752
H	0.359236	-4.653461	-0.666687
C	-2.256115	-4.108326	-0.437788
H	-1.956378	-4.687242	-0.437230
H	-2.433847	-4.821325	-1.251842

H	-3.210140	-3.626144	-0.228629
C	-1.756511	-2.283637	-2.065655
H	-1.016509	-1.588836	-2.472043
H	-2.634231	-1.704119	-1.767986
H	-2.062387	-2.961231	-2.871992
C	-2.233090	-1.477434	1.382305
H	-2.608302	-2.422765	1.787546
H	-1.900870	-0.886029	2.240716
C	-3.349443	-0.752717	0.675570
C	-4.517840	-1.452548	0.341500
H	-4.594686	-2.503958	0.601429
C	-5.600337	-0.834365	-0.274391
H	-6.487554	-1.410351	-0.519147
C	-5.544165	0.530145	-0.541040
H	-6.383504	1.039714	-1.004290
C	-4.416719	1.248988	-0.161063
H	-4.410159	2.325952	-0.307342
C	-3.305242	0.635532	0.437306
C	-2.222830	1.527224	0.995958
H	-1.939786	1.170831	1.993375
H	-2.675151	2.507693	1.154469
C	-1.007567	2.843561	-1.420665
C	-1.911092	4.061317	-1.173912
H	-1.387626	4.867858	-0.653748
H	-2.820377	3.823938	-0.616822
H	-2.228918	4.460384	-2.144120
C	-1.726864	1.829239	-2.328452
H	-1.092405	0.959446	-2.527044
H	-1.939980	2.312435	-3.289412
H	-2.671670	1.474818	-1.916761
C	0.238903	3.310403	-2.187611
H	0.854164	2.464851	-2.501228
H	0.861477	4.012297	-1.630304
H	-0.096919	3.825429	-3.095093
C	0.071695	3.136397	1.572681
C	0.718760	2.271015	2.665169
H	0.013051	1.559352	3.105148
H	1.065977	2.920261	3.477712
H	1.580855	1.714329	2.292951
C	-1.054799	3.957387	2.235292
H	-1.727813	3.349471	2.843129
H	-1.649248	4.532728	1.522221
H	-0.585561	4.677897	2.914541
C	1.109051	4.148122	1.059389
H	0.685967	4.846925	0.334104
H	1.993866	3.683968	0.623812
H	1.451272	4.745043	1.912644
O	5.735070	0.431461	0.392412
C	6.832084	-0.441922	0.059537
H	6.631184	-1.453745	0.417047
H	7.699292	-0.018994	0.563293
H	6.983371	-0.460986	-1.021327
C	4.552252	0.117127	-0.108568
O	4.384951	-0.856679	-0.837541
C	2.361765	1.340374	-0.680547
C	3.465257	1.054060	0.354156
H	3.064128	0.589560	1.267479
H	2.144619	2.402246	-0.679475
H	2.700249	1.100192	-1.693461
H	3.947210	1.978091	0.691372
H	0.940057	-1.483796	-3.375533
C	1.915825	-1.159047	-3.012876
H	2.075792	-0.114916	-3.305540
H	2.689141	-1.783419	-3.470391
O	1.943294	-1.326281	-1.592663
H	2.889094	-1.202363	-1.297400

TS6-1

scf done: -2173.828068

Pd	0.637808	0.070707	-0.263122
P	-0.650406	-1.804402	0.437402
P	-0.820202	1.833930	0.260838
C	0.319112	-2.581560	1.901201
C	0.160005	-1.668453	3.129490
H	-0.844963	-1.696491	3.559417
H	0.426059	-0.632088	2.904798
H	0.845864	-2.017506	3.909506

C	-0.193391	-3.983168	2.268704
H	-1.260089	-3.999227	2.511725
H	0.341474	-4.317971	3.165223
H	-0.000649	-4.720890	1.487712
C	1.818439	-2.652110	1.571719
H	2.241084	-1.659641	1.397080
H	2.041456	-3.259254	0.695714
H	2.338745	-3.093186	2.429873
C	-0.904741	-3.059069	-0.979835
C	0.402491	-3.807395	-1.287555
H	1.259077	-3.138904	-1.364806
H	0.281263	-4.332367	-2.242304
H	0.624063	-4.566976	-0.533895
C	-1.997265	-4.097610	-0.682162
H	-1.826975	-4.654365	0.241444
H	-1.999475	-4.825447	-1.501797
H	-2.991235	-3.653162	-0.649323
C	-1.330808	-2.235520	-2.207546
H	-0.553241	-1.527937	-2.506609
H	-2.255771	-1.678403	-2.031549
H	-1.508346	-2.916068	-3.048535
C	-2.333789	-1.567995	1.212854
H	-2.663497	-2.563694	1.525641
H	-2.138038	-1.011962	2.134736
C	-3.440071	-0.890965	0.445718
C	-4.518995	-1.650718	-0.027295
H	-4.529516	-2.722316	0.146982
C	-5.605225	-1.066766	-0.670431
H	-6.423204	-1.686770	-1.024138
C	-5.647473	0.315819	-0.821519
H	-6.495637	0.794782	-1.300887
C	-4.609399	1.086729	-0.310305
H	-4.677334	2.169570	-0.375209
C	-3.494221	0.509303	0.313734
C	-2.497560	1.425156	0.977583
H	-2.270537	1.060335	1.986941
H	-2.981707	2.393818	1.117356
C	-1.161635	2.727511	-1.391910
C	-2.092787	3.935128	-1.206807
H	-1.637640	4.731608	-0.612948
H	-3.051182	3.669740	-0.753098
H	-2.313946	4.356855	-2.194151
C	-1.812398	1.707453	-2.343755
H	-1.175820	0.828319	-2.483382
H	-1.939689	2.182697	-3.323394
H	-2.792505	1.369698	-2.007693
C	0.146215	3.185650	-2.056478
H	0.804758	2.340119	-2.270077
H	0.702427	3.919951	-1.473658
H	-0.105745	3.653932	-3.014713
C	-0.199413	3.056742	1.634607
C	0.523508	2.194490	2.681051
H	-0.146249	1.458784	3.137136
H	0.891080	2.838374	3.488528
H	1.380675	1.663417	2.256839
C	-1.353544	3.801585	2.334583
H	-2.000400	3.144235	2.918959
H	-1.971616	4.379607	1.642640
H	-0.911680	4.514363	3.039614
C	0.767151	4.136453	1.119024
H	0.277964	4.848611	0.451281
H	1.652830	3.744958	0.616966
H	1.124004	4.705059	1.985345
O	5.897321	0.050056	0.529012
C	7.055805	-0.565733	-0.053368
H	6.774029	-1.466619	-0.603334
H	7.707348	-0.815574	0.783006
H	7.554900	0.126286	-0.735577
C	4.963817	0.457559	-0.339838
O	5.041354	0.314534	-1.540693
C	2.614682	1.377951	-0.531975
C	3.824883	1.555577	0.378266
H	3.580468	0.580989	1.278576
H	1.990021	2.165332	-0.119492
H	2.925108	1.721373	-1.524359
H	4.224124	2.114015	0.739470
H	1.636615	-1.871716	-3.022795

C	2.261551	-1.090260	-2.579416
H	1.952852	-0.123964	-3.003233
H	3.308150	-1.256621	-2.854424
O	2.170614	-1.113647	-1.156866
H	2.436252	0.094590	-0.868749

Complex 7

scf done: -1751.799110

Pd	-0.106054	-1.167619	0.868622
P	1.957784	-0.359768	-0.076526
P	-1.952215	-0.304902	-0.043711
H	-1.422478	-1.715175	1.513802
C	2.889633	-1.803749	-0.905963
C	2.187190	-2.117705	-2.238705
H	2.383774	-1.363555	-3.005747
H	1.103826	-2.226228	-2.119276
H	2.568183	-3.071151	-2.621485
C	4.372740	-1.535399	-1.189772
H	4.524158	-0.637952	-1.797544
H	4.785501	-2.380340	-1.753392
H	4.965542	-1.439673	-0.277212
C	2.736069	-3.036039	0.004280
H	1.678631	-3.289669	0.156931
H	3.201783	-2.906567	0.983087
H	3.211742	-3.901389	-0.471939
C	3.012903	0.502940	1.251351
C	3.529954	-0.549800	2.244999
H	2.721763	-1.167803	2.653603
H	3.999103	-0.034334	3.090831
H	4.284672	-1.208581	1.809376
C	4.193954	1.309149	0.695071
H	4.918670	0.691781	0.162423
H	4.721268	1.783410	1.531137
H	3.868957	2.111052	0.029101
C	2.069053	1.449800	2.015371
H	1.243970	0.903316	2.484205
H	1.644492	2.225363	1.374625
H	2.635435	1.946830	2.811888
C	1.686742	0.858110	-1.466424
H	2.662014	1.157254	-1.864744
H	1.207454	0.265302	-2.251282
C	0.862677	2.093459	-1.181754
C	1.544856	3.315300	-1.079671
H	2.626857	3.318407	-1.175080
C	0.886040	4.525338	-0.897995
H	1.453191	5.448148	-0.824703
C	-0.503946	4.539444	-0.853823
H	-1.046999	5.473599	-0.749235
C	-1.198257	3.343174	-0.988468
H	-2.282082	3.378597	-1.030652
C	-0.551810	2.105103	-1.126575
C	-1.408259	0.884967	-1.393179
H	-0.896446	0.224932	-2.098263
H	-2.333168	1.203737	-1.889264
C	-3.009081	0.624078	1.235405
C	-4.013872	1.591183	0.588245
H	-4.756351	1.088666	-0.032569
H	-3.526535	2.362245	-0.006885
H	-4.555198	2.103377	1.391226
C	-2.028690	1.420932	2.114900
H	-1.350801	0.755574	2.659211
H	-2.605536	1.988827	2.853989
H	-1.431196	2.132363	1.539453
C	-3.777614	-0.361850	2.126554
H	-3.123648	-1.106123	2.591565
H	-4.577262	-0.879310	1.590862
H	-4.246974	0.207165	2.936777
C	-2.937503	-1.619798	-1.021147
C	-2.110979	-2.036691	-2.251016
H	-2.068717	-1.262319	-3.021419
H	-2.588406	-2.911716	-2.705350
H	-1.091744	-2.328718	-1.979535
C	-4.296966	-1.082593	-1.498339
H	-4.214187	-0.152580	-2.068905
H	-4.996586	-0.928195	-0.674164
H	-4.745958	-1.827518	-2.164585
C	-3.153359	-2.874514	-0.159741

H	-3.686618	-2.672796	0.770341
H	-2.204674	-3.358278	0.089376
H	-3.753311	-3.588488	-0.735262

Complex 7a

scf done: -1751.799110

Pd	0.106056	-1.167624	0.868621
P	1.952213	-0.304900	-0.043711
P	-1.957782	-0.359770	-0.076527
H	1.422477	-1.715179	1.513806
C	2.937507	-1.619790	-1.021151
C	2.110989	-2.036679	-2.251026
H	2.068733	-1.262305	-3.021427
H	1.091751	-2.328705	-1.979553
H	2.588417	-2.911704	-2.705358
C	4.296970	-1.082582	-1.498337
H	4.214192	-0.152567	-2.068900
H	4.745965	-1.827504	-2.164584
H	4.996588	-0.928187	-0.674160
C	3.153361	-2.874510	-0.159749
H	2.204676	-3.358275	0.089363
H	3.686616	-2.672793	0.770336
H	3.753317	-3.588480	-0.735269
C	3.009076	0.624078	1.235409
C	3.777611	-0.361851	2.126555
H	3.123646	-1.106125	2.591564
H	4.246967	0.207164	2.936781
H	4.577261	-0.879307	1.590864
C	4.013866	1.591189	0.588252
H	4.756346	1.088676	-0.032563
H	4.555189	2.103382	1.391236
H	3.526526	2.362251	-0.006876
C	2.028683	1.420928	2.114906
H	1.350795	0.755567	2.659214
H	1.431189	2.132360	1.539460
H	2.605528	1.988821	2.853996
C	1.408257	0.884971	-1.393178
H	2.333166	1.203743	-1.889260
H	0.896446	0.224936	-2.098263
C	0.551807	2.105106	-1.126573
C	1.198251	3.343177	-0.988463
H	2.282075	3.378602	-1.030644
C	0.503937	4.539446	-0.853819
H	1.046988	5.473601	-0.749227
C	-0.886048	4.525338	-0.897995
H	-1.453201	5.448147	-0.824705
C	-1.544862	3.315299	-1.079674
H	-2.626863	3.318404	-1.175086
C	-0.862680	2.093460	-1.181755
C	-1.686742	0.858109	-1.466426
H	-1.207454	0.265301	-2.251284
H	-2.662015	1.157250	-1.864746
C	-3.012902	0.502938	1.251351
C	-4.193954	1.309144	0.695074
H	-4.918674	0.691775	0.162433
H	-3.868960	2.111044	0.029098
H	-4.721262	1.783410	1.531141
C	-2.069051	1.449799	2.015370
H	-1.243964	0.903316	2.484200
H	-2.635432	1.946825	2.811890
H	-1.644495	2.225364	1.374625
C	-3.529950	-0.549803	2.245000
H	-2.721757	-1.167806	2.653603
H	-4.284668	-1.208585	1.809378
H	-3.999097	-0.034339	3.090833
C	-2.889630	-1.803751	-0.905963
C	-2.187186	-2.117708	-2.238705
H	-2.383769	-1.363559	-3.005748
H	-2.568180	-3.071153	-2.621485
H	-1.103822	-2.226232	-2.119275
C	-4.372736	-1.535400	-1.189772
H	-4.524154	-0.637952	-1.797541
H	-4.965538	-1.439677	-0.277212
H	-4.785498	-2.380339	-1.753394
C	-2.736066	-3.036041	0.004280
H	-3.201777	-2.906568	0.983087
H	-1.678627	-3.289673	0.156929

H	-3.211740	-3.901390	-0.471939
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Complex 8

scf done: -1830.404709

Pd	-0.063171	-1.344695	-0.547319
P	-1.870150	-0.101497	0.184893
P	1.909393	-0.165578	0.212102
C	-1.125898	-2.944600	-1.322224
H	-1.542110	-3.557840	-0.524189
H	-1.851732	-2.724193	-2.098276
C	0.230607	-3.330640	-1.783661
H	0.369323	-3.299014	-2.865947
H	0.612919	-4.262185	-1.359769
H	1.048832	-2.574758	-1.408877
C	-2.948033	-1.069104	1.449662
C	-1.977014	-1.889030	2.316743
H	-1.276691	-1.253979	2.868752
H	-1.397675	-2.602144	1.722885
H	-2.551733	-2.454546	3.059661
C	-3.772228	-0.161087	2.380708
H	-3.150518	0.414123	3.071041
H	-4.417892	-0.799238	2.994461
H	-4.423549	0.529173	1.839959
C	-3.913642	-2.030653	0.741713
H	-3.420797	-2.656170	-0.004485
H	-4.741981	-1.503043	0.262542
H	-4.351892	-2.699097	1.491803
C	-2.899435	0.621509	-1.254158
C	-3.413597	-0.468971	-2.208135
H	-2.592196	-0.948571	-2.744366
H	-4.045433	0.016403	-2.960820
H	-4.017432	-1.237183	-1.725174
C	-4.099327	1.438875	-0.748641
H	-4.872170	0.805852	-0.304763
H	-4.556268	1.952462	-1.602354
H	-3.825684	2.208867	-0.022942
C	-1.960421	1.516168	-2.083668
H	-1.069416	0.967095	-2.403801
H	-1.637357	2.411455	-1.554044
H	-2.494900	1.835360	-2.986092
C	-1.382925	1.359949	1.261426
H	-2.327592	1.772673	1.624196
H	-0.914675	0.883156	2.130596
C	-0.536285	2.516779	0.784483
C	-1.194899	3.711992	0.456116
H	-2.280762	3.740866	0.493002
C	-0.506419	4.868525	0.109004
H	-1.053185	5.772799	-0.140011
C	0.884870	4.860478	0.122322
H	1.446533	5.758854	-0.114613
C	1.553746	3.696796	0.484190
H	2.637125	3.718672	0.560428
C	0.874041	2.511590	0.802199
C	1.676471	1.335121	1.299237
H	1.200191	0.933516	2.198797
H	2.668626	1.680069	1.608284
C	2.976135	0.394695	-1.266790
C	4.079897	1.397278	-0.902943
H	4.790186	1.009861	-0.171054
H	3.670194	2.335624	-0.528245
H	4.646437	1.637972	-1.810039
C	2.006242	1.061607	-2.259309
H	1.251184	0.353645	-2.617808
H	2.572252	1.416676	-3.128707
H	1.491170	1.921785	-1.823398
C	3.613246	-0.820086	-1.958105
H	2.877078	-1.584874	-2.226603
H	4.395824	-1.286620	-1.355077
H	4.080711	-0.485971	-2.891521
C	2.891252	-1.320020	1.390079
C	2.148765	-1.371686	2.738894
H	2.270313	-0.456166	3.323573
H	2.568014	-2.188133	3.337926
H	1.079907	-1.575546	2.615407
C	4.335516	-0.867659	1.647627
H	4.396536	0.156489	2.028128
H	4.964034	-0.946213	0.757721

H	4.777248	-1.518495	2.411528
C	2.895018	-2.748588	0.820714
H	3.336044	-2.816914	-0.175927
H	1.881707	-3.161829	0.782844
H	3.484372	-3.394071	1.482196

Complex 9

scf done: -1943.681211

Pd	-0.115674	-1.307026	-0.476937
P	-1.910441	0.179481	0.188765
P	1.892334	-0.079293	0.336237
C	0.886259	-2.507459	-1.587114
C	-1.557663	-2.831398	-0.938911
H	-2.534316	-2.429177	-0.697628
H	-1.551952	-3.024712	-2.014925
C	-1.268811	-4.098330	-0.145135
H	-2.094069	-4.811237	-0.277749
H	-1.177415	-3.917646	0.930548
H	-0.356128	-4.606920	-0.469613
O	1.338810	-3.219084	-2.358526
C	-3.116494	-0.485311	1.555285
C	-2.243489	-1.302221	2.521803
H	-1.462087	-0.691230	2.985447
H	-1.767516	-2.152269	2.025842
H	-2.868771	-1.693314	3.332834
C	-3.803340	0.635763	2.361377
H	-3.111414	1.210651	2.980176
H	-4.515591	0.163354	3.046913
H	-4.373588	1.327737	1.736435
C	-4.240494	-1.384162	1.011471
H	-3.884448	-2.258695	0.466220
H	-4.941810	-0.836488	0.378011
H	-4.812831	-1.760377	1.867321
C	-2.833505	0.773476	-1.372648
C	-3.427201	-0.395063	-2.175230
H	-2.649459	-1.067855	-2.540361
H	-3.934027	0.023990	-3.052103
H	-4.166817	-0.978448	-1.624943
C	-3.957871	1.763080	-1.035012
H	-4.782630	1.285992	-0.499077
H	-4.368737	2.159272	-1.970740
H	-3.615905	2.618290	-0.448351
C	-1.785029	1.443648	-2.279530
H	-0.968459	0.752995	-2.515371
H	-1.354773	2.348054	-1.849443
H	-2.267372	1.719619	-3.224525
C	-1.364477	1.739306	1.076924
H	-2.289845	2.262864	1.324345
H	-0.982507	1.358219	2.031290
C	-0.408136	2.770533	0.529012
C	-0.949637	3.958951	0.015363
H	-2.028582	4.051648	-0.073737
C	-0.154280	5.039295	-0.348532
H	-0.610189	5.941252	-0.745058
C	1.220482	4.967031	-0.148108
H	1.859306	5.814415	-0.377185
C	1.769722	3.806799	0.385846
H	2.832890	3.787162	0.605145
C	0.988058	2.684536	0.697278
C	1.648769	1.487456	1.334250
H	1.066235	1.165483	2.202558
H	2.631105	1.779339	1.718678
C	3.131932	0.385660	-1.046122
C	4.178426	1.419342	-0.602412
H	4.753383	1.102403	0.269521
H	3.733194	2.390799	-0.396989
H	4.888911	1.563966	-1.424413
C	2.291903	0.984791	-2.188551
H	1.595347	0.252226	-2.608750
H	2.961890	1.305004	-2.995206
H	1.719821	1.859121	-1.866979
C	3.886403	-0.841662	-1.578677
H	3.231675	-1.649576	-1.905952
H	4.598857	-1.243507	-0.854124
H	4.464124	-0.530117	-2.456486
C	2.701218	-1.222238	1.647161
C	1.767941	-1.262295	2.871282

H	1.772715	-0.330299	3.442943	C	3.875591	-0.664400	-1.575523
H	2.112262	-2.051619	3.549033	H	3.269680	-1.532633	-1.834496
H	0.737111	-1.502159	2.590475	H	4.629879	-0.967745	-0.845359
C	4.090703	-0.749069	2.099536	H	4.412592	-0.367639	-2.483852
H	4.088633	0.278141	2.475701	C	2.790890	-0.898005	1.713321
H	4.839152	-0.827316	1.307577	C	1.893947	-0.907472	2.964182
H	4.427294	-1.388719	2.923836	H	1.846530	0.062611	3.465670
C	2.804464	-2.660425	1.111668	H	2.309247	-1.619203	3.686429
H	3.393915	-2.742502	0.197065	H	0.875929	-1.237334	2.732097
H	1.815771	-3.093080	0.930588	C	4.149709	-0.284625	2.083593
H	3.294652	-3.281868	1.869839	H	4.078602	0.768986	2.369372
				H	4.884204	-0.378797	1.280560
TS9-10				H	4.550543	-0.823253	2.950156
scf done: -1943.673510				C	2.992472	-2.361023	1.287063
Pd	0.024405	-1.254925	-0.419899	H	3.558543	-2.469991	0.361007
P	-1.916537	0.100472	0.265602	H	2.035636	-2.878506	1.171160
P	1.877351	0.075280	0.335368	H	3.550839	-2.879994	2.074533
C	0.961320	-2.594977	-1.333812				
C	-1.063118	-3.142479	-1.255669	Complex 10			
H	-1.995438	-2.675736	-0.957631	scf done: -1943.692203			
H	-1.046497	-3.205354	-2.345133	Pd	0.181400	-1.116136	-0.371679
C	-0.882836	-4.483525	-0.563672	P	-1.996376	-0.122975	0.314303
H	-1.761184	-5.109808	-0.762689	P	1.873279	0.315972	0.334118
H	-0.798665	-4.381027	0.522435	C	1.245147	-2.508913	-1.242181
H	-0.006449	-5.029722	-0.920782	C	-0.036230	-3.292128	-1.627874
O	1.647022	-3.315224	-1.920344	H	-0.970429	-2.853567	-1.226675
C	-3.041984	-0.721642	1.588491	H	-0.110021	-3.198106	-2.717246
C	-2.310459	-0.666343	2.942900	C	0.081013	-4.751387	-1.179916
H	-2.289025	0.336606	3.376309	H	-0.779200	-5.323053	-1.536826
H	-1.285487	-1.045186	2.875909	H	0.119262	-4.835203	-0.090715
H	-2.844835	-1.307562	3.652837	H	0.993544	-5.190426	-1.590521
C	-4.409721	-0.040877	1.744112	O	2.352688	-2.864035	-1.492630
H	-4.335322	1.032521	1.940520	C	-2.883280	-1.220497	1.607062
H	-4.924386	-0.487334	2.603028	C	-2.169877	-1.029539	2.956934
H	-5.051762	-0.191921	0.873317	H	-2.387563	-0.062149	3.417163
C	-3.254904	-2.204200	1.253348	H	-1.084635	-1.140474	2.865848
H	-2.310446	-2.754368	1.261666	H	-2.518709	-1.800732	3.652917
H	-3.746199	-2.360471	0.290700	C	-4.373959	-0.908421	1.794512
H	-3.899969	-2.649936	2.019256	H	-4.552327	0.138209	2.059868
C	-2.899528	0.563645	-1.314029	H	-4.763188	-1.518536	2.618300
C	-3.668996	-0.641509	-1.874236	H	-4.968785	-1.147168	0.909788
H	-3.019756	-1.488104	-2.103878	C	-2.705346	-2.693161	1.200038
H	-4.139320	-0.338388	-2.816914	H	-1.645089	-2.969278	1.165627
H	-4.477103	-0.977769	-1.212656	H	-3.158664	-2.930154	0.235152
C	-3.896355	1.714527	-1.119472	H	-3.183510	-3.334981	1.949154
H	-4.681813	1.485350	-0.398498	C	-3.077449	0.140631	-1.236081
H	-4.385607	1.908518	-2.081031	C	-3.574786	-1.207690	-1.780369
H	-3.408653	2.641067	-0.822051	H	-2.760487	-1.918241	-1.954801
C	-1.841358	0.989331	-2.348056	H	-4.058294	-1.034698	-2.748789
H	-1.149000	0.171046	-2.575798	H	-4.315750	-1.680718	-1.131463
H	-1.258697	1.851987	-2.014097	C	-4.287904	1.058288	-1.013954
H	-2.344124	1.269035	-3.281593	H	-4.966056	0.694945	-0.240278
C	-1.549129	1.722275	1.129927	H	-4.860057	1.116778	-1.947510
H	-2.518135	2.153804	1.401123	H	-3.988808	2.076102	-0.763413
H	-1.088002	1.408639	2.071097	C	-2.156637	0.773027	-2.296779
C	-0.697927	2.804429	0.508036	H	-1.322603	0.110443	-2.554860
C	-1.332095	3.958755	0.025736	H	-1.742715	1.730783	-1.972389
H	-2.415371	4.018897	0.059431	H	-2.734611	0.951726	-3.211411
C	-0.621920	5.059887	-0.439468	C	-1.915714	1.529171	1.182741
H	-1.152767	5.933033	-0.806110	H	-2.937708	1.833292	1.431304
C	0.766603	5.046399	-0.377096	H	-1.423119	1.309023	2.134757
H	1.345156	5.909104	-0.692723	C	-1.207935	2.676124	0.501016
C	1.410956	3.929929	0.143958	C	-1.997131	3.720072	-0.004212
H	2.487926	3.967544	0.272279	H	-3.077261	3.649634	0.083582
C	0.713549	2.788160	0.564340	C	-1.447388	4.865306	-0.567634
C	1.486107	1.673526	1.230284	H	-2.094356	5.650173	-0.947194
H	0.945171	1.343843	2.121853	C	-0.064864	5.008284	-0.590653
H	2.442746	2.070461	1.586836	H	0.393892	5.909464	-0.985657
C	3.049968	0.540254	-1.100180	C	0.730835	4.002307	-0.054737
C	4.025156	1.671353	-0.740074	H	1.800113	4.172812	0.002628
H	4.641485	1.449486	0.132499	C	0.199878	2.813607	0.468935
H	3.513279	2.617728	-0.577722	C	1.140226	1.843930	1.156075
H	4.704828	1.819596	-1.587033	H	0.644578	1.433775	2.039753
C	2.145080	1.008891	-2.253731	H	2.003524	2.406085	1.530221
H	1.511606	0.197297	-2.625306	C	3.004400	0.926331	-1.080712
H	2.774447	1.346637	-3.085358	C	3.772735	2.210803	-0.731640
H	1.502042	1.844349	-1.963437	H	4.410067	2.107245	0.147379

H	3.116147	3.066285	-0.589512
H	4.426567	2.449576	-1.578152
C	2.074981	1.207906	-2.274377
H	1.580759	0.295523	-2.622217
H	2.672996	1.601141	-3.104719
H	1.307465	1.950129	-2.036758
C	4.033794	-0.141055	-1.482139
H	3.588145	-1.107358	-1.712806
H	4.799727	-0.284757	-0.715802
H	4.548205	0.213100	-2.383137
C	2.874975	-0.438253	1.782164
C	1.963789	-0.530356	3.018674
H	1.747579	0.442441	3.468306
H	2.477983	-1.126210	3.781043
H	1.020607	-1.038024	2.794175
C	4.112431	0.395930	2.150862
H	3.872460	1.438188	2.381543
H	4.878551	0.375676	1.373008
H	4.560433	-0.035165	3.053606
C	3.307951	-1.869031	1.427559
H	3.897936	-1.934433	0.513534
H	2.442961	-2.528246	1.316738
H	3.919075	-2.259012	2.249539

Complex 11

scf done: -1943.704468

Pd	-0.463359	-1.032244	-0.231054
P	-1.534337	0.903658	0.418663
P	1.864493	-0.670237	0.311399
C	-1.748971	-2.328586	-1.033036
C	-3.113838	-2.729296	-1.498625
H	-3.837925	-2.380867	-0.755379
H	-3.300222	-2.116906	-2.393254
C	-3.265855	-4.216942	-1.808979
H	-4.279494	-4.416030	-2.165686
H	-3.092842	-4.826652	-0.918547
H	-2.561004	-4.534274	-2.580659
O	-0.751960	-3.028219	-1.126606
C	-2.680803	0.557391	1.915832
C	-1.790088	0.227371	3.126684
H	-1.262239	1.099680	3.520420
H	-1.062210	-0.554462	2.888209
H	-2.424674	-0.152768	3.934980
C	-3.593444	1.738506	2.279610
H	-3.043657	2.670212	2.441555
H	-4.106970	1.503965	3.219298
H	-4.367886	1.916025	1.529676
C	-3.544277	-0.682059	1.638092
H	-2.923503	-1.568359	1.478288
H	-4.204179	-0.555247	0.778371
H	-4.178480	-0.871587	2.511657
C	-2.469951	1.736366	-1.019143
C	-3.734856	0.944576	-1.373080
H	-3.530206	-0.118786	-1.504403
H	-4.129673	1.324933	-2.322133
H	-4.524448	1.060999	-0.626125
C	-2.878576	3.190312	-0.737534
H	-3.521148	3.296446	0.137189
H	-3.442657	3.559658	-1.601779
H	-2.018739	3.846811	-0.619138
C	-1.515028	1.707277	-2.225974
H	-1.281440	0.681024	-2.526309
H	-0.576304	2.229983	-2.025546
H	-1.999800	2.204695	-3.074358
C	-0.386052	2.210596	1.132571
H	-1.036286	3.017563	1.488415
H	0.018069	1.731409	2.028643
C	0.748907	2.816937	0.333907
C	0.569192	4.088634	-0.230172
H	-0.382205	4.593966	-0.101231
C	1.585208	4.756822	-0.904505
H	1.400543	5.740063	-1.326186
C	2.842635	4.170201	-0.994084
H	3.659791	4.681696	-1.493394
C	3.057585	2.936466	-0.390269
H	4.060177	2.518459	-0.396000
C	2.036040	2.236898	0.267684

C	2.404100	0.972745	1.005463
H	1.967088	0.998298	2.008355
H	3.489151	0.940987	1.150252
C	2.824363	-0.929831	-1.318204
C	4.291974	-0.485016	-1.262543
H	4.882553	-1.037797	-0.530736
H	4.391216	0.581567	-1.054561
H	4.746264	-0.660422	-2.244879
C	2.094558	-0.096313	-2.388463
H	1.055497	-0.420252	-2.512024
H	2.602560	-0.232555	-3.350694
H	2.096091	0.972367	-2.160079
C	2.753699	-2.408146	-1.731581
H	1.728202	-2.788663	-1.749162
H	3.352763	-3.053992	-1.085243
H	3.157023	-2.505577	-2.746259
C	2.435809	-1.897484	1.664707
C	2.017289	-1.339994	3.037197
H	2.634951	-0.495480	3.355092
H	2.144746	-2.129062	3.786851
H	0.966477	-1.035905	3.064751
C	3.952100	-2.135292	1.693354
H	4.519676	-1.205070	1.794158
H	4.312628	-2.669093	0.811466
H	4.193309	-2.755686	2.564662
C	1.699592	-3.232005	1.455026
H	1.898472	-3.682522	0.481149
H	0.615552	-3.111516	1.555111
H	2.025377	-3.944414	2.222015

TS10-12

scf done: -1943.644905

Pd	0.004221	-1.215297	-0.412653
P	-1.957277	-0.044936	0.315150
P	1.887670	0.193590	0.328904
C	1.295901	-2.866090	-1.368406
C	-0.021447	-3.065950	-1.706599
H	-1.308208	-1.924886	-0.821932
H	-0.288369	-2.676007	-2.688691
C	-0.714302	-4.336459	-1.237804
H	-0.443515	-4.589293	-0.211156
H	-0.410149	-5.165713	-1.885929
H	-1.799999	-4.233264	-1.287679
O	2.438909	-3.146782	-1.328445
C	-2.898194	-1.038486	1.658242
C	-2.123029	-0.909093	2.981138
H	-2.212563	0.082493	3.432343
H	-1.062567	-1.148596	2.859443
H	-2.537555	-1.624808	3.699706
C	-4.335114	-0.545433	1.882851
H	-4.388619	0.525321	2.100114
H	-4.752473	-1.068550	2.750999
H	-4.988404	-0.761790	1.034579
C	-2.922277	-2.528766	1.285957
H	-1.911146	-2.945438	1.250294
H	-3.412064	-2.724636	0.329591
H	-3.479612	-3.075723	2.055196
C	-3.053796	0.295491	-1.212666
C	-3.681351	-1.002754	-1.740971
H	-2.940273	-1.787892	-1.926348
H	-4.163402	-0.787401	-2.701373
H	-4.451203	-1.401354	-1.075782
C	-4.183938	1.305879	-0.960650
H	-4.903791	0.968290	-0.214016
H	-4.732828	1.450721	-1.898098
H	-3.805725	2.282821	-0.662229
C	-2.112763	0.859175	-2.293916
H	-1.319988	0.148189	-2.549617
H	-1.644025	1.797172	-1.987368
H	-2.693925	1.056502	-3.202413
C	-1.715381	1.598031	1.169746
H	-2.712057	1.945075	1.462699
H	-1.198965	1.340163	2.098786
C	-0.981136	2.722122	0.480087
C	-1.733377	3.798679	-0.011850
H	-2.814721	3.772546	0.081890
C	-1.142277	4.928048	-0.566017

H	-1.760398	5.739712	-0.937153
C	0.244341	5.020539	-0.588102
H	0.735299	5.907925	-0.975685
C	1.003456	3.982861	-0.058678
H	2.078192	4.114314	0.002089
C	0.429184	2.810022	0.454433
C	1.326179	1.800648	1.138746
H	0.835580	1.463568	2.055753
H	2.238145	2.313378	1.460690
C	3.045457	0.743878	-1.096153
C	3.879910	1.992602	-0.776681
H	4.515144	1.871390	0.101771
H	3.266618	2.880881	-0.644978
H	4.541037	2.188495	-1.628863
C	2.114678	1.056448	-2.281420
H	1.564728	0.166733	-2.606779
H	2.714839	1.406799	-3.129536
H	1.389496	1.839359	-2.041450
C	4.020960	-0.367522	-1.507332
H	3.530008	-1.308998	-1.744658
H	4.778675	-0.557945	-0.743228
H	4.552334	-0.037170	-2.407666
C	2.880294	-0.574059	1.781945
C	1.972632	-0.613595	3.023864
H	1.803606	0.371494	3.466581
H	2.459589	-1.226774	3.790571
H	1.005200	-1.077282	2.806203
C	4.160069	0.197343	2.137125
H	3.975592	1.251847	2.363069
H	4.917100	0.136048	1.351893
H	4.597289	-0.248805	3.038212
C	3.241034	-2.027599	1.444501
H	3.846079	-2.126438	0.543856
H	2.343534	-2.640061	1.317767
H	3.812849	-2.450114	2.278951

Complex 12

scf done: -1943.652125

Pd	0.155715	-0.179791	-0.371286
P	-1.960678	-0.457346	0.184765
P	1.698785	0.591103	0.365977
C	2.512828	-2.933261	-1.538479
C	1.203618	-3.130969	-1.279278
H	-0.956323	-2.180731	-0.790720
H	0.635939	-3.070001	-2.211700
C	0.880478	-4.323746	-0.364640
H	-0.202530	-4.413777	-0.286236
H	1.277977	-4.175859	0.641723
H	1.276332	-5.262850	-0.763021
O	3.638996	-2.772638	-1.743330
C	-2.752022	-1.588167	1.519016
C	-2.024377	-1.342755	2.854680
H	-2.283752	-0.384970	3.312645
H	-0.936495	-1.402829	2.746993
H	-2.325066	-2.123483	3.562205
C	-4.251829	-1.316075	1.719932
H	-4.475276	-0.265776	1.928018
H	-4.594469	-1.891048	2.587821
H	-4.852475	-1.639309	0.866532
C	-2.557429	-3.069835	1.163780
H	-1.499485	-3.343143	1.180361
H	-2.970186	-3.339248	0.189828
H	-3.070137	-3.678636	1.917487
C	-3.041001	-0.332225	-1.382054
C	-3.436546	-1.721937	-1.900166
H	-2.574395	-2.383863	-2.027975
H	-3.901896	-1.601938	-2.885147
H	-4.168121	-2.217879	-1.256876
C	-4.321169	0.491654	-1.176164
H	-4.969175	0.095622	-0.393285
H	-4.893908	0.476035	-2.110167
H	-4.104780	1.536067	-0.957229
C	-2.169522	0.361804	-2.444166
H	-1.285740	-0.235863	-2.690669
H	-1.837174	1.352848	-2.123558
H	-2.758787	0.486602	-3.360333
C	-2.071399	1.201321	1.047890

H	-3.133413	1.347488	1.273975
H	-1.583215	1.017542	2.008616
C	-1.523722	2.480500	0.460730
C	-2.427484	3.409045	-0.075997
H	-3.480862	3.152077	-0.127926
C	-2.034898	4.678515	-0.485319
H	-2.766131	5.367354	-0.896944
C	-0.712317	5.067860	-0.306559
H	-0.388012	6.069461	-0.571842
C	0.188734	4.172232	0.258297
H	1.198582	4.513364	0.463673
C	-0.173561	2.865412	0.616567
C	0.854570	1.990988	1.294463
H	0.394050	1.490402	2.151232
H	1.645313	2.628449	1.703535
C	2.621704	1.436227	-1.079831
C	3.301229	2.766150	-0.727743
H	4.068705	2.665862	0.040695
H	2.587936	3.524699	-0.410865
H	3.793584	3.150554	-1.628881
C	1.558080	1.684985	-2.164922
H	1.089848	0.749160	-2.488427
H	2.038520	2.139967	-3.039459
H	0.770951	2.363527	-1.828010
C	3.681667	0.493710	-1.658976
H	3.259777	-0.467479	-1.952065
H	4.513856	0.315789	-0.973165
H	4.101836	0.950743	-2.562596
C	2.911938	-0.021984	1.721545
C	2.101411	-0.257900	3.009121
H	1.802336	0.672031	3.499313
H	2.726209	-0.807480	3.722374
H	1.207325	-0.863837	2.826214
C	4.061139	0.944679	2.034092
H	3.713072	1.946512	2.302268
H	4.766971	1.032028	1.204802
H	4.622167	0.560330	2.894300
C	3.493096	-1.377076	1.294249
H	4.079436	-1.318113	0.376140
H	2.697780	-2.117356	1.157492
H	4.157523	-1.748827	2.083125

TS12-13

scf done: -1943.645508

Pd	0.302830	-0.909865	-0.268277
P	-1.862876	-0.773412	0.278983
P	1.585378	1.024456	0.403074
C	2.016075	-2.974115	-1.915927
C	2.198608	-3.931255	-1.032022
H	-0.536330	-2.153618	-0.713301
H	1.295985	-4.435573	-0.698104
C	3.556272	-4.409995	-0.575255
H	4.361845	-3.816166	-1.012476
H	3.712128	-5.453037	-0.869092
H	3.644555	-4.350781	0.514169
O	1.859299	-2.115293	-2.706167
C	-2.321292	-2.031817	1.644347
C	-1.628022	-1.608950	2.951476
H	-2.068567	-0.715346	3.401445
H	-0.555702	-1.445620	2.808171
H	-1.739627	-2.420198	3.679164
C	-3.837260	-2.101120	1.889961
H	-4.280900	-1.124545	2.105209
H	-4.015782	-2.733637	2.766741
H	-4.374582	-2.553618	1.053763
C	-1.797559	-3.428448	1.274758
H	-0.705300	-3.440712	1.216234
H	-2.195457	-3.800173	0.328906
H	-2.101367	-4.131310	2.058833
C	-2.991931	-0.897106	-1.249020
C	-3.068676	-2.341722	-1.762670
H	-2.079272	-2.772678	-1.945254
H	-3.600626	-2.334785	-2.720665
H	-3.623255	-3.000738	-1.089979
C	-4.419503	-0.395277	-0.977644
H	-4.954449	-1.003370	-0.247487
H	-4.981645	-0.444953	-1.916530

H	-4.442989	0.642558	-0.647780	H	-0.117568	3.480946	-1.755706
C	-2.338588	-0.024237	-2.336072	H	1.306395	4.038733	-2.635800
H	-1.349621	-0.403959	-2.611417	H	1.066353	4.550327	-0.968729
H	-2.236290	1.019201	-2.028754	C	3.234807	2.920677	-1.051354
H	-2.969744	-0.050485	-3.231859	H	3.372025	3.641031	-0.243958
C	-2.178298	0.874955	1.122547	H	3.564471	3.404663	-1.977445
H	-3.224509	0.841368	1.449222	H	3.900298	2.075659	-0.882992
H	-1.570615	0.802174	2.027944	C	1.699783	1.435326	-2.361369
C	-1.916629	2.203349	0.445886	H	0.663083	1.167790	-2.589537
C	-3.003187	2.877513	-0.132050	H	2.248091	0.521831	-2.117991
H	-3.982408	2.409813	-0.118565	H	2.145416	1.862083	-3.267717
C	-2.888115	4.150522	-0.677900	C	2.362655	0.545190	1.052836
H	-3.756197	4.634320	-1.114825	H	3.179294	1.211405	1.353496
C	-1.663510	4.806396	-0.616257	H	1.903807	0.187805	1.979075
H	-1.552810	5.813438	-1.006444	C	2.940338	-0.625519	0.287957
C	-0.586211	4.173147	-0.008076	C	4.200909	-0.470568	-0.307897
H	0.347381	4.718028	0.096036	H	4.709210	0.484753	-0.224538
C	-0.672515	2.873946	0.514230	C	4.852829	-1.512373	-0.957510
C	0.534297	2.327455	1.241545	H	5.827545	-1.347442	-1.406272
H	0.213696	1.850321	2.172756	C	4.260446	-2.769819	-0.984996
H	1.184768	3.158812	1.532954	H	4.759819	-3.608567	-1.460287
C	2.410278	1.851405	-1.101158	C	3.037831	-2.956655	-0.350033
C	2.925352	3.271881	-0.836015	H	2.622510	-3.958855	-0.305757
H	3.687622	3.311273	-0.056754	C	2.348489	-1.909768	0.279445
H	2.121556	3.959203	-0.568094	C	1.097465	-2.248852	1.056905
H	3.379918	3.656391	-1.756567	H	1.128278	-1.735303	2.022487
C	1.340727	1.899353	-2.208896	H	1.099285	-3.320010	1.284739
H	1.015065	0.894989	-2.498177	C	-0.842959	-2.910044	-1.167492
H	1.773389	2.375803	-3.096737	C	-0.315554	-4.343604	-1.020849
H	0.461309	2.478060	-1.916992	H	-0.780543	-4.889268	-0.198745
C	3.569398	0.975535	-1.601875	H	0.766362	-4.375435	-0.890761
H	3.260386	-0.059328	-1.778027	H	-0.539709	-4.892055	-1.943435
H	4.427343	0.981225	-0.925098	C	-0.087465	-2.215799	-2.316283
H	3.915475	1.373576	-2.562864	H	-0.489151	-1.216669	-2.516537
C	2.859270	0.572192	1.751773	H	-0.202277	-2.811133	-3.230184
C	2.099314	0.334069	3.068496	H	0.982581	-2.121181	-2.114028
H	1.736861	1.261228	3.520769	C	-2.333505	-2.967808	-1.539440
H	2.783223	-0.126774	3.790063	H	-2.784400	-1.976168	-1.621949
H	1.254490	-0.350231	2.940046	H	-2.918989	-3.559859	-0.831510
C	3.935335	1.637197	2.002055	H	-2.426626	-3.455010	-2.517286
H	3.507680	2.613661	2.249964	C	-1.738798	-2.338882	1.803288
H	4.611405	1.759752	1.152814	C	-1.190584	-1.739914	3.110541
H	4.547977	1.328374	2.857434	H	-0.291899	-2.251105	3.465914
C	3.520719	-0.758380	1.351658	H	-1.950551	-1.850501	3.892388
H	4.101783	-0.684160	0.430849	H	-0.975892	-0.670688	3.016255
H	2.776929	-1.553816	1.223266	C	-1.865402	-3.857308	1.985377
H	4.207086	-1.072414	2.146923	H	-0.895393	-4.345667	2.120489
Complex 13				H	-2.382942	-4.338201	1.152379
scf done: -1943.657184				H	-2.454460	-4.057554	2.888393
Pd	-0.856380	0.548514	-0.208314	C	-3.127961	-1.723550	1.563188
P	1.037384	1.650256	0.314796	H	-3.589704	-2.058710	0.633245
P	-0.585466	-1.808648	0.369240	H	-3.077959	-0.629994	1.543692
C	-3.751149	1.174077	-1.411578	H	-3.792897	-2.011136	2.386210
C	-4.589480	2.082957	-1.826536	Complex 7.2MeOH			
H	-0.995130	2.053358	-0.591347	scf done: -1983.206656			
H	-4.486812	2.364470	-2.872795	Pd	-0.143508	-1.099579	0.134243
C	-5.655406	2.724469	-0.970069	P	-1.727923	0.740161	0.428791
H	-5.507461	3.807731	-0.929147	P	1.929912	-0.230150	0.416890
H	-5.642349	2.338567	0.051123	H	0.878669	-2.258905	-0.063473
H	-6.645359	2.531987	-1.394356	C	-2.784122	0.492753	2.007960
O	-3.007633	0.322832	-1.045695	C	-1.804787	-0.003476	3.086589
C	0.727995	2.900006	1.733652	H	-1.015629	0.723885	3.302042
C	0.488589	2.105876	3.030066	H	-1.330544	-0.947012	2.795958
H	1.393731	1.627668	3.413506	H	-2.351199	-0.170779	4.022418
H	-0.289779	1.347318	2.902687	C	-3.473321	1.765016	2.524986
H	0.143450	2.800875	3.803566	H	-2.761850	2.530126	2.846933
C	1.914383	3.853052	1.950760	H	-4.076641	1.503143	3.402369
H	2.862733	3.329699	2.104153	H	-4.149529	2.210112	1.791344
H	1.724803	4.440765	2.856064	C	-3.847785	-0.595572	1.792923
H	2.035541	4.562016	1.128524	H	-3.455760	-1.471607	1.269585
C	-0.539813	3.723801	1.458829	H	-4.709037	-0.219173	1.236546
H	-1.430473	3.090160	1.428735	H	-4.219137	-0.922824	2.771297
H	-0.491907	4.286119	0.525250	C	-2.790349	1.029011	-1.131197
H	-0.666527	4.446164	2.273603	C	-3.671849	-0.194618	-1.436741
C	1.772861	2.482302	-1.234702	H	-3.121626	-1.134180	-1.354675
C	0.948275	3.707423	-1.654357	H	-4.041075	-0.101932	-2.465289

H	-4.545948	-0.256880	-0.787393	H	-4.815984	0.085828	1.567101
C	-3.689416	2.269438	-1.060289	C	-3.994031	-2.216192	0.138487
H	-4.468962	2.169249	-0.300511	H	-3.391392	-2.650248	-0.665657
H	-4.195860	2.396870	-2.024566	H	-4.854025	-1.705450	-0.300129
H	-3.135979	3.190668	-0.866202	H	-4.385693	-3.045260	0.738774
C	-1.787802	1.167928	-2.292840	C	-3.168419	0.867867	-1.295162
H	-1.185998	0.260145	-2.406346	C	-3.621186	-0.119107	-2.385477
H	-1.108618	2.013587	-2.173667	H	-2.793393	-0.743174	-2.739704
H	-2.346557	1.318213	-3.224576	H	-3.990809	0.456084	-3.242239
C	-0.953358	2.400054	0.822518	H	-4.430366	-0.773946	-2.062708
H	-1.769939	3.114892	0.953952	C	-4.377037	1.630458	-0.742271
H	-0.521048	2.257288	1.820396	H	-5.153134	0.955519	-0.372164
C	0.075395	3.018039	-0.094131	H	-4.825554	2.228103	-1.544696
C	-0.327060	4.105441	-0.884151	H	-4.108830	2.319953	0.063506
H	-1.366951	4.418596	-0.853461	C	-2.182201	1.846669	-1.961564
C	0.563235	4.817611	-1.679433	H	-1.330123	1.315534	-2.407788
H	0.210964	5.653197	-2.276563	H	-1.794466	2.605328	-1.281166
C	1.910704	4.473627	-1.662967	H	-2.694820	2.362858	-2.781901
H	2.634884	5.038603	-2.241846	C	-1.599506	1.628293	1.362134
C	2.331894	3.418181	-0.862103	H	-2.503059	1.587478	1.806657
H	3.395173	3.208344	-0.798167	H	-1.179355	0.487649	2.119366
C	1.440085	2.654821	-0.093724	C	-0.639711	2.307057	1.095263
C	2.005472	1.598823	0.827604	C	-1.246985	3.564091	0.918280
H	1.504376	1.661706	1.797849	H	-2.332939	3.614674	0.911402
H	3.060596	1.823919	1.018468	C	-0.528835	4.744657	0.787522
C	2.958106	-0.494557	-1.167011	H	-1.050094	5.687814	0.655593
C	4.223574	0.374680	-1.233918	C	0.858787	4.700967	0.875630
H	4.916097	0.195423	-0.410354	H	1.450038	5.609819	0.820482
H	3.989121	1.437400	-1.270382	C	1.481147	3.476361	1.074793
H	4.755523	0.135419	-2.161796	H	2.559020	3.460015	1.206493
C	2.034221	-0.119714	-2.340474	C	0.779929	2.259983	1.161320
H	1.160712	-0.778414	-2.383358	C	1.622985	1.029301	1.451092
H	2.590919	-0.230834	-3.278811	H	1.082657	0.356412	2.122974
H	1.684939	0.914484	-2.280733	H	2.527207	1.343360	1.984738
C	3.370326	-1.965265	-1.322997	C	3.156400	0.809321	-1.249127
H	2.517805	-2.646263	-1.243977	C	4.222809	1.753376	-0.681347
H	4.130390	-2.268137	-0.598379	H	4.981819	1.231602	-0.096629
H	3.805644	-2.094178	-2.320730	H	3.785523	2.538179	-0.062566
C	2.785596	-0.980301	1.961686	H	4.735123	2.248879	-1.514481
C	2.109584	-0.398653	3.217190	C	2.119317	1.624639	-2.045957
H	2.371121	0.647828	3.395394	H	1.390166	0.966964	-2.541758
H	2.454442	-0.964217	4.090048	H	2.628183	2.183897	-2.840228
H	1.020367	-0.492191	3.177207	H	1.582524	2.344744	-1.423553
C	4.287854	-0.661222	2.021087	C	3.812196	-0.198233	-2.205954
H	4.500997	0.409251	1.947507	H	3.092209	-0.920727	-2.604583
H	4.857039	-1.183626	1.248691	H	4.631938	-0.746587	-1.736358
H	4.676772	-0.997472	2.989051	H	4.233219	0.350838	-3.056032
C	2.592410	-2.504384	2.003790	C	3.139315	-1.492745	0.942311
H	2.993434	-3.013524	1.125738	C	2.387245	-1.876854	2.228556
H	1.535794	-2.769243	2.095803	H	2.447897	-1.105468	3.001094
H	3.118348	-2.896269	2.882214	H	2.848734	-2.781525	2.639750
H	-2.474443	-4.489381	0.352107	H	1.334280	-2.112304	2.039016
C	-1.689596	-3.787948	0.652849	C	4.561328	-1.047324	1.314364
H	-0.717753	-4.292851	0.649810	H	4.575346	-0.133058	1.916583
H	-1.903548	-3.434494	1.662423	H	5.194049	-0.894543	0.436403
O	-1.693304	-2.652204	-0.217764	H	5.030249	-1.835527	1.914455
H	-1.591371	-2.974989	-1.148466	C	3.186520	-2.736006	0.036757
H	0.208513	-4.569854	-2.678757	H	3.688111	-2.550937	-0.914775
C	-0.726066	-4.575361	-3.241126	H	2.182580	-3.122327	-0.165076
H	-0.495108	-4.444938	-4.303437	H	3.750681	-3.521394	0.553581
H	-1.226605	-5.538969	-3.091998	H	0.010635	-1.671598	0.261223
O	-1.511649	-3.488260	-2.749981	H	-0.065765	-5.790180	0.757256
H	-2.332418	-3.441141	-3.252155	C	-0.182232	-5.551032	-0.301628
Complex 7a.MeOH				H	0.628656	-6.040608	-0.856205
scf done: -1867.474419				H	-1.141550	-5.960691	-0.643473
Pd	0.001617	-0.533253	-0.703756	O	-0.130331	-4.134514	-0.415149
P	-2.155122	-0.058333	0.019438	H	-0.235643	-3.900690	-1.343569
P	2.146791	-0.136024	0.051417	Complex 8.2MeOH			
C	-3.173494	-1.295426	1.054650	scf done: -2061.787822			
C	-2.180248	-2.172867	1.838017	Pd	0.547055	-0.175030	-0.695715
H	-1.508114	-1.591829	2.478442	P	-0.835772	-1.828544	0.159444
H	-1.579977	-2.803144	1.174996	P	-0.210846	1.903994	0.276093
H	-2.752581	-2.833901	2.499713	C	1.614309	-1.366816	-2.008181
C	-4.114244	-0.596811	2.051187	H	2.165855	-2.173080	-1.533416
H	-3.571849	-0.045150	2.823633	H	1.004087	-1.696902	-2.846589
H	-4.707215	-1.362813	2.564118	C	2.346444	-0.094946	-2.211339

H	2.221368	0.347480	-3.202069
H	3.394349	-0.112589	-1.902352
H	1.927528	0.759048	-1.516723
C	0.117424	-2.917208	1.421607
C	0.497198	-2.038901	2.626196
H	-0.358633	-1.758900	3.246127
H	1.030402	-1.138228	2.308423
H	1.177557	-2.611273	3.266955
C	-0.701752	-4.116843	1.921362
H	-1.678027	-3.835493	2.327084
H	-0.146959	-4.599500	2.734600
H	-0.849837	-4.872794	1.146653
C	1.437267	-3.419006	0.812711
H	2.135917	-2.595565	0.639139
H	1.298396	-3.980087	-0.112641
H	1.906709	-4.098726	1.534025
C	-1.699627	-2.897076	-1.169763
C	-0.729640	-3.910356	-1.798392
H	0.204533	-3.460539	-2.134385
H	-1.216017	-4.350433	-2.676945
H	-0.494679	-4.733462	-1.118639
C	-2.909951	-3.685719	-0.644256
H	-2.658632	-4.368019	0.168724
H	-3.303369	-4.293545	-1.467261
H	-3.721757	-3.039364	-0.316372
C	-2.181424	-1.917503	-2.255490
H	-1.346106	-1.390708	-2.725205
H	-2.873689	-1.170083	-1.858202
H	-2.708697	-2.480210	-3.034963
C	-2.216285	-1.158735	1.244342
H	-2.762075	-2.033563	1.613129
H	-1.684515	-0.753985	2.109564
C	-3.222755	-0.134704	0.762748
C	-4.499228	-0.575178	0.382780
H	-4.714594	-1.638221	0.390231
C	-5.525774	0.301663	0.050136
H	-6.497509	-0.086160	-0.239907
C	-5.304749	1.671172	0.140395
H	-6.099313	2.378144	-0.077859
C	-4.059982	2.128401	0.557568
H	-3.916035	3.195953	0.695622
C	-2.999636	1.258599	0.851128
C	-1.718114	1.855214	1.380304
H	-1.386250	1.291917	2.257827
H	-1.912390	2.874624	1.730412
C	-0.654940	3.065716	-1.179540
C	-1.463539	4.308907	-0.782502
H	-0.923367	4.977026	-0.110756
H	-2.417145	4.050087	-0.322280
H	-1.693977	4.878152	-1.690828
C	-1.493540	2.223287	-2.159599
H	-0.942855	1.344288	-2.513023
H	-1.745452	2.836985	-3.033077
H	-2.429108	1.879201	-1.712770
C	0.617970	3.523396	-1.907144
H	1.241368	2.684679	-2.230285
H	1.230174	4.198240	-1.304178
H	0.325011	4.071042	-2.810466
C	1.087796	2.712106	1.429150
C	1.032808	1.994902	2.789662
H	0.149934	2.265934	3.375296
H	1.909635	2.291222	3.376624
H	1.067708	0.907089	2.683518
C	0.865905	4.211869	1.668001
H	-0.139329	4.434915	2.038364
H	1.046013	4.811791	0.772890
H	1.573167	4.554939	2.432471
C	2.489167	2.476471	0.840939
H	2.601888	2.888060	-0.165402
H	2.748402	1.412207	0.823105
H	3.225386	2.981244	1.478592
H	5.291699	-1.939911	2.149244
C	4.653257	-1.046482	2.209311
H	5.284007	-0.192939	2.497559
H	3.926403	-1.209360	3.009274
O	3.936398	-0.812045	1.014115
H	4.583214	-0.675544	0.298210

H	6.230891	1.499804	-0.737796
C	6.697405	0.601555	-1.145478
H	7.046362	0.819006	-2.161381
H	7.556538	0.336917	-0.517840
O	5.701537	-0.419851	-1.142560
H	6.090994	-1.228715	-1.492592

Complex 9.2MeOH

scf done: -2175.061156

Pd	0.524309	-0.170280	-0.842125
P	-0.914433	-1.872996	0.115850
P	-0.423441	1.900490	0.180797
C	1.687739	0.793788	-2.015336
C	1.709849	-1.725386	-1.754281
H	1.234233	-2.664061	-1.499307
H	1.619421	-1.610998	-2.838967
C	3.163018	-1.716605	-1.303327
H	3.656383	-2.630300	-1.664176
H	3.274941	-1.687733	-0.216051
H	3.730216	-0.870592	-1.700776
O	2.378104	1.250262	-2.804039
C	0.006421	-3.053026	1.343068
C	1.018849	-2.174348	2.094768
H	0.529112	-1.384538	2.674041
H	1.753087	-1.708230	1.432020
H	1.566893	-2.797438	2.811487
C	-0.929465	-3.709505	2.376525
H	-1.363072	-2.995086	3.079466
H	-0.333699	-4.410857	2.971604
H	-1.737959	-4.285812	1.919748
C	0.759342	-4.190727	0.636124
H	1.500113	-3.841165	-0.082865
H	0.082716	-4.889899	0.138745
H	1.302913	-4.761125	1.397971
C	-1.897222	-2.817680	-1.234164
C	-0.998641	-3.515031	-2.268758
H	-0.416704	-2.797927	-2.849326
H	-1.652367	-4.045198	-2.971414
H	-0.322127	-4.255328	-1.838818
C	-2.831782	-3.874355	-0.626268
H	-2.276538	-4.718916	-0.209314
H	-3.473025	-4.272266	-1.421087
H	-3.491145	-3.480351	0.149418
C	-2.706106	-1.759185	-2.006469
H	-2.045738	-1.011216	-2.457509
H	-3.442479	-1.242112	-1.392053
H	-3.242491	-2.257824	-2.822500
C	-2.222438	-1.246928	1.308494
H	-2.714349	-2.145845	1.685505
H	-1.628576	-0.867253	2.148346
C	-3.307706	-0.254539	0.970450
C	-4.600488	-0.748012	0.737225
H	-4.755978	-1.822766	0.703223
C	-5.697815	0.090987	0.582260
H	-6.682273	-0.329165	0.400489
C	-5.524355	1.465044	0.713009
H	-6.371915	2.139914	0.643082
C	-4.254632	1.968262	0.973047
H	-4.142689	3.034573	1.145327
C	-3.127302	1.139258	1.071967
C	-1.800216	1.751730	1.441817
H	-1.348239	1.172316	2.252466
H	-1.969105	2.755049	1.845667
C	-1.091624	3.098426	-1.154621
C	-2.002879	4.199518	-0.589751
H	-1.516894	4.812294	0.171158
H	-2.925615	3.794226	-0.178249
H	-2.287609	4.867111	-1.411404
C	-1.911548	2.231434	-2.127849
H	-1.286364	1.492272	-2.638924
H	-2.357133	2.877215	-2.893877
H	-2.725855	1.703026	-1.624371
C	0.040509	3.781492	-1.934857
H	0.744394	3.080190	-2.383221
H	0.600273	4.494069	-1.324652
H	-0.408178	4.347118	-2.759632
C	0.925957	2.736272	1.257368

C	1.122963	1.880369	2.522013	C	-3.026822	1.489397	0.854058
H	0.289535	1.962245	3.225168	C	-1.668286	1.927017	1.347299
H	2.017050	2.238221	3.044148	H	-1.384448	1.317992	2.210746
H	1.299030	0.828219	2.281059	H	-1.742683	2.954852	1.717855
C	0.563221	4.166945	1.682885	C	-0.500638	3.111751	-1.173628
H	-0.403649	4.230899	2.190584	C	-1.248173	4.378486	-0.729021
H	0.561947	4.867967	0.845025	H	-0.696072	4.972155	0.000657
H	1.319164	4.518820	2.394731	H	-2.234226	4.156177	-0.324687
C	2.269709	2.753433	0.510049	H	-1.402000	5.010767	-1.611118
H	2.215724	3.231429	-0.470179	C	-1.374993	2.353256	-2.188622
H	2.678827	1.744904	0.406321	H	-0.860993	1.472806	-2.587709
H	2.988365	3.325731	1.108778	H	-1.600264	3.018565	-3.030594
H	5.351470	-1.207421	2.898623	H	-2.326496	2.032423	-1.756566
C	4.647602	-0.362352	2.876653	C	0.796343	3.545998	-1.870167
H	5.187707	0.538840	3.203454	H	1.392455	2.705108	-2.25230
H	3.862966	-0.563783	3.611319	H	1.425006	4.177168	-1.237021
O	4.031815	-0.200262	1.616746	H	0.527677	4.141656	-2.750275
H	4.730752	0.002891	0.967004	C	1.179337	2.552827	1.456655
H	6.777727	-1.394421	-0.553458	C	1.097866	1.740488	2.761798
C	7.153459	-0.371335	-0.499425	H	0.214734	1.977218	3.361222
H	7.904570	-0.316114	0.298223	H	1.973449	1.984590	3.373585
H	7.627442	-0.124548	-1.456712	H	1.129910	0.663478	2.573300
O	6.032288	0.468119	-0.239250	C	0.993826	4.039762	1.793075
H	6.340538	1.378633	-0.180657	H	-0.006827	4.274429	2.167941
				H	1.210040	4.690800	0.943160
TS9-10.2MeOH				H	1.701727	4.305114	2.586919
scf done: -2175.054274				C	2.582503	2.328124	0.873163
Pd	0.521656	-0.235119	-0.680608	H	2.713964	2.765436	-0.118259
P	-1.210476	-1.759180	0.190787	H	2.832207	1.263989	0.837735
P	-0.151520	1.882503	0.251636	H	3.312858	2.806509	1.536067
C	2.025714	0.314512	-1.647465	H	5.175433	-2.121600	2.364014
C	1.649289	-1.786245	-1.973353	C	4.357935	-1.399184	2.500420
H	0.980121	-2.535685	-1.569425	H	4.744366	-0.547279	3.077699
H	1.379820	-1.597228	-3.014875	H	3.580599	-1.884309	3.096883
C	3.091779	-2.220329	-1.778373	O	3.778950	-1.001806	1.273161
H	3.204337	-3.245563	-2.152940	H	4.465313	-0.542272	0.750758
H	3.384253	-2.210299	-0.724579	H	7.379949	-0.092240	0.660775
H	3.794452	-1.594765	-2.334417	C	7.025391	0.120449	-0.349303
O	2.945707	0.744139	-2.198651	H	7.600274	0.965812	-0.745199
C	-0.464429	-3.036473	1.415772	H	7.206076	-0.761877	-0.976212
C	-0.057940	-2.286715	2.697438	O	5.640188	0.433650	-0.247508
H	-0.913045	-1.970209	3.300553	H	5.308072	0.651097	-1.125039
H	0.569473	-1.416949	2.479625				
H	0.535745	-2.964737	3.321059	Complex 10.2MeOH			
C	-1.436386	-4.164181	1.790586	scf done: -2175.076692			
H	-2.378533	-3.795770	2.206611	Pd	0.429249	-0.277331	-0.548882
H	-0.968398	-4.784348	2.564114	P	-1.468666	-1.687312	0.229294
H	-1.662163	-4.821178	0.947516	P	0.100693	1.860683	0.306533
C	0.819603	-3.640531	0.826175	C	2.078820	-0.009671	-1.562107
H	1.588315	-2.878158	0.673485	C	1.927079	-1.388205	-2.241458
H	0.653201	-4.172819	-0.112952	H	1.121158	-2.004256	-1.795183
H	1.219725	-4.370322	1.539804	H	1.594956	-1.165836	-3.262857
C	-2.172940	-2.623445	-1.226974	C	3.237293	-2.177827	-2.213643
C	-1.380470	-3.771476	-1.873240	H	3.115840	-3.118260	-2.757262
H	-0.426642	-3.456414	-2.297811	H	3.535665	-2.392260	-1.185011
H	-1.977733	-4.165874	-2.703515	H	4.024879	-1.594322	-2.697814
H	-1.203758	-4.601158	-1.184854	O	3.005950	0.729248	-1.720032
C	-3.526236	-3.196515	-0.780048	C	-0.837106	-3.078205	1.379264
H	-3.442780	-3.911446	0.040438	C	-0.511992	-2.448877	2.745581
H	-3.971085	-3.728358	-1.629111	H	-1.409409	-2.186471	3.312615
H	-4.227619	-2.415226	-0.496172	H	0.120686	-1.561144	2.650944
C	-2.416706	-1.531216	-2.283180	H	0.041734	-3.180443	3.345123
H	-1.474762	-1.152210	-2.693639	C	-1.834143	-4.223031	1.602009
H	-2.980730	-0.685886	-1.878209	H	-2.797937	-3.871780	1.983832
H	-2.998263	-1.952641	-3.111767	H	-1.422759	-4.908132	2.353039
C	-2.524672	-0.987945	1.286914	H	-2.011898	-4.810561	0.698598
H	-3.152233	-1.809955	1.645218	C	0.476879	-3.628281	0.797089
H	-1.954534	-0.647304	2.155893	H	1.251923	-2.855342	0.740689
C	-3.424682	0.134441	0.823723	H	0.350648	-4.072339	-0.192983
C	-4.766895	-0.156493	0.537833	H	0.854011	-4.419353	1.456269
H	-5.111561	-1.182958	0.610669	C	-2.403371	-2.401072	-1.276147
C	-5.695290	0.830820	0.226979	C	-1.560070	-3.480858	-1.971489
H	-6.723814	0.559555	0.009622	H	-0.556859	-3.130334	-2.231169
C	-5.301044	2.163440	0.250623	H	-2.053681	-3.756648	-2.910590
H	-6.013714	2.957623	0.050542	H	-1.464047	-4.392359	-1.377403
C	-3.988975	2.474847	0.588691	C	-3.778278	-2.958631	-0.942073
H	-3.717197	3.520266	0.696341	H	-3.727439	-3.812190	-0.220414

H	-4.218087	-3.399996	-1.861520	H	-1.058004	-1.350194	3.530519
H	-4.470194	-2.242231	-0.565920	H	0.430629	-0.563286	2.947680
C	-2.588413	-1.232263	-2.262580	H	0.505641	-1.852528	4.155267
H	-1.626215	-0.823911	-2.591548	C	-0.520466	-3.879600	2.602563
H	-3.175806	-0.415596	-1.836442	H	-1.608780	-3.792694	2.666527
H	-3.118336	-1.595722	-3.151289	H	-0.161026	-4.140888	3.605205
C	-2.752234	-0.841134	1.290045	H	-0.277778	-4.720008	1.948065
H	-3.494719	-1.587214	1.591900	C	1.671149	-2.820043	2.016895
H	-2.207242	-0.568676	2.198878	H	2.185049	-1.907086	1.703586
C	-3.461587	0.374050	0.741951	H	1.905221	-3.616978	1.309459
C	-4.807646	0.236462	0.372253	H	2.073396	-3.122669	2.991260
H	-5.279433	-0.737047	0.466167	C	-0.647843	-3.187428	-0.843060
C	-5.575247	1.310634	-0.062277	C	0.711100	-3.867013	-1.055382
H	-6.614010	1.160372	-0.339966	H	1.523075	-3.139370	-1.123517
C	-5.007700	2.579394	-0.087536	H	0.684796	-4.426713	-1.997880
H	-5.593679	3.444415	-0.382576	H	0.942825	-4.583466	-0.262736
C	-3.688528	2.740708	0.320113	C	-1.686992	-4.289405	-0.586197
H	-3.291922	3.747889	0.385743	H	-1.457444	-4.897235	0.290438
C	-2.879335	1.662965	0.710596	H	-1.697779	-4.962008	-1.452126
C	-1.507487	1.960341	1.279159	H	-2.699338	-3.902400	-0.475404
H	-1.322567	1.294211	2.125793	C	-1.023563	-2.431143	-2.130615
H	-1.521287	2.973922	1.695417	H	-0.270363	-1.679247	-2.383092
C	0.011922	3.199914	-1.053078	H	-1.989220	-1.926637	-2.049687
C	-0.685142	4.489520	-0.590972	H	-1.086654	-3.144687	-2.961209
H	-0.228069	4.936716	0.292783	C	-2.305498	-1.513459	1.018834
H	-1.745978	4.341532	-0.400978	H	-2.728398	-2.476692	1.321354
H	-0.608144	5.223318	-1.401498	H	-2.206107	-0.926454	1.935867
C	-0.796863	2.585779	-2.208538	C	-3.292258	-0.822603	0.102610
H	-0.283655	1.722544	-2.643791	C	-4.209169	-1.605645	-0.614466
H	-0.916958	3.337415	-2.997631	H	-4.153068	-2.686601	-0.539015
H	-1.795749	2.271204	-1.893223	C	-5.223210	-1.050717	-1.387236
C	1.411903	3.577141	-1.561585	H	-5.909453	-1.696475	-1.926723
H	2.006746	2.716674	-1.865926	C	-5.370719	0.331429	-1.423476
H	1.977951	4.146019	-0.819489	H	-6.174222	0.789814	-1.991984
H	1.288623	4.225228	-2.437176	C	-4.497963	1.123748	-0.686691
C	1.366886	2.304808	1.674408	H	-4.659028	2.197707	-0.664904
C	1.123836	1.379172	2.879076	C	-3.444161	0.581747	0.063572
H	0.208905	1.611270	3.430828	C	-2.609765	1.519738	0.900815
H	1.957296	1.504128	3.579377	H	-2.507004	1.110609	1.910472
H	1.112301	0.327129	2.578700	H	-3.139280	2.471925	1.011431
C	1.254178	3.765992	2.136530	C	-1.000669	2.856607	-1.270758
H	0.248764	4.038219	2.471710	C	-2.145814	3.877525	-1.318700
H	1.570607	4.473172	1.366439	H	-2.053092	4.667893	-0.572579
H	1.923454	3.905112	2.993395	H	-3.122731	3.406261	-1.204377
C	2.795058	2.028014	1.182836	H	-2.140192	4.359985	-2.303676
H	3.045719	2.547622	0.258415	C	-1.234320	1.804299	-2.371664
H	2.963976	0.958733	1.040953	H	-0.411992	1.082213	-2.412805
H	3.493915	2.369961	1.954995	H	-1.288497	2.312581	-3.342354
H	4.914601	-2.795437	2.031626	H	-2.167618	1.253817	-2.231074
C	4.058034	-2.133878	2.222798	C	0.326662	3.570625	-1.573072
H	4.355793	-1.395006	2.979625	H	1.176302	2.883904	-1.533867
H	3.252717	-2.742336	2.643063	H	0.513364	4.411212	-0.899245
O	3.573005	-1.526928	1.040437	H	0.276435	3.980729	-2.589169
H	4.289784	-0.971394	0.669017	C	-0.266350	3.036735	1.789446
H	7.278670	-0.503281	0.343984	C	-0.656265	2.394239	3.132697
C	6.746585	-0.104381	-0.521749	H	-1.727261	2.472354	3.339299
H	7.265699	0.801217	-0.857194	H	-0.136361	2.923951	3.939428
O	6.778481	-0.851948	-1.325067	H	-0.364568	1.342158	3.193639
O	5.418752	0.181898	-0.102427	C	-0.858248	4.451807	1.756729
H	4.923086	0.557250	-0.841519	H	-1.952435	4.446195	1.763225
TS11-13.2MeOH				H	-0.519277	5.031304	0.895536
scf done: -2175.066397				H	-0.535108	4.991443	2.655407
Pd	0.677098	0.047453	-0.095197	C	1.268018	3.114681	1.738983
P	-0.522691	-1.844947	0.515476	H	1.633763	3.555228	0.808629
P	-0.853042	1.885990	0.370941	H	1.715650	2.121841	1.849603
C	2.523549	-0.321587	-0.992941	H	1.625489	3.740508	2.565728
C	2.723289	-0.898141	-2.383229	H	4.918682	-2.033779	-1.085739
H	2.828568	-1.985601	-2.343655	C	4.314523	-2.001743	-0.175295
H	1.791087	-0.705142	-2.922008	H	4.956772	-2.102960	0.701339
C	3.889331	-0.262591	-3.148800	H	3.587207	-2.813704	-0.176470
H	3.960121	-0.686576	-4.154256	O	3.629763	-0.752010	-0.039199
H	4.853090	-0.430179	-2.655835	H	4.204555	0.248345	0.345004
H	3.740259	0.815954	-3.246705	H	6.426519	1.593857	0.668203
O	2.395138	0.978660	-0.895894	C	5.597805	2.006565	0.093313
C	0.161262	-2.580628	2.154515	H	5.539166	3.081962	0.264785
C	-0.014392	-1.516089	3.250814	H	5.735381	1.801556	-0.971910
				O	4.388180	1.397293	0.589035

H	3.579760	1.655490	0.047087
Complex 11.2MeOH			
scf done: -2175.087614			
Pd	0.500626	-0.126493	-0.397445
P	-0.923362	-1.788377	0.322798
P	-0.538761	1.932469	0.335550
C	2.047045	-0.912122	-1.370392
C	2.818291	-2.083078	-1.888866
H	2.812786	-2.848788	-1.108576
H	2.212585	-2.488114	-2.712417
C	4.232739	-1.750127	-2.354343
H	4.728099	-2.656738	-2.710885
H	4.812958	-1.343643	-1.523415
H	4.223274	-1.024390	-3.717837
O	2.366621	0.258896	-1.534487
C	-0.125781	-2.811625	1.732456
C	0.019530	-1.898728	2.962477
H	-0.936403	-1.646112	3.429337
H	0.557193	-0.978319	2.717459
H	0.611101	-2.428281	3.717921
C	-0.945195	-4.049511	2.128136
H	-1.980482	-3.814337	2.392519
H	-0.484992	-4.500091	3.015279
H	-0.948449	-4.814820	1.348386
C	1.291607	-3.245233	1.326271
H	1.940143	-2.384210	1.139778
H	1.299679	-3.895490	0.449898
H	1.725426	-3.817991	2.154526
C	-1.521079	-2.901040	-1.109346
C	-0.408632	-3.856074	-1.558045
H	0.535399	-3.340791	-1.736790
H	-0.712432	-4.326576	-2.500331
H	-0.236510	-4.658859	-0.836816
C	-2.758655	-3.745630	-0.769180
H	-2.607765	-4.408023	0.084080
H	-2.987713	-4.378276	-1.634589
H	-3.639303	-3.134037	-0.584775
C	-1.866790	-1.952436	-2.270870
H	-0.987404	-1.396127	-2.610031
H	-2.642505	-1.231755	-1.998687
H	-2.241247	-2.543524	-3.115083
C	-2.480336	-1.152905	1.166845
H	-3.012029	-2.047229	1.508837
H	-2.101791	-0.665669	2.069529
C	-3.472839	-0.234251	0.484876
C	-4.658918	-0.783927	-0.024183
H	-4.821396	-1.853853	0.052599
C	-5.669019	-0.002814	-0.574889
H	-6.569456	-0.472831	-0.958331
C	-5.528835	1.380370	-0.587585
H	-6.314523	2.014753	-0.986332
C	-4.386069	1.948647	-0.036412
H	-4.314956	3.031052	0.020476
C	-3.343962	1.173242	0.491426
C	-2.203329	1.887270	1.174000
H	-2.006715	1.414611	2.141085
H	-2.500641	2.917896	1.395091
C	-0.751088	3.008170	-1.225171
C	-1.636652	4.244585	-1.019142
H	-1.266027	4.916460	-0.244071
H	-2.666557	3.974578	-0.781516
H	-1.666045	4.812958	-1.956396
C	-1.400206	2.107783	-2.293445
H	-0.753429	1.264190	-2.556097
H	-1.562128	2.698691	-3.203101
H	-2.368614	1.713000	-1.976454
C	0.626834	3.445669	-1.746616
H	1.308195	2.598518	-1.868747
H	1.105679	4.188266	-1.103592
H	0.495088	3.907678	-2.732147
C	0.555432	2.801052	1.644287
C	0.284969	2.148966	3.011779
H	-0.682243	2.436360	3.433424
H	1.053811	2.486416	3.715991
H	0.342624	1.057549	2.970392
C	0.297423	4.308497	1.777461

H	-0.747578	4.537560	2.009349
H	0.587063	4.866743	0.884605
H	0.901384	4.694358	2.607404
C	2.029726	2.549056	1.289102
H	2.307978	2.942144	0.310163
H	2.278260	1.483163	1.312205
H	2.664051	3.048809	2.030833
H	5.706062	-1.580883	1.681778
C	4.726886	-1.252046	2.057980
H	4.893220	-0.495564	2.837472
H	4.241237	-2.113354	2.524447
O	3.881482	-0.783387	1.025051
H	4.306554	-0.006464	0.611166
H	6.794854	1.824027	0.111075
C	6.210818	1.709341	-0.803854
H	6.239483	2.658258	-1.352284
H	6.675079	0.927507	-1.418428
O	4.885247	1.372041	-0.412961
H	4.332810	1.269897	-1.197516

Complex 11'.MeOH			
scf done: -2175.08591951			
Pd	0.769384	-0.401406	0.170238
P	-1.206564	-1.647592	0.361342
P	-0.001109	1.980282	0.504656
C	1.811129	-1.859468	-0.729719
C	2.624671	-2.951147	-0.057026
H	2.902523	-2.608141	0.944194
H	1.933866	-3.784415	0.113093
C	3.834664	-3.410409	-0.866360
H	4.363230	-4.202812	-0.329492
H	4.533691	-2.587497	-1.038052
H	3.530410	-3.802188	-1.840010
O	1.949956	-1.593949	-1.908346
C	-2.723293	-0.580502	0.673605
H	-3.527771	-1.287100	0.903729
H	-2.481082	-0.091405	1.619089
C	-3.256286	0.461571	-0.282137
C	-4.309053	0.135242	-1.150461
H	-4.678502	-0.883960	-1.181722
C	-4.933085	1.084734	-1.951446
H	-5.743628	0.788930	-2.610488
C	-4.534986	2.415409	-1.869344
H	-5.025821	3.179162	-3.464836
C	-3.518901	2.763441	-0.987876
H	-3.236608	3.808917	-0.894111
C	-2.855749	1.810372	-0.200157
C	-1.825049	2.309142	0.778391
H	-2.024085	1.904249	1.778823
H	-1.941498	3.391125	0.871834
H	4.402010	-0.946760	1.271750
C	3.816637	-0.057580	1.526611
H	4.505074	0.759459	1.769719
H	3.204167	-0.270099	2.404261
O	2.951663	0.328333	0.457156
H	3.477019	0.321015	-0.385365
H	5.808184	1.338679	-1.967398
C	5.152410	0.762717	-2.622273
H	4.573058	1.456021	-3.242279
H	5.771225	0.129552	-3.266657
O	4.312422	-0.028992	-1.785474
H	3.712068	-0.569421	-2.319412
C	0.690109	2.865919	2.066914
C	0.430916	2.932680	-1.100084
C	-1.204991	-2.641498	2.012338
C	-1.667774	-2.743931	-1.137759
C	-1.512464	-1.835934	-2.372738
H	-0.484638	-1.481293	-2.484516
H	-2.179120	-0.970965	-2.339490
H	-1.765099	-2.415208	-3.268858
C	-3.099602	-3.302870	-1.083800
H	-3.219247	-4.082032	-0.330497
H	-3.322491	-3.757009	-2.056057
H	-3.859312	-2.543446	-0.908332
C	-0.723064	-3.944237	-1.290982
H	0.315079	-3.648008	-1.438053
H	-1.019302	-4.497232	-2.190117

H	-0.785091	-4.643762	-0.452909	H	1.425304	3.198105	-2.856239
C	-2.386774	-3.611823	2.156963	C	2.377609	1.265638	1.070220
H	-2.395175	-3.994864	3.184248	H	2.888238	2.167363	1.424253
H	-2.294005	-4.476111	1.495496	H	2.192564	0.660284	1.960972
H	-3.359249	-3.143223	1.983629	C	3.319226	0.512172	0.154460
C	0.099629	-3.432190	2.152113	C	4.311703	1.225995	-0.533464
H	0.965931	-2.766573	2.140071	H	4.343905	2.306697	-0.444497
H	0.222677	-4.185561	1.371627	C	5.291465	0.599121	-1.295488
H	0.093223	-3.959691	3.112998	H	6.039584	1.193131	-1.811616
C	-1.245683	-1.630183	3.173656	C	5.324465	-0.789908	-1.351034
H	-0.505228	-0.834472	3.046367	H	6.098544	-1.305372	-1.911339
H	-1.005919	-2.157908	4.103728	C	4.373295	-1.517119	-0.644842
H	-2.231991	-1.180093	3.312815	H	4.441988	-2.601191	-0.638608
C	-0.311832	2.235317	-2.255316	C	3.354407	-0.899153	0.094637
H	-0.071005	1.167751	-2.297922	C	2.424440	-1.775711	0.896153
H	0.015575	2.685617	-3.200261	H	2.351834	-1.390884	1.917998
H	-1.394597	2.339884	-2.196532	H	2.856437	-2.778572	0.981417
C	0.043773	4.416039	-1.046789	C	0.728272	-2.872670	-1.336247
H	0.647377	4.975759	-0.326997	C	1.769929	-3.997634	-0.105560
H	-1.011400	4.573551	-0.808516	H	1.583304	-4.805526	-0.701943
H	0.218511	4.865858	-2.031567	H	2.785530	-3.630183	-1.257480
C	1.929490	2.817632	-1.421855	H	1.738587	-4.434368	-2.416058
H	2.227690	1.777471	-1.570833	C	1.082212	-1.807071	-2.391193
H	2.576789	3.259583	-0.665368	H	0.332469	-1.008785	-2.420144
H	2.114477	3.347654	-2.364078	H	1.110224	-2.280719	-3.380219
C	-0.108480	4.104858	2.506403	H	2.058372	-1.350419	-2.211871
H	0.412207	4.567909	3.353017	C	-0.655135	-3.443844	-1.683984
H	-1.116164	3.860854	2.852432	H	-1.437374	-2.682062	-1.633689
H	-0.185824	4.863440	1.723861	H	-0.936758	-4.282919	-1.042674
C	2.155065	3.282576	1.873211	H	-0.627420	-3.821742	-2.713184
H	2.760696	2.477594	1.453723	C	-0.058812	-3.094026	1.710092
H	2.575041	3.557112	2.848364	C	0.372438	-2.538710	3.079391
H	2.245452	4.161674	1.229459	H	1.429987	-2.718304	3.291393
C	0.620080	1.826209	3.198457	H	-0.200964	-3.051370	3.860406
H	1.228269	0.943937	2.978172	H	0.171251	-1.468681	3.180300
H	-0.404868	1.494144	3.394395	C	0.400981	-4.555922	1.629328
H	0.995268	2.273028	4.126980	H	1.490795	-4.655014	1.634347
Complex 14.MeOH				H	0.009801	-5.072710	0.750241
scf done: -2175.084810				H	0.026833	-5.092197	2.509972
Pd	-0.713199	0.049106	-0.113697	C	-1.591883	-3.026787	1.643956
P	0.651917	1.809217	0.547275	H	-1.990123	-3.387998	0.693301
P	0.648539	-1.953837	0.340015	H	-1.954371	-2.006145	1.798573
C	-2.509078	0.702179	-1.005000	H	-2.015876	-3.653849	2.437495
C	-2.452430	1.184205	-2.445563	H	-4.424922	2.699088	-1.353367
H	-2.327558	2.269883	-2.467605	C	-3.940997	2.559468	-0.382031
H	-1.545175	0.765297	-2.890079	H	-4.666735	2.754109	0.408721
C	-3.666298	0.756984	-3.281290	H	-3.112864	3.264258	-0.279256
H	-3.568526	1.133705	-4.303186	O	-3.512778	1.214583	-0.194079
H	-4.608061	1.138326	-2.875720	H	-4.738026	-0.429404	0.886171
H	-3.736961	-0.332707	-3.328078	H	-6.259949	-2.229106	1.089288
O	-2.566966	-0.679881	-0.948687	C	-5.516390	-2.148979	0.290835
C	0.007582	2.535942	2.207406	H	-5.108343	-3.140213	0.091124
C	0.071067	1.417046	3.260762	H	-5.992698	-1.765950	-0.618537
H	1.090908	1.161895	3.560640	O	-4.422002	-1.324802	0.705518
H	-0.434575	0.513541	2.905846	H	-3.267221	-0.994901	-0.274824
H	-0.449386	1.755061	4.164307	TS14-7a.MeOH			
C	0.795072	3.750106	2.716866	scf done: -2175.058480			
H	1.870357	3.565718	2.794758	Pd	-0.434135	-0.388649	-0.021520
H	0.440190	4.001794	3.723544	P	-0.720127	1.844604	0.433711
H	0.638143	4.633872	2.094024	P	1.687320	-1.413412	0.267162
C	-1.471669	2.919318	2.060322	C	-2.791941	-1.583661	-1.305281
H	-2.070784	2.072452	1.714089	C	-2.566676	-1.259448	-2.744766
H	-1.619968	3.757082	1.377190	H	-3.033710	-0.306205	-2.999643
H	-1.854494	3.230195	3.039849	H	-1.487967	-1.147383	-2.878310
C	0.952808	3.188921	-0.745412	C	-3.094124	-2.388147	-3.654887
C	-0.320935	4.015212	-0.951403	H	-2.889353	-2.130957	-4.696694
H	-1.197033	3.379302	-1.089244	H	-4.172982	-2.533764	-3.549306
H	-0.207604	4.627383	-1.853744	H	-2.595553	-3.333544	-3.429457
H	-0.509716	4.697786	-0.118672	O	-2.008365	-2.428228	-0.747921
C	2.090855	4.162169	-0.402411	C	-1.775328	2.280639	1.988232
H	1.890748	4.753314	0.492172	C	-1.563242	1.132295	2.989526
H	2.204741	4.865469	-1.235992	H	-0.512077	0.984712	3.254224
H	3.053324	3.668961	-0.273983	H	-1.943312	0.191348	2.579762
C	1.289121	2.458407	-2.058143	H	-2.110566	1.347895	3.915499
H	0.483965	1.781038	-2.356325	C	-1.401966	3.597150	2.691004
H	2.209930	1.875336	-1.983701	H	-0.407546	3.562174	3.143189

H	-2.114308	3.776009	3.505645
H	-1.446119	4.463461	2.027725
C	-3.268519	2.317977	1.635901
H	-3.569736	1.447706	1.042663
H	-3.541538	3.225131	1.091410
H	-3.857412	2.310969	2.561397
C	-1.153353	3.007678	-1.026217
C	-2.541703	2.654998	-1.578455
H	-2.613438	1.576166	-1.749309
H	-2.684311	3.159662	-2.541717
H	-3.359706	2.962899	-0.925089
C	-1.110091	4.505668	-0.701993
H	-1.919318	4.805006	-0.029960
H	-1.232493	5.081409	-1.627636
H	-0.162208	4.816605	-0.255284
C	-0.146856	2.678631	-2.144136
H	-0.183631	1.615793	-2.406271
H	0.882083	2.919695	-1.878288
H	-0.407339	3.257827	-3.038706
C	0.952000	2.443214	1.081067
H	0.828023	3.488468	1.377901
H	1.060666	1.874905	2.012302
C	2.231040	2.349429	0.280529
C	2.673998	3.530957	-0.338700
H	2.048181	4.417331	-0.273105
C	3.890532	3.622420	-1.002417
H	4.190061	4.557636	-1.465822
C	4.732340	2.514877	-1.021589
H	5.707767	2.565689	-1.495993
C	4.327313	1.347788	-0.386738
H	5.020942	0.513411	-0.344142
C	3.079713	1.217923	0.246803
C	2.807527	-0.071735	0.985481
H	2.320940	0.157437	1.938369
H	3.768621	-0.535190	1.233039
C	2.455036	-1.945196	-1.401941
C	3.979252	-2.116062	-1.426045
H	4.331817	-2.901062	-0.756104
H	4.499839	-1.191028	-1.178594
H	4.287129	-2.393777	-2.441779
C	2.066792	-0.842933	-2.404355
H	0.978226	-0.729566	-2.462026
H	2.438619	-1.113913	-3.400595
H	2.489683	0.129338	-2.140538
C	1.799937	-3.257376	-1.861526
H	0.709245	-3.230781	-1.765406
H	2.175793	-4.123090	-1.309967
H	2.039998	-3.423052	-2.919014
C	1.946888	-2.775065	1.598684
C	1.611255	-2.137248	2.960538
H	2.403031	-1.474689	3.320400
H	1.491495	-2.929971	3.708268
H	0.676067	-1.565197	2.926310
C	3.363140	-3.362616	1.669778
H	4.143690	-2.600006	1.750474
H	3.586505	-3.995514	0.807731
H	3.442304	-3.997294	2.561039
C	0.949192	-3.919632	1.362426
H	1.122596	-4.446067	0.422857
H	-0.083782	-3.566044	1.368204
H	1.051580	-4.654326	2.170723
H	-5.227094	-0.794374	-2.175343
C	-4.897300	-0.431871	-1.200116
H	-5.725032	-0.471732	-0.494457
H	-4.512317	0.586580	-1.268913
O	-3.892525	-1.302639	-0.645038
H	-1.622344	-1.768444	1.882721
H	-3.084812	-2.604214	3.572276
C	-3.368778	-2.543852	2.519226
H	-3.934288	-3.436452	2.251145
H	-3.979331	-1.653999	2.343815
O	-2.190566	-2.541745	1.699353
H	-2.203795	-2.553558	0.293852

Pd	0.244282	-0.693464	-0.544914
P	-2.141622	-1.368940	0.265567
P	0.325943	1.636014	0.194530
C	2.242449	-0.846818	-0.698584
C	2.741840	-1.743155	0.431588
H	3.383949	-1.101202	1.059715
H	1.907464	-2.090303	1.051178
C	3.592783	-2.916886	-0.066711
H	3.973276	-3.468122	0.797314
H	4.449018	-2.555981	-0.639743
H	3.024156	-3.621000	-0.681296
O	2.949571	-0.465348	-1.598386
C	-1.838810	-2.826655	1.484942
C	-1.084631	-2.248638	2.699190
H	-1.737490	-1.683412	3.369379
H	-0.250553	-1.601678	2.403244
H	-0.667489	-3.075832	3.284963
C	-3.110609	-3.524294	1.986201
H	-3.857491	-2.872963	2.377119
H	-2.840239	-4.200559	2.806143
H	-3.578160	-4.135106	1.210532
C	-0.925509	-3.880519	0.838645
H	0.047460	-3.463056	0.562384
H	-1.365830	-4.342662	-0.048082
H	-0.744365	-4.683542	1.562699
C	-3.505435	-1.802238	-1.017066
C	-3.122574	-3.045008	-1.833871
H	-2.189186	-2.917868	-2.385698
H	-3.906165	-3.226200	-2.578885
H	-3.051858	-3.947238	-1.221441
C	-4.897400	-2.053915	-0.416919
H	-4.950302	-2.982604	0.151467
H	-5.617404	-2.136760	-1.239746
H	-5.240252	-1.241046	0.221841
C	-3.592721	-0.599948	-1.976293
H	-2.625132	-0.352646	-2.421613
H	-3.971562	0.297512	-1.484869
H	-4.280517	-0.847123	-2.793802
C	-2.974624	-0.158723	1.440745
H	-3.804101	-0.685122	1.923396
H	-2.225558	0.009088	2.220237
C	-3.463038	1.168733	0.919639
C	-4.839603	1.363468	0.731783
H	-5.524709	0.554848	0.967604
C	-5.363573	2.570868	0.284062
H	-6.435324	2.681418	0.150162
C	-4.503575	3.637254	0.039751
H	-4.888875	4.594869	-0.296759
C	-3.144210	3.479721	0.282839
H	-2.488636	4.338101	0.162622
C	-2.597314	2.262537	0.718269
C	-1.155827	2.260739	1.164222
H	-1.074873	1.724140	2.116534
H	-0.896211	3.296621	1.394975
C	0.425417	2.756908	-1.353629
C	0.470826	4.252427	-1.013779
H	1.410138	4.534049	-0.531714
H	-0.356457	4.580047	-0.379454
H	0.404670	4.823542	-1.947352
C	-0.824635	2.451201	-2.197446
H	-0.873285	1.391340	-2.464715
H	-0.765969	3.024513	-3.130210
H	-1.756728	2.720429	-1.699514
C	1.653276	2.409397	-2.208066
H	2.597108	2.659398	-1.722554
H	1.598122	2.991301	-3.135881
H	1.683828	1.352502	-2.474944
C	1.674318	2.080998	1.495284
C	1.651967	0.961993	2.550318
H	0.690086	0.898380	3.070308
H	2.415038	1.172916	3.307385
H	1.879910	-0.016654	2.128364
C	1.437088	3.411830	2.235292
H	0.581778	3.376952	2.914585
H	1.317050	4.266306	1.566411
H	2.320964	3.609046	2.852466
C	3.060492	2.154194	0.838495

Complex 15.2MeOH

scf done: -2253.640932

H	3.191422	3.094542	0.295765	H	-0.645887	3.276640	1.530947
H	3.261991	1.333527	0.150357	C	0.570549	2.603966	-1.298789
H	3.831338	2.102049	1.613211	C	0.350681	4.104507	-1.063977
H	6.448034	-1.770690	2.260104	H	1.018229	4.529238	-0.314480
C	6.184349	-0.745205	2.556272	H	-0.677970	4.331269	-0.790348
H	7.109956	-0.153923	2.601768	H	0.549110	4.627397	-2.007242
H	5.761250	-0.3781700	3.564002	C	-0.498953	2.115069	-2.292187
O	5.219698	-0.162469	1.702969	H	-0.348290	1.064465	-2.565312
H	5.569609	-0.171569	0.790592	H	-0.433424	2.712026	-3.209991
H	7.756095	-0.020099	-1.364347	H	-1.512656	2.223769	-1.896492
C	6.792604	0.096916	-1.864460	C	1.957354	2.413595	-1.928615
H	6.635288	1.164173	-2.067886	H	2.750464	2.845702	-1.312323
H	6.831949	-0.444259	-2.817867	H	1.973884	2.940079	-2.890490
O	5.800856	-0.437109	-0.999848	H	2.200087	1.366398	-2.112129
H	4.931296	-0.374948	-1.423176	C	1.789417	1.849084	1.546845
C	0.461557	-2.491866	-2.069619	C	1.339491	1.282223	2.907598
H	-0.318316	-3.199540	-1.822821	H	0.582729	1.897046	3.401551
H	1.480080	-2.856405	-1.983121	H	2.210239	1.252722	3.571673
C	0.195796	-1.330474	-2.745240	H	0.961521	0.257423	2.872619
H	0.998631	-0.744663	-3.181715	C	2.112304	3.341606	1.719291
H	-0.814773	-1.086545	-3.058033	H	1.242725	3.960246	1.959091
				H	2.607186	3.758714	0.839096
TS15-16.2MeOH				H	2.813139	3.442774	2.556119
scf done: -2253.617884				C	3.083874	1.126727	1.165835
Pd	-0.072247	-0.772870	-0.641082	H	3.454559	1.392992	0.176114
P	-2.280636	-1.265610	0.273196	H	2.971220	0.043895	1.210455
P	0.383166	1.506670	0.265164	H	3.867994	1.377245	1.886607
C	2.126289	-1.242470	-0.918137	H	7.392530	-1.758503	1.861104
C	2.343524	-2.360926	0.091759	C	7.058653	-0.784353	2.248132
H	1.888017	-2.040653	1.038060	H	7.898617	-0.078833	2.163318
H	1.758521	-3.227612	-0.235066	H	6.832330	-0.905306	3.311596
C	3.813803	-2.728079	0.294418	O	5.891749	-0.313651	1.609133
H	3.873847	-3.606253	0.943623	H	6.073217	-0.237160	0.653358
H	4.383386	-1.922104	0.766517	H	7.648881	0.538639	-1.886616
H	4.294449	-2.978634	-0.655598	C	6.578108	0.528548	-2.100631
O	2.995666	-0.542336	-1.362679	H	6.201517	1.557478	-2.020118
C	-2.004640	-2.651513	1.573743	H	6.439740	0.182097	-3.133097
C	-1.092618	-2.077209	2.674141	O	5.970761	-0.347709	-1.166168
H	-1.604398	-1.358658	3.319673	H	5.018594	-0.383305	-1.332660
H	-0.201676	-1.597677	2.254684	C	-0.349120	-2.253869	-2.140423
H	-0.755841	-2.897796	3.317919	H	-1.162003	-1.895917	-2.762823
C	-3.293112	-3.171375	2.228478	H	-0.461668	-3.268304	-1.769712
H	-3.908247	-2.378438	2.662325	C	0.963433	-1.788592	-2.423393
H	-3.016427	-3.843192	3.049655	H	1.745800	-2.547562	-2.461024
H	-3.906764	-3.752801	1.536868	H	1.111806	-0.992219	-3.148274
C	-1.264411	-3.836889	0.936423				
H	-0.279617	-3.540358	0.568070	Complex 17			
H	-1.819445	-4.295547	0.116795	scf done: -2059.384031			
H	-1.111982	-4.608506	1.699895	Pd	0.662262	-0.834675	-0.250779
C	-3.700885	-1.738963	-0.937179	C	2.539302	-1.441625	-0.642372
C	-3.534685	-3.144903	-1.539399	C	3.159099	-2.306222	0.457082
H	-2.561321	-3.329933	-1.987936	H	3.364486	-1.666779	1.320063
H	-4.281972	-3.263200	-2.332643	H	2.381313	-3.004074	0.797174
H	-3.730223	-3.929156	-0.803490	C	4.418248	-3.046778	0.012744
C	-5.091996	-1.718114	-0.279296	H	4.806351	-3.649045	0.838531
H	-5.179398	-2.398981	0.568357	H	5.196679	-2.345092	-0.297083
H	-5.824713	-2.039477	-1.028514	H	4.221293	-3.710097	-0.832862
H	-5.390459	-0.723455	0.041991	O	2.988347	-1.414279	-1.762542
C	-3.685961	-0.681374	-2.056322	P	-1.785096	-0.917787	0.367857
H	-2.749028	-0.670883	-2.618384	P	1.313474	1.362169	0.244427
H	-3.850868	0.326059	-1.665992	C	-1.929844	-2.226857	1.759446
H	-4.494831	-0.899703	-2.763363	C	-1.231181	-1.660623	3.009753
C	-3.049602	0.061717	1.353283	H	-1.820165	-0.887127	3.509718
H	-3.951712	-0.383749	1.783098	H	-0.240223	-1.254966	2.778485
H	-2.343778	0.172410	2.181018	H	-1.093579	-2.470879	3.735105
C	-3.389422	1.428760	0.807568	C	-3.366789	-2.614386	2.133167
C	-4.728081	1.742045	0.529473	H	-3.978613	-1.748902	2.404431
H	-5.492584	0.986911	0.676457	H	-3.340016	-3.274224	3.008851
C	-5.127877	3.011367	0.126825	H	-3.875879	-3.161201	1.335784
H	-6.174768	3.209977	-0.081229	C	-1.153050	-3.483138	1.335280
C	-4.181661	4.026486	0.046388	H	-0.101503	-3.245406	1.134393
H	-4.472221	5.036307	-0.226711	H	-1.574875	-3.960516	0.449326
C	-2.860619	3.747795	0.376927	H	-1.175642	-4.216489	2.150076
H	-2.150156	4.567759	0.408913	C	-2.985388	-1.292572	-1.070188
C	-2.430076	2.460893	0.733155	C	-2.853921	-2.750991	-1.533248
C	-1.020405	2.290336	1.240844	H	-1.819220	-3.020601	-1.750195
H	-1.050171	1.705309	2.164882	H	-3.429438	-2.870670	-2.459001

H	-3.270013	-3.456031	-0.808683	C	-3.871265	0.733208	2.649524
C	-4.460355	-1.018974	-0.745771	H	-3.247862	1.511907	3.096517
H	-4.819767	-1.578132	0.120160	H	-4.402235	0.240637	3.472843
H	-5.067149	-1.327204	-1.605399	H	-4.624888	1.213457	2.022091
H	-4.657363	0.040359	-0.584888	C	-3.973900	-1.479593	1.492973
C	-2.546904	-0.372332	-2.224562	H	-3.490011	-2.194379	0.819028
H	-1.526867	-0.596925	-2.551045	H	-4.889948	-1.126013	1.014527
H	-2.596541	0.685932	-1.953931	H	-4.275266	-2.025641	2.394345
H	-3.214633	-0.527677	-3.080538	C	-3.280961	0.804206	-1.069177
C	-2.518656	0.570397	1.236583	C	-3.953153	-0.457881	-1.636835
H	-3.534471	0.307589	1.547508	H	-3.237251	-1.261925	-1.834985
H	-1.933192	0.660654	2.156256	H	-4.428070	-0.200341	-2.590816
C	-2.542368	1.899697	0.526672	H	-4.732572	-0.856248	-0.987192
C	-3.774057	2.409604	0.090201	C	-4.369698	1.818223	-0.694457
H	-4.674232	1.826789	0.260974	H	-5.113887	1.390604	-0.017440
C	-3.889090	3.657218	-0.511786	H	-4.902402	2.127952	-1.601437
H	-4.860864	4.016795	-0.835960	H	-3.967091	2.723328	-0.232955
C	-2.754172	4.448499	-0.656952	C	-2.386421	1.383580	-2.180294
H	-2.820085	5.437058	-1.100930	H	-1.593491	0.682026	-0.463571
C	-1.535033	3.978663	-0.183303	H	-1.903928	2.319091	-1.896493
H	-0.669055	4.631370	-0.241134	H	-3.002129	1.576680	-3.066869
C	-1.394202	2.708160	0.396645	C	-1.439004	1.966915	1.093618
C	-0.068366	2.365496	1.034761	H	-2.311026	2.557127	1.394200
H	-0.238458	1.847226	1.984762	H	-0.969958	1.628103	2.023118
H	0.412680	3.311029	1.297283	C	-0.495892	2.885318	0.344413
C	1.813506	2.325323	-1.332751	C	-1.088196	3.986032	-0.299353
C	2.123332	3.802446	-1.044931	H	-2.170928	4.079036	-0.274852
H	3.078340	3.922493	-0.526920	C	-0.351413	4.977303	-0.933092
H	1.351799	4.316346	-0.469028	H	-0.856523	5.809147	-1.414563
H	2.212768	4.328417	-2.002419	C	1.037549	4.907678	-0.900026
C	0.626854	2.203376	-2.306907	H	1.644815	5.684944	-1.353910
H	0.418169	1.155997	-2.548218	C	1.644417	3.847393	-0.240053
H	0.895242	2.708332	-3.242218	H	2.727424	3.838692	-0.165970
H	-0.289968	2.659379	-1.933199	C	0.920526	2.809575	0.372181
C	3.034095	1.713323	-2.036437	C	1.721098	1.776927	1.140614
H	2.864118	0.680997	-2.338989	H	1.176811	1.494886	2.045753
H	3.945080	1.755330	-1.438782	H	2.653959	2.243176	1.478663
H	3.219652	2.300196	-2.943931	C	3.322365	0.432083	-1.099059
C	2.609510	1.532123	1.653640	C	4.435976	1.455387	-0.834648
C	2.198893	0.538107	2.754891	H	5.160977	1.111501	-0.095922
H	1.237949	0.800383	3.208413	H	4.048902	2.421195	-0.507191
H	2.946852	0.562541	3.555871	H	4.982712	1.629038	-1.769170
H	2.125827	-0.488932	2.389978	C	2.423419	0.948069	-2.237938
C	2.670693	2.930809	2.298422	H	1.642653	0.221762	-2.485998
H	1.774479	3.171720	2.875019	H	3.037813	1.108698	-3.132188
H	2.848976	3.731054	1.577855	H	1.934580	1.893247	-1.992017
H	3.509509	2.939826	3.003997	C	3.959320	-0.890563	-1.554883
C	4.018563	1.194677	1.140501	H	3.217755	-1.680860	-1.701598
H	4.453193	2.029078	0.584573	H	4.717630	-1.251122	-0.854854
H	4.052115	0.313362	0.497766	H	4.463742	-0.724623	-2.514381
H	4.673636	1.005995	1.998801	C	3.076853	-0.759996	1.817732
C	0.820943	-4.100770	-1.708532	C	2.202023	-0.607797	3.075437
H	1.897041	-4.212987	-1.544152	H	2.245863	0.399265	3.499359
H	0.276056	-4.561091	-0.885552	H	2.567925	-1.295535	3.846523
H	0.541271	-4.597369	-2.642494	H	1.154377	-0.861564	2.875217
O	0.437526	-2.717992	-1.754506	C	4.474476	-0.204396	2.117850
H	0.942272	-2.302259	-2.467946	H	4.472522	0.879224	2.270468
TS17-7a				H	5.193952	-0.443570	1.331088
scf done: -2059.338513				H	4.849119	-0.659930	3.042533
Pd	-0.038076	-0.603309	-0.027037	C	3.172193	-2.262663	1.505353
C	0.227183	-3.146416	-0.966022	H	3.744041	-2.480399	0.601897
C	-0.548557	-3.795772	0.132107	H	2.176798	-2.701384	1.388412
H	0.138608	-3.879411	0.978744	H	3.667138	-2.771464	2.341146
H	-1.380782	-3.155402	0.426861	C	-0.419550	-2.314133	-3.367800
C	-1.038163	-5.184257	-0.316892	H	0.564862	-1.845429	-3.370495
H	-1.566431	-5.655979	0.515267	H	-0.374367	-3.306364	-3.813750
H	-0.201028	-5.826297	-0.600731	H	-1.154589	-1.696332	-3.882741
H	-1.729948	-5.109267	-1.159414	O	-0.895919	-2.483095	-2.005745
O	1.282284	-3.343447	-1.451708	H	-0.977219	-1.570319	-1.515769
P	-2.104739	0.345852	0.363653	Complex 11.3MeOH			
P	2.161817	0.098106	0.372037	scf done: -2290.784430			
C	-3.046828	-0.322673	1.894791	Pd	0.227647	-0.174549	-0.330780
C	-1.976876	-0.877319	2.853111	P	-1.369921	-1.772780	0.133565
H	-1.284606	-0.106091	3.204133	P	-0.708849	1.892060	0.508899
H	-1.385809	-1.672015	2.387823	C	1.813680	-1.013556	-1.194082
H	-2.471454	-1.292292	3.739648				

C	2.654521	-2.202902	-1.506902
H	3.038154	-2.477523	-0.509778
H	2.011473	-3.026652	-1.824519
C	3.806475	-1.938069	-2.474647
H	4.335091	-2.874445	-2.671206
H	4.521267	-1.237123	-2.037720
H	3.451125	-1.545141	-3.431606
O	2.163721	0.151875	-1.351721
C	-0.754570	-3.082618	1.389864
C	-0.632634	-2.399360	2.763545
H	-1.600167	-2.179960	3.222381
H	-0.043062	-1.479179	2.705175
H	-0.106003	-3.079941	3.442013
C	-1.688447	-4.295283	1.517393
H	-2.729075	-4.023652	1.717254
H	-1.349609	-4.905220	2.362954
H	-1.659224	-4.934860	0.631927
C	0.649255	-3.563046	0.998383
H	1.380513	-2.752521	1.051233
H	0.683431	-4.007788	0.002236
H	0.960023	-4.338414	1.708746
C	-2.011686	-2.561669	-1.483024
C	-0.935141	-3.449938	-2.118701
H	0.000863	-2.908705	-2.270263
H	-1.289670	-3.771818	-3.104649
H	-0.736078	-4.353403	-1.536916
C	-3.286316	-3.400848	-1.308760
H	-3.141109	-4.272055	-0.669967
H	-3.589770	-3.769125	-2.295742
H	-4.120036	-2.819381	-0.919309
C	-2.303473	-1.396981	-2.445686
H	-1.398358	-0.819212	-2.657246
H	-3.064533	-0.715136	-2.059467
H	-2.670961	-1.806818	-3.393884
C	-2.881822	-1.106933	1.038696
H	-3.480206	-1.987208	1.298175
H	-2.469729	-0.738304	1.982432
C	-3.801712	-0.059576	0.449154
C	-5.022047	-0.473829	-0.105322
H	-5.261246	-1.532357	-0.123882
C	-5.966135	0.425312	-0.588812
H	-6.896734	0.059375	-1.011678
C	-5.720012	1.790103	-0.486932
H	-6.451364	2.513643	-0.833882
C	-4.541720	2.221968	0.111433
H	-4.388704	3.287603	0.256523
C	-3.566543	1.328133	0.576309
C	-2.384255	1.892587	1.324906
H	-2.233598	1.321513	2.246180
H	-2.609907	2.917318	1.637944
C	-0.808222	3.136105	-0.932764
C	-1.596079	4.413955	-0.612791
H	-1.169723	4.987034	0.211563
H	-2.642797	4.205249	-0.386456
H	-1.585822	5.060339	-1.498437
C	-1.506194	2.399850	-2.091045
H	-0.927046	1.531721	-2.421252
H	-1.598786	3.083960	-2.943211
H	-2.510394	2.061309	-1.824631
C	0.608730	3.512611	-1.391239
H	1.223016	2.630644	-1.595006
H	1.131815	4.140638	-0.666443
H	0.533662	4.085072	-2.323318
C	0.427832	2.527694	1.912625
C	0.099693	1.731261	3.188552
H	-0.849156	2.030983	3.641994
H	0.883184	1.923696	3.303156
H	0.082947	0.651587	3.009575
C	0.263095	4.021708	2.222004
H	-0.772458	4.292794	2.450440
H	0.619515	4.660554	1.410702
H	0.861829	4.264990	3.107923
C	1.889533	2.225111	1.541664
H	2.211269	2.705586	0.616393
H	2.070764	1.148495	1.453187
H	2.538944	2.598638	2.342585
H	4.691096	-2.609911	2.688271

C	3.881416	-1.869059	2.756510
H	4.216719	-1.054354	3.414046
H	3.025482	-2.353642	3.234855
O	3.468773	-1.402568	1.488365
H	6.066871	3.022228	-1.891061
C	5.212862	2.471835	-2.290277
H	4.579568	3.174823	-2.844106
H	5.583500	1.704245	-2.981543
O	4.520764	1.909054	-1.181171
H	3.750046	1.419946	-1.501679
H	7.582642	0.066135	-0.206313
C	6.885987	-0.171497	0.607713
H	7.155252	-1.152330	1.006880
H	7.012034	0.572944	1.405262
O	5.547575	-0.243631	0.146088
H	4.239837	-0.967965	1.059552
H	5.290111	0.614891	-0.253574

TS11-14.2MeOH

scf done: -2290.772045

Pd	0.357774	-0.225039	-0.088854
P	-1.361074	-1.724535	0.356039
P	-0.596389	1.919868	0.515049
C	2.027515	-1.026082	-0.995709
C	2.322177	-1.791426	-2.263836
H	2.257590	-2.866425	-2.084224
H	1.495090	-1.551636	-2.942162
C	3.655944	-1.415458	-2.913265
H	3.827055	-2.022531	-3.806312
H	4.499368	-1.568775	-2.233470
H	3.654939	-0.365055	-3.215831
O	2.266142	0.212508	-0.905383
C	-0.981579	-2.821932	1.886775
C	-0.972190	-1.913281	3.128594
H	-1.969535	-1.577324	3.423773
H	-0.330674	-1.039781	2.978566
H	-0.565170	-2.478732	3.974585
C	-1.982250	-3.963099	2.115127
H	-3.020492	-3.622271	2.167217
H	-1.755376	-4.441125	3.075717
H	-1.909246	-4.738728	1.348894
C	0.430703	-3.405794	1.752214
H	1.172512	-2.614074	1.620364
H	0.513193	-4.015847	0.919105
H	0.674750	-3.959210	2.667046
C	-1.811638	-2.792563	-1.162305
C	-0.702982	-3.817586	-1.431793
H	0.288702	-3.363030	-1.392771
H	-0.841834	-4.236712	-2.435257
H	-0.734216	-4.652075	-0.726307
C	-3.145056	-3.547095	-1.056821
H	-3.169451	-4.264650	-0.235736
H	-3.295767	-4.111515	-1.984741
H	-3.998137	-2.877987	-0.953456
C	-1.887393	-1.815342	-2.349756
H	-0.937848	-1.292415	-2.499771
H	-2.668281	-1.062128	-2.215683
H	-2.117375	-2.377272	-3.263118
C	-2.981284	-0.945978	0.910574
H	-3.663011	-1.777412	1.117067
H	-2.734745	-0.513307	1.883805
C	-3.723677	0.089458	0.093950
C	-4.834747	-0.316648	-0.659612
H	-5.098073	-1.368923	-0.686398
C	-5.649956	0.585148	-1.334890
H	-6.499091	0.225132	-1.907838
C	-5.390665	1.946933	-1.227874
H	-6.032443	2.674688	-1.715077
C	-4.318233	2.372267	-0.452136
H	-4.161580	3.438476	-0.316735
C	-3.458825	1.473902	0.196659
C	-2.373299	2.036750	1.081468
H	-2.386413	1.523185	2.047938
H	-2.588699	3.089075	1.293731
C	-0.484358	3.027756	-1.040624
C	-1.287470	4.333555	-0.961320
H	-0.969537	4.986092	-0.147142

H	-2.358725	4.154085	-0.864116
H	-1.142439	4.886828	-1.897034
C	-1.025689	2.183730	-2.209870
H	-0.427024	1.279469	-2.359394
H	-0.976881	2.778285	-3.130512
H	-2.065933	1.884638	-2.061193
C	0.984590	3.363444	-1.337799
H	1.603394	2.464681	-1.385676
H	1.415522	4.050001	-0.605176
H	1.036839	3.858375	-2.315184
C	0.331719	2.718268	1.989842
C	-0.191869	2.082303	3.289742
H	-1.197275	2.423102	3.551829
H	0.469353	2.374382	4.113672
H	-0.191797	0.989314	3.246237
C	0.161872	4.239225	2.104144
H	-0.888472	4.542653	2.151232
H	0.642306	4.779196	1.285288
H	0.635536	4.577848	3.033596
C	1.824120	2.368026	1.871754
H	2.289712	2.757746	0.965133
H	1.976950	1.284101	1.887761
H	2.359092	2.797616	2.727561
H	4.212426	-3.283501	-0.663540
C	3.504599	-3.133074	0.156872
H	3.983306	-3.398321	1.103446
H	2.632262	-3.770929	0.018600
O	3.067468	-1.773271	0.241374
H	6.261181	2.732033	-1.378482
C	5.330208	2.339264	-1.791006
H	4.789572	3.162684	-2.270157
H	5.573093	1.580670	-2.545273
O	4.583456	1.798192	-0.705354
H	3.734069	1.446929	-1.022074
H	6.690894	0.189780	1.786924
C	5.702062	-0.276275	1.839540
H	5.812212	-1.267101	2.285355
H	5.051625	0.332414	2.478362
O	5.161960	-0.440911	0.530479
H	3.907003	-1.162730	0.379701
H	5.074033	0.447338	0.087541

Complex 11'.2MeOH

scf done: -2290.787059

Pd	0.639380	-0.256161	-0.513754
P	0.086554	2.022962	-0.298278
P	-1.655608	-1.364341	-0.595749
C	2.578524	0.095206	-0.909771
C	2.923032	-0.128114	-2.385200
H	2.334286	-0.980828	-2.746616
H	2.538645	0.735047	-2.938291
C	4.412536	-0.318569	-2.657632
H	4.581543	-0.446392	-3.730309
H	4.807432	-1.199046	-2.144770
H	4.987762	0.546708	-2.319517
O	3.463094	0.204789	-0.087153
C	-1.760874	2.375935	-0.311756
H	-1.820991	3.466455	-0.282858
H	-2.061569	2.094325	-1.326550
C	-2.776063	1.853126	0.677212
C	-3.181479	2.697499	1.722451
H	-2.682191	3.652405	1.856072
C	-4.229384	2.371732	2.575631
H	-4.510728	3.051376	3.374193
C	-4.938641	1.194526	2.361018
H	-5.789678	0.938549	2.984767
C	-4.568779	0.360585	1.312228
H	-5.168939	-0.521425	1.110958
C	-3.477763	0.646409	0.478983
C	-3.176940	-0.273529	-0.675006
H	-3.035859	0.319384	-1.583498
H	-4.041708	-0.917309	-0.862978
H	3.526164	-2.525278	-0.517443
C	2.563111	-3.041636	-0.591214
H	2.642556	-4.017929	-0.101267
H	2.322217	-3.206254	-1.642597
O	1.509534	-2.289171	0.005649

H	1.693616	-2.237747	0.999432
H	1.224906	-3.882674	3.208541
C	2.103135	-3.257498	3.382833
H	2.101452	-2.947371	4.433672
H	3.003415	-3.855475	3.190799
O	2.016088	-2.130860	2.521374
H	2.791516	-1.529129	2.668197
C	-1.751837	-2.185969	-2.327691
C	-2.042915	-2.634918	0.783494
C	0.578391	3.147005	-1.780554
C	0.709901	2.702329	1.379771
C	5.387116	-0.685645	2.954601
H	6.001081	0.217933	2.869355
H	5.828283	-1.475278	2.332638
H	5.400458	-1.012307	3.996279
O	4.033176	-0.420711	2.609278
H	3.985123	-0.102662	1.692522
C	-1.621892	-1.952512	2.098232
H	-2.138138	-1.000724	2.253321
H	-0.544115	-1.771780	2.139044
H	-1.882921	-2.607820	2.938496
C	-3.524517	-3.026180	0.878408
H	-3.920792	-3.441784	-0.049965
H	-4.153171	-2.191616	1.185627
H	-3.626612	-3.799817	1.648835
C	-1.220607	-3.920594	0.608546
H	-0.159415	-3.713402	0.466295
H	-1.577730	-4.531670	-0.224782
H	-1.334782	-4.526000	1.516151
C	-2.952303	-3.121058	-2.523337
H	-2.973547	-3.456280	-3.567536
H	-3.909025	-2.627559	-2.328141
H	-2.890696	-4.015981	-1.900429
C	-1.828433	-1.066138	-3.382071
H	-1.066385	-0.296223	-3.221121
H	-2.810208	-0.586322	-3.420001
H	-1.651116	-1.501721	-4.372297
C	-0.451584	-2.962047	-2.585794
H	0.411650	-2.289535	-2.552716
H	-0.490740	-3.405928	-3.587788
H	-0.282707	-3.767104	-1.869592
C	0.145595	1.749626	2.450408
H	0.486466	0.722479	2.283781
H	-0.944136	1.749886	2.496274
H	0.522164	2.066722	3.430039
C	0.253102	4.145352	1.642055
H	0.815923	4.864412	1.040835
H	0.450989	4.385359	2.693151
H	-0.810747	4.312530	1.469586
C	2.238531	2.664002	1.499525
H	2.629583	1.654614	1.398608
H	2.502495	3.023705	2.500906
H	2.744675	3.308861	0.780581
C	2.090181	3.423318	-1.779794
H	2.698227	2.543676	-1.562573
H	2.353527	4.197965	-1.055660
H	2.384249	3.795586	-2.768003
C	-0.141934	4.509304	-1.814659
H	0.292794	5.100188	-2.629231
H	-0.015013	5.086772	-0.897286
H	-1.209755	4.421080	-2.028357
C	0.185284	2.388243	-3.060291
H	0.645075	1.399658	-3.120518
H	0.507119	2.967270	-3.933706
H	-0.897765	2.258427	-3.146376

Complex 14.2MeOH

scf done: -2290.782682

Pd	0.422175	0.129853	-0.340058
P	-0.461470	-1.881377	0.427035
P	-1.185990	1.829154	0.410609
C	2.049714	-0.262543	-1.547654
C	1.711776	-0.598097	-2.999413
H	1.852646	-1.672151	-3.149912
H	0.641578	-0.413586	-3.134379
C	2.461482	0.207568	-4.069327
H	2.079510	-0.060384	-5.058752

H	3.537438	0.018190	-4.073058
H	2.306296	1.279534	-3.926936
O	2.090665	1.109586	-1.352387
C	0.563657	-2.478357	1.939652
C	0.872156	-1.220162	2.767574
H	-0.033296	-0.751249	3.164052
H	1.409677	-0.471152	2.174398
H	1.490633	-1.498478	3.629618
C	-0.163461	-3.486729	2.844044
H	-1.048709	-3.065385	3.326892
H	0.520364	-3.790597	3.645819
H	-0.459869	-4.394646	2.314703
C	1.896052	-3.094700	1.487971
H	2.383554	-2.506019	0.705959
H	1.770290	-4.113785	1.117776
H	2.566291	-3.154652	2.354529
C	-0.684360	-3.262778	-0.874512
C	0.674495	-3.731747	-1.422161
H	1.390308	-2.915915	-1.529767
H	0.519600	-4.181631	-2.409665
H	1.128812	-4.496843	-0.790189
C	-1.441468	-4.499439	-0.370685
H	-0.891498	-5.035808	0.406488
H	-1.568579	-5.194857	-1.208904
H	-2.439983	-4.274207	0.007921
C	-1.474871	-2.607729	-2.022910
H	-0.932778	-1.757216	-2.443975
H	-2.460031	-2.255444	-1.711469
H	-1.619572	-3.345361	-2.821188
C	-2.138027	-1.712659	1.258798
H	-2.406079	-2.717766	1.597332
H	-1.913104	-1.144785	2.168190
C	-3.345021	-1.110050	0.577417
C	-4.295728	-1.978831	0.020634
H	-4.101608	-3.047431	0.029859
C	-5.497774	-1.525708	-0.511213
H	-6.205249	-2.232181	-0.934640
C	-5.797079	-0.168484	-0.453090
H	-6.744544	0.207198	-0.827370
C	-4.881266	0.703575	0.124333
H	-5.146193	1.752627	0.220946
C	-3.643652	0.269332	0.621719
C	-2.747119	1.282079	1.289965
H	-2.390068	0.882017	2.244291
H	-3.332399	2.174756	1.534215
C	-1.758073	2.690717	-1.196383
C	-2.987627	3.597124	-1.050700
H	-2.828284	4.432232	-0.367861
H	-3.870023	3.045463	-0.724153
H	-3.224781	4.022417	-2.033477
C	-2.094802	1.567276	-2.195109
H	-1.227394	0.924368	-2.378975
H	-2.388985	2.018423	-3.150632
H	-2.919144	0.936176	-1.855455
C	-0.594248	3.508650	-1.779593
H	0.327570	2.923515	-1.854104
H	-0.389269	4.413918	-1.202168
H	-0.865992	3.829894	-2.792340
C	-0.486211	3.106672	1.658155
C	-0.467517	2.449934	3.050277
H	-1.466667	2.339614	3.480615
H	0.103593	3.091432	3.731559
H	0.022900	1.472140	3.036884
C	-1.227741	4.411597	1.751730
H	-2.347683	4.243448	1.966283
H	-1.207764	5.015569	0.844927
H	-0.885462	5.014748	2.574756
C	0.968403	3.421363	1.279927
H	1.061425	3.880736	0.294130
H	1.594423	2.525673	1.295083
H	1.381972	4.127156	2.010609
H	4.703329	-0.133000	-2.029229
C	4.308399	-1.102382	-1.710017
H	5.025691	-1.573529	-1.037943
H	4.148768	-1.745399	-2.580196
O	3.098364	-0.945349	-0.949220
H	5.401909	3.280219	0.585495

C	4.883541	2.801917	-0.251745
H	4.387237	3.575583	-0.840279
H	5.619784	2.291049	-0.883471
O	3.880798	1.909184	0.225630
H	2.832189	1.407129	-0.684894
H	5.909916	0.033272	2.993770
C	5.079175	-0.619903	2.721947
H	5.410213	-1.659618	2.819480
H	4.247520	-0.437214	3.412513
O	4.734266	-0.315540	1.373614
H	4.012400	-0.882550	1.068776
H	4.289467	1.166364	0.736641

TS14-7a. 2MeOH

scf done: -2290.765460

Pd	0.437898	-0.027388	-0.099490
P	-0.742510	-1.903111	0.594374
P	-0.617761	2.101144	0.194081
C	2.587735	-0.632045	-1.771117
C	1.969709	-1.204692	-3.014341
H	1.794228	-2.277307	-2.914190
H	0.999436	-0.721686	-3.139186
C	2.854733	-0.910228	-4.240667
H	2.372719	-1.302664	-5.139530
H	3.842993	-1.373015	-4.161225
H	2.990801	0.166545	-4.369040
O	2.453315	0.590457	-1.500273
C	-0.077339	-2.750657	2.189559
C	-0.179894	-1.727382	3.335997
H	-1.201619	-1.621378	3.710353
H	0.175214	-0.735783	3.032562
H	0.434219	-2.068903	4.178185
C	-0.819700	-4.021829	2.622184
H	-1.901698	-3.878361	2.695714
H	-0.466484	-4.322068	3.616701
H	-0.627671	-4.861598	1.950470
C	1.409792	-3.086246	1.990730
H	1.999518	-2.196105	1.753136
H	1.568610	-3.819730	1.196834
H	1.808359	-3.521056	2.916114
C	-1.201945	-3.244947	-0.700291
C	0.044655	-4.070695	-1.038661
H	0.893256	-3.419726	-1.266626
H	-0.155204	-4.687629	-1.923291
H	0.332032	-4.747446	-0.229432
C	-2.327750	-4.217073	-0.315631
H	-2.028890	-4.926773	0.456558
H	-2.605456	-4.802422	-1.200919
H	-3.230939	-3.711744	0.025861
C	-1.617243	-2.471474	-1.965092
H	-0.840822	-1.762114	-2.266458
H	-2.544388	-1.912062	-1.826221
H	-1.773940	-3.180204	-2.787946
C	-2.406410	-1.279364	1.239754
H	-2.938396	-2.130644	1.679786
H	-2.114281	-0.634452	2.072594
C	-3.364940	-0.523363	0.345219
C	-4.437090	-1.235163	-0.217401
H	-4.516331	-2.299931	-0.024288
C	-5.427024	-0.629666	-0.981242
H	-6.235123	-1.225198	-1.395400
C	-5.388275	0.747780	-1.168043
H	-6.164673	1.255720	-1.732268
C	-4.363702	1.477909	-0.579426
H	-4.385021	2.560083	-0.664078
C	-3.331427	0.880341	0.162401
C	-2.355486	1.798509	0.861944
H	-2.164515	1.408631	1.865623
H	-2.838128	2.772612	0.999090
C	-0.850557	2.977430	-1.493322
C	-1.933980	4.062041	-1.560277
H	-1.713364	4.927791	-0.935320
H	-2.919266	3.684150	-1.287000
H	-2.006896	4.420705	-2.594591
C	-1.217457	1.857413	-2.484721
H	-0.442229	1.084043	-2.507585
H	-1.306740	2.282721	-3.492363

H	-2.167438	1.378105	-2.236374
C	0.486737	3.589637	-1.938478
H	1.309595	2.872153	-1.871978
H	0.745987	4.482821	-1.363094
H	0.400958	3.900209	-2.987272
C	-0.005864	3.360157	1.515271
C	-0.258369	2.741236	2.902538
H	-1.308588	2.792177	3.201473
H	0.312588	3.301159	3.653253
H	0.061052	1.693409	2.950055
C	-0.675774	4.739587	1.474560
H	-1.767972	4.681991	1.493754
H	-0.374878	5.317173	0.597377
H	-0.368255	5.314460	2.357172
C	1.510477	3.535114	1.358807
H	1.795379	3.951640	0.391223
H	2.026742	2.579924	1.473686
H	1.881216	4.218090	2.133586
H	3.978471	-2.903424	-2.357238
C	3.805104	-2.665158	-1.305468
H	4.703051	-2.886338	-0.729934
H	2.968081	-3.244865	-0.911751
O	3.566304	-1.264851	-1.116625
H	5.966113	1.647031	0.774063
C	5.410280	1.272405	-0.085614
H	5.662730	1.864596	-0.965149
H	5.632372	0.217622	-0.258598
O	4.005284	1.463159	0.176803
H	3.353136	1.094074	-0.609283
H	4.036931	0.501804	3.688618
C	2.984285	0.485115	3.402244
H	2.476186	-0.294651	3.973561
H	2.533101	1.458134	3.616897
O	2.938428	0.179247	2.002980
H	2.008870	0.101217	1.667383
H	3.659685	0.955612	1.024097

Complex 11'.MeOH.DMBPX

scf done: -1703.536366

Pd	0.747060	-0.038905	0.437761
P	-0.395449	-2.004043	0.365758
P	-0.950909	1.437106	1.365518
C	2.298444	-0.951016	-0.497251
C	3.285685	-1.821885	0.261523
H	3.396215	-1.402076	1.269599
H	2.787027	-2.789619	0.413235
C	4.628550	-2.017074	-0.435413
H	5.268477	-2.677441	0.155637
H	5.152351	-1.065884	-0.564600
H	4.497624	-2.457932	-1.426155
O	2.488753	-0.652012	-1.662301
C	-2.232707	-1.908725	0.620738
H	-2.604118	-2.929092	0.464782
H	-2.380853	-1.686565	1.682495
C	-2.976559	-0.944840	-0.265904
C	-3.467203	-1.392404	-1.498571
H	-3.307701	-2.428165	-1.788842
C	-4.178308	-0.548313	-2.346729
H	-4.552223	-0.921343	-3.295305
C	-4.424694	0.765766	-1.958429
H	-4.992368	1.431851	-2.601034
C	-3.956843	1.218559	-0.727912
H	-4.173519	2.237169	-0.415519
C	-3.228555	0.384918	0.129025
C	-2.735381	0.931906	1.444313
H	-2.837328	0.206518	2.259208
H	-3.319544	1.811878	1.736467
H	3.992740	1.164046	0.578624
C	3.282371	1.855375	1.044981
H	3.672375	2.875514	0.974306
H	3.167258	1.594464	2.098350
O	1.993056	1.789139	0.431506
H	2.060248	2.019646	-0.546566
H	2.489465	3.855251	-2.816825
C	2.652069	2.807460	-3.075069
H	2.278715	2.636660	-4.089813
H	3.727168	2.595078	-3.045764

O	1.928204	2.019802	-2.131509
H	2.050328	1.070446	-2.316568
C	-0.599188	1.998169	3.080373
H	0.398321	2.443578	3.115186
H	-1.329459	2.742978	3.411791
H	-0.620328	1.148164	3.767577
C	-1.019183	2.999875	0.407941
H	-1.702029	3.716157	0.875614
H	-0.017197	3.430264	0.362917
H	-1.353949	2.790648	-0.610807
C	0.063808	-3.213416	1.670339
H	-0.574314	-4.100478	1.604215
H	1.105529	-3.521566	1.569165
H	-0.061853	-2.755983	2.654866
C	-0.236194	-2.936542	-1.203633
H	0.809600	-3.190328	-1.389900
H	-0.826207	-3.857433	-1.164884
H	-0.586602	-2.315034	-2.031116

TS14-7a.MeOH.DMBPX

scf done: -1703.495890

Pd	-0.374147	0.213126	-0.105576
P	0.323998	-1.747703	-1.022029
P	0.912258	2.143393	-0.019756
C	-2.980984	-0.169870	1.083048
C	-2.580574	-0.735932	2.406687
H	-2.331681	-1.794523	2.313247
H	-1.675536	-0.205053	2.712347
C	-3.696708	-0.522568	3.450127
H	-3.365441	-0.919041	4.412430
H	-4.622331	-1.035420	3.173632
H	-3.914577	0.540757	3.572645
O	-2.893631	1.084779	0.911635
C	2.071839	-1.338168	-1.564605
H	2.484773	-2.226709	-2.059150
H	1.961930	-0.566116	-2.332993
C	2.993339	-0.900226	-0.451737
C	3.700997	-1.900680	0.232258
H	3.571656	-2.935347	-0.076114
C	4.579636	-1.609574	1.269547
H	5.113965	-2.410942	1.771157
C	4.785247	-0.282314	1.635832
H	5.481832	-0.029257	2.429526
C	4.110831	0.724153	0.953931
H	4.302704	1.761659	1.216761
C	3.207363	0.448981	-0.083964
C	2.551018	1.627083	-0.762465
H	2.345201	1.427843	-1.819444
H	3.223074	2.493509	-0.727819
H	-4.254601	-2.571312	1.169219
C	-3.764218	-2.271026	0.241704
H	-4.384302	-2.547305	-0.608982
H	-2.775705	-2.727746	0.153163
O	-3.642448	-0.838585	0.168355
H	-1.806467	1.378938	-1.491612
H	-3.141520	1.877202	-3.410747
C	-3.570171	1.487929	-2.485017
H	-4.515712	1.993759	-2.288996
H	-3.735663	0.410468	-2.568324
O	-2.696789	1.800675	-1.386676
H	-2.974974	1.414213	-0.140060
C	1.391823	2.822269	1.624139
H	2.157406	3.599595	1.528624
H	0.509440	3.252191	2.106036
H	1.773730	2.018112	2.257395
C	0.567550	3.685103	-0.974004
H	-0.344115	4.156328	-0.597096
H	1.394839	4.397976	-0.891692
H	0.415403	3.444100	-2.029717
C	-0.372443	-2.404795	-2.601977
H	0.254972	-3.201551	-3.015574
H	-1.376658	-2.802647	-2.431972
H	-0.446749	-1.597999	-3.335979
C	0.567254	-3.302303	-0.056534
H	-0.403330	-3.739345	0.195219
H	1.143782	-4.040656	-0.624345
H	1.093707	-3.078107	0.874138

Complex 15.2MeOH.DMBPX

scf done: -1782.095149

Pd	0.068653	0.950020	-0.112873
P	2.337131	1.560725	0.640669
P	0.014286	-1.312210	0.537506
C	-1.920481	0.725652	-0.433792
C	-2.717540	1.399106	0.672292
H	-3.167853	0.564548	1.235367
H	-2.044344	1.935920	1.351455
C	-3.836508	2.307060	0.149594
H	-4.370960	2.745684	0.996335
H	-4.552969	1.735055	-0.443106
H	-3.454821	3.129609	-0.463541
O	-2.425670	0.203362	-1.402014
C	3.481062	0.272200	1.332722
H	4.432809	0.763135	1.566291
H	3.056072	-0.055011	2.287563
C	3.699033	-0.875962	0.381881
C	4.831402	-0.872054	-0.441952
H	5.543752	-0.054823	-0.357445
C	5.077240	-1.901797	-1.345905
H	5.967030	-1.877319	-1.967616
C	4.187931	-2.969823	-1.427846
H	4.374155	-3.790122	-2.114290
C	3.067399	-2.994364	-0.602539
H	2.395840	-3.848623	-0.642092
C	2.798562	-1.957530	0.300262
C	1.586715	-2.062246	1.188245
H	1.757098	-1.618808	2.174979
H	1.347320	-3.118075	1.364586
H	-6.072501	-0.792175	2.346541
C	-5.338183	-1.604318	2.255301
H	-5.876750	-2.532250	2.017918
H	-4.855517	-1.735640	3.227611
O	-4.330898	-1.313970	1.305456
H	-4.751617	-1.160137	0.433988
H	-6.916007	-1.470020	-1.760424
C	-5.941422	-1.232649	-2.191515
H	-5.466576	-2.168258	-2.514471
H	-6.099341	-0.593165	-3.068318
O	-5.187929	-0.565139	-1.188988
H	-4.317438	-0.319011	-1.539794
C	-0.152620	3.035340	-1.146307
H	0.622785	3.665769	-0.722689
H	-1.174075	3.351036	-0.954647
C	0.126838	2.096848	-2.102916
H	-0.662954	1.629508	-2.683048
H	1.143599	1.927712	-2.446948
C	-1.177011	-1.805197	1.838019
H	-2.216109	-1.659959	1.517717
H	-1.031534	-2.863300	2.079877
H	-1.003409	-1.214289	2.741982
C	-0.396063	-2.354704	-0.909075
H	-0.563004	-3.390950	-0.598999
H	-1.295830	-1.965585	-1.389882
H	0.427017	-2.318279	-1.627030
C	2.267458	2.793554	2.007058
H	3.272837	3.089333	2.322435
H	1.724986	3.686061	1.683696
H	1.738107	2.368452	2.864131
C	3.409749	2.381883	-0.608355
H	2.896318	3.233285	-1.062269
H	4.333980	2.744114	-0.147201
H	3.665246	1.667897	-1.395785

TS15-16.2MeOH.DMBPX

scf done: -1782.079766

Pd	-0.236713	-0.930779	-0.275501
P	-2.238041	-1.582057	0.709548
P	-0.047477	1.323175	0.512807
C	1.968446	-0.849809	-0.842525
C	2.677775	-1.544823	0.298530
H	2.979767	-0.754881	1.000478
H	1.991854	-2.231870	0.805355
C	3.949451	-2.276294	-0.163423

H	4.445506	-2.713703	0.706677
H	4.645636	-1.579018	-0.634885
H	3.732668	-3.091455	-0.862102
O	2.447283	0.042367	-1.505658
C	-3.344418	-0.277374	1.424602
H	-4.262494	-0.784060	1.745005
H	-2.858501	0.092661	2.332779
C	-3.660555	0.827391	0.450714
C	-4.814898	0.739053	-0.336396
H	-5.479136	-0.112768	-0.210429
C	-5.141922	1.731534	-1.256426
H	-6.046307	1.643976	-1.850743
C	-4.314308	2.843241	-1.389885
H	-4.564759	3.633712	-2.090802
C	-3.173288	2.950653	-0.599534
H	-2.549119	3.837154	-0.680644
C	-2.824066	1.953892	0.319591
C	-1.592655	2.129459	1.166302
H	-1.738520	1.751440	2.183787
H	-1.354312	3.194628	1.268543
H	6.000407	0.339467	2.558789
C	5.221760	1.113796	2.599357
H	5.712416	2.097182	2.585706
H	4.695383	1.014620	3.552651
O	4.271467	0.974910	1.561769
H	4.730143	1.033476	0.698845
H	6.914472	1.832535	-1.386746
C	5.928779	1.718871	-1.842185
H	5.463604	2.710451	-1.916698
H	6.060979	1.311727	-2.851944
O	5.181995	0.835408	-1.017406
H	4.302619	0.692208	-1.400530
C	-0.255208	-2.672520	-1.425339
H	-1.129124	-2.652500	-2.071868
H	-0.139837	-3.589193	-0.849055
C	0.933600	-2.013646	-1.911048
H	1.840200	-2.624591	-1.875697
H	0.852332	-1.437218	-2.829538
C	1.133664	1.721569	1.857241
H	2.172128	1.503650	1.581552
H	1.053663	2.784237	2.110418
H	0.884699	1.133191	2.745376
C	0.413429	2.442319	-0.864265
H	0.583181	3.456905	-0.490634
H	1.319505	2.075959	-1.349321
H	-0.393694	2.458498	-1.601428
C	-1.942116	-2.705506	2.131520
H	-2.888985	-2.995021	2.597869
H	-1.425039	-3.606549	1.792091
H	-1.314784	-2.208936	2.876066
C	-3.393484	-2.527971	-0.356102
H	-2.912588	-3.436065	-0.726044
H	-4.286008	-2.810545	0.210651
H	-3.692273	-1.914721	-1.209832

Complex 16.2MeOH

scf done: -2253.678378

Pd	0.122494	0.236540	-0.451750
P	-0.468507	-1.875941	0.298159
P	-1.608045	1.743169	0.332136
C	3.187787	1.604891	-1.028423
C	4.351548	1.957321	-1.914342
H	4.660860	0.999579	-2.360043
H	3.979698	2.568211	-2.747387
C	5.519643	2.625304	-1.201428
H	6.309365	2.858924	-1.919880
H	5.940361	1.970400	-0.435580
H	5.211058	3.559301	-0.723014
O	3.224206	1.619996	0.191758
C	0.705245	-2.422517	1.717107
C	0.446484	-1.519159	2.934631
H	-0.500089	-1.732104	3.438708
H	0.477829	-0.460438	2.661702
H	1.242439	-1.690476	3.668106
C	0.504047	-3.885378	2.140100
H	-0.530087	-4.115749	2.413320
H	1.117953	-4.074361	3.028527

H	0.828992	-4.590947	1.372267
C	2.166277	-2.205649	1.297340
H	2.384766	-1.146564	1.141339
H	2.448932	-2.746292	0.393882
H	2.814153	-2.563671	2.106105
C	-0.581434	-3.210683	-1.064299
C	0.814286	-3.656939	-1.527464
H	1.461479	-2.827864	-1.812240
H	0.693105	-4.296819	-2.409322
H	1.329986	-4.250350	-0.768827
C	-1.351267	-4.470100	-0.632200
H	-0.896441	-4.983419	0.215525
H	-1.351635	-5.172083	-1.474050
H	-2.393631	-4.266084	-0.393068
C	-1.325165	-2.558106	-2.242984
H	-0.777092	-1.700787	-2.642628
H	-2.326838	-2.221522	-1.962311
H	-1.433719	-3.294860	-3.047633
C	-2.125247	-1.892201	1.180749
H	-2.258474	-2.915033	1.548907
H	-1.937154	-1.276172	2.063645
C	-3.415507	-1.436429	0.533930
C	-4.291112	-2.403317	0.018291
H	-3.997279	-3.447144	0.038902
C	-5.552829	-2.084932	-0.471418
H	-6.195784	-2.867130	-0.863240
C	-5.993849	-0.768131	-0.406654
H	-6.989342	-0.498102	-0.745479
C	-5.157424	0.198515	0.139443
H	-5.535288	1.210287	0.253961
C	-3.862550	-0.096553	0.590729
C	-3.068891	1.012354	1.239746
H	-2.649296	0.661048	2.187912
H	-3.744496	1.835613	1.493770
C	-2.333267	2.576080	-1.231186
C	-3.677728	3.282188	-1.004212
H	-3.626442	4.074693	-0.256560
H	-4.463039	2.583077	-0.718027
H	-3.992503	3.744673	-1.947198
C	-2.534026	1.448907	-2.262386
H	-1.583626	0.974266	-2.531800
H	-2.968221	1.873238	-3.175766
H	-3.210379	0.670601	-1.900750
C	-1.343613	3.593567	-1.818333
H	-1.241141	4.487555	-1.198785
H	-1.719131	3.919238	-2.795410
H	-0.348135	3.170304	-1.983892
C	-0.984907	3.052842	1.583940
C	-0.822057	2.365024	2.950753
H	-1.778863	2.133793	3.426708
H	-0.287562	3.045580	3.623117
H	-0.230133	1.447800	2.882140
C	-1.925327	4.253595	1.756611
H	-2.944064	3.959061	2.026886
H	-1.971283	4.883621	0.865253
H	-1.547654	4.881283	2.572521
C	0.404923	3.541194	1.145809
H	0.394274	4.033782	0.171083
H	1.131502	2.723705	1.113959
H	0.768113	4.276534	1.873550
H	6.717481	-1.636367	-1.543407
C	5.765883	-2.153828	-1.357085
H	5.960649	-2.991077	-0.671184
H	5.418692	-2.572393	-2.306029
O	4.763734	-1.281818	-0.874082
H	5.081287	-0.874126	-0.044709
H	6.617810	-0.574108	2.732918
C	5.804913	0.152647	2.671379
H	4.972135	-0.207111	3.290663
H	6.164286	1.104310	3.082241
O	5.447519	0.273154	1.305282
H	4.741960	0.930831	1.197296
C	1.724289	-0.346966	-1.612990
H	1.395928	-0.821986	-2.537499
H	2.535889	-0.886500	-1.127337
C	1.915164	1.134195	-1.724628
H	1.800583	1.503324	-2.747819

H	1.071415	1.710687	-1.154805
Complex 17.2MeOH			
scf done: -2366.945627			
Pd	-0.526260	-1.021106	0.061256
P	0.187854	0.844234	-1.345815
P	-2.957619	-0.496671	0.364579
C	3.757003	-2.567253	0.552731
C	4.631005	-3.775767	0.295809
H	5.656930	-3.490530	0.545765
H	4.327345	-4.541298	1.025147
C	4.546259	-4.359617	-1.117345
H	5.233365	-5.204229	-1.212515
H	4.828115	-3.619707	-1.872981
H	3.543275	-4.727199	-1.353254
O	4.181354	-1.580647	1.132473
C	0.279194	0.095198	-3.113033
C	-1.118113	-0.415368	-3.497648
H	-1.841649	0.862248	-3.668894
H	-1.511352	-1.097600	-2.737760
H	-1.040670	-0.976118	-4.436171
C	0.748983	1.096233	-4.178110
H	0.144890	2.007908	-4.203072
H	0.656142	0.624544	-5.163694
H	1.797454	1.375008	-4.054924
C	1.207544	-1.129020	-3.113376
H	0.836670	-1.899162	-2.430004
H	2.235175	-0.885964	-2.842901
H	1.223688	-1.557535	-4.122253
C	1.796015	1.806031	-0.928337
C	3.065751	1.010413	-1.286881
H	3.076810	-0.014122	-0.916890
H	3.917187	1.530240	-0.830157
H	3.228069	0.984472	-2.368288
C	1.909237	3.144446	-1.680071
H	1.899393	3.033820	-2.765511
H	2.871690	3.587528	-1.403154
H	1.138890	3.862061	-1.400667
C	1.757803	2.116710	0.581918
H	1.643488	1.224057	1.200928
H	0.939382	2.797771	0.831230
H	2.707402	2.588888	0.859329
C	-1.110297	2.178911	-1.579060
H	-0.660894	2.925908	-2.239940
H	-1.894022	1.695658	-2.167205
C	-1.742553	2.890855	-0.402787
C	-1.239893	4.138458	-0.006514
H	-0.355819	4.533910	-0.494268
C	-1.860553	4.918087	0.963420
H	-1.435079	5.877634	1.240699
C	-3.050389	4.477503	1.532118
H	-3.578772	5.087866	2.258006
C	-3.578976	3.255694	1.132437
H	-4.542200	2.949705	1.529932
C	-2.933959	2.431361	0.199072
C	-3.616980	1.153883	-0.221093
H	-3.612555	1.072685	-1.312075
H	-4.671141	1.194632	0.073987
C	-3.119683	-0.474383	2.276761
C	-4.402922	0.196393	2.789741
H	-5.312782	-0.314646	2.475345
H	-4.467108	1.242566	2.495107
H	-4.382935	0.176901	3.885680
C	-1.909934	0.323838	2.800795
H	-0.958653	-0.151816	2.534707
H	-1.960284	0.366665	3.895443
H	-1.896665	1.351074	2.428623
C	-3.055486	-1.894527	2.858395
H	-3.912055	-2.511464	2.577121
H	-3.060065	-1.817401	3.951665
H	-2.141245	-2.425564	2.585243
C	-4.244847	-1.688232	-0.426927
C	-4.481594	-1.277596	-1.891653
H	-5.060409	-0.354783	-1.981418
H	-5.065155	-2.066914	-2.378711
H	-3.554715	-1.166684	-2.458713
C	-5.607620	-1.672042	0.283214

H	-6.041589	-0.669678	0.340476	H	4.732513	4.555344	-1.798265
H	-5.568040	-2.093950	1.289354	C	4.216704	2.708456	-0.825584
H	-6.305289	-2.288550	-0.295644	H	5.098785	2.202635	-1.206417
C	-3.689880	-3.118884	-0.424696	C	3.337925	2.006682	0.012369
H	-3.467131	-3.488168	0.578625	C	3.674306	0.577163	0.365521
H	-2.787752	-3.200222	-1.038850	H	3.540533	0.421956	1.440514
H	-4.438463	-3.792201	-0.857826	H	4.736469	0.401633	0.162432
H	6.957166	3.192116	-0.119110	C	3.006989	-0.730615	-2.297394
C	6.155162	3.578514	0.526637	C	4.419339	-0.278637	-2.699305
H	5.727720	4.460847	0.040528	H	5.202955	-0.957845	-2.362128
H	6.609783	3.907961	1.472860	H	4.645148	0.724649	-2.344318
O	5.117833	2.642986	0.723385	H	4.467413	-0.247274	-3.793922
H	5.508679	1.835328	1.118909	C	1.991949	0.312915	-2.800387
H	7.224848	1.106471	3.330751	H	0.959713	-0.004336	-2.617500
C	6.550504	0.272779	3.121877	H	2.114979	0.432339	-3.883311
H	7.068952	-0.658209	3.385920	H	2.137997	1.293261	-2.339985
H	5.665214	0.375857	3.764523	C	2.719268	-2.069765	-2.992585
O	6.228968	0.319696	1.742561	H	3.459659	-2.837183	-2.754540
H	5.634167	-0.420572	1.541741	H	2.765539	-1.905821	-4.075350
C	1.487836	-1.472197	0.650949	H	1.726777	-2.465264	-2.773292
H	1.344736	-1.612004	1.728788	C	3.699232	-2.347462	0.341983
H	2.023702	-0.540706	0.526243	C	3.832131	-2.131105	1.859821
C	2.306444	-2.614071	0.075618	H	4.539630	-1.338532	2.116246
H	1.900928	-3.605098	0.312115	H	4.211037	-3.055775	2.309269
H	2.345970	-2.576361	-1.020571	H	2.870860	-1.913341	2.333548
C	-0.693254	-2.834363	0.639627	C	5.109853	-2.518628	-0.242491
O	-0.664300	-3.954828	0.869314	H	5.717124	-1.612799	-0.157451
TS17-18.2MeOH				H	5.097508	-2.835464	-1.287442
scf done: -2366.940873				H	5.625710	-3.302616	0.323902
Pd	0.382744	-0.970419	-0.043426	C	2.899536	-3.640582	0.127427
P	-0.042483	1.002959	1.367658	H	2.696875	-3.853187	-0.923487
P	2.750257	-0.857340	-0.405791	H	1.947882	-3.616188	0.666090
C	-4.109333	-2.441662	-0.109502	H	3.478718	-4.481679	0.525479
C	-5.058928	-3.598135	0.111430	C	-6.127392	4.290365	-0.810274
H	-6.072933	-3.189157	0.088921	C	-5.295026	4.334946	-1.527588
H	-4.960221	-4.258752	-0.762544	H	-4.723788	5.245782	-1.324599
C	-4.815193	-4.407685	1.388843	H	-5.721035	4.427973	-2.537790
H	-5.568980	-5.193872	1.479250	O	-4.417312	3.236320	-1.411143
H	-4.888063	-3.777794	2.280878	H	-4.936947	2.417190	-1.540543
H	-3.835535	-4.894673	1.390106	H	-6.845061	1.339177	-3.399853
O	-4.510627	-1.335900	-0.432379	C	-6.418739	0.470373	-2.893338
C	-0.457599	0.403045	3.138930	H	-7.211370	-0.280921	-2.781406
C	0.801682	-0.228509	3.756627	H	-5.627558	0.054511	-3.532854
H	1.562684	0.507850	4.028447	O	-5.929061	0.907420	-1.638257
H	1.250351	-0.972212	3.091056	H	-5.557492	0.145117	-1.170680
H	0.518727	-0.745790	4.680558	C	-1.796195	-1.551568	-0.496573
C	-0.943708	1.526395	4.065831	H	-1.957094	-1.409771	-1.567456
H	-0.221736	2.344283	4.148091	H	-2.082829	-0.629509	-0.005255
H	-1.078612	1.116905	5.074088	C	-2.612845	-2.703659	0.055345
H	-1.903677	1.943290	3.755636	H	-2.379305	-3.661733	-0.424608
C	-1.519748	-0.703811	3.051329	H	-2.427074	-2.856551	1.126197
H	-1.138895	-1.562198	2.487605	C	-0.007499	-2.573063	-0.935014
H	-2.449545	-0.369030	2.589372	O	-0.135843	-3.600210	-1.448557
H	-1.758916	-1.050725	4.063421	Complex 18.2MeOH			
C	-1.420627	2.152349	0.686776	scf done: -2366.962919			
C	-2.844428	1.647060	0.984420	Pd	0.692970	-0.588978	0.636785
H	-3.057945	0.639772	0.624107	P	0.180711	1.728372	1.281052
H	-3.536349	2.310192	0.451088	P	2.722588	-0.946236	-0.432689
H	-3.086636	1.689718	2.049324	C	-3.662009	-2.814717	-0.140927
C	-1.339445	3.580020	1.249572	C	-4.937788	-3.450083	0.361304
H	-1.397809	3.618436	2.340082	H	-5.764698	-2.856451	-0.040932
H	-2.194085	4.140029	0.855487	H	-4.994492	-4.434697	-0.127583
H	-0.441674	4.103686	0.925860	C	-5.060031	-3.623869	1.875847
C	-1.205987	2.211504	-0.837305	H	-6.028065	-4.068844	2.118877
H	-1.260092	1.219360	-1.297783	H	-5.003081	-2.662317	2.395578
H	-0.236238	2.651356	-1.092495	H	-4.288331	-4.283126	2.284132
H	-2.001475	2.821320	-1.280912	O	-3.659232	-2.071542	-1.112637
C	1.423052	2.116111	1.713609	C	0.300805	1.994952	3.168098
H	1.050223	2.929145	2.343937	C	1.788291	2.035157	3.558688
H	2.065409	1.509555	2.358389	H	2.276295	2.967451	3.260820
C	2.269494	2.710973	0.610990	H	2.349833	1.193784	3.140206
C	2.120734	4.072016	0.308413	H	1.867261	1.966480	4.649623
H	1.353120	4.645275	0.817134	C	-0.366925	3.279298	3.676848
C	2.963247	4.736049	-0.576406	H	0.016805	4.175098	3.178806
H	2.809664	5.790780	-0.782802	H	-0.155276	3.388617	4.747244
C	4.030236	4.049004	-1.143258	H	-1.453218	3.259024	3.565159

C	-0.327937	0.768337	3.853559
H	0.189103	-0.155465	3.567730
H	-1.388988	0.652425	3.624172
H	-0.236817	0.875194	4.940944
C	-1.513139	2.238123	0.586790
C	-2.611749	1.494657	1.364508
H	-2.412927	0.416099	1.413421
H	-3.562706	1.633484	0.834942
H	-2.729689	1.867210	2.385456
C	-1.793659	3.746782	0.616372
H	-1.837759	4.155403	1.627022
H	-2.768165	3.921303	0.147595
H	-1.055516	4.317275	0.047284
C	-1.566471	1.758239	-0.876539
H	-1.395631	0.678603	-0.954111
H	-0.829968	2.258873	-1.508780
H	-2.570089	1.962621	-1.267209
C	1.470379	2.893946	0.582400
H	1.187027	3.919310	0.842942
H	2.373237	2.671629	1.158049
C	1.772811	2.824694	-0.896784
C	1.258206	3.850867	-1.704572
H	0.639631	4.615507	-1.243403
C	1.535072	3.943741	-3.062499
H	1.116663	4.755729	-3.649255
C	2.382568	3.007048	-3.645148
H	2.644825	3.073029	-4.696622
C	2.925412	2.001398	-2.855372
H	3.634980	1.317462	-3.309318
C	2.626579	1.863299	-1.490402
C	3.376159	0.804212	-0.705901
H	3.541736	1.156662	0.314999
H	4.371243	0.681735	-1.149716
C	2.586036	-1.801961	-2.129990
C	3.815221	-1.603250	-3.031500
H	4.709810	-2.088474	-2.640867
H	4.048029	-0.553452	-3.209638
H	3.601485	-2.053385	-4.007722
C	1.350018	-1.194673	-2.817920
H	0.436354	-1.384354	-2.248036
H	1.231156	-1.657609	-3.804621
H	1.437023	-0.115864	-2.962878
C	2.359547	-3.310532	-1.949585
H	3.264986	-3.830776	-1.628421
H	2.068473	-3.736299	-2.916784
H	1.562390	-3.539710	-1.236297
C	4.091574	-1.708944	0.667921
C	4.310141	-0.770333	1.867185
H	4.813347	0.162183	1.597733
H	4.953269	-1.281528	2.592117
H	3.368690	-0.537982	2.374665
C	5.425247	-1.896757	-0.069942
H	5.781286	-0.987950	-0.564780
H	5.377636	-2.701225	-0.807335
H	6.187625	-2.182044	0.664373
C	3.621220	-3.061026	1.227412
H	3.416859	-3.800371	0.451955
H	2.726200	-2.961078	1.843394
H	4.420957	-3.466581	1.858000
H	-6.903220	2.622849	-0.244915
C	-6.093505	2.883575	-0.942475
H	-5.695213	3.857378	-0.641924
H	-6.531782	2.999360	-1.945178
O	-5.034295	1.952583	-0.918370
H	-5.395186	1.075932	-1.162457
H	-7.498926	-0.111408	-2.897204
C	-6.571466	-0.688390	-2.913786
H	-6.821955	-1.728344	-3.159719
H	-5.927559	-0.285766	-3.707431
O	-5.978018	-0.580641	-1.629513
H	-5.174612	-1.131357	-1.607971
C	-1.163105	-2.504146	-0.149316
H	-0.886421	-3.092253	-1.033188
H	-1.433512	-1.515763	-0.535845
C	-2.357828	-3.121397	0.576059
H	-2.241252	-4.204401	0.698974
H	-2.443905	-2.726668	1.596746

C	0.097538	-2.441752	0.712775
O	0.419715	-3.235426	1.546892

Complex 17-H*

scf done: -2058.950629

Pd	0.717147	-0.861946	-0.325926
C	2.616750	-1.441735	-0.692271
C	3.106198	-2.488264	0.311666
H	3.007937	-2.081337	1.324207
H	2.366578	-3.296437	0.245169
C	4.522828	-2.988353	0.047829
H	4.794920	-3.764264	0.770556
H	5.255237	-2.178778	0.124937
H	4.605863	-3.408258	-0.957525
O	3.268404	-1.184280	-1.679884
P	-1.729764	-1.003310	0.336324
P	1.231157	1.344321	0.260313
C	-1.848371	-2.291859	1.761586
C	-0.861692	-1.811757	2.841400
H	-1.137151	-0.849412	3.285441
H	0.150716	-1.728583	2.435841
H	-0.842343	-2.544587	3.657660
C	-3.243973	-2.431807	2.385069
H	-3.622821	-1.498912	2.813920
H	-3.193012	-3.162498	3.202553
H	-3.978786	-2.807350	1.667640
C	-1.371275	-3.679922	1.297486
H	-0.473917	-3.625760	0.673744
H	-2.140400	-4.201053	0.724604
H	-1.162601	-4.288883	2.186854
C	-2.904174	-1.435068	-1.113605
C	-2.716612	-2.894802	-1.554655
H	-1.657263	-3.163884	-1.573919
H	-3.139681	-3.011233	-2.560986
H	-3.254655	-3.585301	-0.898474
C	-4.394134	-1.196091	-0.838754
H	-4.761736	-1.757040	0.024725
H	-4.966694	-1.534605	-1.711667
H	-4.629697	-0.140971	-0.693677
C	-2.451674	-0.516883	-2.263958
H	-1.418037	-0.731593	-2.550583
H	-2.526715	0.543137	-2.002531
H	-3.092634	-0.691151	-3.137981
C	-2.582196	0.442764	1.188173
H	-3.610947	0.148462	1.413311
H	-2.072351	0.525590	2.154664
C	-2.603218	1.797382	0.527257
C	-3.829085	2.286939	0.050131
H	-4.711129	1.659671	0.140302
C	-3.965024	3.558494	-0.494155
H	-4.932450	3.895550	-0.855187
C	-2.857501	4.399044	-0.533986
H	-2.938195	5.407805	-0.928639
C	-1.645557	3.944906	-0.027791
H	-0.799560	4.625808	-0.014565
C	-1.478781	2.649054	0.486383
C	-0.151341	2.306351	1.119715
H	-0.319566	1.723477	2.032328
H	0.300568	3.247448	1.442040
C	1.678453	2.402250	-1.274253
C	1.947281	3.881085	-0.964551
H	2.908838	4.018936	-0.461831
H	1.173140	4.355210	-0.358079
H	2.000505	4.434023	-1.910645
C	0.483487	2.263507	-2.236903
H	0.292067	1.210846	-2.467439
H	0.731470	2.773026	-3.176452
H	-0.436252	2.703617	-1.850781
C	2.902878	1.843937	-2.014794
H	2.791427	0.791031	-2.275531
H	3.829177	1.952784	-1.448853
H	3.022526	2.418846	-2.942294
C	2.556884	1.540367	1.647637
C	2.206069	0.504140	2.728773
H	1.226381	0.686542	3.181562
H	2.950743	0.557534	3.532882
H	2.206181	-0.511742	2.329033

C	2.610311	2.920438	2.327332	H	-5.486635	-0.693167	-1.072601
H	1.723166	3.127095	2.932285	O	-2.805030	-1.677102	-1.246653
H	2.746951	3.742925	1.622159	P	0.696235	1.826456	0.524501
H	3.467504	2.933982	3.011967	P	0.009858	-1.715619	0.458369
C	3.958877	1.224914	1.103943	C	2.333269	1.326915	1.268065
H	4.370236	2.063101	0.535429	H	2.941459	2.223247	1.438102
H	3.980274	0.340256	0.464797	H	2.106861	0.906339	2.255160
H	4.635038	1.045943	1.949158	C	3.086493	0.347156	0.405731
C	0.901701	-3.176842	-2.305678	C	4.122456	0.828330	-0.406344
H	0.909068	-2.393739	-3.082401	H	4.361093	1.888861	-0.373267
H	1.938120	-3.553112	-2.231069	C	4.854994	-0.011347	-1.239446
H	0.292658	-4.010816	-2.696844	H	5.652886	0.394590	-1.854740
O	0.370217	-2.759484	-1.082982	C	4.564364	-1.372518	-1.264320
				H	5.131834	-2.047499	-1.898543
Complex 17.DMBPX				C	3.545594	-1.867520	-0.456373
scf done: -1587.828137				H	3.332543	-2.933999	-0.461206
Pd	-0.992590	0.250043	-0.037023	C	2.788433	-1.032897	0.377299
C	-2.622500	-0.854739	-0.503131	C	1.711507	-1.660176	1.226916
C	-3.724688	-0.884762	0.548908	H	1.594172	-1.139715	2.183691
H	-3.351285	-1.497552	1.378944	H	1.989367	-2.694723	1.462909
H	-3.808727	0.124534	0.973343	C	-2.596348	2.189534	-1.621883
C	-5.064764	-1.399813	0.031766	H	-1.875638	2.159169	-2.461525
H	-5.800595	-1.414036	0.840017	H	-3.371855	1.434820	-1.854614
H	-4.968942	-2.413045	-0.365531	H	-3.093742	3.174228	-1.666997
H	-5.452065	-0.768820	-0.772493	O	-2.008373	2.021004	-0.370141
O	-2.759404	-1.287038	-1.621583	C	1.184202	2.844041	-0.922042
P	0.743723	1.885186	0.455173	H	0.260296	3.209481	-1.375966
P	0.025268	-1.728316	0.439789	H	1.716746	2.227885	-1.650461
C	2.323369	1.338762	1.261589	H	1.813610	3.691803	-0.631614
H	2.930448	2.231288	1.451190	C	0.069813	3.072512	1.717023
H	2.053366	0.929879	2.242018	H	-0.078088	2.608959	2.696488
C	3.099587	0.350794	0.429161	H	-0.901011	3.395946	1.331166
C	4.166789	0.819257	-0.348154	H	0.746701	3.927169	1.818035
H	4.416658	1.876971	-0.317043	C	0.224194	-2.732420	-1.048689
C	4.926050	-0.038296	-1.138305	H	-0.754600	-2.781354	-1.535389
H	5.752055	0.352603	-1.724586	H	0.584103	-3.739871	-0.816041
C	4.631453	-1.398954	-1.152474	H	0.927005	-2.237972	-1.723197
H	5.224467	-2.085287	-1.749086	C	-0.848155	-2.864028	1.613256
C	3.581499	-1.880038	-0.376635	H	-1.833327	-3.096990	1.202280
H	3.374778	-2.947517	-0.365707	H	-0.984548	-2.380991	2.584538
C	2.798422	-1.026307	0.412194	H	-0.285668	-3.794126	1.746639
C	1.697840	-1.631165	1.247040				
H	1.558586	-1.105781	2.197625	(MeOH)₉			
H	1.959593	-2.665908	1.499924	scf done: -1041.246583			
C	-3.345722	2.610155	-0.618846	C	-1.052105	2.191461	-1.068260
H	-4.209421	1.941233	-0.675141	H	-1.853932	1.862411	-1.738460
H	-3.185173	2.911938	0.416103	H	-0.916104	3.269353	-1.194554
H	-3.526454	3.499557	-1.228831	H	-1.367588	1.986754	-0.037773
O	-2.141406	1.955940	-1.055011	O	0.184354	1.562584	-1.391602
H	-2.260733	1.663150	-1.968231	H	0.048555	0.588823	-1.337998
C	1.315975	2.851902	-0.996921	C	0.532538	-0.461894	2.105377
H	0.447674	3.273774	-1.508978	H	1.089917	0.431647	1.797980
H	1.846080	2.196456	-1.692144	H	-0.534929	-0.227488	2.097804
H	1.981284	3.666765	-0.694616	H	0.828035	-0.732179	3.127523
C	0.150071	3.186989	1.614235	O	0.748380	-1.555037	1.215511
H	-0.148690	2.736506	2.564726	H	1.723002	-1.662287	1.066097
H	-0.717114	3.695296	1.184884	C	2.315943	3.591358	0.354274
H	0.930066	3.931094	1.804333	H	1.428919	4.032951	0.827822
C	0.300529	-2.681516	-1.096552	H	2.481397	4.094618	-0.608954
H	-0.645703	-2.770023	-1.635559	H	3.177664	3.791817	0.997277
H	0.689090	-3.678980	-0.868764	O	2.190004	2.191476	0.215730
H	1.015190	-2.152889	-1.731159	H	1.433548	1.980539	-0.397792
C	-0.850202	-2.906507	1.543357	C	4.246042	-2.497122	1.310200
H	-1.776438	-3.242487	1.071484	H	3.778863	-3.432440	1.631215
H	-1.091039	-2.430506	2.497238	H	4.559299	-1.943193	2.206080
H	-0.221456	-3.782397	1.731596	H	5.144119	-2.747089	0.728906
				O	3.305966	-1.781397	0.535240
Complex 17-H*.DMBPX				H	3.692701	-0.899130	0.286596
scf done: -1587.401038				C	4.711202	0.725366	-1.460959
Pd	-1.031515	0.250389	0.026515	H	5.184259	1.701641	-1.633712
C	-2.716333	-0.796793	-0.409476	H	3.897531	0.603676	-2.189813
C	-3.929001	-0.346085	0.397993	H	5.459076	-0.049766	-1.650538
H	-3.700840	-0.586776	1.447050	O	4.268958	0.592708	-0.124923
H	-3.936487	0.750116	0.358766	H	3.527400	1.236586	0.022443
C	-5.249844	-0.967858	-0.040728	C	-3.641120	1.318964	2.631174
H	-6.069648	-0.626185	0.599263	H	-4.583126	0.781944	2.825910
H	-5.209595	-2.060061	0.003300	H	-3.894137	2.360903	2.378837

H	-3.071141	1.334013	3.565576
O	-2.849590	0.696524	1.649923
H	-3.352861	0.677099	0.807614
C	-5.460315	0.385619	-1.048469
H	-5.960405	-0.381236	-0.438145
H	-5.682022	0.178586	-2.104775
H	-5.898210	1.356132	-0.796574
O	-4.072202	0.456490	-0.807744
H	-3.659354	-0.415363	-1.033962
C	-2.992805	-2.548403	0.117244
H	-2.932230	-1.858829	0.969061
H	-2.252344	-3.346197	0.254632
H	-3.986309	-3.005887	0.103566
O	-2.809807	-1.878905	-1.123442
H	-1.868889	-1.590777	-1.168938
C	0.597618	-1.936349	-2.031725
H	0.182229	-2.947596	-2.124022
H	1.632873	-2.011767	-1.681257
H	0.586781	-1.465682	-3.018579
O	-0.181627	-1.140365	-1.142960
H	0.139937	-1.319203	-0.198085

H	0.139937	-1.319203	-0.198085
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H⁺ (MeOH)₉

scf done: -1041.246583

C	-1.052105	2.191461	-1.068260
H	-1.853932	1.862411	-1.738460
H	-0.916104	3.269353	-1.194554
H	-1.367588	1.986754	-0.037773
O	0.184354	1.562584	-1.391602
H	0.048555	0.588823	-1.337998
C	0.532538	-0.461894	2.105377
H	1.089917	0.431647	1.797980
H	-0.534929	-0.227488	2.097804
H	0.828035	-0.732179	3.127523
O	0.748380	-1.555037	1.215511
H	1.723002	-1.662287	1.066097
C	2.315943	3.591358	0.354274
H	1.428919	4.032951	0.827822
H	2.481397	4.094618	-0.608954
H	3.177664	3.791817	0.997277
O	2.190004	2.191476	0.215730
H	1.433548	1.980539	-0.397792
C	4.246042	-2.497122	1.310200
H	3.778863	-3.432440	1.631215
H	4.559299	-1.943193	2.206080
H	5.144119	-2.747089	0.728906
O	3.305966	-1.781397	0.535240
H	3.692701	-0.899130	0.286596
C	4.711202	0.725366	-1.460959
H	5.184259	1.701641	-1.633712
H	3.897531	0.603676	-2.189813
H	5.459076	-0.049766	-1.650538
O	4.268958	0.592708	-0.124923
H	3.527400	1.236586	0.022443
C	-3.641120	1.318964	2.631174
H	-4.583126	0.781944	2.825910
H	-3.894137	2.360903	2.378837
H	-3.071141	1.334013	3.565576
O	-2.849590	0.696524	1.649923
H	-3.352861	0.677099	0.807614
C	-5.460315	0.385619	-1.048469
H	-5.960405	-0.381236	-0.438145
H	-5.682022	0.178586	-2.104775
H	-5.898210	1.356132	-0.796574
O	-4.072202	0.456490	-0.807744
H	-3.659354	-0.415363	-1.033962
C	-2.992805	-2.548403	0.117244
H	-2.932230	-1.858829	0.969061
H	-2.252344	-3.346197	0.254632
H	-3.986309	-3.005887	0.103566
O	-2.809807	-1.878905	-1.123442
H	-1.868889	-1.590777	-1.168938
C	0.597618	-1.936349	-2.031725
H	0.182229	-2.947596	-2.124022
H	1.632873	-2.011767	-1.681257
H	0.586781	-1.465682	-3.018579
O	-0.181627	-1.140365	-1.142960

**Atomic coordinates (in Å) of MARI and HETS,
optimised at the B3PW91/ECP1/PCM level,
and corresponding SCF energies (in a.u.).**

Complex 5 (PCM)

scf done: -2058.243532

Pd	-0.598043	-0.695206	0.225436
P	-0.660441	1.697716	0.613182
P	1.629977	-1.305548	0.298126
C	-1.582190	2.155192	2.227645
C	-0.628458	1.904321	3.408259
H	0.170986	2.647324	3.471296
H	-0.179417	0.907961	3.367928
H	-1.203260	1.967800	4.339308
C	-2.054359	3.614346	2.288031
H	-1.240916	4.325710	2.117893
H	-2.451869	3.811242	3.290940
H	-2.856776	3.825300	1.577186
C	-2.786269	1.214868	2.400232
H	-2.465827	0.174349	2.512189
H	-3.499191	1.272106	1.574612
H	-3.323746	1.491647	3.314975
C	-1.502977	2.487441	-0.910375
C	-2.996325	2.132449	-0.939912
H	-3.167885	1.053112	-0.899817
H	-3.417618	2.487076	-1.887860
H	-3.560788	2.608977	-0.135231
C	-1.358471	4.013279	-0.999677
H	-1.846997	4.538028	-0.177702
H	-1.830507	4.350638	-1.930289
H	-0.315731	4.328695	-1.037620
C	-0.837402	1.847963	-2.143519
H	-0.959026	0.760013	-2.143380
H	0.230053	2.071690	-2.200998
H	-1.314367	2.243086	-3.048834
C	0.962236	2.597158	0.824765
H	0.740361	3.653791	1.005426
H	1.368671	2.205616	1.761909
C	1.999394	2.485097	-0.266660
C	2.242262	3.614162	-1.063505
H	1.670980	4.519150	-0.879234
C	3.215278	3.628591	-2.057090
H	3.368292	4.522025	-2.655129
C	4.006885	2.500436	-2.245075
H	4.793238	2.490829	-2.993963
C	3.813917	1.391376	-1.427889
H	4.496636	0.554791	-1.528730
C	2.811982	1.341808	-0.446816
C	2.781657	0.163990	0.502747
H	2.540662	0.528700	1.503891
H	3.792156	-0.252680	0.570407
C	2.222238	-2.237748	-1.260369
C	3.750027	-2.258905	-1.425063
H	4.267359	-2.730009	-0.588789
H	4.169078	-1.265985	-1.575793
C	3.983663	-2.841558	-2.323660
H	1.605091	-1.499475	-2.461815
H	0.512228	-1.527589	-2.438179
H	1.937933	-1.988158	-3.385264
H	1.919213	-0.452804	-2.506401
C	1.736334	-3.695307	-1.259872
H	0.662285	-3.789972	-1.103527
H	2.252654	-4.303850	-0.513301
H	1.962933	-4.128685	-2.241063
C	2.030555	-2.288125	1.899896
C	1.893519	-1.337081	3.101040
H	2.701281	-0.603853	3.162096
H	1.932549	-1.934395	4.018906
H	0.934287	-0.812171	3.091428
C	3.447604	-2.882099	1.902342
H	4.225437	-2.133860	1.726442
H	3.563607	-3.687203	1.173503
H	3.635307	-3.314188	2.892329
C	1.008890	-3.416784	2.102634
H	0.982115	-4.128463	1.275718

H	0.003949	-3.014702	2.254779
H	1.285289	-3.974019	3.005274
O	-4.862475	-2.089110	-0.764695
C	-5.856539	-2.062767	-1.805443
H	-5.886118	-1.078009	-2.276011
H	-6.801803	-2.278785	-1.310803
H	-5.635580	-2.822081	-2.558137
C	-3.609596	-1.849749	-1.151212
O	-3.271147	-1.613664	-2.291694
C	-1.348993	-2.554458	-0.253666
C	-2.659750	-1.903087	0.032561
H	-2.517801	-0.772386	0.277969
H	-1.094355	-3.378935	0.405028
H	-1.186193	-2.775454	-1.307662
H	-3.150727	-2.272050	0.934197

TS5-6 (PCM)

scf done: -2173.885395

Pd	0.638390	0.068325	-0.314037
P	-0.639668	-1.795822	0.420957
P	-0.796164	1.827436	0.258570
C	0.382277	-2.583489	1.842591
C	0.350762	-1.615066	3.037352
H	-0.635829	-1.530415	3.499834
H	0.699951	-0.618982	2.754890
H	1.030864	-1.998102	3.806563
C	-0.176874	-3.943287	2.288680
H	-1.224485	-3.897159	2.598825
H	0.400266	-4.277147	3.159079
H	-0.071100	-4.710754	1.518971
C	1.854516	-2.754573	1.436581
H	2.307824	-1.807593	1.137715
H	1.994721	-3.464173	0.621957
H	2.402551	-3.134079	2.307056
C	-0.959841	-3.044461	-0.989415
C	0.331028	-3.793718	-1.357840
H	1.189581	-3.128618	-1.450373
H	0.172925	-4.296570	-2.319207
H	0.569478	-4.569824	-0.625841
C	-2.036170	-4.085378	-0.644258
H	-1.827533	-4.637235	0.274146
H	-2.069148	-4.814514	-1.462372
H	-3.028832	-3.643743	-0.570376
C	-1.442002	-2.223969	-2.198502
H	-0.679268	-1.521383	-2.543356
H	-2.353624	-1.660819	-1.978808
H	-1.665295	-2.911185	-3.023281
C	-2.290005	-1.559174	1.261515
H	-2.608072	-2.552720	1.590119
H	-2.063819	-0.997239	2.172282
C	-3.421362	-0.887900	0.527622
C	-4.518668	-1.649137	0.100364
H	-4.528618	-2.718027	0.289737
C	-5.621197	-1.067675	-0.518277
H	-6.451918	-1.689037	-0.839138
C	-5.659421	0.313242	-0.690217
H	-6.517027	0.790779	-1.154468
C	-4.602774	1.086546	-0.220405
H	-4.666135	2.168361	-0.300186
C	-3.473334	0.510862	0.379968
C	-2.456382	1.426385	1.010836
H	-2.209055	1.068861	2.017200
H	-2.932436	2.398345	1.152910
C	-1.177695	2.734356	-1.380414
C	-2.105217	3.939156	-1.159488
H	-1.630125	4.733969	-0.579368
H	-3.047714	3.673395	-0.674884
H	-2.357760	4.361068	-2.139251
C	-1.851748	1.719836	-2.320987
H	-1.212095	0.848107	-2.487230
H	-2.014509	2.206078	-3.290036
H	-2.818165	1.372782	-1.955563
C	0.104929	3.207974	-2.082488
H	0.747260	2.368772	-2.359191
H	0.689282	3.918092	-1.497147
H	-0.188589	3.713090	-3.009829
C	-0.144463	3.041167	1.625455

C	0.587498	2.175499	2.661851	H	-0.352617	4.578669	-0.133467
H	-0.072128	1.427563	3.111358	C	1.626947	4.736027	-0.907987
H	0.948541	2.819753	3.472010	H	1.447418	5.716232	-1.339559
H	1.450682	1.660701	2.231871	C	2.885918	4.148147	-0.975355
C	-1.285397	3.789944	2.343774	H	3.711486	4.655233	-1.465897
H	-1.921572	3.133454	2.940141	C	3.089820	2.915539	-0.364069
H	-1.914346	4.369100	1.663165	H	4.090782	2.493947	-0.355104
H	-0.824045	4.500140	3.038837	C	2.056611	2.219561	0.280741
C	0.819185	4.116591	1.097094	C	2.409994	0.951191	1.017475
H	0.325743	4.827874	0.431668	H	1.959686	0.974748	2.014145
H	1.701024	3.720588	0.591800	H	3.492919	0.912354	1.173544
H	1.183265	4.685200	1.960272	C	2.820585	-0.923356	-1.328295
O	5.725167	-0.070385	0.635748	C	4.291438	-0.489323	-1.271894
C	6.925647	-0.691588	0.154650	H	4.878947	-1.053249	-0.546366
H	6.687804	-1.495921	-0.545157	H	4.398164	0.573701	-1.050706
H	7.424739	-1.091594	1.036290	H	4.740588	-0.657457	-2.258244
H	7.564411	0.041772	-0.343273	C	2.097659	-0.074295	-2.391371
C	4.947049	0.496461	-0.299106	H	1.059864	-0.394566	-2.528807
O	5.203153	0.474460	-1.486499	H	2.616470	-0.136692	-3.350129
C	2.593485	1.382632	-0.641272	H	2.099404	0.990540	-2.145649
C	3.762317	1.196055	0.327771	C	2.740434	-2.395985	-1.759758
H	3.475783	0.651904	1.232774	H	1.712000	-2.769545	-1.769571
H	1.962792	2.196651	-0.296371	H	3.343263	-3.050792	-1.125858
H	2.941942	1.692678	-1.633201	H	3.133313	-2.481233	-2.779969
H	4.139470	2.170249	0.672575	C	2.445929	-1.922898	1.641982
H	1.484293	-1.821355	-3.110794	C	2.014384	-1.389843	3.019813
C	2.194205	-1.095731	-2.702013	H	2.608723	-0.531272	3.343349
H	1.944040	-0.107349	-3.112377	H	2.165574	-2.184417	3.759537
H	3.202794	-1.359701	-3.042195	H	0.956312	-1.115324	3.048928
O	2.179657	-1.106101	-1.279276	C	3.964715	-2.143178	1.672954
H	2.416873	0.085616	-0.996272	H	4.520353	-1.207220	1.784567
Complex 11 (PCM)				H	4.332850	-2.664473	0.786409
scf done: -1943.757384				H	4.207489	-2.770175	2.539482
Pd	-0.473064	-1.038422	-0.231372	C	1.729754	-3.265509	1.415517
P	-1.531749	0.905014	0.418305	H	1.950482	-3.707342	0.442303
P	1.862028	-0.681374	0.305762	H	0.643713	-3.159414	1.502686
C	-1.777621	-2.313829	-1.021058	H	2.058050	-3.975295	2.184272
C	-3.152779	-2.668951	-1.487868	TS10-12 (PCM)			
H	-3.864672	-2.323029	-0.732604	scf done: -1943.699241			
H	-3.328749	-2.034750	-2.368085	Pd	-0.000776	-1.213072	-0.405353
C	-3.343462	-4.144629	-1.828168	P	-1.949887	-0.038215	0.323349
H	-4.365676	-4.308855	-2.178315	P	1.888280	0.188038	0.329523
H	-3.177083	-4.776148	-0.951576	C	1.278217	-2.884285	-1.376890
H	-2.655195	-4.460389	-2.615804	C	-0.031553	-3.032081	-1.748243
O	-0.804336	-3.048594	-1.110293	H	-1.325499	-1.901001	-0.797546
C	-2.664091	0.567497	1.926825	H	-0.272137	-2.588300	-2.714137
C	-1.762315	0.222303	3.124891	C	-0.778457	-4.290279	-1.333859
H	-1.218568	1.086324	3.514660	H	-0.543645	-4.580172	-0.308519
H	-1.046925	-0.565995	2.872202	H	-0.485441	-5.108435	-2.000779
H	-2.394094	-0.153987	3.937288	H	-1.857457	-4.145195	-1.411006
C	-3.558518	1.757691	2.304690	O	2.415365	-3.319170	-1.310261
H	-2.995172	2.681152	2.466544	C	-2.897386	-1.026650	1.664996
H	-4.065325	1.520608	3.247615	C	-2.122877	-0.904397	2.988470
H	-4.337027	1.946502	1.561731	H	-2.191844	0.091549	3.433189
C	-3.545003	-0.660693	1.654576	H	-1.068325	-1.167370	2.869042
H	-2.936978	-1.553080	1.481728	H	-2.556006	-1.609082	3.707216
H	-4.217212	-0.522037	0.806454	C	-4.331073	-0.524355	1.888840
H	-4.167041	-0.845283	2.538025	H	-4.376821	0.546332	2.107721
C	-2.477306	1.751134	-1.005315	H	-4.749929	-1.048491	2.755851
C	-3.756496	0.976580	-1.344117	H	-4.983896	-0.736117	1.039061
H	-3.568242	-0.087441	-1.487072	C	-2.929950	-2.516650	1.291664
H	-4.159986	1.368896	-2.284697	H	-1.921289	-2.938459	1.252724
H	-4.531445	1.097954	-0.582959	H	-3.424197	-2.710635	0.337442
C	-2.867501	3.208861	-0.718174	H	-3.488097	-3.057453	2.064930
H	-3.504670	3.318223	0.160023	C	-3.048830	0.308889	-1.201486
H	-3.431184	3.583958	-1.580361	C	-3.681220	-0.986810	-1.730369
H	-2.001858	3.857388	-0.599704	H	-2.942453	-1.771279	-1.924505
C	-1.538148	1.710354	-2.223716	H	-4.167922	-0.764148	-2.686938
H	-1.319032	0.680521	-2.521721	H	-4.447395	-1.386053	-1.061571
H	-0.592306	2.224808	-2.034063	C	-4.175066	1.322895	-0.948716
H	-2.029982	2.211236	-3.066181	H	-4.896996	0.984078	-0.204879
C	-0.373126	2.206737	1.124339	H	-4.719243	1.471796	-1.888509
H	-1.017558	3.019742	1.475898	H	-3.795709	2.297016	-0.643066
H	0.027113	1.730490	2.022917	C	-2.107595	0.866028	-2.285802
C	0.769579	2.803132	0.329710	H	-1.321016	0.148530	-2.540586
C	0.600116	4.072364	-0.244268	H	-1.633630	1.802102	-1.980895

H	-2.692506	1.064486	-3.191893
C	-1.699831	1.603153	1.180776
H	-2.692473	1.953566	1.482192
H	-1.175806	1.341496	2.104133
C	-0.967564	2.723679	0.483779
C	-1.720576	3.800457	-0.008215
H	-2.800484	3.779837	0.099283
C	-1.130967	4.919972	-0.585123
H	-1.751070	5.729952	-0.957466
C	0.256408	5.001490	-0.635011
H	0.747748	5.877670	-1.047642
C	1.017492	3.965627	-0.103266
H	2.094455	4.086835	-0.068848
C	0.443339	2.805641	0.439581
C	1.342832	1.803376	1.129908
H	0.853043	1.477108	2.050342
H	2.255872	2.318117	1.444823
C	3.066727	0.730232	-1.081687
C	3.935391	1.950928	-0.745394
H	4.581956	1.789777	0.117840
H	3.348732	2.850589	-0.573914
H	4.584161	2.154445	-1.605778
C	2.153507	1.079575	-2.270899
H	1.594299	0.206028	-2.620874
H	2.771407	1.438906	-3.102854
H	1.437857	1.868465	-2.022514
C	4.011816	-0.403449	-1.502262
H	3.489145	-1.324856	-1.752028
H	4.757946	-0.625441	-0.735015
H	4.556794	-0.077811	-2.396651
C	2.865129	-0.583797	1.791234
C	1.952360	-0.594821	3.029754
H	1.813195	0.396284	3.468742
H	2.418621	-1.223196	3.797348
H	0.971304	-1.024739	2.807557
C	4.160153	0.159623	2.148298
H	3.997179	1.220280	2.361236
H	4.921292	0.072303	1.369137
H	4.578004	-0.289547	3.057527
C	3.192318	-2.046873	1.461801
H	3.803971	-2.159270	0.566644
H	2.279571	-2.633858	1.324303
H	3.745148	-2.480010	2.304114

11 ` .MeOH (PCM)

scf done: -2175.137305

Pd	0.752255	-0.443897	0.138366
P	-1.279007	-1.586606	0.366534
P	0.097903	1.967821	0.498207
C	1.706289	-1.939992	-0.787384
C	2.466893	-3.072166	-0.123257
H	2.799430	-2.732523	0.861710
H	1.731040	-3.856769	0.082461
C	3.618199	-3.622885	-0.959903
H	4.108943	-4.438610	-0.421718
H	4.363517	-2.850253	-1.165977
H	3.258696	-4.010903	-1.916382
O	1.845962	-1.686024	-1.970737
C	-2.735484	-0.442627	0.693627
H	-3.572219	-1.105369	0.937086
H	-2.456530	0.038552	1.632673
C	-3.226623	0.620708	-0.260718
C	-4.297748	0.339415	-1.123468
H	-4.707890	-0.664000	-1.153981
C	-4.885316	1.314793	-1.922287
H	-5.710859	1.052178	-2.577240
C	-4.428154	2.627536	-1.845189
H	-4.886826	3.411800	-2.440227
C	-3.389895	2.931423	-0.972150
H	-3.057013	3.962492	-0.885322
C	-2.764093	1.950921	-0.186181
C	-1.701077	2.405653	0.778852
H	-1.917302	2.028584	1.786035
H	-1.752388	3.494085	0.853373
H	4.378274	-1.135898	1.280917
C	3.750024	-0.287639	1.569183
H	4.393361	0.520179	1.934947

H	3.078963	-0.595803	2.372098
O	2.958054	0.172116	0.471374
H	3.510338	0.139828	-0.352391
H	5.877332	1.114484	-1.822174
C	5.176150	0.644084	-2.513316
H	4.584147	1.423907	-3.004524
H	5.743190	0.090458	-3.268819
O	4.358745	-0.236925	-1.744947
H	3.726485	-0.689604	-2.321452
C	0.844779	2.822629	2.053104
C	0.572160	2.903247	-1.105063
C	-1.299002	-2.564310	2.026072
C	-1.825754	-2.674596	-1.110781
C	-1.653559	-1.785053	-2.356767
H	-0.614095	-1.470732	-2.481092
H	-2.283878	-0.893379	-2.322044
H	-1.941694	-2.362762	-3.243378
C	-3.280122	-3.168070	-1.024170
H	-3.408539	-3.956773	-0.282276
H	-3.552425	-3.590769	-1.998136
H	-4.000335	-2.381593	-0.805204
C	-0.939327	-3.916885	-1.276804
H	0.107396	-3.668824	-1.450711
H	-1.284268	-4.461772	-2.163686
H	-1.010081	-4.605915	-0.431352
C	-2.530106	-3.465814	2.199790
H	-2.536312	-3.839805	3.230582
H	-2.499731	-4.338493	1.543347
H	-3.477035	-2.942346	2.042844
C	-0.036717	-3.423829	2.149440
H	0.865240	-2.808122	2.121292
H	0.031308	-4.188716	1.373712
H	-0.059552	-3.942842	3.114780
C	-1.263849	-1.544412	3.179422
H	-0.475466	-0.799259	3.039599
H	-1.047894	-2.084493	4.108378
H	-2.217331	-1.030799	3.325191
C	-0.226840	2.266318	-2.257628
H	-0.081231	1.181484	-2.291945
H	0.139195	2.682422	-3.204293
H	-1.296252	2.465930	-2.197914
C	0.281432	4.408302	-1.041383
H	0.935118	4.924662	-0.333148
H	-0.755983	4.632199	-0.778582
H	0.465056	4.846784	-2.029990
C	2.057008	2.694564	-1.445730
H	2.285956	1.639746	-1.613152
H	2.738728	3.080228	-0.688938
H	2.266874	3.226237	-2.382080
C	0.113111	4.103128	2.490959
H	0.664786	4.540264	3.332095
H	-0.903068	3.909934	2.844005
H	0.068637	4.860139	1.704469
C	2.327768	3.161507	1.846247
H	2.886970	2.320764	1.432493
H	2.765593	3.421402	2.817716
H	2.459665	4.028544	1.193149
C	0.730172	1.794948	3.191740
H	1.288155	0.880762	2.972142
H	-0.308962	1.521509	3.401160
H	1.141624	2.229854	4.110827

TS14-7a .MeOH (PCM)

scf done: -2175.116763

Pd	-0.476206	-0.091249	-0.061248
P	0.282901	1.993859	0.496410
P	0.920556	-1.964853	0.258260
C	-3.118280	-0.005940	-1.251748
C	-2.631873	0.256272	-2.638535
H	-2.651347	1.324459	-2.857545
H	-1.589755	-0.075128	-2.674124
C	-3.466354	-0.525645	-3.672565
H	-3.054335	-0.339747	-4.666947
H	-4.513598	-0.212227	-3.674268
H	-3.424355	-1.598983	-3.474348
O	-2.833302	-1.135386	-0.717712
C	-0.471659	2.703139	2.127108

C	-0.763961	1.484743	3.020317	O	-4.054546	-1.661246	1.364255
H	0.141840	0.925725	3.274391	H	-3.364176	-1.322458	0.191788
H	-1.462460	0.794396	2.535609				
H	-1.211553	1.827598	3.962163	11 \ . 2MeOH (PCM)			
C	0.432801	3.666306	2.913082	scf done: -2290.838283			
H	1.334452	3.176862	3.290875	Pd	0.649849	-0.207215	-0.493307
H	-0.121079	4.032955	3.786601	P	0.014513	2.044989	-0.268267
H	0.735890	4.539395	2.330759	P	-1.600701	-1.408729	-0.619746
C	-1.808480	3.402051	1.844576	C	2.572615	0.218562	-0.870204
H	-2.457109	2.802215	1.198368	C	2.935358	0.036256	-2.344497
H	-1.672230	4.385753	1.389073	H	2.360903	-0.810035	-2.739384
H	-2.337749	3.557661	2.793040	H	2.549786	0.910095	-2.879069
C	0.412961	3.366872	-0.838802	C	4.429406	-0.130410	-2.605922
C	-0.988715	3.728146	-1.350223	H	4.605650	-0.236594	-3.679930
H	-1.537563	2.823100	-1.625813	H	4.829232	-1.016518	-2.106403
H	-0.892908	4.348096	-2.249992	H	4.989753	0.737941	-2.250033
H	-1.581761	4.288548	-0.626696	O	3.450423	0.345998	-0.038758
C	1.126664	4.648911	-0.393527	C	-1.843903	2.331042	-0.285957
H	0.544195	5.201499	0.348758	H	-1.945874	3.418089	-0.243481
H	1.257038	5.310272	-1.259454	H	-2.132202	2.051071	-1.304239
H	2.120648	4.463188	0.022817	C	-2.839878	1.755957	0.693204
C	1.155366	2.735798	-2.031029	C	-3.278064	2.570745	1.749446
H	0.636855	1.838256	-2.385223	H	-2.816286	3.542454	1.894975
H	2.183549	2.460109	-1.796408	C	-4.312172	2.193203	2.599229
H	1.180191	3.459139	-2.855968	H	-4.617960	2.851358	3.407124
C	2.056843	1.763481	1.117301	C	-4.974506	0.990723	2.370250
H	2.426120	2.745067	1.428669	H	-5.813396	0.691460	2.991706
H	1.912845	1.185069	2.036794	C	-4.572212	0.185049	1.310455
C	3.132118	1.115594	0.275422	H	-5.135719	-0.718347	1.098608
C	4.053271	1.977781	-0.346355	C	-3.492997	0.523815	0.480094
H	3.913080	3.050186	-0.237285	C	-3.159555	-0.370427	-0.684908
C	5.146608	1.518405	-1.070900	H	-3.036772	0.238824	-1.584723
H	5.828717	2.225213	-1.534805	H	-4.002256	-1.039897	-0.881768
C	5.369316	0.146934	-1.159359	H	3.625325	-2.405954	-0.474118
H	6.230493	-0.244538	-1.693375	C	2.673240	-2.929900	-0.607892
C	4.492997	-0.721693	-0.519473	H	2.751170	-3.930877	-0.171072
H	4.710186	-1.785403	-0.539621	H	2.464886	-3.034534	-1.673211
C	3.361117	-0.279870	0.187704	O	1.591273	-2.224716	-0.001486
C	2.557926	-1.317936	0.937674	H	1.758778	-2.196745	0.990659
H	2.258952	-0.896187	1.900908	H	1.454964	-4.015617	3.090902
H	3.209116	-2.170970	1.159335	C	2.305234	-3.352388	3.262699
C	1.354433	-2.935175	-1.335728	H	2.387882	-3.166914	4.339770
C	2.594920	-3.836386	-1.270142	H	3.217846	-3.855071	2.919303
H	2.477739	-4.666516	-0.572553	O	2.063800	-2.142464	2.555150
H	3.495866	-3.286890	-0.993564	H	2.824796	-1.520804	2.686831
H	2.773494	-4.267180	-2.263737	C	-1.681442	-2.218415	-2.360037
C	1.576332	-1.865896	-2.421552	C	-1.944061	-2.710607	0.744086
H	0.692446	-1.229401	-2.536098	C	0.470291	0.185629	-1.747063
H	1.771542	-2.361556	-3.381276	C	0.604040	2.752624	1.409880
H	2.428697	-1.220126	-2.196109	C	5.381105	-0.715980	2.787481
C	0.144729	-3.786696	-1.751254	H	6.051364	0.135927	2.625771
H	-0.786516	-3.210563	-1.740807	H	5.668763	-1.527952	2.108470
H	0.018422	-4.664393	-1.111639	H	5.501987	-1.061695	3.816184
H	0.300538	-4.151701	-2.774315	O	4.018740	-0.336205	2.621756
C	0.448569	-3.185176	1.668364	H	3.889042	-0.022726	1.708212
C	0.515105	-2.408145	2.996162	C	-1.542914	-2.031996	2.066408
H	1.541266	-2.230788	3.330106	H	-2.103428	-1.108871	2.241532
H	0.020073	-2.999485	3.776129	H	-0.474710	-1.800642	2.094936
H	-0.002831	-1.445495	2.930128	H	-1.761263	-2.714619	2.897427
C	1.333144	-4.432317	1.791880	C	-3.409900	-3.156230	0.840062
H	2.399101	-4.191493	1.850384	H	-3.791033	-3.579648	-0.090792
H	1.180522	-5.130654	0.965070	H	-4.069588	-2.346761	1.149376
H	1.070662	-4.966578	2.714187	H	-3.479986	-3.936907	1.607447
C	-1.013163	-3.616862	1.473123	C	-1.076891	-3.964006	0.551816
H	-1.173112	-4.171730	0.546768	H	-0.025025	-3.716976	0.404374
H	-1.685375	-2.755185	1.473150	H	-1.418205	-4.578237	-0.285884
H	-1.307026	-4.271996	2.303219	H	-1.161530	-4.580629	1.455434
H	-4.935680	1.772301	-2.177743	C	-2.864353	-3.177337	-2.552341
C	-4.526541	1.940822	-1.181364	H	-2.891366	-3.492700	-3.602772
H	-5.317068	2.245196	-0.499453	H	-3.829078	-2.710880	-2.332602
H	-3.737795	2.693061	-1.200048	H	-2.769098	-4.081707	-1.947220
O	-4.018901	0.705803	-0.628182	C	-1.793860	-1.090097	-3.402192
H	-4.024855	-0.952494	2.020696	H	-1.053114	-0.301739	-3.236987
H	-5.793018	-2.479581	2.155919	H	-2.788296	-0.636774	-3.428486
C	-5.412198	-2.112076	1.201115	H	-1.608991	-1.513865	-4.396317
H	-5.384820	-2.930554	0.482164	C	-0.372317	-2.971607	-2.645303
H	-6.050829	-1.308999	0.824174	H	0.479094	-2.286675	-2.674329

H	-0.446554	-3.442488	-3.633133	C	-4.362541	1.586056	-0.538051
H	-0.157242	-3.755146	-1.918129	H	-4.352089	2.668005	-0.628443
C	0.073664	1.784597	2.483862	C	-3.342023	0.962876	0.200411
H	0.443351	0.768309	2.313373	C	-2.334697	1.854405	0.888740
H	-1.015510	1.751465	2.530900	H	-2.144948	1.458741	1.890255
H	0.442015	2.116040	3.462155	H	-2.786567	2.842798	1.029287
C	0.096215	4.178663	1.671538	C	-0.819230	3.006068	-1.468216
H	0.628863	4.915424	1.064602	C	-1.860645	4.132545	-1.506728
H	0.291475	4.426834	2.721448	H	-1.595564	4.981415	-0.875567
H	-0.973706	4.307635	1.503973	H	-2.855393	3.791700	-1.217932
C	2.133114	2.769522	1.533031	H	-1.936212	4.504599	-2.536687
H	2.561701	1.776613	1.415729	C	-1.237900	1.920629	-2.477454
H	2.380825	3.128562	2.539220	H	-0.500903	1.111626	-2.516133
H	2.613686	3.441947	0.821824	H	-1.312100	2.367498	-3.477445
C	1.968939	3.527284	-1.734292	H	-2.208977	1.483130	-2.231429
H	2.614557	2.675856	-1.512737	C	0.536445	3.573416	-1.918114
H	2.191646	4.314490	-1.009855	H	1.330048	2.822254	-1.869894
H	2.251762	3.908492	-2.722189	H	0.837235	4.443883	-1.328279
C	-0.306623	4.515422	-1.790716	H	0.452471	3.905050	-2.961061
H	0.106732	5.116466	-2.609079	C	0.079992	3.313713	1.528918
H	-0.205506	5.102520	-0.876307	C	-0.188274	2.698334	2.914640
H	-1.369064	4.379360	-2.005115	H	-1.233017	2.795660	3.221868
C	0.118321	2.404613	-3.025776	H	0.417863	3.225945	3.660897
H	0.608745	1.430400	-3.072146	H	0.085954	1.638439	2.954102
H	0.435603	2.988241	-3.897716	C	-0.526896	4.721759	1.502916
H	-0.958916	2.240915	-3.122683	H	-1.620449	4.711153	1.537017
TS14-7a.2MeOH (PCM)				H	-0.211810	5.289234	0.623977
scf done: -2290.819091				H	-0.180058	5.275835	2.384679
Pd	0.418870	-0.052641	-0.134754	C	1.601880	3.419243	1.363480
P	-0.813706	-1.863967	0.605838	H	1.899904	3.821355	0.393491
P	-0.593596	2.089945	0.201718	H	2.074325	2.442018	1.481250
C	2.495769	-0.724620	-1.786643	H	2.006421	4.084134	2.137107
C	1.891532	-1.297909	-3.037452	H	3.963020	-2.939664	-2.399077
H	1.741626	-2.375451	-2.950516	C	3.747383	-2.745766	-1.346913
H	0.911957	-0.834351	-3.164065	H	4.631470	-2.957862	-0.748173
C	2.773643	-0.973799	-4.257733	H	2.917379	-3.366149	-1.004115
H	2.303433	-1.374610	-5.159186	O	3.461044	-1.358098	-1.118340
H	3.772005	-1.412003	-4.173244	H	6.068824	1.559555	0.426916
H	2.883560	0.107031	-4.377405	C	5.430878	1.180412	-0.369952
O	2.365626	0.503534	-1.523504	H	5.583137	1.763111	-1.277232
C	-0.133892	-2.694950	2.205573	H	5.625572	0.123081	-0.554042
C	-0.190453	-1.649548	3.335163	O	4.056346	1.377043	0.040750
H	-1.202033	-1.516057	3.728525	H	3.342301	1.009974	-0.671534
H	0.179150	-0.671297	3.008113	H	4.596010	0.517946	3.518117
H	0.438346	-1.987135	4.167631	C	3.512723	0.474196	3.405506
C	-0.890530	-3.943837	2.675666	H	3.110966	-0.289801	4.074578
H	-1.967527	-3.775944	2.770805	H	3.080466	1.448544	3.649201
H	-0.518421	-4.233327	3.666834	O	3.256275	0.114203	2.038950
H	-0.729754	-4.796948	2.012425	H	2.299045	0.027604	1.875007
C	1.341538	-3.062587	1.980752	H	3.822341	0.884393	0.924636
H	1.937638	-2.189258	1.701341	TS17-7a (PCM)			
H	1.472119	-3.819521	1.204434	scf done: -2059.392099			
H	1.756353	-3.471986	2.910498	Pd	-0.037367	-0.619151	-0.030028
C	-1.319157	-3.226165	-0.653159	C	0.194423	-3.150261	-0.897092
C	-0.089719	-4.076018	-0.995306	C	-0.682376	-3.747776	0.153187
H	0.767251	-3.442864	-1.240241	H	-0.090497	-3.778178	1.071633
H	-0.308812	-4.698358	-1.871677	H	-1.549754	-3.110299	0.321032
H	0.195412	-4.747472	-0.181101	C	-1.111995	-5.163866	-0.269629
C	-2.455418	-4.172965	-0.236895	H	-1.731306	-5.588699	0.523786
H	-2.157839	-4.868471	0.548858	H	-0.244142	-5.810379	-0.418177
H	-2.747355	-4.774355	-1.107183	H	-1.700276	-5.141054	-1.189923
H	-3.349321	-3.649057	0.103074	O	1.288274	-3.389197	-1.274227
C	-1.738987	-2.473744	-1.929101	P	-2.101807	0.350290	0.338424
H	-0.949325	-1.794253	-2.262251	P	2.152272	0.095548	0.372918
H	-2.649649	-1.888081	-1.786280	C	-3.066302	-0.290518	1.870654
H	-1.927977	-3.199377	-2.730466	C	-2.015579	-0.877500	2.831250
C	-2.463312	-1.219883	1.271327	H	-1.292788	-0.129776	3.171756
H	-3.008012	-2.064908	1.706937	H	-1.460129	-1.702227	2.375563
H	-2.156916	-0.586124	2.107320	H	-2.527198	-1.262402	3.722054
C	-3.410339	-0.440368	0.385786	C	-3.858544	0.788840	2.627460
C	-4.502657	-1.125734	-0.172915	H	-3.210452	1.542914	3.081219
H	-4.602240	-2.189667	0.015705	H	-4.407354	0.305953	3.445174
C	-5.482308	-0.495504	-0.931769	H	-4.592971	1.297488	1.999618
H	-6.305245	-1.072300	-1.344227	C	-4.031393	-1.416534	1.471321
C	-5.409995	0.881486	-1.119897	H	-3.567515	-2.161184	0.816952
H	-6.174747	1.408854	-1.682981	H	-4.926775	-1.033125	0.976404

H	-4.362790	-1.935922	2.378240
C	-3.274510	0.810282	-1.097385
C	-3.897768	-0.460483	-1.699322
H	-3.143016	-1.204762	-1.968555
H	-4.424122	-0.183851	-2.620601
H	-4.622887	-0.936914	-1.039829
C	-4.396586	1.781598	-0.710259
H	-5.133556	1.314868	-0.051128
H	-4.927662	2.096277	-1.616815
H	-4.024189	2.686353	-0.222553
C	-2.393985	1.441782	-2.190446
H	-1.562069	0.785526	-2.468298
H	-1.972296	2.401608	-1.891912
H	-3.006745	1.606090	-3.084957
C	-1.442148	1.974429	1.071148
H	-2.315007	2.567244	1.362851
H	-0.980977	1.635256	2.004275
C	-0.491301	2.893977	0.334150
C	-1.076913	4.003264	-0.303210
H	-2.159471	4.099216	-0.281607
C	-0.334078	4.995680	-0.929528
H	-0.835655	5.831511	-1.408505
C	1.055447	4.918428	-0.896277
H	1.668211	5.693149	-1.347953
C	1.656088	3.851101	-0.240552
H	2.739033	3.834464	-0.166786
C	0.925650	2.813447	0.366468
C	1.720323	1.778161	1.136664
H	1.169002	1.499081	2.038090
H	2.652456	2.242760	1.478236
C	3.323651	0.426279	-1.092014
C	4.441244	1.444979	-0.827826
H	5.164061	1.096552	-0.088887
H	4.058421	2.411371	-0.496957
H	4.987422	1.616718	-1.763501
C	2.431630	0.942498	-2.236343
H	1.649876	0.219201	-2.488255
H	3.052057	1.100345	-3.127296
H	1.947849	1.890891	-1.991385
C	3.956495	-0.899269	-1.544968
H	3.210591	-1.686511	-1.686050
H	4.714191	-1.258294	-0.843295
H	4.458338	-0.737107	-2.506804
C	3.066763	-0.749974	1.827945
C	2.176068	-0.604805	3.075602
H	2.205237	0.403575	3.497321
H	2.540866	-1.289695	3.850100
H	1.133256	-0.867086	2.862922
C	4.455349	-0.179511	2.141381
H	4.441863	0.905246	2.284893
H	5.185473	-0.419272	1.364214
H	4.820952	-0.626886	3.074132
C	3.183673	-2.252439	1.522133
H	3.782934	-2.462956	0.634605
H	2.198496	-2.705205	1.380622
H	3.664631	-2.750930	2.372667
C	-0.235585	-2.460605	-3.385514
H	0.758471	-2.016591	-3.357140
H	-0.196935	-3.486131	-3.746028
H	-0.921016	-1.865119	-3.985549
O	-0.802299	-2.514101	-2.043407
H	-0.906485	-1.580569	-1.631386
