

Insight into the Electronic Effect of Phosphine Ligand on Rh Catalyzed CO₂ Hydrogenation by Investigating the Reaction Mechanism

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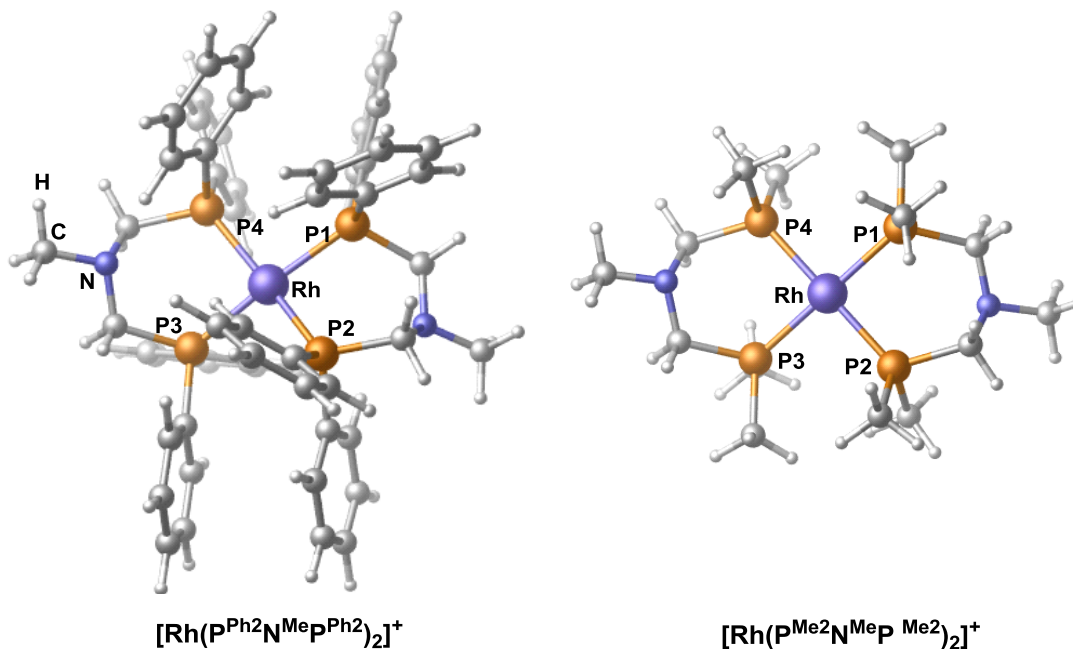
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Complete Reference 44

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

Table S1. Selected bond distances (Å) and angles (°) for catalyst $[\text{Rh}(\text{PN}^{\text{Me}}\text{P})_2]^+$ from both experimental and theoretical investigations.



Parameters	$[\text{Rh}(\text{P}^{\text{Ph}_2\text{N}^{\text{Me}}\text{P}^{\text{Ph}_2})_2]^+$		$[\text{Rh}(\text{P}^{\text{Me}_2\text{N}^{\text{Me}}\text{P}^{\text{Me}_2})_2]^+$	
	Experimental ^a	Theoretical	Theoretical	
Bond (Å)	Rh-P1	2.3268	2.358	2.3416
	Rh-P2	2.3405	2.349	2.3443
	Rh-P3	2.3268	2.350	2.3416
	Rh-P4	2.3405	2.357	2.3443
Angle (°)	P1-Rh-P2	88.02	85.87	87.02
	P2-Rh-P3	91.98	94.75	92.97
	P3-Rh-P4	88.02	86.82	87.02
	P4-Rh-P5	91.98	94.80	92.97
	P1-Rh-P3	180.00	171.31	179.99
	P2-Rh-P4	180.00	166.23	179.99
Dihedral (°)	P1-P2-P3-P4	0.00	-17.03	0.002

^a ref. 42

Table S2. The ΔE_{gas} , ΔG_{gas} , and, ΔE_{sol} of the species involved in the **A1** catalyzed CO_2 hydrogenation.

Species	ΔE_{gas}	ΔG_{gas}	ΔE_{sol}
A1	0.0	0.0	0.0
A1-H₂	-1.1	8.7	8.6
A2	-11.3	0.3	-11.5
A3	-28.8	-1.4	-21.8
A4	-16.7	12.3	-18.7
A5	3.7	15.8	-6.0
A6	0.5	20.5	-8.0
A7	-11.2	17.3	-27.8
A8	-0.3	22.6	-8.1
A9	-2.8	24.7	-23.0
A10	-13.3	8.1	-12.6
A11	-15.9	11.7	-18.6
A12	177.8	187.8	23.3
A13	-33.8	9.5	-30.2
A14	-38.5	3.4	-43.4
A7'	7.9	21.7	-12.9
A8'	9.1	25.4	-13.1
TSA1-2	-0.8	8.6	-0.7
TSA3-4	-1.0	25.9	2.2
TSA6-7	9.5	32.3	-1.5
TSA8-9	3.3	29.2	-6.1
TSA9-7	10.3	36.5	-6.9
TSA10-11	23.7	47.6	11.2
TSA13-14	-11.0	30.6	-9.2
TSA7-8'	18.8	38.8	2.4

Table S3. The ΔE_{gas} , ΔG_{gas} , and, ΔE_{sol} of the species involved in the **B1** catalyzed CO₂ hydrogenation.

Species	ΔE_{gas}	ΔG_{gas}	ΔE_{sol}
B1	0.0	0.0	0.0
B1-H₂	-0.7	9.2	9.7
B2	-13.4	-2.6	-13.2
B3	-26.3	0.3	-20.0
B4	-13.4	16.7	-12.3
B5	6.7	18.3	-4.0
B6	3.2	24.2	-5.9
B7	-11.6	16.6	-29.1
B8	0.7	22.8	-7.6
B9	-1.9	25.2	-21.9
B10	-15.9	4.1	-14.6
B11	-8.2	16.0	-18.3
B12	178.2	188.3	24.6
B13	-24.9	14.6	-28.6
B14	-37.3	2.1	-41.9
B15	15.6	26.1	10.6
B16	-3.6	25.2	-3.2
B17	2.7	28.6	2.9
B18	11.9	33.8	8.5
B19	13.2	34.3	8.7
B20	11.0	34.0	10.1
B21	-14.0	15.2	-16.3
B22	-14.8	11.8	-19.7
B7'	7.7	22.4	-12.8
B8'	12.9	29.1	-8.9
TSB1-2	-0.6	8.9	-0.1
TSB2-15	16.0	24.0	10.4
TSB3-4	-8.5	18.1	-2.9
TSB6-7	11.2	33.9	-0.7
TSB8-9	4.0	29.3	-5.7
TSB9-7	10.8	35.1	-6.5
TSB10-11	22.2	47.7	10.7
TSB13-14	-7.9	34.3	-13.8
TSB16-21	6.0	33.2	10.2
TSB20-22	21.3	45.6	15.5
TSB7-8'	22.5	41.1	6.3

Table S4. The ΔE_{gas} , ΔG_{gas} , and, ΔE_{sol} of the species involved in the **C1** catalyzed CO_2 hydrogenation.

Species	ΔE_{gas}	ΔG_{gas}	ΔE_{sol}
C1	0.0	0.0	0.0
C1-H₂	-1.7	9.2	10.1
C2	-11.3	-0.3	-10.9
C3	-27.6	-1.7	-20.6
C4	-26.2	2.9	-27.1
C5	-7.6	4.3	-15.0
C6	-10.6	9.2	-16.9
C7	-20.7	6.3	-33.1
C8	-12.7	8.9	-18.1
C9	-13.1	14.8	-27.9
C10	-18.6	2.0	-16.7
C11	-8.5	16.4	-16.5
C12	185.8	195.1	31.7
C13	-23.9	14.9	-25.8
C14	-44.7	-2.9	-45.9
C7'	-0.3	10.0	-24.5
C8'	1.6	13.7	-23.3
TSC1-2	-1.2	9.2	-0.4
TSC3-4	-14.7	11.8	-8.4
TSC6-7	-1.9	20.5	-10.1
TSC8-9	-8.1	18.1	-14.4
TSC9-7	2.4	28.3	-8.7
TSC10-11	18.5	45.5	12.4
TSC13-14	-10.4	31.5	-14.2
TSC7-8'	14.9	26.5	-7.4

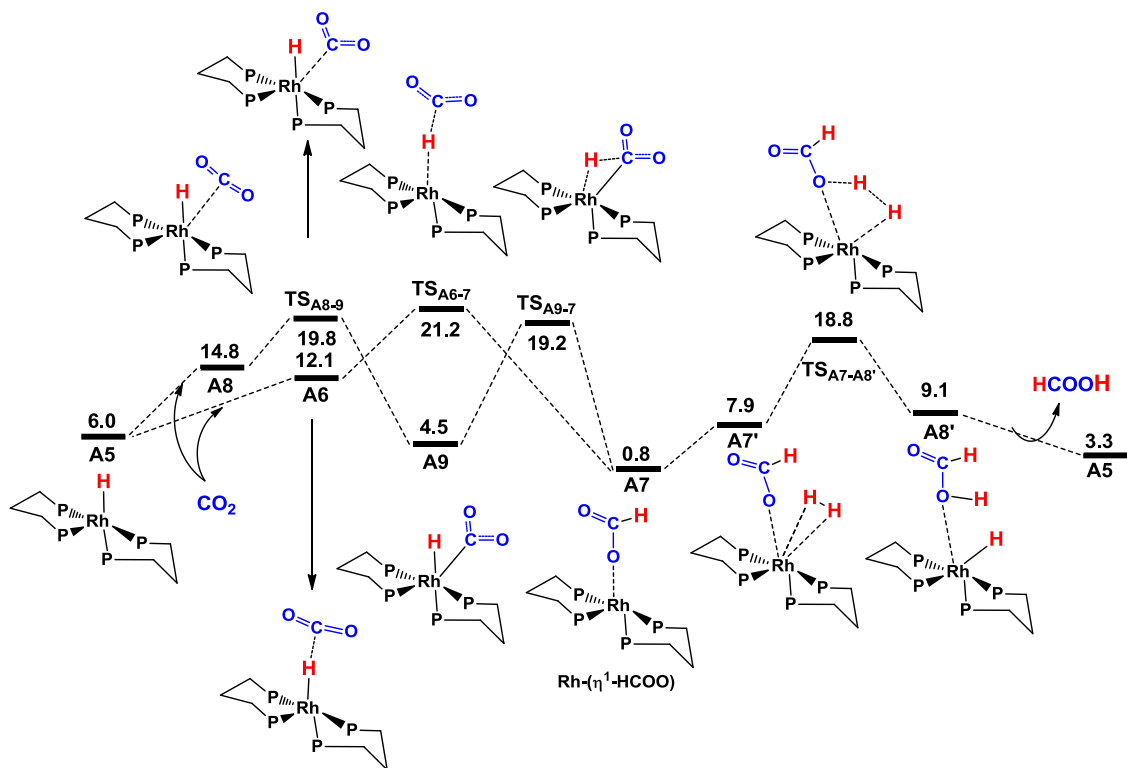


Figure S1. Solvent corrected free energy profile of the σ -bond metathesis route for A5 catalyzed CO_2 hydrogenation.

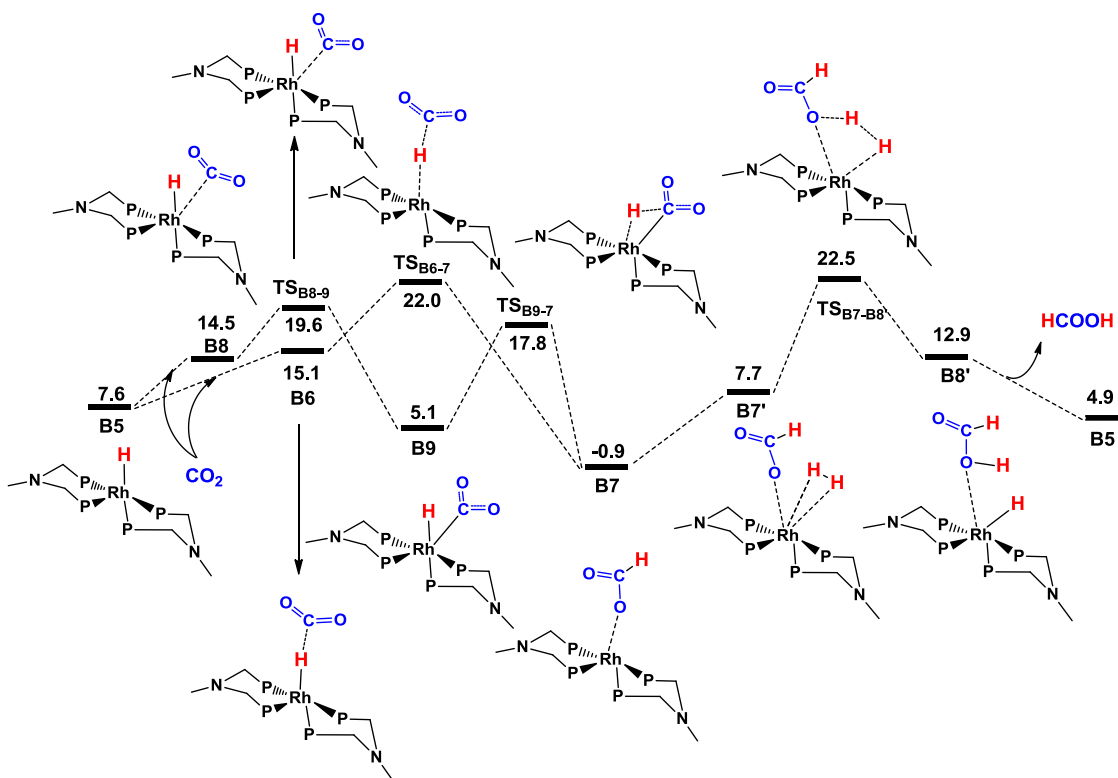


Figure S2. Solvent corrected free energy profile of the σ -bond metathesis route for **B5** catalyzed CO_2 hydrogenation.

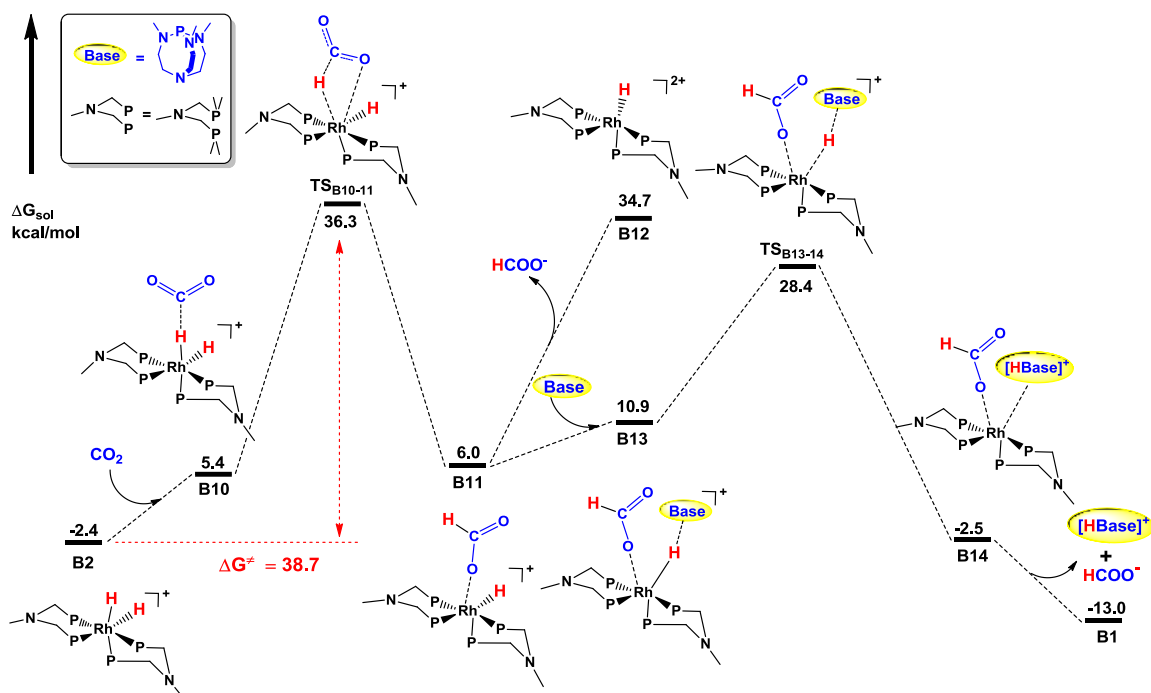


Figure S3. Solvent corrected free energy profile for $[\text{Rh}(\text{PCH}_2\text{N}^{\text{Me}}\text{CH}_2\text{P})_2]^+$ (**B1**) catalyzed CO_2 hydrogenation by the electrophilic attack of CO_2 to the hydride of the Rh dihydride complex.

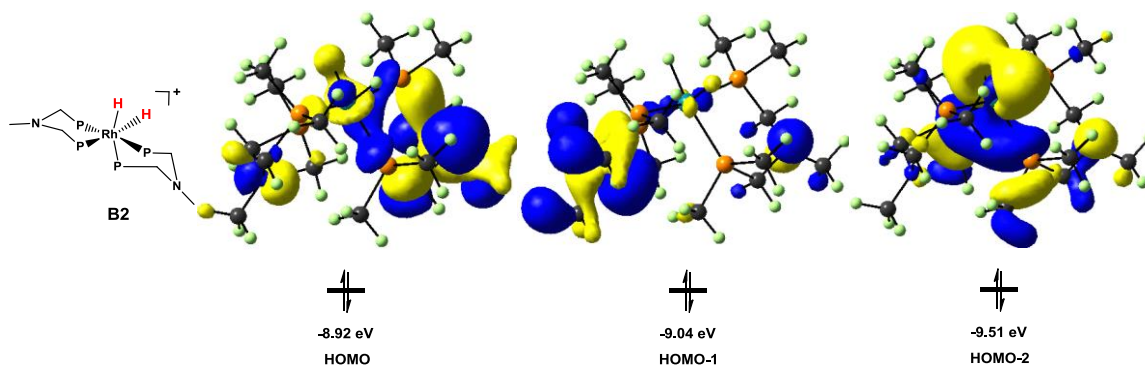


Figure S4. Skeleton diagrams and energies (in eV) of frontier molecular orbitals HOMO, HOMO-1, and HOMO-2 for **B2**.

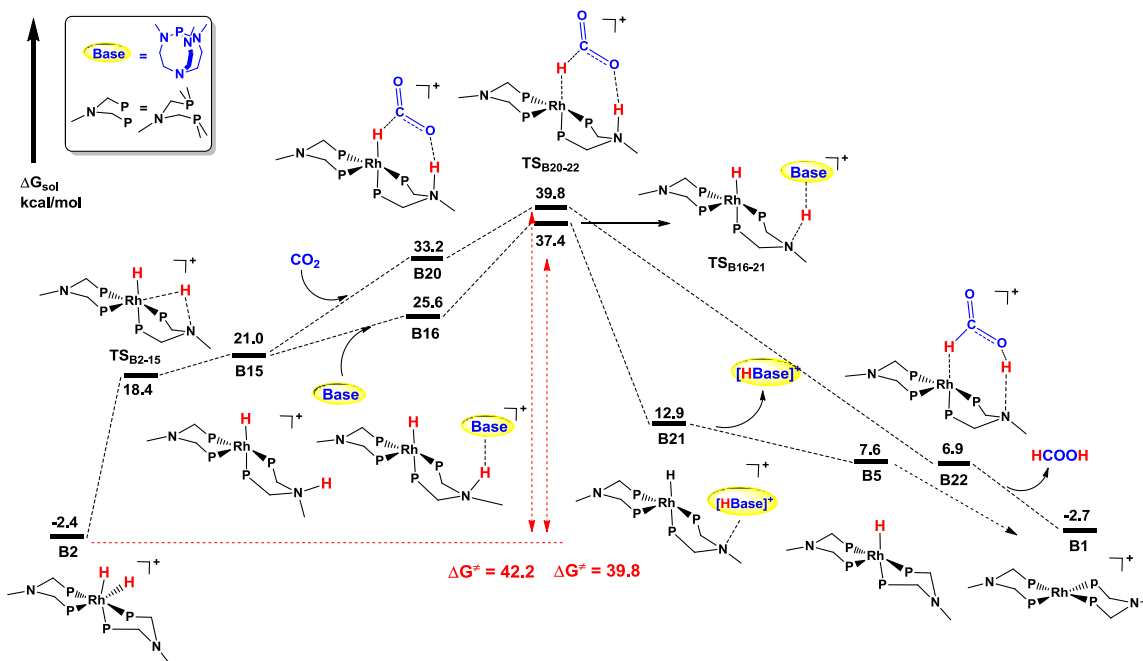


Figure S5. Selected Solvent corrected free energy profiles for outer sphere mechanism of CO₂ hydrogenation catalyzed by [Rh(PCH₂N^{Me}CH₂P)₂]⁺ (**B1**).

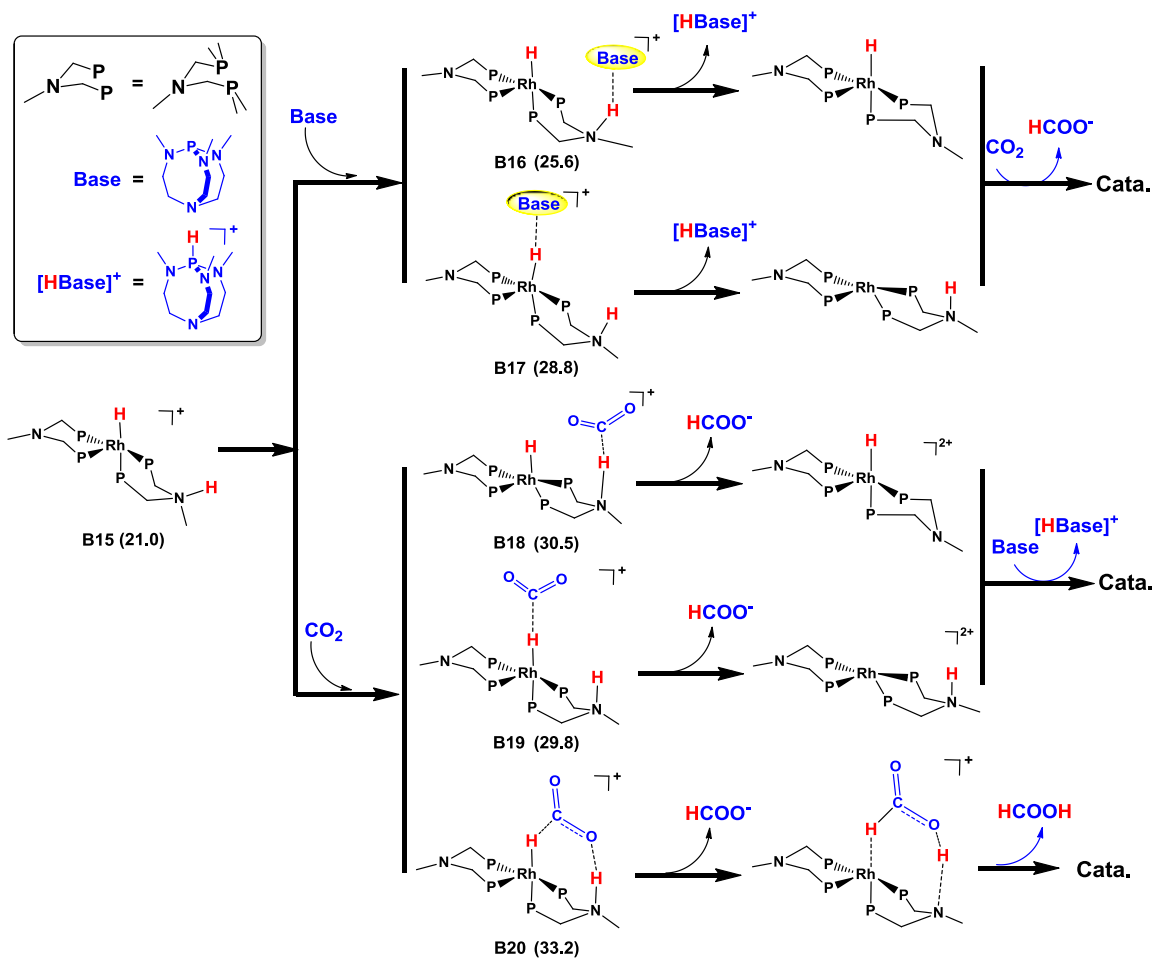


Figure S6. Outline of Proposed Outer Sphere Reaction Mechanism for CO₂ Hydrogenation Catalyzed by [Rh(PCH₂N^{Me}CH₂P)₂]⁺ (B1).

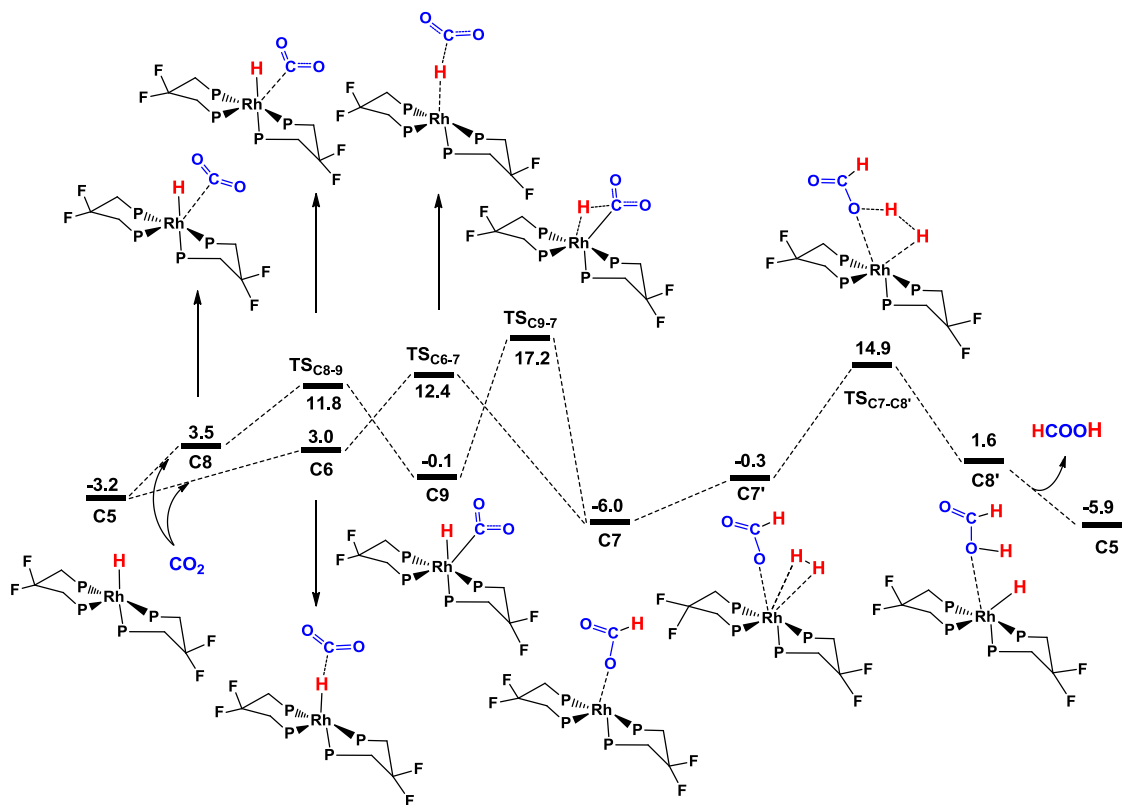


Figure S7. Solvent corrected free energy profile of the σ -bond metathesis route for **C5** catalyzed CO_2 hydrogenation.

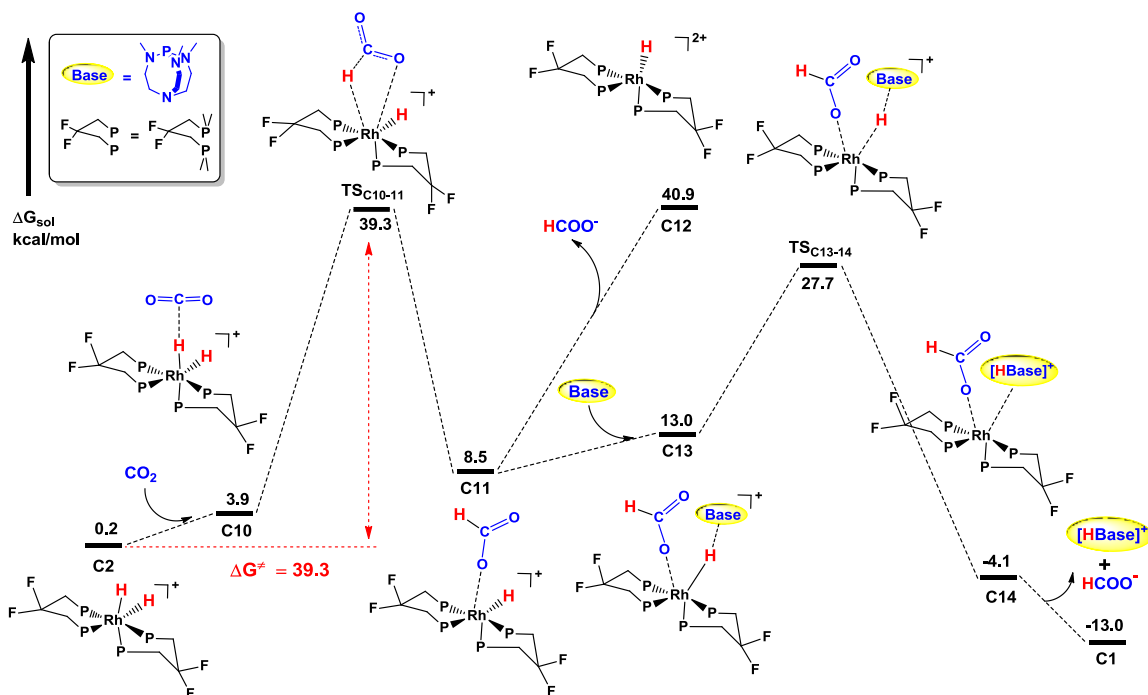


Figure S8. Solvent corrected free energy profile for $[\text{Rh}(\text{PCH}_2\text{CF}_2\text{CH}_2\text{P})_2]^+$ (C1) catalyzed CO₂ hydrogenation by the electrophilic attack of CO₂ to the hydride of the Rh dihydride complex.

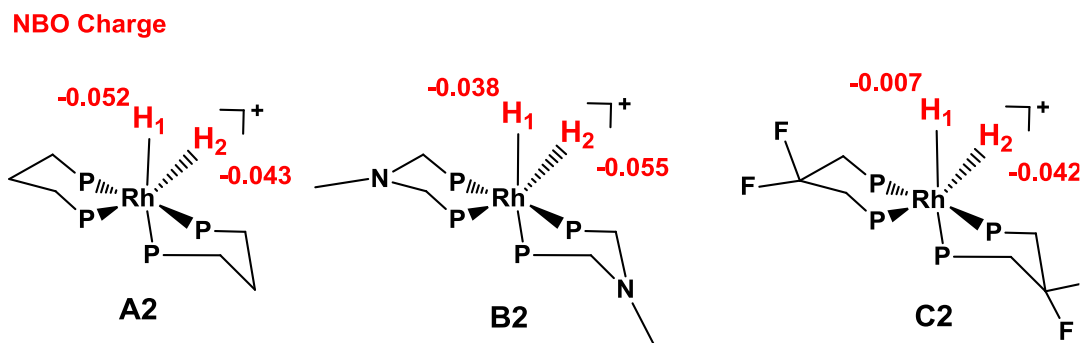
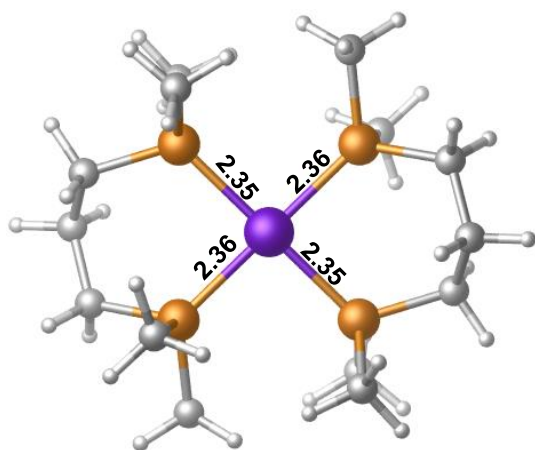
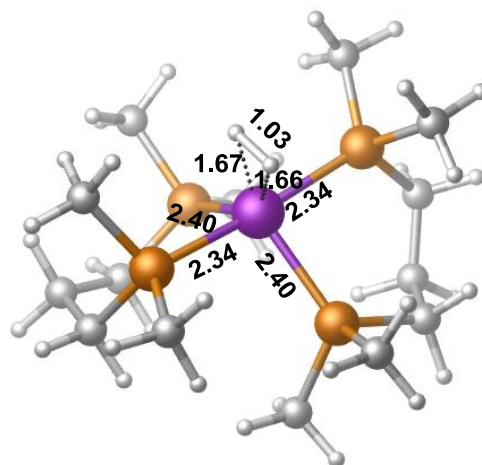


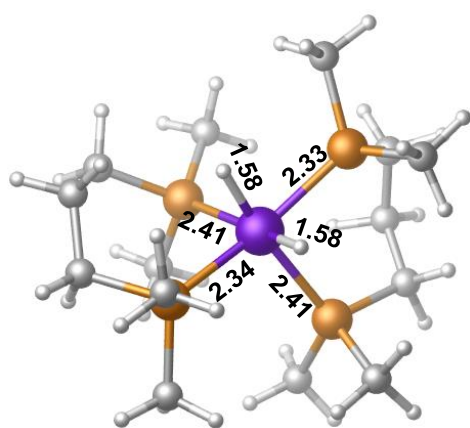
Figure S9. NBO charge distribution on metal H atoms and the selected bond length in **A2**, **B2** and **C2**.



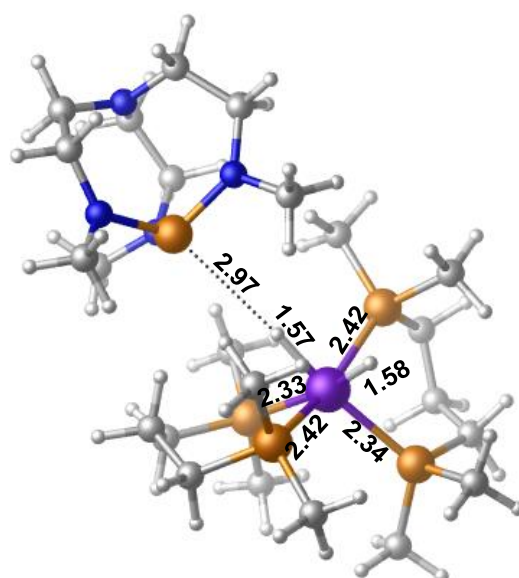
A1



TSA1-2

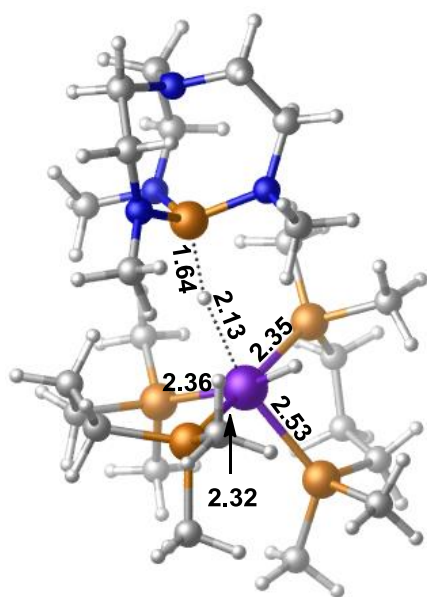


A2

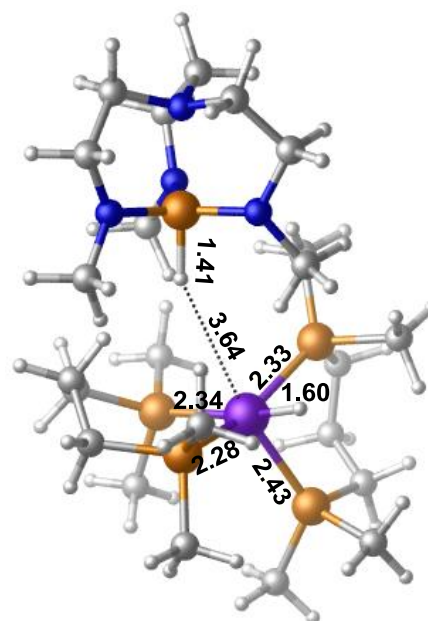


A3

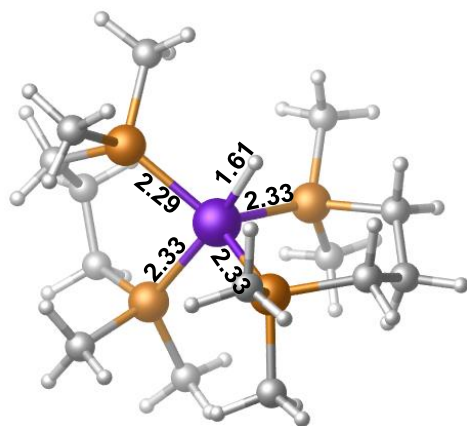
Figure S10 continued



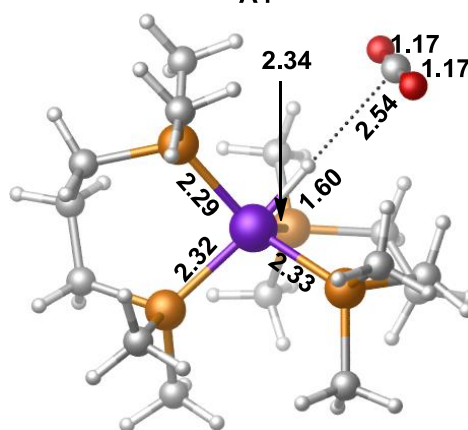
TSA3-4



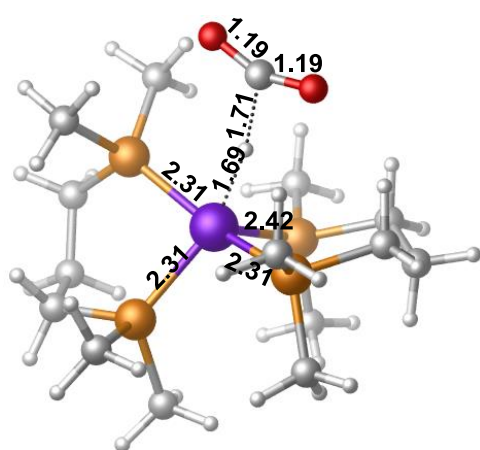
A4



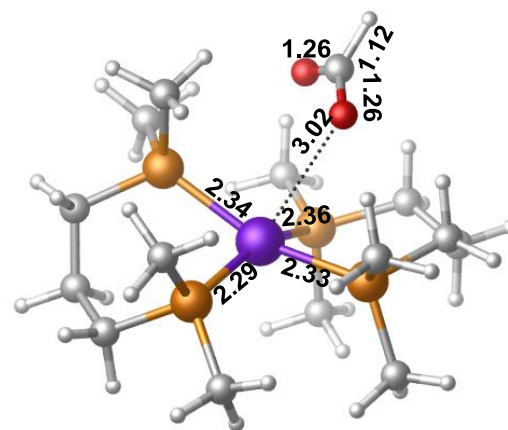
A5



A6



TSA6-7



A7

Figure S10 continued

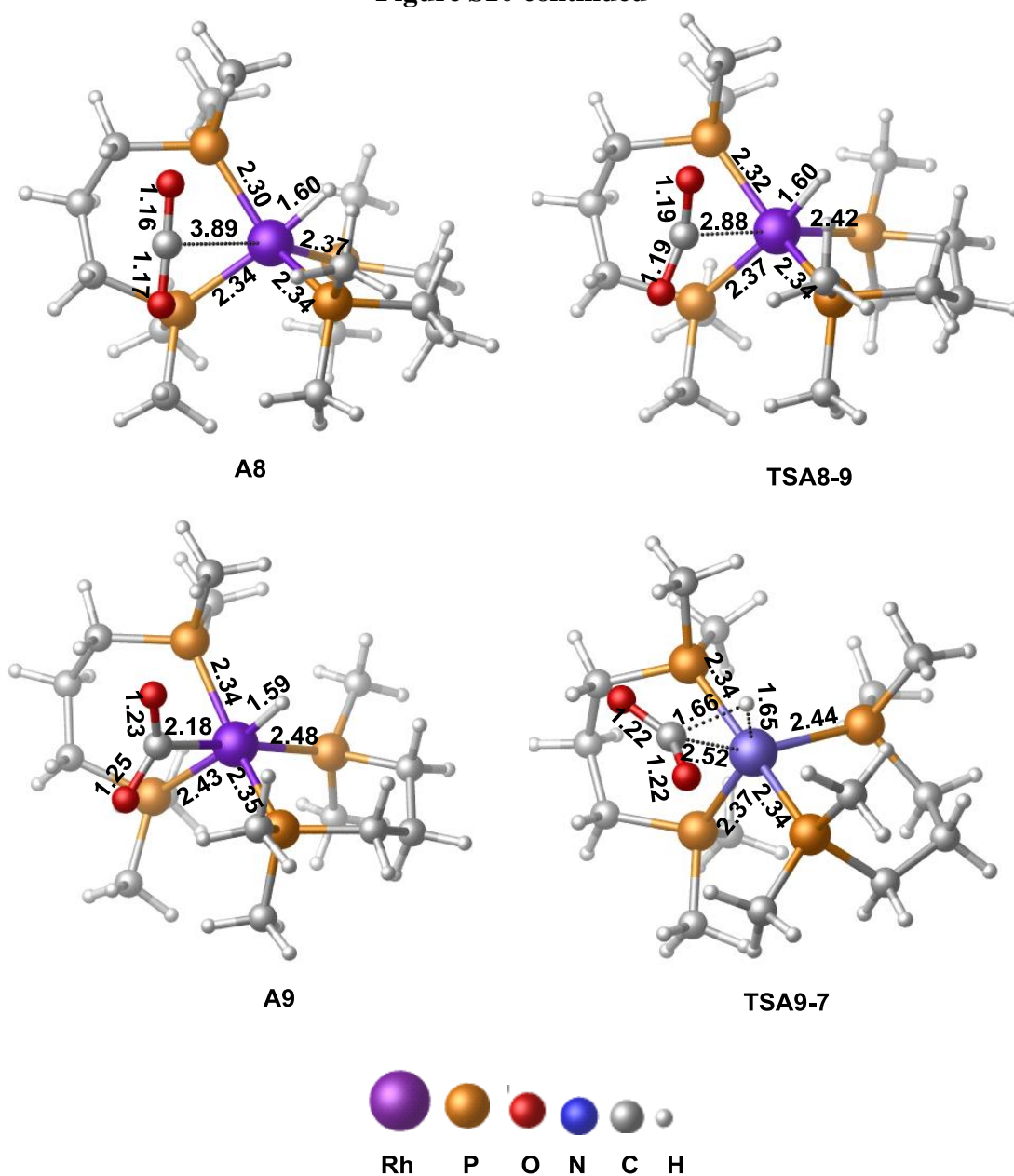


Figure S10. Optimized geometries with selected structural parameters (distances in Å) for the species involved in Figure 1 in the text.

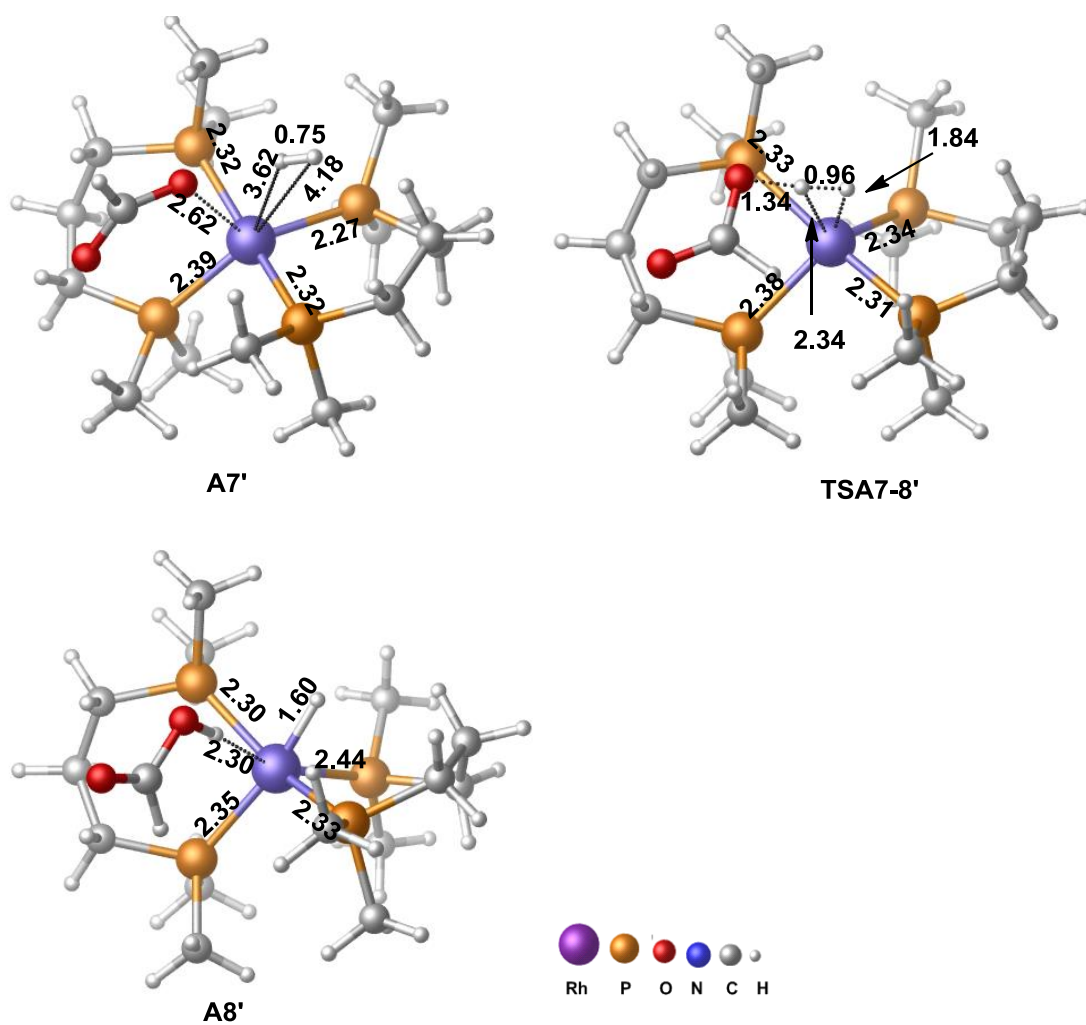
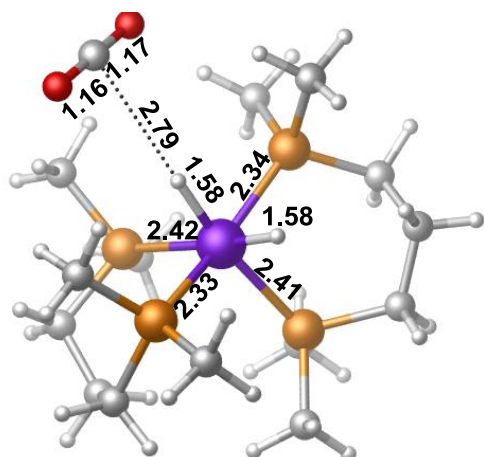
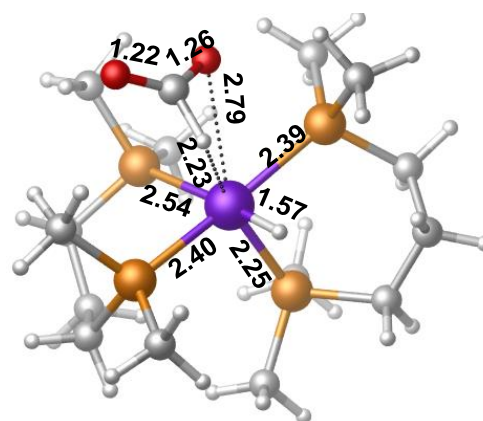


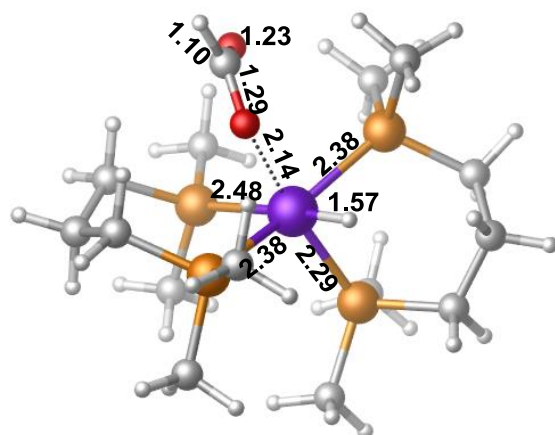
Figure S11. Optimized geometries with selected structural parameters (distances in Å) for the species involved in Figure S1 in the text.



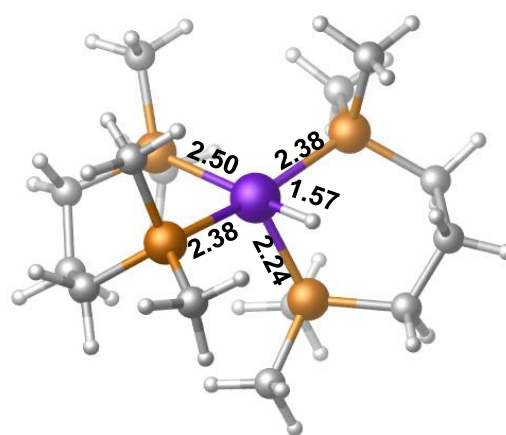
A10



TSA10-11



A11



A12

Figure S12 continued

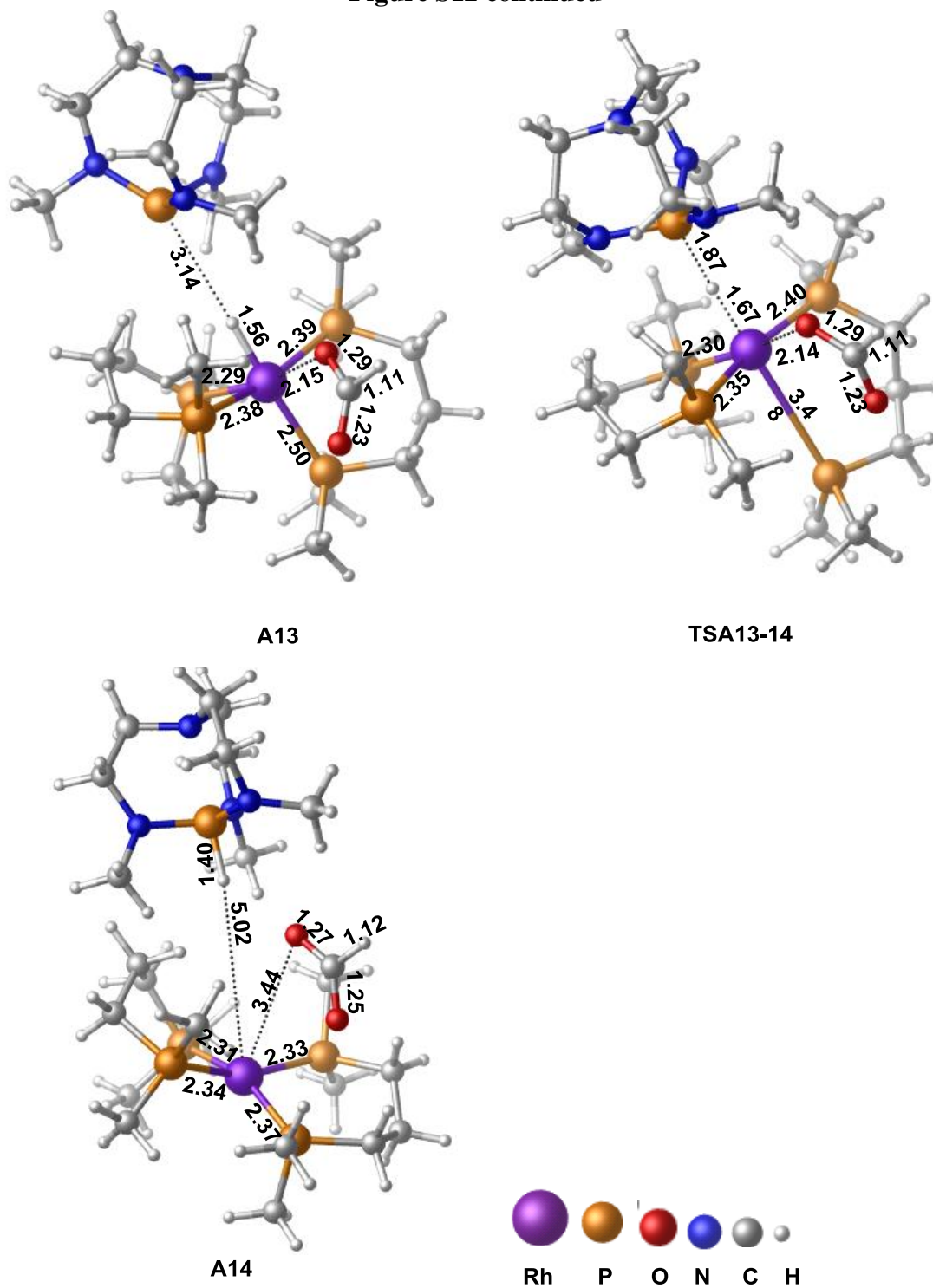
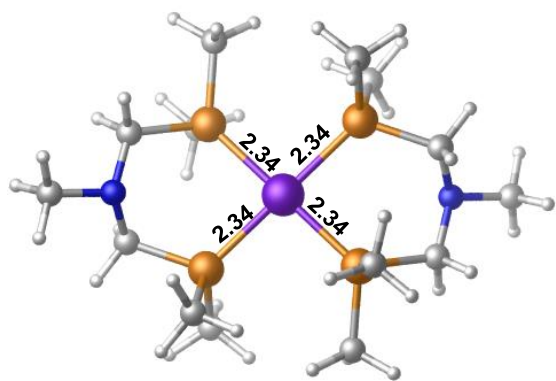
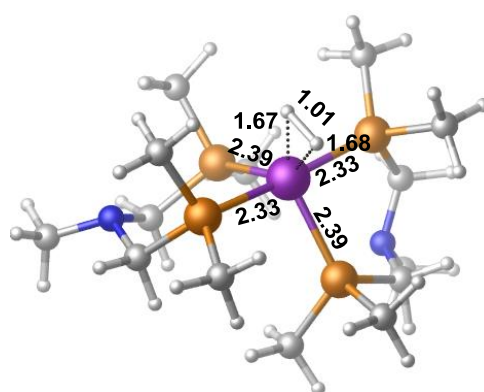


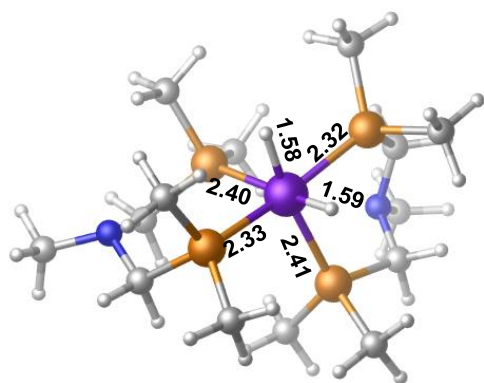
Figure S12. Optimized geometries with selected structural parameters (distances in Å) for the species involved in Figure 2 in the text.



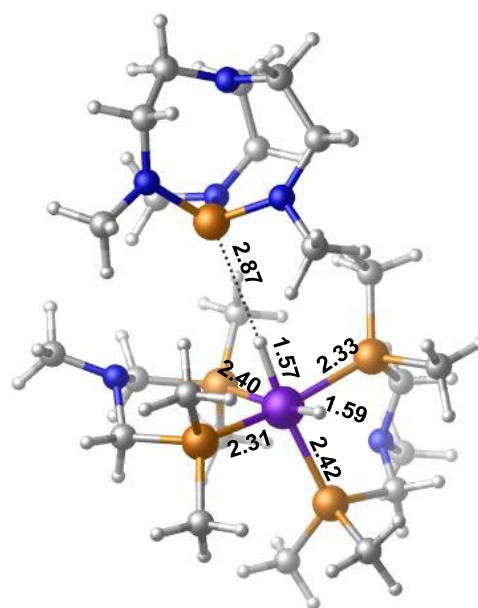
B1



TSB1-2



B2



B3

Figure S13 continued

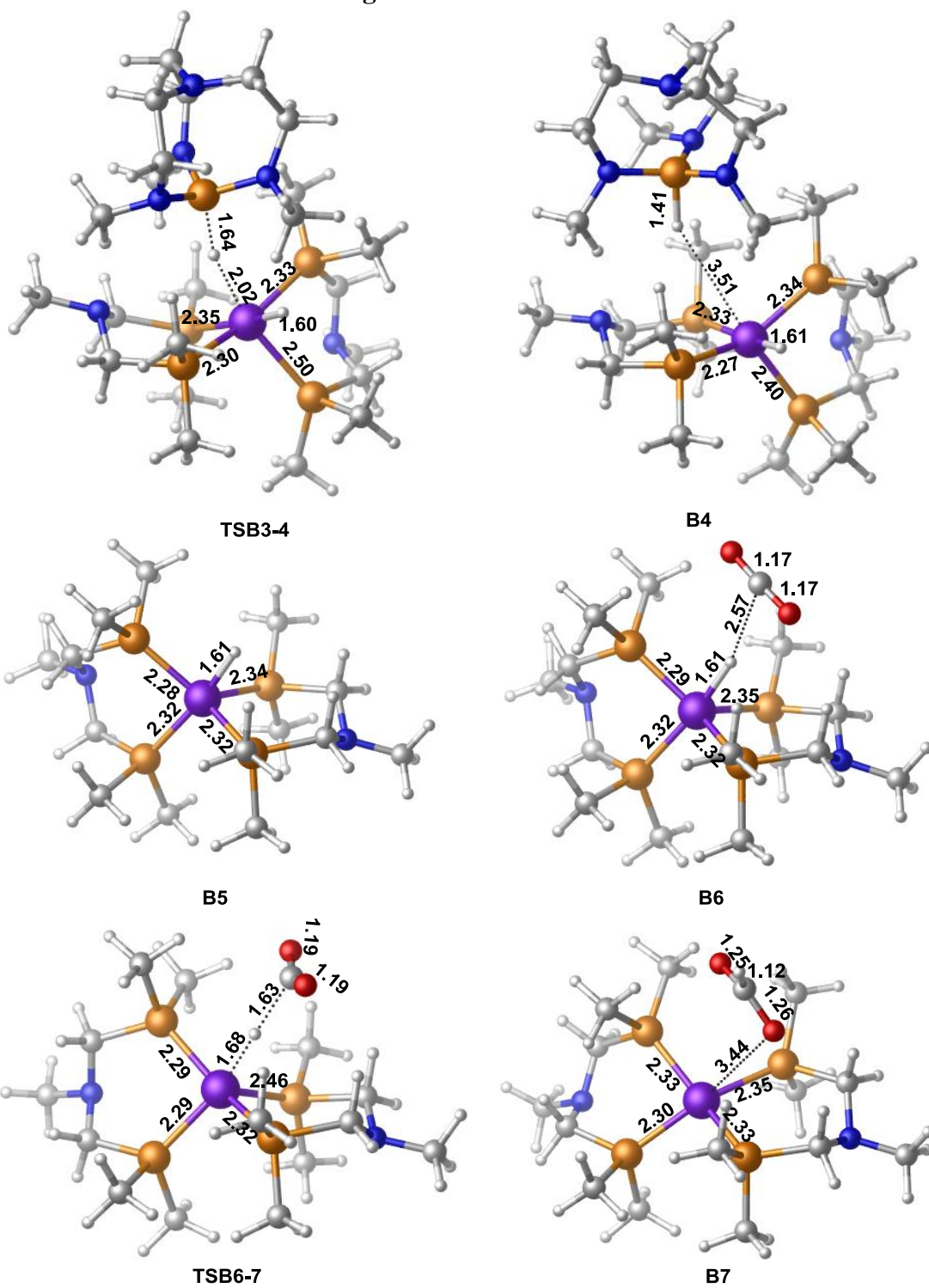


Figure S13 continued

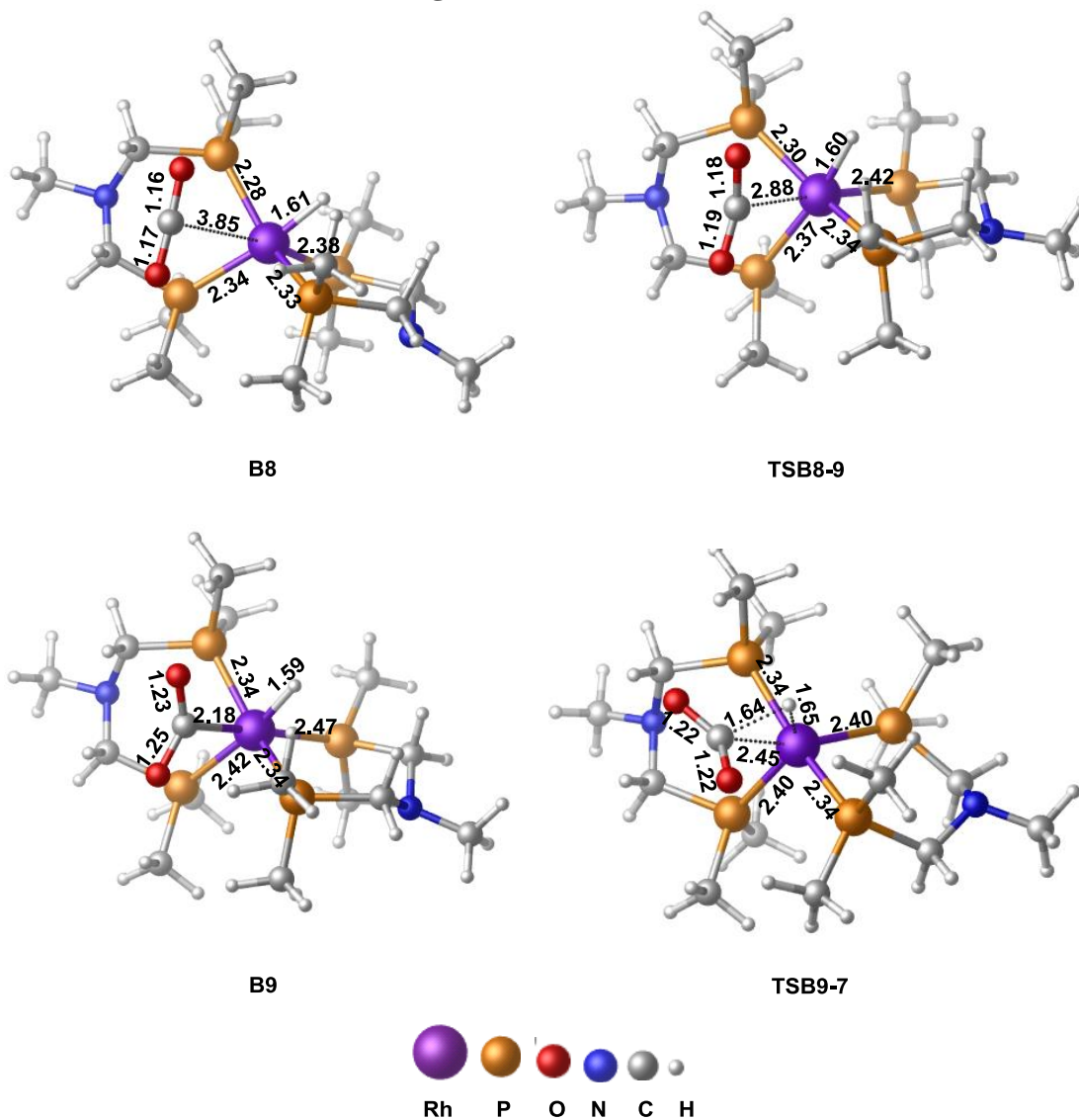


Figure S13. Optimized geometries with selected structural parameters (distances in Å) for the species involved in Figure 3 in the text.

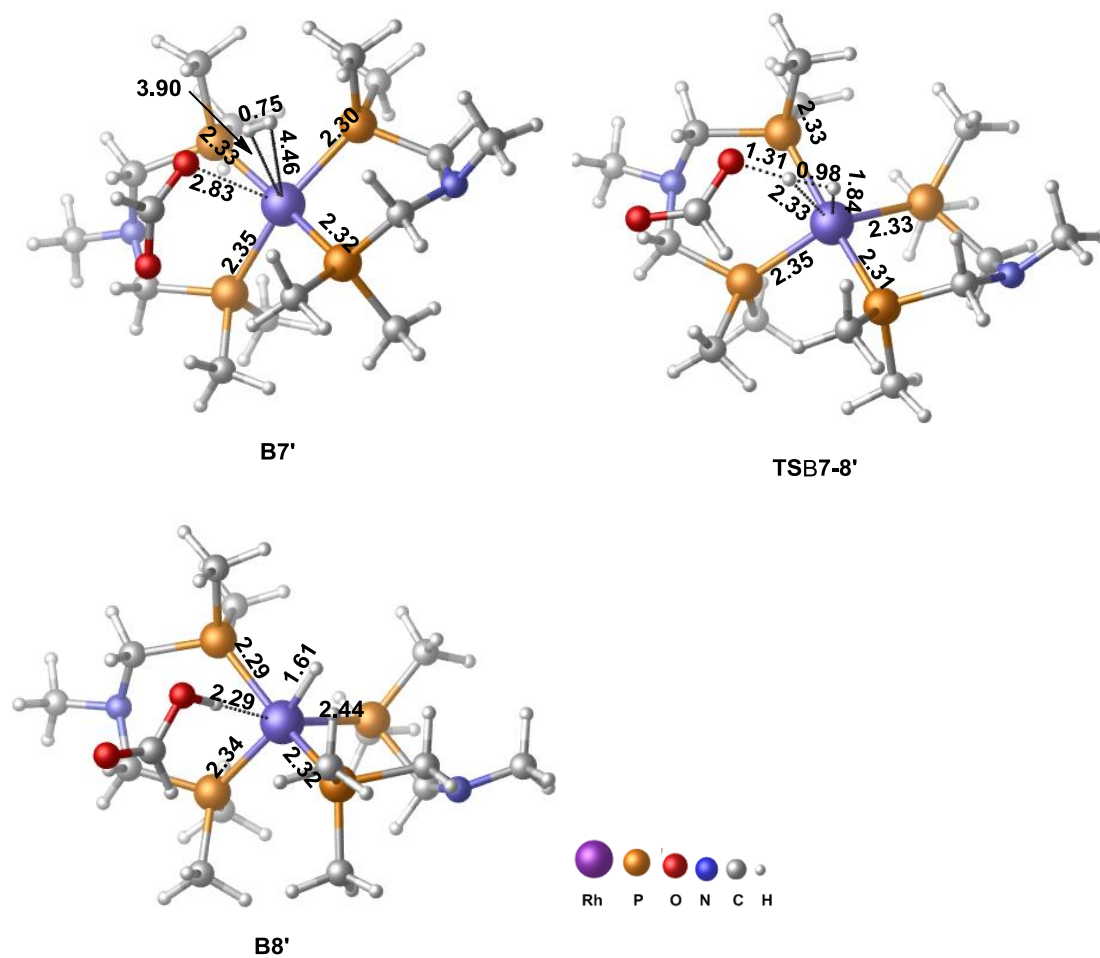
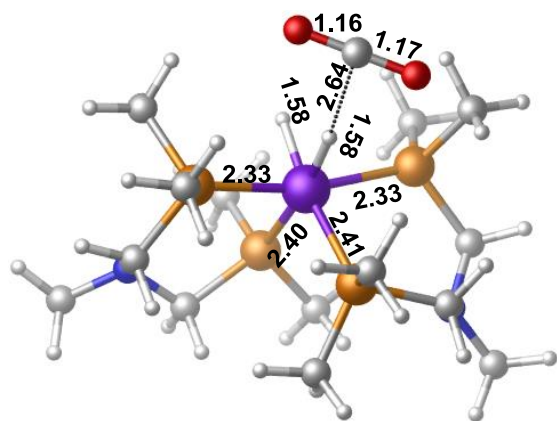
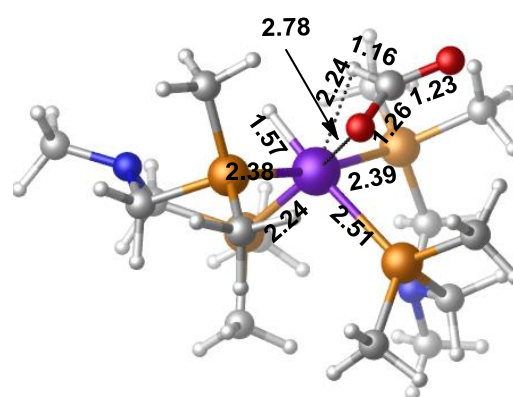


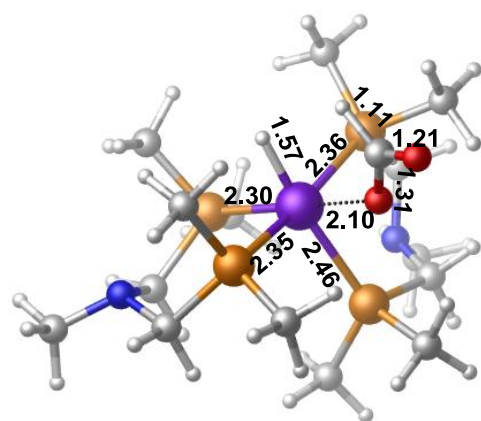
Figure S14. Optimized geometries with selected structural parameters (distances in Å) for the species involved in Figure S2 in the text.



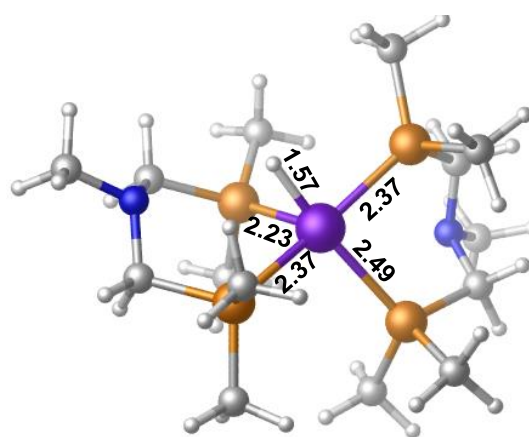
B10



TSB10-11



B11



B12

Figure S15 continued

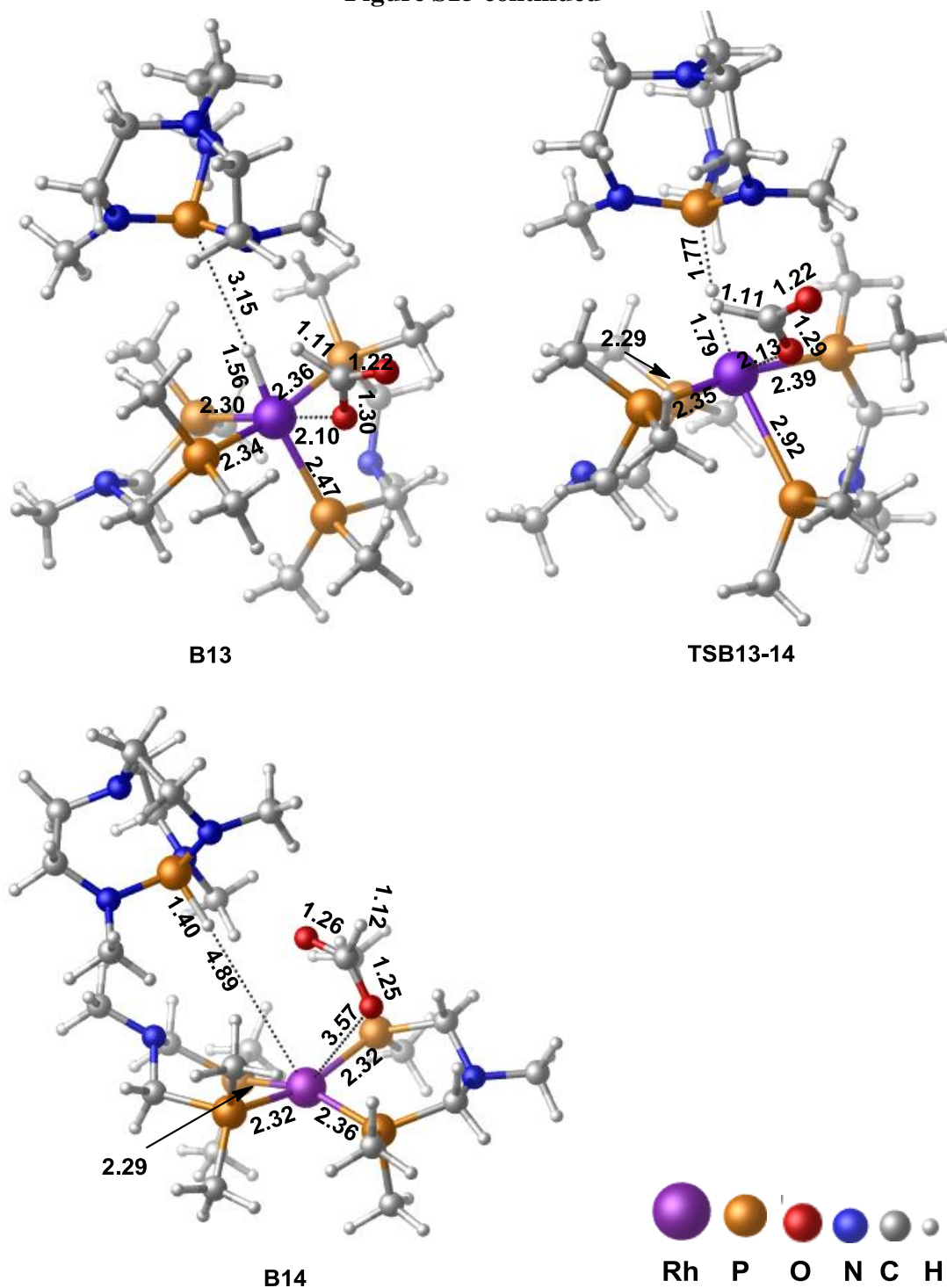


Figure S15. Optimized geometries with selected structural parameters (distances in Å) for the species involved in Figure S3 in the text.

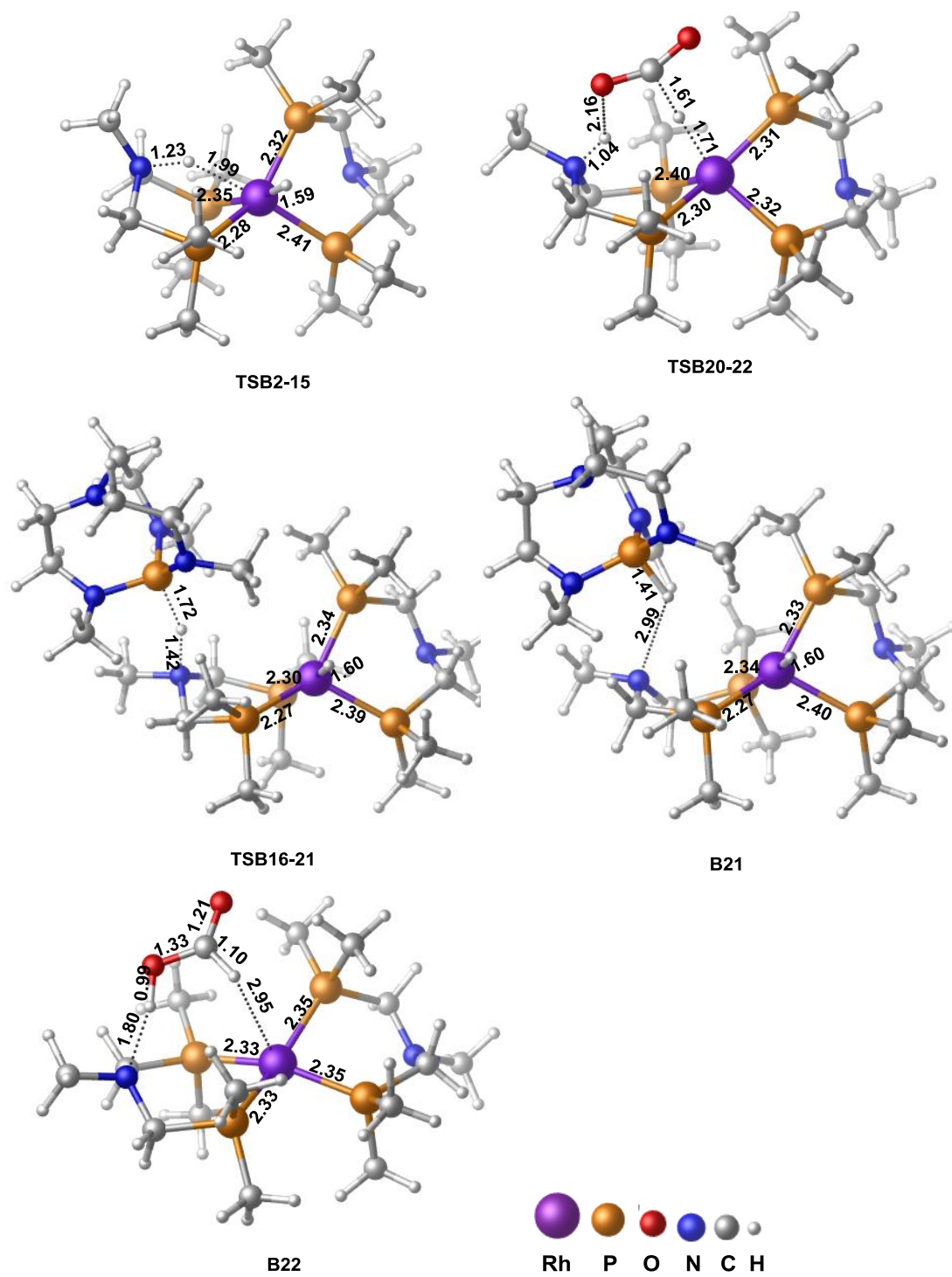


Figure S16. Optimized geometries with selected structural parameters (distances in Å) for the species involved in Figure S5 in the text.

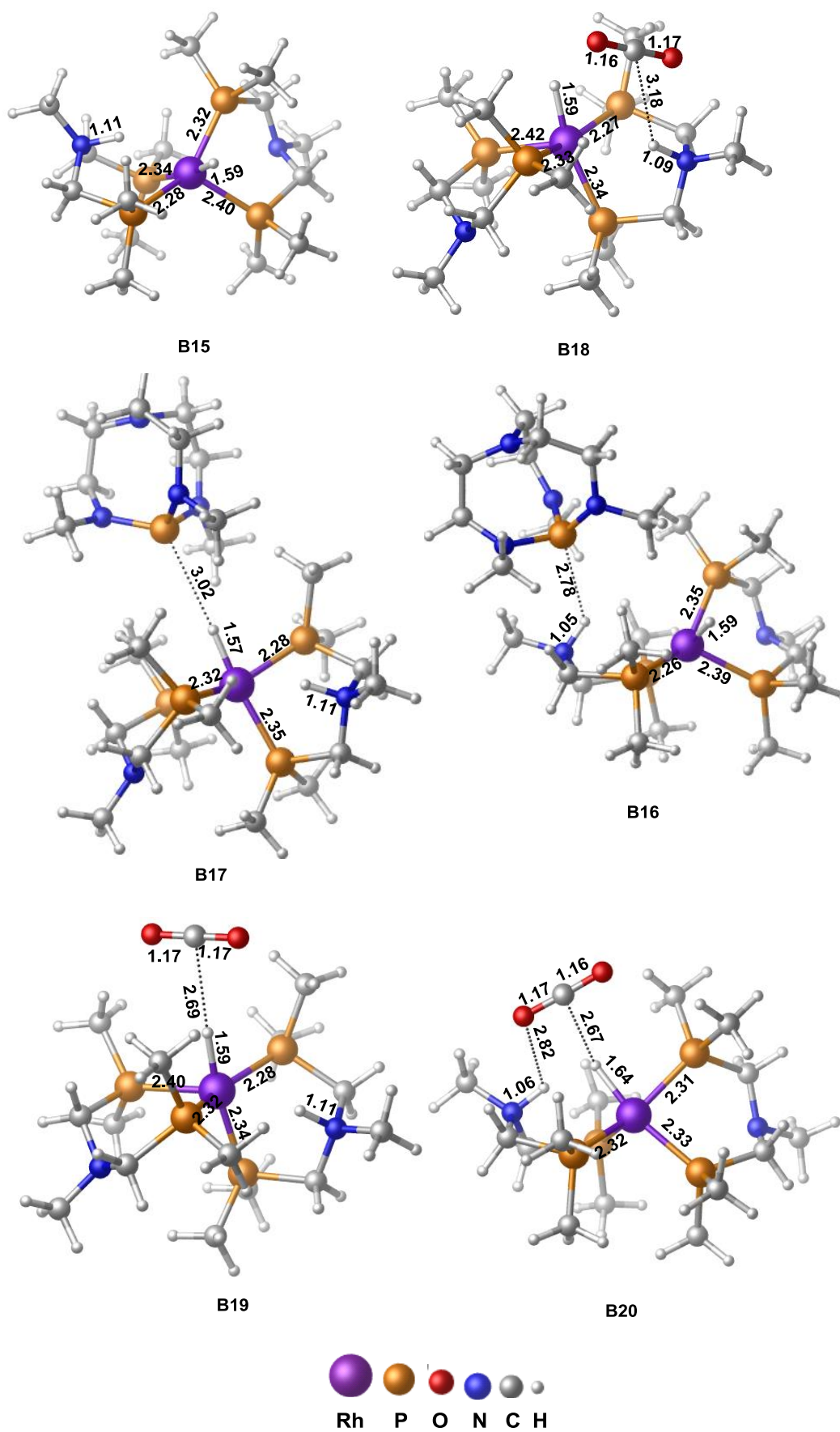
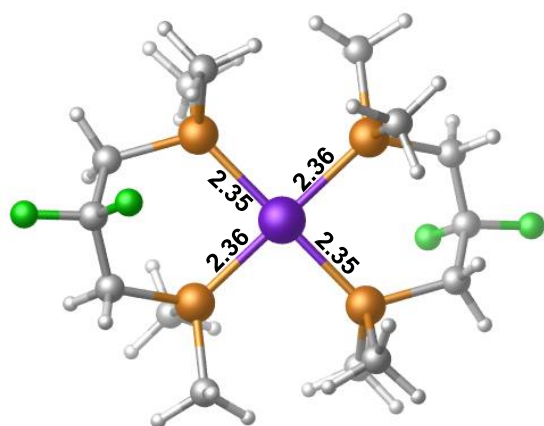
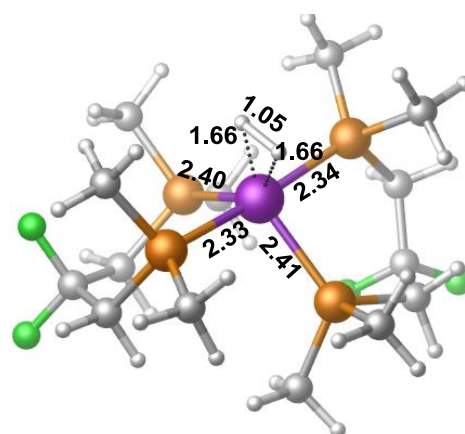


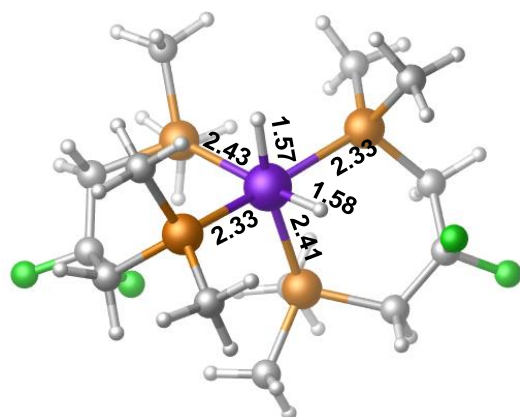
Figure S17. Optimized geometries with selected structural parameters (distances in Å) for the species involved in Figure S6 in the text.



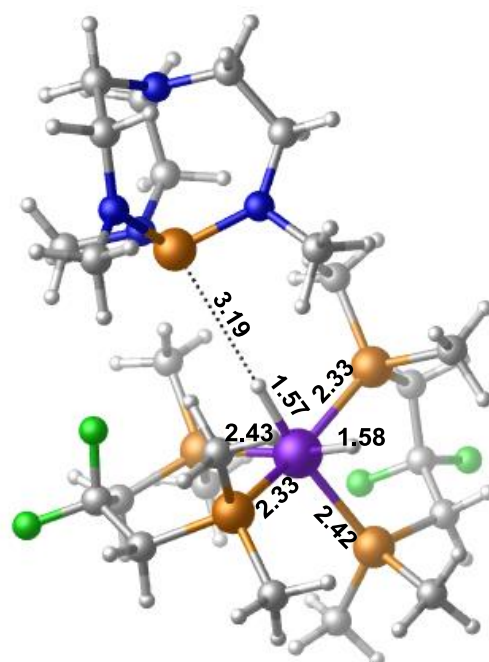
C1



TSC1-2

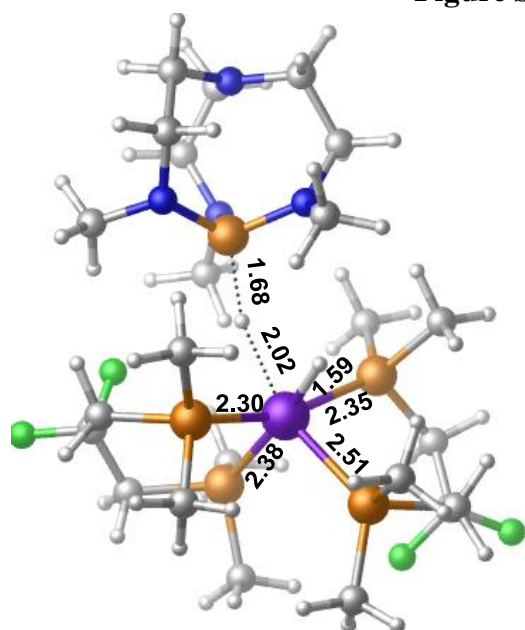


C2

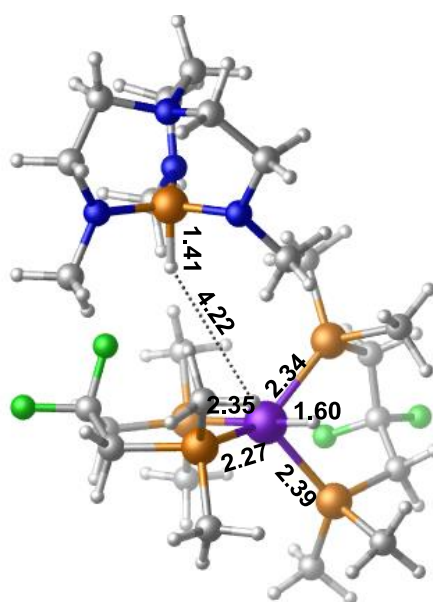


C3

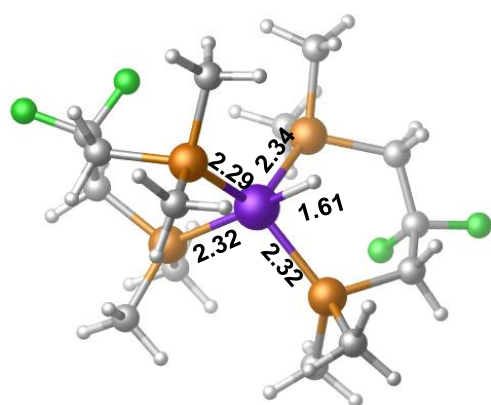
Figure S18 continued



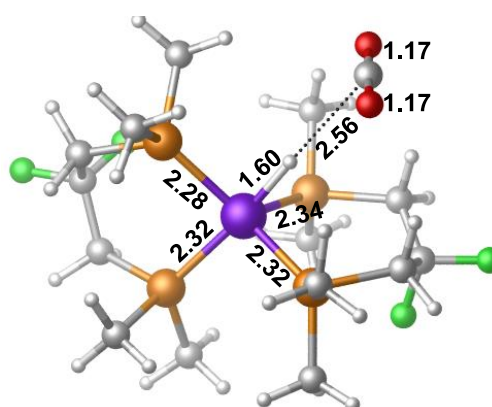
TSC3-4



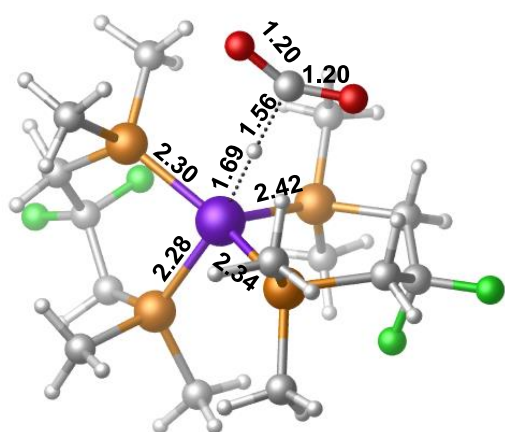
C4



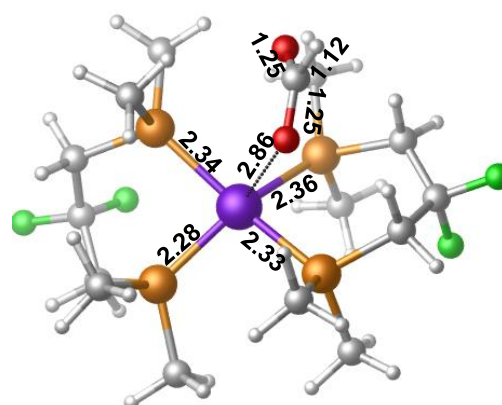
C5



C6



TSC6-7



C7

Figure S18 continued

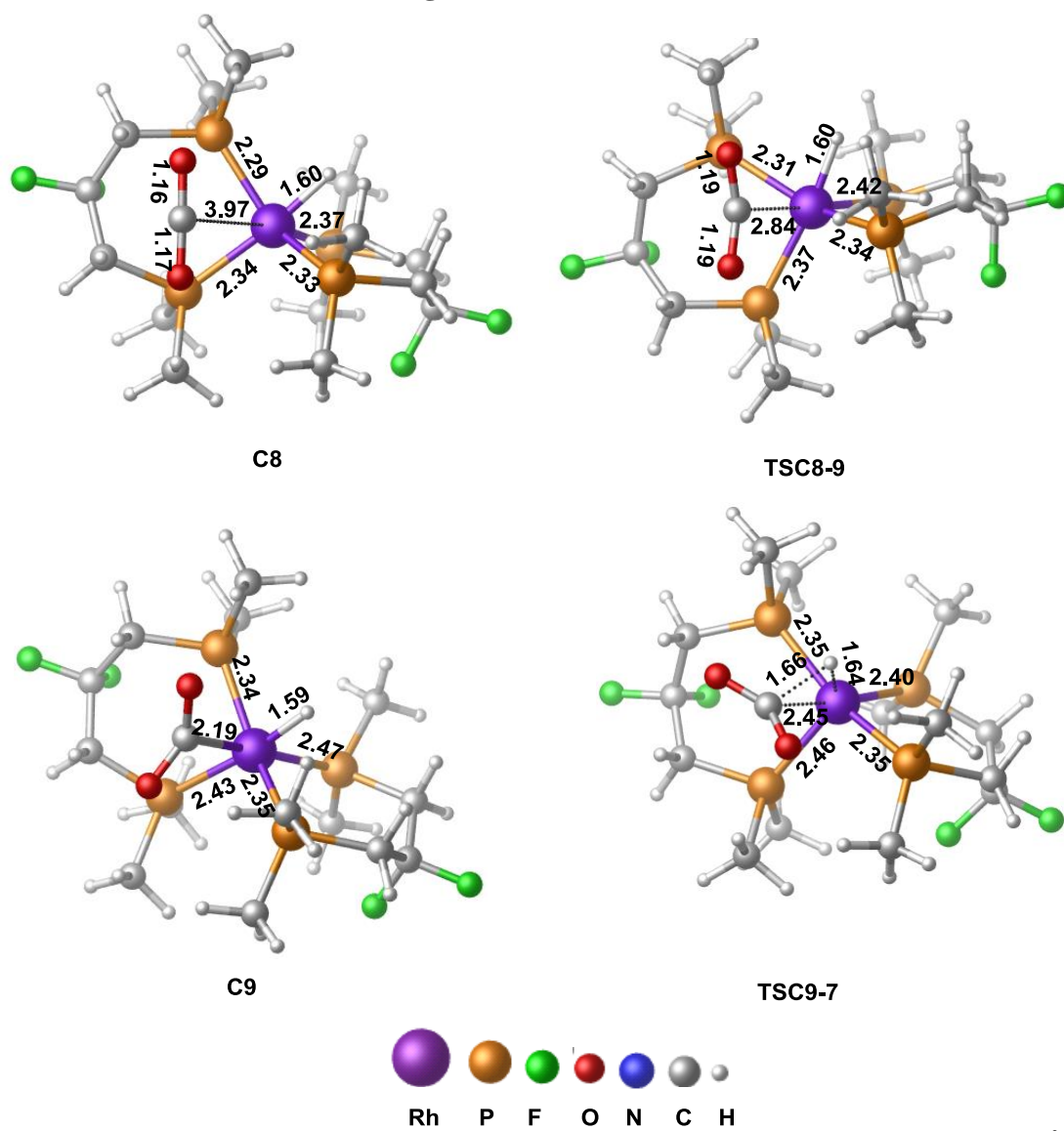


Figure S18. Optimized geometries with selected structural parameters (distances in Å) for the species involved in Figure 4 in the text.

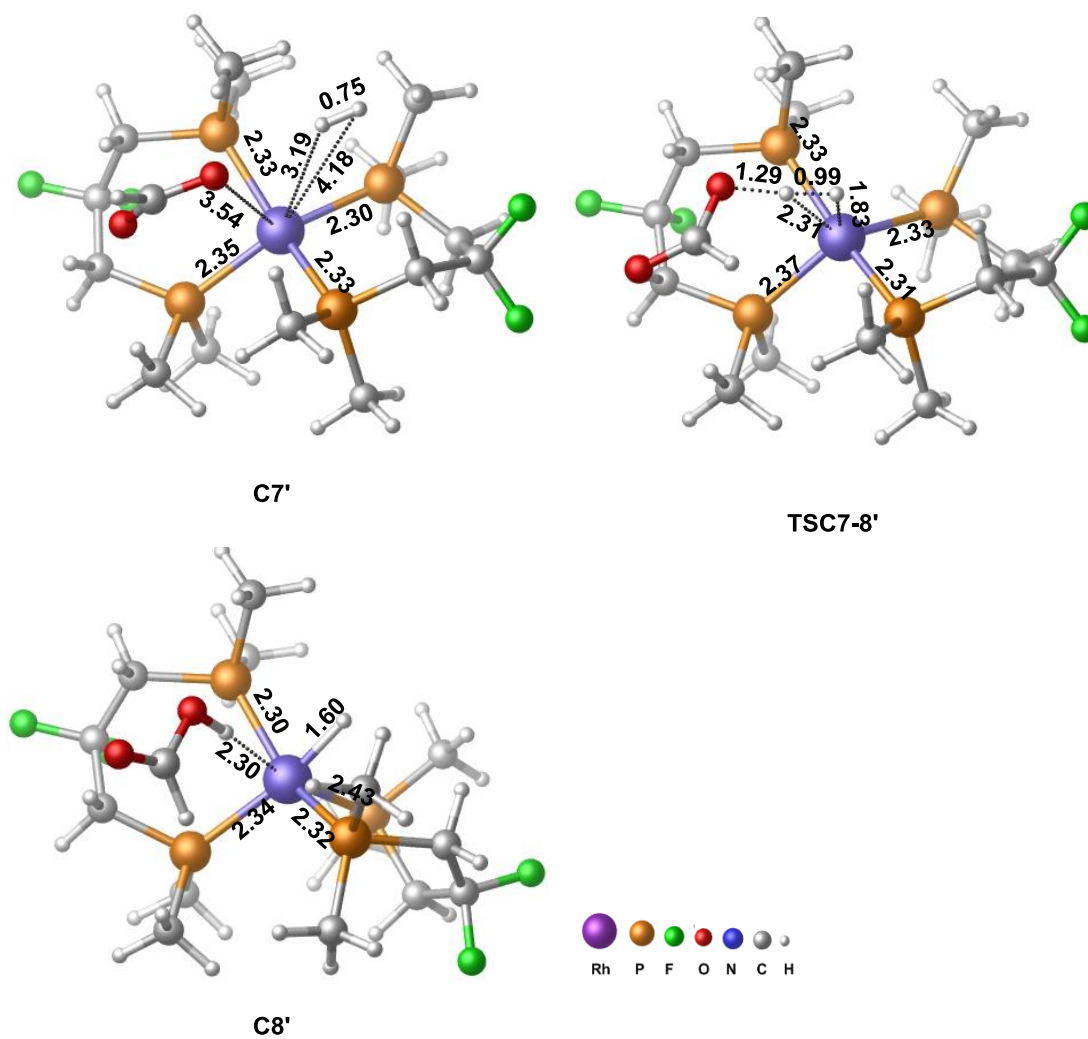
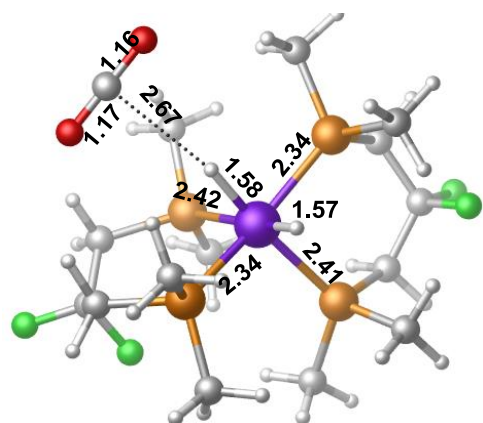
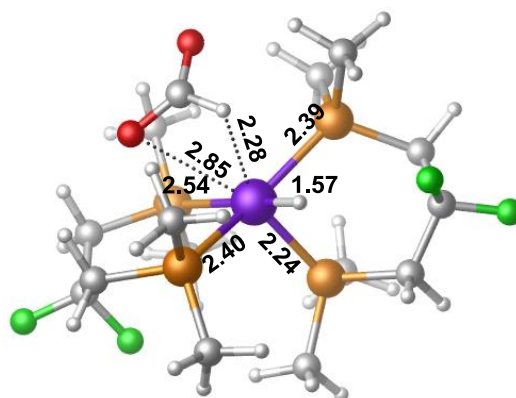


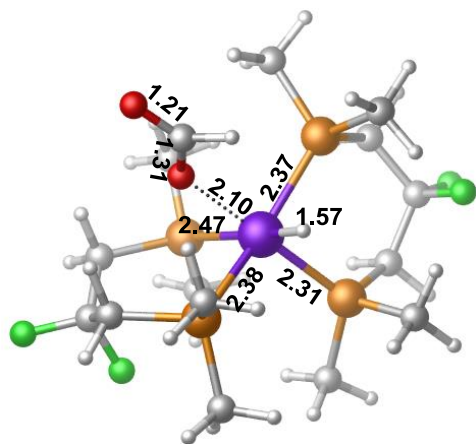
Figure S19. Optimized geometries with selected structural parameters (distances in Å) for the species involved in Figure S7 in the text.



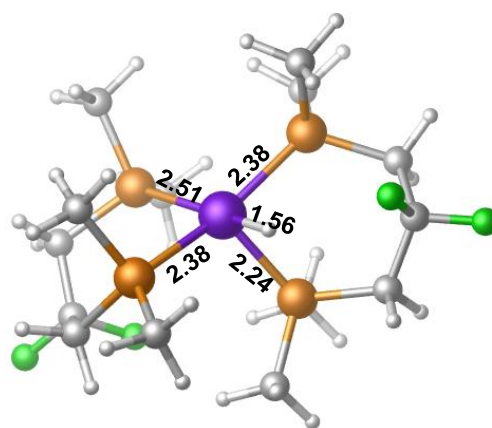
C10



TSC10-11



C11



C12

Figure S20 continued

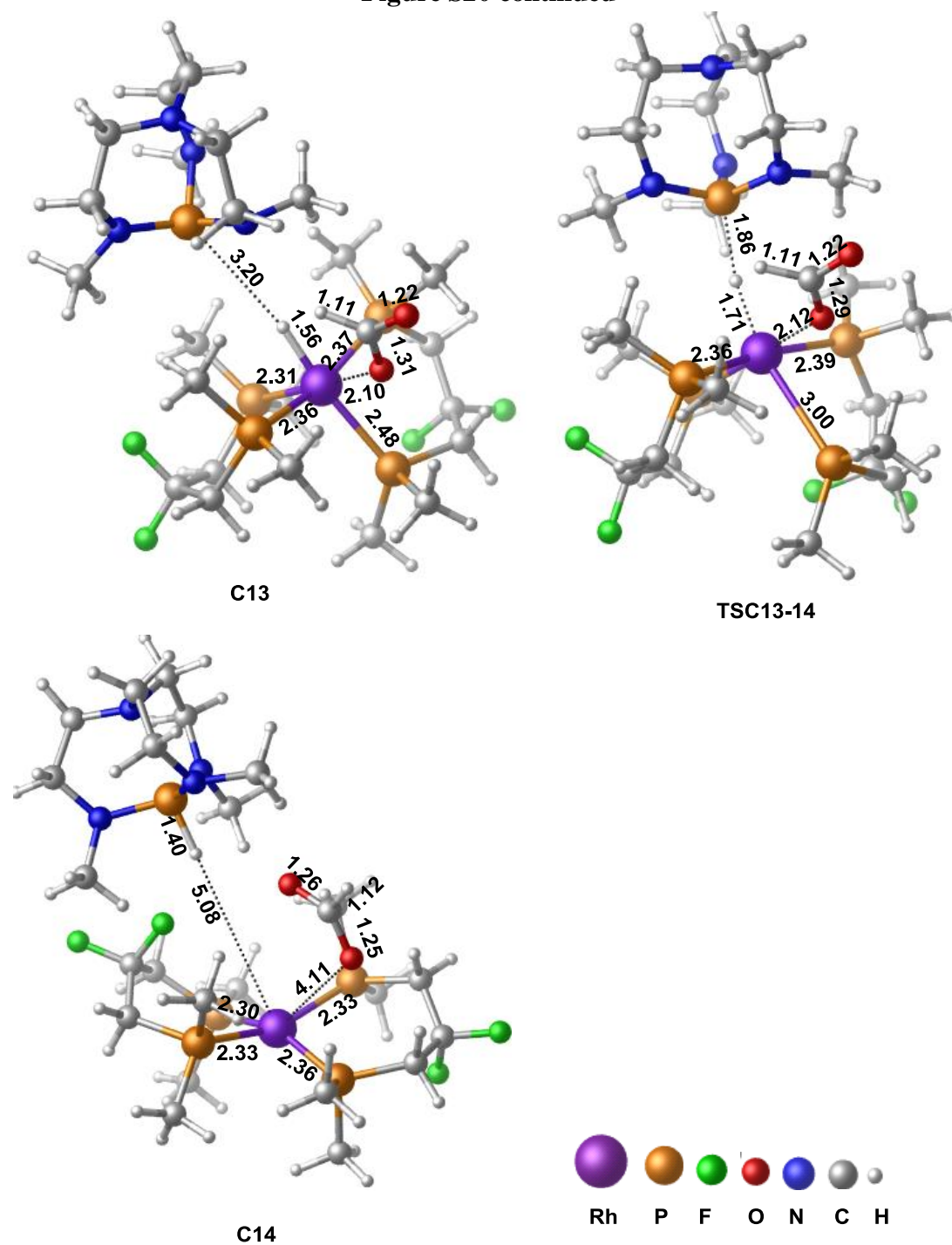


Figure S20. Optimized geometries with selected structural parameters (distances in Å) for the species involved in Figure S8 in the text.

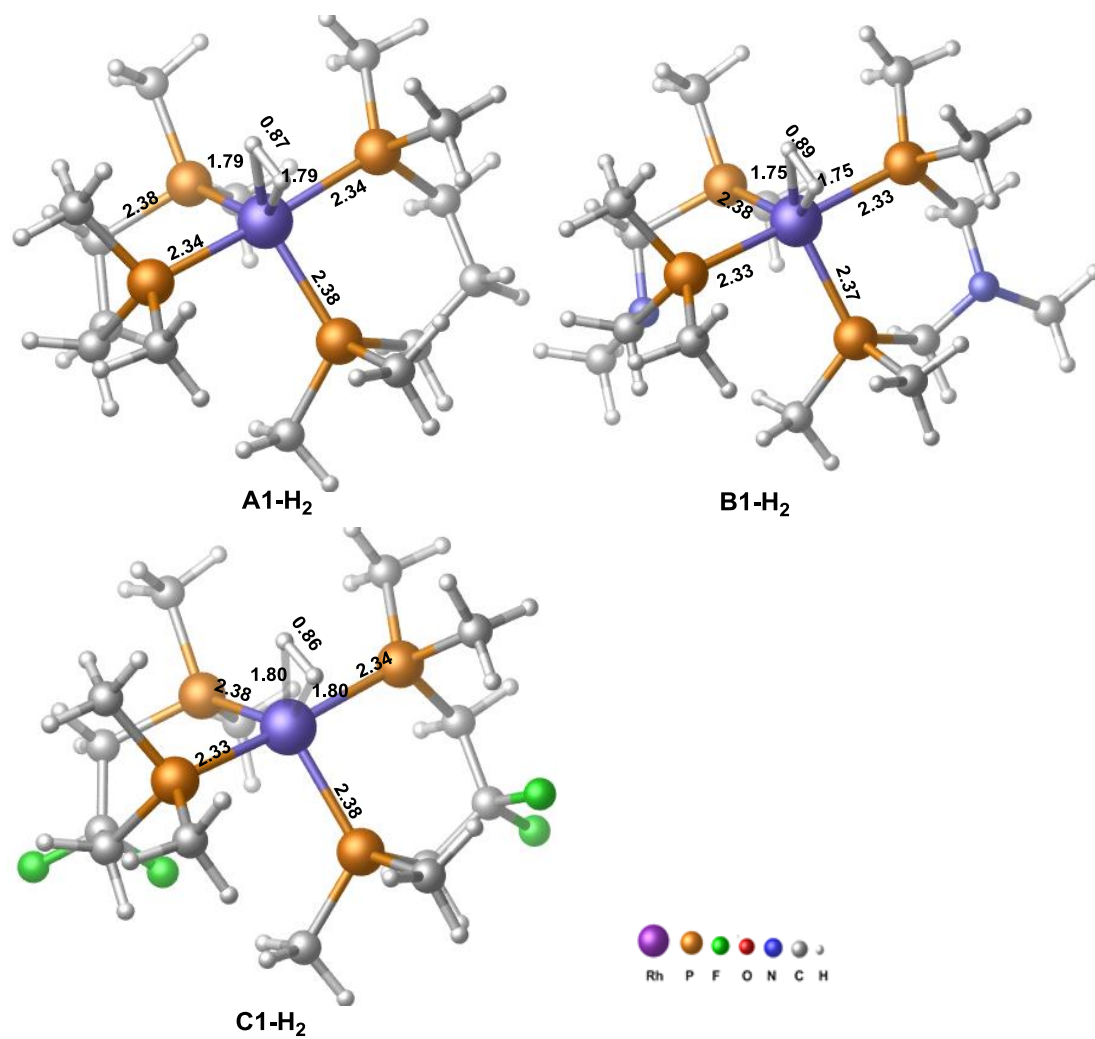


Figure S21. Optimized geometries with selected structural parameters (distances in Å) for the species of sigma-complex **A1-H₂**, **B1-H₂**, and **C1-H₂**.

Cartesian coordinates for all the complexes calculated in this study:

A1**E= -690.67235935 a.u.**

Rh	0.00001400	-0.00000600	-0.00000900
P	1.68986900	1.64375700	-0.12122000
P	1.68041400	-1.63680500	-0.17137700
C	3.36141100	1.33947000	0.65672100
H	4.10800500	1.74388300	-0.03780000
H	3.40526400	1.95972300	1.55744400
C	3.45285500	-1.09613000	-0.10947600
H	4.05976500	-1.99933600	0.01386000
H	3.73068900	-0.66243400	-1.07712800
P	-1.68985800	-1.64372900	0.12131100
P	-1.68043600	1.63678800	0.17131200
C	-3.36122200	-1.33952100	-0.65700700
H	-4.10794800	-1.74399400	0.03733700
H	-3.40480600	-1.95978000	-1.55774100
C	-3.45287900	1.09612600	0.10909500
H	-4.05976000	1.99932900	-0.01439600
C	-3.73092300	0.66247300	1.07670300
C	-1.50280700	-3.39154100	-0.45430000
H	-1.39487000	-3.40874300	-1.54166900
H	-0.64413500	-3.89430000	-0.00951900
H	-2.40417700	-3.95294700	-0.19011600
C	1.70910300	-2.64565500	-1.71194000
H	1.82175800	-1.97545400	-2.56822700
C	2.54467200	-3.35177300	-1.69798600
H	0.77973600	-3.19964000	-1.83843400
C	1.72008000	-2.88578200	1.18970600
H	0.74532600	-3.34563500	1.35019900
H	2.45221900	-3.66969300	0.97457800
H	2.00126400	-2.38486200	2.11958500
C	-1.70931500	2.64530600	1.71208400
H	-2.54466900	3.35167600	1.69804400
H	-1.82244300	1.97492700	2.56817100
C	-0.77981200	3.19896100	1.83901100
C	-1.71996100	2.88603200	-1.18954100
H	-0.74518300	3.34586000	-1.34994700
H	-2.00117100	2.38530000	-2.11951200
H	-2.45205800	3.66994500	-0.97428100
C	1.50274400	3.39142400	0.45482100
H	0.64386800	3.89417900	0.01042700
H	1.39510700	3.40832000	1.54222600
H	2.40396100	3.95302700	0.19053400
C	2.10320000	1.89840600	-1.90274600
H	2.89962000	2.63835400	-2.02740900
H	2.41741000	0.95259000	-2.35032000
C	1.21193000	2.23589300	-2.43752700
H	-2.10341400	-1.89805000	1.90284100
H	-2.41741800	-0.95212700	2.35032400
H	-2.90000500	-2.63781000	2.02753600
H	-1.21224900	-2.23570300	2.43769800
C	-3.71615300	0.10055800	-1.02379300
C	3.71635500	-0.10062400	1.02340800
H	-3.16147000	0.39434700	-1.92316400
H	-4.77464300	0.13294800	-1.30060900
H	3.16180900	-0.39443500	1.92285800
H	4.77489200	-0.13305400	1.30004200

A1-H₂**E= -691.84938001 a.u.**

Rh	0.00648600	0.03619100	-0.59600900
P	-2.16490900	0.91768400	-0.64464300
P	-0.81813400	-1.85747200	0.58099700
C	-3.27231900	0.61037700	0.80006300
C	-2.85518300	1.14874900	1.65905100
H	-4.24165400	1.06917100	0.57415600
H	-2.22443700	-1.54483700	1.75157600
H	-2.50864800	-2.50976600	2.18738900
H	-1.82328600	-0.93239000	2.56854000
P	2.17409100	-0.81505000	-0.77174200
P	0.92325800	1.86732700	0.61637600
C	3.21328700	-0.85700200	0.76733700
H	4.25425600	-0.68804900	0.46741900
H	3.16494900	-1.87359200	1.17055200
C	2.61417500	1.57880300	1.34393200
H	2.74694100	2.30021600	2.15722700
C	3.37121900	1.82513200	0.59055200
C	2.37497000	-2.50850000	-1.46232800
H	1.88244900	-3.25063300	-0.83124600
H	1.91224100	-2.54164000	-2.45204000
H	3.43391500	-2.76740200	-1.55368700
C	0.30082300	-2.75853900	1.74434800
H	0.67766300	-2.06832100	2.50316100
H	-0.23562400	-3.57220900	2.24194000
H	1.15415200	-3.18694100	1.21540500
C	-1.47271800	-3.25878400	-0.42673600

H	-0.68088700	-3.63142800	-1.08162600
H	-1.83830600	-4.07797400	-0.20043900
H	-2.28589400	-2.90705400	-1.06656500
C	1.18838100	3.50100700	-0.19876000
H	1.66693100	4.21290100	0.48119800
H	1.82084000	3.36449900	-1.07981800
H	0.23641300	3.91769500	-0.53377800
C	-0.00016500	2.35188400	2.14264100
H	-1.02683200	2.63437400	1.89875700
H	-0.04080500	1.49873900	2.82562900
H	0.48063300	3.19410000	2.64978200
C	-3.13987900	0.24964300	-2.05485100
H	-2.64524200	0.52270000	-2.99015200
H	-3.18080400	-0.84034000	-2.00362100
H	-4.15760100	0.65097800	-2.05594000
C	-2.36452100	2.72917400	-0.89996600
H	-3.41789300	2.98224200	-1.05046900
H	-1.99217100	3.28505500	-0.03675900
H	-1.79419500	3.03225400	-1.78164700
C	3.18764800	0.15575600	-1.96381100
C	3.24415000	1.20212200	-1.65777300
H	4.19980200	-0.25145100	-2.04534500
H	2.70660200	0.11861300	-2.94445600
H	0.10235600	0.44372500	-2.33589600
H	-0.19349500	-0.36963100	-2.32319400
C	2.80884400	0.14569100	1.85621000
H	3.58175600	0.13547900	2.63073300
H	1.88588100	-0.19631200	2.33884100
C	-3.46618400	-0.86725100	1.16204900
H	-4.26725100	-0.92618000	1.90579200
H	-3.83125400	-1.42792800	0.29283300

A2**E= -691.86562002 a.u.**

Rh	-0.05340300	0.05125600	-0.55835300
P	-2.22854600	0.90973000	-0.67206800
P	-0.78085000	-1.51889000	1.12001300
C	-3.54178200	-0.26627600	-0.09004000
H	-3.67916300	-0.13327400	0.98960100
H	-4.48122500	0.04279900	-0.56096300
C	-2.31161200	-2.43834700	0.58591100
H	-1.96946300	-3.38276900	0.14942500
H	-2.87286600	-2.69596900	1.49213000
P	2.00542300	-0.88513100	-1.10894000
P	1.06251600	1.75836600	0.73208900
C	3.22460200	-1.07050600	0.28602700
H	4.22842100	-0.94645900	-0.13749200
C	3.15942100	-2.10688500	0.63478000
C	2.84084600	1.35624300	1.09685200
H	3.17376800	2.01323700	1.90716400
H	3.44874400	1.61499500	0.22257700
C	1.98857400	-2.55766300	-1.86370300
H	1.48869700	-3.26736600	-1.20224100
H	1.42925100	-2.51204200	-2.80090300
C	3.00569300	-2.96690300	-2.06397200
H	-1.27489200	-0.83425400	2.76249200
H	-1.92646400	0.03389800	2.63737700
H	-1.79374000	-1.58545300	3.36535600
C	-0.38266500	-0.51212700	3.30500400
C	0.28600500	-2.92163600	1.66325000
H	1.18841400	-2.54183500	2.14914600
H	-0.24824800	-3.56431600	2.36933400
H	0.58065800	-3.52366300	0.80092300
C	1.20428700	3.38554000	-0.11239000
H	1.83644300	4.07485000	0.45509200
H	1.62709600	3.23688900	-1.10870500
C	0.21378100	3.83098900	-0.23133300
H	0.47519900	2.24602200	2.41166500
H	-0.59809100	2.44471900	2.40014600
H	0.66515400	1.43671800	3.12040200
C	0.99829500	3.14177300	2.75914600
H	-2.74166600	1.27456400	-2.39471200
H	-2.05457300	2.00824700	-2.82184000
H	-2.66781700	0.36083500	-2.98850900
C	-3.76474900	1.65954400	-2.43333600
C	-2.68485900	2.45174800	0.21962300
H	-3.73527200	2.70045100	0.04209400
H	-2.53380400	2.32211700	1.29399000
H	-2.06542300	3.28286500	-0.12534100
C	2.92925900	0.07862300	-2.37250700
H	3.07715600	1.10592800	-2.03287800
H	3.90066000	-0.37708700	-2.58546600
H	2.33253500	0.11136600	-3.28703900
H	0.21155200	0.97002900	-1.81408200
H	-0.62907200	-0.95293900	-1.63689000
C	-3.22951800	-1.73270100	-0.42310400
C	3.03782700	-0.11998700	1.47808200

H -2.78132000 -1.79505500 -1.42071600
 H -4.16744100 -2.29441400 -0.47233800
 H 2.18222600 -0.45463900 2.07942500
 H 3.91480900 -0.21490900 2.12570600

C -0.06087600 2.89935100 1.31559300
 H -0.64580200 3.71853000 1.74735000
 H -0.75775100 2.30116700 0.71485600
 C 3.80756300 -2.69264700 0.99745500
 H 4.41206600 -3.47990100 1.45872400
 H 3.62589800 -1.95074800 1.78384600

A3

E= -1272.85456367 a.u.

Rh 1.72821600 0.09788300 -0.33584700
 P 1.55825700 2.34135600 -0.92373500
 P 1.36262800 0.46665700 2.02566000
 C 1.03789100 3.49375800 0.42083600
 H 1.92155200 3.75585500 1.01605800
 C 0.69198600 4.41735400 -0.05657200
 H 0.48911100 2.05887800 2.46945300
 H -0.32565600 1.79037000 3.15007200
 H 1.19210000 2.66558400 3.05265600
 P 1.35046100 -2.21158000 -0.43473000
 P 4.11340500 -0.27396900 -0.45807600
 C 2.46786100 -3.31035300 0.57349200
 H 2.64305100 -4.22751200 -0.00153900
 H 1.91055700 -3.60806200 1.46856000
 C 4.60445300 -2.04150200 -0.14494400
 H 5.67738300 -2.05570900 0.07571400
 H 4.47544300 -2.60659300 -1.07544200
 C -0.32155300 -2.84100300 -0.01854200
 H -0.51020700 -2.73179500 1.04981700
 H -1.06551400 -2.24082600 -0.54813000
 H -0.41864300 -3.89512000 -0.29516200
 C 2.74964500 0.52629500 3.24502900
 H 3.44885900 1.32177800 2.97560400
 H 2.36441900 0.72214400 4.25052400
 H 3.28971400 -0.42342500 3.26334200
 C 0.25903200 -0.77996600 2.80788100
 H 0.73024400 -1.76631700 2.76733400
 H 0.06163700 -0.53131000 3.85518800
 -0.68200800 -0.80000600 2.24639600
 C 4.90509200 0.03713800 -2.09045600
 H 5.92937300 -0.34716700 -2.11372200
 H 4.31718500 -0.44411000 -2.87563700
 H 4.92972500 1.11029900 -2.29201300
 C 5.25154300 0.61615300 0.68947100
 H 5.03267500 1.68707400 0.67921200
 H 5.10618600 0.24906800 1.70791700
 H 6.29737900 0.46151700 0.40803600
 C 0.25399800 2.60814600 -2.18569000
 H 0.50624600 2.04412900 -3.08669300
 H -0.69016200 2.21942200 -1.79200000
 C 0.14788400 3.66875500 -2.43204800
 C 3.00755500 3.19955800 -1.65976000
 H 2.78062600 4.25331000 -1.84734200
 H 3.86903200 3.13663000 -0.98991900
 C 3.26241200 2.72095300 -2.60850200
 H 1.56619900 -2.85920300 -2.14428100
 H 2.56565400 -2.62118900 -2.51480400
 H 1.41217300 -3.94185300 -2.18199400
 H 0.84267500 -2.36365700 -2.79566500
 H 1.68916600 -0.04677700 -1.91030700
 H 0.16081900 0.21050000 -0.42019800
 P -2.79201600 0.47738300 -0.31500400
 N -4.15054300 1.57132200 -0.38211800
 N -2.84909400 -0.30353400 1.25736000
 N -2.94273900 -0.82407400 -1.44593100
 C -3.06695600 0.64051300 2.34392300
 C -2.55274000 1.58278800 2.12958000
 H -1.99708900 -0.76841600 -2.55822100
 C -2.49042600 -0.49192700 -3.50052900
 C -3.78951100 2.87717000 -0.92815700
 C -2.72695200 3.07245500 -0.76286200
 C -3.86892400 -1.95139600 -1.57797800
 H -3.44111200 -2.84576200 -1.09846600
 C -3.94582000 -2.19735900 -2.64456000
 H -5.30059500 -1.72583400 -1.07095700
 H -5.84688800 -1.13842600 -1.81409600
 H -5.79195400 -2.71362300 -1.02845400
 C -3.39661100 -1.62646600 1.50536400
 H -2.92966700 -2.32869000 0.81284800
 C -3.09388200 -1.94014400 2.51440500
 C -4.93038300 -1.70814000 1.37432800
 H -5.23621200 -2.76719900 1.38082900
 H -5.40254800 -1.24240000 2.24522500
 C -5.55456100 1.27457400 -0.63622800
 H -5.70709500 1.01858600 -1.69910100
 H -6.13419000 2.19022100 -0.46197500
 C -6.13279000 0.18703000 0.25789300
 H -6.11352900 0.53877200 1.29333800
 H -7.19321600 0.04665500 -0.01567500
 N -5.38285800 -1.04110500 0.18700100
 H -4.12552900 0.88709100 2.50859300
 H -2.65829900 0.22914100 3.27583200
 H -4.36016100 3.66710300 -0.42473800
 H -3.98719300 2.95409100 -2.00946600
 H -1.20362500 -0.04743100 -2.34976100
 H -1.52199000 -1.74883300 -2.71033600

A4

E= -1272.83525136 a.u.

Rh 1.68332000 0.09963600 -0.27425500
 P 1.09330500 2.19016100 -0.96591100
 P 1.89484900 0.79589300 1.95467300
 C 0.48879600 3.40204300 0.32500700
 H 1.36054600 3.95358400 0.69878800
 C -0.15709200 4.14267500 -0.16190300
 H 0.70179500 2.12984100 2.54875800
 H 0.10162100 1.69183200 3.35510900
 H 1.28949100 2.93411400 3.00781900
 P 1.34737300 -2.18880600 0.02618100
 C 3.97430300 -0.29945700 -0.98414400
 P 2.73862100 -3.08721000 0.91269300
 H 2.82239200 -4.09182800 0.47801800
 H 2.41928400 -3.22804800 1.95220900
 C 4.62486700 -1.98209900 -0.48315200
 H 5.72077100 -1.96007400 -0.50048500
 H 4.32033600 -2.71519500 -1.23933000
 C -0.08574000 -3.01598700 0.87386800
 H -0.09072900 -2.73947300 1.93160100
 H -1.02481200 -2.67514200 0.42690300
 H -0.01995200 -4.10738800 0.79924500
 C 3.50116400 1.55342800 2.48669000
 H 3.78096400 2.34365000 1.78477800
 H 3.44771200 1.96816100 3.49863400
 H 4.28287000 0.78959500 2.46245200
 C 1.69925500 -0.42993300 3.33285400
 H 2.46343700 -1.20617500 3.23866500
 H 1.80032300 0.04410900 4.31459600
 C 0.71869200 -0.90813200 3.26701500
 H 4.27014800 -0.35818300 -2.80921800
 H 5.27741700 -0.71066700 -3.05672400
 H 3.52839700 -1.01636400 -3.26934100
 H 4.13231300 0.64216800 -3.22945500
 C 5.41601600 0.75237800 -0.47057200
 H 5.20552800 1.80205400 -0.69367200
 H 5.57501900 0.66233500 0.60681100
 H 6.33676200 0.45694400 -0.98560900
 C -0.17112000 2.36400900 -2.31081400
 H 0.23754500 1.88552000 -3.20525000
 H -1.08742400 1.83140400 -2.04891800
 H -0.40354700 3.41125000 -2.53466300
 C 2.43634900 3.21736300 -1.72349700
 H 2.08692300 4.21450000 -2.01292700
 H 3.25245600 3.31826200 -1.00255400
 C 2.82436200 2.70461000 -2.60778500
 H 1.31460900 -3.12997300 -1.56910600
 H 2.19805500 -2.87519200 -2.15810700
 H 1.28817900 -4.21262100 -1.40544100
 H 0.44146000 -2.82646300 -2.14993500
 H 1.23249200 -0.25617100 -1.77209500
 H -1.92709200 0.55949000 -0.20102800
 P -3.24306900 0.04566000 -0.14419500
 N -4.02605900 1.55657600 -0.02700000
 N -3.00330600 -0.84958500 1.28077500
 C -3.17067700 -0.74838300 -1.63954900
 N -1.91391500 -0.44279900 2.16556500
 H -1.00668200 -0.24530600 1.58294600
 C -1.86487500 -1.10762000 -2.19381600
 H -1.82746200 -0.85609400 -3.25859800
 C -3.34359800 2.76069900 -0.49155000
 H -2.26849200 2.67334000 -0.34651100
 C -4.25311300 -1.60024500 -2.08982600
 H -4.05224900 -2.65306200 -1.83567000
 H -4.34204800 -1.54693300 -3.17984000
 C -5.53770900 -1.10786900 -1.44451800
 H -5.89503000 -0.21462700 -1.96076900
 H -6.33218800 -1.86047700 -1.46224300
 C -4.11283300 -1.51007800 1.93772000
 H -3.75892200 -2.41474600 2.44253800
 H -4.56441700 -0.86486500 2.70778600
 C -5.11891000 -1.88465600 0.86136300
 H -4.75297600 -2.74559300 0.29776300
 H -6.10460500 -2.12738500 1.27085200
 C -5.47179300 1.65147900 -0.09639700
 H -5.80752400 1.82895000 -1.13031600
 H -5.81778600 2.50019400 0.50237400
 C -6.04419200 0.36090500 0.46278800
 H -5.96687600 0.36469300 1.55181800
 H -7.09307400 0.20900100 0.18911000
 N -5.20374800 -0.73338100 -0.05731200
 H -2.17287600 0.44293100 2.76296200
 H -1.69646500 -1.26812600 2.84913500
 H -3.68830300 3.61778700 0.09476700
 H -3.53974700 2.95696700 -1.55432100

H	-1.04547800	-0.58844400	-1.68436300
H	-1.69546300	-2.18657000	-2.08123900
C	-0.23546000	2.73020700	1.49797500
H	-0.88468800	3.46120500	1.99591500
H	-0.88534300	1.93678900	1.11508100
C	4.11548900	-2.40570500	0.90507400
H	4.83292000	-3.09610600	1.36285600
H	4.08370300	-1.52280500	1.55721300

A5**E= -691.41198547 a.u.**

Rh	0.00342500	-0.02473600	-0.34271100
P	-1.78598400	-1.49479500	-0.55994900
P	-1.13867400	1.92220400	0.24524200
C	-3.36077400	-0.58714000	-0.97926800
H	-3.26014500	-0.25264300	-2.01907500
H	-4.19413200	-1.30199900	-0.95004400
C	-2.89266000	1.90547400	-0.39026800
H	-3.42474700	2.77562600	0.01738000
C	-2.83124100	2.04543700	-1.47645900
P	0.97947700	-0.76737200	1.63441000
P	2.06453400	0.07205200	-1.34370000
C	2.52395000	0.14348900	2.17509000
H	3.20597500	-0.57761200	2.64471300
H	2.21850100	0.84601500	2.95950000
C	3.54484800	0.11010200	-0.20096500
H	4.39828300	0.53334700	-0.74418000
H	3.81810900	-0.92137400	0.05560300
C	0.05818200	-0.80359700	3.24002600
H	-0.32915900	0.19430300	3.45863500
H	-0.78935300	-1.48861500	3.15262100
H	0.69741700	-1.13229000	4.06672300
C	-0.59533000	3.55567300	-0.44543000
H	-0.44938300	3.44501800	-1.52332300
H	-1.31943200	4.35687400	-0.25363100
C	0.36639400	3.82777600	-0.00032400
H	-1.44988900	2.43429700	2.00497200
C	-0.49061500	2.57949800	2.51166100
H	-2.03064700	3.36193300	2.07156900
H	-1.99057100	1.63856000	2.52609000
C	2.61809700	-1.22213800	-2.55008200
H	3.62665300	-1.03543700	-2.93782900
H	2.58828900	-2.20001700	-2.06148700
H	1.90815500	-1.24417700	-3.38162900
C	2.39918800	1.59223600	-2.35081100
H	1.62512400	1.67547100	-3.11810700
H	2.32444800	2.47165700	-1.70501400
H	3.38664900	1.57006700	-2.82597300
C	-2.40652900	-2.52387500	0.85901600
H	-1.62052300	-3.20533200	1.19771600
H	-2.66805000	-1.86707800	1.69417100
C	-3.28884300	-3.11305700	0.58289900
H	-1.81674200	-2.77352400	-1.90093900
C	-2.78871200	-3.27479300	-1.98502200
H	-1.57370900	-2.28491100	-2.84819100
H	-1.04104300	-3.51770600	-1.69899700
H	1.59783500	-2.51564000	1.60659000
C	2.30562500	-2.63217200	0.78178700
H	2.08508400	-2.80095300	2.54593200
H	0.75723800	-3.18843300	1.41627100
H	-0.50135500	0.40008000	-1.80774700
C	-3.68292400	0.62148800	-0.08168000
C	3.25836100	0.92170400	1.07300300
H	2.66188700	1.80445300	0.80890300
H	4.20010700	1.29670600	1.49149700
H	-4.75002700	0.84697800	-0.19556400
H	-3.55034400	0.34932100	0.97534100

A6**E= -879.94404708 a.u.**

Rh	0.13252900	0.00574600	-0.10044200
P	-1.30785500	-1.17726500	-1.49879800
P	-0.81854100	-0.49931000	1.97148700
C	-2.99777400	-1.35080700	-0.72836700
H	-3.46037700	-0.35692500	-0.76112500
H	-3.60747100	-2.00455200	-1.36654100
C	-2.64082200	-0.86670600	1.81078000
H	-3.01718800	-1.21847800	2.78105400
H	-3.13325100	0.09238800	1.60829200
P	2.06004300	-1.29001400	-0.20679200
P	1.37615600	1.91017000	-0.40165000
C	3.52771900	-0.65248300	0.76758300
H	4.44355800	-0.88799700	0.20950800
H	3.56616900	-1.23441700	1.69609500
C	3.21007000	1.76829900	-0.07147900
C	3.61524600	2.77117800	0.10906500
C	3.70246700	1.38959300	-0.97602000
H	2.08785300	-3.06647000	0.31591200
H	1.76553800	-3.14621600	1.35685100
H	1.38921900	-3.63504100	-0.30362700
H	3.08787300	-3.50198700	0.21421900

C	-0.90305800	0.80502000	3.28519300
H	-1.30066000	1.71943700	2.83687800
H	-1.53310200	0.50962000	4.13305300
H	0.10825800	1.01418800	3.64664800
C	-0.29717500	-1.94891000	3.01026700
H	0.75786300	-1.83657500	3.27899700
H	-0.89004500	-2.03621300	3.92839400
H	-0.40210900	-2.87077200	2.43022700
C	1.40148000	2.79990100	-2.02732500
H	2.03729900	3.69311100	-2.00981900
H	1.75536700	2.11340700	-2.80165500
H	0.37724400	3.08683800	-2.28191400
C	0.96222300	3.32527600	0.72234200
H	-0.10035000	3.55835400	0.61938700
H	1.13118200	3.01821200	1.75828800
H	1.55680300	4.22005800	0.50493600
C	-1.00472500	-2.95353500	-1.95428800
H	-0.06905300	-3.03780900	-2.51492400
H	-0.90589800	-3.54837100	-1.04144200
H	-1.81792000	-3.36672400	-2.56204400
C	-1.80032900	-0.51288400	-3.15623400
H	-2.60787900	-1.09313300	-3.61896200
H	-2.12033300	0.52460900	-3.03162400
C	-0.92626400	-0.52091200	-3.81401100
H	2.80437700	-1.46958600	-1.89567900
H	2.97037200	-0.47834800	-2.32487100
H	3.74999500	-2.02321200	-1.87864800
H	2.09285000	-1.99200000	-2.54115600
H	-1.08433900	1.04583100	-0.13780600
C	-3.00913200	2.69299100	-0.33010100
O	-3.13839300	2.49014800	-1.47038900
O	-2.91954000	2.92762900	0.80837300
C	-3.01496900	-1.88188800	0.71670900
C	3.49603400	0.84153800	1.12096300
H	-4.02990100	-2.24051800	0.92674900
H	-2.37030000	-2.76896300	0.79599800
H	2.73217700	1.00379000	1.89221800
H	4.45891300	1.10553400	1.57397000

A7**E= -879.96276654 a.u.**

Rh	0.13785600	-0.11778800	0.14407100
P	-1.41453100	-1.80126500	-0.30150600
P	-1.58834600	1.10815400	1.18901200
C	-3.12816800	-1.25617400	-0.73035000
H	-3.01855500	-0.66690900	-1.64626200
H	-3.70093200	-2.16078200	-0.97025500
C	-3.31206200	0.97699100	0.52242200
H	-3.96788400	1.53865800	1.19933900
H	-3.29865100	1.50418000	-0.43700500
P	1.94465400	-1.53000100	0.12925300
P	1.65718000	1.61584300	-0.27080700
C	3.31125700	-1.02676700	1.30541700
H	4.25726100	-1.39630000	0.88777700
H	3.13681200	-1.57755900	2.23591400
C	3.39742400	1.35130000	0.36494100
H	3.83815000	2.33212500	0.57177600
H	4.00638900	0.90020700	-0.42785300
C	1.76723600	-3.28439900	0.69237500
H	1.28813300	-3.29852200	1.67445700
H	1.15684500	-3.86267900	-0.00508200
H	2.75090400	-3.75931100	0.76908700
C	-1.56190700	2.92015400	1.51473200
H	-1.57335900	3.43437900	0.55170400
H	-2.44446200	3.20490700	2.09715900
H	-0.66693900	3.19818700	2.07442400
C	-1.81556400	0.46815500	2.91354300
H	-0.90759100	0.67293300	3.48713500
H	-2.67137600	0.93869100	3.41081300
H	-1.95724100	-0.61510800	2.89772500
C	1.90843000	1.77913400	-2.08629600
H	2.81539400	2.35508300	-2.29865500
H	1.96208900	0.79841200	-2.56081300
H	1.03369100	2.29629700	-2.48304500
C	1.40257700	3.38535600	0.16861700
H	0.45160300	3.70338600	-0.26209600
H	1.39046600	3.52133600	1.25258000
H	2.21325400	3.98594000	-0.25648200
C	-1.79140700	-3.17772400	0.87845000
H	-0.88604400	-3.72467500	1.14416600
H	-2.21625100	-2.76423400	1.79746400
C	-2.51311100	-3.87562400	0.44092500
H	-0.98489600	-2.68643500	-1.85753300
H	-1.76797600	-3.39820900	-2.13825300
H	-0.88399100	-1.91570800	-2.62752800
H	-0.03763000	-3.22075900	-1.75626700
C	2.88419700	-1.82053600	-1.44331200
C	3.32252500	-0.88502900	-1.79795000
H	3.68386900	-2.55669600	-1.30789500
H	2.19110200	-2.17314600	-2.21204000
H	-2.01865300	2.02562600	-3.44459700
H	-1.47737000	1.66876100	-2.53451200
C	-1.17680100	0.44882300	-2.51726400

O	-1.24269700	2.53415400	-1.65499600
C	-3.85424700	-0.44354000	0.34416300
C	3.42220500	0.46859000	1.61816300
H	-4.90986100	-0.36818500	0.05816300
H	-3.84723900	-0.97626400	1.30517000
H	2.59903800	0.75782300	2.28296500
H	4.35209200	0.63602600	2.17404900

A8

E= -879.94541843 a.u.

Rh	0.19114300	-0.13826700	-0.26109700
P	1.14262400	1.99627400	-0.28748400
P	2.17328300	-1.42548100	-0.02771500
C	2.90934800	1.94998400	-0.89175800
H	2.86268600	1.76170000	-1.97155300
H	3.33699100	2.95278300	-0.76019100
C	3.64186700	-0.52913200	-0.74120300
H	4.54739100	-1.11627100	-0.53818500
H	3.50339200	-0.51478000	-1.82917300
P	-0.84086200	-0.35279300	1.83281100
P	-1.55120100	-1.16671400	-1.34873100
C	-2.69700500	-0.51059300	1.84603600
H	-3.11131800	0.47128800	1.58854900
C	-3.00619900	-0.72114800	2.87762800
H	-3.24666900	-1.20704300	-0.58067100
H	-3.86730900	-1.91067600	-1.15043600
C	-3.68768800	-0.21291800	-0.71914400
H	-0.40931300	-1.85952000	2.82702800
H	-0.46617700	-2.74889800	2.19377000
H	0.61913500	-1.76332700	3.18301000
C	-1.07094700	-1.98360100	3.69149800
C	2.33840500	-3.01392200	-0.97305700
H	2.10032300	-2.82210300	-2.02315300
C	3.34793500	-3.43677100	-0.90396200
H	1.61805300	-3.74278800	-0.59086300
C	2.91917300	-1.98271400	1.58370000
C	2.28402300	-2.75190100	2.03118500
H	3.92395200	-2.39862200	1.44349100
H	2.97404200	-1.14005000	2.27946100
C	-1.99602100	-0.59685500	-3.05032100
H	-2.82528900	-1.17504800	-3.47389300
H	-2.26681100	0.46025700	-3.01319400
H	-1.11524800	-0.70080700	-3.68942000
C	-1.33160400	-2.98010200	-1.69038900
H	-0.41565700	-3.11634900	-2.27122100
H	-1.20502600	-3.51321400	-0.74342500
H	-2.17717100	-3.41035700	-2.23977600
C	1.37579100	3.03348000	1.23448700
H	0.40078100	3.29795200	1.65064100
H	1.92344300	2.46057000	1.98816400
H	1.92943200	3.95318100	1.01309500
C	0.53832600	3.31962500	-1.44510700
H	1.28120600	4.11635400	-1.57239400
H	0.31638900	2.86791900	-2.41484700
H	-0.37698100	3.76981100	-1.05297700
C	-0.65402200	0.92892300	3.15451000
H	-1.07877000	1.87234700	2.80507100
H	-1.15768500	0.62857600	4.07970300
H	0.40849100	1.08441800	3.35888500
H	0.73164900	-0.02972900	-1.76564600
C	-2.61353700	2.56649200	-0.30360600
O	-2.27056400	2.91944300	0.75408400
O	-3.00526000	2.26038100	-1.35681100
C	3.82524300	0.90885900	-0.23101300
H	4.86389100	1.20589600	-0.41953900
C	3.70264400	0.93990300	0.86121100
C	-3.27242400	-1.58088200	0.90727200
H	-4.31437600	-1.76386500	1.19621100
H	-2.75102000	-2.53519800	1.06391800

A10

E= -880.39574194 a.u.

Rh	-0.07753600	0.05496500	-0.35933400
P	-0.61055100	2.31369900	-0.03737600
P	-2.36399200	-0.58532400	0.06921100
C	-2.42640200	2.67684100	-0.04716300
H	-2.84965900	2.43254700	0.93429700
H	-2.53998800	3.75884300	-0.17458100
C	-3.60339800	0.50003700	-0.80338100
H	-3.88585100	-0.02632600	-1.72118300
H	-4.50102000	0.53508600	-0.17472900
P	0.71025100	-1.94617400	-1.26731800
P	1.00891000	-0.49842100	1.73274400
C	0.49321200	-3.46726800	-0.21404300
H	1.34303200	-4.13021900	-0.41535800
H	-0.39880600	-3.98734000	-0.57924900
C	1.44194200	-2.30270700	1.88642600
H	1.59844500	-2.51848700	2.94852700
H	2.40537600	-2.47500500	1.39353000
C	0.01668900	-2.46613700	-2.88441000
H	-1.06505300	-2.58924000	-2.81177000
H	0.22453500	-1.68748700	-3.62167700
H	0.46455600	-3.40810400	-3.21426400
C	-2.95784300	-0.53558700	1.81805900
H	-2.68998300	0.41142200	2.29287100
H	-4.04280300	-0.66649900	1.87022800
H	-2.48792500	-1.34561100	2.38195100
C	-2.98711800	-2.24750900	-0.43006300
H	-2.47467500	-3.03200000	0.13193000
H	-4.06153600	-2.32902900	-0.24035900
H	-2.81009300	-2.40590500	-1.49598800
C	2.64930500	0.29284100	1.98900800
H	3.12031500	-0.05557400	2.91275500
H	3.29761100	0.04396600	1.14497600
H	2.53739200	1.37855200	2.03325500
C	0.19171700	-0.20460500	3.36099900
H	-0.20272800	0.81149800	3.41950100
H	-0.63914100	-0.90084600	3.49129200
H	0.90291600	-0.35546500	4.17835800
C	-0.00122700	3.38608400	-1.39510700
H	1.08791400	3.33587100	-1.42679000
H	-0.38902900	3.02014400	-2.34786900
H	-0.31159600	4.42373800	-1.24282900
C	-0.02555800	3.20361100	1.45943700
H	-0.34649700	4.24920000	1.43314900
H	-0.42718900	2.73676700	2.36142800
H	1.06600200	3.17541500	1.49689000
C	2.51112600	-1.92422700	-1.63088300
H	3.08146900	-1.68861800	-0.73006000
H	2.84422200	-2.88734000	-2.02880900
H	2.71155900	-1.13831100	-2.36211800
H	1.31365000	0.62967000	-0.83602200

A9

E= -879.94935964 a.u.

Rh	-0.04766500	-0.06264200	-0.34923300
P	-1.98312700	-1.40397200	-0.35340500
P	-1.37588000	1.93399700	0.27242200
C	-3.52278700	-0.55851300	-0.95079600
H	-3.36402500	-0.35707700	-2.01695800
H	-4.33766800	-1.28959800	-0.88094900
C	-3.04262100	1.94491400	-0.54869900
H	-3.55869900	2.86566700	-0.24828400
H	-2.86687600	2.00760900	-1.62929700
P	1.06982900	-0.48629700	1.76731500
P	1.93527400	0.85552200	-1.19493000
C	2.82809500	-1.04760400	1.57668400
H	2.77679400	-2.02693500	1.09161100
H	3.23387100	-1.19275700	2.58595100
C	3.48742100	-0.03110700	-0.71760000
H	4.32252500	0.48114800	-1.21189700
H	3.41222400	-1.03459700	-1.14828700
C	1.29765400	0.93223400	2.94241700
H	1.59317600	1.83743600	2.40470800

H	-0.55018300	0.38406200	-1.83197000
C	3.76086100	1.98122800	-0.80760300
O	4.25726200	1.04571700	-1.29052200
O	3.26577700	2.91526600	-0.31486800
C	-3.16003200	1.92285800	-1.16803700
H	-4.05216000	2.48702700	-1.45668400
H	-2.52542100	1.88268100	-2.06044400
C	0.36489700	-3.22741600	1.29734500
H	0.40699300	-4.19949100	1.79815900
H	-0.62814700	-2.81589500	1.51977600

A11

E= -880.39991528 a.u.

Rh	-0.10039200	-0.06939900	-0.37116400
P	-2.17700900	1.08968700	-0.34436900
P	-1.18094800	-1.76834000	0.72105600
C	-3.66394200	-0.02754300	-0.27920600
H	-3.94522200	-0.19795900	0.76582500
H	-4.49310100	0.52643300	-0.73074100
C	-2.65760200	-2.39671700	-0.20452000
H	-2.29183600	-3.17817400	-0.87867500
C	-3.30647800	-2.88720700	0.53051800
P	1.91193900	-1.08013500	-1.14961500
P	1.15780900	0.80869300	1.57803700
C	3.36329800	0.05451600	-1.00977000
H	3.12888700	0.92119300	-1.63340700
H	4.20698500	-0.46667400	-1.47727300
C	2.79722500	1.50176300	1.06827800
H	3.26594900	1.90239100	1.97456400
H	2.60286300	2.35256400	0.41023900
C	2.59099900	-2.67100800	-0.52309000
H	2.72304100	-2.64902500	0.56080300
H	1.92418600	-3.49631000	-0.77801400
C	3.56279200	-2.85868200	-0.98898200
H	-1.85537100	-1.31767000	2.37682700
H	-2.34813700	-0.34524900	2.35534600
C	-2.57143400	-2.07264800	2.71337500
H	-1.04235600	-1.26955400	3.10238100
C	-0.30485600	-3.32958600	1.11955300
H	0.59216500	-3.12089600	1.70554500
H	-0.96269400	-3.98340100	1.69929900
H	-0.01965700	-3.84590300	0.20176400
C	0.48679300	2.13203100	2.65796800
H	1.20961500	2.39466800	3.43590700
H	0.27356200	3.00584500	2.04064000
H	-0.43556000	1.79140500	3.13524700
C	1.71378900	-0.43317600	2.83459000
H	0.88392900	-0.73666900	3.47563200
H	2.11953700	-1.32657400	2.35398000
C	2.48913500	-0.00381200	3.47661600
H	-2.43373800	1.96809900	-1.93313600
H	-1.76916800	2.83024500	-1.98104800
C	-2.20712000	1.30096300	-2.76647900
H	-3.46857000	2.31456700	-2.00207900
C	-2.56410300	2.35916500	0.91724400
H	-3.56146700	2.77167600	0.73866300
H	-2.53330500	1.92948900	1.92086800
H	-1.81609500	3.14981100	0.84181300
C	1.80165400	-1.35566200	-2.95565500
H	1.45971000	-0.42527900	-3.41411300
H	2.77117200	-1.64306600	-3.37253800
H	1.06812000	-2.13859500	-3.16103000
H	1.18589300	3.29455800	-2.16421400
C	-0.74438000	-0.68917000	-1.66022400
H	0.71751100	2.66543500	-1.38615500
O	0.71308400	1.41563400	-1.68611900
O	0.26339000	3.18108000	-0.36444500
C	-3.45081200	-1.35821900	-1.01016200
H	-4.42244700	-1.79538300	-1.25865200
H	-2.94377500	-1.17576200	-1.96364000
C	3.75740500	0.50633500	0.40179700
H	3.92163300	-0.36248500	1.05171500
H	4.73310600	0.99675400	0.32324200

A12

E= -690.93775309 a.u.

Rh	-0.07360800	-0.08468700	-0.42765600
P	-2.19606500	0.98512500	-0.58458700
P	-0.96535400	-1.50942400	1.04613300
C	-3.65382600	-0.08634600	-0.20439800
H	-3.93048600	0.06686000	0.84544200
H	-4.49105400	0.28970900	-0.80147100
C	-2.57561400	-2.28441300	0.57699300
H	-2.34100900	-3.29852300	0.23794300
H	-3.14824700	-2.38323600	1.50677500
P	2.01541100	-1.11164200	-0.90819800
P	1.18893300	1.84502900	0.52731600
C	3.35090800	-1.02466100	0.36936200
H	4.30035400	-0.88309400	-0.16023200
H	3.40764800	-2.01173500	0.84043100
C	2.96664600	1.47133500	0.89684200

H	3.30388700	2.22023900	1.62060100
H	3.56413100	1.63207100	-0.00705000
C	2.07333600	-2.83887200	-1.51404700
H	1.88340500	-3.54786200	-0.70713600
H	1.32499300	-2.97887400	-2.29727400
C	3.06386100	-3.04922900	-1.92743900
H	-1.25228900	-0.61933500	2.61891700
H	-1.93286200	0.22202300	2.47671600
H	-1.68737000	-1.30763700	3.35020700
H	-0.30412300	-0.24640900	3.01069300
C	0.09512100	-2.91398900	1.52525400
H	1.07338200	-2.55922100	1.85828500
H	-0.38302300	-3.45117300	2.35046900
H	0.21217500	-3.60081200	0.68586600
C	1.27410200	3.31720700	-0.57062600
H	1.93303900	4.07655000	-0.14002200
H	1.65907500	3.04070500	-1.55555900
H	0.28208100	3.75532100	-0.70251100
C	0.59971800	2.52107600	2.13194300
H	-0.46751500	2.74171400	2.09974300
H	0.78424000	1.79740500	2.92942000
H	1.14321800	3.44003700	2.36911600
C	-2.35708300	1.39363700	-2.36631800
H	-1.54345500	2.05225400	-2.68149700
H	-2.31921700	0.47972900	-2.96365600
H	-3.30776800	1.90218700	-2.55079400
C	-2.59851200	2.54888200	0.28217600
H	-3.58479200	2.89926200	-0.03630900
H	-2.62353200	2.39532200	1.36377400
H	-1.86691500	3.32488200	0.04886100
C	2.63055600	-0.16387600	-2.36143300
H	2.75995000	0.89427700	-2.12588100
H	3.59336700	-0.56677100	-2.68920600
H	1.92007000	-0.25487500	-3.18758800
H	-0.69651900	-1.28120000	-1.23070800
C	-3.40969300	-1.57044600	-0.49243800
H	-4.37269700	-2.08401600	-0.55827900
H	-2.93301100	-1.69488200	-1.47168000
C	3.18235100	0.05307000	1.44878500
H	2.35604200	-0.22052900	2.11933100
H	4.08285000	0.04452900	2.06912500

A13

E= -1461.38937169 a.u.

Rh	1.57165800	0.07556400	-0.06984400
P	1.36392800	2.24429000	-1.06195800
P	1.37437300	1.13474800	1.95297200
C	0.62685900	3.54133600	0.01218600
H	1.41004800	3.99415700	0.62944700
H	0.27509900	4.32776800	-0.66422800
C	-0.13228800	2.19860500	2.09511900
H	-0.95896000	1.52214200	2.34176300
H	0.03318400	2.84830400	2.96251700
P	1.25808600	-2.24224900	0.422110900
P	4.04695000	-0.29547100	0.00222200
C	2.45611900	-3.33460800	-0.47195500
H	2.24981800	-3.18875200	-1.53630600
H	2.16404500	-4.36251300	-0.22577200
C	4.56183900	-1.87744700	-0.80805100
H	5.65420400	-1.93034400	-0.73200400
H	4.31837600	-1.79831400	-1.87107300
C	1.29758200	-2.92528300	2.12862000
H	2.24552600	-2.69368200	2.62029200
H	0.48275100	-2.50870300	2.72292500
H	1.17885700	-4.01215300	2.09164200
C	2.76448700	2.28442500	2.35779500
H	3.19777200	2.71700700	1.45411900
H	2.41658400	3.08995300	3.01022800
H	3.54652000	1.73732700	2.88660500
C	1.26090900	0.17038600	3.51033800
H	2.13426800	-0.47445300	3.62462500
H	1.21421000	0.85767400	4.36020900
H	0.35931800	-0.44442300	3.50766200
C	5.25836100	0.89378900	-0.70116200
H	6.27737700	0.51718700	-0.57041800
H	5.04563500	1.02057600	-1.76336600
H	5.17676300	1.85911400	-0.19532300
C	4.77076700	-0.56277900	1.68822900
H	4.93822300	0.39522800	2.18325900
H	4.10688300	-1.16507400	2.31339600
H	5.73622800	-1.07248500	1.61273700
C	0.14914300	2.15162800	-2.43271000
H	0.45671600	1.40688600	-3.16605100
H	-0.82828600	1.86429700	-2.03484300
H	0.07727300	3.13020600	-2.91596100
C	2.81044300	3.08400800	-1.78528000
H	2.48608500	4.02437600	-2.24078600
H	3.54803400	3.30493000	-1.01040100
H	3.26021500	2.43705800	-2.53958600
C	-0.31493100	-2.87554000	-0.26573800
H	-0.27827000	-2.72170700	-1.34628300
H	-0.41574400	-3.94408700	-0.05171800
H	-1.17754100	-2.32843900	0.12336600

H	1.88355000	-1.14059500	-3.90348200
H	0.01409900	0.17701700	-0.03781000
C	2.14675600	-0.58714000	-2.98342200
O	1.34789200	-0.83010700	-2.00599900
O	3.11811600	0.16821300	-2.97659700
C	-0.53402000	3.01511900	0.85917900
H	-1.14823100	3.85738000	1.19303800
H	-1.18621200	2.39025800	0.24021000
C	3.95048200	-3.14474700	-0.19916100
H	4.15560600	-3.19313500	0.87798300
H	4.47261900	-4.00425600	-0.63243000
P	-3.09368300	0.34232600	0.37156300
N	-3.10036700	-1.33713500	0.88980000
N	-3.14811000	0.36086800	-1.37164800
C	-4.53804900	1.12950000	0.90736300
N	-2.20508400	-0.51319000	-2.04926100
H	-1.23612000	-0.49955800	-1.54294900
C	-4.30473100	2.43873000	1.51082700
H	-4.91025000	2.55513900	2.41835500
C	-2.40114700	-1.46858700	2.16438000
H	-1.52924000	-0.80637400	2.17365400
C	-5.95062600	0.98064100	0.55401400
H	-6.21941800	1.69950600	-0.23623500
H	-6.54395100	1.27238300	1.43156400
C	-6.40195800	-0.42286200	0.14273700
H	-6.46564800	-1.05248400	1.03387900
H	-7.42985000	-0.32928900	-0.24809200
C	-4.35654900	0.66415500	-2.11797100
H	-4.79959200	1.57164400	-1.70169000
H	-4.07346200	0.90516500	-3.15037200
C	-5.38481400	-0.48726200	-2.11412700
H	-6.34993100	-0.11493300	-2.49127500
H	-5.06209400	-1.26917300	-2.80986900
C	-4.16442900	-2.33307500	0.81327200
H	-4.85117400	-2.21537000	1.66894300
C	-3.70855400	-3.32734200	0.92919600
C	-4.95649800	-2.34011100	-0.48714800
H	-4.29106300	-2.62683800	-1.30634300
H	-5.71700200	-3.13675500	-0.40076300
N	-5.53182800	-1.06031700	-0.80477800
H	-2.53536800	-1.56211000	-2.10530800
H	-2.04499200	-0.15231400	-3.07169900
H	-2.05114900	-2.50173000	2.29322700
H	-3.03587000	-1.22251400	3.03071500
H	-3.25376200	2.54376400	1.78849300
H	-4.56320900	3.25992600	0.82409000

H	3.02435600	1.56651600	-3.64042000
C	1.21301300	-1.22252200	2.71906600
H	0.50031900	-1.56171600	1.95987500
H	1.29613600	-1.96713000	3.51749100
H	0.84793300	-0.28290900	3.14201800
H	-0.56429900	-3.65150800	-0.80595900
H	-2.43158400	-0.42678800	-0.38708800
C	-0.05919800	-2.67479700	-0.60615600
O	-0.79067800	-1.77736900	-0.09360000
O	1.14600200	-2.59951500	-0.91066400
C	-0.62445800	2.32501100	-0.09430200
H	-1.62718400	2.76859100	-0.11153000
H	-0.75966000	1.23722200	-0.03242800
C	4.58618500	-2.87730300	0.72388900
H	5.36843900	-2.18098600	1.05701500
H	4.99610600	-3.88038800	0.88297900
P	-3.80398200	-0.32998500	-0.10973100
N	-3.63799900	-0.28057400	1.57056500
N	-4.34444000	-1.72362100	-0.90822100
C	-4.17563800	1.07093800	-0.99563200
N	-3.84742900	-3.00396100	-0.39659900
C	-2.81081600	-2.86979500	-0.06910200
H	-3.33652700	1.36275300	-2.15590800
C	-3.23659800	2.44716100	-2.27206800
H	-2.29831900	-0.10385700	2.13672800
C	-1.53733100	-0.46726800	1.44227400
H	-5.52813100	1.59280200	-1.11545900
H	-6.01945600	1.20221800	-2.02008400
H	-5.48639200	2.68238100	-1.22085100
C	-6.31913500	1.22569200	0.13000700
H	-5.99400000	1.85353700	0.96314300
H	-7.39388200	1.38421700	-0.01605900
C	-5.69125300	-1.66737600	-1.44387900
H	-5.70522300	-1.00019700	-2.31237300
H	-5.97715200	-2.65915200	-1.80152600
C	-6.68763600	-1.17376400	-0.37632400
H	-7.58963500	-0.75915100	-0.83817500
H	-6.99572900	-2.00717700	0.25812200
C	-4.71664400	0.06622500	2.47737300
H	-4.74636500	1.15353000	2.65027200
H	-4.53737300	-0.40500700	3.44913200
C	-6.02195300	-0.45213700	1.90118300
H	-6.05967500	-1.53556600	2.03206900
H	-6.89371000	-0.01250100	2.40066500
H	-6.01429700	-0.16934300	0.46204000
N	-4.44948100	-3.38450000	0.44076400
H	-3.85808900	-3.73890000	-1.20557400
H	-2.21943300	-0.69790100	3.05270600
H	-2.11400200	0.95023200	2.38469200
H	-2.33959300	0.94130300	-2.02212800
H	-3.76510000	0.94741200	-3.07823900

A14

E= -1461.39692298 a.u.

Rh	2.50770000	0.41671700	0.02981900
P	1.41740900	1.38950100	-1.79591400
P	1.88901800	2.26415200	1.26426900
C	0.12733200	2.67379600	-1.38727900
H	0.59282400	3.66247300	-1.30628900
H	-0.55793400	2.72365400	-2.24077200
C	0.10603600	2.80051100	1.16426700
H	-0.38848900	2.39400500	2.05359600
H	0.06314700	3.89416600	1.24788700
P	2.82800700	-0.97096000	1.87177400
P	3.81005900	-1.01647200	-1.32977200
C	3.31628000	-2.72396900	1.56745700
C	2.47482900	-3.20056900	1.05372200
H	3.43906700	-3.20225000	2.54599900
C	4.30711300	-2.70957000	-0.76897500
H	5.18839200	-2.99313300	-1.35688600
H	3.48052600	-3.36694400	-1.05739900
C	3.98618200	-0.54204600	3.24581400
C	5.00097900	-0.45403000	2.84878100
H	3.72041100	0.41062100	3.70346100
H	3.97247500	-1.31800500	4.01742300
C	2.81739100	3.74504900	0.65731500
C	2.67446400	3.88321100	-0.41570200
H	2.50687700	4.65447500	1.18187500
H	3.88347500	3.57722900	0.83019600
C	2.16639300	2.50086400	3.07665900
C	3.23863200	2.50306800	3.28688800
H	1.75015500	3.46203700	3.39426200
H	1.69435700	1.70617500	3.65867600
C	3.38272200	-1.46495200	-3.06662900
H	4.21559000	-2.01101400	-3.52036100
H	2.50298400	-2.11304400	-3.03731900
C	3.17342200	-0.58608600	-3.67913400
C	5.44661600	-0.18584400	-1.54776500
H	5.30278600	0.79729900	-2.00344600
H	5.91116200	-0.03543000	-0.56982300
H	6.11669600	-0.78039400	-2.17716500
C	0.33818800	0.16032600	-2.63591700
C	0.93022900	-0.65218600	-3.05138300
H	-0.31189800	-0.29245300	-1.87984600
H	-0.24619500	0.63519200	-3.43158600
C	2.29345500	2.23582000	-3.18256600
H	1.58875300	2.56894800	-3.95089600
H	2.83332100	3.10414300	-2.79473600

A7'

E= -881.14071614 a.u.

P	1.33350400	1.82215000	-0.43631700
P	1.59398600	-1.13766700	1.11824800
C	3.10645500	1.34450300	-0.62670200
H	3.14666300	0.62598700	-1.45265900
C	3.65760700	2.24292600	-0.92794900
H	3.38279800	-0.75224100	0.81203500
H	3.95937000	-1.17536400	1.64433800
H	3.63637900	-1.30330800	-0.09893600
P	-1.59206900	-1.72409000	-0.03364600
C	-1.85615400	1.48891100	0.50470500
P	-3.31503700	-1.46818900	-0.72587800
H	-4.00199200	-2.07142400	-0.11921000
H	-3.31599000	-1.89996200	-1.73153700
C	-3.57130100	0.77251700	0.49174000
H	-4.29302000	1.59046900	0.59594500
H	-3.69248100	0.13076100	1.37319600
C	-1.02485100	-3.09964700	-1.11029400
H	-0.90506300	-2.69049100	-2.11613400
H	-0.04993500	-3.46655200	-0.79100500
H	-1.75428000	-3.91581400	-1.11813300
C	1.75774800	-2.97923700	1.12533100
H	2.01091700	-3.28207100	0.10616200
H	2.55688300	-3.28418000	1.80939200
H	0.83247800	-3.47004000	1.43481000
C	1.46736800	-0.79371100	2.93719700
H	0.47177400	-1.07641100	3.29016100
H	2.22554300	-1.33477800	3.51516100
C	1.58304300	0.28057500	3.10731300
H	-1.78318500	2.15330400	2.23083500
H	-2.63925900	2.79789300	2.46001100
H	-1.76183600	1.31200300	2.92842200
H	-0.85856700	2.71926600	2.36704300
C	-2.20738000	3.05606000	-0.42940000
C	-1.34415400	3.72477600	-0.39373700
H	-2.40433500	2.81862100	-1.47859100
H	-3.07041100	3.58348200	-0.00945500
C	1.48623500	3.28678800	0.68400500
C	0.52890000	3.80741200	0.76186400
H	1.77120400	2.95943300	1.68744100

H	2.23716800	3.99073000	0.31072200
C	1.00638000	2.59644300	-2.07111000
H	0.04803200	3.11855800	-2.06190700
H	1.79994400	3.30117800	-2.33986100
H	0.94928800	1.78208100	-2.79831300
C	-2.00021400	-2.56428700	1.56393700
H	-2.53481200	-1.86068300	2.20849000
H	-2.62599000	-3.44839300	1.40394000
H	-1.08793400	-2.86368000	2.08331700
H	-1.43939700	-0.43164000	-3.33505300
H	-2.13184700	-0.47857000	-3.62420400
O	0.59681400	-0.49851800	-2.43655600
C	1.50707600	-1.34604000	-2.66866600
H	1.68259300	-1.56757100	-3.74810400
O	2.22086300	-1.95090700	-1.84412900
Rh	-0.14145900	0.08250500	0.00775800
C	-3.81950700	-0.02377200	-0.79666800
H	-4.89160100	-0.04377800	-1.02233000
H	-3.33512100	0.48056200	-1.64120200
C	3.73672200	0.72380400	0.62725900
H	4.82640800	0.80158300	0.53786000
H	3.47320900	1.30173000	1.52434500

A8'

E= -881.14103547 a.u.

P	1.36546200	1.41837200	-1.28902700
P	0.94498300	0.33488000	1.83838700
C	3.11073300	1.44602200	-0.65710800
H	3.54941000	0.46879000	-0.88964000
H	3.66913200	2.19353600	-1.23433400
C	2.78513600	0.60531500	1.76338700
H	3.13340300	0.79859600	2.78567800
H	3.24735900	-0.33651100	1.44508200
P	-1.22719900	-1.99612800	-0.00763000
P	-2.28486600	1.23376600	0.07963400
C	-2.72151200	-2.13057100	-1.12466300
H	-3.42510500	-2.83170100	-0.65680000
H	-2.36336000	-2.60799700	-2.04381800
C	-3.73420100	0.12108700	-0.32809400
H	-4.60328700	0.75235400	-0.55183600
H	-3.99000200	-0.45054800	0.57333500
C	-0.45193000	-3.63554200	-0.38377600
H	0.01637500	-3.60277600	-1.37024400
H	0.32421700	-3.85672200	0.35457900
C	-1.19657300	-4.43888600	-0.35917800
H	0.90799100	-0.97334800	3.14875900
H	1.24024000	-1.92763100	2.72980800
H	1.55400200	-0.71152200	3.99342500
H	-0.11548700	-1.09403200	3.51249500
C	0.45783700	1.79850800	2.86708600
H	-0.57122000	1.66301300	3.20928500
H	1.11002000	1.92877600	3.73762500
H	0.48829600	2.70274500	2.25299600
C	-2.95550800	1.99511300	1.63635900
H	-3.98074200	2.36020900	1.50397600
H	-2.94713800	1.25082600	2.43871900
C	-2.32024800	2.83135700	1.94197100
H	-2.62991300	2.62595600	-1.09665900
H	-1.97501300	3.46749100	-0.85429000
H	-2.39950100	2.29927700	-2.11449200
C	-3.67209300	2.96220600	-1.04894200
H	1.00736000	3.23762800	-1.34309400
H	0.08211300	3.39441300	-1.90303800
H	0.85614700	3.61963000	-0.32939600
H	1.81554500	3.79828000	-1.82562800
C	1.67870500	1.10384100	-3.07876000
H	0.73132300	1.18516400	-3.61742100
H	2.39979100	1.81744100	-3.49219300
H	2.05781200	0.08673700	-3.20280900
C	-1.96994800	-2.41539900	1.64240400
H	-2.47210500	-1.53814800	2.05897800
H	-2.68534100	-3.24141100	1.56903400
H	-1.17296200	-2.70778000	2.33057400
H	1.42239900	-1.31802300	-1.14695700
H	-0.62537900	-0.17620600	-1.73144300
O	2.18343000	-1.88313500	-1.50836000
C	2.78915600	-2.49755600	-0.50732000
H	2.31594100	-2.30379700	0.47389900
O	3.76070100	-3.20426100	-0.63054200
Rh	-0.16287800	0.06805000	-0.22073200
C	-3.44507600	-0.82973500	-1.50037900
H	-4.38953200	-1.10092500	-1.98652700
H	-2.85026300	-0.30213900	-2.25435400
C	3.25390200	1.73886200	0.84147300
H	4.31322800	1.92636600	1.05161400
H	2.73296000	2.67202300	1.09626200

TS_{A1-2}

E= -691.84886007 a.u.

Rh	0.00555000	0.04594800	-0.63855000
P	-2.19740100	0.84089100	-0.70299800

P	-0.73158000	-1.83916000	0.65618900
C	-3.28540000	0.52016100	0.75487400
H	-2.89133300	1.10324000	1.59534300
H	-4.27291900	0.93228500	0.51752600
C	-2.16302100	-1.55536400	1.80110700
H	-2.41369300	-2.51816800	2.26137200
H	-1.80366800	-0.90151400	2.60545600
P	2.19672100	-0.73153900	-0.83866100
P	0.84250000	1.85344500	0.70556200
C	3.24765800	-0.77487900	0.69586100
H	4.27523700	-0.54244000	0.39192000
H	3.25842100	-1.80842700	1.05692200
C	2.55309100	1.60418400	1.39652200
H	2.67287700	2.29182400	2.24046200
C	3.28385400	1.91626400	0.64121900
C	2.41745100	-2.42026100	-1.53015200
H	1.94539600	-3.16303800	-0.88314400
H	1.93859000	-2.46762400	-2.51122400
H	3.47893200	-2.66341800	-1.63433600
C	0.39986400	-2.71458500	1.82517800
H	0.72157100	-2.03294100	2.61590800
H	-0.10713500	-3.56913300	2.28336900
H	1.28688800	-3.08172700	1.30473500
C	-1.33644100	-3.25557600	-0.35981500
H	-0.52223100	-3.61644500	-0.99329800
H	-1.70265100	-4.07818400	0.26240900
H	-2.13752500	-2.91984000	-1.02223900
C	1.04231200	3.50989000	-0.07924400
H	1.52100700	4.21776200	0.60470000
H	1.65379800	3.40715700	-0.97921600
C	0.07269400	3.91098400	-0.37995000
H	-0.08833000	2.27202900	2.24507800
H	-1.11885000	2.54294800	2.00165900
H	-0.11634200	1.39759800	2.90131500
H	0.37366200	3.10724600	2.78026600
C	-3.15913800	0.13378200	-2.10052900
H	-2.67275800	0.41031600	-3.03903000
H	-3.16772200	-0.95628800	-2.03756000
H	-4.18778100	0.50619000	-2.10195300
C	-2.44113700	2.64548400	-0.95647700
H	-3.49721000	2.87135500	-1.12978700
H	-2.10617900	3.20088600	-0.07723200
H	-1.85597400	2.97107700	-1.81980900
C	3.18675800	0.27685200	-2.01567100
H	3.22706000	1.31534900	-1.67999000
H	4.20485300	-0.11173000	-2.11211400
H	2.69803000	0.25795400	-2.99269200
H	0.11739300	0.55503900	-2.21912800
C	-0.20378000	-0.42435300	-2.22249100
C	2.81575200	0.15792000	1.83475900
H	3.59976100	0.14319400	2.59805600
H	1.91624100	-0.24489100	2.31339200
C	-3.42139700	-0.95066900	1.16787300
H	-4.23125700	-1.01652700	1.90144400
H	-3.74872800	-1.55800300	0.31490700

TS_{A3-4}

E= -1272.81021989 a.u.

Rh	1.33483200	0.07024100	-0.23533700
P	1.53144500	2.29529400	-0.85560900
P	1.52930300	0.64922200	2.04398500
C	0.70028500	3.59735800	0.20926100
H	1.45094200	4.34845600	0.48158700
H	-0.04250800	4.11796800	-0.40343500
C	1.03041500	2.40500600	2.45900100
H	0.61734300	2.40386500	3.47393500
H	1.94736500	3.00613600	2.50313600
P	0.84089500	-2.21476900	0.01873800
P	3.67495700	-0.62561800	-0.89760900
C	2.12317500	-3.24817000	0.91076100
H	1.99231700	-4.27604900	0.54898100
H	1.82822300	-3.25746700	1.96693200
C	4.04774800	-2.42751500	-0.60114100
H	5.12422000	-2.58654400	-0.72884700
C	3.55231200	-3.03700100	-1.36416700
H	-0.64200900	-2.93313400	0.85515900
H	-0.80939400	-2.46924800	1.82807200
H	-1.50588600	-2.73994800	0.21991000
H	-0.51892100	-4.01409900	0.97964700
C	3.16090500	0.61074700	2.91640300
C	3.88650300	1.20412300	2.35342300
H	3.08257100	1.01342700	3.93165100
H	3.53063600	-0.41628000	2.97554400
C	0.51632700	-0.33269100	3.23860100
H	0.90245900	-1.35645000	3.26230900
H	0.55852800	0.08067200	4.25128600
H	-0.51869800	-0.37301000	2.89304600
C	4.03719400	-0.48817400	-2.70499300
H	4.99417000	-0.94786300	-2.97268700
H	3.23051800	-0.97159800	-3.26245800
H	4.05878000	0.56461400	-3.00110100
C	5.23950900	0.07007500	-0.17629200
H	5.27633400	1.15506800	-0.28642100

H	5.28184100	-0.16244300	0.89145600
H	6.12244700	-0.36052900	-0.66076400
C	1.03699700	2.76631500	-2.57054000
H	1.64888300	2.18258700	-3.26343300
H	-0.00695600	2.50852100	-2.75559400
C	1.19086600	3.83315700	-2.76063200
H	3.25308800	2.97167600	-0.85625800
H	3.25849400	4.03522400	-1.11418100
H	3.69766200	2.84296100	0.13438000
C	3.86467300	2.43361700	-1.58385100
H	0.68649300	-3.09249900	-1.59973300
H	1.50590900	-2.81935200	-2.26607500
H	0.65782200	-4.17943600	-1.47206000
H	-0.24397600	-2.75972500	-2.06497000
H	0.88128200	-0.17104300	-1.75385800
H	-0.77315700	0.33216000	-0.14148300
P	-2.40724800	0.12478200	-0.13365200
N	-3.21371900	1.57145000	-0.57179100
N	-2.80536600	-0.42095700	1.44035600
N	-2.58711300	-1.13083300	-1.28018400
C	-2.89502400	0.66942000	2.41452800
C	-2.09709400	1.39595700	2.25385200
H	-2.04640500	-0.66246000	-2.56717900
C	-2.75348800	-0.02175900	-3.11426000
H	-2.35712600	2.60418900	-1.14442100
C	-1.31313100	2.35579600	-0.96540800
C	-3.73566700	-2.03281900	-1.41079000
H	-3.66016000	-2.83370200	-0.67007800
H	-3.66254700	-2.52042300	-2.38703400
C	-5.09217100	-1.32845700	-1.28195700
H	-5.25728400	-0.69717300	-2.16007100
H	-5.89574500	-2.08159700	-1.26920600
C	-3.76348600	-1.49321300	1.68788700
H	-3.39170300	-2.40999400	1.23047100
H	-3.78175500	-1.68071600	2.76640300
C	-5.18239900	-1.15683900	1.17995500
H	-5.78154900	-2.07709900	1.12722600
H	-5.68292900	-0.49637100	1.89372700
C	-4.59609200	1.70149800	-1.03488800
C	-4.65513400	1.44641800	-2.10591000
H	-4.88282200	2.75673300	-0.95309200
C	-5.57938000	0.86415800	-0.23028700
H	-5.66655200	1.29077500	0.77243800
H	-6.57291100	0.93144800	-0.70147400
N	-5.10387000	-0.49509200	-0.10161800
H	-3.85063300	1.20899200	2.36847900
H	-2.77257900	0.25401500	3.41906600
H	-2.56616800	3.57838100	-0.68667700
H	-2.50510500	2.69106500	-2.23025500
H	-1.10944100	-0.12061500	-2.40102200
H	-1.80924900	-1.52598000	-3.19465500
C	0.04278700	3.05322500	1.47970900
H	-0.47273900	3.87917900	1.98339000
C	0.72516300	2.32688800	1.19611100
H	3.59822300	-2.84546800	0.80615200
H	4.20509500	-3.68833200	1.15358000
H	3.79961300	-2.02619200	1.50654600

TS_{A8-9}

E= -879.93960211 a.u.

Rh	0.08460100	-0.01829900	-0.27508600
P	1.77759700	1.60204500	-0.23860700
P	1.55945600	-1.91509700	0.03688900
C	3.42372800	0.95998300	-0.82989400
H	3.32697700	0.81378500	-1.91265300
H	4.15819800	1.76153900	-0.67987600
C	3.24737900	-1.60872300	-0.68260400
H	3.87747800	-2.48215200	-0.46916600
C	3.12333100	-1.55635700	-1.77112100
H	-1.01477500	0.12052600	1.82369700
P	-1.86320100	-0.78729600	-1.26832800
C	-2.83220800	0.52164600	1.77825300
H	-2.91959000	1.56364000	1.45501600
H	-3.20271700	0.47052500	2.80990700
C	-3.49715900	-0.17941300	-0.62267600
H	-4.29314900	-0.70053600	-1.17011500
H	-3.57869700	0.88374200	-0.87495300
C	-1.06767100	-1.42002800	2.85526300
H	-1.34373900	-2.27746300	2.23519900
H	-0.07384100	-1.60664600	3.26882400
C	-1.78061400	-1.32878600	3.68201000
C	1.20700900	-3.52782000	-0.81006000
H	1.00052200	-3.33736900	-1.86707100
H	2.05112900	-4.22276800	-0.73024900
C	0.32321800	-3.99360800	-0.36622300
H	2.06585300	-2.58349400	1.69775200
C	1.21208900	-3.08225100	2.16372100
H	2.88693800	-3.30494700	1.61274500
H	2.37646900	-1.76349700	2.35167100
C	-2.06549400	-0.49569400	-3.07519300
H	-3.02067200	-0.88535100	-3.44382400
H	-1.99469100	0.57582600	-3.26646800
H	-1.24217000	-0.99220400	-3.59556100
C	-2.18893200	-2.61453700	-1.21341900
H	-1.41764100	-3.13041700	-1.78979600
H	-2.13928100	-2.97933600	-0.18353700
H	-3.16912200	-2.86107500	-1.63656900
C	2.29339600	2.40491000	1.34714300
H	1.45724100	2.99043600	1.73541100
H	2.55190300	1.64133700	2.08567300
H	3.15333100	3.06671100	1.19746300
C	1.71621500	3.10429500	-1.32489500
H	2.69956100	3.58461700	-1.38312400
H	1.39007300	2.81224500	-2.32542500
H	0.99936400	3.82543800	-0.92510000
C	-0.49282700	1.33361200	3.11549300
H	-0.58195400	2.34080500	2.70318800
H	-1.11745800	1.25171800	4.01136100
H	0.54973100	1.15418000	3.38934500
H	0.62256600	-0.02264900	-1.77931600
O	-1.25235400	2.48403300	-0.78179500
O	-1.26943900	2.97974400	0.30032700
O	-1.47045500	2.46681300	-1.94645800
O	3.93590200	-0.33198200	-0.18362200
C	-3.69849700	-0.37701000	0.88598300
H	-3.54510000	-1.43270100	1.14894900
H	-4.74960100	-0.16769500	1.11742500
H	3.86235600	-0.26265200	0.91086300
H	5.00745900	-0.41642500	-0.40017000

TS_{A9-7}

E= -879.92840207 a.u.

TS_{A6-7}

E= -879.92973130 a.u.

Rh	0.06568600	0.07122700	-0.16321700
P	-1.92415000	-0.70722500	-1.04360000
P	-0.83887000	0.08387000	2.07738500
C	-3.42577400	0.04498500	-0.26139800
H	-3.37237200	1.11886400	-0.46517700
H	-4.30581300	-0.34599800	-0.78764300
C	-2.62917100	0.59424200	2.15082500
C	-2.97545500	0.52794000	3.19116300
H	-2.66005400	1.65241600	1.86335300
P	1.27809900	-1.83291600	-0.65306500
P	2.02354400	1.27813500	0.01682500
C	3.10931500	-1.75208600	-0.31696500
H	3.59772700	-1.22930900	-1.14841200
H	3.50101800	-2.77592300	-0.31560800
C	3.47059800	0.48051800	0.89728300
C	3.51664000	0.91838800	1.90080100
H	4.39041100	0.78195500	0.38021900
C	0.89695500	-3.39115700	0.28485000
H	1.07618800	-3.21511800	1.34908500
H	-0.15507100	-3.65559900	0.16512100
H	1.51652000	-4.23028100	-0.05070600
C	-0.18811900	1.19495900	3.41306900
H	-0.28687800	2.23503000	3.08958700
H	-0.72634000	1.06589100	4.35951500
H	0.87354600	0.98646900	3.57761200
C	-0.91334800	-1.50777300	3.03421500
H	0.10783400	-1.83423700	3.25381200
H	-1.46472200	-1.40841900	3.97693300
H	-1.38203500	-2.28406800	2.42262100
C	2.78064500	1.77874700	-1.59191000
H	3.70671700	2.34650100	-1.44587700
H	2.98929600	0.88845400	-2.19060700
H	2.05367600	2.39311400	-2.12721700

P	-1.17946200	2.01723900	-0.03074300	H	-2.19102600	-2.87913200	0.55042000
P	-2.05295800	-1.21673800	-0.22371800	H	-0.80370400	-3.34553800	1.50412400
P	2.11076100	0.78840700	-0.83689500	C	-0.36562500	-0.88376200	3.27151500
P	0.84226200	-0.72797200	1.80108700	H	0.60789400	-1.37668000	3.25508500
C	-1.85342300	2.81335800	-1.56244900	H	-0.23487500	0.14446700	3.61301800
C	-2.95107100	-1.23159900	-1.82940000	H	-1.00599900	-1.40893500	3.98607500
C	2.44471600	1.06851600	-2.62183500	C	2.91160900	-1.81361200	-1.57882800
C	0.04664700	-2.04761500	2.82438600	H	2.41827400	-2.77972400	-1.66663100
C	-2.15257500	-2.98722100	0.28354700	H	2.68287600	-1.22069700	-2.46628700
C	-0.43438900	3.51884800	0.77441100	C	3.99407100	-1.94796100	-1.49879100
C	0.98342900	0.59838100	3.09217700	C	2.57743500	-2.14639200	1.30075200
C	2.61651300	2.44207800	-0.17049000	H	3.56917800	-2.59476900	1.19070500
H	-0.04979500	-0.44079000	-1.94091200	H	2.53916900	-1.62475400	2.26020700
H	-0.99720300	-1.78893000	3.02374600	H	1.81977300	-2.92920000	1.25838700
H	0.07110600	-2.99313200	2.27739100	C	-3.13755700	-0.59747100	-1.67468700
H	0.56726700	-2.17386500	3.77970600	H	-3.37387100	-1.24685600	-0.83015700
H	1.46937200	0.23968800	4.00650400	H	-4.06151400	-0.16013300	-2.06418200
H	1.55249900	1.44314400	2.69543900	H	-2.67396200	-1.23382400	-2.43154100
H	-0.01981500	0.96002700	3.33795800	H	-0.22377600	-1.50043300	-2.04232700
H	2.39021200	2.54168900	0.89286400	H	0.74874000	0.53776200	-1.72885300
H	2.08451100	3.22850000	-0.71014400	C	-0.45254300	-2.51038500	-1.51129200
H	3.69048400	2.59249100	-0.32143500	O	-1.45366700	-3.09684300	-1.90006500
H	2.34980800	0.11390900	-3.13965800	O	0.37404500	-2.78939000	-0.59905700
H	3.44729100	1.48332900	-2.76947100	C	3.54088500	1.41253700	-0.84458400
H	1.69912100	1.76680400	-3.01144100	H	4.51574700	1.89413000	-0.96282100
H	-2.34793800	-1.81743900	-2.52510500	C	3.29027000	0.99739500	-1.82646800
H	-3.04682600	-0.21585200	-2.21855600	H	-2.76404300	1.41884800	1.54277300
H	-3.94413400	-1.68025600	-1.72018100	H	-1.81165000	1.87286300	1.84206900
H	-1.01968100	3.05838200	-2.22644900	H	-3.53355900	1.93103900	2.12888300
H	-2.49135500	2.10322600	-2.09452300				
H	-2.42360900	3.72433000	-1.34615800				
H	-1.20242400	4.27422400	0.97496000				
H	0.04369900	3.24035300	1.71753700				
H	0.32105200	3.96518700	0.12668800				
H	-2.04874700	-3.07394600	1.36663700				
H	-3.12502000	-3.39784400	-0.00718700				
H	-1.36040000	-3.54180200	-0.21853700				
O	0.63970600	-1.95397700	-1.90510800				
C	1.82904600	-1.88902800	-2.16518700				
O	-0.26399300	-2.76187700	-2.03134100				
C	-2.71908400	1.97063800	1.02063600				
H	-2.38576500	1.80376300	2.05345200				
C	-3.17631100	2.96801900	0.99068400				
H	-3.34631100	-0.52439000	0.91658600				
H	4.22102500	-1.18280800	0.84740400				
H	-2.96131900	-0.61359200	1.94082400				
C	2.58007000	-1.38707600	1.80056100				
C	2.55372300	-2.31765900	1.22135300				
C	2.84447100	-1.64558100	2.83427100				
C	3.55810500	-0.22833300	-0.29496700				
H	4.46489900	0.27678500	-0.64980300				
C	3.47313000	-1.18210100	-0.82094300				
Rh	0.00356300	-0.09587800	-0.32493100				
C	-3.76941200	0.92193800	0.64775600				
H	-4.67647500	1.12890700	1.22802100				
H	-4.06004000	1.03961400	-0.40401300				
C	3.65163000	-0.45392300	1.21967200				
H	4.62980300	-0.90209200	1.42883900				
H	3.64829600	0.50531900	1.75549100				
TS_{A13-14}							
E= -1461.35313747 a.u.							
Rh	0.95212900	0.02015700	0.00205000				
P	0.70808300	2.13499600	-0.98194000				
P	1.11123600	0.88970300	2.12802600				
C	0.68497600	3.60959500	0.12254600				
H	1.71146100	3.82111000	0.44500700				
H	0.35085800	4.47055200	-0.46661700				
C	0.43711400	2.60918100	2.46894000				
H	-0.27212000	2.51170900	3.29736200				
H	1.27710000	3.19908900	2.85398100				
P	1.35619500	-2.29514400	0.48642500				
P	4.38951500	0.33455800	-0.42603700				
C	2.90510300	-2.95203200	-0.28277300				
H	2.83296800	-2.73828200	-1.35294200				
H	2.83797600	-4.04032700	-0.16673900				
C	4.94999600	-1.42813700	-0.64965200				
H	6.03411700	-1.46063200	-0.48826500				
H	4.77058800	-1.68752400	-1.69700100				
C	1.46874800	-3.02841900	2.17722000				
H	2.24566100	-2.53021200	2.76308400				
H	0.51632500	-2.93935600	2.70439500				
H	1.72286800	-4.08977200	2.10007700				
C	2.83165400	1.05096600	2.75244200				
H	3.39090900	1.73191500	2.10949500				
H	2.83947100	1.42462200	3.78084700				
C	3.32329300	0.07589500	2.71557100				
H	0.35810800	-0.03394600	3.53966500				
H	0.87425100	-0.98267300	3.68426500				
H	0.45559400	0.55217700	4.45809000				
C	-0.69838500	-0.24069400	3.36477800				
C	5.16259900	1.07661700	-1.93863700				
H	6.18060700	0.69827100	-2.08071100				
H	4.55836300	0.81483300	-2.80934500				
H	5.21416500	2.16559200	-1.84569400				
C	5.66679900	0.87627300	0.82367800				
H	5.55797100	1.94391200	1.04068300				
H	5.54537700	0.33027200	1.76410200				
H	6.68372200	0.70465000	0.45491100				
C	-0.84187400	2.32776700	-1.94304600				
H	-0.96678000	1.45289400	-2.58403000				
H	-1.69188200	2.36978900	-1.25701300				
P	-0.80763400	3.24155100	-2.54351400				
C	2.01043700	2.56328800	-2.19557600				
H	1.74276400	3.48384900	-2.72282300				
H	2.95342200	2.70961200	-1.66727300				
C	2.14874600	1.74915500	-2.90881100				
C	0.13235000	-3.41308100	-0.31744800				
H	0.20945700	-3.27872100	-1.39821800				
H	0.34858900	-4.45652600	-0.06988100				
H	-0.88875400	-3.17555200	-0.01579800				
H	1.02156000	-1.26686800	-3.83977400				
H	-0.70064800	-0.11258300	0.18004900				
C	1.46542100	-0.89713500	-2.89442300				
O	0.58670500	-0.70517200	-1.97601800				
O	2.67973600	-0.72082000	-2.81971300				
C	-0.23065100	3.38393100	1.32965800				
H	-0.54637600	4.35223300	1.73273800				
H	-1.14583300	2.87527200	1.00607200				
C	4.25466800	-2.44488400	0.26554000				
H	4.14214900	-2.03167300	1.27831000				
H	4.91416100	-3.31064500	0.38139800				
P	-2.55972400	-0.20005800	-0.00968600				
TS_{A10-11}							
E= -880.33684672 a.u.							
Rh	0.12110300	-0.01480700	-0.40278800				
P	2.28813200	-0.97071000	-0.06976100				
P	0.92980700	1.96607700	0.30118700				
C	3.63802400	0.28105400	0.18514900				
H	3.61701100	0.67440600	1.20751300				
C	4.59026500	-0.24877900	0.08125000				
C	2.52089200	2.49661900	-0.48295800				
H	2.24079200	3.05523900	-1.38191700				
H	2.96006600	3.21870400	0.21584200				
P	-2.01529100	0.75861600	-1.16658000				
P	-1.13389400	-0.94216500	1.59519200				
C	-3.04019200	1.70840900	0.06004000				
H	-4.08772800	1.47992000	-0.16804300				
H	-2.91023200	2.77573900	-0.14468900				
C	-2.75312500	-0.07013100	1.91283200				
C	-2.98173800	-0.19701300	2.97606100				
H	-3.54132400	-0.60317100	1.37004000				
C	-2.00987300	1.81378600	-2.66741800				
H	-1.41469900	2.71593200	-2.52203000				
H	-1.57263600	1.24109700	-3.48893700				
H	-3.03102400	2.09951600	-2.93588400				
C	1.25119600	2.01638000	2.11055800				
C	1.75219600	1.10808300	2.44763700				
H	1.86886100	2.88452100	2.35782400				
O	0.30154100	2.10612600	2.64266100				
C	-0.05088200	3.49815400	0.06325100				
H	-0.97681100	3.47337000	0.63670400				
H	0.54877500	4.34508900	0.41009100				
H	-0.27814800	3.64691800	-0.99297500				
C	-1.67668500	-2.69179800	1.49594800				
H	-2.33826300	-2.91926700	2.33750400				

N	-3.18009000	-1.57013500	0.85009700	H	4.76583100	-0.56735300	1.65919700
N	-2.83974800	-0.28412700	-1.68516700	H	3.19833900	0.11541400	2.05539600
N	-3.24094200	1.27339400	0.59874300	C	-3.41329000	1.20544100	-1.07551100
C	-2.38529100	-1.54298400	-2.27347700	H	-4.49404300	1.37290300	-1.14262600
H	-1.43313700	-1.82814500	-1.82943600	H	-2.97386400	1.77240600	-1.90838300
C	-2.98023600	1.34953400	2.03897800				
H	-3.70604400	0.78207800	2.63972300				
C	-2.31122400	-2.05609000	1.91729500				
H	-1.28324300	-1.73342900	1.74103800				
C	-4.53976800	1.86377900	0.24375500				
H	-4.46290000	2.35494800	-0.72741900				
H	-4.74375800	2.66212500	0.96458900				
C	-5.70870800	0.86639700	0.23927200				
H	-5.91643600	0.54352700	1.26410900				
H	-6.61364700	1.38188600	-0.12240700				
C	-3.91553900	0.37828200	-2.40495200				
H	-3.82254200	1.45750400	-2.26975300				
H	-3.75730600	0.19846300	-3.47302400				
C	-5.31500000	-0.12022900	-1.98678500				
H	-6.07993700	0.58263300	-2.34924700				
H	-5.51514600	-1.08098200	-2.46998600				
C	-4.58298800	-1.84716700	1.16401400				
H	-4.89156200	-1.25726800	2.04411000				
C	-4.66299400	-2.90018400	1.46173900				
H	-5.54322100	-1.60784900	0.00758000				
C	-5.33255700	-2.33900500	-0.77772300				
H	-6.56708800	-1.80290800	0.36786300				
N	-5.38815400	-0.28992200	-0.55788400				
C	-3.11306400	-2.35756600	-2.14952600				
H	-2.19956400	-1.38659700	-3.33953800				
H	-2.32884800	-3.15200200	1.95816200				
H	-2.62511000	-1.67819400	2.90327400				
H	-1.98442900	0.95631500	2.25484100				
H	-3.00198800	2.39354900	2.36625600				

B1

E= -801.30555307 a.u.

Rh	-0.00000500	0.00002400	-0.00007800				
P	1.60633100	1.67628000	-0.30496800				
P	1.72086700	-1.54716000	-0.37482700				
C	3.34334700	1.38574900	0.33027400				
H	4.03602600	1.86953500	-0.38787800				
C	3.41729200	1.94001600	1.27167000				
H	3.45070200	-0.87844900	-0.52744000				
H	4.12727900	-1.73769200	-0.47754200				
H	3.61616000	-0.40893200	-1.51253700				
P	-1.60629100	-1.67626900	0.30485800				
C	-1.72088500	1.54714400	0.37490000				
P	-3.34334900	-1.38576700	-0.33028300				
H	-4.03598000	-1.86958900	0.38789300				
H	-3.41734500	-1.93999300	-1.27169800				
C	-3.45068400	0.87835400	0.52758100				
H	-4.12729700	1.73757600	0.47780700				
H	-3.61604400	0.40874500	1.51265100				
N	3.70974300	0.00826800	0.59357500				
N	-3.70977800	-0.00827900	-0.59348700				
C	5.07574400	-0.08040200	1.09689800				
H	5.17278400	0.53593200	1.99474200				
H	5.29870500	-1.11405300	1.37348200				
H	5.82448200	0.25745400	0.35994400				
C	-5.07581200	0.08040000	-1.09681500				
H	-5.29880700	1.11406500	-1.37322600				
H	-5.17289500	-0.53587500	-1.99460400				
C	-5.82450100	-0.25751700	-0.35974900				
H	-1.44023200	-3.41050400	-0.30877500				
H	-1.37825200	-3.41330500	-1.39957400				
H	-0.55071500	-3.89521100	0.09723300				
H	-2.31542400	-3.99422900	-0.00695700				
C	1.64208500	-2.58513900	-1.89545600				
H	1.49566700	-1.94130900	-2.76643000				
H	2.56754000	-3.15519800	-2.02249800				
H	0.80792700	-3.28542200	-1.84751100				
C	2.01613400	-2.74432800	0.99281100				
H	1.08921300	-3.21249200	1.32590800				
H	2.72306600	-3.52306500	0.69099400				
C	2.43319800	-2.18025600	1.83134300				
H	-1.64206400	2.58505000	1.89558200				
H	-2.56764600	3.15485400	2.02284400				
H	-1.49528900	1.94122100	2.76649600				
H	-0.80811600	3.28557200	1.84749500				
C	-2.01629700	2.74437700	-0.99265000				
H	-1.08942000	3.21260700	-1.32577800				
H	-2.43338900	2.18034100	-1.83119200				
H	-2.72324600	3.52306100	-0.69073600				
C	1.44032900	3.41052100	0.30865300				
H	0.55084700	3.89526000	-0.09739300				
H	1.37831200	3.41333200	1.39944900				
H	2.31555600	3.99420700	0.00686100				
C	1.85455400	1.97199400	-2.10964900				
H	2.64629200	2.70442900	-2.29356900				
H	2.10318700	1.03658300	-2.61576100				
H	0.91979800	2.33972900	-2.54081300				
C	-1.85444400	-1.97196700	2.10954900				
H	-2.10315300	-1.03656000	2.61563300				
H	-2.64611700	-2.70446400	2.29350200				
H	-0.91964800	-2.33960600	2.54070700				

B1-H₂

E= -802.48197015 a.u.

Rh	0.01656600	0.18000700	-0.82898900				
P	-2.11461300	1.12194800	-0.69396700				
P	-0.82784300	-1.73647200	0.28775700				
C	-3.17059100	0.68248800	0.76562100				
H	-2.75070000	1.15624000	1.67245800				
H	-4.14797100	1.14320700	0.58688100				
C	-2.19262200	-1.40856200	1.51002200				
H	-2.50728100	-2.38384300	1.89635900				
H	-1.77320800	-0.84202800	2.36271900				
P	2.12915400	-0.74913700	-1.13585700				
P	1.04445800	1.72697600	0.66137800				
C	3.18602800	-0.99379100	0.38378900				
H	4.23856200	-0.80229800	0.09683900				
C	3.11492800	-2.05412100	0.64680600				
C	2.74018300	1.22431000	1.26288300				
H	2.93107400	1.77559100	2.18773000				
H	3.51257700	1.54656600	0.54377400				
C	2.24537800	-2.39496800	-1.94671100				
C	1.70387700	-3.14653400	-1.36840000				
H	1.78387700	-2.32825500	-2.93515000				

TS_{A7-8'}

E= -881.11639513 a.u.

P	-1.10140800	1.93973400	0.41457200				
P	-1.38846200	-0.83632100	-1.35881400				
C	-2.93076100	1.74743300	0.27370700				
H	-3.23304600	1.07392700	1.08338800				
H	-3.37096900	2.73338100	0.46634900				
C	-3.16239300	-0.29303600	-1.24840900				
H	-3.66430300	-0.65308600	-2.15542200				
C	-3.59890700	-0.82965700	-0.39708300				
P	1.50377300	-1.88779400	0.16560300				
P	2.15446700	1.28517000	-0.27051200				
C	3.10939200	-1.81782800	1.11659800				
H	3.81150900	-2.50059300	0.62171800				
C	2.90255700	-2.23836300	2.10607600				
C	3.77257100	0.39392600	-0.01198600				
H	4.57422600	1.14056900	0.01806800				
H	3.97606500	-0.24635700	-0.87867600				
C	0.76843200	-3.38861100	0.93860800				
H	0.50245100	-3.14388800	1.96989400				
H	-0.14117800	-3.68702500	0.41683000				
H	1.48101500	-4.21998000	0.93163500				
C	-1.74623900	-2.64978900	-1.50144700				
H	-2.17039300	-3.00144400	-0.55644900				
H	-2.47882200	-2.83012800	-2.29524100				
C	-0.84582200	-3.22483400	-1.72771400				
H	-1.00364300	-0.43903700	-3.12864600				
H	-0.02847000	-0.86218800	-3.38585900				
H	-1.76208400	-0.82828500	-3.81758100				
H	-0.93131000	0.64588500	-3.24440700				
C	2.43102100	1.96299100	-1.97266000				
C	3.40040900	2.46555000	-2.06720500				
H	2.37762200	1.13932500	-2.68999000				
H	1.63622000	2.67087700	-2.22095200				
C	2.54471100	2.78601400	0.75424300				
H	1.73712200	3.51929300	0.71413400				
H	2.65753200	2.47768000	1.79761500				
C	3.47012700	3.26763200	0.42017500				
H	-0.83816100	3.37581800	-0.72446600				
H	0.16584900	3.78961000	-0.61626200				
H	-0.95543300	3.04525500	-1.75992600				
H	-1.56578400	4.16765400	-0.51975100				
C	-0.96484300	2.69550600	2.08444000				
H	0.08194100	2.89001800	2.32504000				
H	-1.54055500	3.62433400	2.15145800				
H	-1.35460100	1.96632800	2.79970300				
C	2.07780400	-2.54243000	-1.46764300				
C	2.65967300	-1.77369400	-1.98227900				
H	2.69147900	-3.44146300	-1.35055900				
H	1.21800700	-2.78202300	-2.09685200				
H	-0.88361400	-0.40801000	2.13349100				
H	0.05614200	-0.30160800	1.95676200				
O	-2.17252800	-0.49644600	2.47237800				
C	-2.62444400	-1.62449100	2.05621300</				

H	3.28709700	-2.70999100	-2.05874400
C	0.32431000	-2.65538000	1.39986100
H	0.89333800	-1.94168500	2.00167800
H	-0.22254700	-3.34647800	2.04868100
H	1.02673600	-3.24229100	0.80257000
C	-1.58189800	-3.09454600	-0.70149700
H	-0.88929700	-3.40729100	-1.48637800
H	-1.83796300	-3.95642800	-0.07695300
H	-2.48996200	-2.71556900	-1.17651700
C	1.39131500	3.46531700	0.14875100
H	1.93423900	4.01636100	0.92347100
H	1.98076200	3.46041100	-0.77180000
H	0.45410300	3.98562000	-0.06045700
C	0.20344500	1.96246800	2.28728400
H	-0.80916700	2.34635400	2.14154300
H	0.13456700	0.99187100	2.78587400
H	0.75105700	2.66073300	2.92790800
C	-3.19346000	0.64284300	-2.09853500
H	-2.70480500	0.90381000	-3.03985000
H	-3.34506000	-0.43798300	-2.07033100
H	-4.16384300	1.14420900	-2.04031900
C	-2.24814700	2.95651300	-0.68262500
H	-3.29322300	3.27394700	-0.74474600
H	-1.81157500	3.36673300	0.23146500
H	-1.70184200	3.36061300	-1.53828500
C	3.18889100	0.27241600	-2.23951300
H	3.30452300	1.27633700	-1.82487300
H	4.17618800	-0.17890300	-2.37474600
H	2.69844600	0.36513900	-3.21168500
H	0.10970800	0.81813400	-2.45980400
N	-0.23917100	0.00244200	-2.55401400
H	2.78704400	-0.20804700	1.53943300
N	-3.35086500	-0.75185800	0.91992000
C	-4.57354200	-1.05447400	1.66217100
H	-4.54599900	-0.67170700	2.69675100
H	-5.43230600	-0.61293100	1.15053400
H	-4.72392300	-2.13617600	1.69482200
C	3.61645100	-0.53797700	2.69457800
H	4.68122100	-0.29345400	2.54124500
H	3.25543600	0.00315400	3.57269200
H	3.53702200	-1.60891200	2.90315900

B2

E= -802.50220898 a.u.

Rh	-0.00065100	0.28265600	-0.79631900
P	-2.17966200	1.09630200	-0.74599200
P	-0.70151700	-1.70752100	0.34524900
C	-3.22582500	0.55131900	0.69041200
H	-2.85996200	1.04878600	1.60820100
H	-4.23342100	0.93759700	0.50321900
C	-2.13972800	-1.47502600	1.50009500
H	-2.41142200	-2.46908500	1.87018200
H	-1.81181500	-0.88280400	2.37359600
P	2.12549100	-0.46696300	-1.36421500
P	0.92651400	1.53830500	1.03684900
C	3.28977300	-0.85298600	0.05276200
H	4.30490100	-0.52808800	-0.24796500
H	3.32068900	-1.94440600	0.14143200
C	2.71952800	1.13587300	1.33714500
H	2.99373600	1.55098100	2.31221800
H	3.35110700	1.65038900	0.59321300
N	-3.29920500	-0.89555100	0.83238000
N	2.90933400	-0.30972200	1.34702700
C	-4.54852900	-1.30935000	1.46926800
H	-5.39598700	-0.93555700	0.88955300
H	-4.60998600	-2.40022400	1.48144400
H	-4.64133300	-0.94013100	2.50473300
C	3.83101100	-0.75886500	2.38555100
H	3.48370100	-0.40856400	3.36115500
H	3.84889400	-1.85246700	2.40844400
H	4.86197400	-0.39928600	2.22888400
C	2.22750300	-2.01886400	-2.34040700
C	1.75250500	-2.83726400	-1.79377900
H	1.69253400	-1.87752400	-3.28210800
H	3.26762600	-2.28474900	-2.55094700
C	0.47978100	-2.62299200	1.42012600
H	0.98347000	-1.93207000	2.09932100
H	-0.02151200	-3.41837800	1.97987200
H	1.24908200	-3.07766300	0.78908300
C	-1.35532200	-3.02378700	-0.75582700
H	-0.62251900	-3.25825500	-1.53077900
H	-1.59985500	-3.93251100	-0.19747700
H	-2.25758300	-2.64596100	-1.24179200
C	1.01204900	3.36673500	0.85327100
H	1.60295200	3.82101000	1.65446000
H	1.46161500	3.60722700	-0.11309200
H	0.00994000	3.79882900	0.87274700
C	0.24322200	1.32768100	2.73473700
H	-0.82597100	1.55402300	2.73820000
H	0.37638200	0.28726900	3.04383600
H	0.74520100	1.98072900	3.45494800
C	-3.20246500	0.60205000	-2.18225000

B3

E= -1383.48378870 a.u.

Rh	1.57402900	0.17002000	-0.51720300
P	1.25119400	2.38194500	-1.09980900
P	1.30464200	0.58485100	1.83246300
H	0.88878000	3.53033700	0.30927700
C	1.83082000	3.78440700	0.82844500
H	0.50599800	4.46095400	-0.12292100
C	0.48058600	2.20785900	2.29632800
H	-0.31308900	1.95658600	3.00650100
H	1.22409400	2.81454900	2.84997200
P	1.40500700	-2.14868200	-0.46972900
C	3.97450100	-0.06755300	-0.67955300
C	2.62596200	-3.02232500	0.64655000
H	2.90056500	-3.98527300	0.17326100
H	2.08789500	-3.26354200	1.56983000
C	4.55430500	-1.76802900	-0.15883100
H	5.61423500	-1.68897100	0.10239300
H	4.49956300	-2.46520500	-1.01204500
N	-0.11036500	2.96185500	1.20430100
N	3.80183500	-2.23836500	1.00194300
C	-1.04223800	3.96762600	1.70335800
H	-1.51681400	4.47716300	0.86069600
H	-1.83272300	3.48091400	2.28125300
H	-0.55672100	4.72412300	2.34438700
C	4.63554600	-2.96828600	1.95215300
H	5.46371500	-2.33317300	2.27822100
H	4.04286500	-3.22621900	2.83479100
H	5.05186500	-3.89948000	1.53144100
C	-0.18648300	-2.92542600	0.01164300
H	-0.41783800	-2.71184200	1.05525600
H	-0.98085200	-2.48500000	-0.59614900
H	-0.15491400	-4.00810600	-0.14280900
C	2.76477900	0.61873200	2.95498100
H	3.41141900	1.46243500	2.70078400
H	2.46068700	0.71371700	4.00201100
H	3.32145700	-0.31237300	2.81374900
C	0.23341700	-0.63634600	2.69060600
H	0.74718300	-1.60173000	2.71226200
H	0.03199900	-0.33295700	3.72261600
H	-0.70598800	-0.73401100	2.13492000
C	4.69470100	0.06599600	-2.36846000
H	5.74942400	-0.22503700	-2.38803300
H	4.12649900	-0.56651800	-3.05470400
H	4.60881000	1.09812800	-2.71706800
C	5.11872300	0.99001700	0.30918800
H	4.84947800	2.04406600	0.20512900
H	5.03659900	0.71772000	1.36314700
H	6.15630900	0.85467000	-0.01096500
C	-0.19493900	2.62612000	-2.19317700
H	-0.02266800	2.09379800	-3.13184100
H	-1.06372700	2.18286400	-1.69880800
H	-0.37190000	3.68594500	-2.39908300
C	2.59706300	3.27087800	-1.98391700
H	2.32064600	4.31057200	-2.18407000
H	3.51817500	3.25749100	-1.39552300
C	2.78433500	2.76844400	-2.93629300
H	1.69593700	-2.92850700	-2.11069900
H	2.66239100	-2.62085100	-2.51562400
H	1.65992500	-4.02009700	-2.04608800
H	0.92145600	-2.57725900	-2.79681000
H	1.47457800	-0.02991100	-2.08833900
H	0.00473600	0.17646100	-0.53799900
P	-2.85383700	0.22354500	-0.32620600
N	-4.24142000	1.28466100	-0.30690000
N	-2.85969400	-0.59742800	1.23178700
N	-3.03696700	-1.04037800	-1.49341100
C	-3.07142800	0.33593900	2.32866000
H	-2.50408200	1.25411900	2.13741800
C	-2.08348000	-0.97893400	-2.59826100
C	-2.58438700	-0.75857100	-3.55116000
H	-3.91117200	2.64716900	-0.71336800
H	-2.86092000	2.85393900	-0.49162800
C	-3.91926600	-2.20250400	-1.61098800
H	-3.44257100	-3.08615800	-1.15775500
H	-4.01827600	-2.43746500	-2.67850300
C	-5.34276800	-2.03815800	-1.05946000
H	-5.93418300	-1.47043000	-1.78334700
H	-5.79265400	-3.04502000	-1.00682800

C	-3.39166100	-1.92772700	1.47047600
H	-2.93594400	-2.61504600	0.75494000
H	-3.06078200	-2.25716300	2.46584200
C	-4.92718500	-2.02200900	1.37862800
H	-5.22319700	-3.08423200	1.39643000
H	-5.37858200	-1.55727500	2.26110900
C	-5.63110300	0.95823900	-0.59450000
H	-5.75857100	0.70168700	-1.66039100
H	-6.23711000	1.85740600	-0.42595700
C	-6.19354000	-0.14956200	0.28606900
H	-6.18394400	0.19195700	1.32525000
H	-7.24985800	-0.30990800	0.00729300
N	-5.42026800	-1.36248700	0.20358300
H	-4.12216500	0.62820200	2.46584300
H	-2.70673000	-0.10585800	3.26424800
H	-4.52225900	3.36466200	-0.15170900
H	-4.07974200	2.82651800	-1.78777900
H	-1.32801400	-0.21296100	-2.41120400
H	-1.55949500	-1.93996900	-2.71805000

B4

E= -1383.46324012 a.u.

Rh	1.65217400	0.22364000	-0.54044300
P	0.85373500	2.20495500	-1.29726000
P	1.47002400	0.81635600	1.70172300
C	0.44178300	3.55207600	-0.06407800
H	1.36848800	4.12537900	0.12828500
H	-0.25870600	4.24061400	-0.54998500
C	0.84898700	2.53481100	2.09739900
H	0.42328900	2.49908900	3.10624800
H	1.73424800	3.19756000	2.15047200
P	1.35450900	-2.08280700	-0.26853200
P	4.01755300	-0.10900300	-0.77549300
C	2.61884900	-2.87194200	0.88425400
H	2.81816300	-3.90222100	0.52281800
H	2.12269400	-2.97296400	1.85769400
C	4.56421100	-1.78954000	-0.13811800
H	5.63911300	-1.74787500	0.06835200
H	4.43221800	-2.55422900	-0.92287400
N	-0.15573200	3.09658300	1.19376600
C	3.85438000	-2.13143800	1.09519900
N	-0.81881900	4.21935800	1.85624200
H	-1.57258800	4.65233200	1.19156900
H	-1.32189500	3.87031600	2.76319200
H	-0.11248300	5.01980500	2.13683300
C	4.70318400	-2.82577200	2.05335900
C	5.58389600	-2.21698700	2.27748500
H	4.15432300	-2.97843500	2.98829500
H	5.04440200	-3.81266200	1.69147200
C	-0.13127900	-3.01597900	0.35626900
H	-0.48251100	-2.58624100	1.29686800
H	-0.93733500	-2.91616500	-0.37603200
H	0.08574600	-4.08159500	0.49520400
C	2.93798100	0.82433300	2.82582200
H	3.64160000	1.59567900	2.50253500
H	2.66208600	1.01126300	3.86919200
C	3.42862900	-0.14967800	2.73476600
C	0.33341500	-0.22596500	2.72691500
H	0.79871100	-1.20799100	2.85678200
H	0.14738000	0.20300700	3.71764100
H	-0.60665300	-0.36906100	2.19277000
C	4.72084600	-0.17341100	-2.48391300
H	5.76418500	-0.50748400	-2.49996000
H	4.11218300	-0.84259200	-3.09759500
H	4.66162100	0.82464900	-2.92693500
C	5.29282000	0.94006600	0.06816800
H	5.10218600	1.99605000	-0.14089200
H	5.22165000	0.78530400	1.14729900
H	6.30834300	0.68792100	-0.25695900
C	-0.63834400	2.27197400	-2.40387100
H	-0.41844000	1.67860600	-3.29576500
H	-1.50443000	1.82732300	-1.90937800
H	-0.88339500	3.29570500	-2.70799800
C	2.00593900	3.18217000	-2.36889600
H	1.58029400	4.14058900	-2.68682800
H	2.93794700	3.36110000	-1.82650600
C	2.24035800	2.58330900	-3.25307100
H	1.64714000	-3.05068700	-1.82044600
H	2.58660400	-2.73229600	-2.27701200
H	1.67835000	-4.13038000	-1.63940800
H	0.85165700	-2.82259200	-2.53422700
H	1.53177800	-0.11077500	-2.10774900
H	-1.81590800	0.40717700	-0.00552300
P	-3.10325800	-0.17564000	-0.04663600
N	-3.98193200	1.25951600	0.11654800
N	-3.01701200	-1.18282400	1.33415200
N	-2.95242200	-1.02736700	-1.48484200
C	-3.21116400	-0.51144200	2.61949500
H	-2.69142600	0.44978100	2.62114000
C	-1.69565800	-1.03407000	-2.23916700
H	-1.82450400	-0.51880300	-3.19731600
C	-3.28760600	2.54665900	0.09981800
H	-2.22604700	2.42143500	0.33347100

C	-3.99612100	-1.86355400	-2.05850800
H	-3.83021300	-2.92005000	-1.80211900
H	-3.95000700	-1.78822400	-3.14953600
C	-5.35020100	-1.38004300	-1.56882700
H	-5.62013000	-0.46547700	-2.10233500
H	-6.13856800	-2.12176500	-1.74116100
C	-3.70317800	-2.45320800	1.17662400
H	-3.17138100	-3.04791400	0.42855200
H	-3.65708800	-3.00658300	2.11770500
C	-5.16932500	-2.22328100	0.75079400
H	-5.58112000	-3.10965900	0.25906100
H	-5.79026000	-2.01722200	1.62527300
C	-5.41044200	1.34774300	-0.14002200
H	-5.60093200	1.57089700	-1.20063100
H	-5.82922500	2.17763900	0.43795900
C	-6.06919900	0.04906000	0.29293300
H	-6.12568400	0.02368600	1.38298500
H	-7.08612000	-0.04453200	-0.10646400
N	-5.20839700	-1.05542400	-0.14678700
H	-4.26888100	-0.32303800	2.85346600
H	-2.77740200	-1.12832300	3.41106100
H	-3.72174600	3.19534900	0.86803100
H	-3.38716300	3.04227400	-0.87439600
H	-0.87823500	-0.56039800	-1.68363200
H	-1.40304500	-2.07082100	-2.43900600

B5

E= -802.04038939 a.u.

Rh	0.00328100	-0.13815300	-0.41202700
P	-1.85714000	-1.52328800	-0.37585500
P	-1.11062300	1.82806500	0.19805100
C	-3.41639600	-0.56550600	-0.76683500
H	-3.38046300	-0.28505600	-1.83590800
H	-4.26537900	-1.24782600	-0.63792500
C	-2.90049100	1.79031200	-0.34706500
H	-3.39899400	2.67257800	0.07260500
H	-2.92018300	1.89621600	-1.44803300
P	1.13409400	-0.81982500	1.49127000
P	1.98939400	-0.03798400	-1.53072100
C	2.79547300	-0.00372200	1.82517900
H	3.46915100	-0.76654200	2.27010400
H	2.61199600	0.75117400	2.59865600
C	3.54454900	-0.16254800	-0.49649000
H	4.38182300	0.20256100	-1.10188300
H	3.76423100	-1.22130900	-0.26308100
N	-3.62462800	0.59822300	0.09334300
N	3.42834300	0.66462100	0.69872000
C	-5.04419600	0.87747700	0.26347100
H	-5.54643100	-0.00431000	0.67226600
H	-5.17619000	1.69674800	0.97635100
H	-5.54575700	1.15538600	-0.68261500
C	4.69302500	1.25209200	1.10417600
H	5.11703000	1.82750600	0.27610400
H	4.52717200	1.93847400	1.94083800
H	5.43763600	0.49707300	1.42291800
C	0.41671000	-0.66914900	3.19179100
H	0.15835500	0.37438800	3.38606900
H	-0.50080100	-1.26145400	3.24237300
H	1.11193900	-1.02094200	3.96196800
C	-0.64065700	3.44923200	-0.56865300
H	-0.54690600	3.31182300	-1.64922000
H	-1.36582300	4.24572800	-0.36085200
H	0.33828900	3.74669100	-0.18207300
C	-1.36177400	2.36543000	1.95593000
H	-0.38872800	2.53292800	2.42752100
H	-1.95443200	3.28509400	2.03082300
H	-1.87644900	1.56233700	2.49138000
C	2.41604500	-1.26388500	-2.85339700
H	3.40481300	-1.08750600	-3.29405600
H	2.37641500	-2.27184300	-2.43090300
H	1.65597700	-1.20256400	-3.63690200
C	2.34983200	1.54636800	-2.41681400
H	1.52781700	1.75865500	-3.10521600
H	2.38807600	2.34533200	-1.67165200
H	3.29442400	1.51401100	-2.97243100
C	-2.43415700	-2.34988100	1.18139400
H	-1.66958000	-3.04004400	1.54976300
H	-2.59873600	-1.57328300	1.93389400
H	-3.36759800	-2.90516800	1.03305000
C	-2.08933600	-2.90489200	-1.59086500
H	-3.08610900	-3.35953300	-1.53346000
H	-1.92161500	-2.51442900	-2.59820900
H	-1.33343700	-3.67178900	-1.40011200
C	1.61568500	-2.60993600	1.53108100
H	2.18825400	-2.84666200	0.63066600
H	2.20262200	-2.87046100	2.41926700
H	0.70516000	-3.21547300	1.50906400
H	-0.59295800	0.21561700	-1.86291900

B6

E= -990.57296532 a.u.

Rh	0.08418300	0.07477000	-0.17018400	C	1.91954300	-2.74926700	1.31745300
P	-1.76349700	-0.40706500	-1.49506500	H	2.19845900	-2.11399000	2.16197700
C	-0.87000400	-0.58860200	1.86755100	H	0.94634200	-3.19428500	1.52819400
P	-3.35253800	-0.24711400	-0.52245000	H	2.66659700	-3.54068300	1.19226500
H	-3.51940500	0.82561800	-0.32165400	C	-1.62149200	3.01411100	0.99149800
H	-4.16994700	-0.58758000	-1.16938400	H	-1.56183400	3.26379200	-0.07228300
C	-2.72901800	-0.38506100	1.84158300	H	-2.56901100	3.35802700	1.41896300
H	-3.13101700	-0.81735700	2.76612200	H	-0.80432100	3.50127400	1.52661400
H	-2.95011200	0.69873100	1.86472900	C	-1.20863300	0.96011800	2.96740300
P	1.50860500	-1.65112400	-0.76771800	H	-0.16777600	1.18460900	3.21380900
P	1.87117400	1.50384500	-0.13360900	H	-1.86941800	1.60423900	3.55777800
C	3.20000900	-1.68014800	0.05269700	H	-1.40304600	-0.08594800	3.21812000
C	3.93493300	-2.05171200	-0.69272700	C	2.14761500	1.58814600	-2.00312400
H	3.14003000	-2.43494600	0.84549900	H	3.02673100	2.21394500	-2.19079900
C	3.56815100	0.71926300	-0.22598600	H	2.31648500	0.58776000	-2.40819600
H	4.29829800	1.46731500	0.10267500	H	1.26759900	2.02614100	-2.48621800
N	3.82085700	0.47314800	-1.27436800	C	1.57184500	3.32584800	0.13070000
H	-3.37442700	-1.04317400	0.70568600	H	0.72179600	3.68125200	-0.45701700
N	3.64577100	-0.43647600	0.65952900	H	1.40155400	3.50723000	1.19459200
C	-4.73247200	-1.45142100	1.04019700	H	2.47928600	3.85398200	-0.18079700
H	-5.16873200	-2.00296300	0.20223900	C	-1.52261100	-3.36103600	0.11496200
H	-4.71450000	-2.11939200	1.90659300	H	-0.55470900	-3.84289800	-0.04170400
H	-5.39471600	-0.59674900	1.27454900	H	-1.71864500	-3.31948700	1.19024500
C	4.96154600	-0.60483900	1.25108700	C	-2.29579600	-3.96803500	-0.36704600
H	5.24752500	0.30614300	1.78490200	H	-1.51446400	-1.88055400	-2.37471500
H	4.93633100	-1.42568900	1.97497200	H	-2.29177200	-2.58905900	-2.68042200
H	5.74468800	-0.83249800	0.50210700	H	-1.71297100	-0.89940400	-2.81638700
C	1.07171100	-3.43410700	-0.52790900	H	-0.54272300	-2.24152100	-2.71615000
H	0.84520800	-3.61405800	0.52547100	C	1.96754600	-2.86460500	-1.56678300
H	0.17747900	-3.66387200	-1.11241200	C	2.01005800	-2.32115800	-2.51492000
H	1.88330500	-4.09895300	-0.84331400	H	2.86461800	-3.48488100	-1.46868000
C	-0.51637600	0.37811400	3.40957400	H	1.09379600	-3.52044200	-1.59173400
H	-0.64850700	1.44277900	3.19786400	H	-1.89558200	2.24093700	-3.62791900
H	-1.15800600	0.08957500	4.25134000	C	-1.64992300	2.11546500	-2.54444300
H	0.52999400	0.22004700	3.68571700	O	-2.31909400	1.25110300	-1.92352500
C	-0.77679900	-2.31295800	2.54494700	O	-0.73863300	2.85283600	-2.09663100
H	0.27211800	-2.58160900	2.70300700				
H	-1.31665000	-2.41775500	3.49369700				
H	-1.20794700	-2.99908900	1.81027700				
C	2.09735800	2.82715200	-1.41091300				
C	3.03852500	3.37545800	-1.28264300				
H	2.06875700	2.37311200	-2.40502100				
H	1.26458900	3.53089100	-1.33453300				
C	2.09330200	2.49020500	1.41589000				
H	1.16434700	3.02430300	1.62753900				
H	2.28701300	1.78989700	2.23296800				
C	2.91803600	3.20868400	1.34241700				
H	-2.03934000	-2.10670200	-2.18382500				
H	-1.22351900	-2.38183000	-2.85863800				
H	-2.05655600	-2.81043000	-1.34687800				
H	-2.98710100	-2.17971500	-2.72951200				
C	-2.24007000	0.62375800	-2.95973600				
H	-3.20363600	0.32589900	-3.39115400				
H	-2.29049800	1.67068400	-2.65079800				
H	-1.46048900	0.53222000	-3.72109600				
C	1.99103000	-1.70025200	-2.55732400				
H	2.42429500	-0.73696400	-2.83782500				
H	2.70468100	-2.50124600	-2.78095600				
H	1.08811400	-1.84098600	-3.15778900				
H	-0.76051300	1.41348600	0.10128200				
C	-1.75910900	3.77081800	-0.14723100				
O	-2.74148300	3.33795800	-0.60151100				
O	-0.80019000	4.25507400	0.30469600				

B8

E= -990.57691718 a.u.

B7

E= -990.59647902 a.u.

Rh	0.13257800	-0.12206400	0.06344700	C	0.14605700	-0.12614700	-0.30500400
P	-1.52415200	-1.63481600	-0.55172600	P	1.58961300	1.68921700	-0.10942800
P	-1.48054800	1.18865900	1.15256500	P	1.80649100	-1.80378800	-0.01137400
C	-3.31182000	-1.20435100	-0.31741000	C	3.33333700	1.23885000	-0.62386700
H	-3.59195200	-0.50902800	-1.12345000	H	3.33914700	1.12468900	-1.72433700
H	-3.87845500	-2.13367200	-0.44155700	C	3.96973000	2.09909700	-0.38451500
C	-3.28916000	0.77530300	1.03624000	C	3.47591900	-1.19286000	-0.58737800
H	-3.74980700	1.20885900	1.93143500	H	4.21851900	-1.96279000	-0.34562700
H	-3.68267700	1.29764600	0.14977300	H	3.44198200	-1.10431100	-1.68944300
P	1.83055100	-1.65999000	-0.16902400	P	-1.06677300	-0.18297100	1.68998400
P	1.75306200	1.52679100	-0.20327200	P	-1.70780200	-0.76820400	-1.47527100
C	3.59043900	-1.03496700	-0.14963100	C	-2.91231000	0.07361600	1.54721200
H	3.87127200	-0.61299700	-1.13056100	H	-3.10215900	1.13783200	1.30915700
C	4.23313000	-1.90625300	0.01689100	H	-3.33439500	-0.10743400	2.54248500
C	3.42239900	1.27307100	0.60682800	C	-3.40572700	-0.41414400	-0.78661700
H	3.40194600	1.85636100	1.53450200	C	-4.12694800	-0.97186800	-1.39562800
H	4.18836700	1.73269000	-0.05154400	H	-3.62467800	0.66155400	-0.92918600
N	-3.58080400	-0.65405600	1.00858500	N	3.88356100	0.06141700	0.04086900
N	3.76495500	-0.09820400	0.94922300	N	-3.57270300	-0.82265100	0.60476200
C	-4.95963800	-0.90699600	1.40811500	C	5.33384900	0.15020900	0.14892600
H	-5.14366900	-1.98535200	1.43270000	H	5.60820800	1.05825200	0.69380000
H	-5.12745500	-0.51372300	2.41498100	H	5.71469600	-0.70645900	0.71256900
H	-5.69423900	-0.44222100	0.72559800	H	5.83847300	0.17005400	-0.83540400
C	5.08860900	-0.16904800	1.54635400	C	-4.98560500	-0.96125300	0.93155300
H	5.13278800	0.49884300	2.41188700	H	-5.45194600	-1.68011500	0.25173300
H	5.28536500	-1.18705400	1.89526400	H	-5.09564600	-1.34115900	1.95154500
H	5.89120600	0.12462200	0.84446700	H	-5.53452300	-0.00344900	0.85449600
				C	-1.07396700	-1.76752100	2.64603300
				H	-1.32691600	-2.58670100	1.96889500
				H	-0.07449700	-1.94145700	3.05129600
				H	-1.79362700	-1.74507500	3.47160400
				C	1.73949900	-3.34294700	-1.04550800
				H	1.56996900	-3.06126700	-2.08853200
				H	2.65847500	-3.93771300	-0.97611500
				H	0.89465400	-3.95627000	-0.71946600
				C	2.32702100	-2.54826900	1.60778600
				H	1.50699400	-3.14141200	2.02136900
				H	3.20631100	-3.19439800	1.49878200
				H	2.56230500	-1.74044800	2.30645700
				C	-1.95842700	-0.12872600	-3.19049000
				H	-2.87243600	-0.52225900	-3.65032600
				H	-1.99575600	0.96206100	-3.16796600
				H	-1.09477900	-0.42640500	-3.79086200
				C	-1.90388600	-2.58766400	-1.77740300
				H	-1.00082600	-2.96603600	-2.26329800
				H	-2.00918100	-3.08656100	-0.80997900
				H	-2.77550800	-2.81925900	-2.40095100
				C	1.98380700	2.50879100	1.50520200
				H	1.08237800	2.96457700	1.92142700
				H	2.34656000	1.74777200	2.20165200
				H	2.75218400	3.28176800	1.38878200
				C	1.44360000	3.19479300	-1.19058500
				H	2.37454000	3.77474300	-1.21288700
				H	1.18206200	2.88370600	-2.20468900

H	0.65128200	3.84455000	-0.80975200
C	-0.75594200	1.01460400	3.06519100
H	-0.91682200	2.03208300	2.70236900
H	-1.41333760	0.82715800	3.92124200
H	0.28411800	0.92379500	3.38814000
O	0.77982400	-0.05878200	-1.77830900
C	-1.91089200	3.11906200	-0.48616000
O	-1.64725100	3.34350300	0.62828200
O	-2.21419300	2.95901700	-1.59913300

B9

E= -990.58104867 a.u.

Rh	-0.06037200	-0.07832100	-0.38031500
P	-1.89697200	-1.53364300	-0.29753100
P	-1.47689400	1.82081700	0.31660700
C	-3.54326200	-0.74899500	-0.66486800
H	-3.56515500	-0.50429300	-1.74347100
H	-4.29818600	-1.52501700	-0.49590200
C	-3.22605300	1.62709300	-0.29985300
C	-3.79460500	2.48567300	0.07552900
H	-3.21299200	1.69973000	-1.40336900
P	1.19687900	-0.48419700	1.64854100
P	1.82288600	0.97878000	-1.27546400
C	2.98753200	-0.87439800	1.31341000
H	3.02500500	-1.84319900	0.79076600
H	3.46475600	-0.99950600	2.29207800
C	3.43993900	0.17455900	-0.84356500
H	4.22384300	0.75959600	-1.33801100
C	3.44965200	-0.83793900	-1.27721600
N	-3.87292200	0.40511200	0.16184400
C	3.69362000	0.18747600	0.59683300
N	-5.31668600	0.57907900	0.26853100
H	-5.76525500	-0.32623800	0.68680800
H	-5.53953300	1.40670500	0.94783600
H	-5.79591700	0.78703200	-0.70573700
C	5.12474200	0.13140700	0.87050400
H	5.62516500	0.97345200	0.38331500
H	5.29663200	0.21790400	1.94731400
H	5.59183600	-0.80497000	0.51591900
C	1.39590700	0.88987700	2.86999400
H	1.68757800	1.80671000	2.35285600
H	0.44571000	1.05957600	3.38216200
C	2.15865200	0.64885200	3.61755800
H	-1.18058800	3.52599800	-0.34210900
H	-1.01786100	3.47705200	-1.42238200
H	-2.02694900	4.19129900	-0.13746700
H	-0.28715700	3.94835700	0.12392800
C	-1.83928700	2.22337400	2.08661000
H	-0.93679100	2.60651700	2.56890500
H	-2.63056200	2.97623000	2.17383400
H	-2.15623100	1.31351900	2.60267000
C	1.88680100	1.01382200	-3.10715000
H	2.84754500	1.39318400	-3.47075700
H	1.71550200	-0.00913900	-3.44979700
H	1.07942800	1.65443100	-3.47156400
C	2.21687200	2.72698000	-0.83690900
H	1.43967900	3.39064300	-1.21996700
H	2.27652100	2.83057300	0.24871800
C	3.17650300	3.02352200	-1.27269600
H	-2.28133300	-2.44296800	1.25352900
H	-1.42552700	-3.07308000	1.50142400
H	-2.45382400	-1.72608400	2.06028000
H	-3.16973300	-3.07109600	1.13146000
C	-1.95534500	-2.87723600	-1.55299400
H	-2.93011000	-3.37666900	-1.54061900
H	-1.76158100	-2.45367400	-2.54052800
H	-1.16417600	-3.59554700	-1.33144400
C	0.79516200	-1.88350600	2.77595600
C	0.78812000	-2.79746300	2.17950900
H	1.53836900	-1.96275400	3.57635700
H	-0.19031200	-1.72929200	3.22232300
H	-0.68386500	0.11421600	-1.82959300
O	0.89942500	-1.90152000	-1.10354800
C	0.93601500	-2.78055600	-0.22117200
O	1.29351200	-1.90197300	-2.27071700

B10

E= -991.03308083 a.u.

Rh	0.01746900	0.29289700	-0.44961700
P	-1.96223300	1.41094900	0.06824600
P	-1.18529800	-1.77052000	-0.65593700
C	-3.27695600	0.40464600	0.91184900
H	-2.95906900	0.20707200	1.95307900
H	-4.16228700	1.04700800	0.96858000
C	-2.69421500	-1.90715700	0.42112800
H	-3.18712200	-2.84747400	0.15332000
H	-2.38381200	-1.99408400	1.47822000
P	2.01115100	-0.50394200	-1.35227400
O	0.92219800	0.06946600	1.76963000
C	2.89390000	-1.85403700	-0.39595200
H	3.98092400	-1.65333700	-0.46057900

H	2.71213700	-2.78852300	-0.93761500
C	2.54963400	-0.83176400	1.78622600
H	2.77361000	-1.09533000	2.82489800
H	3.35440300	-0.15237700	1.45813400
N	-3.63067200	-0.81275100	0.19823300
C	2.45857700	-2.04226300	0.97868900
N	-5.00801600	-1.21562300	0.47840200
H	-5.68926500	-0.40710500	0.20230600
H	-5.26486500	-2.08773900	-0.12781600
H	-5.17038800	-1.46522800	1.54063700
C	3.13344400	-3.18576800	1.58417200
H	2.72875800	-3.36226500	2.58421300
H	2.94398100	-4.08037400	0.98374400
H	4.22465100	-3.04709800	1.66520500
C	1.91632300	-1.25857800	-3.02384400
H	1.22813200	-2.10737000	-3.01373300
H	1.53352000	-0.51398100	-3.72546500
H	2.89980200	-1.60063100	-3.35957700
C	-0.34397200	-3.36720600	-0.29486600
H	0.19780400	-3.29606300	0.65053600
H	-1.05746200	-4.19628800	-0.27029100
H	0.39098000	-3.56920900	-1.07925100
C	-1.92775700	-2.05829200	-2.31083900
H	-1.16546000	-1.95452100	-3.08561300
H	-2.38711500	-3.04896200	-2.37906100
H	-2.69209400	-1.29606500	-2.47869000
C	1.38700700	1.61528000	2.65190400
H	1.91440500	1.39730800	3.58560100
H	2.03059900	2.21566700	2.00388300
H	0.49807200	2.20442500	2.88510400
C	-0.01219700	-0.87168200	3.04808000
H	-1.00054300	-0.42644100	3.18961000
H	-0.14461000	-1.90189000	2.70647400
H	0.51192300	-0.87879200	4.00853300
C	-2.84393300	2.08302000	-1.38820300
H	-2.17190000	2.75391700	-1.92732600
H	-3.11446900	1.25642200	-2.04818700
C	-3.74691400	2.62387200	-1.09073300
H	-1.87472700	2.84733000	1.20865500
H	-2.85337100	3.32776500	1.29976300
H	-1.55283600	2.52101600	2.20049900
H	-1.15669400	3.57341400	0.82323900
C	3.30665800	0.77570200	-1.57609900
H	3.51820800	1.26519700	-0.62303300
H	4.22631900	0.34571900	-1.98324600
H	2.92606100	1.53582600	-2.26220500
H	0.67671000	1.72898900	-0.49944700
H	-0.37066000	0.60925200	-1.94682800
C	1.56138300	4.21629500	-0.45401500
O	2.59709000	3.82016800	-0.09412900
O	0.52688000	4.61992200	-0.80551600

B11

E= -991.02090528 a.u.

Rh	-0.03844900	0.40736300	-0.38793000
P	-2.22134800	1.01722300	0.23523300
C	-0.73856700	-1.73241200	-0.84750600
P	-3.29570200	-0.32602200	0.92154500
H	-2.95577300	-0.56189900	1.94747500
H	-4.30449200	0.09044800	1.00886000
C	-2.15633800	-2.33767700	0.18694700
H	-2.39273600	-3.33637300	-0.19467800
H	-1.82044400	-2.46137200	1.23189400
P	2.11886800	0.12689400	-1.30877100
H	0.88076000	0.10341900	1.87238900
C	3.29752300	-1.03793800	-0.43591100
H	4.29892900	-0.56798400	-0.45877700
C	3.35711800	-1.94195900	-1.05159600
H	2.69187300	-0.30884700	1.81134500
H	3.00607600	-0.57823500	2.82498500
H	3.26840700	0.58901100	1.53636400
N	-3.33867600	-1.49938500	0.06306400
N	2.91431200	-1.43546700	0.90944000
C	-4.57115300	-2.26520700	0.24969600
H	-5.43184200	-1.61765500	0.06756900
H	-4.60862600	-3.07956200	-0.47775700
H	-4.65868500	-2.69162800	1.26270800
C	3.85573400	-2.41709700	1.44313700
H	3.50225900	-2.77512800	2.41351900
H	3.90747900	-3.27565000	0.76723600
H	4.87288200	-2.01014200	1.56595600
C	2.22140600	-0.47150900	-3.04159400
H	1.77752000	-1.46565200	-3.13342300
H	1.66435300	0.21593800	-3.68247800
H	3.26064000	-0.51545600	-3.37990000
C	0.48669800	-3.08320600	-0.63776900
H	1.08303600	-2.90366100	0.26023500
H	-0.00994000	-4.05644400	-0.58988000
H	1.16635600	-3.09059600	-1.49423300
C	-1.39236000	-1.97735100	-2.54010700
H	-0.67332000	-1.61046900	-3.27466300
H	-1.60112900	-3.03486300	-2.72626300
H	-2.31662500	-1.40435900	-2.64034600

C	0.87359200	1.59578700	2.93957900	Rh	-1.42321300	-0.04952500	0.27708600
H	1.63256700	1.51407000	3.72324100	P	-0.88517900	1.99800300	1.27618500
H	1.06128300	2.47098500	2.31317600	P	-1.69723300	1.01720100	-1.73670800
H	-0.10073600	1.71682300	3.41682000	C	-1.77326400	3.47859500	0.60595000
C	0.25345800	-1.23418600	2.96995500	H	-2.83769100	3.41401000	0.90026500
H	-0.81964100	-1.10578400	3.13530300	H	-1.35270900	4.35611800	1.10783300
H	0.42011900	-2.20630300	2.49779500	C	-2.41610700	2.72686200	-1.61839800
H	0.75992400	-1.21953000	3.93956000	H	-2.45703900	3.10238900	-2.64635400
C	-3.20158700	1.68375300	-1.15833200	H	-3.45744500	2.66012600	-1.25677600
H	-2.66750000	2.53068400	-1.59565700	P	-1.46111100	-2.22388600	-0.63851100
H	-3.31630600	0.90978800	-1.91963300	P	-3.78852900	-0.24126300	0.97262900
H	-4.18693800	2.01604300	-0.81967300	C	-3.08366300	-2.84449200	-1.34005500
C	-2.32467400	2.30866100	1.52824600	H	-3.18826000	-3.90627100	-1.04750100
H	-3.32584600	2.74719300	1.54853900	H	-2.98344900	-2.82434900	-2.43080600
H	-2.11425900	1.86757600	2.50521900	C	-4.44742400	-1.90095400	0.45917400
H	-1.58383100	3.08533700	1.32555200	H	-5.51477100	-1.93910900	0.70069900
C	3.03640400	1.71037800	-1.37852600	H	-3.96423300	-2.69097300	1.05372900
H	3.04592300	2.18660400	-0.39646800	N	-1.59602100	3.63444800	-0.83046400
H	4.05769400	1.54164500	-1.73073600	N	-4.25803000	-2.06432000	-0.98219800
H	2.52794200	2.39009100	-2.06567600	C	-1.78156500	5.02403000	-1.24635500
H	-0.02703900	3.06635000	-1.89303000	H	-1.09044400	5.66473800	-0.69374300
H	-0.49601000	0.71918000	-1.85800600	H	-1.55136800	5.12334300	-2.30992400
C	0.19244200	3.39306500	-0.85270400	H	-2.80932200	5.38511400	-1.07361100
O	0.19597800	4.57089800	-0.55717900	C	-5.44428600	-2.57249100	-1.66437900
O	0.43431700	2.42198800	-0.01320200	H	-6.30000600	-1.92989000	-1.44176000
				H	-5.27980500	-2.54931100	-2.74587200
				H	-5.69534300	-3.60658300	-1.37520200
				C	-0.29558800	-2.55735000	-2.01820800
				H	-0.53867000	-1.93695000	-2.88433300
				H	0.71605800	-2.30074900	-1.69306300
				H	-0.32715500	-3.60991500	-2.31384900
				C	-2.82817100	0.22525400	-2.94828800
				H	-3.70259200	-0.17771900	-2.43123700
				H	-3.12552500	0.93685800	-3.72373200
				H	-2.31018400	-0.60739300	-3.43136900
				C	-0.16060100	1.33457000	-2.67751600
				H	0.52449400	0.48810200	-2.59067900
				H	-0.37941000	1.55072000	-3.72720700
				H	0.32365500	2.20438000	-2.22628700
				C	-4.07896600	-0.24044600	2.78522200
				H	-5.02346100	-0.73525000	3.03040000
				H	-3.24371400	-0.75221900	3.26950700
				H	-4.12767800	0.78718600	3.15393000
				C	-5.11341300	0.86321900	0.32627700
				H	-4.88750400	1.90446200	0.57128300
				H	-5.17624500	0.76465700	-0.76082000
				H	-6.08464600	0.60775800	0.76071900
				C	0.87708900	2.44952700	1.10018700
				H	1.49910000	1.59607200	1.38337600
				H	1.06799400	2.66685200	0.04761200
				H	1.12946000	3.32371900	1.70725500
				C	-1.22677500	2.12638000	3.07065600
				H	-0.85614600	3.07999900	3.45736700
				H	-2.30031300	2.05479000	3.25393400
				H	-0.74021200	1.30700000	3.60205500
				C	-1.01617700	-3.49462900	0.60257600
				H	-1.64920200	-3.39100600	1.48566400
				H	-1.11465400	-4.49458700	0.17108100
				H	0.01288600	-3.33922100	0.93123000
				H	0.84344700	-0.51541400	2.17620100
				H	0.09679400	-0.10877800	-0.08123300
				C	0.03780200	-1.06994800	2.70008500
				O	0.27562200	-1.70372500	3.71316600
				O	-1.13617700	-0.98300700	2.14103800
				P	3.17462800	-0.07827100	-0.76169500
				N	4.13056200	-1.28000100	-1.59732800
				N	2.99473700	-0.66539000	0.87946700
				N	4.03748200	1.41639300	-0.62959000
				C	2.65440800	-2.07999100	0.93267100
				C	1.87959800	-2.29535500	0.18849900
				H	3.45588200	2.52436600	-1.37676400
				H	4.16332200	2.91747500	-2.11943100
				C	3.65592300	-1.52587400	-2.95590600
				C	2.59035500	-1.29237100	-3.03233100
				C	5.20086000	1.84940200	0.14756200
				H	4.88323400	2.24320700	1.12465900
				H	5.65284400	2.70024200	-0.37815400
				C	6.30631700	0.80474200	0.33826500
				H	6.85644600	0.70241200	-0.60128300
				H	7.01799600	1.21018100	1.07885900
				C	3.75782200	-0.19472200	2.02387400
				H	3.70211100	0.89658200	2.05010900
				H	3.26068300	-0.55220300	2.93509500
				C	5.23018900	-0.65480000	2.01792900
				H	5.78844600	-0.09616300	2.78614000
				C	5.28292400	-1.71100800	2.30178200
				H	5.57213700	-1.48972200	-1.52417400
				H	6.09897100	-0.68391000	-2.06513200
				H	5.80869200	-2.41799000	-2.06090600
				C	6.13340900	-1.62265000	-0.11413000
				H	5.71105100	-2.51652000	0.35321500
				H	7.22082800	-1.79227000	-0.20585600
				N	5.82769900	-0.49131000	0.72235300
				H	3.49849200	-2.74804400	0.71310900
				H	2.25885500	-2.32601400	1.92342000

B12

E= -801.57032153 a.u.

Rh	-0.13730200	0.02507500	-0.51553000				
P	-2.10374100	1.33748700	-0.33630000				
P	-0.94719900	-1.25962400	1.11369800				
C	-3.56397600	0.43348100	0.37509500				
H	-3.61616500	0.59503000	1.46571700				
H	-4.45951700	0.89528500	-0.05125800				
C	-2.72817600	-1.76703500	0.91035800				
H	-2.69888300	-2.79423500	0.53295100				
H	-3.16178400	-1.79914500	1.92774100				
P	1.71796900	-1.26615000	-1.23468800				
P	1.51117500	1.73277100	0.23426400				
C	3.15507100	-1.35054300	-0.05655800				
H	4.08648500	-1.35711800	-0.65344700				
H	3.08900800	-2.32690000	0.43512600				
C	3.22714400	1.02859900	0.39594400				
H	3.78054700	1.68714900	1.07197300				
H	3.75892900	1.06450700	-0.56790600				
N	-3.49840500	-0.96290700	-0.01023100				
N	-3.15098900	-0.31518300	0.96531300				
C	-4.80672700	-1.56221500	-0.29330000				
H	-5.30962600	-0.97958900	-1.06767000				
H	-4.66375600	-2.57421900	-0.67844900				
H	-5.45435200	-1.60824100	0.59473500				
C	4.20246700	-0.56516800	1.95887600				
H	4.13696600	0.18101100	2.75360300				
H	4.05180700	-1.54944500	2.40886100				
H	5.21246500	-0.53038000	1.52357600				
C	1.52638100	-2.99692500	-1.80102400				
H	1.28118000	-3.66300300	-0.97340100				
H	0.72976600	-3.04718800	-2.54668500				
C	2.45901100	-3.34192200	-2.25677300				
H	-0.80989600	-0.37489000	2.70866900				
H	-1.27650400	0.61079000	2.66206000				
H	-1.28956800	-0.96145000	3.49795300				
H	0.24886200	-0.25826400	2.94964800				
C	-0.09047400	-2.83581800	1.43719400				
H	0.96823100	-2.64518800	1.62778600				
H	-0.52762300	-3.30146700	2.32605000				
H	-0.20834800	-3.51559400	0.59254900				
C	1.73188100	3.19835400	-0.85441800				
C	2.55928300	3.82123000	-0.50273400				
H	1.93556000	2.89339000	-1.88395100				
H	0.82270200	3.80487200	-0.85482600				
C	1.26603000	2.45881000	1.90334500				
H	0.26245800	2.87112400	2.01409100				
H	1.41797700	1.68496100	2.65869000				
H	1.99354500	3.25829400	2.07041400				
C	-2.59786700	1.68785700	-2.06539600				
H	-1.78962800	2.19173500	-2.60167600				
H	-2.82024800	0.74256400	-2.56568100				
H	-3.48354500	2.32952400	-2.08503900				
C	-2.15530500	2.95495300	0.52357100				
H	-3.13663600	3.41783100	0.38335300				
H	-1.98744100	2.82523300	1.59558000				
H	-1.39708400	3.63257800	0.12496900				
C	2.33319800	-0.43327000	-2.75558400				
H	2.55777600	0.62025100	-2.57772500				
H	3.23862100	-0.92818100	-3.11825400				
H	1.56884600	-0.49760900	-3.53477100				
H	-1.08037500	-1.05434700	-1.15915800				

B13

E= -1572.00849465 a.u.

H	3.79535700	-2.58198100	-3.21846900
H	4.18979700	-0.91910600	-3.70535400
H	2.56280800	2.18893800	-1.90877400
H	3.17284000	3.35492100	-0.71216400

C	-5.56964300	-1.06773600	-1.80023400
H	-5.77951900	-0.08539600	-2.23128000
H	-6.26908600	-1.77837000	-2.27443700
N	-5.74780600	-0.97880200	-0.37438000
H	-4.87807200	1.83105900	-1.74566200
H	-4.50051000	3.14936700	-0.61261800
H	-1.65588900	-2.21247900	-2.05796600
H	-0.96624300	-0.63250000	-1.61807500
H	-1.47707200	-0.71592900	2.12265000
H	-2.85954200	-0.60263500	3.25002500

B14

E= -1572.00955752 a.u. Rh

Rh	1.76207300	0.30656700	-0.47974900
P	0.74504500	2.24816800	-1.04082700
P	2.00505900	0.85859300	1.75363400
C	-0.48265400	2.93405200	0.23696200
H	-0.25256400	3.95437600	0.55689800
H	-1.48689600	2.91484600	-0.18998900
C	0.73092200	2.15076000	2.27274900
H	0.46327600	2.02277200	3.32399300
H	1.14339000	3.15538400	2.14904700
P	1.47956700	-2.01104000	-0.22560100
P	4.05283600	-0.00072300	-1.10323000
C	2.91926500	-2.82263000	0.68115900
C	3.14227400	-3.79229000	0.19314000
H	2.55761900	-3.05654900	1.68867500
C	4.71091000	-1.64387300	-0.47498300
H	5.79649600	-1.55669800	-0.36055800
H	4.54210800	-2.42334100	-1.23832300
N	-0.53340300	2.07561700	1.46265900
N	4.11948500	-2.00448500	0.81566900
C	-1.73502600	2.37975600	2.28995700
C	-2.62944000	2.25967300	1.67153800
H	-1.76905100	1.67701100	3.12391200
H	-1.64876900	3.39997200	2.66778600
C	5.08283800	-2.66061900	1.69360000
H	5.94455500	-2.00587500	1.85046900
H	4.62169400	-2.85000700	2.66810500
H	5.44518300	-3.62383600	1.29323800
C	0.09041900	-2.88880000	0.62982600
H	0.07942900	-2.61694900	1.68823700
H	-0.86270300	-2.58092200	0.19186800
H	0.19091100	-3.97657500	0.54813400
C	3.49769800	1.70277500	2.44085300
C	3.81119500	2.50700700	1.77103200
H	3.33198000	2.10139300	3.44707700
H	4.30022300	0.96178100	2.48810200
C	1.73617900	-0.39348100	3.08746900
C	2.50171200	-1.16490900	2.97049000
H	1.82323800	0.04267200	4.08760700
C	0.75356900	-0.85985700	2.97877300
C	4.46291000	-0.14210100	-2.89798700
H	5.49229300	-0.47565300	-3.06678600
H	3.76979100	-0.83992900	-3.37442400
H	4.32588000	0.83456200	-3.37017800
C	5.41671600	1.12047100	-0.53916000
H	5.17172300	2.15703900	-0.78616300
H	5.52579400	1.04382700	0.54510600
H	6.37233900	0.85960600	-1.00657300
C	-0.32700800	2.33689800	-2.53888200
C	0.28898500	2.09640100	-3.40890800
H	-1.11017100	1.57856200	-2.46270800
H	-0.77620600	3.32562300	-2.67809200
C	1.77517800	3.77066300	-1.27831300
H	1.18449900	4.66178700	-1.51722600
H	2.36326000	3.95336200	-0.37392200
C	2.47738400	3.58035000	-2.09458100
H	1.50531000	-2.93627700	-1.82390400
H	2.39745400	-2.65655400	-2.38913500
H	1.50017500	-4.02005000	-1.66996500
H	0.63521100	-2.64777500	-2.41748600
H	1.39141600	-0.03308700	-1.98928200
H	-0.62755400	1.11060500	1.07194000
P	-2.92609000	-0.04780700	0.01467700
C	-3.08270700	-0.71495000	-1.57043200
N	-4.11060900	1.24194700	0.16998000
N	-3.32779400	-1.19547500	1.25432800
C	-4.18432900	2.15744700	-0.95793700
C	-3.20189400	2.25329400	-1.43137200
C	-2.43396400	-1.16639500	2.40284600
H	-2.22847700	-2.18526100	2.75498700
C	-1.79704500	-1.12235700	-2.13564500
C	-1.74812300	-0.85784000	-3.19981100
C	-4.56908600	-1.89084800	1.59688600
H	-5.09959700	-1.34439400	2.39391300
H	-4.30206500	-2.86398900	2.03104600
C	-5.52390600	-2.14570000	0.43239700
C	-5.10877300	-2.93215800	-0.20302900
H	-6.46145600	-2.54497900	0.85667700
C	-5.34871200	1.08414200	0.91423500
H	-5.10577100	0.68879900	1.90473400
C	-5.78481100	2.07802500	1.07712900
C	-6.38071800	0.16895700	0.21398700
C	-7.15060400	-0.13267400	0.93989400
H	-6.89947300	0.73026900	-0.57034000
C	-4.15829200	-1.48821400	-2.18377100
H	-4.00993700	-2.55867800	-1.96237400
H	-4.06227000	-1.39291800	-3.27347500

B15

E= -802.45587685 a.u.

Rh	-0.21276000	0.28069700	-0.45363400
P	-2.29312300	1.20218800	-0.53911900
P	-0.57508000	-0.62503300	1.67408800
C	-3.50087600	-0.06989600	0.21529200
H	-3.77720400	0.19904900	1.23696300
H	-4.41268800	-0.15838400	-0.37825400
C	-2.13896100	-1.69745100	1.52263900
H	-1.83460900	-2.74685900	1.49674700
H	-2.85794100	-1.55890700	2.33407700
P	1.16691800	-1.39611600	-1.27397300
P	1.62914900	1.74108100	0.01280700
C	2.79908600	-1.57668700	-0.35197700
H	3.59280400	-1.78003400	-1.09777200
C	2.71221500	-2.47742800	0.26620300
C	3.24609000	0.82195200	-0.15508000
H	4.04029300	1.42200400	0.30200200
H	3.50859800	0.71991800	-1.22118400
N	-2.79264800	-1.38921100	0.21921700
N	3.15781500	-0.47122100	0.52679100
C	-3.58559800	-2.50846800	-0.33415000
H	-3.94077300	-2.22888400	-1.32733400
H	-2.94249000	-3.38632300	-0.41677100
H	-4.43402700	-2.72955700	0.31610000
C	4.36768100	-0.79116000	1.27670400
H	4.57643600	0.00310600	1.99859400
H	4.21766300	-1.72166000	1.83306400
H	5.25343300	-0.91848300	0.63051500
C	0.66579600	-3.17697100	-1.35011800
C	0.31606200	-3.51618300	-0.37066000
H	-0.15717100	-3.27391000	-2.06370100
H	1.48926400	-3.82265000	-1.67362100
C	-1.00982600	0.42639200	3.12737800
H	-1.83689800	1.09341900	2.87318100
H	-1.28513100	-0.17119700	4.00166700
C	-0.14847600	1.04873900	3.38210500
H	0.59351800	-1.81940200	2.44798800
H	1.54836200	-1.30298200	2.58125600
H	0.23404100	-2.19847000	3.40886600
H	0.76623300	-2.65791500	1.76868900
C	1.93904500	3.20045900	-1.07051700
H	2.90270400	3.67617600	-0.86088000
H	1.90913800	2.88269400	-2.11592000
H	1.14297500	3.93511000	-0.92181300
C	1.86359100	2.46326300	1.69806700
H	0.96909100	3.01853600	1.99279500
H	2.01681800	1.64540600	2.40908800
C	2.72889100	3.13315000	1.73951000
H	-3.06826000	1.52629500	-2.17940900
H	-2.47688600	2.29113800	-2.68919200
H	-3.02232800	0.61808600	-2.78450600
H	-4.10299400	1.87104200	-2.09130100
C	-2.80985100	2.71900100	0.37990800
H	-3.89060400	2.88836900	0.34045300
H	-2.48573200	2.66031200	1.42142000
H	-2.30549500	3.57513800	-0.07695800
C	1.74187900	-1.15134400	-3.00730900
H	2.20088400	-0.16450600	-3.10226400
H	2.46166700	-1.91800200	-3.31028500
H	0.87550700	-1.17825800	-3.67223100
H	-0.15762000	0.76185100	-1.96509200
H	-1.91384200	-1.16866400	-0.42564200

B16

E= -1383.44759894 a.u.

Rh	1.76207300	0.30656700	-0.47974900
P	0.74504500	2.24816800	-1.04082700
P	2.00505900	0.85859300	1.75363400
C	-0.48265400	2.93405200	0.23696200
H	-0.25256400	3.95437600	0.55689800
H	-1.48689600	2.91484600	-0.18998900
C	0.73092200	2.15076000	2.27274900
H	0.46327600	2.02277200	3.32399300
H	1.14339000	3.15538400	2.14904700
P	1.47956700	-2.01104000	-0.22560100
C	4.05283600	-0.00072300	-1.10323000
P	2.91926500	-2.82263000	0.68115900
H	3.14227400	-3.79229000	0.19314000

H	2.55761900	-3.05654900	1.68867500	H	-4.74992300	-1.83406800	1.55107100
C	4.71091000	-1.64387300	-0.47498300	H	-4.88213300	-2.86114100	0.10519900
H	5.79649600	-1.55669800	-0.36055800	P	-1.65764200	1.15968400	1.79780600
H	4.54210800	-2.42334100	-1.23832300	P	-1.23316200	1.67197700	-1.54261300
N	-0.53340300	2.07561700	1.46265900	C	-2.61194500	2.76074200	1.52686600
C	4.11948500	-2.00448500	0.81566900	H	-2.10410600	3.56677800	2.09316600
N	-1.73502600	2.37975600	2.28995700	H	-3.59476600	2.62115200	1.99200200
H	-2.62944000	2.25967300	1.67153800	C	-1.59432300	3.26643100	-0.63757600
H	-1.76905100	1.67701100	3.12391200	H	-1.70901500	4.06491100	-1.37897900
H	-1.64876900	3.39997200	2.66778600	H	-0.72900200	3.54528800	-0.01355300
C	5.08283800	-2.66061900	1.69360000	N	-2.96429600	-2.78725600	1.01234700
H	5.94455500	-2.00587500	1.85046900	N	-2.82924200	3.13770500	0.13715200
H	4.62169400	-2.85000700	2.66810500	C	-3.03678700	-3.58408800	2.25550300
H	5.44518300	-3.62383600	1.29323800	H	-2.03545700	-3.94259800	2.49961100
C	0.09041900	-2.88880000	0.62982600	H	-3.39520600	-2.94216700	3.06212100
H	0.07942900	-2.61694900	1.68823700	H	-3.71380600	-4.43026400	2.12443100
H	-0.86270300	-2.58099200	0.19186800	C	-3.66843600	4.32735000	0.05769000
H	0.19091100	-3.97657500	0.54813400	C	-3.88851800	4.55343200	-0.98311900
C	3.49769800	1.70277500	2.44085300	H	-4.61831600	4.14107100	0.56895300
H	3.81119500	2.50700700	1.77103200	H	-3.20137500	5.21605400	0.51713700
H	3.33198000	2.10139300	3.44707700	C	-2.42003600	0.64477400	3.40494900
C	4.30022300	0.96178100	2.48810200	H	-3.44479200	0.29876600	3.23854900
H	1.73617900	-0.39348100	3.08746900	H	-1.83777300	-0.18394400	3.81719100
H	2.50171200	-1.16490900	2.97049000	H	-2.43745500	1.46141000	4.13476400
H	1.82323800	0.04267200	4.08760700	C	-4.55489900	-1.03163700	-2.02249600
H	0.75356900	-0.85985700	2.97877300	H	-3.97585800	-1.84805600	-2.46140900
C	4.46291000	-0.14210100	-2.89798700	H	-5.60538800	-1.33015300	-1.95268500
H	5.49229300	-0.47565300	-3.06678600	H	-4.47553400	-0.17198800	-2.69263000
H	3.76979100	-0.83992900	-3.37442400	C	-5.14381400	0.56880700	0.25541900
H	4.32588000	0.83456200	-3.37017800	C	-5.01341500	1.52992300	-0.24959500
C	5.41671600	1.12047100	-0.53916000	H	-6.15687100	0.19144600	0.08877800
H	5.17172300	2.15703900	-0.78616300	H	-4.98992200	0.73709600	1.32456800
H	5.52579400	1.04382700	0.54510600	C	0.40871700	2.07450900	-2.27604500
H	6.37233900	0.85960600	-1.00657300	H	0.42129600	3.08008900	-2.70969900
C	-0.32700800	2.33689800	-2.53888200	H	1.18544100	1.99365300	-1.50925300
H	0.28898500	2.09640100	-3.40890800	H	0.63904200	1.35309900	-3.06428300
H	-1.11017100	1.57856200	-2.46270800	C	-2.35777800	1.89994800	-2.99363500
C	-0.77620600	3.32562300	-2.67809200	H	-2.31669900	1.01822200	-3.63885700
H	1.77517800	3.77066300	-1.27831300	H	-3.38072000	2.01437400	-2.62172500
H	1.18449900	4.66178700	-1.51722600	C	-2.09493200	2.78629900	-3.58097900
H	2.36326000	3.95336200	-0.37392200	H	0.56837100	-3.08699600	-0.16396600
H	2.47738400	3.58035000	-2.09458100	H	1.43467100	-2.46830500	-0.41496700
C	1.50531000	-2.93627700	-1.82390400	H	0.51423800	-3.13965200	0.92643500
H	2.39745400	-2.65655400	-2.38913500	H	0.70666800	-4.09075200	-0.57795600
H	1.50017500	-4.02005000	-1.66996500	C	-0.93003600	-2.80657000	-2.56853100
H	0.63521100	-2.64777500	-2.41748600	H	-0.82050700	-3.88898600	-2.69129100
H	1.39141600	-0.03308700	-1.98928200	H	-1.83597600	-2.46627700	-3.07618800
H	-0.62755400	1.11060500	1.07194000	H	-0.07760200	-2.31383200	-3.04433300
P	-2.92609000	-0.04780700	0.01467700	C	-0.03377700	1.79440500	2.39410800
N	-3.08270700	-0.71495000	-1.57043200	H	0.52795100	2.19329700	1.54611400
N	-4.11060900	1.24194700	0.16998000	H	-0.15330000	2.56678900	3.16025500
N	-3.32779400	-1.19547500	1.25432800	H	0.54697300	0.96415900	2.80199400
C	-4.18432900	2.15744700	-0.95793700	H	-0.00627100	-0.11378800	0.22869100
C	-3.20189400	2.25329400	-1.43137200	H	-2.30205800	-1.90201600	1.14796900
C	-2.43396400	-1.16639500	2.40284600	P	2.99595200	0.18691500	0.11970100
C	-2.22847700	-2.18526100	2.75498700	N	3.50115700	-0.50238300	1.63688800
N	-1.79704500	-1.12235700	-2.13564500	N	3.91234500	1.64303100	-0.13895700
C	-1.74812300	-0.85784000	-3.19981100	N	3.45365000	-0.86531500	-1.19661400
C	4.56908600	-1.89084800	1.59688600	C	3.86147200	2.61283500	0.93861400
H	-5.09959700	-1.34439400	2.39391300	H	2.90010500	2.53702100	1.45756100
H	4.30206500	-2.86398900	2.03104600	C	2.47180100	-0.86385300	-2.27325000
C	-5.52390600	-2.14570000	0.43239700	H	2.39774900	-1.86554300	-2.72098200
C	-5.10877300	-2.93215800	-0.20302900	C	2.41191600	-1.19000400	2.31877700
H	-6.46145600	-2.54497900	0.85667700	H	1.44966900	-0.88359900	1.89807500
C	-5.34871200	1.08414200	0.91423500	C	4.75536100	-1.30309000	-1.70101700
H	-5.10577100	0.68879900	1.90473400	H	5.07469000	-0.65549100	-2.53416700
H	-5.78481100	2.07802500	1.07712900	H	4.62693800	-2.30396800	-2.13859400
C	-6.38071800	0.16895700	0.21398700	C	5.88522100	-1.38903900	-0.67402900
H	-7.15060400	-0.13267400	0.93989400	H	5.69854700	-2.23541000	-0.00814600
H	-6.89947300	0.73026900	-0.57034000	C	6.80745700	-1.62814500	-1.23264400
C	-4.15829200	-1.48821400	-2.18377100	C	5.04400200	1.73855500	-1.03946800
H	-4.00993700	-2.55867800	-1.96237400	H	4.75611000	1.30857300	-2.00248200
C	-4.06227000	-1.39291800	-3.27347500	H	5.24641100	2.80024300	-1.22879200
H	-5.56964300	-1.06773600	-1.80023400	C	6.32365600	1.04973000	-0.51017400
H	-5.77951900	-0.08539600	-2.23128000	H	7.03401600	0.91422400	-1.34011000
H	-6.26908600	-1.77837000	-2.27443700	H	6.81993200	1.70455600	0.21418100
N	-5.74780600	-0.97880200	-0.37438000	C	4.78075600	-1.02148600	2.09721800
H	-4.87807200	1.83105900	-1.74566200	H	4.84702000	-2.10063200	1.87194200
H	-4.50051000	3.14936700	-0.61261800	H	4.80854900	-0.94560400	3.19370600
H	-1.65588900	-2.21247900	-2.05796600	C	6.01095600	-0.30425200	1.56118400
H	-0.96624300	-0.63250000	-1.61807500	H	6.03207200	0.71020200	1.96877700
H	-1.47707200	-0.71592900	2.12265000	H	6.89542800	-0.82727400	1.96762900
H	-2.85954200	-0.60263500	3.25002500	N	6.03688800	-0.20628300	0.12564700
				H	4.64725100	2.47278600	1.69730200
				H	3.95126400	3.62778200	0.53366200
				H	2.42283100	-0.95918000	3.39320500
				H	2.49422100	-2.28482500	2.21267600
				H	1.49036200	-0.58022500	-1.88057000
				H	2.73486400	-0.16009900	-3.08057200

B17

E= -1383.43758577 a.u.

Rh	-1.54641300	-0.19953700	-0.07931200
P	-0.96716800	-2.28432300	-0.79569800
P	-3.84642700	-0.57595700	-0.37861000
C	-2.29398300	-3.48463000	-0.13091500
C	-3.03370900	-3.72495000	-0.89712200
H	-1.85241600	-4.41552700	0.22965500
C	-4.24927500	-2.14011600	0.62902900

B18

E= -990.98884447 a.u.

Rh	0.09429100	-0.02006000	-0.36779900
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P	1.89112400	-1.21225100	-1.07953500	C	-0.59757300	-0.54502400	3.40299900
P	0.10640500	-1.08928300	1.71573700	H	-0.30334700	-1.59036600	3.27245900
C	3.13261600	-1.36550400	0.35532100	H	0.26628800	0.01476700	3.77185600
C	3.10276400	-2.35651200	0.81319700	H	-1.39514300	-0.49566300	4.15187600
H	4.15013500	-1.16785200	0.01397400	C	0.90754700	-3.05973800	-1.78963600
C	1.85066800	-0.86771300	2.43477200	H	1.76029300	-2.58813700	-2.28342400
H	1.79876600	-0.11350500	3.22376700	H	1.13223400	-4.11700000	-1.62012000
H	2.28088000	-1.78258500	2.85088000	C	0.04948200	-2.98445000	-2.46211600
P	-1.11383500	1.87385900	0.24743300	H	-0.67034900	-3.36314100	0.54924700
P	-1.90847600	-0.93019500	-1.36587200	H	-1.63274600	-3.23458600	0.04583200
C	-2.78515800	1.47244200	1.01170100	H	-0.33870800	-4.40158700	0.46214500
H	-3.49314000	2.26776200	0.70562500	H	-0.81574800	-3.11671100	1.60369700
C	-2.65986600	1.56596600	2.09615100	C	-1.94373100	1.98259500	-2.47980700
C	-3.46422300	-0.13575000	-0.69214400	H	-2.91476300	2.01560800	-2.98455800
H	-4.29328200	-0.83553400	-0.84042500	H	-1.87675200	2.80165700	-1.75969000
H	-3.71286600	0.76722200	-1.27648000	H	-1.15428800	2.12514900	-3.22290400
N	2.76444100	-0.33652300	1.38130000	C	-1.98254200	-0.84689400	-2.94667500
N	-3.32331600	0.14587000	0.73667800	H	-1.12102300	-0.89795800	-3.61787100
C	3.92933600	0.38635900	1.94617500	H	-2.12904500	-1.82962100	-2.48788100
H	4.52467300	0.79094800	1.12901100	H	-2.87385300	-0.59447300	-3.53088200
H	3.56420100	1.20780800	2.56453500	C	3.10130300	2.15658400	-0.64163400
C	4.52827500	-0.29689400	2.55089300	H	2.55133900	2.93338400	-1.17972000
C	-4.57631900	-0.04505700	1.46082400	H	3.03706000	2.38470300	0.42414700
H	-4.93685400	-1.06665100	1.31380900	C	4.14401500	2.16974500	-0.97331500
H	-4.40760800	0.10372000	2.53209000	H	2.74617600	0.30490500	-2.74978600
C	-5.36689500	0.65530700	1.14031400	H	3.82653400	0.36899300	-2.91387800
H	-0.55578300	3.15854700	1.45508900	H	2.37346400	-0.65301600	-3.11871000
H	-0.23037900	2.68736700	2.38617800	H	2.25871500	1.09368400	-3.32989900
O	0.28986900	3.70170300	1.02684300	C	-1.63808400	1.85860600	2.34253700
H	-1.35311000	3.87605900	1.67678700	H	-2.07559600	2.40449000	1.50319800
C	-0.08849500	-2.91816300	1.90590600	H	-2.36241600	1.81069500	3.16133600
H	0.57848600	-3.44766500	1.22200700	H	-0.74937500	2.39901900	2.67858000
H	0.11747500	-3.24463200	2.92982800	H	0.18580400	1.71083100	0.07493800
H	-1.11527100	-3.19195500	1.65294100	H	1.91413900	-0.53503800	1.14914900
C	-0.90428200	-0.52217600	3.14855800	C	0.17879900	4.33580600	0.64017400
H	-1.95309800	-0.69339800	2.89108300	O	-0.71518400	4.46432100	-0.09583700
H	-0.66077300	-1.06277600	4.06785200	O	1.07640900	4.21491800	1.37350100
C	-0.75962800	0.54876100	3.30982800				
C	-2.18848500	-0.75161500	-3.18065600				
H	-3.19752800	-1.05570100	-3.47791100				
H	-2.02140200	0.28846300	-3.47213400				
H	-1.46250900	-1.36760200	-3.71846800				
C	-2.33227300	-2.71127000	-1.10487700				
H	-1.48474500	-3.34061800	-1.38831600	Rh	0.00405500	0.07687000	-0.12053600
C	-2.53820500	-2.86950600	-0.04280100	P	1.70749900	-0.70510800	-1.48233600
H	-3.21241600	-3.01343000	-1.68219500	C	0.39371800	-1.41160700	1.69539900
C	2.95992500	-0.59634800	-2.44643500	P	3.28664200	-0.79787100	-0.43136000
C	2.33268600	-0.46953600	-3.33231100	H	3.81158500	-1.75139200	-0.53467100
H	3.37276700	0.37770100	-2.18110300	H	3.95188400	0.00995000	-0.74216300
H	3.77162200	-1.29278700	-2.67707600	C	2.26621000	-1.72769200	1.67107500
C	1.73960700	-2.98530000	-1.57958600	H	2.67753400	-1.85925400	2.67532900
H	2.71271700	-3.46865100	-1.71235700	H	2.47574300	-2.63416700	1.09824500
H	1.14959600	-3.54499300	-0.85099600	P	-1.44606300	1.78274400	0.45019100
C	1.20591700	-3.01653400	-2.53417300	P	-1.75143200	-0.89348200	-1.31118100
H	-1.60092300	2.94540300	-1.17051900	C	-3.13697500	1.21877500	1.03757900
H	-2.06685800	2.33760900	-1.94909600	H	-3.87609700	1.99512700	0.75664800
H	-2.29699000	3.73007900	-0.85882600	C	-3.09086200	1.19756800	2.13218000
H	-0.70342400	3.39918300	-1.59371200	H	-3.44775800	-0.26307400	-0.86083000
H	0.41388400	0.87836500	-1.64416600	H	-4.17097500	-1.01295000	-1.19723100
H	2.10446000	0.32977200	0.82136700	N	-3.67570300	0.66198900	-1.41893900
C	2.54569700	2.96166500	-0.91178800	N	2.98609600	-0.57567800	1.01766500
O	1.73201100	3.70275900	-1.28334200	C	-3.55196000	-0.10076100	0.58170300
O	3.39261300	2.25201700	-0.53187900	N	4.17871100	-0.13009200	1.78135900
				H	4.58062300	0.76831300	1.31274900
				H	3.87786300	0.09390500	2.80576400
				H	4.92766000	-0.92369700	1.78000600
				C	-4.87766300	-0.42720300	1.09268900
				H	-5.13433000	-1.45632700	0.82682700
				H	-4.87450100	-0.35201800	2.18384000
				H	-5.66340900	0.24473100	0.70489100
				C	-0.98148500	2.86502600	1.86722600
				H	-0.73079900	2.24338200	2.73012100
				H	-0.10169500	3.44970900	1.58969200
				H	-1.79282200	3.54919500	2.13484400
				C	-0.13844200	-3.16532700	1.95544800
				H	0.01505100	-3.74098700	1.03876200
				H	0.38657200	-3.65231300	2.78412600
				H	-1.20980600	-3.16723400	2.17504500
				C	0.21867900	-0.75566200	3.41800000
				H	-0.84520500	-0.59586900	3.61527300
				H	0.62367000	-1.42878400	4.18119000
				H	0.71550800	0.21682100	3.48445900
				C	-1.78731900	-0.67999500	-3.14341000
				C	-2.70259100	-1.08888800	-3.58308900
				H	-1.71349400	0.38438400	-3.38009700
				H	-0.92898200	-1.18387300	-3.59561600
				C	-2.02705600	-2.70843400	-1.12450900
				H	-1.10149900	-3.25330800	-1.32450900
				H	-2.32780700	-2.90384200	-0.09193600
				H	-2.80706400	-3.07001200	-1.80161100
				C	2.40985500	0.12151000	-2.97956400
				H	1.64268900	0.12229500	-3.75863500
				H	2.64668900	1.16104800	-2.74342500
				C	3.30347300	-0.38132800	-3.36385400
				H	1.64373900	-2.45399500	-2.09091700
				C	2.58549500	-2.76963700	-2.55051600

B20

E= -990.99028936 a.u.

B19

E= -990.98672439 a.u.

Rh	0.20426500	0.13777500	-0.12619700				
P	2.27885600	0.54289500	-0.97813100				
P	0.51360000	-2.17834200	-0.21611600				
C	3.47675100	-0.68855300	-0.14494800				
H	3.74194400	-1.50762000	-0.81678700				
H	4.39427200	-0.19265600	0.17676700				
C	2.08443500	-2.52895400	0.79797500				
H	1.78390900	-2.94176000	1.76420500				
C	2.78005500	-3.22326900	0.31981100				
P	-1.12178100	0.18026000	1.78205900				
P	-1.66651800	0.38553800	-1.60577900				
C	-2.78117000	-0.68867200	1.58317600				
H	-3.54884100	-0.09609600	2.11870100				
C	-2.69656800	-1.64488600	2.11210400				
C	-3.25809800	0.20519100	-0.64719800				
H	-4.08564400	0.09048200	-1.35572000				
H	-3.46019100	1.12955400	-0.08196400				
N	2.77347900	-1.23334900	1.05952400				
N	-3.17985800	-0.97792100	0.21305200				
C	3.58881000	-1.22825500	2.29433300				
C	3.97948800	-0.22183800	2.45234700				
H	2.95069800	-1.50287600	3.13608600				
H	4.41274400	-1.93865400	2.20566700				
C	-4.40293800	-1.77236300	0.19308200				
H	-4.64840600	-2.04304400	-0.83739000				
H	-4.24771100	-2.69847700	0.75568700				
H	-5.26774100	-1.24570100	0.63222700				

H	1.40203300	-3.12523400	-1.26196500
H	0.85166600	-2.54970000	-2.83873500
C	-1.87897400	3.05192500	-0.81981200
H	-2.29338400	2.56738200	-1.70765000
H	-2.60079900	3.78242800	-0.43952300
H	-0.96279100	3.56813600	-1.11540500
H	1.09613200	1.10193400	0.55715600
C	2.26862300	0.20626200	0.98095100
H	2.47221500	3.19093000	-0.37902300
O	3.38734700	2.46820800	-0.29499000
O	1.58572300	3.93567300	-0.46935800

B21

E= -1383.46410563 a.u.

Rh	1.58608100	0.16348500	-0.52292100
P	0.54452800	2.04210600	-1.24174400
P	1.86211000	1.15814600	1.58001700
C	-0.65412600	2.91059900	-0.07503800
H	-0.49743500	4.00569400	-0.15037700
H	-1.66554900	2.70674900	-0.44051300
C	0.73037200	2.62245000	1.90413800
H	0.62590700	2.72645700	2.98927400
H	1.23096300	3.54339400	1.55169000
P	1.48201200	-2.07226400	0.12397800
P	3.87473600	-0.11676600	-1.17852800
C	2.98477400	-2.61851900	1.12485000
C	3.25064300	-3.65418700	0.82925500
H	2.65861700	-2.66693600	2.17014000
C	4.67005600	-1.57413400	-0.29606900
H	5.74963000	-1.39942100	-0.23825300
H	4.53688100	-2.49027100	-0.89825700
N	-0.59594900	2.46687600	1.31240200
N	4.13883600	-1.73204700	1.05945900
C	-1.62652400	3.13695800	2.09256200
H	-2.60358100	2.93627700	1.63964100
H	-1.63326300	2.74523300	3.11480900
H	-1.48598000	4.23172700	2.14402100
C	5.16057800	-2.15705900	2.00738000
H	5.98329900	-1.43646000	2.01057500
H	4.73499900	-2.18628300	3.01558100
H	5.57325400	-3.15688800	1.78142200
C	0.18336000	2.91765100	1.15203100
H	0.14214400	-2.44543000	2.13662100
H	-0.79354700	-2.79220600	0.67422600
C	0.38737100	-3.98675100	1.28179200
C	3.46236100	1.95635500	2.04630400
H	3.76551600	2.66423300	1.27066900
H	3.39120800	2.48170300	3.00476600
H	4.22295500	1.17448100	2.12442000
C	1.60593500	0.15690400	3.11650700
H	2.37353900	-0.62155600	3.13421500
H	1.70126200	0.76441900	4.02235300
H	0.62505600	-0.32094700	3.10560500
C	4.21229500	-0.57885500	-2.93796100
H	5.25118600	-0.88510800	-3.10266700
H	3.53957300	-1.38610900	-3.23808100
C	3.99315000	0.28389300	-3.57355200
H	5.20525400	1.15453100	-0.94037700
H	4.89081500	2.09960400	-1.39197400
H	5.36868900	1.32366300	0.12574800
H	6.15061800	0.83954400	-1.39581200
C	-0.47583600	2.00706700	-2.78526100
H	0.18784600	1.76853000	-3.62038900
H	-1.21734700	1.20642500	-2.72151700
H	-0.97247800	2.96352700	-2.98313600
C	1.65191400	3.46912200	-1.67153700
H	1.10117800	4.34879900	-2.02287100
H	2.24216900	3.74491200	-0.79247000
H	2.34781900	3.14334400	-2.44958900
C	1.56211000	-3.27668600	-1.28036500
H	2.40660900	-3.02450300	-1.92543600
H	1.66903600	-4.31003200	-0.93405700
H	0.65551700	-3.18717700	-1.88289100
H	1.20349400	-0.41135100	-1.96741100
H	-1.73313000	0.18346500	-0.26406500
P	-3.07514200	-0.24653600	-0.15543700
N	-3.07747600	-1.19288000	-1.55038100
N	-3.90396200	1.25082800	-0.16189700
N	-3.00040200	-0.90105600	1.39561800
C	-4.07543900	1.92405100	-1.44797300
H	-3.17434800	1.80918600	-2.05222900
H	-1.99375000	-0.37644500	2.31593000
C	-1.58953500	-1.20008400	2.91216900
C	-1.79214600	-1.58771600	-2.13723300
H	-1.81408700	-1.41958400	-3.21884700
C	-4.11599400	-1.56470200	2.04888600
H	-4.62968600	-0.87292200	2.73459100
H	-3.73646600	-2.39338400	2.65614700
H	-5.07492100	-2.09026400	0.99261700
C	-4.64459200	-2.97420500	0.51569100
H	-6.04027700	-2.37296900	1.42802400
C	-5.05477400	1.27688900	0.72564000
H	-4.70389600	1.20031800	1.75955500

H	-5.56124700	2.24008500	0.62860300
C	-6.02041100	0.11655500	0.39535000
H	-6.64708100	-0.13104400	1.25765800
H	-6.68865900	0.39899500	-0.42099700
C	-4.17093700	-2.07158200	-1.93493200
H	-3.97113700	-3.09548200	-1.58420100
H	-4.23020600	-2.11830300	-3.02733200
C	-5.47806000	-1.53523300	-1.37629900
H	-5.81016000	-0.69045600	-1.98338600
H	-6.26454600	-2.29911600	-1.39313300
N	-5.21660100	-1.04226800	-0.02156600
H	-4.92355300	1.53483400	-2.02905400
H	-4.23041900	2.99253700	-1.27387700
H	-1.60939600	-2.65401100	-1.95256000
H	-0.95555000	-1.02140400	-1.71315900
H	-1.18383300	0.10851000	1.76365800
H	-2.43495100	0.36494300	2.99595200

B22

E= -991.03132314 a.u.

Rh	-0.15802600	-0.15889600	0.13535700
P	1.34725100	-1.89616400	-0.22250700
P	1.43745000	0.92546600	1.44933600
C	3.11092600	-1.67426300	0.32765400
H	3.21532800	-1.97273600	1.38417500
H	3.71276300	-2.37389400	-0.26092800
C	3.26901800	0.57342200	1.21757900
H	3.74691000	1.53785600	1.02683000
H	3.67967600	0.18393700	2.16499000
P	-1.60647500	1.63781900	-0.31348600
P	-2.01138500	-1.52609200	-0.32495100
C	-3.31497500	1.54785700	0.43012400
H	-3.99997200	2.09922300	-0.24419500
C	-3.26577000	2.10922600	1.36964900
H	-3.68380400	-0.70532300	-0.39748000
H	-4.42483600	-1.50418500	-0.29166300
H	-3.86635400	-0.23385900	-1.37710900
N	3.60600400	-0.31533900	0.10069900
N	-3.79737100	0.21095800	0.72584800
C	5.06201900	-0.31648400	-0.11209400
H	5.30207900	-0.92970200	-0.98382300
H	5.40056600	0.70365300	-0.30868500
H	5.60403400	-0.70790700	0.76152000
C	-5.13772700	0.25189300	1.29993000
H	-5.43490800	-0.75202600	1.61437800
H	-5.13342000	0.89366900	2.18504400
H	-5.89188200	0.63921600	0.59374800
C	-1.27128700	3.42387000	-0.02765400
H	-1.20402700	3.64630800	1.03841400
H	-0.33973100	3.70311400	-0.52451800
H	-2.08389900	4.01722400	-0.45777300
C	1.15346900	0.31532600	3.16673700
H	1.27036300	-0.77077200	3.19944800
H	1.85277900	0.77462700	3.87202300
H	0.13075200	0.55383200	3.46772900
C	1.52599200	2.74392900	1.70953700
H	0.58406400	3.10393900	2.12572200
H	2.32786200	2.98808000	2.41268500
H	1.71645600	3.24771200	0.75872900
C	-2.09266100	-2.62577400	-1.80259700
H	-3.05082900	-3.15246200	-1.84384200
H	-1.97565300	-2.03492200	-2.71521900
H	-1.29397800	-3.37077800	-1.77458700
C	-2.32170500	-2.65354600	1.09551900
H	-1.41883400	-3.19310100	1.38031300
H	-2.63257300	-2.02963100	1.93745900
H	-3.11428300	-3.37075500	0.86125600
C	1.61337600	-2.13679700	-2.03226800
H	0.65686400	-2.20622500	-2.55259400
H	2.15518800	-1.27695900	-2.43463900
H	2.19729800	-3.04151500	-2.22704700
C	1.08599900	-3.62231700	0.37244900
P	1.93495200	-4.25794500	0.10279600
H	0.96718200	-3.63138000	1.45911000
H	0.18523500	-4.04839300	-0.07506100
C	-1.90494200	1.67213700	-2.13602400
H	-2.06324900	0.67000500	-2.53910300
H	-2.77181800	2.29703200	-2.37207200
H	-1.02205300	2.10805100	-2.61226000
H	1.18815100	0.85640000	-2.28473100
H	3.05667800	0.82386500	-1.18516700
C	1.68411500	1.82700900	-2.10412600
O	2.87898800	1.73753400	-1.53628500
O	1.16903100	2.88023000	-2.38840400

B7'

E= -991.77368553 a.u.

P	-1.50168000	1.74205700	0.08098800
P	-1.65261800	-1.36375800	-0.87143300
H	-3.15716700	1.15558400	0.67504100
C	-3.01617600	0.64903300	1.64235900

N	-3.33401100	-0.79926100	0.90416500	H	-3.77024800	-2.15670100	-1.52058900
C	-4.56353700	-1.12747200	1.62399100	H	-2.75123300	-3.34039300	-0.67711400
H	-4.55962500	-0.75293500	2.66191000	H	-4.31330200	-2.84566100	0.03592100
H	-5.42096500	-0.69606900	1.10166000	C	4.34651400	-0.68657200	1.35095900
H	-4.69686600	-2.21171600	1.64542600	H	4.51366700	0.10648300	2.08491200
C	3.63525900	-0.60137000	2.65626700	H	4.20926600	-1.62613000	1.89511400
H	4.69558600	-0.33709400	2.50519500	H	5.25144100	-0.78220500	0.72641900
H	3.27377200	-0.09935100	3.55712800	C	0.75725600	-3.14130500	-1.38824100
H	3.57157400	-1.68049900	2.82442600	H	0.39078400	-3.49951100	-0.42227200
Rh	-0.06603000	0.03143000	-0.49052600	H	-0.04862300	-3.24012300	-2.12047100
P	-1.92591400	1.44299700	-0.19862500	H	1.59905900	-3.76685800	-1.70308800
P	-1.18651000	-1.45706100	0.93511600	C	-1.04393200	0.29708300	3.13957500
C	-3.50324900	0.62252900	0.36325400	H	-1.90321100	0.92824400	2.90170400
H	-3.56241900	0.60858500	1.46609100	H	-1.29268300	-0.33149500	3.99986900
H	-4.32219300	1.26174600	0.01785700	H	-0.21218500	0.95276100	3.40866100
C	-2.99940700	-1.73431700	0.56109400	C	0.61279700	-1.89610400	2.43062700
H	-3.04909300	-2.67083900	-0.00457700	H	1.55273900	-1.36381700	2.60094600
H	-3.53174800	-1.89955000	1.51941400	H	0.23929000	-2.30582600	3.37332800
P	1.75452000	-1.31739500	-1.04794100	H	0.81666800	-2.71628600	1.73816400
P	1.51582600	1.64909100	0.17257500	C	1.85599900	3.21132400	-1.11391600
C	3.22378900	-1.35017600	0.09840200	H	2.79961300	3.72120400	-0.89414600
H	4.12535500	-1.52331200	-0.52239600	H	1.86089300	2.86819300	-2.15175000
H	3.09800500	-2.23342400	0.73461600	H	1.03513100	3.92481600	-1.00187900
C	3.29272300	1.07785200	0.23494900	C	1.71321400	2.53501700	1.67179000
C	3.84864300	1.83943000	0.79080900	H	0.78036900	3.04322900	1.92962800
H	3.74497500	1.03755400	-0.77005500	H	1.88868800	1.73879800	2.40172600
N	-3.62712700	-0.69413400	-0.23573100	H	2.53860600	3.25241300	1.72480800
N	3.36271800	-0.18675400	0.95440000	C	-3.07187300	1.62412200	-2.09323700
C	-5.00619600	-1.04163400	-0.56148000	H	-2.48780200	2.42413000	-2.55512800
H	-5.42276000	-0.29444400	-1.24194900	H	-3.01745800	0.75299000	-2.74954200
H	-5.02551600	-2.00788500	-1.07217100	H	-4.11004200	1.95229800	-1.98595900
H	-5.65249100	-1.10727500	0.33071600	C	-2.80371200	2.67695600	0.52799400
C	4.54504400	-0.30157100	1.80029700	H	-3.88637100	2.83733000	0.52102700
H	4.56625700	0.52311400	2.51719700	H	-2.45584600	2.57589600	1.55822100
H	4.49742000	-1.23660900	2.36534300	H	-2.31907700	3.55772700	0.09724500
H	5.48631400	-0.29350600	1.22414400	C	1.82173400	-1.06122600	-2.99271500
C	1.55563800	-3.11585000	-1.38149800	H	2.25656500	-0.06139000	-3.06078900
H	1.32660600	-3.65688100	-0.46318800	H	2.56655200	-1.80294800	-3.29670300
H	0.73662100	-3.26111800	-2.09028600	H	0.96771200	-1.09833700	-3.67272700
H	2.47392000	-3.52608500	-1.81207700	H	-0.25115400	0.68330000	-1.98379800
C	-1.20717700	-0.82514700	2.67273300	H	-1.74601000	-1.05391200	-0.48720100
H	-1.56488100	0.20662100	2.70448100				
H	-1.83477700	-1.44251600	3.32332600				
H	-0.18146700	-0.83182000	3.05148100				
C	-0.71172600	-3.20955400	1.26534300				
H	0.30283400	-3.24930200	1.67087800				
H	-1.39303100	-3.65501200	1.99718400				
H	-0.75398200	-3.79493800	0.34452200				
C	1.69883000	3.22815400	-0.76482900				
C	2.47735100	3.86992300	-0.34043100				
H	1.94526800	3.00224800	-1.80603600				
H	0.75359800	3.77699100	-0.76188600				
C	1.38477900	2.21398600	1.92320400				
H	0.39670200	2.61645400	2.14154200				
H	1.55776600	1.34321800	2.56053600				
C	2.13414100	2.98042500	2.14554600				
C	-2.44651400	2.14249900	-1.81671700				
H	-1.60305600	2.65464500	-2.28554700				
H	-2.75483900	1.31873800	-2.46495700				
H	-3.27700600	2.84409600	-1.69691400				
C	-1.93591900	2.92446100	0.89617800				
C	-2.90008100	3.43594700	0.81898000				
H	-1.78298600	2.63143900	1.93776500				
H	-1.14997100	3.62716200	0.61117100				
C	2.45791000	-0.76912900	-2.66241800				
C	2.66184500	0.30321600	-2.65391000				
H	3.37655100	-1.31210800	-2.90298300				
H	1.71601300	-0.96102600	-3.44232600				
H	-0.32004500	0.27011300	-2.37086600				
H	-0.78159600	-0.37925700	-2.21598800				

TS_{B3-4}

E= -1383.45533502 a.u.

Rh	1.17373400	0.10587700	-0.38904300				
P	0.75570900	2.18541300	-1.27167100				
P	1.79412700	1.12931800	1.63154300				
C	0.40195300	3.55469400	-0.03882200				
H	1.34237800	4.10094900	0.16360900				
H	-0.26911100	4.26563100	-0.53157300				
C	0.73421600	2.58947800	2.16931600				
H	0.17504200	2.26419600	3.05342700				
H	1.41205300	3.39824500	2.50567400				
P	1.03246600	-2.09836600	0.36549700				
C	3.41711800	-0.46552200	-1.33597100				
P	2.59534300	-2.73847500	1.19497500				
H	2.67790300	-3.82168100	0.97276400				
H	2.42073800	-2.65250500	2.27311800				
C	4.12035700	-2.01512500	-0.55191100				
H	5.20479600	-2.01940800	-0.70187400				
C	3.73413400	-2.91048400	-1.06830300				
N	-0.22900300	3.09297300	1.19488400				
N	3.82862300	-2.03423700	0.88174900				
C	-1.01704100	4.15669300	1.81325400				
H	-1.77083200	4.52269200	1.11019600				
H	-1.53494200	3.76274800	2.69313300				
H	-0.39872700	5.01400600	2.13156700				
C	4.93173000	-2.56711100	1.67243200				
H	5.84074200	-1.99350500	1.47253300				
H	4.70022900	-2.46902600	2.73763200				
H	5.13649900	-3.63186200	1.46246500				
C	-0.17441700	-2.71978100	1.61992200				
H	-0.05589100	-2.17282400	2.55738100				
H	-1.18823500	-2.55773900	1.24907900				
H	-0.02290800	-3.78731100	1.81163500				
C	3.47691400	1.88851500	1.68728400				
H	3.62263400	2.55259900	0.83092500				
H	3.64416600	2.44939300	2.61213600				
H	4.20742500	1.07786900	1.62592900				
C	1.85971300	0.19386500	3.22348800				
H	2.62967200	-0.57618500	3.12914100				
H	2.11581500	0.84677600	4.06378100				
H	0.89904900	-0.28590900	3.42450500				
C	3.39770800	-0.95925100	-3.11754600				
C	4.34553900	-1.40025800	-3.44362100				
H	2.58584400	-1.67052200	-3.28844600				
C	3.19324400	-0.07565900	-3.72884600				
C	4.94289000	0.59182300	-1.32215600				
H	4.73655300	1.55722700	-1.79087500				
H	5.25953100	0.77264900	-0.29286400				
H	5.76539400	0.11102800	-1.86274900				
C	-0.60630500	2.36104000	-2.49989900				
H	-0.34121300	1.75619500	-3.37212700				

TS_{B2-15}

E= -802.45539419 a.u.

Rh	-0.23653300	0.24238500	-0.45953600				
P	-2.30644100	1.20771000	-0.47171400				
P	-0.56919600	-0.70869100	1.66670800				
C	-3.48356300	-0.13169900	0.20832100				
H	-3.77487700	0.09230100	1.23743200				
H	-4.39001100	-0.20214900	-0.39602600				
C	-2.11197500	-1.79453400	1.43033600				
H	-1.78280700	-2.83362600	1.34764800				
C	-2.83060100	-1.71917200	2.25134600				
P	1.22562800	-1.35717100	-1.27628400				
P	1.56552800	1.76964500	-0.00260000				
C	2.83999700	-1.50139100	-0.32151700				
H	3.65419800	-1.67421000	-1.05266200				
C	2.76537500	-2.41068200	0.28525700				
C	3.21802200	0.90371100	-0.09990600				
H	3.96668600	1.53038700	0.39632600				
H	3.53540100	0.81675400	-1.15273100				
N	-2.74037600	-1.41488600	0.14637200				
N	3.14651400	-0.39382100	0.57394300				
C	-3.44663100	-2.50981500	-0.53937900				

H	-1.54252800	1.97171500	-2.09463900
H	-0.73905500	3.40132300	-2.81408300
C	2.12933000	2.99765500	-2.20357400
H	1.84206600	3.98747200	-2.57297200
H	3.00194900	3.10103600	-1.55343800
C	2.40676400	2.37060200	-3.05528400
C	0.74832500	-3.35378200	-0.95509600
H	1.42158300	-3.17947000	-1.79645300
H	0.88161800	-4.37444100	-0.58304400
H	-0.27693500	-3.22727900	-1.30961500
H	0.56816900	-0.46883600	-1.75621300
H	-0.82923300	0.18281100	-0.15320500
P	-2.43742300	-0.15851700	-0.12298100
N	-3.38035500	1.05464400	-0.88834400
N	-2.79833300	-0.48971200	1.50135500
N	-2.55035600	-1.57628900	-1.04908200
C	-1.92966600	0.17144200	2.47266100
H	-1.09669200	0.65164800	1.95622800
C	-2.14263400	-1.44831800	-2.44860100
H	-2.98215200	-1.23198800	-3.12250000
C	-3.33786800	2.32867900	-0.17696500
H	-2.35834100	2.43833100	0.30252400
C	-3.48384200	-2.65533500	-0.74281400
H	-3.22399900	-3.08952400	0.22630000
H	-3.32988400	-3.44821000	-1.48214100
C	-4.96110200	-2.21715100	-0.74582700
H	-5.28485300	-2.05225600	-1.77873900
H	-5.58154500	-3.03308900	-0.34310000
C	-3.87548300	-1.28577800	2.09250400
H	-3.60932000	-2.35074700	2.08659500
C	-3.95750300	-1.00335900	3.14730600
H	-5.24034100	-1.05768200	1.43093800
H	-5.93106500	-1.84773800	1.76814000
H	-5.64169900	-0.10578500	1.78883700
C	-4.61802300	0.76548100	-1.60320800
H	-4.39626900	0.08229000	-2.42780700
H	-4.97769600	1.69508100	-2.05789600
C	-5.69781200	0.14799700	-0.70894400
H	-6.03319100	0.88514000	0.02571400
H	-6.57469600	-0.11814800	-1.31900100
N	-5.14811200	-0.98992900	-0.00547900
H	-2.47862800	0.93893100	3.03439600
H	-1.52570300	-0.55567000	3.18725300
H	-4.10980700	2.40735800	0.60238000
H	-3.46934500	3.15484400	-0.88464700
H	-1.39497900	-0.65819500	-2.54376300
H	-1.67348000	-2.38008000	-2.77985900

TS_{B6-7}

E= -990.56026073 a.u.

Rh	0.13496200	0.02265100	-0.30915700
P	-1.69869700	-1.11030500	-1.16417200
P	-1.03841100	0.40969600	1.81476100
C	-3.32951200	-0.39183500	-0.61795500
C	-3.41561200	0.62999900	-1.02052000
H	-4.11133600	-0.99516000	-1.09356000
C	-2.87364600	0.65132800	1.54175000
H	-3.34224200	0.74214100	2.52920100
H	-3.01779600	1.61959600	1.02713600
P	1.51298700	-1.80247200	-0.16778800
P	1.91406800	1.46865300	-0.39657300
C	3.35801600	-1.56574500	0.08010800
H	3.85154000	-1.70049300	-0.90349300
H	3.69445500	-2.38960700	0.71866900
C	3.64480500	0.79388500	-0.25192000
H	4.28186200	1.61825400	0.08636500
H	4.00033100	0.50429200	-1.26010300
N	-3.52153900	-0.44774000	0.82969100
N	3.75757800	-0.30998700	0.69324400
C	-4.93879800	-0.52142600	1.16290300
H	-5.38685100	-1.39443300	0.67926200
H	-5.05787100	-0.64053400	2.24364300
H	-5.49984200	0.37755000	0.84777300
C	5.10594300	-0.40628200	1.23630000
H	5.36941900	0.53138700	1.73353900
H	5.14641100	-1.20563600	1.98181500
H	5.86601700	-0.61523000	0.45988800
C	1.16410400	-3.00002200	1.20378700
H	1.32706500	-2.48941700	2.15643400
C	0.11647000	-3.30794600	1.16151200
H	1.80323000	-3.88850200	1.15257400
C	-0.77813000	1.92400900	2.85421100
H	-0.85053700	2.81037200	2.21842000
H	-1.51897500	1.99669200	3.65947900
H	0.22077400	1.89888700	3.29712100
C	-1.12245200	-0.87966500	3.14589900
H	-0.11897000	-1.06471400	3.53915400
H	-1.77845800	-0.57861400	3.97137200
H	-1.50192500	-1.80863200	2.71214000
C	2.11874100	2.46997500	-1.93450100
C	3.05145300	3.04575100	-1.91897800
H	2.10586100	1.80771900	-2.80281500
H	1.27697100	3.16126200	-2.01292600

TS_{B8-9}

E= -990.57161146 a.u.

Rh	-0.08049600	-0.01824700	-0.31420300
P	-1.80024100	-1.58526900	-0.07812700
P	-1.56067900	1.84913400	0.08669800
C	-3.46078800	-0.92224500	-0.62141600
H	-3.43510900	-0.81417000	-1.72196600
H	-4.19703400	-1.69975600	-0.38816200
C	-3.27559100	1.50180800	-0.55807600
H	-3.90412300	2.36721400	-0.31618800
H	-3.22195900	1.42988000	-1.66023900
P	1.16549300	-0.13020600	1.69305800
P	1.79448100	0.74046500	-1.41441600
C	2.98973400	-0.47621600	1.49105800
H	3.10931900	-1.52601100	1.17375500
H	3.43510800	-0.38214700	2.48798600
C	3.46162500	0.16231200	-0.81359900
H	4.21834000	0.70116000	-1.39576700
H	3.57755400	-0.91325500	-1.04184000
N	-3.87491300	0.31140900	0.03607500
N	3.67904100	0.45458200	0.60069400
C	-5.32714100	0.41917500	0.08752400
H	-5.74354500	-0.45240200	0.60057400
H	-5.61011700	1.30953000	0.65659500
H	-5.78961900	0.48581400	-0.91496000
C	5.10325500	0.50028100	0.90528300
H	5.59063100	1.25094100	0.27635900
H	5.24893100	0.79014500	1.94999900
C	5.60542800	-0.47123100	0.74100300
H	1.27085900	1.39343000	2.73810900
H	1.55735200	2.24211200	2.11211300
H	0.29113700	1.59494000	3.17767400
C	2.00364600	1.28093200	3.54444000
H	-1.29788000	3.46569100	-0.78515500
H	-1.13996200	3.27790300	-1.85101900
H	-2.15015400	4.14450900	-0.66246900
H	-0.40217800	3.95046100	-0.38789200
C	-2.02742900	2.48630600	1.76584700
H	-1.16144200	2.96269300	2.23211600
H	-2.84243400	3.21778900	1.71286300
H	-2.34421200	1.64489500	2.38785600
C	1.94946600	0.39404500	-3.21650500
H	2.89113400	0.77675600	-3.62534200
H	1.87193100	-0.68098300	-3.38261400
H	1.11074000	0.87750300	-3.72442500
C	2.12070600	2.56352700	-1.40219800
H	1.28379200	3.08199600	-1.87487300
H	2.20989100	2.90505500	-0.36790600
H	3.04247600	2.81033500	-1.94067500
C	-2.26912200	-2.24167300	1.58484300
H	-1.43753000	-2.81961300	1.99363500
H	-2.47898300	-1.40086400	2.25110100
H	-3.15470000	-2.88409900	1.52723600
C	-1.85989400	-3.15077600	-1.06908500
H	-2.85057300	-3.61722300	-1.01621900
H	-1.60949300	-2.93294000	-2.10950900
H	-1.12330400	-3.85731400	-0.67890800
C	0.80559000	-1.39067900	2.99371700
H	0.83236700	-2.38250500	2.53834500
H	1.53705800	-1.34299900	3.80761800
H	-0.19200800	-1.21525200	3.40391600
H	-0.70711200	-0.04650600	-1.78611800
C	1.19306600	-2.53353000	-0.91654900
O	1.35066100	-2.99876800	0.16733600
O	1.25279500	-2.54432400	-2.09950400

TS_{B9-7}

E= -990.56079831 a.u.

P	-1.33253500	1.82512100	0.22082400
P	-2.00117300	-1.40178200	-0.25798700

P	1.82191600	1.11142800	-1.05435800	H	1.21421100	-0.53247100	-3.87693300
P	1.17099000	-0.89217800	1.54993100	H	2.57521900	-1.62978000	-3.55060200
C	-1.79126200	2.95024100	-1.17467800	C	-0.73314500	-2.08190800	2.00183600
C	-2.78662900	-1.62120300	-1.90347600	H	-1.26332900	-1.29377200	2.53875700
C	1.96231300	1.34540600	-2.87097400	H	-1.17350600	-3.05027800	2.25527900
C	0.88347700	-2.58412200	2.23668300	C	0.32026700	-2.07550500	2.29183600
C	-1.99923100	-3.11115900	0.42905400	H	0.07001800	-3.30752600	-0.41398400
C	-0.73674300	3.04017300	1.49308700	H	1.04637400	-3.36950000	0.06417200
C	1.19308100	0.10942800	3.10746700	H	-0.51855000	-4.18592900	-0.13168600
C	2.09318200	2.83965900	-0.45956900	C	0.17856200	-3.29599900	-1.49866600
H	-0.09889900	-0.55475300	-1.95366500	C	2.19309400	2.54105800	1.35383100
H	-0.08102100	-2.61192200	2.74974300	H	2.98471400	2.62788300	2.10417500
H	0.86100400	-3.30806900	1.41859500	H	2.59061900	2.73451500	0.35639500
H	1.66454600	-2.86373300	2.95243000	H	1.42176100	3.29536800	1.52111600
H	1.78860700	-0.36380200	3.89663800	C	0.86023000	0.88275100	3.21157900
H	1.62022800	1.08993700	2.87956800	H	0.09470000	1.64918200	3.34686900
H	0.16888500	0.24833200	3.46597000	H	0.45340000	-0.08334900	3.51223700
H	2.22207200	2.83331700	0.62533000	H	1.70546500	1.12924200	3.86109000
H	1.25060100	3.48152200	-0.72616700	C	-3.11145100	2.01750300	-0.91933500
H	2.99678000	3.25259600	-0.91932800	H	-2.50373000	2.86950900	-1.21715600
H	1.95254100	0.36008800	-3.33843600	H	-3.28692700	1.35733400	-1.77111000
H	2.88422800	1.87680400	-3.12978200	H	-4.06818600	2.37039900	-0.52247600
H	1.10019500	1.91911400	-3.22090100	C	-2.31943400	2.05142800	1.90897000
H	-2.06800000	-2.12570900	-2.55066200	H	-3.33633800	2.43041100	2.04678300
H	-3.01879900	-0.63499400	-2.31000700	H	-2.06004300	1.42835500	2.76865300
H	-3.70385600	-2.21458400	-1.82630600	H	-1.62750700	2.89039900	1.82530600
H	-0.89588400	3.21532300	-1.74296200	C	2.99230400	0.95256800	-2.02260600
H	-2.45565600	2.39339900	-1.84098700	H	3.48680300	1.35133900	-1.13460600
H	-2.29217900	3.86427900	-0.83606200	H	3.75331100	0.55565000	-2.70073500
H	-1.50930600	3.78209200	1.72562100	H	2.45581100	1.78332000	-2.49019100
H	-0.47662100	2.49756600	2.40581800	H	-0.10475000	1.94395600	-1.87871700
H	0.15261700	3.56711900	1.14987000	H	-0.98487800	-0.15293400	-1.67941700
H	-1.85047800	-3.08017200	1.51077700	C	0.27908600	2.84083500	-1.24579600
H	-2.95513300	-3.60115500	0.21754500	O	1.25133700	3.43017200	-1.70369100
H	-1.18983900	-3.66873800	-0.04176300	O	-0.37377000	3.01341600	-0.17924500
O	0.81367500	-1.90385700	-1.79516700				
C	1.95738500	-1.66796800	-2.16147400				
O	0.08205600	-2.88316800	-1.76042000				
C	-3.01579600	1.60007900	0.99648200				
H	-2.86517200	1.38390700	2.07364900				
H	-3.51981700	2.57151600	0.93411900				
C	-3.45063500	-0.75128400	0.71340700				
H	-4.28156300	-1.43177500	0.49651000				
H	-3.23110400	-0.84676000	1.79527800				
N	-3.85493100	0.60098200	0.36006500				
C	-5.26244400	0.82656700	0.66260100				
C	-5.55138100	1.83177200	0.34291000				
H	-5.87662900	0.10907600	0.11153100				
H	-5.48726600	0.72465500	1.74077900				
C	3.00814800	-1.04268400	1.26578200				
C	3.17603700	-1.86651400	0.55080300				
C	3.45792600	-1.33166500	2.22286900				
C	3.48619100	0.41196200	-0.61832100				
H	4.22632600	1.15321700	-0.93966300				
H	3.63612400	-0.50792900	-1.19872900				
N	3.62925400	0.20466900	0.82255000				
C	5.03202100	0.26013700	1.21600000				
H	5.45436700	1.23016500	0.93762200				
H	5.11550200	0.15757300	2.30187900				
H	5.64003800	-0.53240600	0.74341000				
Rh	-0.04799700	-0.11297900	-0.36096500				

TS_{B13-14}
E= -1571.98137596 a.u.

Rh	-0.83942200	-0.01621700	0.12356800
P	-0.83801000	2.04241600	1.26381000
C	-1.55377300	1.09342100	-1.74391000
P	-2.27464600	3.14316100	0.83758400
H	-3.19778300	2.67591800	1.22464200
H	-2.12417400	4.07284300	1.39671200
C	-2.86568400	2.36112900	-1.38078600
H	-3.19516300	2.75710200	-2.34701000
H	-3.72953900	1.85065300	-0.91984300
P	-1.08779900	-2.23058900	-0.74469200
P	-3.43964700	-0.64302400	1.29085200
C	-2.73531000	-2.73355700	-1.49438200
H	-2.81910500	-3.82703300	-1.33834400
H	-2.63887600	-2.58042500	-2.57383700
C	-4.13752300	-2.13849700	0.40113700
H	-5.21188100	-2.17936500	0.60710600
H	-3.71426900	-3.06377300	0.82172700
N	-2.36731900	3.46748300	-0.57626300
C	-3.92811500	-2.03828300	-1.04339000
N	-3.15687200	4.67854200	-0.78908100
H	-2.71057800	5.50933300	-0.23685200
H	-3.14952100	4.93937700	-1.85045300
C	-4.20491200	4.56302100	-0.46328400
H	-5.08855700	-2.48806900	-1.80774600
H	-5.96919200	-1.91240200	-1.51164300
H	-4.91563400	-2.31518200	-2.87458400
H	-5.30460200	-3.56059600	-1.66382100
C	-0.01305300	-2.90732800	-2.08623200
H	-0.15117100	-2.33530800	-3.00719700
H	1.04001900	-2.84543100	-1.80363100
H	-0.26128000	-3.95497900	-2.28268600
C	-2.40339600	0.16010700	-3.08202600
H	-3.26077200	-0.35857100	-2.64469600
H	-2.73934800	0.83964500	-3.87045400
H	-1.72285500	-0.57337800	-3.52221800
C	-0.39130500	2.14698600	-2.70744900
H	0.45470700	1.56341000	-3.07341900
H	-0.90788200	2.59239400	-3.56294500
C	-0.03098000	2.95324500	-2.06576800
H	-3.30059700	-1.30561800	3.01152800
H	-4.10141600	-2.01325800	3.24943000
H	-2.32410900	-1.78444300	3.12865100
H	-3.35549800	-0.48338000	3.73083700
C	-4.99993500	0.35768600	1.40876500
H	-4.81804000	1.28521300	1.95916700
H	-5.34101200	0.62031100	0.40241700
H	-5.79807000	-0.19368100	1.91740000
C	0.55703000	3.22881400	1.14134300
H	1.50525800	2.70273200	1.27780100
H	0.54392600	3.68440500	0.14824000
C	0.45724800	4.01770700	1.89293900
H	-1.09967700	1.90992300	3.08158800
H	-1.47687800	2.85853200	3.47598200
H	-1.81009500	1.11239600	3.30059600
H	-0.16285600	1.67211300	3.58684400

TS_{B10-11}
E= -990.97242797 a.u.

Rh	-0.14629200	0.24881600	-0.41784500
P	-2.23291700	1.06494300	0.37222900
P	-0.79750700	-1.81150700	0.19066900
C	-3.49436600	-0.27182700	0.67959300
C	-3.34830000	-0.77528300	1.65043400
H	-4.46920800	0.22203800	0.73552900
C	-2.53245200	-2.25907600	-0.31912400
H	-2.43167000	-2.76011700	-1.28844300
H	-2.86568200	-3.02259800	0.41302100
P	1.84566800	-0.39954900	-1.56155100
P	1.40351000	0.88720900	1.44861400
C	2.93509000	-1.54783300	-0.56954700
C	3.98620800	-1.27361000	-0.77627800
C	2.79024900	-2.55629800	-0.96903100
C	2.88573700	-0.26551300	1.49552800
C	3.12740000	-0.43033300	2.54943300
H	3.75593800	0.25346600	1.05848800
N	-3.47383900	-1.17584300	-0.45849100
N	2.65031800	-1.56504400	0.86187700
C	-4.78860300	-1.66294100	-0.86063600
H	-5.44531000	-0.81402800	-1.06433800
H	-4.69408000	-2.24087500	-1.78384800
H	-5.26056200	-2.30096600	-0.09467800
C	3.43342100	-2.61906100	1.51019900
C	3.16223200	-2.68382400	2.56714700
H	3.21222300	-3.58427200	1.04450900
H	4.51962700	-2.44740400	1.43732900
C	1.62055800	-1.25803600	-3.16725800
H	0.91286600	-2.08342700	-3.08574100

C	-0.88331700	-3.50719800	0.56548200	H	6.37640300	1.19971000	-0.43738500
H	-1.58341200	-3.32125200	1.38009000	C	-0.67920700	2.18292300	-2.34258900
H	-1.05076600	-4.50312100	0.14529300	H	-0.15055000	1.91980200	-3.26271800
H	0.10837300	-3.44131400	1.00752600	H	-1.46789300	1.44382700	-2.19077500
H	1.17549100	0.25649400	2.56078000	H	-1.12508700	3.17701300	-2.45910500
0	0.89468200	0.07690900	-0.31620900	C	1.45380200	3.70636000	-1.35767500
C	0.72255500	-0.74971200	2.70470500	H	0.79051400	4.57530100	-1.43644400
O	1.13779900	-1.46878200	3.60406900	H	2.21734900	3.89516500	-0.59888600
O	-0.21671800	-1.05538600	1.87646600	H	1.96540800	3.56503600	-2.31380600
P	2.65771800	-0.01994600	-0.27599000	C	1.69446200	-3.01021700	-1.81123900
N	3.21852100	-0.67694900	-1.76838300	H	2.48984100	-2.65505300	-2.47036000
N	2.99975500	-1.03321500	1.02898700	H	1.81422600	-4.08478000	-1.63823300
C	3.29438000	1.55045500	0.02531600	H	0.74488800	-2.82707700	-2.32002100
N	2.61695000	-2.42346900	0.82248300	H	1.58964500	-0.04316700	-2.06666500
H	1.79884000	-2.47381800	0.10462600	H	-1.68193800	0.78104000	0.70898000
C	2.94135000	2.43216000	-1.09103300	P	-3.04332800	-0.07842500	0.11018100
C	3.65955400	2.37413000	-1.92154300	N	-2.88804400	-0.60350100	-1.50601800
C	2.30289300	-0.51875400	-2.89382200	N	-4.21589300	1.16862500	0.24846200
C	1.27757200	-0.42554500	-2.52921900	N	-3.38952800	-1.31403100	1.23180200
C	4.60175600	1.88552700	0.61022100	C	-4.18830900	2.20670300	-0.77336100
H	4.56276700	1.75103400	1.69198700	H	-3.15867000	2.40820300	-1.07850200
H	4.76666200	2.95515400	0.44647200	C	-2.46504700	-1.46534300	2.35104100
C	5.77334400	1.08529300	0.02340700	H	-2.30596900	-2.52880600	2.55856800
H	5.93948300	1.38515300	-1.01606300	C	-1.54642300	-1.09764600	-1.83292900
H	6.69098000	1.33920700	0.57910800	H	-1.32000900	-0.88104900	-2.88251200
C	4.06089800	-0.83808300	2.00254000	C	-4.61978200	-2.09074600	1.41235300
C	3.92691800	0.12945000	2.48843800	H	-5.24939700	-1.62838700	2.18711000
H	3.91852200	-1.58110200	2.79224100	H	-4.33898500	-3.07875600	1.79549400
C	5.45711900	-0.96966400	1.35499500	C	-5.42133100	-2.28271800	0.12683700
H	6.21923000	-0.55112800	2.02787500	H	-4.89051700	-2.98635700	-0.51933700
H	5.69936700	-2.02898000	1.22811200	H	-6.38720600	-2.74678400	0.38393700
C	4.61401900	-0.69305300	-2.21475100	C	-5.50297500	0.91955300	0.87524800
H	4.88435500	0.29402200	-2.62604900	H	-5.32910400	0.47923400	1.86101700
H	4.69280900	-1.40272700	-3.04764400	H	-5.99554900	1.88257600	1.04568400
C	5.61257800	-1.11087500	-1.14108200	C	-6.39394300	-0.00917800	0.01962000
H	5.42790700	-2.15718900	-0.88251800	H	-7.19261700	-0.44032900	0.63828400
H	6.62188800	-1.05901700	-1.58281600	H	-6.88606500	0.56852600	-0.76878700
N	5.48604400	-0.32547400	0.06273700	C	-3.87710100	-1.32759400	-2.30968700
N	3.44381900	-3.03161100	0.43015700	H	-3.70515100	-2.40884700	-2.18805500
H	2.26562300	-2.83774300	1.77291100	C	-3.67963600	-1.10590900	-3.36527600
H	2.35394600	-1.39586400	-3.54914900	H	-5.32851900	-0.99935400	-2.00806000
H	2.54348200	0.37015500	-3.49802300	H	-5.55664200	0.00820500	-2.35658600
H	1.95376200	2.16917700	-1.47405900	N	-5.96659600	-1.69288900	-2.57278800
H	2.89589400	3.46850600	-0.74338800	N	-5.57674900	-1.03624300	-0.57894800
				H	-4.74941400	1.94614700	-1.68106700
				H	-4.60728200	3.13075400	-0.36067100
				H	-1.48651600	-2.18685900	-1.69003200
				H	-0.76937900	-0.62069600	-1.22659000
				H	-1.49421800	-1.04148300	2.09339000
				H	-2.83778700	-0.98763900	3.26872700

TS_{B16-21}

E= -1383.43217554 a.u.

Rh	1.78464400	0.28486500	-0.50848000
P	0.55393800	2.13228300	-0.96300600
P	1.75632000	0.86269700	1.71655900
C	-0.47746300	2.81108900	0.46850900
H	0.11639100	3.55158500	1.02241600
H	-1.34271800	3.34368100	0.06193700
C	0.04859200	1.29828800	2.37226200
H	-0.35244400	0.39882300	2.84592500
H	0.16483800	2.04928700	3.16750800
P	1.72690200	-2.03803200	-0.23964500
P	4.13333600	0.29310600	-0.97177800
C	3.25899300	-2.75701900	0.59630800
C	3.49687200	-3.72403600	0.10864500
H	2.96925500	-2.98723000	1.62834600
C	4.86940500	-1.39657200	-0.65222100
H	5.96222800	-1.31662000	-0.65985800
C	4.60256400	-2.08402500	-1.47181300
N	-0.98711100	1.79310000	1.42257800
N	4.42550400	-1.88666200	0.65489600
C	-2.06612600	2.38861900	2.24388900
C	-2.88179000	2.71613400	1.60139700
H	-2.45256100	1.63030600	2.93093600
H	-1.68515800	3.23547800	2.82601400
C	5.49724000	-2.52085100	1.41109100
H	6.33201000	-1.82328500	1.52266500
H	5.13690300	-2.77736700	2.41256500
H	5.87404100	-3.44419200	0.93592500
C	0.45495400	-2.98752800	0.72735800
H	0.41746400	-2.61080100	1.75319800
H	-0.52924200	-2.83488300	0.27634000
H	0.67130800	-4.06156800	0.75293500
C	2.69733000	2.35577300	2.27677300
H	2.42611900	3.22270100	1.66900100
H	2.52182200	2.58586100	3.33269200
C	3.76306100	2.17057500	2.12798000
H	2.25840800	-0.32341700	3.03932500
C	3.29350000	-0.61171800	2.83251400
H	2.18526400	0.10689900	4.04301600
H	1.64245500	-1.22485300	2.98704900
C	4.69741700	0.58439600	-2.70609900
H	5.76389800	0.37581300	-2.84443400
H	4.10918100	-0.04481400	-3.37900500
H	4.50374400	1.62758800	-2.97114400
C	5.36628700	1.30358200	-0.02608400
H	5.08261600	2.35935100	-0.04196100
H	5.37455000	0.95865500	1.01259400

TS_{B20-22}

E= -990.97386486 a.u.

Rh	0.00011700	0.04609600	-0.24351700
P	1.67175100	-1.32861000	-1.03390500
P	0.63518000	-0.19871800	2.06105300
C	3.32983400	-0.88223800	-0.23509600
H	3.85826800	-1.75958900	0.14748600
C	3.94776300	-0.38915900	-0.98670900
H	2.50372300	-0.50316800	2.10803300
H	2.96414700	-0.06242100	2.99535300
H	2.71202400	-1.57579600	2.11747000
P	-1.57969000	1.73201000	-0.25433600
C	-1.72241100	-1.43285200	-0.74381800
P	-3.21287300	1.37440600	0.58329500
H	-4.00273900	1.92367500	0.03379900
H	-3.15205100	1.81529000	1.58446200
C	-3.45036700	-0.76817500	-0.52848700
H	-4.12283000	-1.63151000	-0.49488000
H	-3.75395500	-0.17011400	-1.40486600
N	3.18240800	0.08918100	0.89692600
N	-3.53931000	-0.03644300	0.72741100
C	4.48600800	0.72961600	1.22897300
H	4.87228700	1.21187700	0.33194800
H	4.32133500	1.47853800	2.00439700
H	5.17614800	-0.03560200	1.58738100
C	-4.82892500	-0.20149600	1.38840100
H	-5.01719400	-1.26285600	1.57067000
H	-4.80873100	0.30849400	2.35560800
H	-5.66728800	0.20939000	0.79960500
C	-1.13293300	3.32112900	0.55562200
H	-0.87559600	3.14785300	1.60272200
H	-0.27026600	3.74592300	0.03885000
C	-1.96283800	4.03254500	0.50331700
H	0.12090500	-1.61749900	3.13135400
H	0.24975800	-2.55778700	2.58900600
H	0.66824900	-1.66309100	4.07858600
H	-0.94476400	-1.50306500	3.34852700
C	0.52874500	1.18561900	3.28678200
H	-0.52800900	1.40409100	3.46626500
H	1.00275300	0.94831600	4.24495800
H	0.98753800	2.08523200	2.86592600
C	-1.84511600	-2.15779600	-2.43649000

H	-2.74513200	-2.77054400	-2.55073100
H	-1.85851900	-1.35139700	-3.17393600
H	-0.97224800	-2.78404000	-2.64081100
C	-1.86178300	-2.92390000	0.33739000
H	-0.90499600	-3.44431900	0.40893600
H	-2.14320400	-2.58023700	1.33641700
H	-2.62037500	-3.62154800	-0.03130300
C	2.16020400	-1.25481100	-2.80700300
H	1.31830700	-1.60035800	-3.41199400
H	2.36363800	-0.21565200	-3.07342700
H	3.03692000	-1.87323600	-3.02443900
C	1.66182300	-3.15008300	-0.73032900
H	2.58275800	-3.62578700	-1.08010200
H	1.53506900	-3.34755700	0.33784500
H	0.81973000	-3.60414500	-1.25887400
C	-2.06646000	2.30710100	-1.93257200
H	-2.46998800	1.47566900	-2.51470000
H	-2.80933500	3.10935300	-1.88132600
H	-1.16675800	2.67307700	-2.43230400
H	1.03540500	1.35277100	-0.62035600
H	2.55465500	0.82139200	0.51456500
C	1.95106800	2.35958800	-1.48281400
O	3.06392800	1.96702100	-1.25255800
O	1.20451600	3.12743000	-1.98902900

C1

E=-1087.54718730 a.u.

Rh	-0.00007300	0.00012500	0.00004200
P	-1.58345000	-1.71591000	-0.33925700
P	-1.67868700	1.58993400	-0.43208800
C	-3.38984700	-1.46296200	0.07818200
H	-3.98538700	-1.85490700	-0.75203800
H	-3.62628300	-2.06203800	0.96139400
C	-3.43551100	1.00626100	-0.62954500
H	-4.10016200	1.86856900	-0.52096100
H	-3.57301900	0.61278100	-1.64165000
P	1.58360900	1.71586100	0.33920700
C	1.67865800	-1.58958500	0.43269400
P	3.38937000	1.46293700	-0.08076000
H	3.98608200	1.85624200	0.74798000
H	3.62414000	2.06088900	-0.96517800
C	3.43554600	-1.00569100	0.62923200
H	4.10021000	-1.86805100	0.52116300
H	3.57340800	-0.61132700	1.64094200
C	1.45605400	3.40758000	-0.39438200
H	1.55884100	3.33754100	-1.48033500
H	0.51021000	3.89546400	-0.16128900
H	2.26731900	4.03237700	-0.00943400
C	-1.53067100	2.50778900	-2.02229200
H	-1.51406500	1.78971500	-2.84603700
H	-2.37229900	3.19326500	-2.15804200
H	-0.60268200	3.07710800	-2.05736600
C	-1.93561400	2.90529500	0.83515600
H	-1.00491200	3.41641500	1.08076900
H	-2.66017800	3.64462700	0.48162600
H	-2.31863300	2.43779400	1.74377600
C	1.53076500	-2.50600300	2.02373300
H	2.37207600	-3.19180000	2.15980900
H	1.51478700	-1.78722300	2.84687400
H	0.60245900	-3.07477000	2.05960200
C	1.93553400	-2.90612200	-0.83337700
H	1.00492500	-3.41771300	-1.07835600
H	2.31834300	-2.43940400	-1.74249000
H	2.66030300	-3.64496900	-0.47925300
C	-1.45618600	-3.40679600	0.39626500
H	-0.50995200	-3.89463600	0.16470300
H	-1.56008000	-3.33551200	1.48203300
H	-2.26684800	-4.03230300	0.01120100
C	-1.66114000	-2.08604600	-2.14460600
H	-2.36933500	-2.89078200	-2.36275600
H	-1.95909600	-1.18698000	-2.69016100
H	-0.66869800	-2.37106200	-2.50169100
C	1.66333900	2.08443300	2.14478700
H	1.96114200	1.18479000	2.68945300
H	2.37225000	2.88854500	2.36290600
H	0.67140800	2.36987700	2.50296700
C	3.85726100	0.05399400	-0.36631000
H	-3.85768100	-0.05425900	0.36489500
F	5.22632400	0.07325900	-0.43175700
F	3.43257100	-0.30627700	-1.62866400
F	-3.43347600	0.30480300	1.62774800
F	-5.22677900	-0.07346300	0.42975600

TS_{B7-8'}

E= -991.74336507 a.u.

P	1.30589000	1.69706000	-0.65988100
P	1.40669200	-0.96579500	1.27310300
C	3.10145500	1.25468300	-0.56489600
H	3.30872600	0.48086200	-1.32039400
H	3.66020900	2.15727700	-0.83689400
C	3.20866500	-0.56357000	1.02288500
H	3.72479500	-0.86851500	1.94097900
H	3.58390900	-1.19568300	0.19929500
P	-1.72470600	-1.71774000	0.04386800
P	-1.93406200	1.49563000	0.38836200
C	-3.33746000	-1.27454400	-0.76538800
H	-3.92920300	-2.19008500	-0.90674500
H	-3.01729900	-0.93381500	-1.76635600
C	-3.56460700	0.66585200	0.81860800
H	-4.30677800	1.44478800	1.02647500
H	-3.37125500	0.17485900	1.78171500
C	-1.30916000	-3.21141600	-0.94802800
H	-1.14210400	-2.90580100	-1.98328300
H	-0.38078200	-3.64789200	-0.57309300
C	-2.10518400	-3.96116100	-0.90139100
H	1.62400900	-2.80361300	1.36134500
H	1.94024800	-3.17422400	0.38239200
H	2.38937000	-3.07191800	2.09749100
H	0.69020100	-3.29515800	1.64351500
C	1.20680700	-0.55145400	3.06548100
H	0.19364400	-0.81172800	3.38418900
H	1.93423600	-1.07427100	3.69695900
H	1.33468200	0.52785700	3.18313900
C	-1.81556700	2.50816800	1.93823700
H	-0.96586000	3.19077200	1.88140000
H	-2.72660600	3.09002500	2.12045600
H	-1.64112000	1.83217100	2.77978800
C	-2.48085800	2.78844700	-0.82299600
H	-1.67645300	3.51419400	-0.97632400
H	-2.68193400	2.30907600	-1.78452500
H	-3.37584500	3.32193100	-0.48410600
C	1.31426600	3.27927300	0.28839800
H	0.35219300	3.78784000	0.19124300
H	1.50226300	3.06232600	1.34237100
H	2.09853300	3.94572700	-0.08454300
C	1.17519100	2.27875600	-2.39905100
H	1.88045100	3.09280900	-2.59645500
H	1.39465800	1.43280200	-3.05435900
H	0.15630800	2.62078100	-2.59551700
C	-2.24913300	-2.48214100	1.64262500
H	-2.58213400	-1.71611600	2.34495000
H	-3.06094700	-3.19829000	1.48448400
H	-1.40011200	-3.00300300	2.09212700
H	0.62763900	-0.67883900	-2.18912500
O	-0.27466700	-0.44167000	-1.90354800
H	1.83338000	-0.90914400	-2.64888200
C	2.25106200	-2.04359100	-2.20934200
H	1.44568900	-2.79262600	-2.03068600
O	3.41227700	-2.35161200	-1.95324300
Rh	-0.20879600	0.01591300	-0.12289600
N	-4.17266500	-0.28355600	-0.09804200
C	3.48008800	0.85317600	0.79073300
N	-5.12574100	0.29404000	-1.02855200
H	-5.83412200	0.93081500	-0.49070400
H	-4.65285200	0.89089000	-1.82901500
H	-5.69426700	-0.51066800	-1.50629000
C	4.88617600	1.14660200	1.04744900
H	5.12716600	0.89898300	2.08558300
H	5.56533500	0.58142600	0.38543200
H	5.07005700	2.21560800	0.90541100

C1-H₂

E= -1088.72523327 a.u.

Rh	0.04433500	0.14143100	-0.82840000
P	-2.00291200	1.27489200	-0.72194300
P	-0.96353400	-1.72826900	0.25214800
C	-3.05799800	1.02569600	0.78000000
H	-2.54815200	1.49013500	1.62927600
H	-4.00921800	1.54806100	0.63507600
C	-2.23334600	-1.31560100	1.55047000
H	-2.67376700	-2.24631100	1.92330000
H	-1.69910000	-0.84432600	2.38171200
P	2.07708400	-0.94502400	-1.16696400
C	1.22623600	1.76857500	0.44161300
H	3.19911200	-1.19032000	0.29426200
H	4.23047000	-1.21646300	-0.07067700
H	2.98864700	-2.16478400	0.74291500
C	2.94772500	1.30117700	1.00423800
H	3.21229300	1.92064000	1.86677800
H	3.66285900	1.53661100	0.21033400
C	2.06703500	-2.61835400	-1.92632700
H	1.50619500	-3.32588900	-1.31423000
H	1.57734700	-2.54828600	-2.90106600
C	3.08449700	-2.99494300	-2.06469000
H	0.08123400	-2.82800900	1.30273700
H	0.79455400	-3.37851700	0.68617300
H	0.63591400	-2.23055200	2.02721700
C	-0.54069500	-3.55844400	1.82814800
H	-1.83542500	-2.96793400	-0.79598200
H	-1.11624900	-3.39465000	-1.50046300
H	-2.27286600	-3.77090900	-0.19522900
H	-2.62737300	-2.48362600	-1.36888400
C	1.62863400	3.40715900	-0.30522600

H	2.23918000	4.01907100	0.36589600	Rh	1.56307900	0.14850100	-0.49342300
H	2.16449700	3.25520200	-1.24566400	P	1.18251100	2.27754500	-1.35586900
H	0.70711600	3.94655600	-0.53183900	P	1.33023300	0.78745200	1.83794600
C	0.46559200	2.25582900	2.04924000	C	1.05698000	3.71203500	-0.18603600
H	-0.51155200	2.71202400	1.87464700	H	2.06805100	4.07578700	0.02079600
H	0.33047400	1.36434800	2.66441900	H	0.51329200	4.51922500	-0.68737000
H	1.09016400	2.97373300	2.58888600	C	1.13698600	2.61546900	2.15071600
C	-3.09794700	0.84919600	-2.13317600	H	0.64313500	2.74222200	3.11937200
H	-2.63032400	1.21868800	-3.04965400	H	2.14052400	3.04306300	2.24187300
H	-3.21183300	-0.23179000	-2.21269400	P	1.29461300	-2.16069900	-0.32151400
H	-4.08382800	1.30766600	-2.02009300	P	3.95374300	-0.11169700	-0.77319700
C	-2.00622700	3.11263300	-0.81596500	C	2.57793900	-3.15813200	0.59312300
H	-3.02904700	3.48980100	-0.90367200	H	2.64953500	-4.13937100	0.11394700
H	-1.54699200	3.55574600	0.07013500	H	2.23219900	-3.32333400	1.61779100
H	-1.43883900	3.42163900	-1.69751900	C	4.56611200	-1.85818700	-0.51373600
C	3.13961900	-0.03307300	-2.36173100	H	5.65337300	-1.83296900	-0.39084500
H	3.30871400	0.99111800	-2.02404100	C	4.35657000	-2.43790900	-1.41796700
H	4.10258100	-0.53201300	-2.50392200	H	-0.26761100	-2.78573500	0.40410600
H	2.61817200	0.01656100	-3.32097700	H	-0.30567800	-2.56241200	1.47164100
H	0.11722400	0.67316000	-2.54736400	H	-1.10209400	-2.26311500	-0.07502200
H	-0.26688600	-0.09135700	-2.59004200	H	-0.36549200	-3.86548800	0.25844500
C	3.12651300	-0.14992400	1.40556900	C	2.58508700	0.47006700	3.14937700
C	-3.38024500	-0.40998700	1.15108800	H	3.54425300	0.92251500	2.89024400
F	-4.07503400	-0.99254200	0.11086900	H	2.24209100	0.89146600	4.09927600
F	-4.26028200	-0.36804200	2.20260300	H	2.73411700	-0.60274100	3.27019300
F	2.11231500	-0.49064100	2.28099800	C	-0.16716000	0.07964500	2.62915400
F	4.28099900	-0.25720200	2.13639600	H	0.04065900	-0.96594200	2.87523300
				H	-0.40657200	0.60429500	3.55877500
				H	-1.02246700	0.11116600	1.94589200
				C	4.60374900	0.14493200	-2.47794300
				H	5.63805400	-0.20064500	-2.56516400
				H	3.97629100	-0.39630800	-3.19023000
				C	4.57040400	1.20599800	-2.73100100
				C	5.13808200	0.87223700	0.23537300
				H	4.91696800	1.93539200	0.10522800
				H	5.02198900	0.61596100	1.28924200
				H	6.17376300	0.68541300	-0.06285200
				C	-0.38746400	2.35921200	-2.29149300
				H	-0.32056300	1.66700800	-3.13477900
				H	-1.20288500	2.02591900	-1.64280700
				H	-0.57876800	3.37040000	-2.66163500
				C	2.39670200	2.96641600	-2.55180300
				H	2.05370400	3.93159200	-2.93593700
				H	3.36979300	3.10325300	-2.07287700
				C	2.50641200	2.27139100	-3.38738300
				H	1.31408500	-2.97253200	-1.97194100
				H	2.27150500	-2.79139000	-2.46565900
				H	1.14705900	-4.05028700	-1.88706100
				H	0.53325600	-2.52668700	-2.59013200
				H	1.42711800	-0.16616400	-2.03578300
				H	-0.00879000	0.14813700	-0.48102300
				H	-3.20256600	0.20229000	-0.44563100
				P	-4.71360400	1.00971600	-0.76636800
				N	-3.18531800	-0.17357700	1.26351800
				N	-3.11487400	-1.35695800	-1.20705100
				C	-3.55350500	0.96487300	2.09443100
				C	-3.13805400	1.88382700	1.67045600
				H	-2.25039500	-1.38188100	-2.38304500
				C	-2.81906900	-1.33678400	-3.32323600
				H	-4.56029100	2.18783400	-1.61620700
				C	-3.54864400	2.58979900	-1.52460600
				H	-3.86466900	-2.60774900	-1.05172000
				H	-3.32477500	-3.28290200	-0.36966600
				H	-3.87534800	-3.11695200	-2.02322300
				C	-5.32791000	-2.48807000	-0.60024300
				H	-5.93453700	-2.17859600	-1.45576600
				H	-5.66692700	-3.50302900	-0.32672000
				C	-3.50589400	-1.46752300	1.83540200
				H	-2.91316900	-2.22917600	1.32418100
				C	-3.17448400	-1.47125500	2.88324900
				H	-5.00284600	-1.83176000	1.76270000
				H	-5.13114600	-2.89413300	2.02684200
				H	-5.55857200	-1.25537300	2.50929400
				C	-6.05171700	0.44822600	-0.89299000
				H	-6.15832800	-0.07753000	-1.85784800
				H	-6.76952500	1.27806800	-0.92576800
				C	-6.46557000	-0.46369500	0.25369400
				H	-6.50846200	0.12656400	1.17332600
				H	-7.49139400	-0.81807300	0.04999000
				N	-5.54519900	-1.55224100	0.46343400
				H	-4.63904800	1.10821300	2.18933700
				H	-3.13106900	0.83368700	3.09817200
				H	-5.26174600	2.97007200	-1.30218900
				H	-4.75065600	1.96947900	-2.67933400
				H	-1.54965400	-0.54316200	-2.35644400
				C	-1.66286000	-2.31062100	-2.40006100
				H	0.37017100	3.44106800	1.13847500
				C	-0.86015700	2.86806000	0.90918300
				F	0.10868200	4.66031200	1.71872300
				F	3.98772200	-2.58772000	0.68633800
				F	4.82617100	-3.62854500	0.99636700
				F	4.04992100	-1.73753200	1.77422200

C2

E=-1088.74051146 a.u.

Rh	0.09797400	0.24233500	0.62277600				
P	2.09655700	1.41563900	0.36651400				
P	0.78051000	-1.36499700	-1.04323100				
C	3.43413800	0.51272100	-0.55702100				
H	3.26110200	0.62588300	-1.63211000				
H	4.39301300	0.98865900	-0.32921400				
C	2.54639700	-1.92927200	-0.83653600				
H	2.54207100	-2.81918300	-0.20066400				
H	2.92385800	-2.23328100	-1.81740100				
P	-1.68851200	-0.90021600	1.58797600				
P	-1.45527700	1.64947100	-0.60467500				
C	-3.12032000	-1.35035100	0.48115900				
H	-4.03637400	-1.33469100	1.08008800				
H	-2.98356700	-2.37693200	0.12907900				
C	-3.21622400	1.02504300	-0.58670100				
H	-3.76787700	1.50095100	-1.40298900				
H	-3.69663600	1.32978200	0.34787200				
C	-1.34406800	-2.50279100	2.40864600				
H	-0.94620900	-3.22062400	1.68972000				
H	-0.59278900	-2.34031500	3.18465500				
H	-2.25167000	-2.91316900	2.86030700				
C	0.75071500	-0.82515500	-2.80616100				
H	1.19810400	0.16567300	-2.91728400				
H	1.28266200	-1.53259000	-3.44863400				
H	-0.28904300	-0.77223100	-3.13606000				
C	-0.03444400	-3.00945200	-1.17380900				
H	-1.09022300	-2.86948300	-1.41332100				
H	0.43013600	-3.61205000	-1.95968100				
H	0.05572500	-3.54710000	-0.22616300				
C	-1.70834800	3.30987900	0.14698900				
H	-2.54206500	3.84150600	-0.32075300				
H	-1.89454000	3.19987000	1.21763900				
H	-0.80063100	3.90453600	0.02289000				
H	-1.25415000	2.07064400	-2.38681600				
C	-0.25982300	2.48674600	-2.56183800				
H	-1.37062300	1.17388000	-2.99599900				
H	-2.00072200	2.80787900	-2.69567800				
C	2.88973700	1.85842100	1.95574200				
H	2.21137700	2.51030100	2.51087900				
H	3.05225000	0.95096100	2.53782100				
C	3.84285000	2.36965400	1.79454900				
C	2.10454500	3.01285700	-0.54277200				
H	3.11964900	3.41298900	-0.61917700				
H	1.69937600	2.88173700	-1.54862900				
H	1.48762700	3.73567400	-0.00385800				
C	-2.50292600	0.04745000	2.93494300				
H	-2.85261400	1.01212400	2.56072400				
H	-3.34475000	-0.50494900	3.36193300				
H	-1.76104600	0.24198500	3.71272700				
H	-0.11212200	1.23672300	1.83141600				
H	0.97333700	-0.56563300	1.64974800				
C	3.56182300	-0.96691200	-0.23147200				
C	-3.35684300	-0.47904300	-0.74390700				
F	4.80476300	-1.37806500	-0.64633200				
F	3.56553900	-1.11831500	1.13655000				
F	-2.50730000	-0.89490000	-1.75981500				
F	-4.61722500	-0.75154500	-1.20373700				

C3

E=-1669.72744369 a.u.

C4

E=-1669.72513643 a.u.

Rh	1.77564900	0.24963900	-0.50817500
F	0.68193600	2.01107100	-1.43631900
P	1.94184100	1.17350300	1.64270500
C	0.08108400	3.42957000	-0.35758900
H	0.82543600	4.23040900	-0.40186100
H	-0.84953100	3.83700300	-0.76639800
C	1.06985400	2.81032100	1.94309400
H	0.77814700	2.87315100	2.99621500
H	1.79828400	3.60701500	1.76273600
P	1.38625400	-2.00236500	0.01676900
F	4.06569500	-0.10173000	-1.08018600
C	2.81278400	-2.92968400	0.82874900
H	2.83682900	-3.94996800	0.43185500
H	2.61766200	-3.00984100	1.90284300
C	4.67456800	-1.82949000	-0.65662500
H	5.76923300	-1.85193400	-0.66677600
H	4.32992300	-2.51992600	-1.43302200
C	0.03844400	-2.70988800	1.08509200
H	0.11415300	-2.27877700	2.08662600
H	-0.93721200	-2.43746900	0.67284600
C	0.10481600	-3.80115600	1.16245700
H	3.57369600	1.68077800	2.34795400
C	4.07743600	2.35400000	1.65013300
H	3.45160900	2.18542700	3.31184100
H	4.19557600	0.79518300	2.48701800
C	1.29709900	0.18744700	3.06878600
H	1.84642600	-0.75765200	3.10867400
H	1.42439200	0.70844500	4.02292100
H	0.23787000	-0.02673500	2.91302800
C	4.43630600	-0.12545800	-2.89128900
H	5.45678900	-0.45955100	-3.10702000
H	3.71922400	-0.77893600	-3.39431600
H	4.30216500	0.88524900	-3.28715400
C	5.51211500	0.88742000	-0.47798900
H	5.33427600	1.94670000	-0.68383500
H	5.62769100	0.75747500	0.59918200
C	6.44026200	0.58012200	-0.97157200
H	-0.83427100	1.74710400	-2.47340900
H	-0.59036900	1.01664100	-3.24910000
H	-1.64408700	1.33940800	-1.86621600
H	-1.17392700	2.67529700	-2.94596300
C	1.65696200	3.00022600	-2.66402200
H	1.09694900	3.84847500	-3.07278800
H	2.57157300	3.36223500	-2.18726800
H	1.94520700	2.33360900	-3.48152400
C	1.19885000	-3.07272100	-1.48615000
H	2.10245500	-2.98133000	-2.09418600
H	1.03871600	-4.12719400	-1.23628900
H	0.37085600	-2.70679500	-2.09510600
H	1.51368400	-0.26491800	-1.99653800
P	-2.41186000	0.31038200	0.04714600
P	-3.68802700	-0.28850100	-0.02128900
N	-4.55937400	1.16961000	-0.02669300
N	-3.53167900	-1.16039100	1.43159800
N	-3.40091100	-1.10762600	-1.48392700
C	-2.58875300	-0.68013200	2.43801600
H	-1.74293000	-0.18652300	1.95738800
C	-2.03160000	-1.48166100	-1.83020400
H	-1.86866100	-1.33822800	-2.90319200
C	-3.89494200	2.41997300	-0.38639800
H	-2.83936000	2.37865900	-0.12297100
C	-4.39742200	-1.99660600	-2.04844700
H	-4.18638500	-3.04249800	-1.77495600
H	-4.37273400	-1.94203500	-3.14180600
C	-5.76047100	-1.55704700	-1.53990500
H	-6.09709000	-0.67558700	-2.08901800
H	-6.51876500	-2.33980500	-1.64068000
C	-4.65116400	-1.90974700	1.96652000
H	-4.28830700	-2.79733900	2.49482300
H	-5.21880500	-1.30965900	2.69477400
C	-5.52196800	-2.33072900	0.79261300
H	-5.05195900	-3.16195800	0.26279100
H	-6.52648600	-2.63676800	1.10125300
C	-5.99690600	1.18647100	-0.20836300
H	-6.26081600	1.34774900	-1.26519600
H	-6.43443500	2.01335400	0.36012100
C	-6.53716900	-0.13585900	0.31020700
H	-6.55730800	-0.12479200	1.40170500
H	-7.54534900	-0.35372500	-0.05585400
N	-5.58670900	-1.17673900	-0.12505100
H	-3.05890400	0.02748500	3.13356400
H	-2.20417600	-1.53340300	3.00472600
H	-4.34190400	3.24096900	0.18174100
H	-3.99435500	2.63442900	-1.45873100
H	-1.29344300	-0.87309900	-1.29876600
H	-1.85034600	-2.53691000	-1.58528100
C	-0.14725100	3.12033700	1.10518700
C	4.21617300	-2.35881500	0.69210600
F	4.38168400	-1.36568600	1.64602700
F	5.09106700	-3.35495800	1.07876500
F	-1.07435900	2.08840100	1.23557900
F	-0.78430700	4.21195200	1.66724800

C5

E=-1088.30481223 a.u.

Rh	-0.00750900	-0.28268200	-0.41695600
P	-1.89567300	-1.61339200	-0.24649800
P	-0.94718600	1.84070100	-0.13333200
C	-3.44708400	-0.65756400	-0.69094200
H	-3.44233100	-0.53626300	-1.77855700
H	-4.33400400	-1.24314200	-0.42353100
C	-2.76595200	1.86789400	-0.58754800
H	-3.22924700	2.79745300	-0.23797200
H	-2.82212400	1.85776700	-1.68054300
P	1.04525500	-0.68792900	1.60821700
F	1.98119400	-0.43174200	-1.53318800
C	2.67898300	0.18620400	1.89710100
H	3.32847800	-0.46061700	2.49567300
H	2.48386600	1.08806400	2.48502300
C	3.55138200	-0.32010000	-0.50780500
H	4.38484800	0.00194100	-1.14051500
C	3.79319300	-1.31876800	-0.12872200
H	0.24125600	-0.30915600	3.22812800
H	0.00715500	0.75650100	3.27772500
H	-0.69679900	-0.86549900	3.29580100
H	0.88092200	-0.57877400	4.07511200
C	-0.38851200	3.20713700	-1.25037200
H	-0.39411900	2.84358200	-2.28139800
H	-1.01397100	4.10389000	-1.17162400
H	0.64207100	3.46345400	-0.98842200
C	-1.00348800	2.76349000	1.47369400
H	0.01995600	2.91233200	1.83144600
H	-1.48804900	3.74071300	1.36887800
H	-1.55517400	2.17379900	2.20950200
C	2.42622600	-1.93863300	-2.51678600
H	3.41391000	-1.86186400	-2.98617100
H	2.39469000	-2.81610800	-1.86517900
H	1.66719400	-2.07178700	-3.29260300
C	2.31474900	0.87327800	-2.80003700
H	1.52073200	0.82786000	-3.55022700
H	2.27569700	1.85187900	-2.31796700
H	3.28635100	0.74355500	-3.28926200
C	-2.45765000	-2.41033200	1.33064600
H	-1.71041500	-3.14101800	1.65386900
H	-2.56157400	-1.64535700	2.10304200
H	-3.41899200	-2.92144900	1.20987500
C	-2.15321600	-3.02908200	-1.41387800
H	-3.16024400	-3.45730600	-1.34549300
H	-1.96832100	-2.68039200	-2.43303200
H	-1.41621500	-3.80416700	-1.18583800
C	1.55576700	-2.44285400	1.91399000
H	2.20489200	-2.77836400	1.10094200
H	2.07122900	-2.57262000	2.87192700
H	0.66141200	-3.07093200	1.89790400
H	-0.58447300	-0.11933400	-1.90801100
C	-3.61806800	0.71998200	-0.07438800
C	3.46919500	0.62670100	0.67357300
F	-4.94312500	1.08491900	-0.27050200
F	-3.48665000	0.62750700	1.30272200
F	2.99232500	1.84905200	0.24453700
F	4.76211500	0.89022000	1.10225500

C6

E=-1276.83655279 a.u.

Rh	0.11024500	0.05763700	-0.29349100
P	-1.68156800	-0.64336400	-1.58907400
P	-0.80154600	-0.21737800	1.84677100
C	-3.30928900	-0.34542200	-0.70839600
H	-3.49059400	0.73301800	-0.74535700
H	-4.12325700	-0.83499100	-1.25505700
C	-2.66608500	-0.03626100	1.82110700
H	-3.09111100	-0.34333700	2.78338900
H	-2.87273400	1.03079500	1.69318600
P	1.57458400	-1.72239900	-0.52217600
P	1.81461000	1.55315100	-0.56408600
C	3.22728500	-1.56919200	0.35190500
H	3.99014300	-2.08727000	-0.23801200
C	3.15015500	-2.08485600	1.31369700
H	3.56881400	0.90340400	-0.40725900
H	4.24986000	1.72662100	-0.16814900
H	3.87836400	0.48925300	-1.37266500
C	1.13945800	-3.43460200	0.01955800
H	0.90232300	-3.42907300	1.08588100
H	0.25013900	-3.76262600	-0.52455000
H	1.95392800	-4.14261800	-0.16618900
C	-0.44391100	1.05878800	3.13779900
H	-0.61063300	2.05038400	2.70941900
H	-1.06021800	0.93705200	4.03596600
C	0.61187500	0.97869200	3.41229500
H	-0.62591200	-1.75270700	2.87039400
H	0.43694300	-1.91292900	3.07739800
H	-1.16411600	-1.67727800	3.82179700
H	-1.01023500	-2.60929800	2.31216300

C	2.01824400	2.47990500	-2.15548500
H	2.87597600	3.16235300	-2.14599000
H	2.12407200	1.76357900	-2.97465300
H	1.10291600	3.05135600	-2.33301300
C	1.87218600	2.96017500	0.63448700
H	0.92069300	3.49540700	0.58213400
H	1.97841200	2.55593700	1.64296200
C	2.69421200	3.65403100	0.42741800
H	-1.92178200	-2.40155400	-2.12730600
H	-1.11143000	-2.68540200	-2.80560300
H	-1.89630400	-3.05622500	-1.25358400
H	-2.87683800	-2.54259500	-2.64494300
C	-2.10321900	0.22481000	-3.16869000
H	-3.06516300	-0.09698100	-3.58492000
H	-2.12452700	1.30143800	-2.98353900
H	-1.31110200	0.02199500	-3.89501900
C	2.14784600	-2.07475600	-2.24835600
H	2.58125600	-1.16777800	-2.67779900
H	2.88100000	-2.88757500	-2.29193300
H	1.27857500	-2.34045700	-2.85575600
H	-0.76563400	1.39979600	-0.26795100
C	-2.21234600	3.51735100	-0.20047100
O	-2.50086900	3.39739800	-1.32309700
O	-1.95028000	3.66869500	0.92525100
C	-3.42426300	-0.78782300	0.74074300
C	3.74763100	-0.17008400	0.64861300
F	-4.77093000	-0.70535900	1.07135200
F	-3.12991200	-2.13881700	0.83018400
F	3.20540000	0.26996200	1.83906000
F	5.10456400	-0.29191200	0.90978600

C7

E=-1276.85273282 a.u.

Rh	0.14726900	0.15353600	0.08363000
P	-1.61389500	1.66013300	0.29522200
P	-1.27879100	-1.26391000	-1.15244200
C	-3.27273100	0.89415100	0.61749300
H	-3.15635100	0.35790000	1.56368600
H	-4.01234600	1.69183100	0.74169100
C	-3.06062500	-1.36483700	-0.62775800
H	-3.62405600	-1.95130400	-1.36106500
H	-3.04812400	-1.91281600	0.31916500
P	1.76758500	1.74997400	0.14237700
P	1.80991800	-1.39241900	0.64713500
C	3.25048400	1.36529600	-0.93463800
H	4.10535800	1.93947000	-0.56241000
H	3.02602500	1.71779100	-1.94514300
C	3.57685300	-0.93184900	0.20130300
H	4.15741600	-1.84534900	0.04573200
H	4.03972100	-0.38875100	1.03068100
C	1.45828700	3.44731100	-0.52432500
H	1.02231000	3.37257200	-1.52326200
O	0.76597200	3.98975100	0.12395300
H	2.39344000	4.01343300	-0.58088200
C	-1.02213000	-3.06789000	-1.40907200
H	-1.07846600	-3.56483900	-0.43879200
H	-1.79412300	-3.46240400	-2.07741300
H	-0.04497100	-3.24193800	-1.86246100
C	-1.38038100	-0.69360200	-2.90659400
H	-0.39565700	-0.83348100	-3.36123600
H	-2.12799000	-1.25683700	-3.47407300
H	-1.62578900	0.36824300	-2.94646500
C	1.93927500	-1.50509300	2.47949200
H	2.89688500	-1.94473100	2.77631200
H	1.81003300	-0.52264000	2.93599600
C	1.12065900	-2.14282600	2.81589700
H	1.82952200	-3.17692800	0.20765900
C	0.89041100	-3.61263800	0.55162700
H	1.94216600	-3.30859200	-0.87000200
H	2.66456000	-3.66798200	0.71719700
C	-2.03618500	2.95949600	-0.94709000
H	-1.21739600	3.67449600	-1.03819700
H	-2.20871400	2.49884600	-1.92114000
H	-2.94238400	3.49533800	-0.64896800
C	-1.46413700	2.61995000	1.85858000
H	-2.36920800	3.20386600	2.05362700
H	-1.30506700	1.89239900	2.65928500
C	-0.60926900	3.29920900	1.80842200
H	2.58876000	2.21184100	1.74014200
C	3.03993800	1.33234300	2.20473500
H	3.35812000	2.97925800	1.60402400
H	1.82341100	2.58455900	2.42691600
H	-2.00656600	-2.08840500	3.46663600
C	-1.43446800	-1.73918800	2.57500000
O	-1.25045400	-0.49604100	2.49313100
O	-1.05007200	-2.62396500	1.77395200
C	-3.80077600	-0.06525300	-0.42280600
C	3.68612800	-0.08623300	-1.04733200
C	-5.10323800	-0.37318700	-0.08027000
F	-3.91041800	0.59450100	-1.64061800
F	2.99316400	-0.70088000	-2.06716100
F	5.00578400	-0.08982800	-1.46515100

C8

E=-1276.84000439 a.u.

Rh	0.15052600	-0.10842200	-0.33555600
P	1.57743600	1.72691500	-0.16642500
P	1.73240600	-1.85875200	-0.09301600
C	3.33244300	1.28532000	-0.66413200
H	3.33910900	1.18952300	-1.75426400
H	4.00149800	2.11085500	-0.39745200
C	3.44676100	-1.31663800	-0.61798700
H	4.18340200	-2.07344300	-0.32681700
H	3.44269500	-1.25723900	-1.71068100
P	-1.01305900	-0.16161200	1.68944800
P	-1.70334500	-0.63683500	-1.57203600
C	-2.85628200	0.15760800	1.60295200
C	-3.41167500	-0.27345300	-0.90199300
H	-4.16315600	-0.81729700	-1.48477600
H	-3.59206900	0.79570200	-1.04382800
C	-0.99771600	-1.73132700	2.66842800
H	-1.22291000	-2.57536200	2.01420600
H	0.00251100	-1.86629900	3.08707400
H	-1.72425500	-1.70711900	3.48667600
C	1.60183400	-3.31379900	-1.23445500
H	1.47053600	-2.94951800	-2.25689900
H	2.48330900	-3.96362600	-1.18886100
H	0.71527600	-3.89538400	-0.96632500
C	2.15613600	-2.75814700	1.47353900
H	1.29088200	-3.34385100	1.79528400
H	3.00664600	-3.43475400	1.33501000
H	2.40209500	-2.03550000	2.25497900
C	-1.90674900	0.13775300	-3.23776900
H	-2.82587900	-0.18923500	-3.73637800
H	-1.90888700	1.22437000	-3.13376200
H	-1.04410000	-0.14520000	-3.84679500
C	-1.91034500	-2.41754000	-2.04291000
H	-1.03405300	-2.72059000	-2.62243900
H	-1.95113800	-3.02652400	-1.13726900
H	-2.81408400	-2.59129900	-2.63735100
C	1.93243900	2.66149500	1.39372700
H	1.02082800	3.15655800	1.73658600
H	2.26771700	1.96441500	2.16435200
H	2.70951400	3.41756200	1.23715300
C	1.41176400	3.15951100	-1.33691900
H	2.32012600	3.77258900	-1.36691500
H	1.19039000	2.77875700	-2.33666900
H	0.58325400	3.79636900	-1.01756500
C	-0.63461900	1.03290300	3.04842000
H	-0.77366900	2.05384400	2.68821700
H	-1.27273500	0.86479000	3.92209900
H	0.41106600	0.90953700	3.34108700
H	0.79328900	-0.05721100	-1.80357900
C	-1.95815600	3.25894000	-0.34582300
O	-1.55063100	3.49079300	0.72193900
O	-2.39821900	3.07239500	-1.40787000
C	3.93461600	0.01815100	-0.08907900
C	-3.64754600	-0.60013600	0.55577000
F	5.30015600	0.07436500	-0.33057800
F	3.82672600	0.03802300	1.29187600
H	-3.30649800	-0.06992900	2.57504100
H	-2.99406200	1.22762000	1.42252300
F	-4.99058000	-0.37722500	0.81908700
F	-3.47502700	-1.95952000	0.75246300

C9

E=-1276.84062978 a.u.

Rh	-0.07081600	-0.11162300	-0.41989500
P	-1.88084500	-1.60901700	-0.32089900
P	-1.44286300	1.86319600	0.16311600
C	-3.55767400	-0.87287300	-0.67128900
H	-3.60552500	-0.68547700	-1.74814300
H	-4.32007700	-1.62065700	-0.42980800
C	-3.21910500	1.67595400	-0.37704000
H	-3.80044400	2.52151100	0.00572500
H	-3.23160100	1.72813300	-1.46997900
P	1.14189400	-0.42763900	1.65941400
P	1.82118400	0.89931000	-1.36624800
C	2.91681100	-0.92745900	1.39624200
H	2.87775000	-1.92700100	0.95501500
C	3.41420400	-0.99144400	2.36977500
C	3.43133500	0.06902900	-0.95555100
H	1.32234700	1.00143800	2.82021600
C	1.58909900	1.90938200	2.27575400
H	0.36905300	1.16341500	3.32949200
H	2.09351000	0.80560700	3.57094900
C	-1.13251200	3.46911100	-0.70432000
H	-0.98732500	3.28711000	-1.77255000
H	-1.96535100	4.16676400	-0.56725500
H	-0.22619400	3.92868300	-0.30402700
C	-1.68291600	2.49916300	1.88480900
H	-0.74335800	2.92881600	2.24111300
H	-2.45885200	3.27062400	1.92140900
H	-1.96896000	1.67981100	2.54718300

C	1.87356300	0.84544200	-3.19796400
H	2.82863800	1.21494400	-3.58437400
H	1.70685500	-0.19255600	-3.49242000
H	1.05821900	1.46305700	-3.58343200
C	2.21153400	2.67412100	-1.03691100
H	1.52965100	3.29997700	-1.61633500
H	2.09547700	2.90298200	0.02385100
C	3.23799300	2.90542600	-1.33488200
C	-2.20287900	-2.59166200	1.19800600
H	-1.31744900	-3.20242000	1.38307500
H	-2.37881700	-1.92947600	2.04741500
H	-3.07216700	-3.24222900	1.06181600
C	-1.92140100	-2.92106700	-1.61126900
H	-2.89078900	-3.42990500	-1.60799600
H	-1.73205200	-2.47346400	-2.58869000
H	-1.12549600	-3.63880400	-1.40578700
C	0.68284600	-1.75197800	2.85270100
C	0.70578400	-2.70572400	2.32354000
H	1.38612200	-1.77262200	3.69118600
H	-0.32324500	-1.57086200	3.23770700
H	-0.68318800	0.02418200	-1.87846900
C	0.89275600	-1.97029700	-1.05079100
O	0.93538900	-2.79940000	-0.12251700
C	1.27854000	-2.02959300	-2.21806000
C	-3.93220600	0.40690400	0.04053400
C	3.77658100	-0.04739500	0.51474600
F	-5.28497000	0.61121500	-0.15856200
F	-3.79861900	0.23330900	1.40800500
H	3.37665400	-0.93431300	-1.38703300
H	4.24813500	0.61277300	-1.44190200
F	3.84154400	1.22684000	1.06643400
F	5.06915600	-0.52465100	0.59573600

C10

E=-1277.27908392 a.u.

Rh	-0.03747500	0.17572100	-0.54583500
P	-1.85595600	1.62323500	-0.30288100
P	-1.50169100	-1.73098600	-0.39220300
C	-3.14384500	1.07987100	0.91798300
H	-2.67904800	1.08624900	1.90942200
C	-3.95825000	1.81160400	0.93034900
H	-2.90948600	-1.52841600	0.80822700
H	-3.58154200	-2.38749800	0.71167300
H	-2.48509200	-1.56100200	1.81562600
P	1.85848200	-0.83256000	-1.47400300
P	0.80022200	0.21687400	1.72682800
C	3.41504800	-0.79995000	-0.46648900
C	3.86605000	0.19037400	-0.57080500
H	4.11394300	-1.53191300	-0.88380800
C	2.63826100	-0.01586500	1.87342100
C	2.87715800	-0.24325000	2.91708300
C	3.11841300	0.93386300	1.62064900
H	1.77845300	-2.59157500	-1.99941500
H	1.74214100	-3.23714700	-1.12059100
H	0.88746800	-2.75436200	-2.61066400
H	2.66203900	-2.85082300	-2.58965600
C	-0.87302900	-3.37050200	0.17164800
C	-0.16572800	-3.25975800	0.99436300
H	-1.69748600	-4.01758800	0.48386300
H	-0.35670500	-3.85666100	-0.65812400
C	-2.35083700	-2.18823200	-1.95580500
H	-1.59576900	-2.46183500	-2.69679500
H	-3.03315900	-3.02960800	-1.80705300
C	-2.91449700	-1.33817500	-2.34078900
H	0.64945200	1.80370200	2.65239300
H	1.22677600	1.77139100	3.58089600
H	1.00270200	2.63442400	2.03763600
H	-0.39825800	1.98157100	2.90945700
C	0.16581600	-0.95967400	2.99577900
H	-0.90439700	-0.79402100	3.14549200
H	0.32646600	-1.99017300	2.67682500
H	0.67225800	-0.80958200	3.95355500
C	-2.78259700	1.93385300	-1.85409500
H	-2.11959600	2.47640100	-2.53252500
C	-3.06781100	0.99525100	-2.32747500
H	-3.67967900	2.52905200	-1.66379700
C	-1.53883500	3.33708300	0.26911500
C	-2.46615200	3.91670200	0.25531200
H	-1.12550500	3.35030100	1.27732800
C	-0.81436600	3.79883100	-0.40527300
C	2.42392200	0.00608200	-3.00309500
H	2.58575800	1.06566400	-2.79808700
H	3.34775300	-0.44212200	-3.37945600
H	1.64261500	-0.07938100	-3.76162400
H	0.79898300	1.49476100	-0.80308500
H	-0.41797500	0.28143900	-2.06964400
C	2.56588200	3.47892900	-0.53535100
O	3.39283500	2.67663000	-0.34856800
C	1.74079000	4.27945400	-0.71159500
C	3.25539100	-1.10042500	1.01103000
C	-3.77506700	-0.28514000	0.69819200
F	-4.40169500	-0.28962600	-0.52998100
F	-4.77938200	-0.41559100	1.62515700

C11

E=-1277.26302527 a.u.

Rh	-0.02784300	0.23010600	-0.42785900
P	-1.96556000	1.51282400	0.02147800
P	-1.29676400	-1.68956600	-0.59894300
C	-3.27615300	0.71069000	1.05265100
H	-2.88169500	0.60670600	2.06823800
H	-4.15213500	1.36573300	1.10010900
C	-2.73314300	-1.78623600	0.57305100
H	-3.28535100	-2.70546100	0.35205700
H	-2.32011000	-1.88813700	1.58139200
P	1.96936600	-0.52300700	-1.47695600
P	0.86396800	-0.02394000	1.86596900
C	3.48961900	-0.05385600	-0.53716400
C	3.57757200	1.03487700	-0.58379700
H	4.35316500	-0.49378600	-1.04608100
C	2.68880200	0.29208400	1.90437900
H	3.05871800	0.06767100	2.91000900
C	2.82622600	1.35979000	1.71317600
C	2.27760500	-2.26635700	-1.96313300
H	2.32002700	-2.91059200	-1.08471500
H	1.49009800	-2.60708900	-2.64065200
H	3.23414200	-2.33267200	-2.48905700
C	-0.51777100	-3.30496000	-0.20576600
C	-0.00923600	-3.26534900	0.75790700
H	-1.28459400	-4.08384900	-0.17473000
H	0.20696500	-3.56931700	-0.97476600
C	-2.01989400	-1.98870400	-2.25415500
H	-1.20404600	-2.11132500	-2.97109900
H	-2.64133100	-2.88811200	-2.25419300
C	-2.62360800	-1.13542800	-2.56352700
C	0.33423900	1.27070500	3.05650900
H	0.89803000	1.19044400	3.99024800
H	0.51509500	2.25144100	2.61154000
C	-0.72911200	1.16119600	3.28620300
H	0.67958900	-1.55680900	2.86951200
H	-0.37939800	-1.79371600	3.00548400
H	1.17792000	-2.39502900	2.38053800
H	1.13011100	-1.42061100	3.85679000
C	-2.83082700	2.04969400	-1.50279000
C	-2.16004300	2.70802500	-2.06067300
H	-3.07590200	1.19175100	-2.12854700
H	-3.74844200	2.59144800	-1.25881900
C	-1.73069900	3.09747300	0.91445600
C	-2.63748600	3.70062200	0.81787400
H	-1.53442100	2.92195200	1.97176800
H	-0.88678800	3.64610800	0.49346400
C	2.24167400	0.36331600	-3.05754600
H	2.18410000	1.44131500	-2.90118200
H	3.22431300	0.11551600	-3.46873900
H	1.46779200	0.07157100	-3.77105900
H	0.37810600	2.88083200	-1.90589300
H	-0.44666900	0.50687500	-1.91074600
C	1.11282200	2.98089000	-1.07666200
O	1.81990600	3.96073700	-0.98244400
O	1.13521900	1.97114300	-0.24494700
C	-3.74460800	-0.65366100	0.58443200
C	3.53910200	-0.48329100	0.91747400
F	-4.29168400	-0.53375800	-0.67464600
F	-4.77180100	-1.04004900	1.40257800
F	3.21844700	-1.83358400	1.00236900
F	4.83865900	-0.39191200	1.32964900

C12

E=-1087.79980410 a.u.

Rh	0.10905300	0.05530500	0.49356900
P	2.03056100	1.44979800	0.33506200
P	0.95609200	-1.22024000	-1.13554700
C	3.56178000	0.67559200	-0.36134700
H	3.62320500	0.89330300	-1.43250800
H	4.42991100	1.14438900	0.11340500
C	2.73387400	-1.70564000	-0.98428200
C	2.76941200	-2.70908900	-0.54969200
H	3.14179500	-1.77135200	-1.99813600
P	-1.66952600	-1.29486500	1.31141700
P	-1.59154900	1.75734700	-0.21143800
C	-3.20271400	-1.44103700	0.28121900
H	-4.07323300	-1.44381900	0.94539400
C	-3.18858900	-2.40712500	-0.23242300
C	-3.32446100	1.08525700	-0.31586500
H	-3.88637100	1.69703900	-1.02833800
C	-3.82281400	1.18705100	0.65287300
H	-1.36472100	-3.01199400	1.86355600
H	-1.19591100	-3.67582300	1.01487600
H	-0.48878100	-3.03368600	2.51598400
C	-2.23182300	-3.37960300	2.41955600
C	0.80178300	-0.32087400	-2.71897400
H	1.29064300	0.65409100	-2.67371900

H	1.25484900	-0.91233700	-3.52057600
H	-0.25744800	-0.18096000	-2.94136100
C	0.12351400	-2.81233500	-1.43167300
H	-0.94079900	-2.64826500	-1.61214700
H	0.56222500	-3.27510200	-2.32143400
C	0.27305700	-3.48090200	-0.58283300
H	-1.79984900	3.18001000	0.93452700
H	-2.63164300	3.81510400	0.61726800
H	-1.98859100	2.83582700	1.95443400
H	-0.89036300	3.78581900	0.94416800
C	-1.38535900	2.54613700	-1.85631200
H	-0.40834700	3.02361800	-1.93616500
H	-1.48302400	1.79543000	-2.64205300
H	-2.15791600	3.30664700	-2.00122300
C	2.43686600	1.85924600	2.07361000
H	1.58802100	2.36057200	2.54653300
H	2.66626400	0.94366700	2.62158800
H	3.30151800	2.52822300	2.11072800
C	2.01675200	3.06089600	-0.53666700
H	2.97940200	3.56129300	-0.39646600
H	1.85324000	2.92157600	-1.60781600
C	1.23384700	3.70816300	-0.13587800
H	-2.20408000	-0.45457800	2.85695700
H	-2.52801200	0.57016700	2.66304600
C	-3.03170900	-1.00160000	3.31786900
H	-1.37225700	-0.42891700	3.56620500
H	1.03269700	-1.01414200	1.15621600
C	-3.40575300	-0.36481600	-0.77421700
C	3.66423600	-0.82572000	-0.15281600
F	-4.61193700	-0.57594700	-1.35335500
F	3.46059400	-1.10071000	1.17878100
F	4.93424000	-1.21256000	-0.43406900
F	-2.46342100	-0.56183300	-1.78209900

C13

E=-1858.24840360 a.u.

Rh	-1.34871400	-0.05399600	0.27921400
P	-0.63660000	1.88231700	1.41773600
P	-1.50207500	1.12154500	-1.70104200
C	-1.41875500	3.47815300	0.89626500
H	-2.46350000	3.45722000	1.22297300
H	-0.92563000	4.30591700	1.41640000
C	-2.13122200	2.85676300	-1.52635500
H	-2.12246700	3.32264600	-2.51704200
C	-3.17421100	2.79262700	-1.20163600
P	-1.49631700	-2.19980300	-0.71076300
P	-3.71766300	-0.10314800	0.99553100
C	-3.13763200	-2.83212600	-1.33434400
H	-3.15762100	-3.90668100	-1.13049100
H	-3.17775500	-2.71561900	-2.42091800
C	-4.47965100	-1.76621900	0.65982800
H	-5.53249700	-1.73705400	0.95796000
H	-3.97298500	-2.49050000	1.30634100
C	-0.41582200	-2.53318700	-2.15834100
C	-0.71437600	-1.92764900	-3.01708600
H	0.61522100	-2.27907500	-1.89868600
H	-0.46749900	-3.58849300	-2.44048700
C	-2.67130200	0.53339000	-2.98725000
H	-3.69105400	0.51978400	-2.60376500
H	-2.61681300	1.18472400	-3.86405700
H	-2.41606700	-0.48258100	-3.29373700
C	0.06815400	1.26609500	-2.62664000
H	0.28921000	0.29378100	-3.07419500
H	-0.00617400	2.02014400	-3.41422400
C	0.89049800	1.49883400	-1.94968300
C	-3.95547200	-0.03405900	2.81556600
H	-4.92023000	-0.46475400	3.09759300
H	-3.14104500	-0.58119100	3.29586600
H	-3.94007200	1.00704300	3.14697900
C	-4.98007700	1.09462800	0.39326300
H	-4.70144100	2.09604900	0.73548800
H	-5.03611300	1.09230700	-0.69605500
H	-5.97073600	0.85893000	0.79206300
C	1.16106200	2.18035300	1.30087200
H	1.68655400	1.29199800	1.66229800
H	1.44075100	2.32447700	0.25828900
H	1.45073000	3.05922100	1.88339100
C	-0.94813200	1.92420800	3.22273700
H	-0.51455500	2.83503300	3.64494700
H	-2.01776600	1.90408600	3.43101500
C	-0.49204400	1.05561000	3.69978000
H	-1.01054000	-3.50974300	0.47406100
C	-1.61874600	-3.44649300	1.37798200
H	-1.11696900	-4.49188900	0.00533700
H	0.02747200	-3.36483100	0.77647500
H	0.87537900	-0.77492100	2.15920100
H	0.16689400	-0.20011000	-0.07403100
C	0.02672300	-1.29532100	2.64843100
O	0.20540000	-2.00448400	3.62046300
P	-1.13765400	-1.08421000	2.09516900
P	3.31124500	-0.00704600	-0.67469400
N	4.08175500	-1.17542600	-1.72319000

N	3.09154800	-0.81802000	0.86798000
N	4.34744100	1.33964300	-0.35913800
C	2.60725800	-2.18166800	0.71578800
H	1.78510600	-2.19224100	-0.00877300
C	3.88577900	2.61137500	-0.90683500
H	4.62711900	3.03585200	-1.59636300
C	3.54264200	-1.13877500	-3.07976000
C	2.51243900	-0.77231600	-3.06354300
H	5.57654300	1.51022900	0.41991200
H	5.33765100	1.78135400	1.45883800
H	6.11310300	2.37306600	0.00632600
C	6.54581800	0.32355300	0.39938000
H	7.05677000	0.30401500	-0.56719700
H	7.31993500	0.51531000	1.16276400
C	3.93917100	-0.61583700	2.03250100
H	4.01921000	0.45817500	2.21621600
C	3.42960600	-1.04410000	2.90542000
H	5.34180200	-1.23975100	1.88579400
H	5.99012900	-0.87640300	2.69884600
H	5.27102300	-2.32575500	2.00629400
C	5.48914300	-1.56163100	-1.75289700
H	6.09328400	-0.75067700	-2.19564100
H	5.59271200	-2.41877000	-2.43125500
C	6.07125600	-1.96687600	-0.40452800
H	5.56950800	-2.87348500	-0.05532000
H	7.13140000	-2.23018100	-0.56567500
N	5.90986100	-0.94723500	0.59921500
H	3.36519600	-2.88677000	0.34826000
H	2.22804200	-2.54633300	1.67660600
H	3.54453500	-2.14547800	-3.51603200
H	4.12464400	-0.48245400	-3.74692300
H	2.95772700	2.47174100	-1.46652600
H	3.70037200	3.35133700	-0.11409700
C	-1.39300900	3.79282600	-0.58734700
C	-4.43235800	-2.24660000	-0.77973400
F	-4.82628400	-1.20133300	-1.59955700
F	-5.40146900	-3.20232500	-0.93822100
F	-0.08367200	3.89912100	-1.00369400
F	-1.93691300	5.04070600	-0.75119300

C14

E=-1858.28168693 a.u.

Rh	2.32876800	0.60754200	-0.00811400
P	1.14337500	1.67329900	-1.70101000
P	1.86392800	2.39948900	1.36292800
C	-0.02063700	3.05998200	-1.21455100
H	0.52585500	4.00817000	-1.20916400
H	-0.79852900	3.13864000	-1.98045800
C	0.14871200	3.14695200	1.36225000
H	-0.39938900	2.74669300	2.22024400
H	0.23556300	4.22961400	1.49916200
P	2.72707400	-0.91861800	1.71297000
P	3.55787900	-0.70653200	-1.53837700
C	3.25931900	-2.63186000	1.25704400
H	2.41282500	-3.10190000	0.74784300
H	3.49132600	-3.18359000	2.17284100
C	4.17015700	-2.40867300	-1.11613000
H	5.08161600	-2.60026200	-1.69116300
C	3.38592400	-3.09821700	-1.43945300
H	3.82848300	-0.58111700	3.15335600
H	4.83108600	-0.33731300	2.79779200
H	3.44610600	0.25117800	3.74318600
H	3.88797900	-1.46205500	3.79908200
H	2.90002000	3.82791000	0.81254000
C	2.73168100	4.03950500	-0.24544900
H	2.69283600	4.72803500	1.39995900
H	3.95213200	3.55711000	0.93048300
C	2.16723400	2.49337900	3.18111700
H	3.23439600	2.36746500	3.37567600
H	1.85724800	3.46820100	3.56983300
H	1.61559400	1.71166100	3.70905200
C	3.00408100	-1.11845100	-3.24731500
H	3.80721000	-1.64128700	-3.77551500
H	-2.13678000	-1.77789900	-3.16359900
H	2.74362500	-0.22682700	-3.81954700
C	5.12982200	0.20931200	-1.84588700
H	4.90277300	1.20023800	-2.24773900
H	5.66002500	0.33482300	-0.89957400
H	5.77403700	-0.32565100	-2.55031300
C	-0.02534800	0.49441700	-2.48618700
H	0.53120000	-0.23889400	-3.06935800
H	-0.54478100	-0.05612100	-1.69544100
H	-0.73061200	1.01459900	-3.14213600
C	1.95072400	2.52851800	-3.12360900
H	1.21212900	2.89323300	-3.84399800
H	2.53853400	3.37382700	-2.75513900
C	2.63370100	1.84836400	-3.63478600
H	1.10266000	-1.30438100	2.48051900
H	0.42812400	-1.61988100	1.67659100
H	1.19507200	-2.09347100	3.23364600
H	0.69148600	-0.40557900	2.94803200
H	-0.56020500	-3.59813600	-1.39074500
H	-2.62954800	-0.45389000	-0.42671700

C	-0.09787300	-2.69630300	-0.92197000
O	-0.88003900	-1.94084400	-0.28533400
O	1.13330700	-2.55428200	-1.09082700
C	-0.69381100	2.89013900	0.13082900
C	4.45556600	-2.69612000	0.33538800
P	-3.99143500	-0.56442500	-0.11055000
N	-3.76379500	-0.84186800	1.53818600
N	-4.43181200	-1.82073500	-1.16348000
N	-4.53753000	0.93015100	-0.69293600
C	-3.85727900	-3.14100900	-0.89176500
H	-2.83569200	-3.00879500	-0.51905700
C	-3.77539500	1.56748600	-1.76277300
C	-3.73385700	2.64762600	-1.59077500
H	-2.43203000	-0.63462600	2.11152500
H	-1.66602500	-0.73099900	1.34140300
C	-5.92715300	1.35067700	-0.63679400
H	-6.44080500	1.12929500	-1.58573800
H	-5.97217900	2.43609700	-0.49522000
C	-6.61592500	0.65260700	0.52501100
H	-6.29238900	1.10833000	1.46385400
H	-7.70646800	0.74420800	0.45917000
C	-5.79085100	-1.75927600	-1.66694200
H	-5.87615200	-0.92284600	-2.36879800
C	-6.00544000	-2.67065100	-2.22983100
H	-6.79940200	-1.59185400	-0.51125700
C	-7.73850500	-1.15589400	-0.86705200
H	-7.03250600	-2.56491000	-0.07438700
C	-4.83503400	-0.84255200	2.51664000
H	-4.97022400	0.16214800	2.94697300
H	-4.56607300	-1.50751700	3.34400300
C	-6.10308900	-1.35229000	1.85570400
H	-6.02274900	-2.43374300	1.72731300
H	-6.99402800	-1.13857500	2.45874100
N	-6.18310100	-0.74722500	0.52308300
H	-4.44354200	-3.71209800	-0.15725600
H	-3.81247100	-3.70676300	-1.82629500
H	-2.24573300	-1.41134600	2.86029900
H	-2.35939000	0.34993200	2.59209900
H	-2.75357800	1.18807700	-1.77627500
H	-4.23264100	1.37746100	-2.74360500
F	5.00297600	-3.95389500	0.41994300
F	5.45036000	-1.84103100	0.79344500
F	-1.22953300	1.62227900	0.21292100
F	-1.78495600	3.73759600	0.18123000

C7'

E= -1278.03402868 a.u.

P	-1.50404000	1.59996500	0.61000600
P	-1.59315600	-1.35187900	-1.02497400
C	-3.25916700	1.02562400	0.74846800
H	-3.27195600	0.27857700	1.54912900
C	-3.89374200	1.87449100	1.02066800
H	-3.40469000	-1.05034200	-0.74226800
H	-3.96272200	-1.42847300	-1.60485000
C	-3.66722800	-1.62745300	0.14798300
P	1.68608600	-1.59840200	-0.05077500
P	1.71072800	1.67163000	-0.41164000
C	3.24766200	-0.95292300	0.72651600
H	3.90963800	-1.77744900	1.00758900
H	2.91310800	-0.46384500	1.64653800
C	3.33973900	0.99653900	-1.00394700
H	4.03145900	1.80705200	-1.25345600
H	3.10767100	0.46012100	-1.92903600
C	1.29973700	-2.90102400	1.17883600
H	0.98557100	-2.40507000	2.10358100
H	0.46465800	-3.50973300	0.83227600
H	2.17099100	-3.54130800	1.34701500
C	-1.61375000	-3.17978000	-0.80603800
H	-1.75794300	-3.38337000	0.25788100
H	-2.43750600	-3.61834600	-1.37803000
H	-0.67669100	-3.61937600	-1.15643400
C	-1.47978300	-1.20518000	-2.86582500
H	-0.47298400	-1.48364800	-3.18880500
H	-2.21039000	-1.84805800	-3.36794100
H	-1.65829300	-0.16631200	-3.15145900
C	1.38872100	2.79236900	-1.84264800
H	0.45036600	3.32736000	-1.69668500
H	2.20073700	3.51491700	-1.97227900
H	1.28997800	2.18844200	-2.74811400
C	2.23529100	2.85668700	0.90082900
H	1.40580900	3.52990300	1.13468200
H	2.49261900	2.30690900	1.80905600
H	3.09695200	3.45050800	0.58225300
C	-1.72174500	3.30120300	-0.07687000
H	-0.79793800	3.87155200	0.05356300
H	-1.96751100	3.25251400	-1.13965400
H	-2.52428000	3.82587700	0.45028100
C	-1.13652000	1.93597300	2.37539900
H	-1.94007900	2.51628300	2.84010800
H	-1.00592700	0.97106900	2.87745100
H	-0.19719000	2.48809100	2.45417700
C	2.30685200	-2.55427000	-1.50301400
H	2.69703100	-1.87957000	-2.26839800

C8'

E= -1278.03218831 a.u.

P	1.70498700	-0.92052900	1.49118400
P	1.04901100	0.00598000	-1.68067400
C	3.42459300	-0.58040100	0.85663300
H	3.65153500	0.45911000	1.11310200
H	4.14337500	-1.22569900	1.37264600
C	2.90610100	0.18544900	-1.56960000
H	3.34043300	0.04978900	-2.56580200
H	3.11942200	1.21066000	-1.25129600
P	-1.65957600	1.67578900	0.20069900
P	-1.73489600	-1.78866600	0.06162000
C	-3.33811100	1.01548700	0.68866500
H	-4.05583300	1.83289700	0.81405600
C	-3.18362800	0.55285200	1.66723400
H	-3.20682200	-1.11934200	-0.87701500
H	-3.92095400	-1.90726000	-1.13978500
H	-2.79307700	-0.71674700	-1.80703500
C	-1.59093600	3.07273700	1.40923000
H	-1.47071200	2.65967100	2.41336800
H	-0.72059500	3.69939100	1.20185100
C	-2.49190900	3.69360300	1.36518700
H	0.76149300	1.34622200	-2.92362500
H	0.93050200	2.32700100	-2.47352500
H	1.42342900	1.23473200	-3.78820200
H	-0.27525900	1.30089900	-3.26554900
C	0.90787000	-1.45580600	-2.80620700
H	-0.11490500	-1.49477900	-3.19355700
H	1.60266100	-1.39213800	-3.64953500
H	1.10684400	-2.37232100	-2.24857300
C	-1.49772600	-3.35026500	-0.91160900
H	-0.65297600	-3.90332700	-0.49085300
H	-2.38895200	-3.98692700	-0.88590700
H	-1.26059800	-3.11494600	-1.95159500
C	-2.53742600	-2.50269600	1.56819800
H	-1.80803100	-3.13913500	2.07812700
H	-2.81789300	-1.70295400	2.25653500
C	-3.42474100	-3.09581800	1.32518500
C	1.72389400	-2.76135800	1.65916300
H	0.81485400	-3.06347400	2.18745000
H	1.71868400	-3.21395700	0.66564400
H	2.59811300	-3.11847300	2.21312200
C	1.96144400	-0.41541800	3.24518100
H	2.83311300	-0.90959800	3.68678600
H	2.09033000	0.66831100	3.29291200
H	1.06463100	-0.68003000	3.81071500
C	-2.08154700	2.60405300	-1.34314900
H	-2.31733700	1.90711500	-2.15064000
H	-2.94560700	3.25636100	-1.18487700
H	-1.22735900	3.21420700	-1.64818200
H	1.24544400	1.71897800	1.05825800
C	-0.62152600	0.12818300	1.87121300
O	1.93174800	2.42397400	1.30848800
C	1.95527700	3.37678600	0.39096000
H	1.19558400	3.23861000	-0.40263500
O	2.71869600	4.31040300	0.39963400
Rh	-0.08927600	-0.02484700	0.36846500
C	-4.00929500	-0.00960500	-0.21173500
C	3.63848300	-0.75211900	-0.63031900
F	-5.01241600	-0.60157600	0.53635200
F	-4.67526200	0.67249800	-1.21723300
F	3.35681500	-2.06273700	-0.98641900
F	4.98977200	-0.60625900	-0.87745700

TS_{c1-2}

E= -1088.72437411 a.u.

Rh	0.03827400	0.16199700	-0.86674600
P	-2.03883400	1.23479200	-0.77047100
P	-0.89834900	-1.71920700	0.30731500
C	-3.06251200	0.97719600	0.75316100
H	-2.54764900	1.46457700	1.58632000
H	-4.02496200	1.48116500	0.61642000
C	-2.19513300	-1.33056300	1.58441500
H	-2.61967900	-2.26710300	1.96118200

H	-1.68638100	-0.83741400	2.41911800	H	2.59093600	0.35352600	-2.70142600
P	2.09255600	-0.87437200	-1.22869700	H	3.19441100	-1.27963900	-3.08860700
P	1.16050100	1.75172300	0.54615200	H	1.53835600	-0.79946800	-3.52265700
C	3.21657500	-1.13633300	0.23149200	H	-0.44484000	0.30129900	-2.48394500
H	4.24673700	-1.13558400	-0.13789100	H	-0.89840600	-0.30526700	-2.30203800
C	3.02515600	-2.12778800	0.65060500	C	-3.72991300	-0.66169800	-0.02353500
H	2.90997100	1.32157300	1.04105900	C	3.53446400	-0.29793400	0.76099700
H	3.18532900	1.91586800	1.91779600	F	4.84474200	-0.42869400	1.14154300
C	3.58938300	1.60821600	0.23258000	F	2.80428100	-0.38328800	1.93014200
C	2.08502200	-2.54354800	-1.99296900	F	-3.45177100	-0.75226500	-1.37255400
H	1.52736000	-3.24953300	-1.37516600	F	-5.06832200	-0.93603800	0.09313500
H	1.58936700	-2.47449000	-2.96439300				
H	3.10259000	-2.91862400	-2.13439000				
C	0.14677000	-2.82545500	1.34791900				
H	0.89962200	-3.32084600	0.73054800				
H	0.65873100	-2.24620300	2.11635000				
H	-0.46656100	-3.59981000	1.81768500				
C	-1.73409900	-2.95506600	-0.77305500	Rh	1.10514600	0.11413400	-0.33413300
H	-0.99264800	-3.37136000	-1.46024000	P	0.50182700	1.97761900	-1.53965800
H	-2.18054600	-3.76513600	-0.18896700	P	1.88483100	1.49500800	1.44660700
H	-2.51265500	-2.47422900	-1.36606600	C	-0.24001500	3.45190700	-0.64780500
C	1.49689800	3.41917900	-0.16645500	H	0.19826100	4.36514100	-1.061696500
H	2.11383900	4.02581700	0.50340000	C	-1.31055900	3.48878000	-0.86231100
H	2.00636000	3.30337800	-1.12627300	H	1.30258800	3.27757600	1.42266600
H	0.55813200	3.94406400	-0.34942800	H	1.32852300	3.67514300	2.44175800
C	0.41353900	2.17431000	2.17780200	H	2.01623900	3.86072500	0.83161300
H	-0.56330100	2.63978800	2.02146000	P	1.04986700	-1.98789900	0.72189400
H	0.27742700	1.26148000	2.76078200	C	3.25667100	-0.55523000	-1.43323400
H	1.03992700	2.87070600	2.74274400	C	2.66654400	-2.63671600	1.41127600
C	-3.14682600	0.78610300	-2.16110800	H	2.58208100	-3.72581200	1.47784700
H	-2.69091300	1.14924900	-3.08584300	H	2.77601100	-2.26318400	2.43407800
H	-3.25109100	-0.29656400	-2.22847200	C	3.95651400	-2.18371500	-0.82221700
H	-4.13516500	1.23727400	-2.04034800	H	4.98513600	-2.30120900	-1.17817000
C	-2.06579400	3.07105600	-0.85371200	C	3.37109600	-3.00543400	-1.24603500
H	-3.09173100	3.43543400	-0.95734000	H	-0.00207800	-2.41977500	2.17656200
H	-1.63165900	3.50664600	0.04907100	H	0.21417000	-1.75430500	3.01523800
H	-1.48209800	3.39670700	-1.71801400	H	-1.05421800	-2.30716200	1.90260600
C	3.15043100	0.06210700	-2.40513900	H	0.17426900	-3.45456700	2.48662500
C	3.31442700	1.07949600	-2.04426500	C	3.68864000	1.86735700	1.56807600
H	4.11544000	-0.42988300	-2.55689100	H	4.03969400	2.27464900	0.61624000
H	2.62596400	0.13043600	-3.36136600	C	3.89082100	2.59316300	2.36191700
H	0.15743500	0.78203500	-2.40209600	H	4.23767600	0.94804700	1.77142900
H	-0.29863400	-0.15802700	-2.45827600	C	1.53399100	1.02498600	3.19742000
C	3.13988800	-0.13687500	1.38020700	H	1.96318800	0.03647600	3.38444900
C	-3.35689100	-0.45607900	1.15615000	H	1.97742300	1.73595900	3.90085500
F	-4.03545900	-1.07616800	0.12760800	H	0.45745800	0.98047200	3.37009800
F	-4.24217800	-0.40637700	2.20317400	C	3.00789000	-1.01948400	-3.20547300
F	2.15377200	-0.53459900	2.26439200	H	3.90057200	-1.47457400	-3.64602800
F	4.31219400	-0.23944500	2.08262000	H	2.16703600	-1.71383500	-3.27839900
Rh	-0.05861300	0.07998700	-0.43933200	H	2.75094400	-0.12594700	-3.78140000
P	-1.89434200	1.53229200	-0.13308900	C	4.81700900	0.43448000	-1.56584600
P	-1.14374900	-1.44321100	0.96445500	H	4.59068500	1.42009800	-1.98180200
C	-3.50206400	0.77029000	0.42683500	H	5.25493300	0.56577600	-0.57473800
H	-3.55954200	0.80829100	1.51916800	H	5.55023900	-0.05834300	-2.21269800
H	-4.32088000	1.38312800	0.03742700	C	-0.72386900	1.80246700	-2.90216900
C	-2.96903600	-1.74654900	0.71633100	H	-0.34940300	1.06692400	-3.61907800
H	-3.09089900	-2.67119400	0.14474000	H	-1.67253000	1.44201700	-2.49268200
H	-3.44843100	-1.89410100	1.68951800	H	-0.89065500	2.75413500	-3.41612100
P	1.66403200	-1.32156000	-1.15928100	C	1.89478600	2.81093500	-2.42369700
P	1.57692000	1.68579800	0.09537200	H	1.56162200	3.68611400	-2.98999400
C	3.18956300	-1.49188000	-0.11475600	H	2.65445200	3.11906700	-1.69969100
C	4.04160500	-1.69082500	-0.77197200	C	2.35419400	2.09820400	-3.11292300
H	3.07256800	-2.35805900	0.54255300	H	0.56679300	-3.37516700	-0.39630500
C	3.34751300	1.08291600	0.15580300	H	1.07213400	-3.29033400	-1.36003700
H	3.92954400	1.79068800	0.75344700	H	0.77495900	-4.35246300	0.04963300
C	3.77589100	1.08537600	-0.85089400	H	-0.50701700	-3.27907300	-0.56742700
C	1.34322700	-3.07966000	-1.59221100	H	0.44856000	-0.70133700	-1.52558600
H	1.20129200	-3.67970300	-0.69348900	H	-0.89802700	0.15261800	-0.06755400
H	0.43886300	-3.13982500	-2.20280000	P	-2.52981800	-0.24497300	-0.04036200
C	2.18454600	-3.49053300	-2.15730000	N	-3.58830900	0.78677100	-0.89984400
H	-1.08173700	-0.79381600	2.69242700	N	-3.02584000	-0.46529300	1.57865000
H	-1.49501400	0.21632400	2.73863700	N	-2.52359100	-1.75479000	-0.81940700
H	-1.62790800	-1.43763900	3.38868500	C	-2.10045700	0.08778700	2.57544400
H	-0.03360800	-0.73903200	2.99759800	H	-1.09665300	0.15206100	2.15418900
C	-0.60537200	-3.18051700	1.26138200	C	-2.10167800	-1.77926900	-2.21743200
H	0.44973400	-3.19462400	1.54766300	C	-2.94902100	-1.80400300	-2.91498600
H	-1.19029300	-3.62684000	2.07104100	C	-3.71350700	2.15003200	-0.39040100
H	-0.74278600	-3.77959600	0.35905500	H	-2.91911100	2.36310800	0.32886900
C	1.81685400	3.20376600	-0.92645200	C	-3.35187500	-2.87442000	-0.38804200
C	2.63059300	3.82889800	-0.54652000	H	-3.19501500	-3.02812400	0.68496900
H	2.02596700	2.92695700	-1.96294700	H	-2.99256500	-3.77576100	-0.89814500
C	0.89320400	3.78946800	-0.91798800	C	-4.84566500	-2.65175400	-0.65451200
C	1.44158200	2.40076500	1.79034300	H	-5.02678500	-2.58390100	-1.73229600
H	0.56170200	3.03815900	1.86282300	H	-5.41636800	-3.52131300	-0.29313300
H	1.35511500	1.59425700	2.51927600	C	-4.42611500	-0.32993100	2.00577300
H	2.32393900	3.00290900	2.02588300	H	-4.44280300	-0.43480200	3.09583200
C	-2.36490800	2.29724300	-1.73817900	H	-4.79368800	0.68382700	1.78568000
H	-1.49887500	2.81919800	-2.15282900	C	-5.36768600	-1.36776500	1.40113500
H	-2.67141600	1.51934000	-2.43898000	H	-5.11790000	-2.35484600	1.80275900
H	-3.18515300	3.00803700	-1.60474600	H	-6.39143800	-1.14155800	1.73813300
C	-1.89035900	3.00027000	0.97897400	C	-4.72699900	0.30930600	-1.68167500
C	-2.87196700	3.48247200	0.95969400	H	-4.37344700	-0.39936200	-2.43466100
H	-1.66060400	2.71032500	2.00683300	H	-5.13666500	1.16377500	-2.23176900
H	-1.14771400	3.72620900	0.63941100	C	-5.82062000	-0.35745800	-0.83477200
C	2.32257900	-0.70238900	-2.76739800	H	-6.27021200	0.38219400	-0.16339000
C				H	-6.62433000	-0.70733400	-1.50149600

TS_{C3-4}
E= -1669.70688968 a.u.

N	-5.27426800	-1.42324400	-0.03465400
H	-2.40178100	1.09384300	2.89230600
H	-2.07310600	-0.56515700	3.45427000
H	-4.67210200	2.30988700	0.11918300
H	-3.64222200	2.87411200	-1.21122100
H	-1.49037000	-0.90408000	-2.44079500
H	-1.48454500	-2.66381300	-2.40577900
C	-0.07763500	3.52218300	0.85830000
C	3.96993900	-2.32509200	0.68757700
F	4.50515400	-1.16657700	1.22936400
F	4.86773200	-3.31278600	1.02030600
F	-0.96892500	2.64959800	1.46157800
F	-0.49695700	4.77270700	1.25491600

TS_{C6-7}

E= -1276.82273222 a.u.

Rh	0.06853100	0.24144100	-0.36530500
P	-1.88912500	-0.18714000	-1.56609900
P	-0.78825400	-0.15801800	1.86772400
C	-3.43285500	-0.01859800	-0.52698000
H	-3.58877100	1.05110300	-0.36217800
H	-4.28950900	-0.41003300	-1.08590200
C	-2.65293400	-0.04068500	1.95997200
H	-3.01090800	-0.47384000	2.90064800
H	-2.90326100	1.02441400	1.95406500
P	1.20101200	-1.67149800	-0.86648500
P	2.05992100	1.39409200	-0.33540600
C	2.75110500	-2.01238000	0.12962300
H	3.43433000	-2.60329000	-0.48880200
H	2.46845100	-2.62975900	0.98754000
C	3.64287300	0.40255200	-0.20743300
H	4.43923300	1.03763400	0.19258800
H	3.94944900	0.08245400	-1.20841700
C	0.41120500	-3.32887700	-0.67025400
H	-0.06242900	-3.39802700	0.31075700
H	-0.35772200	-3.45961600	-1.43300600
H	1.15043200	-4.12936400	-0.77703600
C	-0.38602800	1.04898900	3.21060400
H	-0.57106600	2.06482800	2.85212900
H	-0.97259800	0.87279600	4.11916200
C	0.67646400	0.95522800	3.45151700
H	-0.49652300	-1.74359000	2.77967800
H	0.58171700	-1.90068900	2.87612200
H	-0.94470400	-1.72859600	3.77935200
H	-0.93005400	-2.57400600	2.21805400
C	2.46175700	2.44442200	-1.79713900
H	3.43082100	2.94471400	-1.69238600
H	2.45431700	1.82985600	-2.70088600
H	1.67202300	3.19538300	-1.88275400
C	2.30566100	2.60359600	1.03428000
H	1.50233000	3.34152600	0.98755700
H	2.26084000	2.08070300	1.99085000
H	3.26877000	3.11646100	0.94332400
C	-2.26753500	-1.77056800	-2.44697700
H	-1.47676800	-1.99979800	-3.16701100
H	-2.34353700	-2.58236800	-1.72140100
C	-3.21862500	-1.69397700	-2.98382500
C	-2.31879900	1.02525300	-2.89236400
H	-3.31125000	0.83537500	-3.31600100
H	-2.28740300	2.03549300	-2.47957500
H	-1.56530200	0.95853200	-3.68122500
C	1.85355800	-1.83551000	-2.59087600
H	2.52535700	-1.00325500	-2.81431600
H	2.37957800	-2.78340200	-2.74853900
H	1.01153200	-1.76902700	-3.28455700
C	-0.60199100	1.78672600	-0.29496000
H	-1.21880000	3.14641800	-0.10072700
O	-2.31025100	2.93879700	0.34843900
O	-0.39123100	3.92697700	-0.46874400
C	-3.42429000	-0.69901500	0.83124100
C	3.52810700	-0.82414300	0.67330600
F	4.80441500	-1.26839400	0.97008400
F	2.99378400	-0.45816600	1.89336600
F	-4.74202700	-0.80157300	1.24122500
F	-3.00440600	-2.01787500	0.68960700

TS_{C8-9}

E= -1276.83262132 a.u.

Rh	0.08756300	0.05590100	-0.34964500
P	1.79327500	1.64660200	-0.12495000
P	1.49589900	-1.88710300	-0.02994300
C	3.47962800	0.99930900	-0.61159000
H	3.48703200	0.92576900	-1.70332600
H	4.23328500	1.73915900	-0.32213200
C	3.25425500	-1.58420700	-0.58769000
H	3.88107000	-2.43917800	-0.31140600
C	3.23735700	-1.51698000	-1.67970700
P	-1.11201600	0.13999700	1.69472500
P	-1.79644400	-0.64939600	-1.49259800
C	-2.92408800	0.57904400	1.55792300
H	-2.97149100	1.63977700	1.29937600

H	-3.39441500	0.44643000	2.53800600
C	-3.45960500	-0.02479200	-0.91693400
H	-4.25518000	-0.53494600	-1.47094700
H	-3.51297100	1.04039100	-1.15949400
C	-1.20751300	-1.39908000	2.71580500
H	-1.48676900	-2.24870300	2.08965000
H	-0.22320800	-1.58942300	3.15028500
H	-1.93900300	-1.29985500	3.52378300
C	1.20429900	-3.38763100	-1.07959500
H	1.07435500	-3.08322900	-2.12169500
H	2.03305000	-4.10132500	-1.01264600
H	0.28811900	-3.88352000	-0.74949100
C	1.81737500	-2.73834400	1.58625600
H	0.90084900	-3.23372900	1.91663600
H	2.60946600	-3.48951400	1.49612600
H	2.11194100	-2.00380100	2.33856100
C	-1.91837400	-0.22896400	-3.28159800
C	-2.85887100	-0.58317300	-3.71651300
H	-1.82321700	0.84953300	-3.40796800
H	-1.07911500	-0.70836500	-3.79254100
C	-2.13894000	-2.46658200	-1.59177800
H	-1.35572200	-2.93119500	-2.19538600
H	-2.12646900	-2.91266100	-0.59592000
C	-3.10872200	-2.66440800	-2.05915600
C	2.18980100	2.43944600	1.49508000
H	1.33725400	3.04918000	1.80224200
H	2.37198700	1.67218500	2.24955900
H	3.07490300	3.07887900	1.41612500
C	1.85365300	3.14571900	-1.21374200
H	2.84185000	3.61722200	-1.17732100
H	1.61437700	2.86303700	-2.24079600
H	1.11105500	3.87226000	-0.87596000
C	-0.68359400	1.35352400	3.01777600
H	-0.72465600	2.36163500	2.60221300
H	-1.37957600	1.27731800	3.85931900
H	0.32942700	1.15573400	3.37549100
H	0.71441600	0.09546500	-1.81904700
C	-1.15416200	2.56485000	-0.85864900
O	-1.30152700	3.00851100	0.23810200
O	-1.23748400	2.62541300	-2.04020100
C	3.92464900	-0.33564100	-0.05594300
C	-3.76033600	-0.18966800	0.55807800
F	-5.07889400	0.18036100	0.75470100
F	-3.72620000	-1.53853800	0.87826400
F	3.83443300	-0.31627900	1.32633900
F	5.28025800	-0.45446500	-0.31530600

TS_{C9-7}

E= -1276.81588493 a.u.

Rh	-0.05558700	-0.18976100	-0.57251000
P	-2.10504100	-1.33259600	-0.57703900
P	-1.12132500	1.93271300	-0.24003500
C	-3.68571500	-0.36836800	-0.32657800
H	-4.00141500	0.03548700	-1.29285400
H	-4.45948600	-1.06625300	0.00691800
C	-2.95747800	2.02877100	0.14369200
H	-3.12115000	2.82789000	0.87341700
H	-3.47988900	2.31228200	-0.77426300
P	0.82718500	-0.77977200	1.64577700
P	1.96278000	0.75606000	-1.32844700
C	2.69047700	-0.90767000	1.69943900
H	2.95344800	-1.84413500	1.19873700
H	3.01306400	-0.97116700	2.74421900
C	3.52345300	0.21587100	-0.47136200
C	0.51850900	0.22419500	3.17210200
H	0.95874100	1.21614300	3.05632300
H	-0.56028500	0.32936300	3.31732800
C	0.95364000	-0.25339700	4.05645200
H	-1.14922000	3.23451800	-1.56421300
H	-1.49031300	2.78708400	-2.50124000
H	-1.81694600	4.05756400	-1.28750800
H	-0.15248500	3.64517900	-1.71855400
C	-0.50374800	2.93474500	1.19127200
H	0.58788800	2.95495000	1.20365900
H	-0.88754600	3.95989500	1.15883200
H	-0.83993900	2.45849200	2.11482900
C	2.39302900	0.33098300	-3.06543100
H	3.35922400	0.76401500	-3.34433600
H	2.42929800	-0.75522600	-3.15465900
C	1.61274900	0.72150700	-3.72290900
C	2.25157300	2.58372000	-1.39553100
H	1.66742800	3.00895200	-2.21364200
H	1.98581700	3.07668300	-0.45986100
H	3.30822900	2.77934100	-1.59920300
C	-2.42268000	-2.70090800	0.61416400
H	-1.60346600	-3.41670700	0.56008300
H	-2.50510400	-2.28809700	1.62189700
H	-3.36193900	-3.20225000	0.35979000
C	-2.52992700	-2.11132400	-2.18854200
H	-3.52111100	-2.57483500	-2.14900500
H	-2.50582500	-1.34762800	-2.96899700
H	-1.77431800	-2.86780800	-2.40286300
C	0.48511600	-2.46582200	2.32647300

H	0.58915200	-3.21139100	1.53459000
H	1.17260800	-2.70042500	3.14603700
H	-0.53618500	-2.50385300	2.71058800
H	0.14498600	-1.06944400	-1.94342200
C	0.90817400	-2.35203100	-1.22227900
O	0.09835600	-3.24968000	-1.05916900
O	2.11551100	-2.25604000	-1.38163700
C	-3.62224900	0.77580900	0.65662500
C	3.47852400	0.20204600	1.03915200
F	-4.91501600	1.10652200	1.01929300
F	-3.01964200	0.36655900	1.83211800
H	3.73492500	-0.79615900	-0.81972800
H	4.33780600	0.87953900	-0.77758000
F	3.02932700	1.43661300	1.49991000
F	4.78064900	0.11765700	1.49296900

TS_{C10-11}

E= -1277.21999613 a.u.

Rh	-0.14968000	0.07725400	-0.33808700
P	-2.15888500	1.34771800	-0.05500200
P	-1.07362800	-1.45143100	1.01956000
C	-3.63678300	0.35792700	0.49585100
H	-3.66852400	0.29194600	1.58672900
H	-4.53645000	0.89478100	0.18035500
C	-2.70176900	-2.07899700	0.41408800
H	-2.51410500	-2.78622900	-0.39801300
C	-3.16370600	-2.63139600	1.23790600
P	1.54968500	-1.17702200	-1.47797200
P	1.47130200	1.12669900	1.30813600
C	3.31911300	-0.78363500	-1.12136900
H	3.59014600	0.07910100	-1.73302900
H	3.92652900	-1.64125600	-1.42704600
C	3.25056700	0.89663400	0.84045400
H	3.86054300	1.10741100	1.72410100
H	3.47105500	1.63925400	0.07074300
C	1.53766400	-3.01539600	-1.44816100
H	1.86566300	-3.39490100	-0.47998800
H	0.53715500	-3.38969400	-1.67838600
H	2.22684500	-3.38448100	-2.21307400
C	-1.44171100	-0.85134000	2.72182400
H	-1.64478300	0.21878500	2.74936400
H	-2.30185800	-1.39372400	3.12377600
O	-0.58254800	-1.05420200	3.36130100
C	-0.17416600	-3.00156700	1.37610000
H	0.85852400	-2.77180800	1.64861200
H	-0.66492900	-3.50697400	2.21302700
C	-0.18151600	-3.66561600	0.51257000
H	1.41569600	2.95160400	1.50719300
C	2.30566500	3.29009200	2.04589600
H	1.36141400	3.43132100	0.52745600
H	0.53351900	3.22833800	2.08916700
C	1.51474300	0.58982300	3.07552800
H	0.59231500	0.87694600	3.58404000
H	1.66244500	-0.48938700	3.15591000
H	2.34629900	1.08581200	3.58418700
C	-2.71494700	2.07102900	-1.63986100
H	-1.97410200	2.81452200	-1.94607000
H	-2.81039300	1.28999000	-2.39431300
C	-3.68267100	2.55832800	-1.49138200
H	-2.15166200	2.77544900	1.08638100
C	-3.13666400	3.24968900	1.11237200
H	-1.86726100	2.47977200	2.09902400
H	-1.41988300	3.48735400	0.69400900
C	1.41979900	-0.84088600	-3.27487900
H	1.51245600	0.23177600	-3.44519800
H	2.22198800	-1.36384300	-3.80404100
H	0.45465300	-1.19570400	-3.64311800
H	-0.11839500	1.45464700	-2.16324600
H	-1.01999300	-0.60362300	-1.44682500
C	0.61431800	2.23093500	-1.71602900
O	1.78045500	1.78000400	-1.57513200
O	0.12312500	3.32322200	-1.42419100
C	3.64340100	-0.47250700	0.32626500
C	-3.70978500	-1.04372700	-0.09012600
F	4.99233500	-0.61553100	0.48928000
F	3.07257200	-1.45677100	1.13812300
F	-3.60095500	-0.95700800	-1.45582300
F	-4.96022600	-1.54188600	0.15411800

TS_{C13-14}

E= -1858.22695066 a.u.

Rh	-0.71806400	-0.06087900	0.11127900
P	-0.74184300	1.91204700	1.40524100
P	-1.36907400	1.19186700	-1.70102700
C	-2.28677100	2.91119800	1.14196500
H	-3.11290000	2.29913300	1.51201800
C	-2.23751500	3.81577500	1.75675800
H	-2.83019500	2.27390300	-1.32564700
H	-3.15140400	2.78009400	-2.24161700
H	-3.63918600	1.61196900	-1.00423900
F	-0.98453400	-2.20021800	-0.91606200

P	-3.29353900	-0.85557700	1.42892400
C	-2.64179100	-2.64636000	-1.65923700
H	-2.68742100	-3.74025900	-1.67513200
H	-2.65930600	-2.31877500	-2.70187000
C	-4.07812000	-2.28118000	0.49066600
H	-5.14750200	-2.32223100	0.71852100
H	-3.64321000	-3.22778700	0.82117800
C	0.07949000	-2.75349400	-2.31773100
H	-0.09819600	-2.13877500	-3.20282300
H	1.13380000	-2.66107600	-2.04853000
H	-0.13067600	-3.79727500	-2.56836000
C	-1.96684200	0.40564700	-3.25539300
H	-2.89931800	-0.12790700	-3.07754600
H	-2.13817800	1.17329000	-4.01507600
H	-1.21204300	-0.28850600	-3.63235300
C	-0.16182900	2.37775400	-2.42334900
H	0.63734400	1.81915100	-2.91495700
H	-0.65578900	3.01364400	-3.16265600
C	0.26716700	3.01763200	-1.65527400
H	-2.99304200	-1.67610300	3.05652500
H	-3.79465100	-2.37164400	3.32258300
H	-2.02830200	-2.18936600	3.02943500
H	-2.93441400	-0.91447900	3.83919800
C	-4.81604700	0.13437700	1.80664400
H	-4.57086700	0.92787900	2.51921400
H	-5.20602500	0.59411700	0.89462000
H	-5.60148200	-0.48487900	2.25128200
C	0.60840500	3.15159500	1.33194100
H	1.56233300	2.63456800	1.47236200
H	0.61731200	3.65185400	0.36289500
H	0.47542700	3.90763900	2.11097400
C	-0.90738800	1.64017100	3.21720400
H	-1.25487400	2.55831400	3.69917700
H	-1.61279600	0.83183800	3.41129100
H	0.05320600	1.35976500	3.65044200
C	-0.76674700	-3.57320600	0.28740900
H	-1.46911600	-3.46094000	1.11291900
H	-0.91970400	-4.53606200	-0.20857900
H	0.22383000	-3.52642600	0.73453900
H	1.33232400	-0.00450900	2.53146300
H	0.93374700	0.08077900	-0.31163300
C	0.84932100	-1.00189800	2.61420400
O	1.23549100	-1.79187800	3.46339100
O	-0.10223100	-1.22607500	1.76976300
P	2.79312800	-0.01464900	-0.26808200
N	3.39635300	-0.52358700	-1.80540600
N	3.13068100	-1.16099500	0.93226600
N	3.44983300	1.59429900	0.20709200
C	2.74696600	-2.52005100	0.57926300
H	1.92367700	-2.49417200	-0.13462200
C	3.16142100	2.50173500	-0.83227600
C	3.93189800	2.53185000	-1.61547300
H	2.49568600	-0.29046400	-2.92890400
H	1.46173700	-0.25981200	-2.57649100
C	4.74286500	1.76797300	0.86061300
H	4.67535300	1.51689200	1.91928300
H	4.91361200	2.84869900	0.82140800
C	5.92929900	1.03599400	0.21680700
H	6.11913300	1.45225000	-0.77752100
H	6.83239600	1.22830900	0.81923300
C	4.18047000	-1.07859200	1.93493400
H	4.04678100	-0.16706000	2.51880900
H	4.02176700	-1.89780500	2.64217900
C	5.58694900	-1.15375800	1.30075700
H	6.33868100	-0.82061700	2.03093100
H	5.82257200	-2.19573000	1.06386300
C	4.79976100	-0.47329800	-2.22467900
H	5.06814300	0.55907300	-2.50482500
H	4.90056500	-1.07248700	-3.13799700
C	5.78626300	-1.01220600	-1.19425100
H	5.60097400	-2.08135600	-1.05832400
H	6.79969700	-0.91052800	-1.61801800
N	5.65065100	-0.37059600	0.09045100
H	3.56978600	-3.08323400	0.11727900
H	2.40364800	-3.03644100	1.48164700
H	2.58236400	-1.10284300	-3.65984100
H	2.71633200	0.65650000	-3.44817200
H	2.20681800	2.27568400	-1.30873700
H	3.08322700	3.49741900	-0.38478200
C	-2.63382500	3.34401900	-0.26768100
C	-3.93444600	-2.16732500	-1.01312300
F	-4.16792200	-0.84586500	-1.37683000
F	-4.95041300	-2.87238900	-1.60958300
F	-1.67688200	4.24115800	-0.70363000
F	-3.80009700	4.06515300	-0.19646300

TS_{C7-8'}

E= -1278.00669451 a.u.

P	1.40601300	-1.64124800	0.81453500
P	1.40602600	0.98749300	-1.27509600
C	3.19370800	-1.15568700	0.75588000
H	3.32002000	-0.37685800	1.51508900
H	3.80329900	-2.02609500	1.01887400

C	3.22638700	0.77268400	-0.94542800	H	-2.68853000	-2.35319500	1.84021100
H	3.78800300	1.08279700	-1.83327700	H	-3.08834700	-3.54205400	0.57360100
H	3.47738200	1.45119900	-0.11994200	C	1.44847200	-3.30756700	0.02213200
P	-1.73478000	1.64042300	0.00483300	H	0.50889900	-3.83426000	0.20593400
P	-1.80103200	-1.61048400	-0.30387800	H	1.59911800	-3.20171700	-1.05325200
C	-3.30292900	1.12129200	0.85435700	H	2.26760400	-3.90315900	0.43544300
H	-3.95356000	1.98019300	1.04438800	C	1.27219800	-2.08132100	2.59550100
H	-2.97220600	0.71792000	1.81513100	H	2.00789800	-2.84362500	2.87063200
C	-3.47104900	-0.92859200	-0.78513800	H	1.43704000	-1.17674400	3.18443100
H	-4.18206600	-1.74388500	-0.95353100	H	0.26483200	-2.45133800	2.80082300
H	-3.32322100	-0.42570000	-1.74472700	C	-2.33916500	2.31674900	-1.60562300
C	-1.37086000	3.18552500	0.93216300	H	-2.52149800	1.51204900	-2.31984800
H	-1.20241800	2.93159700	1.98106800	H	-3.26099700	2.88942000	-1.46991200
H	-0.45568800	3.63575000	0.54158200	H	-1.57705500	2.97403700	-2.02995200
H	-2.19172900	3.90450400	0.84913000	H	0.74998300	0.86625100	2.10540300
C	1.47017800	2.82642700	-1.48284000	H	-0.16138500	0.51501900	1.92857900
H	1.73837000	3.29025500	-0.53009100	O	1.95265400	1.22798100	2.40869100
H	2.22676400	3.10274800	-2.22437400	C	2.16592900	2.47387900	2.15190200
H	0.50551200	3.21358800	-1.81825300	H	1.32449400	3.15366100	2.40950000
C	1.26670400	0.46512400	-3.04436900	O	3.17853100	2.94472900	1.64266800
H	0.26364300	0.71728900	-3.40138500	Rh	-0.15617300	-0.03136800	0.18287900
H	2.01178200	0.95562700	-3.68015400	C	-4.14008000	0.06085300	0.15284600
H	1.39359800	-0.61717600	-3.11099900	C	3.68939800	-0.61152100	-0.56447200
C	-1.58126900	-2.67533200	-1.80360900	F	-4.82213700	-0.64631200	1.12271400
H	-0.67304000	-3.27106800	-1.70501800	F	-5.12380000	0.70551100	-0.57788800
H	-2.43275200	-3.34588500	-1.96254800	F	3.37290100	-1.50512500	-1.58546200
H	-1.45796400	-2.02581600	-2.67432300	F	5.06661600	-0.60529800	-0.52746100
C	-2.31231000	-2.86983300	0.95390700				
H	-1.44496100	-3.46324100	1.25507600				