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Supporting Information
Carbon-Hydrogen Activation of Cycloalkanes by
Cyclopentadienylcarbonylrhodium – A Lifetime Enigma

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Energy Scaling Procedure for BMK Free Energies

$\Delta E_e(\text{BMK})$ and $\Delta E_e(\text{CCSD(T)//BMK})$ were calculated for each transition state,

$$E_e^{TS} - E_e^{\sigma\text{-complex}}$$

A ratio of $\Delta E_e(\text{BMK})$ and $\Delta E_e(\text{CCSD(T)//BMK})$ was calculated by

$$\frac{\Delta E_e(\text{BMK})}{\Delta E_e(\text{CCSD(T)//BMK})}$$

which yielded a scaling factor for that specific species. As shown below, the cyclopentane data yielded 10 different scaling factors, each specific to one of the ten optimized activations that were calculated. The 10 scaling factors were averaged along with the 12 cyclohexane species, and the resultant scaling factor was calculated to be 0.68 for the CpRh(CO) reactions with all four cycloalkanes.

Calculated Scaling Factors	
Cyclopentane	Cyclohexane
0.693	0.686
0.691	0.669
0.688	0.668
0.691	0.687
0.689	0.687
0.690	0.670
0.685	0.667
0.690	0.686
0.689	0.685
0.690	0.666
	0.668
	0.684

The same method was used for the Cp*Rh(CO) transition state species, the CpRh(CO) migration barriers, and the Cp*Rh(CO) migration barriers, where the scaling factors were calculated to be 0.73, 1.24 and 1.24, respectively.

S-1. Unscaled activation energies (kcal/mol) for the CpRh(CO) reactions*

		CpRh(CO) - BMK Energies					
		ΔG σ -complexes	ΔE	ΔH	ΔS (cal)	ΔG	ΔG^a
Cyclopentane		N/A	10.19	7.23	-5.04	8.73	
Cyclohexane	C-H_{ax}	0.00	10.88	8.20	-6.89	10.25	10.25
	C-H_{eq}	0.11	10.17	7.66	-6.49	9.59	9.70
TS - σ-com^b	C-H_{eq} - C-H_{ax}		10.27	7.80	-6.37	9.70	
Cycloheptane	C2-H4	0.20	10.94	8.10	-6.75	10.11	10.31
	C3-H5	0.43	11.11	8.43	-6.80	10.46	10.89
	C4-H7	0.31	10.95	8.57	-5.88	10.32	10.63
	C1-H1	0.00	10.69	8.26	-7.70	10.56	10.56
	C2-H3	0.14	10.82	8.18	-6.84	10.22	10.36
	C3-H6	0.35	11.16	8.86	-6.07	10.67	11.02
	C4-H8	0.24	11.54	8.86	-7.10	10.97	11.21
TS - σ-com^b	C1-H1 - C1-H2		10.69	8.26	-7.70	10.56	
	C2-H4 - C2-H3		10.68	8.13	-6.85	10.17	
	C3-H5 - C3-H6		10.53	8.02	-8.45	10.54	
	C4-H7 - C4-H8		11.23	8.77	-5.45	10.39	
Cyclooctane	C1-H1	1.33	16.54	13.71	-3.16	14.65	15.98
	C1-H2	0.28	11.69	9.24	-6.41	11.15	11.43
	C2-H3	0.75	11.32	8.52	-5.75	10.24	10.99
	C2-H4	0.39	10.43	7.95	-6.57	9.91	10.30
	C3-H6	0.08	12.83	10.64	-6.29	12.52	12.60
	C3-H5	0.07	11.33	8.49	-3.97	9.67	9.74
	C4-H7	0.16	12.82	10.40	-6.17	12.24	12.40
	C4-H8	0.22	11.62	9.01	-7.12	11.13	11.35
	C5-H9	0.00	11.47	8.97	-6.50	10.91	10.91
	C5-H10	0.62	11.65	8.72	-4.71	10.12	10.74
TS - σ-com^b	C1-H2 - C1-H2		11.69	9.24	-6.41	11.15	
	C2-H4 - C2-H4		10.43	7.95	-6.57	9.91	
	C3-H5 - C3-H5		11.33	8.49	-3.97	9.67	
	C4-H8 - C4-H7		11.95	9.35	-6.18	11.19	
	C5-H10 - C5-H9		11.38	8.74	-6.72	10.74	

* The BMK energies reported in the manuscript are scaled with CCSD(T) energies.

^aFree energies of activation calculated for each species where the zero-relative energy is the lowest energy σ -complex of each cycloalkane.

^bActivation barriers calculated from the lowest energy σ -complex species to the lowest energy transition state of a CH₂ group.

S-2. Scaled activation energies (kcal/mol) for the CpRh(CO) reactions

CpRh(CO) - Scaled Energies

		ΔG	ΔG^a
Cyclopentane		5.94	
Cyclohexane	C-H_{ax}	6.97	6.97
	C-H_{eq}	6.52	6.60
TS - σ-com^b	C-H_{eq} - C-H_{ax}	6.60	
Cycloheptane	C2-H4	6.87	7.01
	C3-H5	7.11	7.41
	C4-H7	7.02	7.23
	C1-H1	7.18	7.18
	C2-H3	6.95	7.04
	C3-H6	7.26	7.49
	C4-H8	7.46	7.62
TS - σ-com^b	C1-H1 - C1-H2	7.18	
	C2-H4 - C2-H3	6.92	
	C3-H5 - C3-H6	7.17	
	C4-H8 - C4-H7	7.07	
Cyclooctane	C1-H1	9.96	10.87
	C1-H2	7.58	7.77
	C2-H3	6.96	7.47
	C2-H4	6.74	7.00
	C3-H6	8.51	8.57
	C3-H5	6.58	6.62
	C4-H7	8.32	8.43
	C4-H8	7.57	7.72
	C5-H9	7.42	7.42
	C5-H10	6.88	7.30
TS - σ-com^b	C1-H2 - C1-H2	7.58	
	C2-H4 - C2-H4	6.74	
	C3-H5 - C3-H5	6.58	
	C4-H8 - C4-H7	7.61	
	C5-H10 - C5-H9	7.30	

^aFree energies of activation calculated for each species where the zero-relative energy is the lowest energy σ -complex of each cycloalkane.

^bActivation barriers calculated from the lowest energy σ -complex species to the lowest energy transition state of a CH₂ group.

S-3. Unscaled activation energies (kcal/mol) for the Cp*Rh(CO) reactions*

		Cp*Rh(CO) - BMK Energies					
		ΔG σ -complexes	ΔE	ΔH	ΔS (cal)	ΔG	ΔG^{1a}
Cyclopentane		N/A	9.6	6.82	-5.45	8.44	
Cyclohexane	C-H_{ax}	0	11.1	8.45	-6.69	10.45	10.45
	C-H_{eq}	0.07	10.34	7.8	-5.68	9.49	9.56
TS - σ-com^b	C-H_{eq} - C-H_{ax}		10.47	7.95	-5.38	9.56	
Cycloheptane	C2-H4	0.86	11.3	8.13	-5.22	9.69	10.55
	C3-H5	1.47	11.39	8.86	-7.92	11.22	12.69
	C4-H7	0.72	11.08	8.92	-8.6	11.48	12.20
	C1-H1	0.00	10.82	8.72	-9.75	11.62	11.62
	C2-H3	0.87	10.94	8.26	-7.39	10.46	11.33
	C3-H6	0.79	11.4	9.33	-7.81	11.66	12.45
	C4-H8	1.39	11.76	9.03	-5.76	10.75	12.14
TS - σ-com^b	C1-H1 - C1-H2		10.82	8.72	-9.75	11.62	
	C2-H4 - C2-H3		11.3	8.13	-5.22	9.69	
	C3-H5 - C3-H6		12.15	9.62	-4.57	10.98	
	C4-H7 - C4-H8		11.42	8.92	-8.39	11.42	
Cyclooctane	C1-H1	1.52	16.72	14.24	-6.83	16.28	17.8
	C1-H2	1.21	11.74	8.95	-6.38	10.85	12.1
	C2-H3	1.16	11.55	8.68	-6.42	10.6	11.8
	C2-H4	0.49	10.56	7.71	-8.22	10.16	10.7
	C3-H6	0.80	13.19	10.18	-2.99	11.08	11.9
	C3-H5	0.00	11.78	9.26	-8.49	11.8	11.8
	C4-H7	1.31	13.29	10.86	-5.43	12.48	13.8
	C4-H8	1.23	12.3	9.47	-7.82	11.81	13.0
	C5-H9	2.07	11.71	8.47	-2.76	9.29	11.4
	C5-H10	1.08	11.66	8.95	-9.53	11.79	12.9
TS - σ-com^b	C1-H2 - C1-H2		11.74	8.95	-6.38	10.85	
	C2-H4 - C2-H4		10.56	7.71	-8.22	10.16	
	C3-H5 - C3-H5		11.78	9.26	-8.49	11.8	
	C4-H8 - C4-H7		12.3	9.47	-7.82	11.81	
	C5-H10 - C5-H9		11.98	8.91	-4.58	10.27	

* The BMK energies reported in the manuscript are scaled with CCSD(T) energies.

^aFree energies of activation calculated for each species where the zero-relative energy is the lowest energy σ -complex of each cycloalkane.

^bActivation barriers calculated from the lowest energy σ -complex species to the lowest energy transition state of a CH₂ group.

S-4. Scaled activation energies (kcal/mol) for the Cp*Rh(CO) reactions

Cp*Rh(CO) - Scaled Energies

		ΔG	ΔG^{1a}
Cyclopentane		6.16	
Cyclohexane	C-H_{ax}	7.63	7.63
	C-H_{eq}	6.93	6.98
TS - σ-com^b	C-H_{eq} - C-H_{ax}	6.98	
Cycloheptane	C2-H4	7.07	7.70
	C3-H5	8.19	9.26
	C4-H7	8.38	8.91
	C1-H1	8.48	8.48
	C2-H3	7.64	8.27
	C3-H6	8.51	9.09
	C4-H8	7.85	8.86
TS - σ-com^b	C1-H1 - C1-H2	8.48	
	C2-H4 - C2-H3	7.07	
	C3-H5 - C3-H6	8.02	
	C4-H8 - C4-H7	8.34	
Cyclooctane	C1-H1	11.88	12.99
	C1-H2	7.92	8.80
	C2-H3	7.74	8.58
	C2-H4	7.42	7.77
	C3-H6	8.09	8.67
	C3-H5	8.61	8.61
	C4-H7	9.11	10.07
	C4-H8	8.62	9.52
	C5-H9	6.78	8.29
	C5-H10	8.61	9.40
TS - σ-com^b	C1-H2 - C1-H2	7.92	
	C2-H4 - C2-H4	7.42	
	C3-H5 - C3-H5	8.61	
	C4-H8 - C4-H7	8.62	
	C5-H10 - C5-H9	7.50	

^aFree energies of activation calculated for each species where the zero-relative energy is the lowest energy σ-complex of each cycloalkane.

^bActivation barriers calculated from the lowest energy σ-complex species to the lowest energy transition state of a CH₂ group.

S-5. Unscaled migration barriers (kcal/mol) for the CpRh(CO) reactions*

CpRh(CO) - BMK Energies						
	σ -complex	ΔE	ΔH	ΔS (cal)	ΔG	
Cyclohexane						
1,1-migrations	C-H _{eq} - C-H _{ax}	0.89	0.19	-1.61	0.67	
	C-H _{ax} - C-H _{eq}	0.99	0.39	-1.28	0.77	
Cycloheptane						
1,1-migrations	C1-H1 - C1-H2	0.84	-0.47	-0.07	-0.45	
	C1-H2 - C1-H1	0.84	-0.47	-0.07	-0.45	
	C2-H3 - C2-H4	0.87	-0.25	-3.49	0.79	
	C2-H4 - C2-H3	0.61	-0.22	-3.59	0.85	
	C3-H5 - C3-H6	0.60	-0.47	-1.11	-0.14	
	C3-H6 - C3-H5	1.19	-0.06	0.54	-0.22	
	C4-H7 - C4-H8	1.07	0.94	-3.05	1.85	
	C4-H8 - C4-H7	0.78	0.74	-3.49	1.78	
1,2-migrations	C1-H2 - C2-H3	7.16	6.38	0.50	6.23	
	C2-H3 - C1-H2	7.15	6.40	1.07	6.08	
	C1-H1 - C2-H3	7.14	6.25	-0.84	6.50	
	C2-H3 - C1-H1	3.48	2.92	-2.42	3.64	
	C3-H5 - C2-H3	8.29	7.82	1.81	7.28	
	C2-H3 - C3-H5	4.38	4.36	-1.68	4.86	
	C2-H4 - C3-H6	8.05	7.51	-2.38	8.22	
	C3-H6 - C2-H4	4.41	4.55	-4.60	5.92	
	C3-H5 - C4-H7	7.65	6.99	0.81	6.75	
	C4-H7 - C3-H5	4.10	3.84	-1.31	4.23	
	C3-H6 - C4-H8	3.93	3.61	-2.32	4.30	
	C4-H8 - C3-H6	7.29	6.50	-0.23	6.57	
	C4-H8 - C3-H6	7.28	6.66	0.27	6.58	
	C3-H6 - C4-H8	4.01	3.72	-0.50	3.87	
	1,3-migrations	C1-H1 - C3-H5	7.04	6.17	0.20	6.11
		C3-H5 - C1-H1	6.70	5.89	0.44	5.76
C2-H4 - C4-H8		7.29	6.16	0.84	5.91	
C4-H8 - C2-H4		6.73	5.89	0.30	5.80	
1,4-migrations	C3-H5 - C2-H4	7.16	5.95	0.87	5.69	
	C2-H4 - C3-H5	7.16	5.81	-0.37	5.92	
	C3-H5 - C4-H8	7.39	6.39	0.64	6.20	
	C4-H8 - C3-H5	7.12	6.18	-0.70	6.39	
Cyclooctane						
1,1-migrations	C1-H1 - C1-H2	0.59	-0.27	-0.97	0.02	
	C1-H2 - C1-H1	0.52	-0.35	-1.28	0.03	
	C2-H3 - C2-H4	0.45	-0.07	-3.05	0.84	
	C2-H4 - C2-H3	0.77	0.27	-2.11	0.90	
	C3-H5 - C3-H6	1.03	0.32	-1.95	0.90	
	C3-H6 - C3-H5	0.76	0.34	-3.96	1.52	
C4-H7 - C4-H8	0.97	0.53	-3.15	1.47		

	C4-H8 - C4-H7	0.68	0.19	-3.29	1.17
	C5-H9 - C5-H10	0.49	-0.60	-1.61	-0.12
	C5-H10 - C5-H9	0.62	-0.75	1.41	-1.17
1,2-migrations	C1-H2 - C2-H3	7.06	6.36	-0.94	6.64
	C3-H3 - C1-H2	3.70	3.26	-1.74	3.78
	C3-H5 - C2-H4	4.30	4.20	-2.42	4.92
	C2-H4 - C3-H5	7.96	7.71	-2.05	8.32
	C2-H4 - C3-H6	3.97	3.54	0.23	3.47
	C3-H6 - C2-H4	7.55	6.98	0.34	6.88
	C2-H3 - C3-H5	7.82	7.20	0.50	7.05
	C3-H5 - C2-H3	3.94	3.61	-2.48	4.35
	C3-H5 - C4-H7	7.36	6.93	-0.27	7.01
	C4-H7 - C3-H5	3.97	3.72	-1.54	4.18
	C4-H8 - C5-H10	6.92	6.19	-0.34	6.29
	C5-H10 - C4-H8	3.22	2.87	-4.23	4.13
1,3-migrations	C3-H6 - C5-H10	6.93	6.39	0.07	6.37
	C5-H10 - C3-H6	6.88	6.16	0.87	5.90
	C2-H3 - C4-H7	6.16	5.21	-2.01	5.81
	C4-H7 - C2-H3	6.46	5.62	-2.45	6.35
1,4-migrations	C1-H1 - C4-H7	6.92	5.82	0.10	5.79
	C4-H7 - C1-H1	7.23	6.36	-2.01	6.96

*The σ -complex listed first is the zero-relative energy for each row.

S-6. Scaled migration barriers (kcal/mol) for the CpRh(CO) reactions*

CpRh(CO) - Scaled Energies

	σ -complex	ΔG
Cyclohexane		
1,1-migrations	C-H _{eq} - C-H _{ax}	0.83
	C-H _{ax} - C-H _{eq}	0.95
Cycloheptane		
1,1-migrations	C1-H1 - C1-H2	-0.56
	C1-H2 - C1-H1	-0.56
	C2-H3 - C2-H4	0.98
	C2-H4 - C2-H3	1.05
	C3-H5 - C3-H6	-0.17
	C3-H6 - C3-H5	-0.27
	C4-H7 - C4-H8	2.29
	C4-H8 - C4-H7	2.21
1,2-migrations	C1-H2 - C2-H3	7.73
	C2-H3 - C1-H2	7.54
	C1-H1 - C2-H3	8.06
	C2-H3 - C1-H1	4.51
	C3-H5 - C2-H3	9.03
	C2-H3 - C3-H5	6.03
	C2-H4 - C3-H6	10.19
	C3-H6 - C2-H4	7.34
	C3-H5 - C4-H7	8.37
	C4-H7 - C3-H5	5.25
	C3-H6 - C4-H8	5.33
	C4-H8 - C3-H6	8.15
	C4-H8 - C3-H6	8.16
	C3-H6 - C4-H8	4.80
1,3-migrations	C1-H1 - C3-H5	7.58
	C3-H5 - C1-H1	7.14
	C2-H4 - C4-H8	7.33
	C4-H8 - C2-H4	7.19
1,4-migrations	C3-H5 - C2-H4	7.06
	C2-H4 - C3-H5	7.34
	C3-H5 - C4-H8	7.69
	C4-H8 - C3-H5	7.92
Cyclooctane		
1,1-migrations	C1-H1 - C1-H2	0.02
	C1-H2 - C1-H1	0.04
	C2-H3 - C2-H4	1.04
	C2-H4 - C2-H3	1.12
	C3-H5 - C3-H6	1.12
	C3-H6 - C3-H5	1.88
	C4-H7 - C4-H8	1.82

	C4-H8 - C4-H7	1.45
	C5-H9 - C5-H10	-0.15
	C5-H10 - C5-H9	-1.45
1,2-migrations	C1-H2 - C2-H3	8.23
	C3-H3 - C1-H2	4.69
	C3-H5 - C2-H4	6.10
	C2-H4 - C3-H5	10.32
	C2-H4 - C3-H6	4.30
	C3-H6 - C2-H4	8.53
	C2-H3 - C3-H5	8.74
	C3-H5 - C2-H3	5.39
	C3-H5 - C4-H7	8.69
	C4-H7 - C3-H5	5.18
	C4-H8 - C5-H10	7.80
	C5-H10 - C4-H8	5.12
1,3-migrations	C3-H6 - C5-H10	7.90
	C5-H10 - C3-H6	7.32
	C2-H3 - C4-H7	7.20
	C4-H7 - C2-H3	7.87
1,4-migrations	C1-H1 - C4-H7	7.18
	C4-H7 - C1-H1	8.63

*The σ -complex listed first is the zero-relative energy for each row.

S-7. Unscaled migration barriers (kcal/mol) for the Cp*Rh(CO) reactions*

Cp*Rh(CO) - BMK Energies						
	σ-complex	ΔE	ΔH	ΔS (cal)	ΔG	
Cyclohexane						
1,1-migrations	C-H_{eq} - C-H_{ax}	1.15	1.33	-3.36	2.33	
	C-H_{ax} - C-H_{eq}	1.02	1.17	-3.66	2.26	
Cycloheptane						
1,1-migrations	C2-H3 - C2-H4	0.98	0.45	-3.66	1.54	
	C2-H4 - C2-H3	0.58	0.40	-3.83	1.54	
	C3-H5 - C3-H6	0.60	0.32	-5.40	1.93	
	C3-H6 - C3-H5	1.34	0.61	-2.15	1.25	
	C4-H7 - C4-H8	1.32	0.34	-0.20	0.40	
	C4-H8 - C4-H7	0.91	0.02	-1.85	0.57	
	1,2-migrations	C1-H1 - C2-H3	6.66	6.45	-3.09	7.37
		C2-H3 - C1-H1	2.92	2.61	-3.42	3.63
		C3-H5 - C2-H3	7.39	6.84	2.48	6.10
		C2-H3 - C3-H5	3.08	2.85	-3.29	3.83
C2-H4 - C3-H6		7.42	7.13	-4.33	8.42	
C3-H6 - C2-H4		3.72	3.55	-4.60	4.92	
C3-H5 - C4-H7		7.52	6.61	2.25	5.94	
C4-H7 - C3-H5		3.96	3.26	-0.44	3.39	
C3-H6 - C4-H8		3.08	2.50	-2.15	3.14	
C4-H8 - C3-H6		6.42	5.93	-0.60	6.11	
1,3-migrations	C4-H8 - C3-H6	6.37	5.90	-0.97	6.19	
	C3-H6 - C4-H8	3.28	2.90	-2.21	3.56	
	C1-H1 - C3-H5	5.88	5.43	-6.04	7.23	
	C3-H5 - C1-H1	6.45	5.58	-0.60	5.76	
	C2-H4 - C4-H8	6.33	5.26	-3.02	6.16	
	C4-H8 - C2-H4	5.63	4.99	-4.40	6.30	
	1,4-migrations	C3-H5 - C4-H8	6.95	6.07	-0.70	6.28
		C4-H8 - C3-H5	6.82	5.87	-3.42	6.89
	Cyclooctane					
	1,1-migrations	C1-H1 - C1-H2	0.66	-0.37	-0.20	-0.31
C1-H2 - C1-H1		0.54	-0.57	-1.51	-0.12	
C2-H3 - C2-H4		0.59	0.17	-6.17	2.01	
C2-H4 - C2-H3		1.08	0.72	-4.06	1.93	
C3-H5 - C3-H6		1.13	0.99	-6.04	2.79	
C3-H6 - C3-H5		0.86	0.55	-4.23	1.81	
C4-H7 - C4-H8		1.10	0.44	-3.32	1.43	
C4-H8 - C4-H7		0.83	0.01	-2.52	0.76	
C5-H9 - C5-H10		0.51	-0.21	-2.85	0.64	
C5-H10 - C5-H9		0.76	-0.06	-1.31	0.33	
1,2-migrations	C1-H2 - C2-H3	6.91	6.42	-2.72	7.23	
	C2-H3 - C1-H2	3.30	2.76	-3.02	3.66	
	C3-H5 - C2-H4	3.03	2.81	-3.36	3.81	

	C2-H4 - C3-H5	7.05	7.03	-2.11	7.66
	C2-H4 - C3-H6	2.88	2.31	-2.01	2.91
	C3-H6 - C2-H4	6.67	6.52	-3.49	7.56
	C2-H3 - C3-H5	6.65	6.02	-0.37	6.13
	C3-H5 - C2-H3	3.17	2.72	-2.11	3.35
	C3-H5 - C4-H7	6.47	5.90	-2.25	6.57
	C4-H7 - C3-H5	3.26	2.46	0.37	2.35
	C4-H8 - C5-H10	6.09	5.37	1.31	4.98
	C5-H10 - C4-H8	2.73	2.14	0.00	2.14
1,3-migrations	C3-H6 - C5-H10	6.02	5.66	-1.68	6.16
	C5-H10 - C3-H6	5.99	5.55	-2.21	6.21
	C2-H3 - C4-H7	5.51	4.47	-3.46	5.50
	C4-H7 - C2-H3	5.92	5.04	-2.48	5.78
1,4-migrations	C1-H1 - C4-H7	6.34	5.49	-2.55	6.25
	C4-H7 - C1-H1	6.66	5.85	-2.05	6.46

*The σ -complex listed first is the zero-relative energy for each row.

S-8. Scaled migration barriers (kcal/mol) for the Cp*Rh(CO) reactions*

Cp*Rh(CO) - Scaled Energies

	σ -complex	ΔG
Cyclohexane		
1,1-migrations	C-H _{eq} - C-H _{ax}	2.89
	C-H _{ax} - C-H _{eq}	2.80
Cycloheptane		
1,1-migrations	C2-H3 - C2-H4	1.91
	C2-H4 - C2-H3	1.91
	C3-H5 - C3-H6	2.39
	C3-H6 - C3-H5	1.55
	C4-H7 - C4-H8	0.50
	C4-H8 - C4-H7	0.71
1,2-migrations	C1-H1 - C2-H3	9.14
	C2-H3 - C1-H1	4.50
	C3-H5 - C2-H3	7.56
	C2-H3 - C3-H5	4.75
	C2-H4 - C3-H6	10.44
	C3-H6 - C2-H4	6.10
	C3-H5 - C4-H7	7.37
	C4-H7 - C3-H5	4.20
	C3-H6 - C4-H8	3.89
	C4-H8 - C3-H6	7.58
	C4-H8 - C3-H6	7.68
	C3-H6 - C4-H8	4.41
	C1-H1 - C3-H5	8.97
	C3-H5 - C1-H1	7.14
1,3-migrations	C2-H4 - C4-H8	7.64
	C4-H8 - C2-H4	7.81
1,4-migrations	C3-H5 - C4-H8	7.79
	C4-H8 - C3-H5	8.54
Cyclooctane		
1,1-migrations	C1-H1 - C1-H2	-0.38
	C1-H2 - C1-H1	-0.15
	C2-H3 - C2-H4	2.49
	C2-H4 - C2-H3	2.39
	C3-H5 - C3-H6	3.46
	C3-H6 - C3-H5	2.24
	C4-H7 - C4-H8	1.77
	C4-H8 - C4-H7	0.94
	C5-H9 - C5-H10	0.79
	C5-H10 - C5-H9	0.41
1,2-migrations	C1-H2 - C2-H3	8.97
	C2-H3 - C1-H2	4.54
	C3-H5 - C2-H4	4.72

	C2-H4 - C3-H5	9.50
	C2-H4 - C3-H6	3.61
	C3-H6 - C2-H4	9.37
	C2-H3 - C3-H5	7.60
	C3-H5 - C2-H3	4.15
	C3-H5 - C4-H7	8.15
	C4-H7 - C3-H5	2.91
	C4-H8 - C5-H10	6.18
	C5-H10 - C4-H8	2.65
1,3-migrations	C3-H6 - C5-H10	7.64
	C5-H10 - C3-H6	7.70
	C2-H3 - C4-H7	6.82
	C4-H7 - C2-H3	7.17
1,4-migrations	C1-H1 - C4-H7	7.75
	C4-H7 - C1-H1	8.01

*The σ -complex listed first is the zero-relative energy for each row.

CpRh(CO)

Final Energy = -416.7848101000

C	0.4762650	-1.2580000	0.8942080
C	1.4990180	-0.9226180	-0.0141310
C	1.5985530	0.5234190	-0.0960110
C	0.6442310	1.0983780	0.7661770
C	-0.1486580	-0.0039650	1.2847560
Rh	-0.5004280	-0.0978560	-0.7966550
C	-2.3573040	-0.0005070	-0.9492000
O	-3.4929960	0.0558560	-1.0778270
H	0.4848450	2.1495470	0.9552830
H	-0.9555220	0.0920800	1.9986500
H	0.1719100	-2.2489540	1.1968190
H	2.1272520	-1.6196190	-0.5524450
H	2.3123990	1.0624070	-0.7046540

Cp*Rh(CO)

Final Energy = -613.2659243940

C	0.5189330	-1.1937970	0.7745900
C	1.4989760	-0.7336360	-0.1311570
C	1.5025270	0.7327820	-0.1256040
C	0.5248350	1.1909250	0.7838780
C	-0.1968820	-0.0014250	1.2372920
Rh	-0.5530250	0.0079900	-0.8316030
C	-2.4077670	0.0130740	-1.0141850
O	-3.5467040	0.0163800	-1.1601980
C	2.4702890	-1.5775300	-0.9193920
H	3.4533460	-1.5974580	-0.4318950
H	2.1186320	-2.6082240	-1.0099170
H	2.6166260	-1.1830090	-1.9296570
C	-1.2621250	-0.0029530	2.3058450
H	-0.8047300	-0.0086970	3.3033010
H	-1.8976500	0.8832210	2.2312190
H	-1.9029340	-0.8846260	2.2234670
C	0.2560770	-2.6099230	1.2142280
H	0.5699410	-3.3280620	0.4523920
H	0.8048680	-2.8374440	2.1378410
H	-0.8066390	-2.7737750	1.4095850
C	2.4780780	1.5779760	-0.9072010
H	2.1326840	2.6116460	-0.9872950
H	3.4619010	1.5871300	-0.4209350
H	2.6205760	1.1923620	-1.9214530
C	0.2691910	2.6048990	1.2345350
H	0.8178710	2.8220070	2.1607170

H	0.5882010	3.3272890	0.4788800
H	-0.7928980	2.7730900	1.4295990

Cyclopentane

Final Energy = -196.4534173880

C	-2.9867630	-1.7477050	0.2269060
C	-1.4908750	-1.3847440	-0.0462440
C	-0.6782830	-2.6412990	0.3557040
C	-1.6618980	-3.8019270	0.1096300
C	-2.9883260	-3.2406570	0.6617050
H	-3.4284270	-1.1081810	0.9958590
H	-3.5821660	-1.6128510	-0.6809140
H	-1.1717820	-0.4949340	0.5030020
H	-1.3444370	-1.1756140	-1.1107460
H	0.2563370	-2.7368830	-0.2042990
H	-0.4250670	-2.6021860	1.4220340
H	-1.7524530	-3.9897400	-0.9677380
H	-1.3579510	-4.7367470	0.5896400
H	-3.8677620	-3.7825750	0.3028390
H	-2.9806780	-3.3131210	1.7553760

Cyclohexane

Final Energy = -235.7553811270

C	-3.4516880	-3.8483730	0.4286730
C	-1.9956750	-3.7021270	0.9132400
C	-1.2561980	-2.5979390	0.1319090
C	-2.0087140	-1.2551080	0.2164980
C	-3.4647270	-1.4013540	-0.2680690
C	-4.2042040	-2.5055420	0.5132610
H	-0.2346970	-2.4845140	0.5120270
H	-1.9965730	-3.4470890	1.9820810
H	-1.4657350	-4.6561220	0.8140110
H	-3.4505660	-4.1946780	-0.6141810
H	-3.9722260	-4.6120730	1.0173740
H	-2.0098350	-0.9088030	1.2593510
H	-3.9946670	-0.4473590	-0.1688410
H	-3.4638290	-1.6563920	-1.3369110
H	-4.2871670	-2.2058540	1.5671760
H	-5.2257050	-2.6189660	0.1331440
H	-1.1732350	-2.8976270	-0.9220050
H	-1.4881760	-0.4914080	-0.3722040

Cycloheptane

Final Energy = -275.0382451330

C	-3.4516880	-3.8483730	0.4286730
C	-1.9956750	-3.7021270	0.9132400
C	-1.2561980	-2.5979390	0.1319090
C	-2.0087140	-1.2551080	0.2164980
C	-3.4647270	-1.4013540	-0.2680690
C	-4.2042040	-2.5055420	0.5132610
H	-0.2346970	-2.4845140	0.5120270
H	-1.9965730	-3.4470890	1.9820810
H	-1.4657350	-4.6561220	0.8140110
H	-3.4505660	-4.1946780	-0.6141810
H	-3.9722260	-4.6120730	1.0173740
H	-2.0098350	-0.9088030	1.2593510
H	-3.9946670	-0.4473590	-0.1688410
H	-3.4638290	-1.6563920	-1.3369110
H	-4.2871670	-2.2058540	1.5671760
H	-5.2257050	-2.6189660	0.1331440
H	-1.1732350	-2.8976270	-0.9220050
H	-1.4881760	-0.4914080	-0.3722040

Cyclooctane

Final Energy = -314.3253531330

C	-0.0123090	1.6089380	0.6470480
C	-1.1919430	1.3287460	-0.3214120
C	1.3960210	-1.3129390	0.0760970
C	-1.9463620	-0.0000180	-0.0871860
C	-0.0122830	-1.6089260	0.6470560
C	-1.1919220	-1.3287680	-0.3214100
H	-0.1700310	1.0546750	1.5774430
H	-2.3228760	-0.0000200	0.9454310
H	2.1248710	-1.3425820	0.8968110
H	-0.1700060	-1.0546250	1.5774290
H	-0.0275270	2.6677210	0.9294580
H	1.6638980	-2.1349770	-0.6005110
H	-2.8327520	-0.0000240	-0.7340940
H	-0.0274900	-2.6676990	0.9295000
C	1.3960010	1.3129520	0.0760960
H	2.1248470	1.3426100	0.8968140
H	1.6638710	2.1349960	-0.6005090
C	1.5706110	0.0000080	-0.7103080
H	0.8911950	0.0000040	-1.5702350
H	2.5822160	0.0000170	-1.1347800
H	-1.9299760	2.1318230	-0.2134560
H	-1.9299360	-2.1318640	-0.2134550

H	-0.8435850	-1.3814170	-1.3608640
H	-0.8436050	1.3814000	-1.3608640

CpRh(CO)-Cyclopentane σ -complex

Final Energy = -613.2574546130

C	-1.1812100	2.8617500	-0.9704050
C	-2.4088220	2.2679410	-0.6130650
C	-2.5520260	2.3215830	0.8303250
C	-1.4093230	2.9470730	1.3719600
C	-0.4990330	3.1713140	0.2676610
Rh	-0.7153500	1.0354930	0.3404580
C	1.0309760	0.4435420	0.5786430
O	2.1053820	0.0758700	0.7290960
C	-3.0300710	-1.8083530	0.1924580
C	-1.5484430	-1.3590130	0.0117860
C	-0.6671620	-2.6333430	0.1759340
C	-1.6702470	-3.8059510	0.0971880
C	-2.9334920	-3.2363340	0.7729370
H	-3.5973160	-1.1257410	0.8306240
H	-3.5276740	-1.8380920	-0.7825850
H	-1.3038850	-0.6787140	0.8873160
H	-1.3949770	-0.9014720	-0.9675810
H	0.1193320	-2.6895350	-0.5806120
H	-0.1787590	-2.6317380	1.1559970
H	-1.8897560	-4.0459400	-0.9501830
H	-1.2945990	-4.7135100	0.5776240
H	-3.8317090	-3.8305830	0.5836420
H	-2.7814120	-3.1925350	1.8581570
H	-3.4112170	1.9716980	1.3859830
H	-1.2162270	3.1549330	2.4140850
H	0.4633620	3.6584590	0.3440420
H	-0.7910190	2.9961590	-1.9684880
H	-3.1440410	1.8645200	-1.2963760

CpRh(CO)-Cyclopentane TS

Final Energy = -613.2418966020

C	-1.4000720	2.7918070	-0.8925670
C	-2.5443380	2.0755980	-0.4379280
C	-2.4987820	2.0129860	1.0015190
C	-1.3158870	2.6521370	1.4392220
C	-0.6007150	3.0785490	0.2606070
Rh	-0.7287230	0.8506980	0.1143500
C	1.0414360	0.2704750	0.2207230
O	2.1225950	-0.0911340	0.2677130
C	-2.8828900	-1.5407940	0.0321290

C	-1.4337690	-1.2091150	0.4617330
C	-0.6600770	-2.5037820	0.1290960
C	-1.6204890	-3.6027000	0.6314410
C	-3.0439450	-3.0748840	0.2834180
H	-3.6150050	-0.9463460	0.5858600
H	-3.0240950	-1.3170330	-1.0310820
H	-1.4088700	-1.0902180	1.5504020
H	-0.9615350	-0.4445580	-0.7488780
H	-0.5128920	-2.5982700	-0.9546730
H	0.3242100	-2.5447380	0.6041980
H	-1.4162940	-4.5796800	0.1845640
H	-1.5125350	-3.7085330	1.7162760
H	-3.4331460	-3.5684270	-0.6117100
H	-3.7489090	-3.2785320	1.0937960
H	-3.2435710	1.5497260	1.6338700
H	-0.9901890	2.7755360	2.4618950
H	0.3425730	3.6072460	0.2565400
H	-1.1527760	3.0257460	-1.9175790
H	-3.3400270	1.6877190	-1.0583140

CpRh(CO)-Cyclopentane Product

Final Energy = -613.2656296120

C	-1.4990110	2.7145360	-0.9061080
C	-2.5916450	1.9294160	-0.3984820
C	-2.4536940	1.8685770	1.0274300
C	-1.2650550	2.5500550	1.3925080
C	-0.6707980	3.0714450	0.1865680
Rh	-0.7275990	0.7689650	0.0090210
C	0.9981220	0.1444750	0.3542020
O	2.0527960	-0.2369320	0.5298310
C	-2.8367930	-1.4534440	-0.0053480
C	-1.4446190	-1.1183760	0.5756420
C	-0.6496750	-2.3921170	0.2152720
C	-1.6299760	-3.5558240	0.5210220
C	-3.0600310	-2.9509300	0.3471560
H	-3.6342470	-0.8139110	0.3862970
H	-2.8155310	-1.3246820	-1.0938430
H	-1.5318660	-1.0807920	1.6724340
H	-0.5345910	0.0377990	-1.3561350
H	-0.4045950	-2.3798140	-0.8532150
H	0.2889940	-2.4904690	0.7690870
H	-1.4618270	-4.4147270	-0.1350230
H	-1.4892900	-3.9034530	1.5492300
H	-3.6331160	-3.4667720	-0.4287970
H	-3.6269440	-3.0408940	1.2788110
H	-3.1171490	1.3464400	1.7029420

H	-0.8832400	2.6752050	2.3958200
H	0.2424590	3.6472030	0.1284880
H	-1.3190580	2.9512830	-1.9451120
H	-3.4057390	1.5196160	-0.9778770

CpRh(CO)-Cyclohexane Axial σ -complex

Final Energy = -613.2659243940

C	-1.2345550	2.7868010	-1.1640140
C	-2.4753880	2.4492040	-0.5862890
C	-2.4349630	2.7885820	0.8245480
C	-1.1750530	3.3465360	1.1229410
C	-0.3801810	3.2317940	-0.0815040
Rh	-0.8224560	1.1922440	0.4187210
C	0.8584570	0.4096010	0.5142940
O	1.8923320	-0.0811580	0.5731410
C	-1.9565390	-0.9329910	1.3629520
C	-3.4553410	-1.1778030	1.0999640
C	-3.6593210	-2.1797480	-0.0527870
C	-2.9053900	-3.4983860	0.2126000
C	-1.4055590	-3.2456970	0.4654440
C	-1.1943020	-2.2476890	1.6199240
H	-4.7276610	-2.3749670	-0.1958380
H	-3.9072950	-1.5785900	2.0175060
H	-3.9580600	-0.2300920	0.8795730
H	-1.5455030	-0.5483090	0.3688240
H	-1.8168210	-0.2437700	2.1996740
H	-3.3410950	-3.9913900	1.0925720
H	-3.0352980	-4.1825680	-0.6329100
H	-0.8933700	-4.1881610	0.6867340
H	-0.9470600	-2.8405280	-0.4471860
H	-1.5682390	-2.6859610	2.5552210
H	-0.1281330	-2.0450300	1.7631670
H	-3.2879730	-1.7326860	-0.9853980
H	-0.8413660	3.7228190	2.0787000
H	0.6331610	3.5912740	-0.1964490
H	-0.9490260	2.6724510	-2.1993860
H	-3.3280000	2.0321390	-1.1047020
H	-3.2551900	2.6623330	1.5187130

CpRh(CO)-Cyclohexane Equatorial σ -complex

Final Energy = -652.5591185350

C	-1.0848430	2.8405830	-1.2516260
C	-2.3500020	2.4465000	-0.7738360
C	-2.4688460	2.8482820	0.6162860
C	-1.2771220	3.4972190	1.0024880
C	-0.3654180	3.3810970	-0.1157490

Rh	-0.7401700	1.3452730	0.4512640
C	0.9635430	0.6739000	0.7629150
O	2.0115440	0.2528830	0.9562190
C	-1.8087320	-0.9809970	0.7638560
C	-3.3116750	-1.1069390	1.0809820
C	-3.9009130	-2.3735910	0.4292100
C	-3.1206800	-3.6337650	0.8520070
C	-1.6209750	-3.4964340	0.5244780
C	-1.0185580	-2.2375090	1.1788910
H	-4.9584520	-2.4729060	0.6973200
H	-3.4472030	-1.1615340	2.1695000
H	-3.8434270	-0.2142240	0.7347840
H	-1.6750540	-0.8156850	-0.3115490
H	-1.4176950	-0.1336880	1.4161120
H	-3.2411540	-3.7864970	1.9332820
H	-3.5362150	-4.5181440	0.3568750
H	-1.0758390	-4.3860030	0.8581640
H	-1.4928310	-3.4327760	-0.5646850
H	-1.0551270	-2.3427350	2.2714020
H	0.0346530	-2.1278910	0.9011690
H	-3.8558580	-2.2711260	-0.6636200
H	-1.0573800	3.9303890	1.9670790
H	0.6319300	3.7974310	-0.1519030
H	-0.6965150	2.7041550	-2.2502130
H	-3.1230100	1.9537420	-1.3482170
H	-3.3431670	2.7012420	1.2358690

CpRh(CO)-Cyclohexane Axial TS

Final Energy = -652.5589475720

C	-1.4049260	2.5112470	-1.1670910
C	-2.5983610	2.1698240	-0.4668160
C	-2.4564660	2.5868240	0.9057630
C	-1.1672510	3.1415100	1.0703040
C	-0.4906580	3.0367840	-0.2002640
Rh	-0.9293430	0.9328230	0.4266780
C	0.7589910	0.1911810	0.6911380
O	1.7970760	-0.2627170	0.8299130
C	-1.9042070	-0.7698130	1.4812620
C	-3.3847860	-1.0063140	1.1065250
C	-3.5503300	-1.9262390	-0.1189940
C	-2.8211420	-3.2690150	0.0891510
C	-1.3365800	-3.0544820	0.4460030
C	-1.1881790	-2.1259760	1.6670450
H	-4.6147390	-2.1014850	-0.3112150
H	-3.8759530	-1.4817950	1.9693660
H	-3.8966380	-0.0537230	0.9386540

H	-1.3806760	-0.5222440	0.0314070
H	-1.8624460	-0.2297420	2.4312530
H	-3.3095540	-3.8181330	0.9059990
H	-2.9091420	-3.8898930	-0.8092440
H	-0.8551880	-4.0169000	0.6514080
H	-0.8137960	-2.6158650	-0.4144710
H	-1.6420590	-2.6226270	2.5379310
H	-0.1316240	-1.9787990	1.9087420
H	-3.1436680	-1.4253000	-1.0077150
H	-0.7512620	3.5457910	1.9817750
H	0.5136330	3.3811820	-0.4054920
H	-1.2057890	2.3495600	-2.2162320
H	-3.4835070	1.7263820	-0.9012520
H	-3.2066220	2.4782070	1.6772200

CpRh(CO)-Cyclohexane Equatorial TS

Final Energy = -652.5418100480

C	-1.1106250	2.7323730	-1.1386930
C	-2.3869430	2.2859770	-0.7246600
C	-2.5520690	2.6125410	0.6695980
C	-1.3862620	3.3027620	1.1105070
C	-0.4640070	3.3068730	0.0162280
Rh	-0.8272960	1.1575980	0.5287390
C	0.8912990	0.4528200	0.6985430
O	1.9483300	0.0398670	0.8190800
C	-1.7182300	-0.8804390	0.4829280
C	-3.2089780	-0.9371970	0.8809470
C	-3.8633820	-2.2565290	0.4185220
C	-3.1050470	-3.4786140	0.9681540
C	-1.6175430	-3.4236960	0.5737900
C	-0.9612520	-2.1063450	1.0380860
H	-4.9117050	-2.2821560	0.7378050
H	-3.3013640	-0.8532100	1.9730280
H	-3.7478460	-0.0860710	0.4528290
H	-1.6534310	-0.9195740	-0.6109520
H	-1.2599080	0.0718530	1.5870630
H	-3.1875190	-3.4913200	2.0636750
H	-3.5616560	-4.4052320	0.6028300
H	-1.0779400	-4.2764760	1.0013750
H	-1.5294730	-3.5048260	-0.5181750
H	-0.9584480	-2.0752100	2.1368810
H	0.0850940	-2.0836930	0.7187950
H	-3.8622880	-2.2943770	-0.6793730
H	-1.2079390	3.6967190	2.1002280
H	0.5246660	3.7447190	0.0283250
H	-0.6849940	2.6404520	-2.1274010

H	-3.1146640	1.7775400	-1.3423550
H	-3.4337700	2.4131190	1.2624100

CpRh(CO)-Cyclohexane Axial Product

Final Energy = -652.5427552920

C	-1.4463700	2.5165250	-1.1523470
C	-2.6326000	2.1159920	-0.4448650
C	-2.4341980	2.4220160	0.9411640
C	-1.1272950	2.9476340	1.1041360
C	-0.5138290	2.9967430	-0.1997960
Rh	-0.9743660	0.7898990	0.2730610
C	0.6903420	0.0345010	0.6394350
O	1.7172090	-0.4203620	0.8076580
C	-1.9073680	-0.6645790	1.5061200
C	-3.3754170	-0.9388790	1.0955910
C	-3.5055850	-1.8600300	-0.1338040
C	-2.7651060	-3.1939030	0.0890730
C	-1.2978090	-2.9651800	0.5033310
C	-1.2124870	-2.0293870	1.7247320
H	-4.5648720	-2.0533540	-0.3408620
H	-3.8742840	-1.4372270	1.9436760
H	-3.9234920	-0.0068590	0.9240060
H	-1.0524080	-0.3386610	-0.7971080
H	-1.9193740	-0.1500140	2.4760540
H	-3.2746250	-3.7553170	0.8847150
H	-2.8137930	-3.8103760	-0.8158270
H	-0.8231740	-3.9251220	0.7380080
H	-0.7441550	-2.5308250	-0.3372690
H	-1.7209020	-2.5318180	2.5639820
H	-0.1710530	-1.9054340	2.0374650
H	-3.0906580	-1.3553860	-1.0140450
H	-0.6793510	3.2732210	2.0320670
H	0.4842770	3.3525270	-0.4154750
H	-1.2817450	2.4257070	-2.2164880
H	-3.5355780	1.7217360	-0.8876700
H	-3.1431200	2.2311650	1.7352340

CpRh(CO)-Cyclohexane Equatorial Product

Final Energy = -652.5624387590

C	-1.0450650	2.5735590	-1.0698320
C	-2.3446310	2.1319910	-0.7076300
C	-2.6000630	2.5287460	0.6440930
C	-1.4581610	3.2730980	1.1019610
C	-0.4969370	3.2797960	0.0606910
Rh	-0.8760590	1.0962230	0.7047030
C	0.8329350	0.3513660	0.7964020

O	1.8879750	-0.0576240	0.8900890
C	-1.7088750	-0.8108530	0.3349660
C	-3.1713530	-0.8721310	0.8346480
C	-3.8650390	-2.2036820	0.4663190
C	-3.0790660	-3.4093750	1.0092310
C	-1.6246620	-3.3710470	0.5096180
C	-0.9366310	-2.0358550	0.8729890
H	-4.8906150	-2.2086510	0.8549690
H	-3.1812210	-0.7560970	1.9269210
H	-3.7582650	-0.0429310	0.4262980
H	-1.7216120	-0.8882600	-0.7633320
H	-0.9954650	0.5944630	2.1789050
H	-3.0849630	-3.3789110	2.1076000
H	-3.5618460	-4.3476270	0.7123930
H	-1.0540870	-4.2085910	0.9285310
H	-1.6163010	-3.4935620	-0.5823730
H	-0.8556210	-1.9623540	1.9663270
H	0.0847930	-2.0554010	0.4794820
H	-3.9367360	-2.2832820	-0.6273290
H	-1.3414780	3.7168540	2.0803450
H	0.4800930	3.7411970	0.1045150
H	-0.5642180	2.4296740	-2.0267560
H	-3.0100890	1.5491230	-1.3295600
H	-3.5105380	2.3553990	1.1985720

CpRh(CO)-Cyclohexane 1,1-migration

Final Energy = -652.5646817780

C	2.5034030	-0.8639690	1.3112090
C	1.7028660	-1.8434480	0.6910820
C	1.8964950	-1.7581510	-0.7458990
C	2.8258030	-0.7342550	-1.0199880
C	3.1050930	-0.0869670	0.2451680
Rh	1.0045670	0.2334760	-0.0205280
C	0.8453660	2.0813150	0.0916750
O	0.7359030	3.2199770	0.1577730
C	-1.5133530	-0.0441530	-0.4796020
C	-2.1657120	-1.4372220	-0.5688700
C	-3.3086160	-1.5740710	0.4564750
C	-4.3444920	-0.4442540	0.2923930
C	-3.6810370	0.9434530	0.3954930
C	-2.5404980	1.0951870	-0.6297280
H	-3.7924390	-2.5512450	0.3503230
H	-2.5673640	-1.5777580	-1.5815300
H	-1.4128640	-2.2167580	-0.4101610
H	-1.0614170	0.0514450	0.5361870
H	-0.7495610	0.0588600	-1.2792180

H	-4.8291900	-0.5400660	-0.6889640
H	-5.1318600	-0.5430850	1.0475860
H	-4.4262030	1.7322030	0.2455230
H	-3.2750030	1.0758580	1.4076680
H	-2.9579270	1.0644220	-1.6452140
H	-2.0481050	2.0662540	-0.5143440
H	-2.8884180	-1.5334670	1.4707930
H	3.1983880	-0.4374210	-1.9892630
H	3.8010520	0.7285040	0.3868860
H	2.5987000	-0.6787110	2.3709870
H	1.0692220	-2.5613950	1.1940400
H	1.4283280	-2.4046770	-1.4761710

CpRh(CO)-Cyclohexane 1,2-migration

Final Energy = -652.5575479020

C	-2.7326300	-1.0207940	-1.0809720
C	-1.8540960	-1.9301200	-0.4619200
C	-1.8884630	-1.7157380	0.9744810
C	-2.7869240	-0.6678830	1.2542600
C	-3.2135260	-0.1411860	-0.0311800
Rh	-1.1200580	0.2124280	-0.0224650
C	-0.9931440	2.0557980	-0.2400350
O	-0.8900010	3.1892580	-0.3679260
C	1.9301120	0.4102290	0.6354400
C	1.8306230	-0.5065140	-0.6033810
C	3.1171570	-0.4401370	-1.4510250
C	4.3562980	-0.7840960	-0.6012940
C	4.4556630	0.1292880	0.6367730
C	3.1699240	0.0643970	1.4846840
H	3.0405800	-1.1207310	-2.3058610
H	1.6658430	-1.5414960	-0.2758310
H	0.9692090	-0.2249080	-1.2327830
H	1.9969820	1.4558880	0.3074880
H	1.0229950	0.3291810	1.2570240
H	4.2885850	-1.8304090	-0.2729370
H	5.2642620	-0.6988490	-1.2084880
H	5.3223210	-0.1513350	1.2454920
H	4.6177260	1.1649900	0.3083530
H	3.0556330	-0.9495130	1.8917080
H	3.2427740	0.7461870	2.3387560
H	3.2262410	0.5743740	-1.8572650
H	-3.0562320	-0.2831690	2.2268170
H	-3.9306670	0.6567300	-0.1680080
H	-2.9519080	-0.9417390	-2.1354430
H	-1.2639670	-2.6861350	-0.9624270
H	-1.3337040	-2.2918590	1.7027420

CpRh(CO)-Cycloheptane σ -complex (1)

Final Energy = -691.8424544170

C	1.1075220	-1.0396630	3.4026480
C	2.0953350	-0.6775480	2.4651510
C	2.1957390	0.7697780	2.4269960
C	1.2681400	1.3094900	3.3420860
C	0.5014920	0.1936130	3.8587670
Rh	0.0781260	0.1814950	1.7530260
C	-1.7726650	0.3336140	1.6945950
O	-2.9137500	0.4297660	1.6562190
C	0.2226340	-0.2317150	-0.7878870
C	-1.0831880	-0.2622580	-1.6165970
C	-0.9526990	-0.8830180	-3.0255450
C	1.5379380	0.0601330	-1.5474420
C	-0.4873100	0.1233090	-4.0999040
C	1.4414420	1.1330800	-2.6542720
C	0.9857070	0.5659040	-4.0155500
H	0.0970360	0.6526330	-0.0788100
H	-1.8302480	-0.8138310	-1.0364190
H	-1.9370350	-1.2617910	-3.3226550
H	-0.6557900	-0.3120240	-5.0922600
H	1.9032730	-0.8709610	-1.9981810
H	2.4324010	1.5807190	-2.7900010
H	0.3330830	-1.1882950	-0.2672150
H	-1.4762060	0.7560120	-1.7253860
H	-0.2828530	-1.7530490	-3.0012570
H	2.2898230	0.3558080	-0.8079080
H	-1.1331410	1.0097710	-4.0379730
H	0.7757120	1.9475150	-2.3380380
H	1.6321380	-0.2875850	-4.2622490
H	1.1609930	1.3197660	-4.7924530
H	2.8935100	1.3319470	1.8213090
H	2.7041350	-1.3590420	1.8860680
H	0.8090440	-2.0406520	3.6773110
H	-0.2778130	0.2664110	4.6049040
H	1.1078580	2.3544220	3.5633060

CpRh(CO)-Cycloheptane σ -complex (2)

Final Energy = -691.8428781360

C	1.0322450	-0.8363970	3.5974530
C	2.0341410	-0.6826660	2.6177830
C	2.1959870	0.7304080	2.3315080
C	1.2885870	1.4578980	3.1286890
C	0.4757830	0.4811610	3.8251520
Rh	0.0587050	0.1164760	1.7497200
C	-1.7839110	0.3244410	1.6371160

O	-2.9200170	0.4506430	1.5561270
C	1.5774580	-0.7649420	-1.3840660
C	0.1951070	-0.7211700	-0.6904980
C	-1.0465000	-0.6876890	-1.6107970
C	1.7065190	0.0674130	-2.6795040
C	-1.4331030	0.7316120	-2.0774810
C	1.0146640	1.4500760	-2.6575500
C	-0.4699900	1.3957160	-3.0800940
H	2.3275710	-0.4270530	-0.6595240
H	0.1225720	-1.5823100	-0.0191990
H	-1.8953430	-1.1090390	-1.0613510
H	-2.4306040	0.6943030	-2.5305810
H	1.3004880	-0.5042180	-3.5232440
H	1.5381590	2.1123120	-3.3561840
H	1.8215050	-1.8086030	-1.6160820
H	0.1617690	0.2733730	-0.1372340
H	-0.8750180	-1.3426490	-2.4753930
H	2.7749800	0.1926630	-2.8879310
H	-1.5243960	1.3695300	-1.1877550
H	1.1113030	1.9118540	-1.6651830
H	-0.5298150	0.8667990	-4.0411880
H	-0.8257240	2.4160250	-3.2666770
H	2.9165780	1.1495280	1.6423470
H	2.6154990	-1.4784600	2.1714750
H	0.6928490	-1.7614650	4.0396460
H	-0.3014510	0.7145220	4.5398500
H	1.1706150	2.5309410	3.1629350

CpRh(CO)-Cycloheptane σ -complex (3)

Final Energy = -691.8424936710

C	1.2455640	-0.6852200	3.7682380
C	2.1525310	-0.4036960	2.7244650
C	2.1045260	1.0180780	2.4377280
C	1.1637790	1.6211600	3.2958790
C	0.5358430	0.5473630	4.0391940
Rh	0.0362590	0.1000170	1.9998690
C	-1.8208580	0.0565960	2.0191460
O	-2.9663780	0.0245180	2.0222700
C	1.4871070	-0.5896720	-1.1460300
C	0.1153600	-0.1816030	-0.5576600
C	-1.1292290	-0.4381800	-1.4381190
C	1.6478590	-0.3671030	-2.6663060
C	-1.4130410	0.7165860	-2.4222020
C	1.0677140	0.9576460	-3.2126910
C	-0.4247900	0.8586890	-3.5953070
H	2.2615680	-0.0250850	-0.6132910

H	-0.0207460	-0.8485720	0.3547130
H	-2.0013750	-0.5503920	-0.7856110
H	-2.4201510	0.5873160	-2.8361070
H	1.1791880	-1.1970590	-3.2093760
H	1.6268150	1.2390900	-4.1120980
H	1.6758120	-1.6481460	-0.9302830
H	0.1274920	0.8850210	-0.3062730
H	-1.0199880	-1.3875650	-1.9782120
H	2.7179140	-0.4232120	-2.8956380
H	-1.4334180	1.6538770	-1.8496580
H	1.2217510	1.7689140	-2.4880470
H	-0.5456450	0.0015220	-4.2717230
H	-0.7060340	1.7482900	-4.1715910
H	2.7150260	1.5267670	1.7037350
H	2.8053480	-1.1159260	2.2382630
H	1.0613690	-1.6456260	4.2265780
H	-0.2168890	0.6774670	4.8045670
H	0.9069270	2.6691730	3.3438640

CpRh(CO)-Cycloheptane σ -complex (4)

Final Energy = -691.8418936690

C	1.1065750	-1.0415150	3.5494970
C	2.0445160	-0.6672230	2.5624180
C	2.1484850	0.7797000	2.5304100
C	1.2446540	1.3084470	3.4726610
C	0.5095490	0.1855430	4.0253040
Rh	0.0048200	0.1682220	1.9370080
C	-1.8356960	0.4215780	1.9365370
O	-2.9708940	0.5773250	1.9256900
C	1.9064450	-1.7347240	-1.8114090
C	1.4151290	-0.3624130	-1.2972360
C	0.0451450	-0.3847730	-0.5831680
C	0.8276010	-2.6525480	-2.4342690
C	-1.1594530	-0.2171250	-1.5356410
C	-0.2533260	-1.9433640	-3.2825110
C	-1.4443830	-1.4266980	-2.4460880
H	2.6957720	-1.5514940	-2.5502650
H	2.1753890	0.0427350	-0.6207810
H	0.0187480	0.5538440	0.0578260
H	-2.0592290	-0.0093260	-0.9458750
H	0.3200620	-3.2120920	-1.6384380
H	-0.6458030	-2.6584700	-4.0141570
H	2.3813380	-2.2789510	-0.9860420
H	1.3455090	0.3425580	-2.1345790
H	-0.0697530	-1.3075640	-0.0004240
H	1.3400090	-3.4028030	-3.0466210

H	-0.9798930	0.6709690	-2.1560150
H	0.1905850	-1.1227790	-3.8621090
H	-1.8151520	-2.2576670	-1.8310860
H	-2.2644380	-1.1518880	-3.1202200
H	2.8186120	1.3467280	1.8989990
H	2.6316230	-1.3443500	1.9559060
H	0.8319960	-2.0452950	3.8379140
H	-0.2400530	0.2559190	4.8014840
H	1.0806860	2.3520010	3.6984600

CpRh(CO)-Cycloheptane σ -complex (5)

Final Energy = -691.8428133040

C	1.1734210	-0.7927770	3.3777580
C	2.0911360	-0.3547400	2.3972510
C	1.9898260	1.0878360	2.2691210
C	0.9851480	1.5428500	3.1435820
C	0.3923710	0.3652750	3.7486870
Rh	-0.0234370	0.1186950	1.6555330
C	-1.8790480	0.0639830	1.5904950
O	-3.0232390	0.0256630	1.5427230
C	1.8973570	-1.8710970	-1.3896770
C	1.5463600	-0.3698520	-1.4984320
C	0.1809980	0.0432890	-0.9069680
C	0.7319190	-2.8610290	-1.6278300
C	-1.0054980	-0.1056760	-1.8840540
C	-0.2754890	-2.4678170	-2.7332840
C	-1.4109770	-1.5507300	-2.2277910
H	2.7033620	-2.0794890	-2.1032140
H	2.3417490	0.2042260	-1.0101060
H	0.2263340	1.0907250	-0.5949550
H	-1.8771300	0.4114050	-1.4666610
H	0.1741150	-2.9979220	-0.6927270
H	-0.7356790	-3.3821340	-3.1243560
H	2.3101910	-2.0696490	-0.3930440
H	1.5510060	-0.0651190	-2.5521660
H	-0.0360290	-0.6795040	-0.0508710
H	1.1676200	-3.8387630	-1.8613550
H	-0.7362750	0.4268840	-2.8061680
H	0.2452780	-1.9993620	-3.5794260
H	-1.8575240	-2.0174680	-1.3392780
H	-2.2036800	-1.5074570	-2.9840690
H	2.5967620	1.7021940	1.6179780
H	2.7958990	-0.9777300	1.8628440
H	1.0282780	-1.8048180	3.7253940
H	-0.3888360	0.3775940	4.4962730
H	0.6688900	2.5650180	3.2919730

CpRh(CO)-Cycloheptane σ -complex (6)

Final Energy = -691.8424481510

C	1.0820310	-0.8039210	3.7173620
C	2.0236050	-0.6870660	2.6763610
C	2.1674580	0.7168520	2.3372880
C	1.3285500	1.4763310	3.1814860
C	0.5563340	0.5263470	3.9527320
Rh	-0.0031890	0.1141030	1.9220070
C	-1.8544640	0.2676770	1.9549740
O	-2.9963670	0.3629060	1.9672020
C	0.9463040	0.9847360	-3.3404790
C	1.5610630	0.7898060	-1.9336600
C	1.3361100	-0.5949020	-1.2867130
C	-0.4292470	0.3222030	-3.5875870
C	-0.0094000	-0.7085860	-0.5371180
C	-1.4365050	0.4007200	-2.4177560
C	-1.2822860	-0.7519770	-1.4041920
H	0.8633630	2.0624500	-3.5252930
H	2.6365550	0.9857060	-2.0065180
H	2.1379100	-0.7840030	-0.5646500
H	-0.0001080	-1.5967680	0.1017410
H	-0.2854420	-0.7356970	-3.8416050
H	-2.4527620	0.3513020	-2.8240740
H	1.6451580	0.6002750	-4.0932230
H	1.1645860	1.5507450	-1.2489320
H	1.4000970	-1.3899110	-2.0415150
H	-0.8673490	0.7862980	-4.4782060
H	-0.0953070	0.2690890	0.0467740
H	-1.3567690	1.3689650	-1.9051010
H	-1.2927050	-1.7021670	-1.9550700
H	-2.1507600	-0.7695980	-0.7364780
H	2.8399250	1.1111270	1.5872800
H	2.5686130	-1.4998580	2.2153410
H	0.7624570	-1.7137180	4.2039790
H	-0.1691760	0.7831370	4.7123240
H	1.2255820	2.5512420	3.1973960

CpRh(CO)-Cycloheptane σ -complex (7)

Final Energy = -691.8419548350

C	1.2612570	-0.7317190	3.8224030
C	2.1328200	-0.4252800	2.7575450
C	2.0660980	1.0018170	2.5010720
C	1.1593310	1.5854470	3.4085910
C	0.5588070	0.4939080	4.1465710
Rh	-0.0141870	0.0933270	2.1168750
C	-1.8665740	-0.0089080	2.2155290

O	-3.0091480	-0.0742260	2.2731110
C	0.9997710	0.2665050	-3.7065870
C	1.6218420	0.6059430	-2.3321490
C	1.2865320	-0.3744060	-1.1854760
C	-0.4464630	-0.2805890	-3.6815370
C	-0.0384780	-0.0267600	-0.4720540
C	-1.3962000	0.3821980	-2.6581760
C	-1.3405870	-0.2705450	-1.2603160
H	1.0312290	1.1720830	-4.3243160
H	2.7091350	0.6584390	-2.4569980
H	2.0864340	-0.3341810	-0.4383810
H	-0.1053490	-0.7438620	0.4104450
H	-0.4269670	-1.3587000	-3.4782060
H	-2.4255570	0.2886540	-3.0218630
H	1.6327950	-0.4708720	-4.2148300
H	1.3059970	1.6104720	-2.0239860
H	1.2573740	-1.4074440	-1.5559920
H	-0.8629230	-0.1738930	-4.6893000
H	-0.0002180	1.0268310	-0.1707350
H	-1.1920930	1.4586750	-2.5846870
H	-1.4928870	-1.3513150	-1.3803370
H	-2.1773400	0.0965860	-0.6557580
H	2.6467860	1.5278400	1.7549910
H	2.7709370	-1.1248710	2.2348360
H	1.0929160	-1.7028460	4.2640920
H	-0.1661380	0.6036420	4.9414130
H	0.9049170	2.6318950	3.4902860

CpRh(CO)-Cycloheptane TS (1)

Final Energy = -691.8256072590

C	1.0781260	-0.9704390	3.1409290
C	2.0841750	-0.5928990	2.2149580
C	2.1873420	0.8432400	2.2061780
C	1.2388070	1.3618390	3.1291160
C	0.5057560	0.2436570	3.6551790
Rh	0.1145670	0.2838510	1.4516980
C	-1.7404860	0.4509960	1.3544380
O	-2.8737360	0.5769680	1.3133470
C	0.2339600	-0.4811240	-0.6362890
C	-1.0647920	-0.4334220	-1.4753360
C	-0.9337660	-0.9076630	-2.9431070
C	1.5324900	-0.1284670	-1.4066500
C	-0.4931270	0.2089570	-3.9141950
C	1.4400570	1.0648240	-2.3843830
C	0.9756230	0.6579520	-3.7985420
H	0.1361270	0.9238690	0.0090310

H	-1.8099430	-1.0503490	-0.9625240
H	-1.9160570	-1.2677160	-3.2700870
H	-0.6689450	-0.1227480	-4.9447810
H	1.8533810	-1.0118820	-1.9755630
H	2.4313250	1.5233430	-2.4740820
H	0.3508200	-1.5044610	-0.2662430
H	-1.4768210	0.5835780	-1.4911020
H	-0.2530750	-1.7664570	-3.0123330
H	2.3237940	0.0595470	-0.6746720
H	-1.1476330	1.0764720	-3.7531820
H	0.7787960	1.8415460	-1.9751520
H	1.6277490	-0.1531830	-4.1505030
H	1.1328160	1.4996800	-4.4839350
H	2.8857350	1.4221740	1.6184870
H	2.6849630	-1.2675730	1.6199900
H	0.7731290	-1.9768190	3.3878010
H	-0.2916510	0.3035040	4.3832510
H	1.0708770	2.4029590	3.3626420

CpRh(CO)-Cycloheptane TS (2)

Final Energy = -691.8252679510

C	1.1235990	-1.1559910	3.4311380
C	2.0644690	-0.7921750	2.4424660
C	2.0728800	0.6456930	2.3375760
C	1.1766990	1.1749200	3.3133400
C	0.5323570	0.0617520	3.9348080
Rh	-0.0003780	-0.0251950	1.7584250
C	-1.8392570	-0.3312740	1.7722020
O	-2.9673500	-0.5023180	1.7983490
C	1.4670410	0.0276350	-1.0060790
C	0.1030460	-0.4319020	-0.4352660
C	-1.1075530	-0.1876410	-1.3708430
C	1.6545740	-0.1453600	-2.5337030
C	-1.1495240	1.1825000	-2.0855400
C	1.1253560	1.0486390	-3.3577570
C	-0.4070540	1.1825060	-3.4384560
H	1.6418140	1.0842570	-0.7667870
H	0.1490370	-1.5110980	-0.2620130
H	-2.0280310	-0.3317540	-0.7990080
H	-2.1953240	1.4492730	-2.2740520
H	1.1946890	-1.0815410	-2.8759600
H	1.5170880	0.9793950	-4.3799150
H	2.2501080	-0.5306550	-0.4825030
H	-0.2461240	0.8001900	0.4389270
H	-1.1125150	-0.9716230	-2.1398650
H	2.7284350	-0.2401900	-2.7327990

H	-0.7466550	1.9675700	-1.4302610
H	1.5442300	1.9690710	-2.9282240
H	-0.8071950	0.3588730	-4.0454040
H	-0.6433770	2.1071510	-3.9789170
H	2.7032780	1.2226890	1.6757640
H	2.6639400	-1.4717210	1.8527990
H	0.8751340	-2.1597780	3.7445530
H	-0.2178040	0.1199070	4.7113740
H	0.9775790	2.2192310	3.5039200

CpRh(CO)-Cycloheptane TS (3)

Final Energy = -691.8250034230

C	1.3220260	-0.8826240	3.4637820
C	2.1694980	-0.3898670	2.4252510
C	2.0726010	1.0474210	2.3974730
C	1.1124810	1.4379590	3.3569280
C	0.6118430	0.2378270	3.9886030
Rh	0.0497800	0.0813560	1.8228250
C	-1.7955850	0.3518830	1.8241460
O	-2.9258170	0.5071440	1.8450560
C	1.4742650	-0.3065100	-0.9307490
C	0.0957810	0.1676730	-0.4082920
C	-1.1142920	-0.2785770	-1.2697950
C	1.6414260	-0.3716520	-2.4682440
C	-1.4109560	0.6810740	-2.4449760
C	1.0626280	0.8203040	-3.2628500
C	-0.4248420	0.6362820	-3.6263780
H	2.2367130	0.3676050	-0.5230200
H	-0.1924400	-0.9330900	0.6428940
H	-2.0129520	-0.3174420	-0.6480270
H	-2.4146470	0.4624550	-2.8302130
H	1.1842480	-1.2933510	-2.8490440
H	1.6275290	0.9291130	-4.1957710
H	1.7038830	-1.3012890	-0.5298990
H	0.0848240	1.2615920	-0.3954130
H	-0.9598760	-1.3017270	-1.6390890
H	2.7147100	-0.4623560	-2.6726310
H	-1.4510480	1.7036180	-2.0453260
H	1.2043480	1.7549720	-2.7033700
H	-0.5308660	-0.3267940	-4.1443930
H	-0.7183120	1.4086850	-4.3477350
H	2.6195080	1.7059380	1.7371690
H	2.8303250	-0.9858320	1.8117670
H	1.1962710	-1.9152400	3.7543540
H	-0.1244100	0.2062280	4.7797620
H	0.7985650	2.4482490	3.5774930

CpRh(CO)-Cycloheptane TS (4)

Final Energy = -691.8242205850

C	1.0398880	-1.0077840	3.3785530
C	2.0109880	-0.6661130	2.4023880
C	2.1508180	0.7672650	2.3704320
C	1.2521890	1.3199490	3.3209240
C	0.5171050	0.2261020	3.8959000
Rh	0.0288450	0.2433120	1.7130680
C	-1.8157540	0.5002090	1.7085880
O	-2.9429980	0.6786030	1.7270600
C	1.9097860	-1.7615570	-1.7262250
C	1.3787490	-0.4567900	-1.0887890
C	0.0221460	-0.5949980	-0.3533120
C	0.8692390	-2.6238600	-2.4800080
C	-1.1674260	-0.3317660	-1.3049950
C	-0.2191520	-1.8367160	-3.2436800
C	-1.4177100	-1.4334470	-2.3575460
H	2.7194330	-1.4890290	-2.4145990
H	2.1498560	-0.0821510	-0.4098790
H	0.0163090	0.8294010	0.2462410
H	-2.0917350	-0.2159040	-0.7316550
H	0.3663940	-3.2950730	-1.7727870
H	-0.6024620	-2.4698120	-4.0521540
H	2.3690310	-2.3807860	-0.9451440
H	1.2687360	0.3123820	-1.8638690
H	-0.0726870	-1.6091190	0.0507280
H	1.4100770	-3.2733260	-3.1775380
H	-1.0011820	0.6261870	-1.8165940
H	0.2152070	-0.9509390	-3.7260300
H	-1.7793230	-2.3359150	-1.8459440
H	-2.2391390	-1.0952050	-3.0013800
H	2.8364350	1.3210930	1.7446720
H	2.5688540	-1.3629240	1.7911540
H	0.7237940	-2.0030790	3.6543370
H	-0.2467380	0.3162710	4.6561160
H	1.1176070	2.3680220	3.5451510

CpRh(CO)-Cycloheptane TS (5)

Final Energy = -691.8250387560

C	1.2301370	-0.8291410	3.1737430
C	2.1071910	-0.2939410	2.1838390
C	1.8986740	1.1302710	2.1092080
C	0.8537320	1.4688450	2.9962660
C	0.3986290	0.2445980	3.6160760
Rh	0.0112810	0.0031040	1.4177110
C	-1.8464710	0.0473390	1.2666670

O	-2.9845130	0.0482290	1.1818550
C	1.8740780	-1.8883650	-1.2560880
C	1.5758270	-0.3740540	-1.3666240
C	0.2491990	0.1676290	-0.7840980
C	0.7101340	-2.8710660	-1.5450570
C	-0.9449830	-0.0331500	-1.7433780
C	-0.3273280	-2.4200650	-2.5960100
C	-1.4076800	-1.4733210	-2.0289980
H	2.6996300	-2.1012840	-1.9460240
H	2.4116420	0.1599640	-0.8989470
H	0.3694720	1.2514680	-0.6899020
H	-1.8015670	0.5405030	-1.3727890
H	0.1723370	-3.0844250	-0.6135170
H	-0.8317450	-3.3128400	-2.9833830
H	2.2532440	-2.1072930	-0.2513070
H	1.5926190	-0.0880020	-2.4280920
H	-0.0475480	-1.0023040	0.2090420
H	1.1516710	-3.8236140	-1.8596480
H	-0.6592620	0.4290970	-2.7005210
H	0.1721050	-1.9511950	-3.4547980
H	-1.8159640	-1.9200510	-1.1123180
H	-2.2404390	-1.4176500	-2.7404770
H	2.4374190	1.8135590	1.4671910
H	2.8578890	-0.8460470	1.6362810
H	1.1632480	-1.8616410	3.4835480
H	-0.3865550	0.1713820	4.3558870
H	0.4490790	2.4559660	3.1678440

CpRh(CO)-Cycloheptane TS (6)

Final Energy = -691.8239812300

C	1.0307780	-0.6412780	3.5442920
C	1.9606820	-0.6914420	2.4827330
C	2.1170610	0.6444530	1.9641700
C	1.3362810	1.5352220	2.7608750
C	0.6034010	0.7328270	3.6844880
Rh	-0.0343570	0.0833930	1.6259810
C	-1.8895450	-0.0722880	1.7450940
O	-3.0253330	-0.1442680	1.8293490
C	1.0134370	1.0588210	-3.0718430
C	1.6017720	0.7338860	-1.6765760
C	1.3113310	-0.6846590	-1.1339050
C	-0.3770390	0.4608980	-3.3898970
C	-0.0348750	-0.8635290	-0.3915290
C	-1.3957560	0.4482350	-2.2269340
C	-1.2701740	-0.7937520	-1.3171560
H	0.9650130	2.1500360	-3.1701390

H	2.6869270	0.8814980	-1.7300200
H	2.1163490	-0.9744580	-0.4517120
H	-0.0362210	-1.8644550	0.0505070
H	-0.2582320	-0.5702730	-3.7456100
H	-2.4063020	0.4463350	-2.6507890
H	1.7110080	0.7155780	-3.8454950
H	1.2357940	1.4656190	-0.9479050
H	1.3421970	-1.4062910	-1.9646390
H	-0.7953870	1.0214810	-4.2336020
H	-0.2781790	0.5893650	0.1578960
H	-1.3145270	1.3693060	-1.6336520
H	-1.2496990	-1.6803450	-1.9682120
H	-2.1750850	-0.8865560	-0.7083610
H	2.7714660	0.9306650	1.1522870
H	2.4511150	-1.5781660	2.1054270
H	0.6853720	-1.4766340	4.1364800
H	-0.0981980	1.0983180	4.4215660
H	1.2627860	2.6063020	2.6429080

CpRh(CO)-Cycloheptane TS (7)

Final Energy = -691.8246136010

C	1.2556380	-0.7644910	3.6665020
C	2.1339040	-0.4266750	2.6015950
C	1.9935050	0.9819500	2.3327250
C	1.0361300	1.5221540	3.2285080
C	0.5256050	0.4252360	4.0055070
Rh	0.0103200	-0.0538170	1.8823930
C	-1.8420000	-0.2593060	1.9433210
O	-2.9716900	-0.4067970	2.0090280
C	1.0030490	0.1462460	-3.6236000
C	1.6460500	0.6123380	-2.2977180
C	1.2918700	-0.2325830	-1.0499480
C	-0.4589970	-0.3433880	-3.5177650
C	0.0068600	0.2478700	-0.3296750
C	-1.3569730	0.4659070	-2.5561430
C	-1.3066370	-0.0256850	-1.0899960
H	1.0547570	0.9766930	-4.3382710
H	2.7338370	0.6195470	-2.4324580
H	2.1233400	-0.1693410	-0.3417870
H	-0.0370450	-0.9782680	0.6055750
H	-0.4729520	-1.3922640	-3.1959320
H	-2.3975870	0.3762350	-2.8889840
H	1.6062680	-0.6633080	-4.0521300
H	1.3610280	1.6526300	-2.0972380
H	1.2029730	-1.2942240	-1.3187280
H	-0.8938350	-0.3320930	-4.5235060

H	0.0961550	1.3319920	-0.1955910
H	-1.1089800	1.5343930	-2.6080110
H	-1.5211430	-1.1034420	-1.0890470
H	-2.1247350	0.4515220	-0.5414790
H	2.5423670	1.5341720	1.5818420
H	2.8107410	-1.1009920	2.0960970
H	1.1278030	-1.7411090	4.1099020
H	-0.2267150	0.4994480	4.7788460
H	0.7209560	2.5532960	3.2922450

CpRh(CO)-Cycloheptane Product (1)

Final Energy = -691.8460620180

C	0.9576140	-0.9139800	3.0435780
C	1.9897260	-0.6549890	2.1010580
C	2.2073350	0.7572930	2.0417980
C	1.3298380	1.3751800	2.9998950
C	0.5515680	0.3520380	3.5962300
Rh	0.1121120	0.3896590	1.3309880
C	-1.7542840	0.3304610	1.2594930
O	-2.8894290	0.3498830	1.2558710
C	0.2401120	-0.5641630	-0.5577290
C	-1.0361020	-0.4816100	-1.4298210
C	-0.8875500	-0.9258180	-2.9083730
C	1.5223470	-0.1437070	-1.3247000
C	-0.4689640	0.2224780	-3.8516420
C	1.3973250	1.0901890	-2.2494880
C	0.9776370	0.7264560	-3.6898880
H	-0.0486680	1.6462430	0.4202130
H	-1.8074790	-1.0991640	-0.9558910
H	-1.8577620	-1.3034530	-3.2524640
H	-0.6088080	-0.0954530	-4.8923300
H	1.8501070	-0.9899250	-1.9473960
H	2.3696740	1.5937390	-2.3017590
H	0.3683000	-1.6193770	-0.2797300
H	-1.4267330	0.5434950	-1.4352760
H	-0.1842550	-1.7651500	-2.9896260
H	2.3349350	0.0221120	-0.6126230
H	-1.1602970	1.0607280	-3.6891010
H	0.6962840	1.8159640	-1.8180140
H	1.6689010	-0.0422270	-4.0621300
H	1.1115390	1.6016130	-4.3378200
H	2.9406650	1.2648430	1.4324070
H	2.4911240	-1.3950340	1.4924000
H	0.5692820	-1.8843620	3.3174630
H	-0.2191550	0.4975850	4.3408860
H	1.2574460	2.4338060	3.2039050

CpRh(CO)-Cycloheptane Product (2)

Final Energy = -691.8455222250

C	0.9884850	-1.1165860	3.3227270
C	1.9517730	-0.8286610	2.3247940
C	2.0910960	0.5965300	2.2297360
C	1.2413170	1.1833060	3.2270780
C	0.5420510	0.1371640	3.8794190
Rh	-0.0241270	0.1211720	1.6468800
C	-1.8361970	-0.3214240	1.6358170
O	-2.9460240	-0.5597060	1.6706610
C	1.4836810	0.0254690	-0.9571250
C	0.1562640	-0.5222780	-0.3698080
C	-1.0477300	-0.2814100	-1.3168520
C	1.6767750	-0.1193700	-2.4906630
C	-1.1368150	1.1158080	-1.9766790
C	1.1126880	1.0733460	-3.2931260
C	-0.4231930	1.1804950	-3.3439220
H	1.5864870	1.0903380	-0.7151730
H	0.2603310	-1.6119560	-0.2744350
H	-1.9829520	-0.4960010	-0.7944870
H	-2.1915070	1.3679000	-2.1359960
H	1.2443400	-1.0626750	-2.8485330
H	1.4893360	1.0260220	-4.3224870
H	2.3145500	-0.4796490	-0.4529250
H	-0.4866980	1.4274780	0.9256260
H	-1.0025050	-1.0230090	-2.1276510
H	2.7527970	-0.1780880	-2.6943860
H	-0.7349870	1.8802930	-1.2995910
H	1.5211920	1.9952900	-2.8567190
H	-0.8184480	0.3712060	-3.9730270
H	-0.6864800	2.1192320	-3.8469990
H	2.7654460	1.1282890	1.5752710
H	2.4643040	-1.5567430	1.7117120
H	0.6587260	-2.1002540	3.6260450
H	-0.1868030	0.2563570	4.6689050
H	1.1225370	2.2410510	3.4145040

CpRh(CO)-Cycloheptane 1,1-Migration (1)

Final Energy = -691.8411409050

C	2.9141130	-0.7933520	1.2659060
C	1.9872690	-1.7856140	0.8906070
C	1.9950580	-1.9058490	-0.5565070
C	2.9291590	-0.9915040	-1.0822870
C	3.4085920	-0.2051180	0.0370080
Rh	1.3109760	0.2270370	-0.0147610
C	1.2684020	2.0769320	-0.1711210

O	1.2334480	3.2181730	-0.2680230
C	-1.2626290	0.0561110	-0.0470970
C	-2.2202530	1.2583470	-0.2171410
C	-3.4733790	1.2309820	0.6857390
C	-1.8925890	-1.3463450	0.1303990
C	-4.6460050	0.4291530	0.0825260
C	-3.1852620	-1.6022900	-0.6758310
C	-4.4612350	-1.0992190	0.0330070
H	-0.6222310	0.0348600	-0.9563620
H	-1.6470160	2.1714130	-0.0249290
H	-3.8120550	2.2622880	0.8355170
H	-5.5565790	0.6441250	0.6546810
H	-2.1125530	-1.5163210	1.1917710
H	-3.2867560	-2.6834400	-0.8241010
H	-0.6535430	0.2541320	0.8635320
H	-2.5483130	1.3207280	-1.2619720
H	-3.2180440	0.8426560	1.6810300
H	-1.1352060	-2.0885520	-0.1442890
H	-4.8257320	0.8019110	-0.9351750
H	-3.1057980	-1.1594990	-1.6776450
H	-4.4601260	-1.4949540	1.0579930
H	-5.3378800	-1.5324460	-0.4634820
H	1.4043130	-2.6104890	-1.1264390
H	1.3855310	-2.3828490	1.5623970
H	3.1570830	-0.4784220	2.2700680
H	4.1602210	0.5699900	-0.0235210
H	3.1857120	-0.8505630	-2.1219090

CpRh(CO)-Cycloheptane 1,1-Migration (2)

Final Energy = -691.8414906170

C	2.4507100	-1.0467790	1.3548270
C	1.6479900	-1.9148230	0.5887120
C	1.9910390	-1.7467410	-0.8121970
C	3.0152740	-0.7835790	-0.9174630
C	3.2135580	-0.2500460	0.4141420
Rh	1.1782400	0.2573510	-0.0296300
C	1.1468190	2.0980680	0.2193480
O	1.1223120	3.2330010	0.3740950
C	-2.2195600	1.4268920	-0.7237850
C	-3.6718950	1.1739140	-0.2606360
C	-3.8293980	0.2698170	0.9837390
C	-1.2889350	0.1924090	-0.6712990
C	-3.8928990	-1.2360790	0.6450160
C	-1.9067330	-1.1723970	-1.0469890
C	-2.5813260	-1.8755710	0.1493570
H	-2.2463080	1.8199120	-1.7468970

H	-4.1308070	2.1496550	-0.0661610
H	-4.7628570	0.5362160	1.4919910
H	-4.2265340	-1.7879940	1.5319790
H	-0.9146470	0.1029060	0.3737130
H	-1.1109280	-1.8234120	-1.4251040
H	-1.7739770	2.2135850	-0.1041560
H	-4.2469340	0.7292510	-1.0824340
H	-3.0220890	0.4653870	1.7025410
H	-0.4493920	0.4026560	-1.3737830
H	-4.6699250	-1.3796930	-0.1182900
H	-2.6225730	-1.0438320	-1.8694470
H	-1.8578990	-1.9058230	0.9764810
H	-2.7882670	-2.9185730	-0.1190850
H	1.5558460	-2.3036970	-1.6311650
H	0.9146940	-2.6119820	0.9713740
H	2.4506560	-0.9423790	2.4298840
H	3.9497590	0.4947430	0.6836910
H	3.5050350	-0.4522100	-1.8211760

CpRh(CO)-Cycloheptane 1,1-Migration (3)

Final Energy = -691.8409727050

C	-3.1452060	-0.6268870	-0.8058750
C	-2.2482460	-1.7065690	-0.6966060
C	-1.8539730	-1.8415770	0.6946670
C	-2.5185580	-0.8559380	1.4538160
C	-3.2197120	-0.0151580	0.5064790
Rh	-1.1620210	0.2233000	-0.0430640
C	-0.9224890	2.0642280	0.0177740
O	-0.7628600	3.1984060	0.0522490
C	3.1417020	1.4979070	0.1875190
C	3.6878100	0.3627560	1.0860020
C	4.1190270	-0.9303090	0.3549480
C	2.2565770	1.0527680	-0.9985320
C	2.9598710	-1.9283760	0.1381970
C	1.2901400	-0.1142240	-0.6985140
C	1.9022090	-1.5160770	-0.9031840
H	2.5730160	2.1905220	0.8192940
H	4.5367370	0.7629100	1.6512920
H	4.8819880	-1.4340080	0.9590990
H	3.3723490	-2.8986000	-0.1640640
H	2.8913960	0.7461950	-1.8388930
H	0.4389320	-0.0243400	-1.4118520
H	3.9815990	2.0742370	-0.2184120
H	2.9318650	0.0935340	1.8346150
H	4.5966840	-0.6879150	-0.6039210
H	1.6879080	1.9213370	-1.3475400

H	2.4654060	-2.0897710	1.1058190
H	0.9429480	-0.0282600	0.3565120
H	2.3498200	-1.5435570	-1.9057110
H	1.0990380	-2.2624380	-0.8989340
H	-1.1902180	-2.6029260	1.0821390
H	-1.9211030	-2.3485090	-1.5033540
H	-3.6308180	-0.2752760	-1.7043300
H	-3.8499130	0.8244180	0.7659840
H	-2.4587380	-0.7085550	2.5220050

CpRh(CO)-Cycloheptane 1,1-Migration (4)

Final Energy = -691.8407347420

C	2.7083440	-0.8342390	1.3766790
C	1.9075400	-1.8259230	0.7767810
C	2.1380060	-1.8053590	-0.6572140
C	3.0847130	-0.8035060	-0.9495670
C	3.3448110	-0.1091310	0.2951070
Rh	1.2549060	0.2285480	-0.0343960
C	1.1248360	2.0812460	-0.0132210
O	1.0362660	3.2236360	-0.0019030
C	-4.4977180	0.4454420	0.4675510
C	-4.3406840	-0.9872340	-0.0926940
C	-3.0618890	-1.7418030	0.3370660
C	-3.2133840	1.3069340	0.5142760
C	-1.8538770	-1.4671290	-0.5838750
C	-2.2465390	1.1335850	-0.6782380
C	-1.2660310	-0.0456560	-0.4955400
H	-5.2541470	0.9616060	-0.1358820
H	-5.2226060	-1.5630780	0.2093680
H	-3.2624720	-2.8188190	0.3079460
H	-1.0535690	-2.1806460	-0.3557030
H	-2.6580620	1.0912370	1.4357040
H	-1.6565960	2.0490690	-0.7913910
H	-4.9057500	0.3904870	1.4840220
H	-4.3645870	-0.9563590	-1.1893300
H	-2.8075640	-1.5025780	1.3783530
H	-3.5136860	2.3579460	0.5869200
H	-2.1607210	-1.6624790	-1.6202190
H	-2.8068560	1.0079190	-1.6140930
H	-0.8199020	0.0720180	0.5196780
H	-0.4866110	0.0415010	-1.2857890
H	1.6782120	-2.4751180	-1.3716090
H	1.2518880	-2.5139690	1.2933540
H	2.7812020	-0.6077390	2.4301910
H	4.0486830	0.7023280	0.4197060
H	3.4835020	-0.5504450	-1.9208550

CpRh(CO)-Cycloheptane 1,2-Migration (1)

Final Energy = -691.8310611640

C	2.7625820	-0.8695830	1.4243350
C	1.7379940	-1.7786240	1.0889890
C	1.8076520	-2.0616810	-0.3336260
C	2.8632050	-1.3191000	-0.8926700
C	3.3791570	-0.4746200	0.1713610
Rh	1.3749820	0.1926850	-0.0323140
C	1.5647380	2.0098800	-0.3831540
O	1.6602890	3.1314560	-0.5945910
C	-1.6303040	1.0021540	0.2300600
C	-2.9712610	1.3153200	0.9371110
C	-3.7894600	0.0902320	1.4034030
C	-1.6130430	-0.2500500	-0.6772500
C	-4.6998540	-0.4920690	0.2997530
C	-2.8640190	-0.4527870	-1.5620260
C	-3.9856470	-1.2353720	-0.8453420
H	-1.3460990	1.8798560	-0.3620630
H	-2.7559990	1.9630120	1.7939040
H	-4.4298720	0.3993780	2.2372690
H	-5.4181500	-1.1832780	0.7571330
H	-1.4828560	-1.1483020	-0.0616750
H	-2.5758660	-1.0169250	-2.4560420
H	-0.8465420	0.8806270	0.9984570
H	-3.6021450	1.9082070	0.2631660
H	-3.1239670	-0.6885970	1.7993790
H	-0.7206030	-0.1873680	-1.3246310
H	-5.2910270	0.3323220	-0.1219110
H	-3.2386780	0.5172360	-1.9147720
H	-3.5533650	-2.1667350	-0.4544000
H	-4.7408260	-1.5322880	-1.5832110
H	1.1565220	-2.7432640	-0.8642120
H	1.0359750	-2.2283900	1.7782930
H	2.9997780	-0.4880820	2.4063580
H	4.2205040	0.1984650	0.0774140
H	3.1862810	-1.3205610	-1.9232430

CpRh(CO)-Cycloheptane 1,2-Migration (2)

Final Energy = -691.8310914780

C	-2.5903970	-1.5120480	-0.8339490
C	-1.4253340	-2.0757470	-0.2817500
C	-1.3795260	-1.7636410	1.1363850
C	-2.5170360	-1.0048220	1.4720410
C	-3.2060240	-0.7286080	0.2236760
Rh	-1.3259860	0.2221490	-0.0432640
C	-1.7870970	1.9860190	-0.4092840

O	-2.0499460	3.0775380	-0.6347430
C	1.6270050	1.1793730	0.4136800
C	2.8303700	0.9041380	1.3448910
C	4.2005490	0.7613320	0.6425420
C	1.6414620	0.4292600	-0.9432640
C	4.4917240	-0.6768160	0.1607480
C	2.1282630	-1.0357990	-0.8972480
C	3.6599040	-1.1681090	-1.0394920
H	0.7129380	0.9275710	0.9805770
H	2.8757780	1.7138810	2.0812200
H	4.9849530	1.0419670	1.3544540
H	5.5526740	-0.7572840	-0.1051780
H	2.2749490	0.9785090	-1.6511280
H	1.6630980	-1.5836570	-1.7246000
H	1.5606410	2.2540230	0.2087740
H	2.6456340	-0.0137520	1.9166310
H	4.2791210	1.4675330	-0.1948900
H	0.6305910	0.4673730	-1.3860310
H	4.3340200	-1.3568950	1.0090300
H	1.7862000	-1.5209190	0.0274410
H	3.9650390	-0.6153890	-1.9384850
H	3.9125490	-2.2193780	-1.2236850
H	-0.6072130	-2.0903820	1.8198400
H	-0.6889070	-2.6652190	-0.8110820
H	-2.9268600	-1.5841490	-1.8576470
H	-4.1396660	-0.1899700	0.1351700
H	-2.7897930	-0.6380710	2.4505450

CpRh(CO)-Cycloheptane 1,2-Migration (3)

Final Energy = -691.8296498920

C	-3.1801880	-0.8568480	-0.8103020
C	-2.2297600	-1.8633460	-0.5435050
C	-1.8958630	-1.8367070	0.8685900
C	-2.6197030	-0.7989960	1.4839370
C	-3.3274990	-0.1035380	0.4209860
Rh	-1.2917250	0.1916670	-0.0802540
C	-1.1482690	2.0449800	-0.1119660
O	-1.0576140	3.1864900	-0.1339760
C	2.4097260	1.5508020	-0.0177170
C	3.4925810	1.0078870	0.9432380
C	4.5133330	0.0271770	0.3230930
C	1.8347380	0.5366520	-1.0339900
C	4.0348580	-1.4406380	0.3435790
C	1.6192170	-0.9032110	-0.5099090
C	2.8825370	-1.7873530	-0.6177270
H	1.5932060	1.9582140	0.5895790

H	4.0214000	1.8680730	1.3686020
H	5.4457470	0.0829690	0.8962470
H	4.8806030	-2.0979740	0.1073970
H	2.4928170	0.4785690	-1.9102380
H	0.8387190	-1.3837300	-1.1135880
H	2.8190720	2.3969030	-0.5823420
H	3.0088810	0.5045650	1.7899020
H	4.7631540	0.3317290	-0.7023060
H	0.8857440	0.9378350	-1.4220560
H	3.7313220	-1.6848150	1.3707710
H	1.2613880	-0.8837500	0.5310340
H	3.2450470	-1.7227450	-1.6528560
H	2.6017620	-2.8346710	-0.4532180
H	-1.2088350	-2.5131850	1.3586400
H	-1.8348950	-2.5696700	-1.2616040
H	-3.6536890	-0.6419960	-1.7567280
H	-4.0065110	0.7256840	0.5662440
H	-2.6106530	-0.5301040	2.5299240

CpRh(CO)-Cycloheptane 1,2-Migration (4)

Final Energy = -691.8300508660

C	2.5473460	-1.0839030	1.3036570
C	1.7107340	-1.9277290	0.5472960
C	2.0199530	-1.7575340	-0.8601620
C	3.0479470	-0.8035560	-0.9887920
C	3.2914980	-0.2839370	0.3455330
Rh	1.2788370	0.2635940	-0.0228160
C	1.3016770	2.1079240	0.2241030
O	1.3031440	3.2424560	0.3790990
C	-3.2418860	1.5811580	-0.2824800
C	-4.3812090	0.5653850	-0.0411740
C	-4.0694320	-0.5696410	0.9598600
C	-1.8128500	0.9958910	-0.4069390
C	-3.3903380	-1.7897110	0.3021230
C	-1.6936060	-0.3809680	-1.1007280
C	-1.9349330	-1.5747370	-0.1511330
H	-3.4757760	2.1411280	-1.1958010
H	-5.2576630	1.1268930	0.3016370
H	-5.0092740	-0.9092940	1.4095990
H	-3.4066830	-2.6322700	1.0041380
H	-1.3683460	0.9063410	0.5966790
H	-0.6764020	-0.4755680	-1.5163840
H	-3.2360410	2.3157600	0.5313070
H	-4.6723040	0.1082160	-0.9953260
H	-3.4506620	-0.1910960	1.7848390
H	-1.2077510	1.7294930	-0.9515680

H	-3.9965730	-2.0948290	-0.5618470
H	-2.3692980	-0.4354140	-1.9649790
H	-1.3007090	-1.4348760	0.7349800
H	-1.5860400	-2.4938260	-0.6384740
H	1.5474570	-2.2976990	-1.6696410
H	0.9731640	-2.6137240	0.9411190
H	2.5851520	-0.9976590	2.3794720
H	4.0459260	0.4482380	0.5995450
H	3.5196270	-0.4730460	-1.9023460

CpRh(CO)-Cycloheptane 1,2-Migration (5)

Final Energy = -691.8301850200

C	-3.1819820	-0.6816310	-0.7600130
C	-2.2191500	-1.7054310	-0.8042070
C	-1.7071170	-1.9133690	0.5376910
C	-2.3818480	-1.0533270	1.4311290
C	-3.2042370	-0.1887450	0.6097630
Rh	-1.2382810	0.2595020	-0.0378540
C	-1.1700920	2.1127220	0.1143390
O	-1.1165400	3.2526660	0.2082550
C	4.0457420	0.8491590	0.6903830
C	3.7221890	-0.5750640	1.1982400
C	3.5234370	-1.6489170	0.1040610
C	3.2904260	1.3062550	-0.5784560
C	2.0721100	-1.7166010	-0.4193130
C	1.8083680	0.8773030	-0.6728670
C	1.6161970	-0.5281010	-1.2871970
H	3.8399540	1.5548110	1.5042000
H	4.5298610	-0.8830360	1.8716630
H	3.7721220	-2.6296470	0.5251460
H	1.9411310	-2.6353050	-1.0041540
H	3.8027010	0.9224450	-1.4700800
H	1.2813550	1.5969840	-1.3091060
H	5.1209870	0.9236500	0.4872650
H	2.8135460	-0.5455590	1.8126870
H	4.2216860	-1.4841630	-0.7275660
H	3.3579000	2.3979510	-0.6380050
H	1.4040510	-1.8015920	0.4484470
H	1.3388690	0.9244510	0.3241960
H	2.1509110	-0.5531650	-2.2466890
H	0.5522880	-0.6733770	-1.5431610
H	-0.9616530	-2.6496210	0.8071880
H	-1.9055520	-2.2509740	-1.6837510
H	-3.7577080	-0.2938770	-1.5876090
H	-3.8713830	0.5764940	0.9826630
H	-2.2603410	-1.0008960	2.5027510

CpRh(CO)-Cycloheptane 1,2-Migration (6)

Final Energy = -691.8308086150

C	-2.9797830	-0.8225230	-1.1336220
C	-2.3371600	-1.8147310	-0.3704710
C	-2.4447290	-1.4681820	1.0354510
C	-3.1599890	-0.2603660	1.1542790
C	-3.3779530	0.2175320	-0.1993230
Rh	-1.2627840	0.2011200	-0.0270180
C	-0.8049520	1.9563520	-0.4377630
O	-0.5245090	3.0379200	-0.6893220
C	3.9330320	1.1685630	0.4728700
C	4.5928710	-0.1818890	0.1063860
C	3.8810040	-0.9982730	-0.9966220
C	2.3881170	1.1867410	0.4758670
C	2.7599670	-1.9093780	-0.4514840
C	1.7104550	-0.0627760	1.0815290
C	1.4894940	-1.1975800	0.0548180
H	4.2988540	1.4709000	1.4616670
H	5.6264370	0.0193000	-0.1966660
H	4.6201610	-1.6408200	-1.4883800
H	2.4629850	-2.6217030	-1.2305630
H	2.0239710	1.3087700	-0.5519410
H	0.7268650	0.2309830	1.4869660
H	4.2760280	1.9392690	-0.2277650
H	4.6607670	-0.8117440	1.0024410
H	3.4864780	-0.3311490	-1.7744580
H	2.0590790	2.0809320	1.0164610
H	3.1773990	-2.5064050	0.3710670
H	2.2843800	-0.4352100	1.9410070
H	0.9564830	-0.7754600	-0.8173440
H	0.8304250	-1.9571910	0.4918080
H	-2.0603570	-2.0630520	1.8532630
H	-1.8574830	-2.7041210	-0.7564810
H	-3.0951760	-0.7987820	-2.2071630
H	-3.9255330	1.1124600	-0.4620410
H	-3.4326570	0.2483080	2.0670410

CpRh(CO)-Cycloheptane 1,2-Migration (7)

Final Energy = -691.8308269680

C	3.2567970	-0.2014560	0.9793560
C	2.5623740	-1.4280280	0.9302560
C	2.3306980	-1.7858030	-0.4577220
C	2.8498520	-0.7685290	-1.2771440
C	3.3180760	0.2822240	-0.3869740
Rh	1.2361710	0.2129040	0.0097430
C	0.6921590	1.9461100	-0.3851630

O	0.3588420	3.0158720	-0.6224830
C	-4.4525640	0.0392000	-0.6705670
C	-3.4759080	-1.0370930	-1.1992220
C	-2.7793950	-1.8992440	-0.1219620
C	-4.0107890	0.7915410	0.6067540
C	-1.4812700	-1.2635890	0.4215010
C	-2.5053960	1.1299920	0.6968810
C	-1.6664120	-0.0128250	1.3068620
H	-4.6207810	0.7656190	-1.4746990
H	-4.0312620	-1.6878340	-1.8838920
H	-2.5201870	-2.8697930	-0.5596550
H	-0.9254350	-2.0137810	0.9959750
H	-4.2805160	0.2014200	1.4916820
H	-2.3787120	2.0141070	1.3314040
H	-5.4259250	-0.4254060	-0.4713810
H	-2.6971150	-0.5581560	-1.8058760
H	-3.4673750	-2.1076750	0.7088180
H	-4.5964100	1.7151910	0.6726290
H	-0.8567660	-1.0060920	-0.4542280
H	-2.1161740	1.4045750	-0.2922850
H	-2.1337200	-0.3138850	2.2545880
H	-0.6708430	0.3771180	1.5839170
H	1.8399540	-2.6889780	-0.7942990
H	2.2821090	-2.0333020	1.7821160
H	3.6101700	0.3124560	1.8609060
H	3.8108750	1.1910450	-0.7045890
H	2.8503520	-0.7392580	-2.3568330

CpRh(CO)-Cycloheptane 1,3-Migration (1)

Final Energy = -691.8312528300

C	3.0318000	-0.1971990	1.0561970
C	2.3536250	-1.4228410	0.9020700
C	2.1989460	-1.6984500	-0.5154450
C	2.7730240	-0.6429780	-1.2488640
C	3.1778340	0.3577420	-0.2770940
Rh	1.0708520	0.2576280	-0.0162330
C	0.5259030	2.0129790	-0.2952950
O	0.1702290	3.0887740	-0.4637790
C	-1.7011570	-0.3737870	1.6253310
C	-2.6237170	0.8172620	1.2462370
C	-3.9180250	0.4728630	0.4767650
C	-1.7988730	-1.6374450	0.7510000
C	-3.6957000	0.2635180	-1.0379010
C	-1.6820920	-1.3784880	-0.7644930
C	-3.0291100	-1.0636610	-1.4453720
H	-0.6505860	-0.0177940	1.6123530

H	-2.8836600	1.3493430	2.1675580
H	-4.6139840	1.3104630	0.6003170
H	-4.6622600	0.3257160	-1.5522710
H	-2.7459120	-2.1544470	0.9476740
H	-1.2498660	-2.2592740	-1.2520800
H	-1.8853060	-0.6642710	2.6664220
H	-2.0644620	1.5381130	0.6384380
H	-4.4119030	-0.4042060	0.9151460
H	-1.0047650	-2.3231150	1.0696240
H	-3.0915940	1.1006260	-1.4136060
H	-0.9664050	-0.5511240	-0.9595760
H	-3.7163080	-1.8921940	-1.2246190
H	-2.8877280	-1.0598650	-2.5327010
H	1.7319750	-2.5822160	-0.9289330
H	2.0264740	-2.0744630	1.7011810
H	3.3261270	0.2722590	1.9831450
H	3.6834040	1.2843110	-0.5128460
H	2.8418150	-0.5583830	-2.3233160

CpRh(CO)-Cycloheptane 1,3-Migration (2)

Final Energy = -691.8312528340

C	-2.7730350	-0.6429440	-1.2488730
C	-2.1989770	-1.6984340	-0.5154650
C	-2.3536510	-1.4228350	0.9020520
C	-3.0318120	-0.1971850	1.0561910
C	-3.1778320	0.3577720	-0.2770940
Rh	-1.0708540	0.2576220	-0.0162260
C	-0.5258760	2.0129650	-0.2952880
O	-0.1701850	3.0887550	-0.4637670
C	2.6237010	0.8172500	1.2462470
C	3.9180100	0.4728830	0.4767610
C	3.6956740	0.2635480	-1.0379050
C	1.7011640	-0.3738210	1.6253310
C	3.0291240	-1.0636500	-1.4453760
C	1.7989030	-1.6374730	0.7509930
C	1.6821120	-1.3785060	-0.7644990
H	2.8836400	1.3493270	2.1675720
H	4.6139560	1.3104930	0.6003180
H	4.6622260	0.3257870	-1.5522870
H	2.8877490	-1.0598650	-2.5327060
H	0.6505850	-0.0178450	1.6123550
H	1.0048090	-2.3231600	1.0696140
H	2.0644250	1.5380940	0.6384600
H	4.4119050	-0.4041830	0.9151280
H	3.0915330	1.1006380	-1.4135930
H	1.8853120	-0.6643070	2.6664220

H	3.7163440	-1.8921630	-1.2246130
H	2.7459520	-2.1544570	0.9476640
H	0.9664150	-0.5511470	-0.9595580
H	1.2498920	-2.2592890	-1.2520950
H	-2.0265140	-2.0744680	1.7011600
H	-1.7320170	-2.5822010	-0.9289640
H	-2.8418180	-0.5583370	-2.3233250
H	-3.6833870	1.2843500	-0.5128410
H	-3.3261360	0.2722690	1.9831420

CpRh(CO)-Cycloheptane 1,4-Migration (1)

Final Energy = -691.8314585480

C	-2.6086680	-0.8275200	-1.1762210
C	-1.7651340	-1.8097630	-0.6184980
C	-1.8251510	-1.7199270	0.8295390
C	-2.6860200	-0.6640750	1.1791430
C	-3.0808560	-0.0233970	-0.0657490
Rh	-0.9774390	0.2700310	-0.0081760
C	-0.8098680	2.1205300	-0.0442370
O	-0.6850720	3.2587660	-0.0708750
C	2.6992820	1.3691760	0.6525040
C	2.1238090	0.2225100	1.5125650
C	2.7636110	-1.1680180	1.3077180
C	3.0555110	1.0116820	-0.8099890
C	2.1280680	-1.9689330	0.1511100
C	2.0932020	0.0374560	-1.5225490
C	2.4140970	-1.4490770	-1.2696830
H	1.9750770	2.1926360	0.6578190
H	2.2026210	0.5178920	2.5648110
H	2.6399870	-1.7504010	2.2276690
H	2.4615580	-3.0122160	0.2085210
H	4.0598860	0.5711930	-0.8440160
H	2.1420170	0.2180970	-2.6022000
H	3.6035130	1.7582060	1.1355120
H	1.0352810	0.1302360	1.3356760
H	3.8456950	-1.0663590	1.1490850
H	3.1168370	1.9457650	-1.3788670
H	1.0400210	-1.9806980	0.3096740
H	1.0399780	0.2558400	-1.2510330
H	3.4755920	-1.6073780	-1.5044060
H	1.8465170	-2.0633300	-1.9793730
H	-1.3017650	-2.3712490	1.5162250
H	-1.1901430	-2.5415080	-1.1702530
H	-2.8089980	-0.6586960	-2.2238130
H	-3.7716330	0.8049930	-0.1456200
H	-2.9579920	-0.3483910	2.1756100

CpRh(CO)-Cycloheptane 1,4-Migration (2)

Final Energy = -691.8310895370

C	-2.7724740	-0.4831840	-1.2473830
C	-2.0988460	-1.6184570	-0.7613440
C	-2.1495880	-1.6053280	0.6893720
C	-2.8713070	-0.4713490	1.1135310
C	-3.1454130	0.3035130	-0.0825090
Rh	-1.0244850	0.2812490	0.0064900
C	-0.6053160	2.0930830	-0.0368850
O	-0.3536230	3.2099370	-0.0665230
C	3.5117060	0.8106200	-0.8336790
C	2.9620880	1.0715570	0.5889200
C	2.9915760	-0.1223890	1.5680860
C	3.2104210	-0.5751940	-1.4518560
C	1.7729950	-1.0601810	1.4329370
C	1.8098790	-1.1610130	-1.1634090
C	1.7337750	-1.9336700	0.1682110
H	3.1149490	1.5908970	-1.4940060
H	3.5267210	1.9073980	1.0166790
H	3.0018980	0.2686970	2.5915600
H	1.7181630	-1.7149660	2.3111160
H	3.9531050	-1.3020450	-1.0994380
H	1.5370890	-1.8450300	-1.9748450
H	4.6002520	0.9434810	-0.8272350
H	1.9256250	1.4242260	0.5220340
H	3.9200560	-0.6967540	1.4460810
H	3.3565390	-0.4976300	-2.5348700
H	0.8573870	-0.4364320	1.4740370
H	1.0475870	-0.3566230	-1.1908000
H	2.5674180	-2.6480960	0.1983910
H	0.8125240	-2.5287190	0.1890250
H	-1.7273720	-2.3666210	1.3318620
H	-1.6269480	-2.3857460	-1.3603390
H	-2.9290150	-0.2115830	-2.2809020
H	-3.7086320	1.2264190	-0.1110140
H	-3.1134900	-0.1946380	2.1288370

CpRh(CO)-Cyclooctane σ -complex (1)

Final Energy = -731.1297780220

C	2.5534430	-0.9649190	1.5304860
C	1.9215420	-1.8950440	0.6777200
C	2.4555630	-1.7449620	-0.6637120
C	3.4003400	-0.7000070	-0.6513670
C	3.3785850	-0.1324340	0.6834110
Rh	1.3955920	0.2124590	-0.0612310
C	1.2442720	2.0636780	-0.0175670

O	1.1442760	3.2051000	0.0031270
H	3.9826490	-0.3430140	-1.4881630
H	4.0152520	0.6711560	1.0272270
H	2.3981320	-0.8469600	2.5926690
H	1.1916370	-2.6356780	0.9763840
H	2.1811290	-2.3491010	-1.5174970
C	-1.1088570	-0.0118280	-0.6351150
C	-1.9680980	1.2128160	-1.0455970
C	-3.6570270	-1.6817360	0.5600910
C	-2.8557600	1.7910830	0.0776570
C	-3.5654910	-0.3704490	1.3786560
C	-4.0039140	0.9142780	0.6265550
H	-0.9672560	0.0025690	0.4486460
H	-2.2035120	2.0717170	0.9162290
H	-3.1403760	-2.4795850	1.1095930
H	-2.5529090	-0.2328730	1.7713160
H	-0.1302700	0.1136190	-1.2008690
H	-4.7133790	-1.9764810	0.5160890
H	-3.2922930	2.7261920	-0.2939460
H	-4.2032630	-0.5007550	2.2600390
C	-1.6291280	-1.3988010	-1.0830130
H	-1.0599800	-2.1735440	-0.5537770
H	-1.4048420	-1.5237940	-2.1499650
C	-3.1373100	-1.6458110	-0.8900030
H	-3.7019400	-0.9004330	-1.4611010
H	-3.3724650	-2.6122960	-1.3521640
H	-1.2999680	2.0169100	-1.3717990
H	-4.5761880	1.5437900	1.3170310
H	-4.6959950	0.6552080	-0.1850160
H	-2.5789450	0.9567060	-1.9197780

CpRh(CO)-Cyclooctane σ -complex (2)

Final Energy = -731.1299722500

C	2.4531280	-0.9250680	1.5017450
C	1.8274040	-1.8715990	0.6620470
C	2.3328660	-1.7056800	-0.6888650
C	3.2576960	-0.6443380	-0.6948050
C	3.2447170	-0.0747160	0.6387870
Rh	1.2354380	0.2237400	-0.0497820
C	1.0331050	2.0681800	0.0440080
O	0.9074880	3.2059310	0.0991760
H	3.8187520	-0.2774730	-1.5417630
H	3.8695460	0.7425420	0.9720080
H	2.3131870	-0.8080080	2.5661580
H	1.1213330	-2.6293350	0.9741200
H	2.0532790	-2.3137730	-1.5386370

C	-1.0930930	-0.0613350	-1.1426010
C	-2.0618710	1.1376100	-1.3141880
C	-3.1528270	-1.6780020	0.8804990
C	-2.6162790	1.7637090	-0.0147310
C	-2.8635380	-0.3166690	1.5582200
C	-3.5361510	0.9106940	0.8875610
H	-0.6858890	0.0128630	-0.0907700
H	-1.7660150	2.1053220	0.5904720
H	-2.4750390	-2.4342550	1.2979300
H	-1.7842150	-0.1455580	1.6332520
H	-0.3019190	0.0283570	-1.8954870
H	-4.1672080	-1.9868900	1.1640080
H	-3.1666700	2.6688430	-0.2990270
H	-3.2159010	-0.3939020	2.5928040
C	-1.7008210	-1.4780590	-1.2976550
H	-0.9819140	-2.2117260	-0.9112450
H	-1.7964410	-1.6768910	-2.3727270
C	-3.0789860	-1.7244170	-0.6572770
H	-3.8053860	-1.0205400	-1.0785680
H	-3.4132820	-2.7191110	-0.9767270
H	-1.5265580	1.9334710	-1.8441330
H	-3.9049190	1.5783220	1.6741980
H	-4.4237880	0.5930480	0.3256450
H	-2.8876590	0.8370890	-1.9711820

CpRh(CO)-Cyclooctane σ -complex (3)

Final Energy = -731.1294926380

C	-3.2363860	-0.8333840	-0.9464880
C	-2.1726260	-1.7571080	-0.8720820
C	-1.8196110	-1.9472770	0.5232450
C	-2.6613140	-1.1420370	1.3166520
C	-3.4598060	-0.3535780	0.4012790
Rh	-1.4502440	0.2580410	-0.0350870
C	-1.5035450	2.0932370	0.2458340
O	-1.5299000	3.2256080	0.4194420
H	-2.6651700	-1.0722930	2.3944640
H	-4.2277820	0.3498900	0.6922170
H	-3.7404400	-0.4947920	-1.8396260
H	-1.7150160	-2.2698010	-1.7073230
H	-1.0547980	-2.6214580	0.8852620
C	1.6953620	-0.9959000	-1.0808210
C	1.0937400	0.2750720	-0.4282790
C	4.5367280	-0.6758640	0.5112680
C	1.9307880	1.5695230	-0.5484310
C	4.3629150	0.6162870	-0.3260370
C	3.2878000	1.6090440	0.1899660

H	2.4194720	-0.6951840	-1.8434320
H	2.1104240	1.7651860	-1.6142190
H	5.1487400	-1.3863880	-0.0596810
H	4.1533710	0.3686880	-1.3712730
H	0.9035690	-1.5327440	-1.6142890
H	5.1207500	-0.4197650	1.4045400
H	1.3199660	2.4017780	-0.1804600
H	5.3346820	1.1222390	-0.3350950
C	2.3382400	-1.9864240	-0.0828760
H	2.8918730	-2.7458410	-0.6499900
H	1.5279350	-2.5177920	0.4339710
C	3.2571090	-1.3840550	0.9968800
H	2.6790660	-0.6969410	1.6253460
H	3.5628240	-2.2004670	1.6624890
H	0.1607060	0.5177700	-1.0316860
H	3.6706740	2.6292590	0.0751940
H	3.1297120	1.4695430	1.2666390
H	0.8732650	0.0872040	0.6296890

CpRh(CO)-Cyclooctane σ -complex (4)

Final Energy = -731.1300111980

C	3.3334720	-0.3065180	0.8277360
C	2.4782140	-1.4014350	1.0538120
C	2.0086240	-1.8891810	-0.2298090
C	2.5997260	-1.1199750	-1.2568490
C	3.3198860	-0.0524030	-0.6003090
Rh	1.2836730	0.2718720	-0.0080370
C	0.9987940	2.0491990	-0.4678430
O	0.8197780	3.1447960	-0.7518410
H	2.4767920	-1.2538380	-2.3213070
H	3.9036340	0.7073520	-1.1016240
H	3.8526020	0.2757520	1.5749690
H	2.2208070	-1.8235310	2.0157230
H	1.3558760	-2.7403810	-0.3690550
C	-1.7012030	-1.3376330	1.1819740
C	-1.0539170	0.0663210	1.0629690
C	-4.0734220	-0.6559080	-0.9960530
C	-1.9976800	1.2811260	1.2166240
C	-4.2071180	0.3919230	0.1361280
C	-3.1070150	1.4862380	0.1627050
H	-2.6090040	-1.2473730	1.7861240
H	-2.4707110	1.2042980	2.2054070
H	-4.7606910	-1.4873730	-0.7916060
H	-4.2451720	-0.1045370	1.1109690
H	-1.0256900	-1.9884230	1.7487940
H	-4.4237240	-0.1918370	-1.9269350

H	-1.3760570	2.1835750	1.2417140
H	-5.1838600	0.8730090	0.0141460
C	-2.0110220	-2.0524130	-0.1552130
H	-2.6374810	-2.9283880	0.0569340
H	-1.0649390	-2.4387370	-0.5552890
C	-2.6649780	-1.2153310	-1.2711860
H	-1.9953840	-0.3948530	-1.5538910
H	-2.7297350	-1.8532290	-2.1611130
H	-0.2928600	0.1700160	1.8432390
H	-3.5755130	2.4503290	0.3891780
H	-2.6595410	1.6001710	-0.8326140
H	-0.6170080	0.1313090	0.0144850

CpRh(CO)-Cyclooctane σ -complex (5)

Final Energy = -731.1292121630

C	3.0887540	-0.6132850	1.3871240
C	2.1737040	-1.6512680	1.1133690
C	2.2291520	-1.9634450	-0.3030760
C	3.1740000	-1.1125800	-0.9133230
C	3.6191000	-0.1878280	0.1097670
Rh	1.5186960	0.2097740	-0.0643440
C	1.4697060	2.0139970	-0.5047590
O	1.4331320	3.1265640	-0.7770700
H	3.4595580	-1.1016930	-1.9549040
H	4.3667350	0.5808560	-0.0298760
H	3.3015860	-0.1723420	2.3497520
H	1.5533380	-2.1603750	1.8390170
H	1.6601980	-2.7407780	-0.7948160
C	-4.2062660	0.5396270	1.0232890
C	-4.7276040	-0.0917340	-0.2945730
C	-1.0613230	0.1011590	0.2248490
C	-4.1609160	-1.4888620	-0.6338900
C	-1.6954960	-1.3117220	0.2341570
C	-2.6529770	-1.6182390	-0.9468680
H	-3.8663410	-0.2546650	1.6952610
H	-4.3940080	-2.1633750	0.2019250
H	-0.5984110	0.2935300	1.1997660
H	-2.2201240	-1.4723590	1.1809160
H	-5.0414880	1.0238250	1.5413340
H	-0.3043760	0.0708910	-0.6267340
H	-4.7143350	-1.8743880	-1.4991340
H	-0.8709300	-2.0320020	0.2240980
C	-3.1019180	1.6100530	0.8511940
H	-2.6701250	1.8396920	1.8339080
H	-3.5792390	2.5350450	0.5033030
C	-1.9673460	1.2932580	-0.1406820

H	-2.3870310	1.1367560	-1.1403050
H	-1.3329590	2.1829330	-0.2188860
H	-5.8150780	-0.2046020	-0.2203860
H	-2.4855230	-2.6531680	-1.2655200
H	-2.3943300	-0.9954950	-1.8124650
H	-4.5569090	0.5946060	-1.1336910

CpRh(CO)-Cyclooctane σ -complex (6)

Final Energy = -731.1297147220

C	2.9606370	-0.7139700	1.4492260
C	2.0567200	-1.7310240	1.0787120
C	2.1895880	-1.9736830	-0.3457530
C	3.1735910	-1.1078980	-0.8634500
C	3.5667030	-0.2348430	0.2237500
Rh	1.4782260	0.1955110	-0.0334640
C	1.4561390	2.0284900	-0.3321100
O	1.4334630	3.1598370	-0.5133990
H	3.5195030	-1.0548330	-1.8852480
H	4.3271150	0.5316340	0.1634930
H	3.1182700	-0.3157960	2.4407260
H	1.3952200	-2.2694890	1.7436690
H	1.6426200	-2.7212490	-0.9044330
C	-3.6713650	0.7288190	1.2421450
C	-4.6593250	0.0402640	0.2633580
C	-1.0463710	0.0047130	-0.5457340
C	-4.3082410	-1.4135140	-0.1252900
C	-1.6892680	-1.3622480	-0.1998380
C	-3.0187780	-1.6708360	-0.9372440
H	-3.1293320	-0.0350920	1.8087930
H	-4.2537320	-2.0096060	0.7963720
H	-0.3724220	0.2636800	0.3385900
H	-1.8456390	-1.4487830	0.8797900
H	-4.2417440	1.2964980	1.9855370
H	-0.4992000	-0.1036660	-1.4882540
H	-5.1494820	-1.8195660	-0.7007120
H	-0.9518720	-2.1304980	-0.4557310
C	-2.6771600	1.7142220	0.5843440
H	-1.9209000	2.0070730	1.3245470
H	-3.2240410	2.6300660	0.3266440
C	-1.9697760	1.2300980	-0.6935270
H	-2.7118050	1.0158490	-1.4703330
H	-1.3634240	2.0575190	-1.0792320
H	-5.6500250	0.0089240	0.7305770
H	-3.0210060	-2.7341220	-1.2025440
H	-3.0580380	-1.1272300	-1.8892970
H	-4.7765070	0.6504480	-0.6414110

CpRh(CO)-Cyclooctane σ -complex (7)

Final Energy = -731.1294794850

C	-2.8107230	-0.9838490	-1.3423000
C	-2.0186120	-1.8936840	-0.6112490
C	-2.3157950	-1.7391390	0.8003530
C	-3.2894530	-0.7316620	0.9504590
C	-3.5082750	-0.1709630	-0.3678400
Rh	-1.4332260	0.2362800	0.0131140
C	-1.3193200	2.0837000	-0.1480700
O	-1.2388120	3.2226420	-0.2458950
H	-3.7354200	-0.3920520	1.8736810
H	-4.2183630	0.6101840	-0.6022200
H	-2.8376560	-0.8632440	-2.4152010
H	-1.3260090	-2.6123420	-1.0281360
H	-1.8791620	-2.3260670	1.5974140
C	2.3800570	-1.7106150	-0.5577560
C	1.6291440	-1.3744790	0.7569240
C	4.2595280	0.9965600	-0.3930770
C	1.0232640	0.0453870	0.8316330
C	2.7929480	1.4891440	-0.4497520
C	1.9691430	1.2679910	0.8456180
H	1.9926600	-1.0813840	-1.3654610
H	0.4423440	0.1617520	-0.1451130
H	4.6746310	1.0096810	-1.4092070
H	2.2683420	1.0315290	-1.2946950
H	2.1408980	-2.7396270	-0.8478850
H	4.8385070	1.7300640	0.1827980
H	0.3869960	0.1027090	1.7204510
H	2.8205530	2.5616000	-0.6700240
C	3.9232770	-1.6080930	-0.4835470
H	4.3279630	-1.6547530	-1.5028850
H	4.2944660	-2.5023580	0.0336660
C	4.5144340	-0.3839560	0.2412330
H	4.1705590	-0.3751970	1.2820240
H	5.6006710	-0.5267550	0.2952140
H	0.7981830	-2.0770090	0.8800650
H	1.3433270	2.1487320	1.0229570
H	2.6372000	1.1915940	1.7126750
H	2.2872750	-1.5288700	1.6211280

CpRh(CO)-Cyclooctane σ -complex (8)

Final Energy = -731.1290503230

C	3.0454470	-0.8371760	1.3043820
C	2.1472070	-1.8156110	0.8362710
C	2.2565730	-1.8916820	-0.6094360
C	3.2350790	-0.9708390	-1.0399260

C	3.6344340	-0.2211880	0.1319530
Rh	1.5458370	0.2238590	-0.0670080
C	1.5213020	2.0792980	-0.1367410
O	1.5026020	3.2242980	-0.1811610
H	3.5665300	-0.8023430	-2.0538590
H	4.3905210	0.5517340	0.1491530
H	3.2158500	-0.5509880	2.3318640
H	1.4968960	-2.4283800	1.4460310
H	1.7049220	-2.5744410	-1.2416580
C	-2.8195270	-1.7890390	0.4806750
C	-1.6610070	-1.2933950	-0.4244970
C	-4.5019250	1.0252080	0.2077440
C	-1.0544960	0.0726260	-0.0265540
C	-3.1371990	1.3887070	0.8413850
C	-1.9257420	1.3462180	-0.1268690
H	-2.7295680	-1.3295690	1.4695950
H	-0.6831830	-0.0006150	1.0029110
H	-5.2384970	0.8895860	1.0103980
H	-2.9340550	0.7495450	1.7058760
H	-2.7002270	-2.8658590	0.6441310
H	-4.8419170	1.8901240	-0.3762560
H	-0.2220820	0.2432410	-0.7856360
H	-3.2279910	2.4040540	1.2424900
C	-4.2417430	-1.5701470	-0.0898410
H	-4.9738300	-1.7665180	0.7042400
H	-4.4153210	-2.3318120	-0.8610160
C	-4.5374100	-0.1990360	-0.7262110
H	-3.8546910	-0.0347920	-1.5677920
H	-5.5397950	-0.2491610	-1.1686620
H	-0.8443330	-2.0214440	-0.3818440
H	-1.2706850	2.1946550	0.0939330
H	-2.2628510	1.4862260	-1.1611700
H	-1.9851030	-1.2649330	-1.4720980

CpRh(CO)-Cyclooctane σ -complex (9)

Final Energy = -731.1295127900

C	-3.2259530	-0.5645470	-0.7210400
C	-2.2970120	-1.6224760	-0.7663100
C	-1.7894280	-1.8543100	0.5738230
C	-2.4060480	-0.9431390	1.4555800
C	-3.2019930	-0.0530100	0.6351170
Rh	-1.1976020	0.2744630	-0.0529400
C	-0.9672140	2.1042680	0.1683650
O	-0.8159050	3.2322250	0.3033880
H	-2.2589390	-0.8715720	2.5231370
H	-3.8237870	0.7488360	1.0089800

H	-3.7925930	-0.1620380	-1.5477490
H	-2.0222110	-2.1920090	-1.6441020
H	-1.0806420	-2.6246270	0.8468700
C	3.3011800	1.2447290	-0.4033320
C	2.9507720	0.9943540	1.0877900
C	1.6368790	-1.4151650	-1.4364700
C	3.2658250	-0.4232400	1.6171760
C	2.7259980	-1.9227650	-0.4620790
C	2.4750760	-1.6191920	1.0394390
H	4.0879980	0.5493460	-0.7115970
H	4.3367350	-0.6160470	1.4620310
H	2.0115980	-1.5005910	-2.4648580
H	3.7051900	-1.5293440	-0.7514370
H	3.7371910	2.2448840	-0.5028370
H	0.7731300	-2.0877000	-1.3658520
H	3.1114590	-0.4152540	2.7031850
H	2.7920350	-3.0076590	-0.6014460
C	2.1119890	1.1823440	-1.3914480
H	2.5023620	1.1596560	-2.4172480
H	1.5419190	2.1146550	-1.3006720
C	1.1131390	0.0193990	-1.2283750
H	0.7341490	0.0786330	-0.1634690
H	0.3071940	0.1852720	-1.9540690
H	3.5310870	1.6935590	1.7000300
H	2.7659150	-2.4996450	1.6235130
H	1.4021380	-1.4796240	1.2250780
H	1.8981400	1.2391230	1.2783030

CpRh(CO)-Cyclooctane σ -complex (10)

Final Energy = -731.1293011060

C	-3.2872080	-0.8435880	-0.7286450
C	-2.2496190	-1.7973810	-0.6596510
C	-1.7966530	-1.8980340	0.7157820
C	-2.5370140	-0.9909980	1.4991350
C	-3.3798060	-0.2452580	0.5855720
Rh	-1.3892350	0.2414280	-0.0541310
C	-1.3385900	2.0907520	0.1111220
O	-1.3052030	3.2319790	0.2097080
H	-2.4503160	-0.8322470	2.5640500
H	-4.0945420	0.5121320	0.8768620
H	-3.8489220	-0.5576610	-1.6055630
H	-1.8771640	-2.3915040	-1.4833710
H	-1.0318680	-2.5742670	1.0733880
C	3.3717510	1.4482290	-0.4027940
C	3.5011920	0.9560620	1.0629280
C	1.6125770	-1.1874470	-1.3275260

C	4.0331540	-0.4844930	1.2381650
C	2.9738710	-1.7168040	-0.8171480
C	3.1701380	-1.6578400	0.7210820
H	4.0604820	0.8834370	-1.0383470
H	5.0170840	-0.5462790	0.7525290
H	1.6521620	-1.0832990	-2.4194130
H	3.7960160	-1.1885420	-1.3088890
H	3.7048540	2.4903300	-0.4603020
H	0.8508510	-1.9478140	-1.1161730
H	4.2112700	-0.6472520	2.3083550
H	3.0520560	-2.7581550	-1.1489210
C	1.9400630	1.4086830	-0.9890190
H	1.9900810	1.5747440	-2.0726740
H	1.3807380	2.2545410	-0.5726320
C	1.1201210	0.1342980	-0.7069860
H	1.0140340	0.0107970	0.3756490
H	0.1237900	0.3350910	-1.2192230
H	4.2005840	1.6149740	1.5894950
H	3.6665100	-2.5799400	1.0437300
H	2.1945570	-1.6537340	1.2245660
H	2.5410920	1.0674610	1.5830040

CpRh(CO)-Cyclooctane TS (1)

Final Energy = -731.1115070140

C	2.6500570	-0.7131090	1.5113010
C	1.8270230	-1.7349970	0.9880530
C	2.1152870	-1.8677400	-0.4181030
C	3.1716340	-0.9671640	-0.7498830
C	3.4481740	-0.1993070	0.4224650
Rh	1.3161960	0.2182790	-0.1235830
C	1.1946250	2.0757170	0.0110930
O	1.1432500	3.2130410	0.0872910
H	3.6314030	-0.8451620	-1.7195580
H	4.1884100	0.5846810	0.5032470
H	2.6727290	-0.3659270	2.5342940
H	1.0913740	-2.3053860	1.5381010
H	1.6536330	-2.5781090	-1.0894670
C	-0.9039730	0.0541040	-0.3059880
C	-1.7502910	1.2284170	-0.8759830
C	-3.6064980	-1.7198530	0.3908030
C	-2.8437100	1.7658250	0.0764200
C	-3.7147270	-0.4233310	1.2289360
C	-4.0461870	0.8573400	0.4194930
H	-1.0060950	0.0660280	0.7798700
H	-2.3571360	2.0619970	1.0164190
H	-3.1729110	-2.5121520	1.0153740

H	-2.7953210	-0.2614730	1.8009010
H	0.2701710	0.3210310	-1.2937530
H	-4.6253160	-2.0474780	0.1460000
H	-3.2389470	2.6898200	-0.3643830
H	-4.5011820	-0.5873350	1.9744330
C	-1.3128610	-1.3425690	-0.8390190
H	-0.8457780	-2.1098290	-0.2094990
H	-0.8924090	-1.4764520	-1.8441570
C	-2.8259480	-1.6350970	-0.9343860
H	-3.3020300	-0.8991140	-1.5909770
H	-2.9359960	-2.6000560	-1.4450560
H	-1.1037670	2.0782390	-1.1110690
H	-4.7424570	1.4687320	1.0048030
H	-4.5839370	0.5892090	-0.4991080
H	-2.1948950	0.9324400	-1.8347280

CpRh(CO)-Cyclooctane TS (2)

Final Energy = -731.1093941350

C	2.5615330	-1.0581400	1.4860640
C	1.7125300	-1.9133120	0.7214350
C	2.1241730	-1.8513540	-0.6590170
C	3.1727870	-0.9107600	-0.7614560
C	3.4122070	-0.3805420	0.5611410
Rh	1.3101000	0.1936770	0.0336020
C	1.4138160	2.0391850	-0.2099370
O	1.4952680	3.1706420	-0.3359740
H	3.6958920	-0.6265240	-1.6632190
H	4.1646440	0.3530040	0.8158100
H	2.5256310	-0.9054720	2.5547050
H	0.9372030	-2.5541210	1.1172800
H	1.6889300	-2.4122950	-1.4744050
C	-0.7715590	0.1495270	-0.7856160
C	-1.6919060	1.3948420	-0.7102600
C	-4.0008980	-1.5327230	-0.1120910
C	-2.5197590	1.6198870	0.5779290
C	-4.0226550	-0.5047170	1.0401040
C	-3.9354730	0.9870630	0.6373240
H	-0.1385890	0.4462160	0.5988700
H	-1.9441890	1.3006170	1.4581830
H	-3.9572080	-2.5355330	0.3326350
H	-3.2183670	-0.7218190	1.7533420
H	-0.3946280	0.1170830	-1.8130550
H	-4.9540120	-1.4778060	-0.6534860
H	-2.6530940	2.7022250	0.6867770
H	-4.9562970	-0.6640280	1.5922190
C	-1.4515980	-1.2060010	-0.4798080

H	-1.5350120	-1.3418610	0.6036490
H	-0.7828440	-1.9998720	-0.8241230
C	-2.8510780	-1.3845860	-1.1324320
H	-3.0653420	-0.5407610	-1.7943540
H	-2.8492740	-2.2706620	-1.7762040
H	-1.0620200	2.2742880	-0.8721340
H	-4.5033630	1.5604070	1.3788980
H	-4.4462040	1.1477300	-0.3222690
H	-2.3812150	1.3783680	-1.5637150

CpRh(CO)-Cyclooctane TS (3)

Final Energy = -731.1111542300

C	-3.3056830	-0.7124500	-0.7630800
C	-2.2562990	-1.6435830	-0.9846010
C	-1.6764640	-1.9725730	0.2905580
C	-2.3786370	-1.2710200	1.3079890
C	-3.3424260	-0.4382210	0.6490780
Rh	-1.3444260	0.2510470	-0.0918740
C	-1.4043990	2.0839490	0.2363410
O	-1.4738440	3.2069860	0.4270870
H	-2.1981720	-1.3251840	2.3715240
H	-4.0352200	0.2324710	1.1387070
H	-3.9421880	-0.2702030	-1.5155200
H	-1.9521770	-2.0465530	-1.9402460
H	-0.8573880	-2.6617610	0.4461150
C	1.4644420	-1.0052680	-0.8685010
C	0.8857280	0.2194750	-0.1071390
C	4.5050110	-0.6140390	0.2778490
C	1.6674200	1.5315230	-0.3583500
C	4.1578470	0.6770030	-0.5062010
C	3.1221230	1.6137810	0.1695920
H	2.0704090	-0.6502020	-1.7075490
H	1.6836140	1.7357290	-1.4382150
H	5.0463630	-1.2979810	-0.3889940
H	3.8183260	0.4313210	-1.5168510
H	0.6555720	-1.5838980	-1.3237130
H	5.2102380	-0.3432410	1.0741980
H	1.1185450	2.3604650	0.0984070
H	5.0951480	1.2287090	-0.6400050
C	2.2823730	-1.9834690	0.0082070
H	2.7645290	-2.7196800	-0.6487400
H	1.5778110	-2.5467410	0.6354880
C	3.3401490	-1.3702400	0.9449550
H	2.8475320	-0.7091820	1.6665850
H	3.7706260	-2.1860650	1.5387550
H	-0.2186530	0.5790770	-1.1489220

H	3.4411060	2.6506400	0.0118430
H	3.1305570	1.4629760	1.2563900
H	0.8962550	0.0171190	0.9681900

CpRh(CO)-Cyclooctane TS (4)

Final Energy = -731.1096852570

C	2.8317380	-0.7837910	1.1032800
C	1.9129440	-1.7559440	0.5998600
C	1.9406290	-1.7219690	-0.8366810
C	2.8141880	-0.6762950	-1.2266670
C	3.3378650	-0.0730080	-0.0241100
Rh	1.1101150	0.2635020	-0.0312900
C	0.9424450	2.0852800	-0.3840960
O	0.8543030	3.1966170	-0.6279050
H	3.0483450	-0.3794790	-2.2388450
H	4.0441250	0.7453010	0.0084740
H	3.0646330	-0.5939610	2.1407420
H	1.3434230	-2.4545330	1.1969400
H	1.3767480	-2.3636900	-1.4983330
C	-1.4575520	-1.1444450	1.3243840
C	-0.7955380	0.2447790	1.1231390
C	-3.8704800	-0.8047490	-0.9209410
C	-1.7939870	1.4251130	1.0370920
C	-3.9776260	0.4077360	0.0349730
C	-2.8510290	1.4704020	-0.0888320
H	-2.3719180	-0.9882200	1.9095110
H	-2.3394930	1.4427550	1.9930360
H	-4.5567060	-1.5885640	-0.5738910
H	-4.0267540	0.0627130	1.0726960
H	-0.7979910	-1.7375570	1.9684870
H	-4.2363160	-0.4943300	-1.9081140
H	-1.2188080	2.3559510	1.0074850
H	-4.9431480	0.8876000	-0.1600790
C	-1.7772730	-2.0361820	0.0976420
H	-2.3873160	-2.8769410	0.4544710
H	-0.8355600	-2.4729090	-0.2562400
C	-2.4690150	-1.4072220	-1.1278370
H	-1.8113180	-0.6542650	-1.5737620
H	-2.5583070	-2.1961040	-1.8856020
H	-0.2214810	0.4411350	2.0335680
H	-3.3069540	2.4656590	-0.0448220
H	-2.3671420	1.4100230	-1.0714750
H	-0.4115250	0.1806780	-0.4101970

CpRh(CO)-Cyclooctane TS (5)

Final Energy = -731.1112009830

C	3.0203440	-0.4287350	1.3353810
C	2.1218290	-1.5135500	1.1958490
C	2.1133140	-1.9268530	-0.1845920
C	3.0246860	-1.1052950	-0.9025360
C	3.5284870	-0.1304360	0.0209150
Rh	1.3190720	0.2010580	-0.1054590
C	1.2164520	2.0012440	-0.5723530
O	1.1852820	3.0984360	-0.8853490
H	3.2575890	-1.1700430	-1.9552290
H	4.2406080	0.6484760	-0.2150080
H	3.2572300	0.0998670	2.2471730
H	1.5382940	-1.9616310	1.9887680
H	1.5424480	-2.7489120	-0.5929890
C	-4.1327160	0.3999600	0.9057330
C	-4.4178140	-0.1651240	-0.5099090
C	-0.8238220	0.1258810	0.5349630
C	-3.7513400	-1.5225140	-0.8274120
C	-1.4525040	-1.2861220	0.4094300
C	-2.2094810	-1.5748380	-0.9148750
H	-3.9083820	-0.4289250	1.5842290
H	-4.0782270	-2.2489740	-0.0702440
H	-0.5320540	0.2751500	1.5801730
H	-2.1274480	-1.4518080	1.2561570
H	-5.0490610	0.8570550	1.2960340
H	-0.0734360	0.0460010	-0.8260910
H	-4.1524280	-1.8788340	-1.7844920
H	-0.6518820	-2.0205020	0.5288480
C	-3.0266280	1.4819540	0.9835920
H	-2.7408310	1.6235560	2.0341250
H	-3.4699580	2.4326440	0.6595440
C	-1.7502690	1.2905560	0.1342350
H	-2.0268750	1.2072660	-0.9230770
H	-1.1835620	2.2222150	0.2167740
H	-5.4988220	-0.3119780	-0.6149030
H	-1.9454850	-2.5818800	-1.2568240
H	-1.8609660	-0.8947720	-1.7028480
H	-4.1404790	0.5741420	-1.2721960

CpRh(CO)-Cyclooctane TS (6)

Final Energy = -731.1130103890

C	2.6650510	-0.8650480	1.4886620
C	1.8348180	-1.8287710	0.8422250
C	2.1711690	-1.8535900	-0.5593130
C	3.1582190	-0.8701320	-0.7935070

C	3.4257940	-0.2181680	0.4666700
Rh	1.2710260	0.1936770	0.0119970
C	1.2290020	2.0288790	-0.3078770
O	1.2089570	3.1575820	-0.4760580
H	3.6186330	-0.6333530	-1.7418900
H	4.1448180	0.5743370	0.6220790
H	2.6735960	-0.6272900	2.5421800
H	1.1188960	-2.4772530	1.3274750
H	1.7286030	-2.5014900	-1.3033110
C	-3.2533140	0.7565540	1.2627490
C	-4.3444520	0.0378470	0.4254850
C	-0.8055790	-0.0357810	-0.7701360
C	-4.0332030	-1.4228240	0.0296000
C	-1.4363860	-1.3854340	-0.3349880
C	-2.8435360	-1.6932210	-0.9188730
H	-2.6387200	0.0136140	1.7819360
H	-3.8705050	-1.9994680	0.9510030
H	-0.1836070	0.3782990	0.5845840
H	-1.4808070	-1.4646110	0.7562840
H	-3.7367470	1.3428490	2.0522190
H	-0.4277300	-0.1749640	-1.7885310
H	-4.9338580	-1.8419640	-0.4365470
H	-0.7466990	-2.1720390	-0.6576900
C	-2.3562380	1.7249020	0.4598080
H	-1.5469170	2.0830600	1.1088110
H	-2.9548420	2.6076130	0.1999390
C	-1.7625310	1.1743160	-0.8494810
H	-2.5854340	0.9076320	-1.5238470
H	-1.2307070	1.9915770	-1.3485200
H	-5.2735360	0.0144640	1.0063260
H	-2.8784890	-2.7598070	-1.1695810
H	-2.9870160	-1.1606490	-1.8668840
H	-4.5696440	0.6261600	-0.4735650

CpRh(CO)-Cyclooctane TS (7)

Final Energy = -731.1109204580

C	-2.7119540	-0.9727200	-1.3090040
C	-1.9752800	-1.8630790	-0.4748010
C	-2.3048130	-1.5758030	0.8986810
C	-3.2059510	-0.4863140	0.9219210
C	-3.4096470	-0.0718350	-0.4447300
Rh	-1.2256030	0.2236850	-0.0342070
C	-1.0011600	2.0687120	-0.1704900
O	-0.8669990	3.1963370	-0.2840490
H	-3.6432910	-0.0305170	1.7983700
H	-4.0525740	0.7365940	-0.7647620

H	-2.6995630	-0.9446520	-2.3886020
H	-1.3219340	-2.6551490	-0.8132330
H	-1.9168860	-2.0997010	1.7617610
C	2.0861550	-1.7140700	-0.5765120
C	1.3797320	-1.4231610	0.7757540
C	3.9871970	0.9630030	-0.3761650
C	0.7510840	-0.0175360	0.9598630
C	2.5181040	1.4542350	-0.3540150
C	1.7439880	1.1701630	0.9618530
H	1.6899020	-1.0476850	-1.3481290
H	0.2622740	0.1305320	-0.5339470
H	4.3602820	1.0203480	-1.4071670
H	1.9698620	1.0358820	-1.2029740
H	1.8222820	-2.7262030	-0.9038440
H	4.5903470	1.6714580	0.2063360
H	0.2754790	-0.0156450	1.9461160
H	2.5367800	2.5358890	-0.5269160
C	3.6329530	-1.6371620	-0.5517120
H	3.9994530	-1.6572070	-1.5865260
H	4.0108350	-2.5516690	-0.0762260
C	4.2685640	-0.4436720	0.1870410
H	3.9792980	-0.4761490	1.2434520
H	5.3555660	-0.5915540	0.1773580
H	0.5815130	-2.1568850	0.9224940
H	1.1827320	2.0644510	1.2464790
H	2.4637060	1.0054190	1.7757530
H	2.0882560	-1.5886340	1.5998040

CpRh(CO)-Cyclooctane TS (8)

Final Energy = -731.1107753880

C	2.9473000	-0.7629720	1.2722760
C	2.0564190	-1.7686230	0.8274780
C	2.1516520	-1.8619520	-0.6076560
C	3.1256780	-0.9246920	-1.0527910
C	3.5602120	-0.1928910	0.0998720
Rh	1.3719420	0.2142140	-0.1141780
C	1.3297580	2.0768390	-0.1384890
O	1.3455420	3.2173090	-0.1757460
H	3.4406440	-0.7591560	-2.0725660
H	4.2945650	0.6009930	0.0995210
H	3.1153420	-0.4560650	2.2943070
H	1.4098000	-2.3670230	1.4548890
H	1.6076940	-2.5571700	-1.2314880
C	-2.6800500	-1.7925570	0.5506660
C	-1.4035330	-1.2975920	-0.1861620
C	-4.3012710	1.0072720	0.0419930

C	-0.8205730	0.0550630	0.2997100
C	-3.0378420	1.3472800	0.8685830
C	-1.6968650	1.3136340	0.0822340
H	-2.7321140	-1.3333900	1.5416420
H	-0.6402140	-0.0290270	1.3779190
H	-5.1486840	0.8784400	0.7282490
H	-2.9649850	0.6958290	1.7437830
H	-2.5811730	-2.8690730	0.7316570
H	-4.5415300	1.8789010	-0.5805670
H	0.0493810	0.2758110	-0.9725080
H	-3.1783950	2.3582430	1.2675900
C	-4.0085000	-1.5827400	-0.2162940
H	-4.8459000	-1.7790620	0.4661610
H	-4.0680530	-2.3473840	-1.0017380
C	-4.2131330	-0.2139680	-0.8910300
H	-3.4189790	-0.0502010	-1.6284860
H	-5.1447660	-0.2621060	-1.4681760
H	-0.6222370	-2.0497700	-0.0518490
H	-1.1083150	2.1773700	0.3988180
H	-1.8899700	1.4608270	-0.9883440
H	-1.5893460	-1.2576780	-1.2671650

CpRh(CO)-Cyclooctane TS (9)

Final Energy = -731.1031492230

C	3.1616730	-0.3184660	0.6421140
C	2.3218300	-1.4366080	0.8429800
C	1.7695310	-1.8225440	-0.4311000
C	2.3122650	-0.9665470	-1.4339770
C	3.1103330	0.0102560	-0.7617620
Rh	1.0078910	0.2602210	-0.0042500
C	0.7216280	2.0938600	-0.1699310
O	0.5557870	3.2142680	-0.3081090
H	2.1145570	-1.0122900	-2.4948350
H	3.6513010	0.8171000	-1.2368510
H	3.7204400	0.2116060	1.3998770
H	2.1110760	-1.9130030	1.7908260
H	1.1068090	-2.6593500	-0.6025430
C	-3.0757330	1.1715220	0.4728860
C	-2.8610480	0.9369890	-1.0457780
C	-1.2994910	-1.4240950	1.4240040
C	-3.1728350	-0.4919000	-1.5464850
C	-2.4350880	-1.9419430	0.5026240
C	-2.3237440	-1.6721630	-1.0216230
H	-3.8388790	0.4726600	0.8291490
H	-4.2250420	-0.7067550	-1.3112360
H	-1.6576520	-1.5420870	2.4582500

H	-3.3995890	-1.5661300	0.8573170
H	-3.5127920	2.1676010	0.6079480
H	-0.4471460	-2.1043720	1.3280150
H	-3.1011050	-0.4869440	-2.6413930
H	-2.4728220	-3.0261360	0.6613140
C	-1.8436940	1.1289350	1.4185600
H	-2.2418370	1.0701530	2.4428040
H	-1.3369890	2.0972720	1.3605540
C	-0.7673370	0.0239640	1.2993790
H	-0.5135000	0.1072460	-0.3142400
H	-0.1220360	0.1722630	2.1717850
H	-3.5396110	1.6064080	-1.5874940
H	-2.6777550	-2.5649390	-1.5507260
H	-1.2766380	-1.5458100	-1.3156320
H	-1.8519100	1.2338650	-1.3481150

CpRh(CO)-Cyclooctane TS (10)

Final Energy = -731.1106780680

C	-3.2183770	-0.9322220	-0.6425730
C	-2.1275530	-1.8433220	-0.5648220
C	-1.6477440	-1.8615560	0.7944310
C	-2.4140170	-0.9447440	1.5520600
C	-3.3451900	-0.3198260	0.6464350
Rh	-1.3139560	0.2236070	-0.1101480
C	-1.3170380	2.0797160	0.0607200
O	-1.3624230	3.2160210	0.1553900
H	-2.3063840	-0.7300500	2.6053250
H	-4.0773170	0.4284540	0.9174700
H	-3.8051780	-0.7044020	-1.5202550
H	-1.7525900	-2.4542450	-1.3738240
H	-0.8344840	-2.4705920	1.1653320
C	3.1731180	1.4891300	-0.3882330
C	3.5829710	0.9240860	0.9976740
C	1.3581230	-1.0987830	-1.1793140
C	4.1724960	-0.5038040	0.9867230
C	2.8005830	-1.6190670	-0.9405720
C	3.2593660	-1.6672710	0.5404580
H	3.7411310	0.9821340	-1.1731900
H	5.0602080	-0.5014600	0.3387660
H	1.2255280	-0.9085000	-2.2528770
H	3.5205600	-1.0389820	-1.5244000
H	3.4717370	2.5422440	-0.4437060
H	0.6741480	-1.9173970	-0.9325290
H	4.5342740	-0.7271660	1.9982860
H	2.8354400	-2.6326460	-1.3565180
C	1.6541770	1.4517230	-0.6987710

H	1.5045790	1.7158680	-1.7542440
H	1.1921630	2.2542260	-0.1154800
C	0.9070420	0.1414870	-0.3757410
H	1.0333270	-0.0670870	0.6894700
H	-0.3076290	0.4404290	-1.3035680
H	4.3497520	1.5781520	1.4282480
H	3.8242960	-2.5926470	0.7011960
H	2.3858820	-1.7305420	1.2021760
H	2.7302400	0.9704210	1.6870190

CpRh(CO)-Cyclooctane Product (1)

Final Energy = -731.1317175340

C	2.5941090	-0.5991860	1.5181120
C	1.7560130	-1.6346650	1.0369590
C	2.0694330	-1.8619510	-0.3454360
C	3.1582740	-0.9923010	-0.6919080
C	3.4655550	-0.1982030	0.4411080
Rh	1.2970910	0.2378350	-0.2058720
C	1.0542920	2.0620340	0.1174650
O	0.9341240	3.1752910	0.3049580
H	3.6288230	-0.9243980	-1.6624790
H	4.2274120	0.5669790	0.4926270
H	2.5967810	-0.1956330	2.5209260
H	0.9850610	-2.1380530	1.6030740
H	1.6159320	-2.6017380	-0.9881890
C	-0.8180160	0.0211190	-0.1701640
C	-1.6412230	1.1218950	-0.9039680
C	-3.5551470	-1.7196490	0.4555590
C	-2.8054410	1.7319010	-0.0853830
C	-3.7561800	-0.3639270	1.1772760
C	-4.0292860	0.8484060	0.2503630
H	-1.0449010	0.0852420	0.8985160
H	-2.3921220	2.1144250	0.8590850
H	-3.1401340	-2.4433940	1.1700970
H	-2.8958320	-0.1396600	1.8153160
H	0.9816620	0.5805220	-1.6969160
H	-4.5470260	-2.1009210	0.1791960
H	-3.1730340	2.6102190	-0.6319170
H	-4.6061050	-0.4872500	1.8586730
C	-1.1927280	-1.3996040	-0.6662600
H	-0.7602620	-2.1486840	0.0081260
H	-0.7254130	-1.5604150	-1.6462930
C	-2.6973270	-1.7223510	-0.8245480
H	-3.1462070	-1.0514940	-1.5641180
H	-2.7660100	-2.7268640	-1.2623130
H	-1.0037360	1.9596550	-1.1952490

H	-4.7602500	1.5013160	0.7417230
H	-4.5093510	0.5096510	-0.6767540
H	-2.0213640	0.7245020	-1.8536000

CpRh(CO)-Cyclooctane Product (6)

Final Energy = -731.1297299340

C	2.9497950	-0.7606700	1.4382190
C	2.0711940	-1.7714370	0.9943860
C	2.2376850	-1.9368400	-0.4386750
C	3.2114890	-1.0230850	-0.8878750
C	3.5672180	-0.2045080	0.2532300
Rh	1.4755610	0.1980870	-0.0231620
C	1.4276020	2.0378700	-0.2744700
O	1.3903980	3.1727250	-0.4294270
H	3.5744970	-0.9059380	-1.8983790
H	4.3127270	0.5787890	0.2486300
H	3.0817450	-0.4150640	2.4528580
H	1.4071070	-2.3563980	1.6162820
H	1.7170330	-2.6637990	-1.0475150
C	-3.6887420	0.7937120	1.1786180
C	-4.6626580	0.0452420	0.2301510
C	-1.0412850	-0.0347720	-0.5352880
C	-4.3059950	-1.4291260	-0.0649460
C	-1.6869600	-1.3790460	-0.1143470
C	-3.0077810	-1.7339440	-0.8461300
H	-3.1569380	0.0667020	1.8008140
H	-4.2610000	-1.9675710	0.8920260
H	-0.3745780	0.2690020	0.3405510
H	-1.8552870	-1.3989310	0.9668290
H	-4.2701940	1.4066280	1.8761450
H	-0.4873330	-0.1974910	-1.4659570
H	-5.1408190	-1.8706910	-0.6233070
H	-0.9454200	-2.1602020	-0.3139500
C	-2.6835930	1.7373100	0.4772080
H	-1.9360710	2.0715120	1.2086820
H	-3.2248810	2.6376680	0.1600000
C	-1.9621360	1.1799260	-0.7621730
H	-2.6964470	0.9230980	-1.5333880
H	-1.3505660	1.9834590	-1.1881220
H	-5.6593020	0.0408850	0.6856210
H	-3.0066250	-2.8113770	-1.0463720
H	-3.0372060	-1.2487220	-1.8296390
H	-4.7688760	0.5989440	-0.7115300

CpRh(CO)-Cyclooctane 1,1-Migration (1)

Final Energy = -731.1290194150

C	2.4868320	-0.9221920	1.5399730
C	1.8781120	-1.8800480	0.7019850
C	2.4137970	-1.7385760	-0.6404910
C	3.3402540	-0.6784650	-0.6427270
C	3.2982150	-0.0865350	0.6810450
Rh	1.3116050	0.2092830	-0.0652390
C	1.1190630	2.0563320	-0.0155860
O	0.9920430	3.1948300	0.0109500
H	3.9205470	-0.3259430	-1.4827870
H	3.9185170	0.7339430	1.0148220
H	2.3243030	-0.7883840	2.5992110
H	1.1625580	-2.6306600	1.0100200
H	2.1532250	-2.3612990	-1.4854950
C	-1.0873970	-0.0567770	-0.9062500
C	-1.9814470	1.1807570	-1.1781760
C	-3.4459760	-1.6664350	0.7048010
C	-2.6626110	1.7871680	0.0676390
C	-3.1971490	-0.3524280	1.4857110
C	-3.7239980	0.9380960	0.8031550
H	-0.8056440	-0.0412900	0.1660630
H	-1.8778400	2.0590610	0.7873180
H	-2.8695650	-2.4728220	1.1770720
H	-2.1323270	-0.2353900	1.7130780
H	-0.1825960	0.0431660	-1.5497750
H	-4.5031020	-1.9346120	0.8287050
H	-3.1342320	2.7292920	-0.2371690
H	-3.6890810	-0.4644590	2.4584020
C	-1.6930170	-1.4423400	-1.2365610
H	-1.0617080	-2.2186780	-0.7856490
H	-1.6384220	-1.5904810	-2.3225300
C	-3.1566810	-1.6574840	-0.8086590
H	-3.7888780	-0.9075830	-1.2970580
H	-3.4789170	-2.6242220	-1.2144970
H	-1.3617150	1.9679430	-1.6214160
H	-4.1633160	1.5833480	1.5720530
H	-4.5442110	0.6902770	0.1169650
H	-2.7341500	0.9260160	-1.9343120

CpRh(CO)-Cyclooctane 1,1-Migration (2)

Final Energy = -731.1287903630

C	3.2964620	-0.5585940	0.9157440
C	2.3245220	-1.5731310	1.0152910
C	1.9036880	-1.9434130	-0.3238660
C	2.6247370	-1.1706220	-1.2581090

C	3.3973170	-0.2174660	-0.4899740
Rh	1.3716120	0.2704860	0.0031670
C	1.2715680	2.0770200	-0.4162530
O	1.2023400	3.1913950	-0.6735840
H	2.5607080	-1.2268150	-2.3346970
H	4.0816940	0.5093590	-0.9055630
H	3.8186520	-0.0781760	1.7301240
H	1.9652370	-2.0249850	1.9300110
H	1.1840220	-2.7165510	-0.5573430
C	-1.6859920	-1.1640100	1.1283830
C	-1.0785770	0.2131600	0.7619390
C	-4.3151440	-0.6956600	-0.7786110
C	-1.9925460	1.4468350	0.9429170
C	-4.3174030	0.4567680	0.2563750
C	-3.2406150	1.5528580	0.0385620
H	-2.5136060	-1.0067330	1.8263640
H	-2.3211270	1.4730600	1.9908780
H	-4.9641660	-1.5011640	-0.4106850
H	-4.2252610	0.0570710	1.2710630
H	-0.9383820	-1.7501580	1.6747670
H	-4.7843500	-0.3217640	-1.6977480
H	-1.3817620	2.3440930	0.7892550
H	-5.3088690	0.9211200	0.2137240
C	-2.1515580	-2.0140000	-0.0773930
H	-2.7379850	-2.8628650	0.2972370
H	-1.2589510	-2.4411960	-0.5526840
C	-2.9491480	-1.2868640	-1.1768680
H	-2.3276070	-0.4999760	-1.6193690
H	-3.1234770	-2.0065500	-1.9860410
H	-0.2099350	0.3950050	1.4333200
H	-3.6899080	2.5311200	0.2428120
H	-2.9356120	1.5789810	-1.0151180
H	-0.7544560	0.1867840	-0.3029870

CpRh(CO)-Cyclooctane 1,1-Migration (3)

Final Energy = -731.1278445480

C	2.9658860	-0.9684160	1.2823340
C	2.1232410	-1.8941660	0.6334340
C	2.3295260	-1.7872790	-0.8001960
C	3.2969400	-0.7928290	-1.0445800
C	3.6012010	-0.1907520	0.2380660
Rh	1.5191420	0.2266420	-0.0272790
C	1.4493550	2.0794130	0.0856840
O	1.3965890	3.2221260	0.1536560
H	3.6849710	-0.4864610	-2.0048240
H	4.3308410	0.5906330	0.4008510

H	3.0655600	-0.8159190	2.3468710
H	1.4556150	-2.5948010	1.1167550
H	1.8388110	-2.3961130	-1.5477340
C	-2.6653340	-1.7105860	0.6437480
C	-1.6689480	-1.3560520	-0.4915540
C	-4.4507770	1.0221420	0.1931450
C	-1.0511560	0.0585330	-0.4080550
C	-3.0197460	1.4894850	0.5536760
C	-1.9617950	1.2983820	-0.5643860
H	-2.4413670	-1.1011910	1.5246330
H	-0.5705370	0.1424750	0.5936540
H	-5.0594340	1.0116430	1.1066860
H	-2.6755760	0.9953920	1.4673020
H	-2.4952440	-2.7482090	0.9517430
H	-4.8967940	1.7811130	-0.4625610
H	-0.2910420	0.1291670	-1.2180270
H	-3.0807080	2.5548490	0.8012100
C	-4.1622960	-1.5871830	0.2688800
H	-4.7621860	-1.6560470	1.1856600
H	-4.4298270	-2.4618740	-0.3380580
C	-4.5852170	-0.3352130	-0.5226100
H	-4.0349140	-0.3022480	-1.4699880
H	-5.6389170	-0.4601540	-0.8004470
H	-0.8347870	-2.0651800	-0.4640780
H	-1.3048700	2.1739760	-0.5815570
H	-2.4511750	1.2708610	-1.5458910
H	-2.1477850	-1.4906840	-1.4694180

CpRh(CO)-Cyclooctane 1,1-Migration (4)

Final Energy = -731.1281358930

C	-3.0540980	-1.1469180	-1.0085700
C	-2.1655090	-1.9568290	-0.2720890
C	-2.2726440	-1.6134800	1.1346740
C	-3.2105800	-0.5731280	1.2715010
C	-3.6089860	-0.1932300	-0.0709550
Rh	-1.5097610	0.2355080	-0.0367160
C	-1.4506130	2.0473030	-0.4375340
O	-1.4089290	3.1648160	-0.6874270
H	-3.5249700	-0.0995240	2.1899790
H	-4.3482340	0.5588080	-0.3104060
H	-3.2311390	-1.1785170	-2.0734430
H	-1.5361310	-2.7391340	-0.6750640
H	-1.7303750	-2.0935200	1.9381520
C	1.9847730	1.3087360	-0.0671260
C	3.1549810	1.4065610	0.9460250
C	2.5663450	-1.9130570	-0.6487650

C	4.5245980	0.9054800	0.4344270
C	3.8397720	-1.1362710	-1.0583880
C	4.6919520	-0.5986860	0.1218790
H	2.3846700	1.3323800	-1.0853390
H	4.7764240	1.4723210	-0.4727440
H	1.9528640	-2.0872370	-1.5424900
H	3.5807560	-0.3086950	-1.7263010
H	1.3580500	2.2016560	0.0252120
H	2.8734620	-2.9035000	-0.2885530
H	5.2794250	1.1780240	1.1824700
H	4.4512940	-1.8185520	-1.6591990
C	1.0551460	0.0821130	0.1145880
H	0.4753440	-0.0345330	-0.8297660
H	0.3801320	0.3274370	0.9672800
C	1.6929320	-1.2799840	0.4494460
H	2.2747210	-1.1856260	1.3727830
H	0.8798590	-1.9784630	0.6793530
H	3.2859820	2.4609550	1.2138650
H	5.7508410	-0.7543440	-0.1133490
H	4.4979570	-1.1913550	1.0251830
H	2.8913340	0.8933660	1.8793210

CpRh(CO)-Cyclooctane 1,1-Migration (5)

Final Energy = -731.1285269100

C	-3.2909810	-0.6417340	-0.6965940
C	-2.3349150	-1.6751760	-0.7474940
C	-1.8098110	-1.8897160	0.5893960
C	-2.4415570	-0.9924300	1.4737700
C	-3.2686530	-0.1258330	0.6580840
Rh	-1.2886790	0.2603030	-0.0531580
C	-1.1216940	2.0968050	0.1678570
O	-1.0119910	3.2296730	0.3007910
H	-2.2877730	-0.9147830	2.5399790
H	-3.9100540	0.6585480	1.0358530
H	-3.8761990	-0.2576370	-1.5190730
H	-2.0527310	-2.2395850	-1.6261610
H	-1.0782060	-2.6400260	0.8580610
C	3.3510370	1.3283540	-0.4496060
C	3.2002360	0.9952680	1.0585180
C	1.6356090	-1.3358360	-1.3931560
C	3.6146500	-0.4359680	1.4701810
C	2.8560740	-1.8571440	-0.5978060
C	2.7893070	-1.6292450	0.9360930
H	4.1073590	0.6722270	-0.8914080
H	4.6617780	-0.5867680	1.1723910
H	1.8700220	-1.3517000	-2.4653520

H	3.7790840	-1.4189790	-0.9891830
H	3.7449080	2.3453740	-0.5536090
H	0.8068860	-2.0395290	-1.2466790
H	3.5996540	-0.4849200	2.5660240
H	2.9316760	-2.9317750	-0.7981220
C	2.0411410	1.2707080	-1.2714570
H	2.2845370	1.3096700	-2.3410030
H	1.4635220	2.1770110	-1.0539220
C	1.1190260	0.0638880	-1.0102730
H	0.8786030	0.0552620	0.0729170
H	0.2016230	0.2440980	-1.6147180
H	3.8347900	1.6817660	1.6300280
H	3.1730250	-2.5251870	1.4369910
H	1.7438990	-1.5336880	1.2584050
H	2.1732480	1.1979390	1.3892920

CpRh(CO)-Cyclooctane 1,2-Migration (1)

Final Energy = -731.1182267640

C	2.5474630	-1.0080050	1.5831450
C	1.6018740	-1.8442760	0.9484550
C	1.9868390	-2.0366570	-0.4375340
C	3.1404100	-1.2725320	-0.6873630
C	3.4290380	-0.5376760	0.5364450
Rh	1.5335460	0.2095140	-0.0559890
C	1.8584220	2.0208540	-0.3351060
O	2.0360590	3.1393980	-0.5042600
H	3.6838630	-1.2003220	-1.6181060
H	4.2808770	0.1125350	0.6822220
H	2.5662600	-0.7166920	2.6226770
H	0.7525200	-2.3159310	1.4244590
H	1.4647330	-2.6597650	-1.1508230
C	-1.8201590	-1.3136320	-0.4095020
C	-1.4217620	0.0008760	-1.1290220
C	-4.6149630	-0.0382390	0.7706890
C	-1.4318030	1.2781310	-0.2547990
C	-3.4635970	0.8277900	1.3378190
C	-2.7810190	1.7721000	0.3138160
H	-1.6315600	-1.2071500	0.6634250
H	-0.7502460	1.1195800	0.6010760
H	-4.8805120	-0.8038570	1.5114170
H	-2.7046390	0.1944500	1.8073060
H	-1.1562900	-2.1176940	-0.7470650
H	-5.4984430	0.6046810	0.6655380
H	-1.0000490	2.0944990	-0.8459500
H	-3.8851550	1.4309350	2.1495650
C	-3.2734010	-1.7850440	-0.6588770

H	-3.5091480	-2.5903910	0.0490370
H	-3.3139300	-2.2350620	-1.6592940
C	-4.3769770	-0.7122720	-0.5938790
H	-4.1786180	0.0575280	-1.3484620
H	-5.3178020	-1.1867220	-0.8985600
H	-0.3993830	-0.1093230	-1.5329600
H	-2.5816100	2.7333810	0.7999910
H	-3.4681180	1.9916940	-0.5134380
H	-2.0529960	0.1517830	-2.0142060

CpRh(CO)-Cyclooctane 1,2-Migration (2)

Final Energy = -731.1172780380

C	2.8131970	-0.7674280	1.5481190
C	2.1474880	-1.8302130	0.9100850
C	2.5418570	-1.8583060	-0.4862500
C	3.4686740	-0.8215380	-0.7209430
C	3.5425780	-0.0570340	0.5109280
Rh	1.5251800	0.1690990	-0.0852220
C	1.3349380	2.0174460	-0.1729840
O	1.2131430	3.1545410	-0.2341600
H	3.9756290	-0.5985370	-1.6479930
H	4.1884760	0.7943660	0.6772720
H	2.7510850	-0.4923380	2.5906420
H	1.4593380	-2.5224880	1.3760700
H	2.2020290	-2.5833430	-1.2136870
C	-1.4239370	-0.9044780	-0.3998630
C	-1.5655960	0.4719570	-1.1068030
C	-4.5206740	-0.8357560	0.7185110
C	-2.0758510	1.6273090	-0.2175860
C	-3.8126410	0.4052070	1.3148440
C	-3.5260210	1.5530830	0.3106490
H	-1.3069880	-0.7465440	0.6770030
H	-1.4015560	1.7184500	0.6450910
H	-4.4869090	-1.6505860	1.4536900
H	-2.8788180	0.1132040	1.8054670
H	-0.5009550	-1.3928750	-0.7441030
H	-5.5816730	-0.5866600	0.5873110
H	-1.9683340	2.5595990	-0.7853010
H	-4.4566110	0.7861160	2.1153970
C	-2.5699790	-1.9112150	-0.6738840
H	-2.4857720	-2.7452130	0.0347490
H	-2.4106790	-2.3378600	-1.6724610
C	-4.0056950	-1.3543330	-0.6372840
H	-4.1082850	-0.5657950	-1.3911500
H	-4.6772370	-2.1587700	-0.9618130
H	-0.5840050	0.7741290	-1.5047700

H	-3.7260000	2.5090070	0.8074640
H	-4.2289990	1.5006420	-0.5306490
H	-2.2020010	0.3715000	-1.9951880

CpRh(CO)-Cyclooctane 1,2-Migration (3)

Final Energy = -731.1178098670

C	-2.8630430	-1.5144970	-0.7399830
C	-1.7047740	-2.0794370	-0.1758210
C	-1.6425470	-1.7130190	1.2282520
C	-2.7675890	-0.9286810	1.5467030
C	-3.4605310	-0.6851060	0.2941950
Rh	-1.5698380	0.2278340	-0.0221270
C	-2.0127860	1.9723290	-0.4845440
O	-2.2688660	3.0514740	-0.7701430
H	-3.0270840	-0.5243470	2.5138840
H	-4.3872650	-0.1369860	0.1922410
H	-3.2079000	-1.6169590	-1.7583250
H	-0.9841090	-2.7016240	-0.6891740
H	-0.8684840	-2.0237670	1.9171390
C	1.4459920	0.6615810	0.5314180
C	1.4218760	0.3995390	-1.0028960
C	4.6364400	-0.0756150	0.8002320
C	1.9778970	-0.9712070	-1.4465030
C	3.9363770	-1.3446620	0.2555850
C	3.4792050	-1.2645290	-1.2250270
H	1.4603580	-0.2956110	1.0601510
H	1.3971800	-1.7513920	-0.9342610
H	4.7249570	-0.1595550	1.8913220
H	3.0802360	-1.6076500	0.8846890
H	0.5153590	1.1619990	0.8462430
H	5.6624200	-0.0645980	0.4102620
H	1.7659720	-1.0869250	-2.5165310
H	4.6451580	-2.1732490	0.3638710
C	2.6013570	1.5674370	1.0240050
H	2.6448960	1.5185840	2.1195360
H	2.3468710	2.6045040	0.7714930
C	3.9995890	1.2809360	0.4445350
H	3.9732290	1.3939950	-0.6451550
H	4.6718270	2.0691040	0.8049700
H	0.3844080	0.4456420	-1.3760460
H	3.6823450	-2.2281000	-1.7058760
H	4.0866750	-0.5277260	-1.7656000
H	1.9418110	1.2098890	-1.5288760

CpRh(CO)-Cyclooctane 1,2-Migration (4)

Final Energy = -731.1170420410

C	3.4694270	-0.2628000	1.1572350
C	2.5872790	-1.3447680	1.3504870
C	2.3118230	-1.9633580	0.0662810
C	3.0090840	-1.2613140	-0.9341670
C	3.6324650	-0.1232800	-0.2786430
Rh	1.5652580	0.2310500	0.0104860
C	1.3203840	1.9038490	-0.7657090
O	1.1602470	2.9336310	-1.2402930
H	3.0310000	-1.4835910	-1.9908150
H	4.2740830	0.5990710	-0.7647540
H	3.8899710	0.3784530	1.9175570
H	2.1989930	-1.6864790	2.3006430
H	1.6817620	-2.8296390	-0.0845090
C	-1.4557300	-0.7156070	0.5781810
C	-1.5603650	0.8330650	0.4936650
C	-4.4559030	-1.1814770	-0.6738280
C	-2.8164250	1.4516640	1.1492280
C	-4.6409580	-0.3543940	0.6218780
C	-4.1961000	1.1295930	0.5316350
H	-2.0452510	-1.0693150	1.4296590
H	-2.8333020	1.1485170	2.2052710
H	-4.6051310	-2.2438300	-0.4398960
H	-4.1244630	-0.8361810	1.4580300
H	-0.4214580	-1.0061980	0.8232770
H	-5.2611860	-0.9052060	-1.3667590
H	-2.6913750	2.5412900	1.1453080
H	-5.7064290	-0.3908760	0.8751300
C	-1.8467500	-1.4773030	-0.7107330
H	-1.9326830	-2.5466860	-0.4771440
H	-1.0146870	-1.3812900	-1.4204000
C	-3.1254070	-1.0104730	-1.4314130
H	-3.0108390	0.0368060	-1.7326970
H	-3.2008700	-1.5776990	-2.3671570
H	-0.6987400	1.2757120	1.0139830
H	-4.9278400	1.7466070	1.0653650
H	-4.2255830	1.4681760	-0.5116840
H	-1.4915110	1.1556810	-0.5525350

CpRh(CO)-Cyclooctane 1,2-Migration (5)

Final Energy = -731.1179174850

C	-3.2974810	-0.9453250	-1.0063480
C	-2.4903890	-1.9115150	-0.3784330
C	-2.4718580	-1.6471560	1.0493220
C	-3.2829700	-0.5266550	1.3186710

C	-3.6898990	-0.0020930	0.0281250
Rh	-1.5772490	0.1850970	-0.0234650
C	-1.3347080	1.9907580	-0.3958740
O	-1.1828700	3.1027490	-0.6250960
H	-3.5008910	-0.0972450	2.2852500
H	-4.3448980	0.8456130	-0.1204620
H	-3.5311810	-0.8761860	-2.0585120
H	-1.9753320	-2.7275060	-0.8671290
H	-1.9456230	-2.2421710	1.7839040
C	3.5996080	1.4886080	-0.1047920
C	4.5808040	0.5707390	0.6709200
C	1.3166620	-0.8864490	-0.3700760
C	4.8900960	-0.7891910	0.0047490
C	2.5882880	-1.4027940	-1.0862090
C	3.7450580	-1.8172980	-0.1380660
H	3.6302870	1.2321300	-1.1682130
H	5.2985770	-0.5929840	-0.9964170
H	0.6480130	-0.4495600	-1.1325160
H	2.9508460	-0.6564510	-1.7987390
H	3.9558940	2.5227490	-0.0425180
H	0.7937990	-1.7558340	0.0485480
H	5.6975080	-1.2656490	0.5748150
H	2.2893560	-2.2679980	-1.6880050
C	2.1379380	1.4885410	0.4071270
H	1.5036280	1.9849230	-0.3380370
H	2.0946740	2.1145910	1.3072890
C	1.5260330	0.1247460	0.7766180
H	2.1269350	-0.3442990	1.5642740
H	0.5470240	0.3188430	1.2500410
H	5.5381980	1.0941710	0.7730470
H	4.1946990	-2.7400280	-0.5217890
H	3.3455530	-2.0699490	0.8526080
H	4.2190240	0.4119590	1.6948180

CpRh(CO)-Cyclooctane 1,2-Migration (6)

Final Energy = -731.1181940660

C	3.3148750	-0.2279210	1.3485060
C	2.6066240	-1.4398850	1.2241240
C	2.6491730	-1.8728040	-0.1621000
C	3.3635310	-0.9196880	-0.9096930
C	3.6706210	0.1726620	0.0003670
Rh	1.5485410	0.1646300	-0.0465240
C	1.1392510	1.8774700	-0.6453050
O	0.8811370	2.9302030	-1.0152970
H	3.5876370	-0.9553700	-1.9656520
H	4.2471160	1.0509320	-0.2564970

H	3.4949280	0.3315720	2.2544270
H	2.1367290	-1.9873960	2.0303330
H	2.2096420	-2.7847030	-0.5430210
C	-1.4812670	-0.0379680	0.8336310
C	-2.1014700	1.3293540	0.4469810
C	-3.8470070	-1.7694580	-0.6285080
C	-3.5900780	1.5104320	0.8196150
C	-4.5483680	-0.9002620	0.4449770
C	-4.6392600	0.6147370	0.1221630
H	-2.0552180	-0.4837850	1.6518140
H	-3.6893840	1.3703560	1.9051540
H	-3.6415140	-2.7610930	-0.2043480
H	-4.0665990	-1.0328500	1.4187090
H	-0.4790690	0.1355410	1.2617380
H	-4.5598330	-1.9299940	-1.4475620
H	-3.8569340	2.5559650	0.6219520
H	-5.5620960	-1.2989710	0.5638810
C	-1.3394860	-1.0526390	-0.3309710
H	-1.0621710	-2.0322240	0.0783230
H	-0.5002370	-0.7387410	-0.9783830
C	-2.5579380	-1.2089170	-1.2600000
H	-2.7743750	-0.2452620	-1.7339590
H	-2.2676360	-1.8816500	-2.0759840
H	-1.5458300	2.1217120	0.9605210
H	-5.6226440	0.9790540	0.4403370
H	-4.6013490	0.7710900	-0.9633170
H	-1.9597870	1.5151840	-0.6252310

CpRh(CO)-Cyclooctane 1,3-Migration (1)

Final Energy = -731.1182553310

C	2.9577720	-1.0715530	1.3367970
C	1.8786940	-1.8983220	0.9709760
C	1.8815770	-2.0653810	-0.4721490
C	2.9616090	-1.3391250	-1.0099560
C	3.5569010	-0.6109930	0.0972720
Rh	1.5895850	0.1791240	-0.0063990
C	1.8715370	1.9993030	-0.2571820
O	2.0209330	3.1235280	-0.4170280
H	3.2535820	-1.2794960	-2.0480190
H	4.4326080	0.0197030	0.0263760
H	3.2440020	-0.7781960	2.3359470
H	1.1715320	-2.3587560	1.6478450
H	1.1806820	-2.6721800	-1.0293640
C	-2.6318810	0.5607550	-1.6394470
C	-3.1667610	-0.8929560	-1.5544280
C	-2.5446950	0.9331720	1.6296390

C	-4.4215560	-1.0933440	-0.6746600
C	-4.0166070	0.6231070	1.2615750
C	-4.3035750	-0.8439610	0.8459670
H	-3.4438990	1.2615860	-1.4223390
H	-5.2182040	-0.4447480	-1.0650110
H	-2.4135850	2.0210190	1.6916960
H	-4.3596000	1.2960860	0.4700290
H	-2.3290400	0.7712110	-2.6710250
H	-2.3596320	0.5437930	2.6388070
H	-4.7699230	-2.1236490	-0.8194730
H	-4.6222030	0.8697790	2.1407420
C	-1.4103110	0.8685630	-0.7406700
H	-1.2368750	1.9518160	-0.7317120
H	-0.5272270	0.4221180	-1.2338270
C	-1.4576760	0.3447100	0.7101280
H	-1.5378130	-0.7474780	0.7017550
H	-0.4877250	0.5696870	1.1900250
H	-3.4347230	-1.2237650	-2.5642070
H	-5.2573010	-1.1511850	1.2896890
H	-3.5463580	-1.5117200	1.2765460
H	-2.3672700	-1.5682560	-1.2234860

CpRh(CO)-Cyclooctane 1,4-Migration (1)

Final Energy = -731.1196662920

C	-2.6730660	-0.9276730	-1.3830300
C	-1.6540270	-1.8280540	-1.0196610
C	-1.6780570	-1.9836760	0.4226280
C	-2.7470990	-1.2308700	0.9570390
C	-3.2836720	-0.4636270	-0.1444840
Rh	-1.2741060	0.2267100	-0.0237240
C	-1.4338880	2.0801720	-0.0046480
O	-1.4949690	3.2237990	0.0102950
H	-3.0524460	-1.1749470	1.9911900
H	-4.1264910	0.2114510	-0.0844910
H	-2.9289530	-0.6033950	-2.3811460
H	-0.9658670	-2.3231180	-1.6906530
H	-1.0053490	-2.6182370	0.9847250
C	2.1185490	-1.7366370	0.1415140
C	2.2341740	-1.1367990	1.5672060
C	3.1193510	1.0170460	-1.3296270
C	1.5436650	0.2261580	1.7914820
C	1.8662410	1.4131330	-0.5095550
C	2.0570030	1.4623670	1.0259770
H	1.2223140	-1.3415940	-0.3486750
H	0.4622890	0.1096970	1.5638930
H	2.8116810	0.7816570	-2.3565490

H	1.0317680	0.7332140	-0.7564070
H	1.9545910	-2.8172760	0.2248350
H	3.7601460	1.9055050	-1.3991280
H	1.5776630	0.4506420	2.8648760
H	1.5426370	2.3969920	-0.8652480
C	3.3554560	-1.5351150	-0.7659870
H	3.0911480	-1.8222270	-1.7921170
H	4.1316850	-2.2400070	-0.4408560
C	3.9867340	-0.1309350	-0.7796710
H	4.3291450	0.1229830	0.2299950
H	4.8942770	-0.1820610	-1.3936220
H	1.7819380	-1.8364680	2.2793070
H	1.5102350	2.3265140	1.4198580
H	3.1127430	1.6376010	1.2663860
H	3.2911800	-1.0622120	1.8539270

CpRh(CO)-Cyclooctane 1,4-Migration (2)

Final Energy = -731.1184925480

C	-2.8724280	-0.6514450	-1.2368770
C	-2.2040810	-1.7103960	-0.5922980
C	-2.3025070	-1.5239460	0.8441460
C	-3.0341460	-0.3484540	1.1005380
C	-3.2786120	0.2703800	-0.1912840
Rh	-1.1588570	0.2722600	-0.0380000
C	-0.7329650	2.0757480	-0.1877770
O	-0.4621030	3.1859430	-0.2672340
H	-3.3035190	0.0536310	2.0659980
H	-3.8435220	1.1792280	-0.3481530
H	-3.0014050	-0.5133140	-2.3001220
H	-1.7109220	-2.5422450	-1.0773970
H	-1.9005100	-2.1991330	1.5876020
C	3.6793850	0.2664510	-0.9569260
C	2.8511070	1.3817670	-0.2676780
C	1.7811660	-2.1447620	0.2394080
C	2.6151220	1.2020620	1.2490690
C	2.3826390	-1.4061210	1.4600160
C	1.7892790	-0.0049850	1.7458080
H	4.3140070	-0.2272160	-0.2146730
H	3.5974190	1.1562820	1.7401800
H	2.4037100	-3.0204290	0.0144200
H	3.4682870	-1.3222470	1.3538260
H	4.3676080	0.7260460	-1.6749320
H	0.7961440	-2.5330050	0.5313290
H	2.1294430	2.1123440	1.6219160
H	2.2192030	-2.0468800	2.3335810
C	2.8476140	-0.7798190	-1.7375060

H	3.4970020	-1.6227230	-2.0089740
H	2.5279610	-0.3213390	-2.6818120
C	1.5848680	-1.3266840	-1.0479570
H	0.8968970	-0.4812500	-0.8596820
H	1.0500920	-1.9547290	-1.7700010
H	3.3776140	2.3349740	-0.3883750
H	1.6743420	0.1162130	2.8287470
H	0.7545740	0.0574860	1.3560450
H	1.8923010	1.5102800	-0.7857480

Cp*Rh(CO)-Cyclopentane σ -complex

Final Energy = -809.7369702520

C	-1.1031690	2.8028680	-0.9302180
C	-2.3352500	2.2050850	-0.5800910
C	-2.4888780	2.2608750	0.8750600
C	-1.3536090	2.9027000	1.4272710
C	-0.4232800	3.1127690	0.3243790
Rh	-0.6533380	0.9923340	0.3999660
C	1.0871090	0.3675110	0.5936700
O	2.1622010	-0.0179270	0.7172620
C	-3.0289360	-1.8632400	0.5866360
C	-1.6256380	-1.3733610	0.1050590
C	-0.7402400	-2.6408510	-0.0522510
C	-1.7554930	-3.8001240	-0.1347210
C	-2.8473950	-3.3742930	0.8667730
H	-3.3808340	-1.3152020	1.4645850
H	-3.7670130	-1.7180420	-0.2093320
H	-1.1944030	-0.7468400	0.9455490
H	-1.7073890	-0.8432100	-0.8458880
H	-0.0811910	-2.5758250	-0.9215060
H	-0.1066160	-2.7710050	0.8317440
H	-2.1802120	-3.8589300	-1.1444530
H	-1.3102380	-4.7710030	0.0998310
H	-3.7789770	-3.9366770	0.7589180
H	-2.4816240	-3.5248580	1.8893250
C	-1.1425570	3.3164640	2.8599870
H	-0.0903970	3.2396940	3.1455300
H	-1.4553720	4.3580600	3.0131870
H	-1.7209750	2.6894720	3.5436280
C	-3.7289830	1.8270810	1.6176660
H	-3.5042730	1.5849300	2.6599700
H	-4.4856460	2.6222340	1.6115480
H	-4.1800650	0.9436830	1.1562070
C	-3.3773660	1.6580730	-1.5242880
H	-3.8105370	0.7270630	-1.1432060
H	-4.2010650	2.3704260	-1.6586730

H	-2.9489800	1.4508800	-2.5085930
C	-0.5762940	3.0862740	-2.3128570
H	-1.0129540	2.4098660	-3.0523380
H	-0.8142600	4.1143900	-2.6165850
H	0.5096720	2.9701180	-2.3551560
C	0.8816750	3.8658320	0.4310290
H	1.5658050	3.5868360	-0.3747050
H	0.7105440	4.9478130	0.3690710
H	1.3815400	3.6576450	1.3806610

Cp*Rh(CO)-Cyclopentane TS

Final Energy = -809.7216850040

C	-1.2304490	2.9607460	-0.9383010
C	-2.4293130	2.3015710	-0.5162540
C	-2.4276330	2.2304490	0.9348380
C	-1.2151740	2.7996070	1.4096400
C	-0.4399010	3.1907420	0.2440160
Rh	-0.7004880	0.9907540	0.0874590
C	1.0453660	0.3431570	0.2352150
O	2.1197450	-0.0411860	0.3065840
C	-2.7486160	-1.6150580	-0.3109850
C	-1.5282240	-1.0323430	0.4411020
C	-0.5842570	-2.2500370	0.5694890
C	-1.5189590	-3.4988480	0.6606150
C	-2.9588100	-2.9733050	0.3909690
H	-3.6296120	-0.9685480	-0.2614930
H	-2.5099190	-1.7718820	-1.3711880
H	-1.8743740	-0.7528080	1.4438830
H	-0.9943540	-0.3090050	-0.7678610
H	0.0565050	-2.3270730	-0.3158000
H	0.0757830	-2.1562760	1.4356940
H	-1.2340090	-4.2440810	-0.0877880
H	-1.4516310	-3.9841850	1.6379090
H	-3.5560140	-3.6710360	-0.2031920
H	-3.4854090	-2.8128700	1.3382470
C	-0.8187960	3.0291550	2.8466270
H	0.2656270	2.9764190	2.9725570
H	-1.1453780	4.0203660	3.1868860
H	-1.2658080	2.2843760	3.5100810
C	-3.5490520	1.6762380	1.7757310
H	-3.2020470	1.4222750	2.7808120
H	-4.3614900	2.4063830	1.8757670
H	-3.9713470	0.7701700	1.3297890
C	-3.5899620	1.9293780	-1.4065670
H	-4.1843320	1.1222190	-0.9718680
H	-4.2552890	2.7900140	-1.5506850

H	-3.2471540	1.5999310	-2.3909120
C	-0.8834670	3.3798860	-2.3436900
H	-1.3346230	2.7100920	-3.0800710
H	-1.2467270	4.3960120	-2.5461880
H	0.1972810	3.3732300	-2.5058400
C	0.8770700	3.9285040	0.2872970
H	1.4542890	3.7646140	-0.6261310
H	0.7092110	5.0075970	0.3909430
H	1.4889150	3.6036480	1.1328360

Cp*Rh(CO)-Cyclopentane Product

Final Energy = -809.7466615460

C	-2.0255810	-0.7387270	-0.8541000
C	-1.0694910	-1.6358090	-0.2403550
C	-0.8959100	-1.2168620	1.1302140
C	-1.6686320	-0.0362320	1.3402540
C	-2.3730640	0.2568040	0.1027760
Rh	-0.1257220	0.3900580	-0.3063760
C	0.2166550	2.2269680	-0.3702740
O	0.4045210	3.3452300	-0.4513350
C	2.5534250	-1.1652600	-0.4491950
C	1.8963070	0.0750600	0.1953060
C	2.9491870	1.1620750	-0.1190450
C	4.3198260	0.4718010	0.1239510
C	4.0547850	-1.0558510	-0.0675570
H	2.1162040	-2.1127130	-0.1230470
H	2.4376500	-1.1100570	-1.5378530
H	1.8939630	-0.0710100	1.2877170
H	0.4770380	0.3957730	-1.7596680
H	2.8649020	1.4584720	-1.1717790
H	2.8321700	2.0647720	0.4885250
H	5.0891830	0.8446530	-0.5586260
H	4.6690990	0.6722880	1.1416070
H	4.7041110	-1.4964390	-0.8300750
H	4.2450970	-1.5931650	0.8671180
C	-1.8503130	0.6989540	2.6456640
H	-2.0340660	1.7640690	2.4820330
H	-2.7058100	0.2955270	3.2019840
H	-0.9656100	0.6074500	3.2805480
C	-0.0644680	-1.9240280	2.1672290
H	0.2315510	-1.2434070	2.9693150
H	-0.6358820	-2.7455700	2.6161750
H	0.8455850	-2.3446180	1.7324320
C	-0.5774510	-2.9230720	-0.8560170
H	0.2665730	-3.3341030	-0.2989410
H	-1.3755920	-3.6761040	-0.8555040

H	-0.2534720	-2.7739570	-1.8894410
C	-2.5896090	-0.8908500	-2.2435380
H	-1.8540210	-1.3346590	-2.9185340
H	-3.4708740	-1.5445290	-2.2264230
H	-2.8924640	0.0722380	-2.6612390
C	-3.3896730	1.3568110	-0.0816150
H	-3.4851460	1.6377550	-1.1332640
H	-4.3758980	1.0289860	0.2697040
H	-3.1189470	2.2532190	0.4826340

Cp*Rh(CO)-Cyclohexane Axial σ -complex

Final Energy = -849.0385121160

C	-1.1794290	2.8452510	-1.0085400
C	-2.4574220	2.5001320	-0.5115730
C	-2.4701350	2.7198640	0.9357290
C	-1.2063940	3.2159400	1.3351280
C	-0.3528510	3.1623080	0.1531380
Rh	-0.8943120	1.1246410	0.4609860
C	0.7423730	0.2552810	0.5761680
O	1.7526810	-0.2874270	0.6503540
C	-2.1999640	-1.0202870	1.2155560
C	-3.5871160	-1.4122290	0.6680270
C	-3.4630790	-2.4459690	-0.4679370
C	-2.6659670	-3.6844070	-0.0110030
C	-1.2802780	-3.2883640	0.5371280
C	-1.4029330	-2.2562470	1.6743220
H	-4.4581810	-2.7417510	-0.8177410
H	-4.1779330	-1.8391030	1.4898950
H	-4.1203940	-0.5223400	0.3166520
H	-1.6496640	-0.6088790	0.3058760
H	-2.2943690	-0.2988220	2.0311380
H	-3.2295670	-4.2043770	0.7759880
H	-2.5559600	-4.3887620	-0.8427440
H	-0.7449280	-4.1753410	0.8924730
H	-0.6782400	-2.8565530	-0.2740660
H	-1.9297320	-2.7110640	2.5245820
H	-0.4125820	-1.9566650	2.0305350
H	-2.9492210	-1.9797510	-1.3198970
C	-3.6622210	2.1091400	-1.3315750
H	-4.3144920	1.4221920	-0.7852850
H	-4.2614890	2.9927190	-1.5868460
H	-3.3680630	1.6218990	-2.2648900
C	-3.6850440	2.5296490	1.8103210
H	-4.4013820	3.3491200	1.6714080
H	-4.2075160	1.5968420	1.5727200
H	-3.4113350	2.4993260	2.8681300

C	-0.8023570	3.7210660	2.6959260
H	-0.9274010	4.8102840	2.7592710
H	-1.4075640	3.2692170	3.4861740
H	0.2453430	3.4938450	2.9085850
C	1.0567270	3.7006360	0.0848230
H	1.0491480	4.7837550	-0.0901270
H	1.5964200	3.5139800	1.0169820
H	1.6202670	3.2327940	-0.7266390
C	-0.7449910	2.9101390	-2.4493280
H	-0.8614260	3.9283340	-2.8441320
H	0.3048610	2.6280230	-2.5616570
H	-1.3399280	2.2385180	-3.0737910

Cp*Rh(CO)-Cyclohexane Equatorial σ -complex

Final Energy = -849.0383047280

C	-1.0336100	2.7911040	-1.0153270
C	-2.3229310	2.3917880	-0.5881290
C	-2.4984980	2.7748640	0.8138120
C	-1.3104590	3.3960960	1.2623390
C	-0.3460400	3.2874610	0.1711950
Rh	-0.7785070	1.2589320	0.6641110
C	0.8873750	0.5583470	1.0953120
O	1.9177570	0.1240780	1.3599570
C	-1.9019400	-1.0984270	0.7203170
C	-3.3600890	-1.3675090	1.1429470
C	-3.9540650	-2.5396120	0.3373340
C	-3.0853340	-3.8053060	0.4737880
C	-1.6288430	-3.5286330	0.0527110
C	-1.0250710	-2.3578850	0.8535020
H	-4.9775050	-2.7422520	0.6718440
H	-3.3862830	-1.6113640	2.2135010
H	-3.9651500	-0.4648240	1.0064920
H	-1.8827170	-0.7556380	-0.3211510
H	-1.5074950	-0.3283480	1.4559720
H	-3.1008030	-4.1407910	1.5198340
H	-3.5057900	-4.6183090	-0.1281700
H	-1.0170050	-4.4270670	0.1884070
H	-1.6026790	-3.2832670	-1.0178320
H	-0.9564560	-2.6387970	1.9129780
H	-0.0079430	-2.1445770	0.5106840
H	-4.0134410	-2.2547250	-0.7221690
C	-3.4018160	1.7664600	-1.4380920
H	-3.9119620	0.9554000	-0.9072980
H	-4.1641050	2.5061380	-1.7132260
H	-2.9878720	1.3525440	-2.3611570
C	-3.7896080	2.6475280	1.5842620

H	-4.4432730	3.5079150	1.3908470
H	-4.3425220	1.7489720	1.2968510
H	-3.6077620	2.5990010	2.6611460
C	-1.0750330	4.0701860	2.5885370
H	-1.2704330	5.1484590	2.5156380
H	-1.7305430	3.6625660	3.3625790
H	-0.0424980	3.9411820	2.9226780
C	1.0246510	3.9220680	0.1710360
H	0.9619050	4.9785480	-0.1182780
H	1.4831980	3.8714530	1.1620960
H	1.6936790	3.4194950	-0.5323750
C	-0.4662740	2.7380560	-2.4101340
H	-0.6111120	3.6967450	-2.9258660
H	0.6061220	2.5275290	-2.3949400
H	-0.9492610	1.9609760	-3.0083200

Cp*Rh(CO)-Cyclohexane Axial TS

Final Energy = -849.0208846100

C	-1.2451270	2.6954760	-0.9781370
C	-2.5303160	2.3495460	-0.4557300
C	-2.5251450	2.5961130	0.9758900
C	-1.2337120	3.0596310	1.3462140
C	-0.4159540	3.0535870	0.1448780
Rh	-1.0155580	0.9404720	0.4701680
C	0.6206600	0.1038300	0.7660050
O	1.6338810	-0.4052630	0.9177460
C	-2.1548690	-0.8013580	1.2910720
C	-3.4922000	-1.1985910	0.6214510
C	-3.3046120	-2.1626560	-0.5668000
C	-2.5081590	-3.4158150	-0.1507780
C	-1.1662280	-3.0369360	0.5080350
C	-1.3851130	-2.0767550	1.6934730
H	-4.2819940	-2.4524110	-0.9687830
H	-4.1167360	-1.6940200	1.3804560
H	-4.0364700	-0.3073780	0.2963460
H	-1.4871560	-0.4674900	-0.0744360
H	-2.3822850	-0.2303480	2.1973000
H	-3.1054370	-3.9973650	0.5651550
H	-2.3364000	-4.0603210	-1.0200490
H	-0.6478230	-3.9389840	0.8513700
H	-0.5151670	-2.5595950	-0.2359510
H	-1.9834800	-2.6014450	2.4544530
H	-0.4315550	-1.8242280	2.1646110
H	-2.7694190	-1.6436590	-1.3735310
C	-3.7419930	2.0039970	-1.2883810
H	-4.5444660	1.5877040	-0.6754750

H	-4.1365690	2.9038490	-1.7767370
H	-3.5014020	1.2768720	-2.0692890
C	-3.7124900	2.4338370	1.8903720
H	-4.3917160	3.2910380	1.8058870
H	-4.2848890	1.5329740	1.6487840
H	-3.3989950	2.3582340	2.9349180
C	-0.7942030	3.5346630	2.7085970
H	-0.9548800	4.6153770	2.8146810
H	-1.3505720	3.0350390	3.5058740
H	0.2684280	3.3400090	2.8744120
C	1.0026570	3.5646410	0.0590870
H	1.0108730	4.6523050	-0.0832580
H	1.5622940	3.3437380	0.9717310
H	1.5380710	3.1121940	-0.7794440
C	-0.8590100	2.7356430	-2.4342650
H	-1.0595770	3.7272870	-2.8611760
H	0.2034820	2.5213150	-2.5740330
H	-1.4267170	2.0018090	-3.0124690

Cp*Rh(CO)-Cyclohexane Equatorial TS

Final Energy = -849.0217600050

C	-1.0953940	2.6640690	-0.9564930
C	-2.4029670	2.3093890	-0.5174350
C	-2.5422370	2.6843710	0.8783860
C	-1.3143580	3.2796420	1.3026810
C	-0.3937430	3.1990710	0.1899540
Rh	-0.9001980	1.1119850	0.7231830
C	0.7793190	0.3957310	1.0883600
O	1.8179140	-0.0180650	1.3303470
C	-1.7921960	-0.9139510	0.4286610
C	-3.2619170	-1.1207230	0.8615070
C	-3.8681910	-2.3912560	0.2307860
C	-3.0286650	-3.6346760	0.5760720
C	-1.5638190	-3.4401550	0.1443200
C	-0.9530570	-2.1640460	0.7628010
H	-4.9016130	-2.5202130	0.5733500
H	-3.3142040	-1.2054960	1.9564470
H	-3.8598610	-0.2479840	0.5840590
H	-1.7797030	-0.7791790	-0.6613210
H	-1.4608620	-0.0526870	1.6376120
H	-3.0663990	-3.8042350	1.6610070
H	-3.4515530	-4.5256530	0.0984790
H	-0.9634140	-4.3118810	0.4292160
H	-1.5180430	-3.3655830	-0.9507920
H	-0.8940890	-2.2864220	1.8536690
H	0.0721500	-2.0399250	0.4027340

H	-3.9048720	-2.2708230	-0.8607360
C	-3.4810740	1.7324440	-1.4023750
H	-4.4008070	1.5462490	-0.8436870
H	-3.7224040	2.4305780	-2.2122960
H	-3.1686300	0.7874750	-1.8623980
C	-3.8111660	2.6154420	1.6928090
H	-4.4238330	3.5111440	1.5293260
H	-4.4168790	1.7455120	1.4286710
H	-3.5883560	2.5510260	2.7608380
C	-1.0452750	3.9314010	2.6350880
H	-1.2978800	4.9993720	2.6035070
H	-1.6385900	3.4696030	3.4283670
H	0.0077570	3.8463310	2.9147740
C	0.9969970	3.7872720	0.1631290
H	0.9610570	4.8425250	-0.1339910
H	1.4718410	3.7322290	1.1460480
H	1.6381170	3.2608340	-0.5487930
C	-0.5764710	2.5576420	-2.3677950
H	-0.7992440	3.4705770	-2.9360090
H	0.5064320	2.4104290	-2.3871360
H	-1.0376640	1.7171680	-2.8946880

Cp*Rh(CO)-Cyclohexane Axial Product

Final Energy = -849.0433266480

C	1.9724400	0.6030590	-1.1305920
C	1.3122440	1.5798090	-0.2909710
C	1.4202740	1.1289220	1.0739250
C	2.0634500	-0.1453180	1.0771750
C	2.4129120	-0.4643090	-0.2979160
Rh	0.1349480	-0.3269140	-0.1608740
C	-0.3781420	-2.1160340	-0.2741020
O	-0.6682300	-3.2084520	-0.4016150
C	-1.6353160	0.1328830	0.9316270
C	-2.2960040	1.4707810	0.5172060
C	-3.1489830	1.3731700	-0.7635230
C	-4.2132370	0.2646160	-0.6473840
C	-3.5769310	-1.0825180	-0.2522900
C	-2.7510970	-0.9336530	1.0404580
H	-3.6340320	2.3371900	-0.9585590
H	-2.9591420	1.7939800	1.3377550
H	-1.5477290	2.2596510	0.3958770
H	-0.8068390	-0.1550490	-1.3988010
H	-1.2230840	0.2642220	1.9413890
H	-4.9467120	0.5494050	0.1200060
H	-4.7622580	0.1656710	-1.5909890
H	-4.3577080	-1.8392810	-0.1119530

H	-2.9341280	-1.4322120	-1.0690560
H	-3.4437430	-0.6233820	1.8405430
H	-2.3463560	-1.9024110	1.3511100
H	-2.4961960	1.1601290	-1.6176410
C	0.8569380	2.9432620	-0.7522670
H	0.2606980	3.4444710	0.0131100
H	1.7235790	3.5812650	-0.9664500
H	0.2519140	2.8793660	-1.6608250
C	0.9525150	1.8924020	2.2842480
H	1.6865890	2.6612190	2.5542310
H	-0.0036150	2.3893320	2.0988800
H	0.8253180	1.2332040	3.1462890
C	2.4598170	-0.9513960	2.2903010
H	3.4479300	-0.6449620	2.6562640
H	1.7458770	-0.8227270	3.1076450
H	2.5089570	-2.0185660	2.0585870
C	3.2090370	-1.6688280	-0.7367570
H	4.2831860	-1.4788060	-0.6205870
H	2.9632480	-2.5520530	-0.1411440
H	3.0226010	-1.9072650	-1.7867430
C	2.2067700	0.7496860	-2.6123050
H	3.1360480	1.3030090	-2.7984700
H	2.2902280	-0.2230060	-3.1030210
H	1.3884210	1.2971410	-3.0862040

Cp*Rh(CO)-Cyclohexane Equatorial Product

Final Energy = -849.0455893060

C	1.5766630	-0.2913570	1.4704540
C	0.9879290	-1.4532390	0.8652590
C	1.4646200	-1.5554770	-0.4823000
C	2.4064090	-0.4754250	-0.7025500
C	2.4707130	0.2949350	0.5006050
Rh	0.3383760	0.3940490	-0.3277990
C	0.0780190	2.2323860	-0.4717590
O	-0.0409640	3.3546920	-0.6132750
C	-1.7049470	0.1189550	0.1593830
C	-2.3002880	-1.0958480	-0.5874600
C	-3.7299540	-1.4406230	-0.1129910
C	-4.6674180	-0.2303180	-0.2710960
C	-4.0984250	0.9952010	0.4653830
C	-2.6604370	1.3223250	0.0021670
H	-4.1169800	-2.2989620	-0.6758800
H	-2.3279350	-0.8702990	-1.6617970
H	-1.6583150	-1.9747060	-0.4717490
H	-1.6724520	-0.1222900	1.2346230
H	-0.2416170	0.3867700	-1.7906520

H	-4.7699290	0.0061190	-1.3393030
H	-5.6705810	-0.4687780	0.1012310
H	-4.7471210	1.8663290	0.3127920
H	-4.0872480	0.7912530	1.5452520
H	-2.6887010	1.6296920	-1.0531110
H	-2.2965950	2.1822210	0.5749150
H	-3.6992090	-1.7383880	0.9447230
C	0.0938670	-2.4298560	1.5837590
H	-0.2225850	-3.2404980	0.9245240
H	0.6357610	-2.8746030	2.4265640
H	-0.8034780	-1.9450730	1.9824760
C	1.1886610	-2.6827930	-1.4463140
H	1.9089810	-3.4978990	-1.3024090
H	0.1843390	-3.0899830	-1.3086210
H	1.2673390	-2.3413670	-2.4811460
C	3.2436230	-0.2824930	-1.9422390
H	4.1534000	-0.8942040	-1.8941890
H	2.6910010	-0.5716980	-2.8395070
H	3.5473360	0.7605980	-2.0600080
C	3.3728520	1.4784590	0.7499100
H	4.3243530	1.1442920	1.1811020
H	3.5957860	2.0158270	-0.1750480
H	2.9205160	2.1846730	1.4510020
C	1.4083090	0.1168800	2.9126870
H	2.1005840	-0.4358970	3.5609940
H	1.6015920	1.1837000	3.0521350
H	0.3913990	-0.0868360	3.2608720

Cp*Rh(CO)-Cyclohexane 1,1-Migration

Final Energy = -849.0366720690

C	1.8858050	-0.5231090	1.3860220
C	1.1296320	-1.5426960	0.7627680
C	1.4240450	-1.5395900	-0.6729180
C	2.3565130	-0.5124420	-0.9415150
C	2.5390880	0.2177160	0.3108500
Rh	0.4733280	0.4772870	-0.1075100
C	0.2845880	2.3238700	-0.1670390
O	0.1626750	3.4659620	-0.2045530
C	-2.1062180	0.1777930	-0.5355100
C	-2.8139690	-1.1712190	-0.7641200
C	-3.9256070	-1.3930170	0.2796970
C	-4.9273760	-0.2211770	0.2840650
C	-4.2130450	1.1254590	0.5134170
C	-3.1013790	1.3548680	-0.5289170
H	-4.4460010	-2.3363700	0.0802210
H	-3.2541080	-1.1761430	-1.7705740

H	-2.0898260	-1.9919610	-0.7298520
H	-1.6173000	0.1490500	0.4642530
H	-1.3589500	0.3387370	-1.3401410
H	-5.4494090	-0.1919310	-0.6823040
H	-5.6905390	-0.3806910	1.0536960
H	-4.9354110	1.9482470	0.4780460
H	-3.7692380	1.1331460	1.5183560
H	-3.5514140	1.4457770	-1.5268320
H	-2.5760250	2.2936370	-0.3269720
H	-3.4700240	-1.4824010	1.2756270
C	0.2509430	-2.5616380	1.4464460
H	-0.6584390	-2.7589920	0.8701880
H	0.7775390	-3.5175450	1.5619570
H	-0.0512540	-2.2228340	2.4405840
C	0.9093020	-2.5648570	-1.6530820
H	1.5067670	-3.4843390	-1.6037820
H	-0.1277800	-2.8399210	-1.4408000
H	0.9531730	-2.1905110	-2.6792180
C	3.0558490	-0.2234440	-2.2438740
H	4.0362510	-0.7173840	-2.2754070
H	2.4734160	-0.5817380	-3.0966650
H	3.2194520	0.8487910	-2.3782780
C	3.5419420	1.3280840	0.5178820
H	4.5389190	0.9160320	0.7180540
H	3.6130950	1.9664420	-0.3666940
H	3.2625550	1.9601520	1.3648810
C	2.0224450	-0.2439290	2.8601690
H	2.9075790	-0.7481220	3.2705970
H	2.1307070	0.8264800	3.0526670
H	1.1497530	-0.5952450	3.4167050

Cp*Rh(CO)-Cyclohexane 1,2-Migration

Final Energy = -849.0285622960

C	-2.2313130	-0.8071920	-1.0018280
C	-1.3164200	-1.6836350	-0.3833190
C	-1.2479300	-1.3605030	1.0445900
C	-2.1453400	-0.3022850	1.3232040
C	-2.6457280	0.1518320	0.0273970
Rh	-0.5703330	0.4853600	-0.1133890
C	-0.4250510	2.2851150	-0.5597250
O	-0.3130780	3.3963870	-0.8284970
C	5.0518290	0.4713930	0.4554040
C	3.7878840	0.6791920	1.3128710
C	2.5312810	0.7942560	0.4274310
C	2.3853390	-0.4346710	-0.4952880
C	3.6499960	-0.6433920	-1.3522530

C	4.9059830	-0.7560140	-0.4659670
H	1.6374320	0.9114240	1.0610220
H	3.6704500	-0.1732590	1.9957700
H	3.8929630	1.5750060	1.9343040
H	5.2195150	1.3657070	-0.1601500
H	5.9306890	0.3584450	1.0998880
H	2.2137380	-1.3285380	0.1203500
H	1.5104250	-0.3237340	-1.1584110
H	3.5418720	-1.5382360	-1.9747850
H	3.7632380	0.2099970	-2.0342440
H	4.8315880	-1.6625370	0.1505920
H	5.7986750	-0.8686930	-1.0912090
H	2.6037090	1.7004830	-0.1881870
C	-0.4327070	-2.1400030	2.0471900
H	-0.2839970	-1.5696040	2.9675900
H	-0.9324240	-3.0812390	2.3096690
H	0.5534280	-2.3959850	1.6469120
C	-2.5390610	0.2451330	2.6699630
H	-2.7375150	1.3187670	2.6198090
H	-3.4495410	-0.2463860	3.0383550
H	-1.7510550	0.0863930	3.4107420
C	-3.7175040	1.1978550	-0.1619320
H	-3.6638900	1.6424560	-1.1591680
H	-4.7138680	0.7537580	-0.0431890
H	-3.6173140	2.0029400	0.5706190
C	-2.7252390	-0.8401250	-2.4242710
H	-2.0083610	-1.3385110	-3.0818900
H	-3.6774290	-1.3830760	-2.4914690
H	-2.8896760	0.1683700	-2.8121010
C	-0.5742290	-2.8256590	-1.0310580
H	-1.0498680	-3.7858150	-0.7939180
H	-0.5556690	-2.7188230	-2.1187010
H	0.4617810	-2.8793700	-0.6821540

Cp*Rh(CO)-Cycloheptane σ -complex (1)

Final Energy = -888.3218465140

C	0.9693320	-0.9782220	3.3937990
C	2.0104610	-0.6626490	2.4873000
C	2.2023810	0.7885940	2.4709510
C	1.2669180	1.3759840	3.3529610
C	0.4064350	0.2954770	3.8275990
Rh	0.0893580	0.3053250	1.7190410
C	-1.7410760	0.5887350	1.5643160
O	-2.8727870	0.7643000	1.4717950
C	0.3260540	-0.2057720	-0.8310380
C	-1.0105480	-0.3947490	-1.5860150

C	-0.8981620	-1.0269400	-2.9912400
C	1.5633850	0.1758150	-1.6764930
C	-0.5948200	-0.0016600	-4.1052250
C	1.3090670	1.2137200	-2.7920960
C	0.8315700	0.5799740	-4.1157640
H	0.1733550	0.6915760	-0.1478510
H	-1.6613640	-1.0077020	-0.9541830
H	-1.8562250	-1.5044140	-3.2256110
H	-0.7788490	-0.4692590	-5.0800650
H	1.9793510	-0.7307580	-2.1334640
H	2.2451610	1.7475310	-2.9911770
H	0.5590980	-1.1206690	-0.2773720
H	-1.5152560	0.5740020	-1.6863780
H	-0.1466740	-1.8279510	-2.9946890
H	2.3301290	0.5524200	-0.9905140
H	-1.3174730	0.8208660	-4.0159170
H	0.5891440	1.9692610	-2.4494460
H	1.5411340	-0.2132460	-4.3889030
H	0.8883380	1.3319480	-4.9120470
C	3.3152040	1.5005760	1.7412160
H	4.2084210	1.5755330	2.3748430
H	3.6064070	0.9624710	0.8349530
H	3.0224990	2.5137130	1.4523370
C	1.1783040	2.8232590	3.7603710
H	1.7394890	2.9998950	4.6877950
H	1.5906950	3.4792910	2.9892990
H	0.1424280	3.1240690	3.9362720
C	-0.6639300	0.4492940	4.8821590
H	-0.2247110	0.4153100	5.8870100
H	-1.1894090	1.4020850	4.7768950
H	-1.4059690	-0.3504050	4.8119630
C	0.5238050	-2.3447350	3.8456250
H	1.0217770	-2.6264400	4.7830260
H	-0.5547240	-2.3737600	4.0202620
H	0.7609640	-3.1078480	3.0996160
C	2.8682250	-1.6398430	1.7211850
H	3.8490460	-1.7614300	2.1977190
H	2.3959690	-2.6243930	1.6697580
H	3.0438560	-1.2985530	0.6952750

Cp*Rh(CO)-Cycloheptane σ -complex (2)

Final Energy = -888.3221401920

C	1.0304440	-0.9301110	3.5160950
C	2.0707090	-0.6715290	2.5922700
C	2.1981590	0.7760880	2.4139720
C	1.2246040	1.4158630	3.2162800

C	0.4046430	0.3571860	3.7981610
Rh	0.1156070	0.1261100	1.7007580
C	-1.7239770	0.2956470	1.5098440
O	-2.8628800	0.3971480	1.3938120
C	1.6950040	-0.5072900	-1.5871310
C	0.3726310	-0.6411200	-0.7937950
C	-0.9210880	-0.7902300	-1.6254220
C	1.6174150	0.3016670	-2.9013060
C	-1.5260050	0.5560050	-2.0778410
C	0.7508090	1.5807190	-2.8492100
C	-0.7388210	1.3186210	-3.1601270
H	2.4393900	-0.0472410	-0.9268860
H	0.4677670	-1.4975510	-0.1182310
H	-1.6656270	-1.3075670	-1.0108820
H	-2.5414310	0.3779440	-2.4506240
H	1.2308860	-0.3406450	-3.7022880
H	1.1307210	2.2898490	-3.5933050
H	2.0692050	-1.5111230	-1.8217470
H	0.2578020	0.3343730	-0.2260180
H	-0.7258920	-1.4333200	-2.4941060
H	2.6418420	0.5609640	-3.1916360
H	-1.6333490	1.1960950	-1.1922100
H	0.8538060	2.0736440	-1.8727340
H	-0.7956550	0.7640480	-4.1069230
H	-1.2419820	2.2774850	-3.3332510
C	3.2945190	1.4525980	1.6280320
H	4.1894870	1.5867340	2.2494580
H	3.5910110	0.8595280	0.7585980
H	2.9821430	2.4383150	1.2728960
C	1.0703180	2.8938560	3.4615500
H	1.6101390	3.1945420	4.3695310
H	1.4672290	3.4777960	2.6269790
H	0.0204970	3.1679150	3.5927940
C	-0.6863260	0.5794890	4.8189400
H	-0.2608250	0.6714230	5.8260520
H	-1.2466560	1.4936430	4.6058850
H	-1.3955910	-0.2523130	4.8277980
C	0.6339400	-2.2550970	4.1139410
H	1.1423380	-2.4164650	5.0739100
H	-0.4426970	-2.3007490	4.2967640
H	0.8944590	-3.0870520	3.4545380
C	2.9881300	-1.6880820	1.9575110
H	3.9623820	-1.7062500	2.4620640
H	2.5634240	-2.6937560	2.0128430
H	3.1706240	-1.4592340	0.9024740

Cp*Rh(CO)-Cycloheptane σ -complex (3)

Final Energy = -888.3214349120

C	1.1797560	-0.7021420	3.7963970
C	2.1079350	-0.4509950	2.7581760
C	2.0646410	0.9742950	2.4249120
C	1.1111480	1.6076020	3.2551970
C	0.4559760	0.5456700	4.0137190
Rh	0.0057890	0.0463920	1.9943370
C	-1.8501310	-0.0101830	1.9872930
O	-2.9988430	-0.0465130	1.9855350
C	1.3160140	-0.9687300	-1.2889800
C	0.1173140	-0.2594690	-0.6149480
C	-1.1862610	-0.1872210	-1.4419840
C	1.4721890	-0.7093860	-2.8047570
C	-1.2337510	1.0475980	-2.3669840
C	1.2036790	0.7411090	-3.2672530
C	-0.2834550	1.0164920	-3.5793450
H	2.2302010	-0.6497720	-0.7753450
H	-0.1038870	-0.8924900	0.2988380
H	-2.0371410	-0.1304570	-0.7564960
H	-2.2579620	1.1724480	-2.7380540
H	0.8012790	-1.3757660	-3.3606350
H	1.7786450	0.9281430	-4.1812120
H	1.2369300	-2.0507550	-1.1297120
H	0.4019270	0.7647200	-0.3476540
H	-1.3156200	-1.1090770	-2.0238460
H	2.4894710	-1.0035440	-3.0867840
H	-1.0167470	1.9354950	-1.7575780
H	1.5741830	1.4548840	-2.5187670
H	-0.6286430	0.2484230	-4.2849450
H	-0.3670940	1.9762610	-4.1033850
C	2.9767900	1.6443170	1.4269760
H	3.9860170	1.7685680	1.8395560
H	3.0713730	1.0554170	0.5089600
H	2.6026280	2.6338620	1.1521240
C	0.8205110	3.0815400	3.3684310
H	1.3943890	3.5284510	4.1912080
H	1.0841800	3.6128310	2.4502900
H	-0.2390410	3.2636370	3.5653790
C	-0.5567770	0.7732550	5.1110990
H	-0.0548560	1.0136150	6.0566580
H	-1.2265020	1.6017030	4.8655760
H	-1.1712320	-0.1162710	5.2727970
C	0.9829580	-1.9865580	4.5582570
H	1.5788960	-1.9859380	5.4807980
H	-0.0640840	-2.1266270	4.8385250

H	1.2880220	-2.8512540	3.9631230
C	3.0990190	-1.4346960	2.1857720
H	4.0520330	-1.3845000	2.7281150
H	2.7274780	-2.4604980	2.2541370
H	3.3113190	-1.2254740	1.1338120

Cp*Rh(CO)-Cycloheptane σ -complex (4)

Final Energy = -888.3212727700

C	1.0372400	-0.9459210	3.5287820
C	2.0160440	-0.6101740	2.5618440
C	2.1300280	0.8473670	2.4832190
C	1.1996150	1.4168540	3.3812890
C	0.4231410	0.3105640	3.9383260
Rh	0.0049520	0.2220790	1.8520530
C	-1.8358180	0.4559080	1.7870140
O	-2.9751110	0.6022110	1.7499110
C	1.9344140	-1.6067190	-2.1050690
C	1.3758970	-0.2824690	-1.5339030
C	0.0792830	-0.4124770	-0.7033690
C	0.8890090	-2.6251820	-2.6160880
C	-1.2078960	-0.3602030	-1.5555870
C	-0.3204460	-2.0258290	-3.3689290
C	-1.4702570	-1.6005500	-2.4304280
H	2.6210240	-1.3546460	-2.9223590
H	2.1577440	0.1830370	-0.9239240
H	0.0399600	0.5249000	-0.0652250
H	-2.0707220	-0.2165850	-0.8967820
H	0.5059480	-3.2108670	-1.7709360
H	-0.7131370	-2.7823950	-4.0576080
H	2.5415370	-2.1019520	-1.3375310
H	1.1779120	0.4181210	-2.3542960
H	0.0961770	-1.3286520	-0.1003620
H	1.4086630	-3.3394710	-3.2644910
H	-1.1524540	0.5300780	-2.1962500
H	-0.0025320	-1.1780390	-3.9908620
H	-1.7129790	-2.4518490	-1.7802540
H	-2.3681130	-1.4036240	-3.0284560
C	3.1686860	1.5889850	1.6779700
H	4.1130410	1.6598980	2.2331850
H	3.3858280	1.0812530	0.7341010
H	2.8397910	2.6049300	1.4437330
C	2.9007980	-1.5723110	1.8082250
H	3.0684120	-1.2382440	0.7796020
H	3.8838690	-1.6589150	2.2880830
H	2.4576690	-2.5709830	1.7684960
C	0.6954670	-2.3144720	4.0578650

H	0.9288740	-3.0948800	3.3287780
H	1.2630940	-2.5312220	4.9727690
H	-0.3675320	-2.3923310	4.3000520
C	-0.6035520	0.4512480	5.0371800
H	-1.3031190	-0.3887610	5.0345050
H	-0.1162890	0.4826330	6.0197290
H	-1.1840820	1.3702050	4.9206820
C	1.0418940	2.8722650	3.7359300
H	-0.0029400	3.1213720	3.9376790
H	1.6233010	3.1170380	4.6348790
H	1.3889160	3.5188240	2.9258000

Cp*Rh(CO)-Cycloheptane σ -complex (5)

Final Energy = -888.3225259070

C	1.2652350	-0.8503650	3.4494850
C	2.2006920	-0.4078930	2.4830710
C	2.0344830	1.0352960	2.2947910
C	0.9948470	1.4870500	3.1391330
C	0.4178350	0.2959320	3.7564780
Rh	0.0982400	-0.0282760	1.6739900
C	-1.7432620	-0.2360070	1.5413880
O	-2.8816580	-0.3654260	1.4513580
C	1.7192640	-2.1571680	-1.6313840
C	1.6120120	-0.6154420	-1.6425510
C	0.3819430	-0.0251750	-0.9157710
C	0.3917020	-2.9327880	-1.8098090
C	-0.8785430	0.0751950	-1.8003310
C	-0.6200500	-2.3227380	-2.8075260
C	-1.5445040	-1.2632090	-2.1686400
H	2.4208950	-2.4507700	-2.4214060
H	2.5292980	-0.2056060	-1.2041210
H	0.6249530	0.9788820	-0.5563060
H	-1.6183420	0.7028510	-1.2909880
H	-0.1065940	-3.0289890	-0.8369500
H	-1.2538270	-3.1281030	-3.1954100
H	2.1720080	-2.4748250	-0.6840600
H	1.5845850	-0.2527010	-2.6773770
H	0.1472940	-0.7571220	-0.0754620
H	0.6420100	-3.9532840	-2.1203980
H	-0.5932210	0.6045910	-2.7196840
H	-0.0955360	-1.8984540	-3.6745890
H	-1.9939400	-1.6985510	-1.2659270
H	-2.3744050	-1.0493000	-2.8525590
C	2.9119670	1.8820520	1.4062100
H	3.8792640	2.0817170	1.8844160
H	3.1175530	1.3822510	0.4539680

H	2.4429120	2.8442520	1.1844680
C	3.2970430	-1.2276870	1.8483700
H	3.4612230	-0.9398790	0.8055690
H	4.2467030	-1.0859560	2.3802510
H	3.0574290	-2.2940730	1.8683290
C	0.5564270	2.9073840	3.3848530
H	1.0587310	3.3209780	4.2694760
H	0.7923780	3.5524590	2.5345750
H	-0.5212470	2.9655810	3.5574880
C	-0.6521300	0.3122940	4.8225540
H	-0.2123560	0.5035730	5.8093650
H	-1.3934160	1.0917510	4.6277770
H	-1.1779340	-0.6450160	4.8681560
C	1.1658710	-2.2195730	4.0694840
H	1.7240070	-2.2590520	5.0145090
H	0.1277610	-2.4850080	4.2846900
H	1.5756510	-2.9856050	3.4060180

Cp*Rh(CO)-Cycloheptane σ -complex (6)

Final Energy = -888.3217232530

C	1.0919480	-0.9011200	3.6319400
C	2.0615520	-0.6737790	2.6294430
C	2.1117570	0.7621630	2.3422720
C	1.1827680	1.4261100	3.1799880
C	0.4451560	0.3830250	3.8830480
Rh	0.0123170	0.0055990	1.8322770
C	-1.8440100	0.0389670	1.7887820
O	-2.9927050	0.0627080	1.7630910
C	0.7894300	1.2117740	-3.3964500
C	1.4990400	0.9414410	-2.0469040
C	1.3880350	-0.5007200	-1.5052260
C	-0.5412890	0.4618060	-3.6382100
C	0.0968620	-0.7510030	-0.6959660
C	-1.4963820	0.3679490	-2.4264200
C	-1.2063760	-0.8399550	-1.5113290
H	0.6112480	2.2909910	-3.4742640
H	2.5562710	1.2061320	-2.1622850
H	2.2412750	-0.6989250	-0.8485960
H	0.2021140	-1.6642970	-0.1034050
H	-0.3285330	-0.5579820	-3.9835160
H	-2.5231800	0.2668430	-2.7949000
H	1.4714280	0.9567070	-4.2166450
H	1.1042720	1.6192310	-1.2786000
H	1.4523500	-1.2296350	-2.3238880
H	-1.0548840	0.9576020	-4.4696060
H	-0.0195410	0.1826210	-0.0542030

H	-1.4693770	1.2977140	-1.8418630
H	-1.1660890	-1.7454060	-2.1321160
H	-2.0397570	-0.9758460	-0.8138390
C	0.9906300	2.9112080	3.3442070
H	-0.0552650	3.1566330	3.5450090
H	1.5896600	3.2896930	4.1832950
H	1.2931600	3.4543000	2.4452220
C	3.1013260	1.4135930	1.4071760
H	2.7736510	2.4163860	1.1211230
H	4.0866770	1.5031800	1.8822850
H	3.2325730	0.8326640	0.4895520
C	2.9934180	-1.7008650	2.0351800
H	3.2290640	-1.4753660	0.9912660
H	3.9435800	-1.7271700	2.5840360
H	2.5583720	-2.7032350	2.0715660
C	0.7903190	-2.1973030	4.3380320
H	1.0462510	-3.0583770	3.7149510
H	1.3657210	-2.2746470	5.2702700
H	-0.2693700	-2.2732890	4.5945270
C	-0.5766240	0.6321650	4.9673110
H	-1.2514720	-0.2206810	5.0781740
H	-0.0826960	0.7992930	5.9326580
H	-1.1847360	1.5124840	4.7434170

Cp*Rh(CO)-Cycloheptane σ -complex (7)

Final Energy = -888.3213062040

C	1.2167610	-0.8636970	3.7475710
C	2.1075020	-0.5192620	2.7065280
C	1.9470740	0.9064580	2.4141770
C	0.9858280	1.4553830	3.2991390
C	0.4215200	0.3296050	4.0320120
Rh	-0.0458360	-0.1205200	2.0026740
C	-1.8805380	-0.4130880	2.0420010
O	-3.0149920	-0.5939520	2.0676740
C	1.0296120	0.3108950	-3.8592760
C	1.7384200	0.3752040	-2.4856520
C	1.2311380	-0.6277920	-1.4251760
C	-0.4940010	0.0494640	-3.8253260
C	0.0253020	-0.0897250	-0.6236710
C	-1.2736330	0.7789090	-2.7078410
C	-1.3158340	-0.0014670	-1.3761930
H	1.2210180	1.2548810	-4.3836740
H	2.8104540	0.2189280	-2.6508410
H	2.0394490	-0.8353750	-0.7160380
H	-0.1325190	-0.8464760	0.2077140
H	-0.6790520	-1.0271540	-3.7223560

H	-2.3091090	0.9210220	-3.0368070
H	1.4952030	-0.4746930	-4.4666130
H	1.6421180	1.3861070	-2.0695550
H	0.9761980	-1.5882310	-1.8919240
H	-0.9038810	0.3315470	-4.8015490
H	0.2839370	0.9054200	-0.2422220
H	-0.8609630	1.7838450	-2.5462180
H	-1.6804410	-1.0162710	-1.5836250
H	-2.0488190	0.4629690	-0.7079210
C	0.6119960	2.9043660	3.4744970
H	-0.4461160	3.0130290	3.7258660
H	1.1963440	3.3624800	4.2837160
H	0.7976070	3.4787680	2.5631060
C	2.7726810	1.6611000	1.4004560
H	2.3249980	2.6308790	1.1679670
H	3.7879460	1.8410320	1.7755150
H	2.8657720	1.1026830	0.4625880
C	-0.5745400	0.4460150	5.1613740
H	-0.0645030	0.6790630	6.1044380
H	-1.3023000	1.2381500	4.9667870
H	-1.1257910	-0.4878630	5.2995660
C	1.1144320	-2.1860620	4.4610410
H	1.7317840	-2.1853310	5.3693120
H	0.0845280	-2.3979670	4.7590610
H	1.4546020	-3.0071150	3.8245240
C	3.1524090	-1.4148750	2.0879030
H	3.3644470	-1.1307160	1.0535280
H	4.0975000	-1.3482430	2.6424580
H	2.8342250	-2.4609460	2.0911490

Cp*Rh(CO)-Cycloheptane TS (1)

Final Energy = -888.3051046460

C	0.9321360	-0.9366170	3.2521640
C	2.0181530	-0.6754010	2.3706910
C	2.2126300	0.7614470	2.2929670
C	1.2557410	1.3916840	3.1477510
C	0.4120940	0.3496070	3.6790730
Rh	0.1421250	0.2979060	1.4806040
C	-1.7123930	0.4185240	1.3330790
O	-2.8500870	0.5180500	1.2752220
C	0.3614890	-0.4355830	-0.6212020
C	-0.9610250	-0.5858330	-1.4072520
C	-0.8278040	-1.0454510	-2.8801530
C	1.5597690	0.0831000	-1.4589190
C	-0.6000200	0.1177550	-3.8698250
C	1.2574650	1.2492100	-2.4278990

C	0.7915050	0.7760520	-3.8209820
H	0.1791070	0.9495630	0.0354480
H	-1.5887780	-1.2977550	-0.8617240
H	-1.7603920	-1.5476110	-3.1625460
H	-0.7728600	-0.2409920	-4.8919210
H	1.9687620	-0.7502360	-2.0465980
H	2.1689300	1.8428850	-2.5611240
H	0.6474180	-1.4257080	-0.2489630
H	-1.5134060	0.3623700	-1.4074840
H	-0.0319370	-1.7952270	-2.9810170
H	2.3525850	0.3825070	-0.7676250
H	-1.3657310	0.8815310	-3.6768230
H	0.5119460	1.9255330	-1.9866970
H	1.5372500	0.0670410	-4.2062010
H	0.7929090	1.6299200	-4.5095280
C	3.3600850	1.4602210	1.6041910
H	4.1561460	1.6841180	2.3255120
H	3.7971720	0.8376480	0.8200750
H	3.0428360	2.4033870	1.1507340
C	1.1871710	2.8597770	3.4808210
H	1.8015550	3.0869250	4.3621000
H	1.5529290	3.4702000	2.6510810
H	0.1628930	3.1724220	3.6987260
C	-0.6867960	0.5474630	4.6960900
H	-0.2801150	0.5017200	5.7138070
H	-1.1717310	1.5190670	4.5718710
H	-1.4558910	-0.2244750	4.6091240
C	0.4429190	-2.2866140	3.7132500
H	0.9583560	-2.5951540	4.6320220
H	-0.6295190	-2.2712930	3.9235740
H	0.6215630	-3.0556170	2.9570390
C	2.8665670	-1.7047930	1.6685120
H	3.8000960	-1.8832170	2.2161350
H	2.3405520	-2.6597040	1.5853630
H	3.1314100	-1.3807270	0.6573060

Cp*Rh(CO)-Cycloheptane TS (2)

Final Energy = -888.3035741010

C	1.0938970	-1.0057230	3.3803500
C	2.0845860	-0.6350380	2.4338650
C	2.1338450	0.8158900	2.3677700
C	1.2024790	1.3409690	3.3207910
C	0.4995410	0.2184200	3.8874960
Rh	0.0508090	0.1912470	1.7190780
C	-1.8038810	0.0427540	1.7450210
O	-2.9446870	-0.0247840	1.7978150

C	1.4516760	0.1198830	-1.1373600
C	0.1406250	-0.3462410	-0.4567080
C	-1.1174080	-0.2384290	-1.3528720
C	1.5781560	-0.1833130	-2.6509140
C	-1.2548650	1.0630210	-2.1767030
C	0.9585360	0.9085900	-3.5502150
C	-0.5803640	0.9755580	-3.5621650
H	1.5883040	1.2004060	-1.0014810
H	0.2535930	-1.4056570	-0.1987430
H	-2.0068030	-0.3758130	-0.7337770
H	-2.3193210	1.2712900	-2.3316360
H	1.1464050	-1.1648010	-2.8863170
H	1.3031500	0.7617840	-4.5812330
H	2.2815360	-0.3563660	-0.6084530
H	-0.1358680	0.9451310	0.3361870
H	-1.1147590	-1.0830720	-2.0549730
H	2.6449950	-0.2512590	-2.8947950
H	-0.8546350	1.9160740	-1.6112800
H	1.3575930	1.8797160	-3.2264010
H	-0.9734680	0.0872660	-4.0754060
H	-0.8823440	1.8398600	-4.1662670
C	3.1478230	1.6355750	1.6064100
H	4.0391910	1.8093210	2.2224510
H	3.4677240	1.1370060	0.6895710
H	2.7377290	2.6103760	1.3287810
C	1.0283080	2.7894030	3.6991300
H	1.6995800	3.0587160	4.5252370
H	1.2528120	3.4487970	2.8569290
H	0.0042640	2.9959780	4.0201810
C	-0.5239480	0.2914720	4.9955060
H	-0.0305690	0.2730230	5.9750460
H	-1.1124710	1.2103720	4.9331500
H	-1.2160430	-0.5538500	4.9549430
C	0.7787500	-2.4097130	3.8305750
H	1.4012760	-2.6911200	4.6903120
H	-0.2671320	-2.5097340	4.1320930
H	0.9671390	-3.1317920	3.0310370
C	2.9702230	-1.6053240	1.6896680
H	3.5224330	-2.2345420	2.3970960
H	2.3909260	-2.2698460	1.0372970
H	3.7039420	-1.0829070	1.0720000

Cp*Rh(CO)-Cycloheptane TS (3)

Final Energy = -888.3033754020

C	1.1245230	-0.7825110	3.6366070
C	2.0788900	-0.5228260	2.5992690

C	2.1185330	0.9103550	2.3645510
C	1.1576580	1.5274080	3.2083380
C	0.4962810	0.4727350	3.9564340
Rh	0.0351530	0.0755910	1.8276640
C	-1.8042130	0.3670650	1.8155340
O	-2.9345410	0.5377930	1.8540820
C	1.4061950	-0.5331220	-0.9697080
C	0.1184460	0.1213190	-0.4118930
C	-1.1501180	-0.1490170	-1.2603260
C	1.5475900	-0.5723410	-2.5111910
C	-1.3410100	0.8695000	-2.4077460
C	1.1213940	0.7091800	-3.2616580
C	-0.3822480	0.7337700	-3.6053990
H	2.2604430	0.0126190	-0.5570550
H	-0.2130770	-0.9505380	0.6441880
H	-2.0390790	-0.0950170	-0.6274470
H	-2.3685020	0.7873720	-2.7836980
H	0.9691390	-1.4134650	-2.9129530
H	1.6833590	0.7709000	-4.2007950
H	1.4939200	-1.5626410	-0.6008020
H	0.2654600	1.2073140	-0.3954210
H	-1.1267300	-1.1729890	-1.6578630
H	2.5972190	-0.7964890	-2.7355010
H	-1.2489950	1.8783810	-1.9827320
H	1.3927410	1.5995080	-2.6782870
H	-0.6194420	-0.1908190	-4.1494970
H	-0.5803940	1.5596580	-4.2996290
C	3.0604460	1.6500670	1.4455550
H	3.6774110	2.3515240	2.0191310
H	3.7353600	0.9636400	0.9298410
H	2.5205470	2.2278480	0.6861580
C	0.9302940	3.0106450	3.3555000
H	1.5781800	3.4274620	4.1380000
H	1.1515030	3.5375310	2.4229660
H	-0.1043590	3.2336720	3.6286620
C	-0.5214900	0.6942840	5.0498840
H	-0.0202230	0.8819430	6.0073590
H	-1.1579580	1.5562380	4.8327020
H	-1.1688220	-0.1774280	5.1745360
C	0.8696750	-2.1083240	4.3065430
H	1.5335690	-2.2398590	5.1711530
H	-0.1609000	-2.1830330	4.6625210
H	1.0463020	-2.9394750	3.6191560
C	3.0366280	-1.5413740	2.0295860
H	3.9196530	-1.6382410	2.6738400
H	2.5665270	-2.5257280	1.9554330

H	3.3797250	-1.2616720	1.0317400
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Cp*Rh(CO)-Cycloheptane TS (4)

Final Energy = -888.3033574810

C	0.9740180	-0.9085810	3.3369490
C	2.0006990	-0.5682800	2.4019450
C	2.1544850	0.8729940	2.3794390
C	1.1980120	1.4305610	3.2794370
C	0.4280600	0.3311640	3.8287300
Rh	0.0551080	0.3303470	1.6389460
C	-1.7734910	0.6773800	1.5892250
O	-2.8921620	0.9155530	1.5943720
C	1.9456800	-1.5973300	-1.9665360
C	1.3298120	-0.3737790	-1.2469840
C	0.0718790	-0.6415540	-0.3785570
C	0.9543950	-2.5975790	-2.6033920
C	-1.2230140	-0.5729480	-1.2202590
C	-0.2973580	-1.9669450	-3.2503380
C	-1.4343990	-1.7135620	-2.2391210
H	2.6176760	-1.2154430	-2.7457870
H	2.1163290	0.0764370	-0.6346950
H	0.0639750	0.8154190	0.1237270
H	-2.0945600	-0.5718070	-0.5604950
H	0.6170870	-3.3142990	-1.8441530
H	-0.6777330	-2.6510710	-4.0177380
H	2.5796810	-2.1469390	-1.2602840
H	1.0643870	0.3902370	-1.9897340
H	0.1512110	-1.6348820	0.0816280
H	1.5007880	-3.1846170	-3.3504760
H	-1.2384610	0.3888960	-1.7516480
H	-0.0329970	-1.0362310	-3.7702170
H	-1.6164640	-2.6490820	-1.6925730
H	-2.3588020	-1.4944110	-2.7882900
C	3.2281610	1.6412830	1.6488530
H	4.1181910	1.7540020	2.2810480
H	3.5381740	1.1325870	0.7329150
H	2.8824290	2.6407790	1.3730710
C	2.8638930	-1.5684840	1.6747960
H	3.4257330	-1.1016430	0.8628510
H	3.5881730	-2.0204600	2.3632980
H	2.2633490	-2.3777220	1.2458890
C	0.5898270	-2.3025600	3.7626000
H	0.7018540	-3.0130830	2.9382610
H	1.2253130	-2.6492780	4.5882050
H	-0.4484800	-2.3456580	4.1012390
C	-0.6297710	0.4585220	4.8988290

H	-1.3415530	-0.3698350	4.8542860
H	-0.1689930	0.4531820	5.8941990
H	-1.1924250	1.3899550	4.7965910
C	1.0653450	2.8828790	3.6621090
H	0.0385010	3.1265670	3.9460280
H	1.7131830	3.1201640	4.5161060
H	1.3465050	3.5391940	2.8346740

Cp*Rh(CO)-Cycloheptane TS (5)

Final Energy = -888.3042614250

C	1.2705130	-0.8833950	3.3259190
C	2.2210660	-0.4308260	2.3553400
C	2.0414790	0.9994110	2.1713080
C	0.9619130	1.4241630	2.9899670
C	0.4362200	0.2431640	3.6541470
Rh	0.1542240	-0.1189590	1.4834800
C	-1.7017680	-0.1529040	1.3409950
O	-2.8430770	-0.1920440	1.2775170
C	1.6800670	-2.1220460	-1.4305250
C	1.5926290	-0.5779170	-1.4393010
C	0.3996220	0.1033470	-0.7230870
C	0.3747610	-2.9136280	-1.7023340
C	-0.8611990	0.1370530	-1.6147010
C	-0.6455650	-2.2492400	-2.6509670
C	-1.5414540	-1.2027110	-1.9530220
H	2.4306420	-2.4039650	-2.1792370
H	2.5281280	-0.1977240	-1.0137650
H	0.6911560	1.1499570	-0.5771280
H	-1.6046350	0.7993370	-1.1585030
H	-0.1346000	-3.1148770	-0.7523660
H	-1.2962770	-3.0325800	-3.0568570
H	2.0770110	-2.4493310	-0.4627940
H	1.5784530	-0.2279350	-2.4814070
H	0.1374060	-1.0973330	0.2416030
H	0.6578190	-3.8933450	-2.1042100
H	-0.5666690	0.6129620	-2.5629600
H	-0.1343090	-1.7960460	-3.5112400
H	-1.9540010	-1.6522120	-1.0406200
H	-2.3988330	-0.9816200	-2.6004260
C	2.8982390	1.8874830	1.3060850
H	3.7629640	2.2620850	1.8678650
H	3.2803810	1.3508630	0.4335900
H	2.3346750	2.7533520	0.9462590
C	3.3652310	-1.2436320	1.8011330
H	3.6458900	-0.9175220	0.7966530
H	4.2504660	-1.1427230	2.4417970

H	3.1094930	-2.3050240	1.7497940
C	0.4820850	2.8394170	3.1922830
H	1.0106970	3.3131250	4.0296740
H	0.6531020	3.4504210	2.3020060
H	-0.5873350	2.8696580	3.4162110
C	-0.6578190	0.2498360	4.6953250
H	-0.2442930	0.4803100	5.6848560
H	-1.4194090	1.0007340	4.4694090
H	-1.1539580	-0.7220250	4.7565090
C	1.1913320	-2.2618490	3.9304580
H	1.8240850	-2.3305660	4.8250880
H	0.1682190	-2.5076840	4.2256660
H	1.5264860	-3.0249760	3.2234860

Cp*Rh(CO)-Cycloheptane TS (6)

Final Energy = -888.3026933320

C	0.9872510	-0.8950270	3.4977920
C	2.0270200	-0.7633890	2.5414670
C	2.1487840	0.6436370	2.1987610
C	1.2251720	1.3892300	2.9994930
C	0.4462760	0.4362750	3.7397540
Rh	0.0679450	0.0053250	1.5914360
C	-1.7847190	-0.1786800	1.5565050
O	-2.9258530	-0.2555760	1.5599380
C	0.6169290	1.3976810	-3.1614850
C	1.3791350	1.1882150	-1.8296260
C	1.4788650	-0.2670760	-1.3183530
C	-0.6179700	0.4979880	-3.4040150
C	0.2744830	-0.7884540	-0.4941670
C	-1.4975130	0.1942870	-2.1691750
C	-0.9926710	-1.0105090	-1.3447260
H	0.3083300	2.4490410	-3.2084950
H	2.3913320	1.5897820	-1.9581260
H	2.3746990	-0.3538140	-0.6983220
H	0.5623020	-1.7677290	-0.0945110
H	-0.2923740	-0.4604080	-3.8278130
H	-2.5100490	-0.0411300	-2.5159510
H	1.3097970	1.2485810	-3.9986690
H	0.9144670	1.7974680	-1.0450170
H	1.6321970	-0.9455690	-2.1715320
H	-1.2297340	0.9745750	-4.1785720
H	-0.0986020	0.5957390	0.1367280
H	-1.5898470	1.0840390	-1.5319600
H	-0.7811260	-1.8265160	-2.0525480
H	-1.7987320	-1.3731720	-0.7009540
C	1.1335610	2.8911510	3.0768930

H	0.1180280	3.2186220	3.3135380
H	1.8020200	3.2808060	3.8561690
H	1.4222770	3.3516990	2.1281950
C	3.2375390	1.2539800	1.3470400
H	2.8400850	1.9924010	0.6443120
H	3.9757080	1.7578780	1.9829850
H	3.7679950	0.4921620	0.7712620
C	2.8885600	-1.8711970	1.9912720
H	2.9898040	-1.8024390	0.9031290
H	3.8973420	-1.8328040	2.4204690
H	2.4639980	-2.8509210	2.2237520
C	0.5527480	-2.1544450	4.2054670
H	0.7375160	-3.0414600	3.5944090
H	1.0979610	-2.2765860	5.1502210
H	-0.5144920	-2.1298380	4.4402700
C	-0.6040970	0.7709390	4.7718060
H	-1.3612680	-0.0143430	4.8429710
H	-0.1472310	0.8846260	5.7626990
H	-1.1139160	1.7063340	4.5271490

Cp*Rh(CO)-Cycloheptane TS (7)

Final Energy = -888.3041081730

C	1.1939280	-0.8868310	3.5721570
C	2.1116060	-0.4685780	2.5605470
C	1.9580380	0.9632020	2.3679640
C	0.9373090	1.4295060	3.2436680
C	0.4122170	0.2691000	3.9383950
Rh	0.0052970	-0.0897120	1.7927060
C	-1.8539810	-0.2050820	1.7829040
O	-2.9933630	-0.2999650	1.8100140
C	0.9832070	-0.0298960	-3.7530460
C	1.7433940	0.2675470	-2.4406950
C	1.2411990	-0.5023330	-1.1959610
C	-0.5472950	-0.1877380	-3.6078760
C	0.1155620	0.2317810	-0.4221780
C	-1.2160770	0.7902400	-2.6172030
C	-1.2400730	0.2871970	-1.1534660
H	1.1973710	0.7772990	-4.4642000
H	2.8040400	0.0429950	-2.6041680
H	2.0814310	-0.6450200	-0.5107640
H	-0.0649310	-0.9912170	0.4908670
H	-0.7835240	-1.2108940	-3.2898780
H	-2.2591120	0.9382910	-2.9208130
H	1.3833160	-0.9472160	-4.2019650
H	1.6922450	1.3414970	-2.2215950
H	0.9111050	-1.5115130	-1.4796200

H	-0.9963400	-0.0706030	-4.6006540
H	0.4613490	1.2609880	-0.2628190
H	-0.7376970	1.7771960	-2.6728390
H	-1.7015070	-0.7102320	-1.1499590
H	-1.9089150	0.9378190	-0.5817720
C	0.5126200	2.8596270	3.4647180
H	-0.5384890	2.9200130	3.7582340
H	1.1080830	3.3247560	4.2610440
H	0.6388990	3.4599970	2.5599470
C	2.7887690	1.8050000	1.4332260
H	2.2983330	2.7580960	1.2181550
H	3.7701470	2.0248130	1.8711230
H	2.9586660	1.2950100	0.4794750
C	-0.6246730	0.3097470	5.0357490
H	-0.1521550	0.5253170	6.0019150
H	-1.3728190	1.0846550	4.8496120
H	-1.1473560	-0.6460820	5.1237920
C	1.1085160	-2.2608710	4.1850570
H	1.7730900	-2.3395100	5.0556240
H	0.0927590	-2.4864970	4.5193860
H	1.4034780	-3.0311930	3.4676900
C	3.1979860	-1.3263740	1.9576940
H	3.6062150	-0.8762490	1.0497580
H	4.0276290	-1.4417770	2.6666160
H	2.8304330	-2.3249370	1.7052990

Cp*Rh(CO)-Cycloheptane Product (1)

Final Energy = -888.3272683320

C	0.8605450	-0.8958840	3.1044970
C	1.9897880	-0.6376660	2.2644600
C	2.2284550	0.7803130	2.2468410
C	1.2751660	1.4001570	3.1450510
C	0.4301090	0.3742530	3.6582760
Rh	0.1763230	0.4614770	1.3842570
C	-1.6849450	0.4556260	1.2366390
O	-2.8199330	0.5135790	1.1930390
C	0.3811000	-0.4844520	-0.5080240
C	-0.9237590	-0.6452020	-1.3230760
C	-0.7628960	-1.1569620	-2.7787540
C	1.5389290	0.1282930	-1.3422000
C	-0.5788490	-0.0186260	-3.8048560
C	1.1557930	1.2568780	-2.3286840
C	0.7618840	0.7359650	-3.7279440
H	0.0891200	1.7389900	0.4703700
H	-1.5781230	-1.3341620	-0.7764930
H	-1.6672620	-1.7127890	-3.0540900

H	-0.6903390	-0.4221200	-4.8191170
H	2.0226360	-0.6680080	-1.9288720
H	2.0178520	1.9228590	-2.4524250
H	0.6965780	-1.4977110	-0.2216370
H	-1.4616240	0.3097480	-1.3732790
H	0.0697840	-1.8701540	-2.8447580
H	2.3083130	0.5033770	-0.6631660
H	-1.4007490	0.6968520	-3.6647070
H	0.3506350	1.8709190	-1.9057600
H	1.5651910	0.0757440	-4.0833030
H	0.7224800	1.5787490	-4.4294520
C	3.4129910	1.4818450	1.6285510
H	4.1836690	1.6660440	2.3876110
H	3.8664360	0.8790940	0.8385540
H	3.1277560	2.4447760	1.1965810
C	1.2624630	2.8597150	3.5223080
H	1.9548770	3.0466880	4.3529930
H	1.5708420	3.4844420	2.6804390
H	0.2675100	3.1856670	3.8348510
C	-0.6666170	0.5495880	4.6800890
H	-0.2743660	0.3824560	5.6907300
H	-1.0872010	1.5574810	4.6466690
H	-1.4819060	-0.1609770	4.5203040
C	0.3159860	-2.2529280	3.4783820
H	0.8436900	-2.6596720	4.3503880
H	-0.7468870	-2.2004220	3.7282740
H	0.4286090	-2.9657800	2.6574050
C	2.8120140	-1.6745970	1.5464440
H	3.7022090	-1.9265130	2.1355610
H	2.2420300	-2.5938250	1.3905620
H	3.1434700	-1.3155010	0.5687190

Cp*Rh(CO)-Cycloheptane Product (2)

Final Energy = -888.3257055570

C	0.9663470	-0.9501080	3.2143590
C	2.0521060	-0.5908740	2.3542110
C	2.2107450	0.8370000	2.3905260
C	1.2548300	1.3597610	3.3486560
C	0.4884210	0.2635310	3.8437310
Rh	0.1442260	0.4437060	1.5888740
C	-1.7140900	0.4002980	1.4894930
O	-2.8504810	0.4423750	1.4572240
C	1.5022520	0.1882910	-1.1007520
C	0.3009790	-0.4391320	-0.3436460
C	-0.9674170	-0.5350730	-1.2261420
C	1.6011400	-0.0851830	-2.6252190

C	-1.3497110	0.7461730	-2.0053210
C	0.7951350	0.9191360	-3.4798120
C	-0.7389260	0.7806660	-3.4225370
H	1.4966190	1.2764530	-0.9673920
H	0.5651610	-1.4774180	-0.0936770
H	-1.8130370	-0.8718810	-0.6203570
H	-2.4400290	0.7973640	-2.1063250
H	1.3030120	-1.1154800	-2.8586140
H	1.1076390	0.8316020	-4.5280120
H	2.4209010	-0.1660360	-0.6229860
H	-0.0305380	1.7602300	0.7481310
H	-0.8177790	-1.3347290	-1.9662940
H	2.6545800	0.0028620	-2.9184170
H	-1.0459360	1.6359490	-1.4387750
H	1.0741650	1.9319010	-3.1576630
H	-1.0345760	-0.1410600	-3.9423050
H	-1.1800890	1.6100540	-3.9894120
C	3.3086340	1.6375130	1.7343670
H	4.1937250	1.6839560	2.3813130
H	3.6077680	1.2001660	0.7795650
H	2.9807650	2.6615720	1.5386900
C	1.1632370	2.7969550	3.7959100
H	1.8768700	2.9932750	4.6060060
H	1.3903290	3.4805710	2.9744370
H	0.1630760	3.0379230	4.1639680
C	-0.5789750	0.3296880	4.9082710
H	-0.1396040	0.1526220	5.8975760
H	-1.0642490	1.3085570	4.9280020
H	-1.3511830	-0.4275570	4.7485400
C	0.5358560	-2.3597070	3.5361300
H	1.1354900	-2.7741140	4.3571000
H	-0.5138420	-2.3994110	3.8387980
H	0.6589560	-3.0150700	2.6692890
C	2.9208240	-1.5783670	1.6190550
H	3.3985710	-2.2545320	2.3375430
H	2.3437430	-2.1913700	0.9185240
H	3.7102390	-1.0741710	1.0584520

Cp*Rh(CO)-Cycloheptane 1,1-Migration (1)

Final Energy = -888.3207450460

C	1.9361670	-0.7187180	1.3624810
C	1.2656110	-1.6319120	0.5149400
C	1.6878490	-1.3949790	-0.8680220
C	2.6046730	-0.3207870	-0.8805920
C	2.6584820	0.1967900	0.4857230
Rh	0.6309330	0.4953760	-0.0708070

C	0.4251840	2.3313770	0.1141210
O	0.3019630	3.4680770	0.2288590
C	-2.8214280	1.5006630	-0.8763070
C	-4.2781600	1.3086600	-0.3968590
C	-4.4505160	0.5043250	0.9122240
C	-1.9056890	0.2631400	-0.7238560
C	-4.5398720	-1.0209530	0.6872080
C	-2.5481720	-1.1142060	-0.9980650
C	-3.2370340	-1.7148550	0.2455540
H	-2.8417570	1.8095990	-1.9281620
H	-4.7201110	2.3040690	-0.2771280
H	-5.3785860	0.8246800	1.3989280
H	-4.8835090	-1.4997590	1.6121130
H	-1.5321570	0.2435900	0.3211460
H	-1.7658870	-1.8073030	-1.3261890
H	-2.3650050	2.3287900	-0.3225990
H	-4.8618320	0.8125810	-1.1824850
H	-3.6386320	0.7392740	1.6137870
H	-1.0602250	0.4073270	-1.4320400
H	-5.3179370	-1.2085610	-0.0654100
H	-3.2595720	-1.0368120	-1.8307980
H	-2.5172550	-1.6915120	1.0754620
H	-3.4579930	-2.7728120	0.0572610
C	1.2967380	-2.2554730	-2.0443650
H	1.9228670	-3.1557580	-2.0933510
H	0.2570970	-2.5875490	-1.9735450
H	1.4122320	-1.7149360	-2.9875650
C	3.4031030	0.1919170	-2.0504930
H	4.3928040	-0.2830340	-2.0820300
H	2.9012120	-0.0171450	-2.9987490
H	3.5551640	1.2722060	-1.9845650
C	3.6072830	1.2730990	0.9578690
H	4.5946560	0.8484560	1.1782190
H	3.7366030	2.0473460	0.1970160
H	3.2376280	1.7556540	1.8664340
C	1.9370260	-0.6884550	2.8686250
H	2.7917340	-1.2506060	3.2683050
H	2.0078520	0.3353740	3.2446150
H	1.0253900	-1.1313440	3.2780480
C	0.3774770	-2.7727840	0.9478130
H	0.9482920	-3.7084640	1.0057920
H	-0.0599220	-2.5859540	1.9321470
H	-0.4431540	-2.9350410	0.2427920

Cp*Rh(CO)-Cycloheptane 1,1-Migration (2)

Final Energy = -888.3203702050

C	-2.6020270	-0.5018920	-0.7815720
C	-1.6735890	-1.5481800	-0.5850080
C	-1.2282890	-1.5211000	0.8101390
C	-1.8984180	-0.4732600	1.4858730
C	-2.6437000	0.2579710	0.4665860
Rh	-0.6262580	0.4588270	-0.1664750
C	-0.4115330	2.2980930	-0.3147260
O	-0.2738930	3.4354260	-0.4052410
C	3.6929510	1.6775200	0.2462020
C	4.2194320	0.4995200	1.1004970
C	4.6978860	-0.7443660	0.3157690
C	2.8614150	1.2898500	-0.9974040
C	3.5627370	-1.7409090	-0.0083940
C	1.8980240	0.0990130	-0.7953550
C	2.5421610	-1.2770520	-1.0644360
H	3.0886690	2.3250830	0.8925320
H	5.0396420	0.8764550	1.7215220
H	5.4417210	-1.2741060	0.9216280
H	4.0011490	-2.6862430	-0.3508410
H	3.5332170	1.0355080	-1.8264180
H	1.0631610	0.2141760	-1.5213340
H	4.5399890	2.2865900	-0.0915150
H	3.4381120	0.1786930	1.8011030
H	5.2115060	-0.4414530	-0.6065800
H	2.2985990	2.1713220	-1.3217080
H	3.0305460	-1.9657850	0.9266350
H	1.5178360	0.1225930	0.2481900
H	3.0298110	-1.2344280	-2.0475520
H	1.7547080	-2.0354670	-1.1438540
C	-0.2921900	-2.5354950	1.4208700
H	-0.8039530	-3.4918640	1.5872300
H	0.5654600	-2.7334890	0.7693360
H	0.0925640	-2.1887550	2.3833050
C	-1.8749770	-0.1627660	2.9598800
H	-0.9573990	-0.5269150	3.4293220
H	-1.9371040	0.9134530	3.1400620
H	-2.7239430	-0.6365450	3.4706930
C	-3.5976140	1.3947880	0.7476480
H	-3.7385870	2.0212350	-0.1370810
H	-4.5798920	1.0093660	1.0482810
H	-3.2253150	2.0331530	1.5531520
C	-3.4223530	-0.2258800	-2.0142890
H	-4.4065810	-0.7076610	-1.9410970
H	-3.5864690	0.8458650	-2.1516490

H	-2.9293100	-0.6064130	-2.9127210
C	-1.2946940	-2.6109550	-1.5868830
H	-1.9511050	-3.4856070	-1.4914450
H	-1.3767690	-2.2404560	-2.6122720
H	-0.2688710	-2.9583380	-1.4360110

Cp*Rh(CO)-Cycloheptane 1,1-Migration (3)

Final Energy = -888.3196422180

C	2.2765400	-0.4511740	1.2941120
C	1.5451930	-1.5280930	0.7439470
C	1.6904720	-1.4951830	-0.7135920
C	2.5250660	-0.4092890	-1.0667380
C	2.7744590	0.3316060	0.1650580
Rh	0.6636990	0.4457530	-0.0468820
C	0.3472020	2.2746710	0.0079600
O	0.1528700	3.4068640	0.0410070
C	-5.1529520	0.6438490	0.3228560
C	-5.0049370	-0.8458600	-0.0647120
C	-3.7524680	-1.5622080	0.4895810
C	-3.8533420	1.4834300	0.3152880
C	-2.5109880	-1.4106810	-0.4160600
C	-2.8532730	1.1602580	-0.8172480
C	-1.8959910	0.0003600	-0.4666550
H	-5.8788690	1.0995320	-0.3614440
H	-5.9051910	-1.3716000	0.2727480
H	-3.9699220	-2.6328950	0.5769600
H	-1.7362700	-2.1091070	-0.0800860
H	-3.3314720	1.3634740	1.2729390
H	-2.2471800	2.0492800	-1.0180660
H	-5.5951310	0.7119600	1.3242010
H	-4.9945640	-0.9405700	-1.1579270
H	-3.5265060	-1.2084670	1.5043340
H	-4.1339830	2.5408790	0.2599160
H	-2.7893610	-1.7174980	-1.4333380
H	-3.3872640	0.9320160	-1.7492950
H	-1.4697330	0.2210820	0.5366490
H	-1.0891010	-0.0105370	-1.2337530
C	1.1320050	-2.5416800	-1.6470800
H	1.7281170	-3.4620070	-1.6030870
H	0.1027650	-2.8064860	-1.3861370
H	1.1337370	-2.1901240	-2.6819550
C	3.0725080	-0.0725030	-2.4293290
H	4.0699310	-0.5111550	-2.5667700
H	2.4269330	-0.4550430	-3.2241780
H	3.1632930	1.0081550	-2.5653690
C	3.7104390	1.5110940	0.2851200

H	4.7493370	1.1715580	0.3809280
H	3.6470320	2.1576720	-0.5940530
H	3.4723160	2.1169440	1.1633310
C	2.5311430	-0.1653240	2.7508810
H	3.4881240	-0.5995460	3.0699770
H	2.5728540	0.9096050	2.9441080
H	1.7447910	-0.5883020	3.3815730
C	0.8562590	-2.6278480	1.5140420
H	1.5402990	-3.4698560	1.6818070
H	0.5113170	-2.2768770	2.4903070
H	-0.0097320	-3.0184560	0.9727190

Cp*Rh(CO)-Cycloheptane 1,2-Migration (1)

Final Energy = -888.3109896360

C	-2.3617830	-1.0707770	-0.8246130
C	-1.2932260	-1.7379040	-0.1916920
C	-1.1931300	-1.2612510	1.1910390
C	-2.2147240	-0.3143610	1.4290950
C	-2.8489750	-0.0722530	0.1328130
Rh	-0.8531960	0.5226810	-0.2017490
C	-0.9786930	2.2694390	-0.8296170
O	-1.0267910	3.3507180	-1.2147010
C	2.2222840	1.1173240	0.3320880
C	3.4632650	1.0558410	1.2530990
C	4.8294630	1.0260950	0.5299730
C	2.2911910	0.2570050	-0.9552390
C	5.2854980	-0.3997660	0.1526210
C	2.9607490	-1.1264390	-0.8035240
C	4.4946760	-1.0817150	-0.9798870
H	1.3510710	0.8172920	0.9375560
H	3.4211510	1.9183930	1.9270890
H	5.5856710	1.4555700	1.1968160
H	6.3424330	-0.3732480	-0.1391510
H	2.8285100	0.8129220	-1.7336440
H	2.5551880	-1.7971370	-1.5692080
H	2.0431590	2.1579960	0.0385250
H	3.3990060	0.1679020	1.8943050
H	4.8053570	1.6671130	-0.3615220
H	1.2712710	0.1254180	-1.3547160
H	5.2301000	-1.0237150	1.0552230
H	2.7028520	-1.5706400	0.1685080
H	4.7095660	-0.5691530	-1.9274410
H	4.8706910	-2.1060360	-1.0913180
C	-0.2018770	-1.7946720	2.1962850
H	-0.1311810	-1.1392360	3.0680380
H	-0.4949880	-2.7926590	2.5459790

H	0.7992700	-1.8827940	1.7605040
C	-2.5996040	0.3229320	2.7383800
H	-2.9396630	1.3517050	2.5948320
H	-3.4152900	-0.2348480	3.2176280
H	-1.7564050	0.3447240	3.4337420
C	-4.0690640	0.7912590	-0.0775750
H	-4.1407700	1.1283400	-1.1149480
H	-4.9826010	0.2317080	0.1599860
H	-4.0402570	1.6773790	0.5618680
C	-2.9299820	-1.3281370	-2.1953740
H	-2.1838230	-1.7732770	-2.8586330
H	-3.7831530	-2.0172970	-2.1382220
H	-3.2804510	-0.4030290	-2.6599640
C	-0.4401250	-2.8377870	-0.7729270
H	-0.8164290	-3.8237950	-0.4710600
H	-0.4332150	-2.8015120	-1.8655510
H	0.5954410	-2.7634480	-0.4285750

Cp*Rh(CO)-Cycloheptane 1,2-Migration (2)

Final Energy = -888.3107381720

C	-2.6582130	-0.5015360	-0.8436890
C	-1.7409600	-1.5518600	-0.6171850
C	-1.3493980	-1.5436140	0.7942280
C	-2.0213720	-0.4895660	1.4507610
C	-2.7290110	0.2563050	0.4075670
Rh	-0.7155920	0.4564180	-0.1587180
C	-0.4732790	2.2967900	-0.2501760
O	-0.3195840	3.4340400	-0.3081270
C	3.0939110	1.7068240	-0.2504390
C	4.1613430	1.2049250	0.7487640
C	5.1175200	0.1119270	0.2197490
C	2.4370080	0.6261110	-1.1404330
C	4.5646790	-1.3181380	0.4004180
C	2.1641930	-0.7368540	-0.4611070
C	3.3741150	-1.6971790	-0.5001520
H	2.3155690	2.2276150	0.3188090
H	4.7430250	2.0730860	1.0783370
H	6.0634360	0.1764740	0.7694990
H	5.3695600	-2.0410890	0.2193770
H	3.0633360	0.4409120	-2.0224070
H	1.3422420	-1.2324450	-0.9948940
H	3.5425940	2.4591730	-0.9099840
H	3.6654420	0.8175990	1.6478020
H	5.3609330	0.2947780	-0.8356900
H	1.4968610	1.0361940	-1.5401900
H	4.2714560	-1.4387620	1.4522100

H	1.8335130	-0.5889630	0.5780900
H	3.7159860	-1.7614990	-1.5423040
H	3.0413220	-2.7049890	-0.2213820
C	-0.4418250	-2.5705230	1.4247630
H	-0.0758250	-2.2319310	2.3973820
H	-0.9711100	-3.5200200	1.5747900
H	0.4282550	-2.7768000	0.7931070
C	-2.0483180	-0.1868800	2.9260330
H	-2.0933160	0.8894700	3.1100400
H	-2.9269470	-0.6442600	3.4002230
H	-1.1578080	-0.5744320	3.4276370
C	-3.6820750	1.3976940	0.6665640
H	-3.7971900	2.0258680	-0.2205970
H	-4.6731720	1.0153130	0.9414140
H	-3.3268200	2.0311980	1.4834810
C	-3.4439490	-0.2205260	-2.0973200
H	-2.9288640	-0.6035300	-2.9821880
H	-4.4323350	-0.6970930	-2.0508080
H	-3.5978590	0.8522190	-2.2384690
C	-1.3100560	-2.5999950	-1.6135560
H	-0.2707420	-2.9026230	-1.4539600
H	-1.9289190	-3.5017550	-1.5209170
H	-1.4001770	-2.2342730	-2.6398200

Cp*Rh(CO)-Cycloheptane 1,2-Migration (3)

Final Energy = -888.3104804020

C	2.2235720	-0.6174940	1.2502890
C	1.4422790	-1.6048760	0.6154710
C	1.5841950	-1.4490440	-0.8334260
C	2.4933120	-0.3979050	-1.1042370
C	2.7801820	0.2251060	0.1847130
Rh	0.7068650	0.5063280	-0.0153680
C	0.4963720	2.3320360	0.2657440
O	0.3610440	3.4595180	0.4380870
C	-3.9296760	1.6676890	-0.4220480
C	-5.0454850	0.6467690	-0.1037950
C	-4.7048050	-0.4046590	0.9758850
C	-2.4861770	1.1123480	-0.4893230
C	-3.9949000	-1.6503870	0.4047530
C	-2.3229100	-0.3024720	-1.0896920
C	-2.5444700	-1.4364610	-0.0661440
H	-4.1707790	2.1452360	-1.3794040
H	-5.9351390	1.2101670	0.1997110
H	-5.6356490	-0.7364560	1.4497610
H	-3.9916390	-2.4424830	1.1634850
H	-2.0503710	1.0998980	0.5213740

H	-1.2977770	-0.3949980	-1.4852420
H	-3.9477510	2.4664530	0.3287310
H	-5.3264080	0.1135380	-1.0209070
H	-4.0966520	0.0474430	1.7710290
H	-1.8877280	1.8215900	-1.0714080
H	-4.5932410	-2.0290050	-0.4353530
H	-2.9866860	-0.4322460	-1.9552850
H	-1.9084900	-1.2348460	0.8077650
H	-2.1868080	-2.3802510	-0.4972430
C	0.9510000	-2.3692830	-1.8485970
H	0.9433240	-1.9168010	-2.8435860
H	1.5016080	-3.3163600	-1.9125420
H	-0.0824760	-2.6097720	-1.5808320
C	3.0779330	0.0004830	-2.4340860
H	3.2616260	1.0769320	-2.4797430
H	4.0350600	-0.5097390	-2.6069210
H	2.4085560	-0.2578220	-3.2586830
C	3.7901280	1.3248560	0.4059070
H	3.5749310	1.8815060	1.3217830
H	4.8002230	0.9055930	0.4954080
H	3.7911380	2.0339900	-0.4258760
C	2.4935330	-0.4680430	2.7243740
H	1.6830890	-0.8944620	3.3212030
H	3.4229880	-0.9832340	3.0014980
H	2.5995840	0.5828140	3.0050640
C	0.6817810	-2.7189850	1.2901280
H	1.3113750	-3.6133080	1.3842040
H	0.3577590	-2.4304440	2.2939080
H	-0.2061260	-3.0019110	0.7194660

Cp*Rh(CO)-Cycloheptane 1,2-Migration (4)

Final Energy = -888.3105207800

C	-2.4992080	-0.4860250	-1.0056010
C	-1.5770180	-1.5103750	-0.6847890
C	-1.3765240	-1.5424410	0.7657800
C	-2.1406780	-0.5100220	1.3476130
C	-2.7402620	0.2405760	0.2382300
Rh	-0.6756750	0.5047140	-0.0607970
C	-0.4659080	2.3501130	0.0409930
O	-0.3311260	3.4892570	0.0994690
C	4.7001340	0.9648110	0.6496290
C	4.3045570	-0.4228750	1.2055070
C	4.0748360	-1.5297770	0.1510570
C	3.9825460	1.4098400	-0.6456340
C	2.6332840	-1.5491320	-0.4025810
C	2.4866150	1.0347440	-0.7523680

C	2.2537010	-0.3791710	-1.3289110
H	4.5170450	1.7083950	1.4345790
H	5.0872430	-0.7401500	1.9038190
H	4.2674080	-2.5029950	0.6167770
H	2.4712950	-2.4871940	-0.9489840
H	4.4949930	0.9795880	-1.5157060
H	1.9917620	1.7549330	-1.4124580
H	5.7803400	0.9817860	0.4600550
H	3.3890170	-0.3290390	1.8028880
H	4.7964130	-1.4323710	-0.6712960
H	4.0931470	2.4958060	-0.7372720
H	1.9434010	-1.5618250	0.4523990
H	2.0051300	1.1265850	0.2354560
H	2.8179810	-0.4614070	-2.2680480
H	1.1933640	-0.4859870	-1.6108750
C	-0.5919400	-2.5973300	1.5060900
H	-0.1704730	-2.2040740	2.4356000
H	-1.2377170	-3.4469130	1.7633950
H	0.2304860	-2.9859720	0.9003600
C	-2.3543610	-0.2444650	2.8143250
H	-2.4543150	0.8250490	3.0157520
H	-3.2695670	-0.7381120	3.1677720
H	-1.5187730	-0.6216960	3.4098000
C	-3.7437730	1.3557630	0.4047100
H	-3.7760280	1.9941590	-0.4820010
H	-4.7492230	0.9463430	0.5643890
H	-3.4965810	1.9852260	1.2636170
C	-3.1325400	-0.1973760	-2.3413650
H	-2.5023430	-0.5451470	-3.1640080
H	-4.1046500	-0.7010580	-2.4281100
H	-3.2990230	0.8740010	-2.4792770
C	-0.9768370	-2.5089790	-1.6442150
H	0.0663240	-2.7260090	-1.3944730
H	-1.5263210	-3.4583320	-1.6130860
H	-1.0056960	-2.1370240	-2.6717560

Cp*Rh(CO)-Cycloheptane 1,2-Migration (5)

Final Energy = -888.3115110240

C	-2.1402930	0.5652330	1.3491210
C	-1.5329550	1.5903670	0.5941330
C	-1.8457790	1.3848770	-0.8227560
C	-2.6598220	0.2368250	-0.9513400
C	-2.7253240	-0.3661700	0.3804690
Rh	-0.6735670	-0.4459430	-0.0809330
C	-0.2572140	-2.2503380	0.0753900
O	0.0060770	-3.3652700	0.1626580

C	4.5451050	-1.3806870	-0.0235870
C	5.1890460	0.0237540	0.0469030
C	4.3990980	1.0852840	0.8459990
C	3.0076740	-1.4199960	-0.1806510
C	3.3423510	1.8225190	-0.0044360
C	2.4052770	-0.3539510	-1.1224920
C	2.1133370	0.9915180	-0.4204030
H	5.0056080	-1.9234430	-0.8580940
H	6.1909580	-0.0869080	0.4767670
H	5.1031640	1.8345340	1.2256530
H	2.9878980	2.7036040	0.5448910
H	2.5308450	-1.3105750	0.8017190
H	1.4557780	-0.7374360	-1.5319510
H	4.8042000	-1.9408320	0.8829480
H	5.3401120	0.4087870	-0.9695810
H	3.9276220	0.6294850	1.7268950
H	2.7290370	-2.4186610	-0.5335840
H	3.8367370	2.2004120	-0.9100400
H	3.0570960	-0.1938450	-1.9922170
H	1.5126270	0.7823090	0.4823920
H	1.4915280	1.6106030	-1.0789320
C	-0.7587350	2.7705840	1.1264090
H	-1.3817950	3.6738800	1.1346020
H	-0.4132490	2.5913710	2.1477120
H	0.1194180	2.9852100	0.5092480
C	-1.4571670	2.3379960	-1.9261400
H	-1.4720190	1.8443100	-2.9013200
H	-2.1500370	3.1882880	-1.9674890
H	-0.4536280	2.7449560	-1.7703680
C	-3.3545600	-0.2660100	-2.1892690
H	-3.4082560	-1.3575630	-2.1996550
H	-4.3814040	0.1200320	-2.2419230
H	-2.8309570	0.0514790	-3.0948030
C	-3.5856950	-1.5519450	0.7441870
H	-3.2143960	-2.0478800	1.6447980
H	-4.6183510	-1.2335880	0.9347580
H	-3.6035070	-2.2894050	-0.0625110
C	-2.2151800	0.4376170	2.8481940
H	-1.3867590	0.9581240	3.3354730
H	-3.1518700	0.8670780	3.2279310
H	-2.1794910	-0.6095810	3.1590260

Cp*Rh(CO)-Cycloheptane 1,2-Migration (6)

Final Energy = -888.3115970740

C	2.6580460	0.0616290	-0.9479820
C	1.9130860	1.2623120	-0.9138070

C	1.6170900	1.6005960	0.4810890
C	2.1578430	0.6020110	1.3163390
C	2.6845590	-0.4379190	0.4272140
Rh	0.6307020	-0.4247090	-0.0403150
C	0.0980950	-2.1783820	0.2709990
O	-0.2326180	-3.2632850	0.4542410
C	-5.0421030	-0.1222950	0.7242230
C	-4.0332630	0.9680800	1.1535550
C	-3.3616980	1.7516700	0.0028840
C	-4.6527190	-0.9592050	-0.5172030
C	-2.0917190	1.0613540	-0.5400780
C	-3.1560790	-1.3268660	-0.6342260
C	-2.3207580	-0.2379920	-1.3402240
H	-5.1939910	-0.7948860	1.5769900
H	-4.5557190	1.6680040	1.8153650
H	-3.0745550	2.7429980	0.3717020
H	-1.5415530	1.7650420	-1.1768930
H	-4.9428580	-0.4200740	-1.4279400
H	-3.0626410	-2.2499170	-1.2168700
H	-6.0147920	0.3450540	0.5277670
H	-3.2408870	0.5136700	1.7614040
H	-4.0743940	1.9196260	-0.8161290
H	-5.2537290	-1.8752980	-0.5069650
H	-1.4448150	0.8466840	0.3307110
H	-2.7357780	-1.5469420	0.3558740
H	-2.8131850	0.0113540	-2.2902920
H	-1.3382950	-0.6577990	-1.6152060
C	1.5731110	2.1453720	-2.0891610
H	0.5855240	2.6022080	-1.9733930
H	2.3002490	2.9617500	-2.1864330
H	1.5737510	1.5807300	-3.0250230
C	0.9167360	2.8640790	0.9147410
H	0.5688480	2.7893310	1.9481540
H	1.5909760	3.7272260	0.8466870
H	0.0485380	3.0776410	0.2831880
C	2.2217340	0.5894640	2.8211290
H	2.1079330	-0.4235060	3.2154530
H	3.1873240	0.9778240	3.1715600
H	1.4336720	1.2082810	3.2579070
C	3.4699450	-1.6417110	0.8884160
H	3.4492910	-2.4371320	0.1388980
H	4.5184320	-1.3716230	1.0666700
H	3.0634860	-2.0464460	1.8190120
C	3.3215550	-0.5790470	-2.1385980
H	2.8171930	-0.3060870	-3.0692500
H	4.3692330	-0.2592690	-2.2180430

H 3.3113260 -1.6691460 -2.0604830

Cp*Rh(CO)-Cycloheptane 1,3-Migration (1)

Final Energy = -888.3122257720

C	2.4439850	0.0330440	-1.0646890
C	1.7759310	1.2637350	-0.8839660
C	1.6074390	1.5016790	0.5527970
C	2.1821420	0.4275790	1.2686330
C	2.5702130	-0.5645750	0.2672020
Rh	0.4814030	-0.4155350	-0.0006080
C	-0.1263370	-2.1640020	0.1730880
O	-0.5223980	-3.2377330	0.2777080
C	-2.2795350	0.5319140	-1.5722880
C	-3.1564540	-0.7456950	-1.4342560
C	-4.4469560	-0.6217030	-0.5950610
C	-2.4660950	1.6301160	-0.5097040
C	-4.2015770	-0.6662370	0.9297780
C	-2.3280340	1.1498040	0.9481780
C	-3.6416720	0.6232350	1.5577770
H	-1.2149170	0.2218840	-1.5740360
H	-3.4189980	-1.0858190	-2.4417670
H	-5.0935290	-1.4673880	-0.8562110
H	-5.1455620	-0.9033500	1.4352160
H	-3.4464200	2.1064970	-0.6342570
H	-1.9682980	1.9781030	1.5695210
H	-2.4441180	0.9832370	-2.5578700
H	-2.5588160	-1.5538540	-0.9971690
H	-5.0044060	0.2850630	-0.8643410
H	-1.7234620	2.4122930	-0.7103130
H	-3.5179730	-1.4989520	1.1443480
H	-1.5456730	0.3652720	1.0207930
H	-4.3954440	1.4186190	1.4742390
H	-3.4918830	0.4494220	2.6300680
C	1.0120670	2.7589840	1.1362630
H	1.7408680	3.5794040	1.1196820
H	0.1374950	3.0885190	0.5666060
H	0.6993950	2.6074120	2.1726010
C	2.3830530	0.3111640	2.7568420
H	2.2845040	-0.7248320	3.0909160
H	3.3839720	0.6609380	3.0431130
H	1.6506990	0.9094900	3.3051360
C	3.3279810	-1.8355050	0.5658310
H	3.1833260	-2.5768340	-0.2243650
H	4.4032960	-1.6321570	0.6457450
H	2.9978430	-2.2802630	1.5081880
C	2.9581690	-0.5591570	-2.3506110

H	2.3985050	-0.1852890	-3.2118650
H	4.0157330	-0.3037360	-2.4999060
H	2.8765490	-1.6490230	-2.3471280
C	1.3711730	2.2412840	-1.9594480
H	0.3828510	2.6681490	-1.7613040
H	2.0821020	3.0752880	-2.0186960
H	1.3354380	1.7588680	-2.9394350

Cp*Rh(CO)-Cycloheptane 1,3-Migration (2)

Final Energy = -888.3122229600

C	-2.1974580	0.3944200	1.2630710
C	-1.6183350	1.4842750	0.5752810
C	-1.7683260	1.2737390	-0.8673360
C	-2.4294090	0.0446170	-1.0808460
C	-2.5689370	-0.5798280	0.2374090
Rh	-0.4762600	-0.4126510	-0.0011460
C	0.1511790	-2.1570200	0.1485590
O	0.5641250	-3.2258120	0.2378310
C	3.1813390	-0.6716010	-1.4944470
C	4.4312040	-0.6128690	-0.5903560
C	4.1216640	-0.7296430	0.9187160
C	2.2782440	0.5968000	-1.5472590
C	3.6072550	0.5550240	1.5924750
C	2.4832170	1.6639060	-0.4570360
C	2.3242520	1.1547280	0.9884740
H	3.5006370	-0.9040020	-2.5160890
H	5.0748420	-1.4548770	-0.8703540
H	5.0316040	-1.0433740	1.4442480
H	3.4344880	0.3459970	2.6549840
H	1.2181280	0.2715460	-1.5208200
H	1.7539930	2.4628220	-0.6417060
H	2.5834350	-1.5309750	-1.1697440
H	5.0141400	0.2965390	-0.7868640
H	3.3877310	-1.5344870	1.0629920
H	2.3951690	1.0848420	-2.5219360
H	4.3946570	1.3206180	1.5498670
H	3.4719670	2.1266980	-0.5661910
H	1.5095560	0.4017680	1.0386390
H	1.9962230	1.9818660	1.6288990
C	-1.3511300	2.2739700	-1.9169630
H	-1.3075430	1.8141980	-2.9073950
H	-2.0590240	3.1113260	-1.9635950
H	-0.3633020	2.6930010	-1.6997740
C	-2.9253810	-0.5247070	-2.3841270
H	-2.8425060	-1.6143780	-2.3988860
H	-3.9811970	-0.2678090	-2.5429640

H	-2.3548320	-0.1353050	-3.2312130
C	-3.3232700	-1.8601570	0.5023760
H	-3.0034510	-2.3195510	1.4412690
H	-4.4007990	-1.6645150	0.5709620
H	-3.1631540	-2.5863970	-0.2987760
C	-2.4148050	0.2480000	2.7462520
H	-1.6943820	0.8427920	3.3138950
H	-3.4221600	0.5832720	3.0271840
H	-2.3103710	-0.7930650	3.0623180
C	-1.0317200	2.7307410	1.1899570
H	-1.7577310	3.5535820	1.1723910
H	-0.7398870	2.5610700	2.2295740
H	-0.1450160	3.0661890	0.6427960

Cp*Rh(CO)-Cycloheptane 1,4-Migration (1)

Final Energy = -888.3114335760

C	-2.1033370	0.4671310	1.2411300
C	-1.4065800	1.5284060	0.6140720
C	-1.5562480	1.4138970	-0.8388520
C	-2.3015430	0.2507260	-1.1196710
C	-2.5380410	-0.4179770	0.1663350
Rh	-0.4402670	-0.4570760	-0.0136150
C	-0.0589160	-2.2743520	-0.0095100
O	0.1840080	-3.3972380	0.0004200
C	3.4832910	-1.5200020	-0.4163680
C	2.8640170	-0.5569120	-1.4543950
C	3.3608260	0.9043540	-1.4091660
C	3.7424380	-0.9374820	0.9931760
C	2.5892640	1.7747940	-0.3943720
C	2.6674440	0.0274610	1.5391120
C	2.8666630	1.4888760	1.0919190
H	2.8263560	-2.3932850	-0.3303860
H	3.0405070	-0.9775850	-2.4507690
H	3.2314830	1.3495380	-2.4020420
H	2.8015530	2.8338220	-0.5884240
H	4.7020360	-0.4048820	0.9979110
H	2.6934460	0.0003470	2.6344300
H	4.4375380	-1.8962550	-0.8044280
H	1.7651120	-0.5461100	-1.3459170
H	4.4372550	0.9353200	-1.1930430
H	3.8617000	-1.7784890	1.6850540
H	1.5145020	1.6330600	-0.5871760
H	1.6520150	-0.3235380	1.2684220
H	3.8998750	1.7794040	1.3268110
H	2.2185840	2.1388980	1.6922950
C	-1.0860880	2.4417560	-1.8383970

H	-1.8214300	3.2510560	-1.9348040
H	-0.1393050	2.8970030	-1.5358350
H	-0.9434740	1.9991030	-2.8277430
C	-2.8107100	-0.2136560	-2.4590060
H	-2.8214550	-1.3045370	-2.5241060
H	-3.8361620	0.1411410	-2.6280700
H	-2.1868680	0.1637680	-3.2733540
C	-3.4176220	-1.6310880	0.3484360
H	-3.1734330	-2.1618260	1.2722760
H	-4.4732450	-1.3353420	0.3960590
H	-3.3023740	-2.3317600	-0.4826970
C	-2.3765980	0.2877690	2.7114510
H	-1.6069980	0.7689540	3.3207700
H	-3.3441520	0.7300940	2.9845820
H	-2.4051990	-0.7701010	2.9848300
C	-0.7447460	2.6915150	1.3125930
H	0.1260770	3.0508500	0.7572160
H	-1.4427400	3.5329190	1.4099900
H	-0.4123510	2.4134600	2.3165490

Cp*Rh(CO)-Cyclooctane σ -complex (1)

Final Energy = -927.6091537510

C	1.8785750	-0.4037600	1.5874830
C	1.1128120	-1.4311200	0.9871620
C	1.6373480	-1.6912320	-0.3547140
C	2.7213870	-0.8152850	-0.5931880
C	2.7888230	0.0839280	0.5554590
Rh	0.8656020	0.4661400	-0.2743200
C	0.9094490	2.2893720	-0.6261230
O	0.9340550	3.4176390	-0.8432810
C	-1.6776230	0.2889530	-0.8221860
C	-2.5116080	1.5947680	-0.8765650
C	-4.1367870	-1.5408100	0.2575280
C	-3.2397750	1.9396560	0.4405060
C	-3.9134970	-0.4396400	1.3253790
C	-4.3619100	0.9909920	0.9226990
H	-1.4688800	0.0474550	0.2225860
H	-2.4839950	2.0155020	1.2347250
H	-3.5834410	-2.4408230	0.5584620
H	-2.8637630	-0.4158480	1.6364140
H	-0.7237060	0.4691670	-1.4065730
H	-5.1988170	-1.8168910	0.2788810
H	-3.6705690	2.9424880	0.3321830
H	-4.4728760	-0.7466450	2.2162430
C	-2.3076900	-0.9359900	-1.5257150
H	-1.7186600	-1.8275170	-1.2773570

H	-2.2169440	-0.7984680	-2.6107050
C	-3.7906210	-1.1999380	-1.2050850
H	-4.3916410	-0.3444780	-1.5319170
H	-4.1157510	-2.0421340	-1.8281900
H	-1.8478510	2.4332380	-1.1094520
H	-4.8196830	1.4676090	1.7968300
H	-5.1542660	0.9357670	0.1651560
H	-3.2311870	1.5384790	-1.7025730
C	1.7999540	0.1006600	3.0050880
H	2.5361150	-0.4098490	3.6402640
H	2.0043550	1.1731460	3.0562230
H	0.8106020	-0.0697640	3.4372930
C	3.8728250	1.1113100	0.7809700
H	3.5371710	1.8972290	1.4626740
H	4.7643790	0.6437760	1.2172220
H	4.1677030	1.5874110	-0.1577990
C	1.1879390	-2.8202950	-1.2496430
H	1.7529000	-3.7353600	-1.0294580
H	0.1291560	-3.0505420	-1.1048150
H	1.3380730	-2.5790460	-2.3054490
C	-0.0082800	-2.2140140	1.6266260
H	-0.8654250	-2.3175320	0.9510470
H	0.3196090	-3.2263560	1.8938680
H	-0.3604800	-1.7240380	2.5380680
C	3.6547940	-0.8176490	-1.7751610
H	3.9882810	0.1936740	-2.0210640
H	4.5473600	-1.4214990	-1.5630770
H	3.1710170	-1.2350070	-2.6621760

Cp*Rh(CO)-Cyclooctane σ -complex (2)

Final Energy = -927.6090451650

C	1.8701330	-0.5157270	1.5104410
C	1.2548570	-1.5477780	0.7587690
C	1.7971170	-1.5318240	-0.6022390
C	2.7207770	-0.4690990	-0.7045590
C	2.6728940	0.2513560	0.5668580
Rh	0.6892930	0.4531210	-0.1809570
C	0.4704450	2.2936110	-0.3007350
O	0.3316700	3.4323000	-0.3717360
C	-1.6954810	0.1282990	-1.2498960
C	-2.6512420	1.3478600	-1.3224520
C	-3.6425460	-1.5503990	0.8018250
C	-3.1207010	1.9240530	0.0324770
C	-3.3046900	-0.2227870	1.5248650
C	-3.9969810	1.0424700	0.9511770
H	-1.2452420	0.1385450	-0.2170380

H	-2.2306370	2.2271880	0.5993830
H	-2.9372210	-2.3240720	1.1341330
H	-2.2211570	-0.0625360	1.5512620
H	-0.9226410	0.2398580	-2.0188170
H	-4.6345780	-1.8753580	1.1409370
H	-3.6748080	2.8467270	-0.1787700
H	-3.6043170	-0.3464370	2.5716060
C	-2.3447470	-1.2602310	-1.4604510
H	-1.6204580	-2.0342570	-1.1786780
H	-2.5203870	-1.3817980	-2.5370390
C	-3.6777260	-1.5261680	-0.7380810
H	-4.4242610	-0.7989350	-1.0756270
H	-4.0442810	-2.5026810	-1.0779540
H	-2.1337510	2.1584280	-1.8474590
H	-4.3046230	1.6783410	1.7889090
H	-4.9237660	0.7627770	0.4340940
H	-3.5180580	1.0876550	-1.9428780
C	1.7479180	-0.2600050	2.9898700
H	2.5598360	-0.7566700	3.5380340
H	1.7996830	0.8083310	3.2147740
H	0.8002230	-0.6382280	3.3821200
C	0.3123790	-2.5999520	1.2916140
H	0.8637600	-3.4941950	1.6094930
H	-0.2517820	-2.2296750	2.1522530
H	-0.4078780	-2.9150010	0.5310590
C	1.4875710	-2.5605350	-1.6614140
H	2.0553810	-3.4831510	-1.4852570
H	0.4270100	-2.8280320	-1.6689570
H	1.7457190	-2.1931750	-2.6579700
C	3.6136920	-0.1364070	-1.8715700
H	4.6016950	-0.5998530	-1.7489510
H	3.1899360	-0.4956100	-2.8129600
H	3.7622960	0.9425090	-1.9630130
C	3.5929020	1.3888380	0.9428890
H	4.5589860	1.0048410	1.2936330
H	3.7820380	2.0440110	0.0884800
H	3.1623080	1.9981560	1.7418210

Cp*Rh(CO)-Cyclooctane σ -complex (3)

Final Energy = -927.6082997100

C	-2.8267670	-0.2221230	-0.9489180
C	-1.9132740	-1.2996690	-1.0082790
C	-1.5338610	-1.6654090	0.3577320
C	-2.2189020	-0.8231380	1.2652590
C	-2.9152520	0.1701370	0.4558880
Rh	-0.8685850	0.4962460	-0.0256840

C	-0.6481140	2.3037250	0.3398480
O	-0.5137980	3.4228040	0.5646570
C	2.3356850	-1.0503160	-0.9237330
C	1.7418850	0.3011370	-0.4522080
C	5.2320640	-0.4806260	0.5247130
C	2.5755490	1.5610050	-0.7855670
C	5.0216680	0.6610990	-0.4998390
C	3.9544110	1.7160140	-0.1059910
H	3.0224670	-0.8651980	-1.7549630
H	2.7225300	1.5924600	-1.8738790
H	5.8389570	-1.2681990	0.0589600
H	4.7784360	0.2500120	-1.4845510
H	1.5322650	-1.6707340	-1.3362310
H	5.8317710	-0.0823050	1.3532410
H	1.9728850	2.4398640	-0.5314490
H	5.9878830	1.1629380	-0.6228520
C	3.0333570	-1.8747470	0.1841880
H	3.5883180	-2.6966870	-0.2869450
H	2.2525740	-2.3412780	0.7978370
C	3.9683000	-1.1103390	1.1399970
H	3.3959860	-0.3369690	1.6649330
H	4.2917960	-1.8138930	1.9168170
H	0.7939680	0.4587250	-1.0515600
H	4.3242070	2.7087790	-0.3858490
H	3.8323580	1.7403440	0.9840190
H	1.5352030	0.2667860	0.6238610
C	-2.2567370	-0.9289650	2.7675230
H	-2.3308020	0.0569840	3.2334830
H	-3.1237160	-1.5186610	3.0944740
H	-1.3575630	-1.4143880	3.1560120
C	-0.6732180	-2.8521710	0.7137370
H	-0.2255360	-2.7364050	1.7046130
H	-1.2679600	-3.7746820	0.7194230
H	0.1365410	-2.9922950	-0.0079280
C	-1.4962170	-2.0542130	-2.2471700
H	-0.4605950	-2.3994540	-2.1800970
H	-2.1263100	-2.9410290	-2.3935800
H	-1.5825360	-1.4297420	-3.1401710
C	-3.5879490	0.4007970	-2.0897960
H	-3.0598490	0.2723390	-3.0381340
H	-4.5796560	-0.0599370	-2.1915460
H	-3.7338920	1.4723000	-1.9316440
C	-3.8666140	1.2099910	0.9993180
H	-3.9661330	2.0538630	0.3115500
H	-4.8641480	0.7791770	1.1512420
H	-3.5188090	1.6006560	1.9592380

Cp*Rh(CO)-Cyclooctane σ -complex (4)

Final Energy = -927.6095552430

C	-2.7205110	-0.0758460	0.9472890
C	-1.9603240	1.1102410	1.0725970
C	-1.6622910	1.6258300	-0.2648710
C	-2.2277780	0.7522800	-1.2222430
C	-2.7679670	-0.3829170	-0.4789560
Rh	-0.6870500	-0.4415170	-0.0308760
C	-0.1851560	-2.1502630	-0.5580210
O	0.1261330	-3.2092380	-0.8781250
C	2.3386600	1.4402530	0.9412610
C	1.6388490	0.0611650	1.0675380
C	4.7249670	0.2847680	-1.0058660
C	2.5342970	-1.1311060	1.4735050
C	4.7988180	-0.5360140	0.3052430
C	3.6579040	-1.5680200	0.5090010
H	3.2308870	1.4356990	1.5746480
H	2.9887620	-0.8852870	2.4435310
H	5.4369260	1.1182900	-0.9424110
H	4.8396610	0.1326630	1.1710180
H	1.6805630	2.2107120	1.3607560
H	5.0772960	-0.3564850	-1.8239360
H	1.8770840	-1.9908990	1.6464810
H	5.7585500	-1.0646050	0.2985890
C	2.6958500	1.8785600	-0.4987810
H	3.3455420	2.7616920	-0.4426120
H	1.7689290	2.2058850	-0.9865180
C	3.3431330	0.8255700	-1.4185290
H	2.6493610	-0.0110450	-1.5596200
H	3.4487470	1.2816140	-2.4105580
H	0.8535170	0.1315780	1.8266340
H	4.0853540	-2.4859790	0.9272760
H	3.2274850	-1.8555130	-0.4583570
H	1.2183810	-0.1621450	0.0390700
C	-0.9937370	2.9511880	-0.5343820
H	-1.7112250	3.7751460	-0.4282020
H	-0.1757440	3.1390240	0.1676670
H	-0.5836530	2.9928300	-1.5467990
C	-2.2959710	0.9455380	-2.7145280
H	-3.2474540	1.4123090	-3.0025290
H	-1.4860710	1.5880820	-3.0695440
H	-2.2206390	-0.0087300	-3.2419050
C	-3.5700170	-1.5064210	-1.0920870
H	-4.6188670	-1.2096320	-1.2170080
H	-3.1784860	-1.7800790	-2.0753810
H	-3.5457940	-2.3998000	-0.4625610

C	-3.3733000	-0.8746040	2.0453560
H	-4.4191330	-0.5676390	2.1794670
H	-3.3675750	-1.9432220	1.8160600
H	-2.8597680	-0.7367280	3.0003870
C	-1.5894930	1.8160530	2.3537760
H	-2.2577040	2.6657410	2.5424790
H	-1.6541540	1.1417380	3.2117610
H	-0.5682000	2.2094150	2.3127250

Cp*Rh(CO)-Cyclooctane σ -complex (5)

Final Energy = -927.6084386020

C	-2.4865780	0.0404270	1.3791270
C	-1.6579310	1.1803150	1.2333490
C	-1.8001720	1.7035310	-0.1266700
C	-2.6877450	0.8649870	-0.8372600
C	-3.0173730	-0.2469790	0.0522160
Rh	-0.9125070	-0.4207660	-0.2172040
C	-0.7228120	-2.1110280	-0.9634130
O	-0.6069960	-3.1580630	-1.4227960
C	4.8041610	-0.5632610	1.0885140
C	5.3704780	-0.1025930	-0.2805120
C	1.6858230	-0.1520300	0.1582310
C	4.8469010	1.2578880	-0.7934550
C	2.3592920	1.2365800	0.0274980
C	3.3500980	1.3845630	-1.1565800
H	4.4716730	0.3122020	1.6552820
H	5.0786980	2.0196290	-0.0358020
H	1.1872890	-0.2198050	1.1321270
H	2.8668960	1.4922920	0.9626930
H	5.6146080	-1.0044370	1.6793410
H	0.9487330	-0.1784950	-0.7059250
H	5.4288450	1.5274590	-1.6835960
H	1.5549420	1.9702990	-0.0883940
C	3.6744010	-1.6184920	1.0130050
H	3.2118360	-1.7190890	2.0034830
H	4.1344640	-2.5897930	0.7907590
C	2.5742640	-1.3943630	-0.0413900
H	3.0263230	-1.3590050	-1.0386220
H	1.9219210	-2.2739020	-0.0375860
H	6.4586820	-0.0069050	-0.1935450
H	3.2160730	2.3795980	-1.5954680
H	3.0942270	0.6726370	-1.9512130
H	5.1992530	-0.8781890	-1.0377000
C	-2.7858090	-0.7305670	2.6385650
H	-3.6971450	-0.3511050	3.1198690
H	-2.9397460	-1.7915720	2.4258780

H	-1.9696320	-0.6517590	3.3614220
C	-4.0362030	-1.3184190	-0.2565180
H	-3.8539220	-2.2201130	0.3340270
H	-5.0498750	-0.9648870	-0.0300330
H	-4.0064270	-1.5990200	-1.3126830
C	-3.2299560	1.0799440	-2.2258660
H	-3.3800140	0.1306880	-2.7462870
H	-4.1980370	1.5972490	-2.1883700
H	-2.5483610	1.6873990	-2.8271820
C	-1.2068750	3.0004340	-0.6198000
H	-1.0107590	2.9687180	-1.6951250
H	-1.8914960	3.8366560	-0.4271220
H	-0.2665900	3.2302240	-0.1113850
C	-0.8366890	1.8426960	2.3128190
H	0.1434650	2.1534380	1.9358590
H	-1.3398590	2.7397690	2.6948430
H	-0.6709020	1.1670130	3.1558670

Cp*Rh(CO)-Cyclooctane σ -complex (6)

Final Energy = -927.6087803090

C	2.4467240	-0.3494920	1.3603640
C	1.6698600	-1.4529600	0.9314110
C	1.8330730	-1.6090390	-0.5156510
C	2.7010410	-0.5968770	-0.9854800
C	2.9772050	0.2737680	0.1539410
Rh	0.8659000	0.4317260	-0.0833450
C	0.6109360	2.2536480	-0.3379130
O	0.4536840	3.3813760	-0.4939850
C	-4.3002130	1.0264410	1.0522680
C	-5.2976370	0.2101690	0.1878110
C	-1.6772880	-0.0312890	-0.5659690
C	-4.9776350	-1.2945220	0.0414970
C	-2.3590480	-1.3104460	-0.0151970
C	-3.6898630	-1.7071930	-0.7069380
H	-3.7794980	0.3531060	1.7408380
H	-4.9411580	-1.7351880	1.0476470
H	-1.0027570	0.3253680	0.2790890
H	-2.5260690	-1.2205160	1.0624980
H	-4.8623330	1.7193920	1.6880560
H	-1.1178550	-0.3015470	-1.4676600
H	-5.8248650	-1.7700040	-0.4683520
H	-1.6412550	-2.1284040	-0.1361830
C	-3.2792010	1.8701420	0.2536680
H	-2.5211210	2.2631710	0.9437060
H	-3.8029770	2.7435560	-0.1550650
C	-2.5741310	1.1699550	-0.9210800

H	-3.3156600	0.8502350	-1.6612030
H	-1.9470140	1.9112020	-1.4283390
H	-6.2918570	0.2758790	0.6440210
H	-3.7146090	-2.7992970	-0.7959490
H	-3.7116370	-1.3244870	-1.7346590
H	-5.3947130	0.6685060	-0.8047360
C	1.2562330	-2.7443570	-1.3249740
H	1.8740240	-3.6463240	-1.2280290
H	0.2476520	-3.0049760	-0.9908390
H	1.2016520	-2.4883190	-2.3864290
C	3.2622910	-0.4385620	-2.3745420
H	4.2508350	-0.9109510	-2.4500490
H	2.6130740	-0.9012450	-3.1224480
H	3.3768950	0.6156410	-2.6392810
C	3.9542510	1.4256350	0.1376390
H	4.9799350	1.0646370	0.2841100
H	3.9192060	1.9609260	-0.8148900
H	3.7330700	2.1428980	0.9323300
C	2.7083510	0.0950590	2.7757140
H	3.6346200	-0.3539350	3.1586990
H	2.8151000	1.1810070	2.8374220
H	1.8937470	-0.1977470	3.4430750
C	0.9168410	-2.4160350	1.8166780
H	1.5277750	-3.3011260	2.0359710
H	0.6466720	-1.9503060	2.7679740
H	-0.0046070	-2.7640840	1.3416020

Cp*Rh(CO)-Cyclooctane σ -complex (7)

Final Energy = -927.6086947230

C	2.3833560	-0.6105140	1.2736450
C	1.7084410	-1.6055640	0.5285690
C	1.9285010	-1.3526320	-0.8968830
C	2.7473310	-0.2072510	-1.0369040
C	2.9161840	0.3423930	0.3045060
Rh	0.8101830	0.4355720	-0.0050320
C	0.4176920	2.2317890	0.2608790
O	0.1698440	3.3424050	0.4218150
C	-3.0733950	-1.5346830	0.7552060
C	-2.3132970	-1.4161170	-0.5915670
C	-4.8416910	1.1924290	0.1869240
C	-1.6396010	-0.0499060	-0.8543390
C	-3.3566640	1.6305160	0.1804790
C	-2.5379660	1.1894030	-1.0606860
H	-2.6596060	-0.8128250	1.4664490
H	-1.0615640	0.1504440	0.1068920
H	-5.2569810	1.3736910	1.1868480

H	-2.8514340	1.2843440	1.0878210
H	-2.8722700	-2.5205700	1.1888360
H	-5.3902750	1.8543000	-0.4957240
H	-0.9861660	-0.1482130	-1.7267880
H	-3.3420190	2.7238940	0.2398210
C	-4.6115940	-1.3827540	0.6633660
H	-5.0140270	-1.2619910	1.6775200
H	-5.0209520	-2.3275820	0.2827870
C	-5.1544530	-0.2557740	-0.2359420
H	-4.8138730	-0.4169180	-1.2652840
H	-6.2458890	-0.3603830	-0.2711750
H	-1.5194400	-2.1698180	-0.6152310
H	-1.8781880	2.0098550	-1.3594210
H	-3.2053610	1.0093640	-1.9129270
H	-2.9803170	-1.6548310	-1.4293390
C	1.4414710	-2.2540340	-2.0048860
H	2.0607610	-3.1571290	-2.0762660
H	0.4101960	-2.5797030	-1.8345950
H	1.4754830	-1.7470240	-2.9726770
C	3.3514700	0.3462400	-2.3013100
H	4.3678510	-0.0426520	-2.4488970
H	2.7597340	0.0759440	-3.1797050
H	3.4149530	1.4367920	-2.2661770
C	3.8081390	1.5116350	0.6493410
H	4.8504340	1.1855970	0.7546150
H	3.7725840	2.2793020	-0.1281190
H	3.5041160	1.9760820	1.5910690
C	1.0042600	-2.8168620	1.0889550
H	0.1668430	-3.1254750	0.4571780
H	1.6926620	-3.6692710	1.1556720
H	0.6133990	-2.6216490	2.0909290
C	2.5530810	-0.5423730	2.7687510
H	3.4989140	-1.0098400	3.0737900
H	2.5648070	0.4921840	3.1209130
H	1.7410180	-1.0615530	3.2844700

Cp*Rh(CO)-Cyclooctane σ -complex (8)

Final Energy = -927.6082702120

C	2.3419030	-0.3747010	1.4215700
C	1.5346820	-1.4333130	0.9391960
C	1.8175800	-1.6400380	-0.4824870
C	2.7785750	-0.6875240	-0.8898400
C	3.0118060	0.1890780	0.2558320
Rh	0.9499300	0.4752910	-0.1850990
C	0.8493600	2.2935810	-0.5461190
O	0.7907270	3.4194250	-0.7691650

C	-3.4356100	-1.6990640	0.2376640
C	-2.3219720	-1.1102220	-0.6675940
C	-5.0957560	1.1425390	0.3598550
C	-1.6739280	0.1924090	-0.1445860
C	-3.6956360	1.4237770	0.9569820
C	-2.5313610	1.4758340	-0.0676120
H	-3.2871730	-1.3530090	1.2651550
H	-1.2673600	-0.0024330	0.8557990
H	-5.7929250	0.9304520	1.1810460
H	-3.4596110	0.6936300	1.7371150
H	-3.3217090	-2.7884810	0.2737470
H	-5.4517200	2.0674330	-0.1120220
H	-0.8583800	0.4134780	-0.9020400
H	-3.7529130	2.3907250	1.4687440
C	-4.8844640	-1.4090030	-0.2252440
H	-5.5739530	-1.6837360	0.5836600
H	-5.1108420	-2.0824840	-1.0619600
C	-5.1979590	0.0244590	-0.6944820
H	-4.5625000	0.2754440	-1.5514420
H	-6.2242910	0.0273420	-1.0816140
H	-1.5157320	-1.8449350	-0.7616190
H	-1.8548190	2.2889020	0.2122150
H	-2.9129870	1.7296060	-1.0640860
H	-2.7022090	-0.9539020	-1.6845600
C	1.2793040	-2.7799520	-1.3121990
H	1.9390700	-3.6544580	-1.2409770
H	0.2897390	-3.0942950	-0.9697580
H	1.1982340	-2.5058600	-2.3676150
C	3.4687270	-0.6010670	-2.2257980
H	4.4231820	-1.1439990	-2.2043770
H	2.8544760	-1.0345090	-3.0193600
H	3.6821040	0.4358230	-2.4973050
C	4.0597470	1.2757820	0.3049910
H	5.0435270	0.8539670	0.5459290
H	4.1409350	1.7903780	-0.6560750
H	3.8183860	2.0235340	1.0649940
C	2.5032950	0.0884000	2.8463020
H	3.3672530	-0.3982340	3.3183940
H	2.6616430	1.1686470	2.8972630
H	1.6196340	-0.1467150	3.4453670
C	0.6021210	-2.2978500	1.7523680
H	1.0505160	-3.2787790	1.9535890
H	0.3691710	-1.8326340	2.7135770
H	-0.3438840	-2.4731570	1.2281980

Cp*Rh(CO)-Cyclooctane σ -complex (9)

Final Energy = -927.6088913640

C	2.7220230	0.2309080	-0.7709420
C	1.9047810	1.3824950	-0.7130680
C	1.4233630	1.5496320	0.6601330
C	1.9463470	0.5030830	1.4557960
C	2.6390890	-0.4011690	0.5431900
Rh	0.6294320	-0.4470260	-0.1434540
C	0.2237520	-2.2578200	-0.0809790
O	-0.0236240	-3.3795910	-0.0410890
C	-3.8397430	-1.3249050	-0.6425260
C	-3.4768560	-1.2837830	0.8661840
C	-2.2878790	1.4974510	-1.3095130
C	-3.8182720	0.0332050	1.5996510
C	-3.3631120	1.8310380	-0.2476730
C	-3.0688070	1.3212120	1.1886960
H	-4.6474750	-0.6131080	-0.8402450
H	-4.8963790	0.2176070	1.4900350
H	-2.6974150	1.6987750	-2.3080350
H	-4.3394490	1.4560700	-0.5693840
H	-4.2511210	-2.3117230	-0.8817640
H	-1.4510090	2.1933020	-1.1774030
H	-3.6435790	-0.1272960	2.6707160
H	-3.4592240	2.9225590	-0.2273840
C	-2.6642710	-1.0878970	-1.6208270
H	-3.0682250	-0.9333560	-2.6300380
H	-2.0654800	-2.0048460	-1.6658560
C	-1.7020840	0.0726530	-1.3019260
H	-1.3038720	-0.1063130	-0.2603700
H	-0.8941320	0.0407190	-2.0427270
H	-4.0320230	-2.0791030	1.3759020
H	-3.3666960	2.1001170	1.8996720
H	-1.9885830	1.1846510	1.3303380
H	-2.4163410	-1.5251390	1.0089600
C	0.6318790	2.7383010	1.1478520
H	1.2835440	3.6122700	1.2754290
H	-0.1556350	3.0193670	0.4422260
H	0.1571630	2.5306290	2.1102420
C	1.6562100	2.3663660	-1.8297830
H	0.6382030	2.7655810	-1.7956640
H	2.3428820	3.2195090	-1.7572050
H	1.8009350	1.9025750	-2.8090750
C	3.5424550	-0.2565630	-1.9366820
H	3.1212350	0.0776750	-2.8884570
H	4.5710930	0.1228490	-1.8732130
H	3.5919560	-1.3481410	-1.9591560

C	3.4488650	-1.6018600	0.9724850
H	3.5505390	-2.3229710	0.1571980
H	4.4566140	-1.2977620	1.2818690
H	2.9785520	-2.1150540	1.8153410
C	1.8453720	0.3463950	2.9506650
H	1.7833320	-0.7065420	3.2367880
H	2.7264930	0.7757620	3.4460960
H	0.9599720	0.8517890	3.3448960

Cp*Rh(CO)-Cyclooctane σ -complex (10)

Final Energy = -927.6084929080

C	-2.7985060	-0.5970980	-0.6740740
C	-1.7859630	-1.5782140	-0.5759040
C	-1.2389150	-1.5488050	0.7819560
C	-1.9231510	-0.5627830	1.5317280
C	-2.7962420	0.1321730	0.5918280
Rh	-0.8541140	0.4904730	-0.1953230
C	-0.8025380	2.3433310	-0.3060410
O	-0.7815740	3.4904740	-0.3710950
C	3.9264910	1.6459230	-0.3054990
C	4.0135130	1.0483610	1.1238910
C	2.2860430	-0.9433880	-1.4973540
C	4.5829350	-0.3855830	1.2127570
C	3.6383710	-1.4818860	-0.9703490
C	3.7752180	-1.5381120	0.5743010
H	4.6534360	1.1471550	-0.9535080
H	5.5859390	-0.3832180	0.7635400
H	2.3734110	-0.7449880	-2.5732830
H	4.4658460	-0.8995960	-1.3863070
H	4.2343350	2.6968220	-0.2721030
H	1.5395690	-1.7397300	-1.3928920
H	4.7253180	-0.6248430	2.2740020
H	3.7558920	-2.4926140	-1.3771700
C	2.5179980	1.6178020	-0.9459730
H	2.6020090	1.8683480	-2.0111690
H	1.9238520	2.4155760	-0.4869040
C	1.7226660	0.3068340	-0.7947040
H	1.5751440	0.0944050	0.2691810
H	0.7377060	0.4976260	-1.3232000
H	4.6699060	1.6850190	1.7276280
H	4.2853200	-2.4695110	0.8447560
H	2.7817620	-1.5969800	1.0375440
H	3.0297550	1.0920810	1.6086240
C	-0.1969450	-2.5090080	1.3006030
H	-0.6398520	-3.4894240	1.5172820
H	0.6032080	-2.6674380	0.5705940

H	0.2596710	-2.1369940	2.2218020
C	-1.8049740	-0.2800180	3.0068350
H	-2.5742400	-0.8250170	3.5701750
H	-0.8293510	-0.5844870	3.3947790
H	-1.9301420	0.7849370	3.2186340
C	-3.7993590	1.1947190	0.9742880
H	-4.7248000	0.7369940	1.3455090
H	-3.4061060	1.8445050	1.7605570
H	-4.0554060	1.8243090	0.1181310
C	-3.7297780	-0.3556950	-1.8330730
H	-4.6667640	-0.9129140	-1.6998220
H	-3.9831960	0.7033490	-1.9257780
H	-3.2809740	-0.6755130	-2.7770820
C	-1.4243080	-2.5973160	-1.6285610
H	-2.0233050	-3.5090180	-1.5059820
H	-1.6026590	-2.2115950	-2.6358200
H	-0.3728820	-2.8897250	-1.5633470

Cp*Rh(CO)-Cyclooctane TS (1)

Final Energy = -927.5897375420

C	2.1287470	-0.1507020	1.4576300
C	1.3470930	-1.2954520	1.1492620
C	1.6133610	-1.6609280	-0.2305810
C	2.6197850	-0.7823100	-0.7500500
C	2.8842770	0.2000640	0.2616670
Rh	0.7391100	0.4226550	-0.2751950
C	0.5729680	2.2773390	-0.3641970
O	0.5198710	3.4183860	-0.4179740
C	-1.4865540	0.1705530	-0.4551490
C	-2.3514420	1.3305920	-1.0240110
C	-4.1287780	-1.5701330	0.4176000
C	-3.3933350	1.9056220	-0.0376060
C	-4.2224700	-0.2456100	1.2162070
C	-4.5829590	1.0118530	0.3830930
H	-1.5718500	0.1820670	0.6333070
H	-2.8621570	2.2240650	0.8705020
H	-3.6405080	-2.3282170	1.0449020
H	-3.2903000	-0.0606040	1.7590400
H	-0.3153590	0.3538930	-1.4537510
H	-5.1516280	-1.9304740	0.2470660
H	-3.8053850	2.8193180	-0.4845500
H	-4.9884220	-0.3916560	1.9866170
C	-1.9186550	-1.2237240	-0.9683460
H	-1.4087510	-1.9904220	-0.3766770
H	-1.5668030	-1.3538070	-2.0008180
C	-3.4328320	-1.5252220	-0.9566080

H	-3.9569600	-0.8150630	-1.6048360
H	-3.5699200	-2.5073610	-1.4269090
H	-1.7159770	2.1653440	-1.3297780
H	-5.2527390	1.6418910	0.9796020
H	-5.1595440	0.7194820	-0.5040920
H	-2.8513440	0.9992860	-1.9431880
C	2.2438110	0.5391810	2.7946170
H	3.0715740	0.1165890	3.3784600
H	2.4352940	1.6086930	2.6758810
H	1.3289050	0.4305190	3.3821870
C	3.9320330	1.2848320	0.1850970
H	3.6571210	2.1521410	0.7910010
H	4.8963900	0.9133690	0.5533820
H	4.0737630	1.6272390	-0.8430520
C	1.1327850	-2.9178080	-0.9179580
H	1.9415870	-3.6580990	-0.9543290
H	0.2960620	-3.3713670	-0.3825750
H	0.8098380	-2.7223240	-1.9445040
C	0.4280190	-2.0371810	2.0862570
H	-0.5405220	-2.2485140	1.6212560
H	0.8669480	-2.9967550	2.3862690
H	0.2411840	-1.4576040	2.9934400
C	3.3057110	-0.9151580	-2.0851570
H	3.6103370	0.0578730	-2.4786180
H	4.2052740	-1.5388820	-1.9974130
H	2.6455900	-1.3820230	-2.8208400

Cp*Rh(CO)-Cyclooctane TS (2)

Final Energy = -927.5876625100

C	2.3395290	-0.4602620	1.3307630
C	1.5065230	-1.5195290	0.8492010
C	1.6444340	-1.5838800	-0.5951760
C	2.5314990	-0.5533150	-1.0105740
C	2.9113370	0.1886360	0.1753830
Rh	0.7212650	0.4385390	-0.0034010
C	0.5903720	2.2860430	-0.1783180
O	0.5374240	3.4265020	-0.2517500
C	-1.3560630	0.1230570	-0.7860090
C	-2.2922650	1.3440370	-0.9548800
C	-4.6037150	-1.4287550	0.0808050
C	-3.1302270	1.7933280	0.2666410
C	-4.6525070	-0.2230920	1.0454540
C	-4.5503100	1.1854190	0.4127280
H	-0.7499170	0.5130430	0.5812710
H	-2.5671110	1.6244580	1.1949570
H	-4.5892780	-2.3414520	0.6909480

H	-3.8722240	-0.3197930	1.8098160
H	-0.9558520	-0.0956850	-1.7841220
H	-5.5387050	-1.4590000	-0.4933350
H	-3.2577090	2.8790310	0.1890800
H	-5.6032400	-0.2918500	1.5874750
C	-2.0419250	-1.1651600	-0.2640280
H	-2.1577330	-1.1108470	0.8238050
H	-1.3589510	-1.9976330	-0.4455590
C	-3.4202960	-1.4727270	-0.9124480
H	-3.6118950	-0.7739180	-1.7315260
H	-3.4014330	-2.4666600	-1.3726230
H	-1.6784060	2.1856830	-1.2851170
H	-5.1212250	1.8708740	1.0497740
H	-5.0520930	1.1950920	-0.5649300
H	-2.9805180	1.1520250	-1.7876990
C	2.6188530	-0.1218390	2.7728930
H	3.4827680	-0.6884430	3.1444380
H	2.8395670	0.9413260	2.8965500
H	1.7633310	-0.3595200	3.4100160
C	0.7717120	-2.5163930	1.7126120
H	1.4146470	-3.3759040	1.9411770
H	0.4666980	-2.0647260	2.6601150
H	-0.1276930	-2.8935740	1.2211070
C	1.0362130	-2.6169260	-1.5125460
H	1.8247880	-3.1779110	-2.0271680
H	0.4294610	-3.3354420	-0.9570940
H	0.4008680	-2.1589810	-2.2801360
C	3.0358030	-0.3299970	-2.4135800
H	3.9500170	-0.9102880	-2.5965070
H	2.2916430	-0.6379530	-3.1536990
H	3.2696880	0.7225800	-2.5927580
C	3.9220590	1.3103080	0.2109330
H	4.9379930	0.9076190	0.3050000
H	3.8834480	1.9090230	-0.7029440
H	3.7466050	1.9788510	1.0576250

Cp*Rh(CO)-Cyclooctane TS (3)

Final Energy = -927.5890252340

C	-2.7949810	-0.3868500	-0.7859020
C	-1.8391790	-1.4448570	-0.8289440
C	-1.3258800	-1.6371160	0.5123350
C	-1.9829490	-0.7238870	1.3941410
C	-2.8432300	0.0977330	0.5797700
Rh	-0.7817020	0.4755010	-0.1544940
C	-0.7517110	2.3359490	-0.0995160
O	-0.7947020	3.4786930	-0.0807240

C	2.0781980	-0.8639650	-0.9087630
C	1.4673780	0.3002060	-0.0766920
C	5.1889060	-0.4002310	0.1731660
C	2.2307470	1.6426180	-0.2039420
C	4.7376570	0.8992370	-0.5318420
C	3.7043820	1.7371340	0.2636290
H	2.5788460	-0.4375620	-1.7849740
H	2.1936530	1.9627870	-1.2549310
H	5.7563770	-1.0159540	-0.5371060
H	4.3383800	0.6736440	-1.5255230
H	1.2681570	-1.4785630	-1.3140400
H	5.8898460	-0.1283440	0.9732500
H	1.6808970	2.3990940	0.3619870
H	5.6341760	1.5052650	-0.7044160
C	3.0284260	-1.8390070	-0.1635250
H	3.5424130	-2.4541030	-0.9151150
H	2.4076710	-2.5287040	0.4197130
C	4.0727810	-1.2517880	0.8028130
H	3.5605950	-0.6729620	1.5796280
H	4.5473570	-2.0918070	1.3253360
H	0.4206160	0.5927600	-1.1776650
H	3.9736060	2.7963400	0.1768900
H	3.7731940	1.5022400	1.3329390
H	1.4240480	0.0074730	0.9789220
C	-1.8485670	-0.6835220	2.8950060
H	-2.0418200	0.3182680	3.2870500
H	-2.5598350	-1.3715470	3.3708210
H	-0.8430890	-0.9765550	3.2105870
C	-0.3792320	-2.7271220	0.9450120
H	0.3275500	-2.3686750	1.6998520
H	-0.9362720	-3.5656650	1.3809810
H	0.1953620	-3.1150740	0.1009740
C	-1.5265570	-2.3024710	-2.0303070
H	-0.5092190	-2.6993500	-1.9905370
H	-2.2126490	-3.1575170	-2.0826180
H	-1.6264750	-1.7337070	-2.9583370
C	-3.6614150	0.0845590	-1.9263090
H	-3.1586700	-0.0518910	-2.8871580
H	-4.6037430	-0.4779200	-1.9558920
H	-3.9095530	1.1443580	-1.8281430
C	-3.7943800	1.1517670	1.0945490
H	-3.9968090	1.9117350	0.3354580
H	-4.7519770	0.6971640	1.3764480
H	-3.3907880	1.6573640	1.9755500

Cp*Rh(CO)-Cyclooctane TS (4)

Final Energy = -927.5882093920

C	-2.6635480	-0.2704280	0.7896280
C	-1.9914390	0.9251490	1.1511700
C	-1.6037370	1.6154510	-0.0671740
C	-2.0903690	0.8671050	-1.1875590
C	-2.6673420	-0.3414630	-0.6647290
Rh	-0.5319590	-0.3767930	-0.0605700
C	-0.0205060	-2.1065210	-0.5204420
O	0.2894750	-3.1621960	-0.8326550
C	2.0736160	1.3247670	1.0807400
C	1.3441410	-0.0484520	1.1175000
C	4.5758050	0.4294230	-0.9134650
C	2.2857630	-1.2594250	1.3215090
C	4.5678940	-0.5811300	0.2586880
C	3.3813350	-1.5838890	0.2814690
H	2.9425720	1.2543610	1.7466130
H	2.7990970	-1.0992730	2.2827810
H	5.2843300	1.2356300	-0.6813940
H	4.5970600	-0.0466480	1.2137420
H	1.4141860	2.0675590	1.5461280
H	4.9731280	-0.0800430	-1.8007820
H	1.6649110	-2.1497520	1.4597860
H	5.5080940	-1.1417440	0.2086090
C	2.5035700	1.9303130	-0.2798780
H	3.1353580	2.8036360	-0.0683690
H	1.6018680	2.3160890	-0.7697880
C	3.2190140	1.0359620	-1.3119520
H	2.5449360	0.2335620	-1.6288200
H	3.3804370	1.6488320	-2.2079280
H	0.7281530	-0.0271020	2.0232040
H	3.7703970	-2.5742940	0.5426500
H	2.9442550	-1.6932570	-0.7179880
H	0.9624400	-0.0182620	-0.4123780
C	-1.0363110	3.0126410	-0.1185420
H	-1.8409890	3.7515500	-0.0139520
H	-0.3201470	3.1892110	0.6880030
H	-0.5297950	3.2047610	-1.0673840
C	-2.0456440	1.2867300	-2.6345230
H	-2.9474360	1.8523300	-2.9033120
H	-1.1793490	1.9220250	-2.8358190
H	-1.9841300	0.4206360	-3.2981800
C	-3.3726970	-1.4012650	-1.4772880
H	-4.4340310	-1.1505920	-1.5965990
H	-2.9351350	-1.4932710	-2.4745770
H	-3.3142960	-2.3803220	-0.9945690

C	-3.3208750	-1.2618120	1.7169600
H	-4.3800850	-1.0133390	1.8624110
H	-3.2711880	-2.2770490	1.3150340
H	-2.8407330	-1.2685890	2.6988550
C	-1.7417620	1.4351140	2.5467600
H	-2.4673050	2.2127030	2.8160320
H	-1.8235520	0.6314010	3.2832910
H	-0.7421460	1.8728680	2.6383550

Cp*Rh(CO)-Cyclooctane TS (5)

Final Energy = -927.5902337210

C	-2.4432240	-0.1315190	1.2698050
C	-1.6684590	1.0624260	1.2948530
C	-1.7198710	1.6737070	-0.0212380
C	-2.5394140	0.8591320	-0.8614730
C	-2.9251760	-0.2963190	-0.0874830
Rh	-0.7145250	-0.3617690	-0.2315680
C	-0.4543600	-2.0529550	-0.9634610
O	-0.3282130	-3.0834340	-1.4434750
C	4.7239690	-0.4973810	0.9016460
C	5.0297490	-0.0045430	-0.5361490
C	1.4074480	-0.1901520	0.4735030
C	4.3921610	1.3496310	-0.9179280
C	2.0779990	1.2003740	0.3086960
C	2.8525610	1.4226590	-1.0191540
H	4.5172850	0.3675090	1.5395690
H	4.7273620	2.1025500	-0.1907900
H	1.0833130	-0.2785310	1.5175590
H	2.7474340	1.3840910	1.1560120
H	5.6276840	-0.9573220	1.3175410
H	0.6827140	-0.0133880	-0.8927650
H	4.8056530	1.6563800	-1.8869480
H	1.2925530	1.9561880	0.3852470
C	3.5921470	-1.5486520	1.0244560
H	3.2934560	-1.6264130	2.0781590
H	4.0188870	-2.5247860	0.7586610
C	2.3262560	-1.3836000	0.1522040
H	2.6166550	-1.3559990	-0.9049120
H	1.7471990	-2.3025490	0.2769710
H	6.1142620	0.1154290	-0.6401440
H	2.6060070	2.4178570	-1.4060960
H	2.5006590	0.7145100	-1.7804220
H	4.7416390	-0.7717540	-1.2660740
C	-2.7618790	-1.0285490	2.4393990
H	-3.6780270	-0.6985200	2.9462500
H	-2.9145180	-2.0619680	2.1178840

H	-1.9544190	-1.0259410	3.1765120
C	-3.8666370	-1.3832380	-0.5492100
H	-3.6697090	-2.3267250	-0.0333970
H	-4.9069410	-1.1010100	-0.3459340
H	-3.7714060	-1.5618180	-1.6232880
C	-2.9772870	1.1851880	-2.2661730
H	-3.1440480	0.2784350	-2.8530350
H	-3.9154860	1.7556680	-2.2574430
H	-2.2251490	1.7853440	-2.7848680
C	-1.1780770	3.0344360	-0.3875540
H	-0.7766880	3.0462070	-1.4047140
H	-1.9735260	3.7882730	-0.3307610
H	-0.3834280	3.3488750	0.2929070
C	-0.9746800	1.6395220	2.5024510
H	-0.0246720	2.1112670	2.2357220
H	-1.5999700	2.4010940	2.9844780
H	-0.7648020	0.8631050	3.2433440

Cp*Rh(CO)-Cyclooctane TS (6)

Final Energy = -927.6128298680

C	2.3149320	-0.5366070	1.2645500
C	1.5047430	-1.5826330	0.6729300
C	1.6287180	-1.4696340	-0.7584140
C	2.4370950	-0.3309010	-1.0533170
C	2.8738150	0.2392740	0.2084660
Rh	0.5988010	0.4029850	0.1083970
C	0.3893610	2.2259200	-0.2165660
O	0.3094010	3.3503780	-0.3684780
C	-3.7457170	1.0014290	1.1453650
C	-4.8373310	0.1817210	0.4081750
C	-1.2716810	0.0094310	-0.8271210
C	-4.5107530	-1.3095340	0.1715090
C	-1.9157410	-1.2644340	-0.2198560
C	-3.3245490	-1.6619830	-0.7536060
H	-3.1229810	0.3311170	1.7464810
H	-4.3299340	-1.7785750	1.1491480
H	-0.3369930	0.6563930	1.3470760
H	-1.9655390	-1.1825030	0.8703890
H	-4.2311940	1.6769350	1.8593600
H	-0.9589560	-0.2551620	-1.8499700
H	-5.4106090	-1.7895550	-0.2345860
H	-1.2361930	-2.0978310	-0.4197170
C	-2.8561320	1.8723320	0.2302760
H	-2.0570990	2.3088630	0.8393270
H	-3.4663630	2.7125770	-0.1285910
C	-2.2591660	1.1843480	-1.0135840

H	-3.0953360	0.8394680	-1.6369900
H	-1.7658750	1.9568860	-1.6156920
H	-5.7595590	0.2123300	1.0002100
H	-3.3446990	-2.7505950	-0.8863430
H	-3.4879220	-1.2385260	-1.7522060
H	-5.0791280	0.6639090	-0.5481350
C	1.0624540	-2.4107300	-1.7908800
H	1.8616600	-2.7715200	-2.4477760
H	0.5941970	-3.2781640	-1.3208740
H	0.3078060	-1.9229120	-2.4180890
C	2.8891870	0.0902900	-2.4298380
H	3.8110370	-0.4336080	-2.7141200
H	2.1283720	-0.1398920	-3.1808410
H	3.0910600	1.1638030	-2.4756580
C	3.8401480	1.3889650	0.3555960
H	4.8743290	1.0263820	0.3084910
H	3.7112400	2.1251550	-0.4424900
H	3.7079950	1.9015750	1.3115790
C	2.5742980	-0.3646980	2.7401550
H	3.4059600	-1.0057690	3.0595510
H	2.8366050	0.6685990	2.9794130
H	1.6937360	-0.6312200	3.3289650
C	0.8769280	-2.7294590	1.4373550
H	0.9979500	-3.6695180	0.8898020
H	1.3716020	-2.8509400	2.4052090
H	-0.1900520	-2.5836440	1.6198490

Cp*Rh(CO)-Cyclooctane TS (7)

Final Energy = -927.5901195520

C	2.2125940	0.7280700	-1.2467570
C	1.5909400	1.6315500	-0.3269280
C	1.9029140	1.1994890	1.0248120
C	2.6681050	0.0051690	0.9432710
C	2.8084980	-0.3228760	-0.4670010
Rh	0.6304270	-0.3947090	-0.0384840
C	0.2352550	-2.2003260	-0.2666610
O	-0.0060180	-3.3045900	-0.4410930
C	-2.7267780	1.5535780	-0.6791510
C	-2.0009590	1.3640620	0.6806310
C	-4.5729400	-1.1399750	-0.2680050
C	-1.3381930	-0.0127080	0.9511980
C	-3.0949000	-1.6019050	-0.2191920
C	-2.3184530	-1.2036820	1.0660930
H	-2.3229680	0.8477100	-1.4113030
H	-0.8495280	-0.1577250	-0.5335500
H	-4.9509290	-1.2810470	-1.2891990

H	-2.5589000	-1.2393000	-1.1006410
H	-2.4844510	2.5484190	-1.0714990
H	-5.1599420	-1.8133920	0.3700720
H	-0.8414100	0.0753820	1.9245770
H	-3.0935750	-2.6936990	-0.3098730
C	-4.2715940	1.4486540	-0.6363590
H	-4.6458550	1.3882870	-1.6668620
H	-4.6643500	2.3871370	-0.2236240
C	-4.8792170	0.2992970	0.1908980
H	-4.5864480	0.4154940	1.2402890
H	-5.9690870	0.4249410	0.1765980
H	-1.2153810	2.1192380	0.7606090
H	-1.7485520	-2.0659980	1.4223210
H	-3.0379710	-0.9754100	1.8650390
H	-2.7012980	1.5755840	1.5010980
C	1.5122880	1.9291750	2.2845670
H	2.1556460	2.8028710	2.4460600
H	0.4778340	2.2843820	2.2408380
H	1.6040240	1.2809560	3.1597760
C	3.2925550	-0.7542670	2.0873490
H	4.3139440	-0.4003460	2.2781160
H	2.7182930	-0.6312380	3.0091640
H	3.3475800	-1.8243510	1.8716270
C	3.6412420	-1.4583550	-1.0127570
H	4.6943080	-1.1602940	-1.0877120
H	3.5899150	-2.3385400	-0.3665100
H	3.3040160	-1.7546380	-2.0092700
C	0.9257740	2.9328410	-0.7118700
H	0.4655310	3.4163990	0.1528830
H	1.6666040	3.6304190	-1.1213280
H	0.1498610	2.7835990	-1.4692520
C	2.2716170	0.8918080	-2.7434700
H	3.1628670	1.4627580	-3.0361230
H	2.3126040	-0.0748710	-3.2517380
H	1.3940330	1.4283220	-3.1140940

Cp*Rh(CO)-Cyclooctane TS (8)

Final Energy = -927.5896074520

C	-2.3346120	0.2324160	1.3452820
C	-1.5604610	1.3733000	0.9867050
C	-1.7481800	1.6307040	-0.4301570
C	-2.6514070	0.6528300	-0.9473650
C	-2.9568500	-0.2564520	0.1307800
Rh	-0.7737260	-0.4202770	-0.2072080
C	-0.6055790	-2.2495120	-0.5072410
O	-0.5433900	-3.3715480	-0.7196380

C	3.2851960	1.7117450	0.3585450
C	2.0351820	1.1519640	-0.3749390
C	4.8922030	-1.1371670	0.1289760
C	1.4123670	-0.1407620	0.2175100
C	3.6089740	-1.3936070	0.9545920
C	2.2773500	-1.4219320	0.1505240
H	3.3018370	1.3425880	1.3876730
H	1.2010670	0.0585870	1.2762080
H	5.7279410	-0.9665190	0.8206520
H	3.5272520	-0.6716530	1.7718630
H	3.1878000	2.8008940	0.4385010
H	5.1307470	-2.0590460	-0.4173330
H	0.5537970	-0.3030390	-1.0643250
H	3.7341290	-2.3684850	1.4398220
C	4.6368290	1.4272220	-0.3426910
H	5.4543440	1.6677670	0.3496920
H	4.7328970	2.1256170	-1.1842250
C	4.8440770	0.0064340	-0.8999580
H	4.0688250	-0.2099980	-1.6437190
H	5.7920450	-0.0002760	-1.4521070
H	1.2542980	1.9157620	-0.3575750
H	1.6736950	-2.2377380	0.5530750
H	2.4793050	-1.6863110	-0.8959820
H	2.2653840	1.0011880	-1.4374630
C	-1.2509060	2.8411550	-1.1833260
H	-2.0459310	3.5938240	-1.2581870
H	-0.4050500	3.3111530	-0.6765480
H	-0.9355310	2.5832010	-2.1981060
C	-3.2318610	0.6255150	-2.3378850
H	-4.1623500	1.2069790	-2.3808480
H	-2.5356370	1.0533120	-3.0640130
H	-3.4613660	-0.3944990	-2.6560730
C	-3.9441240	-1.3971190	0.0577290
H	-4.9561680	-1.0424700	0.2883040
H	-3.9642020	-1.8421150	-0.9403380
H	-3.6964020	-2.1867730	0.7718500
C	-2.5320060	-0.3300420	2.7307310
H	-3.3870390	0.1464690	3.2276920
H	-2.7238480	-1.4055610	2.6990840
H	-1.6508040	-0.1696730	3.3575480
C	-0.7431060	2.2208370	1.9281560
H	-1.3131130	3.0983490	2.2573330
H	-0.4559920	1.6565090	2.8195040
H	0.1743620	2.5816090	1.4537100

Cp*Rh(CO)-Cyclooctane TS (9)

Final Energy = -927.5822528700

C	2.6466390	-0.0645950	-0.7023250
C	1.9609210	1.1642340	-0.8832970
C	1.4481950	1.5902380	0.4070270
C	1.8757800	0.6491170	1.3988190
C	2.5448000	-0.4164860	0.7068610
Rh	0.4547780	-0.3907380	-0.0588180
C	0.0095220	-2.1946890	0.0323010
O	-0.2480320	-3.3048010	0.1268180
C	-3.5938120	-1.2774740	-0.7182700
C	-3.4080670	-1.2420910	0.8219500
C	-1.9090100	1.4988950	-1.2529050
C	-3.7998890	0.0869110	1.5067240
C	-3.0893240	1.8330270	-0.3046560
C	-2.9949890	1.3626480	1.1708600
H	-4.3936140	-0.5795470	-0.9854220
H	-4.8560200	0.2869110	1.2754680
H	-2.2413240	1.7618010	-2.2688960
H	-4.0250740	1.4624730	-0.7344190
H	-3.9730690	-2.2680570	-0.9944940
H	-1.0895810	2.1850750	-1.0216060
H	-3.7500160	-0.0669940	2.5920620
H	-3.1784720	2.9258740	-0.3162490
C	-2.3605370	-1.0353530	-1.6348380
H	-2.7609400	-0.8181250	-2.6371250
H	-1.8207250	-1.9813200	-1.7370090
C	-1.3229280	0.0682330	-1.3236470
H	-1.0527290	-0.1158660	0.2706910
H	-0.6553050	0.0788920	-2.1937960
H	-4.0560780	-2.0134100	1.2546670
H	-3.3951480	2.1592460	1.8093180
H	-1.9476980	1.2365160	1.4679800
H	-2.3883500	-1.5221120	1.0998200
C	0.8092390	2.9259740	0.7081390
H	1.5262310	3.5801240	1.2193790
H	0.4971900	3.4350880	-0.2066330
H	-0.0686670	2.8229870	1.3536810
C	1.8073910	1.9259910	-2.1747970
H	0.7870130	2.3012480	-2.3023620
H	2.4838140	2.7891340	-2.2026500
H	2.0390350	1.2933740	-3.0353210
C	3.4112020	-0.8422430	-1.7448020
H	3.0008430	-0.6803330	-2.7447980
H	4.4657170	-0.5380740	-1.7611790
H	3.3796950	-1.9160700	-1.5432400

C	3.2301570	-1.5941360	1.3580920
H	3.2409390	-2.4665970	0.6994860
H	4.2710540	-1.3463540	1.6001180
H	2.7285170	-1.8807890	2.2859150
C	1.6988140	0.7935410	2.8882080
H	1.6311150	-0.1801110	3.3800470
H	2.5473660	1.3337950	3.3286430
H	0.7889210	1.3523840	3.1235410

Cp*Rh(CO)-Cyclooctane TS (10)

Final Energy = -927.5897855400

C	-2.7487500	-0.6497890	-0.5886850
C	-1.7059380	-1.6169330	-0.4615900
C	-1.1377740	-1.4989840	0.8694720
C	-1.8203230	-0.4597980	1.5647390
C	-2.7699310	0.1169650	0.6351470
Rh	-0.7772540	0.4563850	-0.2686060
C	-0.7723270	2.3127500	-0.4116840
O	-0.8162920	3.4508600	-0.5145480
C	3.7172350	1.6487680	-0.3751800
C	4.1118510	1.0304740	0.9926950
C	1.9696890	-0.8631270	-1.3553590
C	4.7053970	-0.3940280	0.9356930
C	3.3858490	-1.4360610	-1.0649310
C	3.8001620	-1.5372360	0.4260410
H	4.2741780	1.1586220	-1.1788380
H	5.6051350	-0.3659740	0.3050980
H	1.9241030	-0.5734880	-2.4142380
H	4.1460650	-0.8657460	-1.6062240
H	4.0327560	2.6983280	-0.3952410
H	1.2547190	-1.6841480	-1.2447540
H	5.0482600	-0.6576130	1.9442930
H	3.4077150	-2.4397640	-1.5054370
C	2.1978830	1.6433240	-0.6763360
H	2.0408320	2.0074320	-1.7006230
H	1.7399980	2.3836340	-0.0129230
C	1.4558480	0.3073680	-0.4828800
H	1.5347480	0.0122600	0.5678230
H	0.2670560	0.4991420	-1.4577510
H	4.8673400	1.6698460	1.4635460
H	4.3577780	-2.4702690	0.5680840
H	2.9102480	-1.6196840	1.0622480
H	3.2457410	1.0436360	1.6669740
C	-0.0667650	-2.3872640	1.4488950
H	-0.5067760	-3.2873330	1.8957950
H	0.6452260	-2.7115800	0.6852760

H	0.4955450	-1.8684400	2.2309740
C	-1.6404580	-0.0702740	3.0101920
H	-2.3226510	-0.6387630	3.6557280
H	-0.6202530	-0.2660190	3.3511550
H	-1.8446180	0.9922580	3.1652140
C	-3.7742690	1.1932300	0.9727230
H	-4.6726020	0.7513670	1.4209490
H	-3.3639910	1.9124920	1.6863060
H	-4.0815840	1.7439130	0.0799780
C	-3.6942500	-0.5047640	-1.7534100
H	-4.5833350	-1.1333640	-1.6119700
H	-4.0314650	0.5283910	-1.8683230
H	-3.2164450	-0.8059110	-2.6892730
C	-1.3946180	-2.7000070	-1.4660400
H	-2.1126930	-3.5244860	-1.3717050
H	-1.4484890	-2.3227390	-2.4908460
H	-0.3968490	-3.1178970	-1.3146550

Cp*Rh(CO)-Cyclooctane Product (6)

Final Energy = -927.6128298640

C	2.3149380	-0.5366040	1.2645470
C	1.5047550	-1.5826330	0.6729230
C	1.6287280	-1.4696270	-0.7584210
C	2.4370990	-0.3308870	-1.0533190
C	2.8738150	0.2392850	0.2084670
Rh	0.5988000	0.4029820	0.1083990
C	0.3893460	2.2259170	-0.2165550
O	0.3093730	3.3503740	-0.3684650
C	-3.7457200	1.0014370	1.1453540
C	-4.8373340	0.1817210	0.4081730
C	-1.2716810	0.0094180	-0.8271180
C	-4.5107570	-1.3095370	0.1715200
C	-1.9157420	-1.2644400	-0.2198400
C	-3.3245490	-1.6619950	-0.7535880
H	-3.1229830	0.3311320	1.7464760
H	-4.3299430	-1.7785700	1.1491630
H	-0.3369910	0.6563800	1.3470830
H	-1.9655430	-1.1824980	0.8704040
H	-4.2311970	1.6769500	1.8593430
H	-0.9589540	-0.2551860	-1.8499620
H	-5.4106120	-1.7895590	-0.2345760
H	-1.2361940	-2.0978390	-0.4196910
C	-2.8561370	1.8723310	0.2302540
H	-2.0571060	2.3088730	0.8393010
H	-3.4663710	2.7125700	-0.1286240
C	-2.2591670	1.1843330	-1.0135960

H	-3.0953340	0.8394470	-1.6370010
H	-1.7658740	1.9568640	-1.6157110
H	-5.7595610	0.2123350	1.0002090
H	-3.3446980	-2.7506090	-0.8863130
H	-3.4879200	-1.2385500	-1.7521930
H	-5.0791330	0.6639000	-0.5481410
C	1.0624690	-2.4107220	-1.7908910
H	1.8616790	-2.7715100	-2.4477840
H	0.5942110	-3.2781560	-1.3208890
H	0.3078240	-1.9229020	-2.4181030
C	2.8891870	0.0903120	-2.4298380
H	3.8110400	-0.4335800	-2.7141230
H	2.1283730	-0.1398690	-3.1808420
H	3.0910560	1.1638270	-2.4756520
C	3.8401400	1.3889820	0.3556030
H	4.8743230	1.0264050	0.3085040
H	3.7112330	2.1251710	-0.4424830
H	3.7079790	1.9015900	1.3115850
C	2.5743030	-0.3647010	2.7401530
H	3.4059770	-1.0057580	3.0595430
H	2.8365910	0.6686000	2.9794170
H	1.6937460	-0.6312430	3.3289620
C	0.8769470	-2.7294670	1.4373420
H	0.9979730	-3.6695220	0.8897850
H	1.3716230	-2.8509490	2.4051950
H	-0.1900330	-2.5836580	1.6198390

Cp*Rh(CO)-Cyclooctane Product (8)

Final Energy = -927.6130679080

C	-2.1023540	-0.0032580	1.4344550
C	-1.4951730	1.2532250	1.0983430
C	-1.8796340	1.6019570	-0.2386770
C	-2.7827160	0.5774300	-0.7226650
C	-2.9120700	-0.4050610	0.3053700
Rh	-0.7228580	-0.3291800	-0.3686310
C	-0.3840560	-2.1072020	-0.8096130
O	-0.2132240	-3.1807850	-1.1442480
C	3.1965640	1.7855710	0.1300650
C	1.9180060	1.1435830	-0.4867670
C	4.7747250	-1.0826180	0.2789410
C	1.2885620	-0.0454950	0.2821030
C	3.4995010	-1.2055280	1.1462430
C	2.1568090	-1.3267060	0.3649140
H	3.2346270	1.5697490	1.2015880
H	1.1442160	0.2818990	1.3221000
H	5.6212270	-0.8212070	0.9283570

H	3.4348720	-0.3705020	1.8498060
H	3.1133450	2.8767740	0.0543940
H	5.0003120	-2.0751420	-0.1328740
H	-0.0945610	-0.0781200	-1.7894080
H	3.6223760	-2.1017970	1.7661210
C	4.5312890	1.3904460	-0.5493770
H	5.3656290	1.7199430	0.0845130
H	4.6141690	1.9599020	-1.4844230
C	4.7196580	-0.0967030	-0.9020510
H	3.9311300	-0.4075710	-1.5962600
H	5.6593270	-0.1910530	-1.4607960
H	1.1554540	1.9252390	-0.5615230
H	1.5607550	-2.0909740	0.8733820
H	2.3541200	-1.7178330	-0.6421630
H	2.1160680	0.8429490	-1.5224720
C	-1.5736280	2.9015530	-0.9405470
H	-2.3776480	3.6281490	-0.7677060
H	-0.6434840	3.3426780	-0.5741350
H	-1.4740390	2.7575540	-2.0192960
C	-3.5235390	0.6161530	-2.0355800
H	-4.4488550	1.1982160	-1.9395750
H	-2.9150170	1.0787970	-2.8165620
H	-3.7927620	-0.3876660	-2.3731560
C	-3.8044650	-1.6212670	0.2631600
H	-4.7816180	-1.3895390	0.7042220
H	-3.9722300	-1.9587290	-0.7624860
H	-3.3747360	-2.4531680	0.8272570
C	-2.0446470	-0.6894470	2.7773330
H	-2.7990950	-0.2801610	3.4611710
H	-2.2299160	-1.7624170	2.6818260
H	-1.0650710	-0.5641860	3.2462960
C	-0.6511610	2.1034220	2.0103170
H	-1.2529290	2.9217350	2.4239270
H	-0.2578540	1.5210600	2.8466590
H	0.1965810	2.5444530	1.4777920

Cp*Rh(CO)-Cyclooctane 1,1-Migration (1)

Final Energy = -927.6082982600

C	1.8011900	-0.4724940	1.5705870
C	1.1123090	-1.4977890	0.8808230
C	1.6932260	-1.6441030	-0.4568890
C	2.7275680	-0.6937750	-0.6047790
C	2.7078710	0.1334390	0.6000390
Rh	0.7904030	0.4645700	-0.2538100
C	0.7517960	2.3040090	-0.5094540
O	0.7257990	3.4422420	-0.6658180

C	-1.6827390	0.2697690	-1.0727530
C	-2.5623360	1.5465950	-1.0694450
C	-3.8881090	-1.5575660	0.4858630
C	-3.1060120	1.9535500	0.3173020
C	-3.5480710	-0.3816550	1.4364240
C	-4.1073150	1.0044280	1.0155590
H	-1.3335900	0.1051840	-0.0363700
H	-2.2466770	2.1034120	0.9857320
H	-3.2682590	-2.4222490	0.7588620
H	-2.4651180	-0.3077730	1.5851840
H	-0.8114520	0.4437490	-1.7419170
H	-4.9263900	-1.8553440	0.6808620
H	-3.5871470	2.9337320	0.2138180
H	-3.9570810	-0.6427780	2.4190040
C	-2.3607820	-1.0227180	-1.5827390
H	-1.7060610	-1.8759110	-1.3653090
H	-2.4352150	-0.9631350	-2.6761000
C	-3.7698960	-1.3073770	-1.0304000
H	-4.4431080	-0.4922010	-1.3178970
H	-4.1511690	-2.1982880	-1.5444940
H	-1.9661570	2.3867080	-1.4413050
H	-4.4545220	1.5240100	1.9156900
H	-4.9967830	0.8719950	0.3860360
H	-3.3893980	1.4242770	-1.7795280
C	1.6569190	-0.0727220	3.0158850
H	2.4087760	-0.5792070	3.6358060
H	1.7904360	1.0043350	3.1450120
H	0.6702420	-0.3355270	3.4060950
C	0.0275490	-2.3886750	1.4358740
H	0.4250160	-3.3775750	1.6970930
H	-0.4174130	-1.9567070	2.3361660
H	-0.7765110	-2.5420600	0.7081350
C	1.3236490	-2.7297090	-1.4374240
H	1.8738680	-3.6538600	-1.2179060
H	0.2574880	-2.9683180	-1.3905740
H	1.5567410	-2.4364020	-2.4644490
C	3.6910930	-0.5592790	-1.7546710
H	4.6141330	-1.1197510	-1.5546760
H	3.2596760	-0.9443850	-2.6823140
H	3.9662960	0.4850410	-1.9222850
C	3.7253820	1.2017560	0.9238920
H	4.6349520	0.7548700	1.3443240
H	4.0086030	1.7625810	0.0292920
H	3.3315260	1.9138590	1.6538420

Cp*Rh(CO)-Cyclooctane 1,1-Migration (2)

Final Energy = -927.6076882160

C	-2.7818320	0.0484990	0.9639340
C	-1.9440510	1.1798280	1.0868580
C	-1.6044790	1.6611550	-0.2542460
C	-2.2385850	0.8332240	-1.2102650
C	-2.8565450	-0.2578080	-0.4628500
Rh	-0.7908140	-0.4727400	-0.0252300
C	-0.4431990	-2.2246380	-0.5358260
O	-0.2258020	-3.3088160	-0.8486610
C	2.3276380	1.2164230	0.9337310
C	1.7062290	-0.1900540	0.7447890
C	5.0237450	0.4319280	-0.7680660
C	2.5902910	-1.3914020	1.1523150
C	4.9630640	-0.5499230	0.4282360
C	3.8743790	-1.6515730	0.3340720
H	3.1192740	1.1542450	1.6861780
H	2.8731820	-1.2606350	2.2060270
H	5.6740920	1.2749950	-0.4998660
H	4.8399910	-0.0001460	1.3666740
H	1.5723720	1.8906350	1.3537920
H	5.5203070	-0.0838780	-1.6000600
H	1.9697860	-2.2938500	1.1094200
H	5.9461960	-1.0289290	0.4967880
C	2.8607270	1.8700690	-0.3629230
H	3.4500460	2.7565230	-0.0940540
H	1.9967920	2.2341390	-0.9337910
C	3.6861220	0.9746390	-1.3064830
H	3.0660750	0.1390580	-1.6503710
H	3.9057720	1.5616750	-2.2067080
H	0.8047600	-0.2646730	1.3934470
H	4.2950740	-2.5915270	0.7085940
H	3.6154440	-1.8391450	-0.7154240
H	1.4192820	-0.3075970	-0.3198010
C	-0.8383960	2.9305220	-0.5337290
H	-1.4880810	3.8079690	-0.4201440
H	0.0014110	3.0556930	0.1560790
H	-0.4409590	2.9378050	-1.5521470
C	-2.3008970	1.0337950	-2.7018230
H	-3.2149270	1.5737230	-2.9833410
H	-1.4459990	1.6128070	-3.0607630
H	-2.3029010	0.0778600	-3.2316380
C	-3.7426690	-1.3212190	-1.0673520
H	-4.7679550	-0.9486590	-1.1846810
H	-3.3798830	-1.6252110	-2.0527210
H	-3.7789440	-2.2123250	-0.4351570

C	-3.4892700	-0.6974420	2.0652540
H	-4.5109900	-0.3169530	2.1970450
H	-3.5585550	-1.7649540	1.8414420
H	-2.9670340	-0.5904780	3.0195270
C	-1.5426790	1.8732170	2.3658660
H	-2.1845380	2.7427390	2.5569460
H	-1.6225680	1.2021770	3.2249450
H	-0.5110350	2.2353030	2.3194540

Cp*Rh(CO)-Cyclooctane 1,1-Migration (3)

Final Energy = -927.6068984000

C	2.3077430	-0.4903700	1.4015160
C	1.5130620	-1.5127400	0.8316610
C	1.8012380	-1.5918220	-0.6025680
C	2.7613920	-0.6086280	-0.9258240
C	2.9808460	0.1737230	0.2886020
Rh	0.9240780	0.4896730	-0.1308710
C	0.8172870	2.3363890	-0.2816770
O	0.7511960	3.4802320	-0.3722050
C	-3.2228600	-1.6338820	0.3834590
C	-2.3063170	-1.1226930	-0.7591880
C	-5.0451140	1.1129680	0.3843820
C	-1.6805150	0.2694920	-0.5237830
C	-3.5958510	1.5515130	0.7066180
C	-2.6064160	1.5066870	-0.4880740
H	-2.9450870	-1.1362750	1.3178570
H	-1.1659690	0.2370770	0.4631410
H	-5.5935470	0.9866740	1.3270560
H	-3.1921230	0.9568390	1.5319770
H	-3.0271140	-2.7000710	0.5467420
H	-5.5360280	1.9390490	-0.1462020
H	-0.9407630	0.4362600	-1.3363470
H	-3.6465120	2.5789890	1.0831440
C	-4.7424380	-1.4844420	0.1256860
H	-5.2799860	-1.6707180	1.0645450
H	-5.0463730	-2.2822040	-0.5643990
C	-5.2214040	-0.1507160	-0.4787960
H	-4.7357960	0.0028630	-1.4493010
H	-6.2908710	-0.2540160	-0.6997220
H	-1.4772520	-1.8246610	-0.8915610
H	-1.9605110	2.3888570	-0.4425690
H	-3.1541430	1.5820950	-1.4357070
H	-2.8524800	-1.1234940	-1.7106960
C	0.5926770	-2.4564070	1.5673400
H	-0.3561040	-2.5909470	1.0368270
H	1.0511720	-3.4475410	1.6748870

H	0.3633510	-2.0820450	2.5680930
C	1.2731040	-2.6574000	-1.5323080
H	1.1394580	-2.2759770	-2.5486500
H	1.9689340	-3.5049290	-1.5809670
H	0.3119580	-3.0493590	-1.1898010
C	3.4589560	-0.4157320	-2.2466360
H	3.6789100	0.6388590	-2.4310430
H	4.4107150	-0.9636330	-2.2661350
H	2.8460610	-0.7807220	-3.0752350
C	4.0248540	1.2552830	0.4353930
H	3.7768790	1.9369060	1.2532760
H	5.0080280	0.8168390	0.6473330
H	4.1109950	1.8482510	-0.4789970
C	2.4607700	-0.1438700	2.8597590
H	1.5793930	-0.4384670	3.4351890
H	3.3307120	-0.6563560	3.2917990
H	2.6049370	0.9305770	2.9989430

Cp*Rh(CO)-Cyclooctane 1,1-Migration (4)

Final Energy = -927.6071227440

C	-2.4323610	-0.7570360	-1.1890610
C	-1.6266130	-1.6467940	-0.4390560
C	-1.8178460	-1.3752160	0.9879070
C	-2.7200950	-0.2976850	1.1220430
C	-3.0032740	0.1819560	-0.2301090
Rh	-0.9114620	0.4918210	-0.0231970
C	-0.7475210	2.3233520	-0.2769220
O	-0.6506250	3.4576440	-0.4345530
C	2.6342800	1.4135620	-0.2591620
C	3.8367820	1.6491780	0.6917800
C	3.1751230	-1.8619880	-0.3697990
C	5.1864340	1.0608640	0.2214590
C	4.4396790	-1.1699870	-0.9311170
C	5.3329300	-0.4749440	0.1306830
H	3.0030010	1.2778710	-1.2805400
H	5.4150030	1.4836770	-0.7668380
H	2.5296770	-2.1587700	-1.2073670
H	4.1636530	-0.4447300	-1.7028500
H	2.0202550	2.3188170	-0.2851670
H	3.4875310	-2.7915830	0.1238610
H	5.9659290	1.4320950	0.8984930
H	5.0263880	-1.9396050	-1.4448290
C	1.6998370	0.2394460	0.1293260
H	1.0880010	-0.0056570	-0.7664980
H	1.0454220	0.6076680	0.9523490
C	2.3463780	-1.0583670	0.6479080

H	2.9649080	-0.8280630	1.5222050
H	1.5428430	-1.7047410	1.0182930
H	3.9838370	2.7303810	0.7923710
H	6.3827680	-0.6768230	-0.1101060
H	5.1621050	-0.9250740	1.1170500
H	3.5995270	1.2874570	1.7000750
C	-0.7959240	-2.7834680	-0.9836290
H	0.1638890	-2.8669400	-0.4637130
H	-1.3171200	-3.7416040	-0.8631200
H	-0.5879790	-2.6465360	-2.0479180
C	-1.2542540	-2.2140100	2.1085640
H	-1.9214750	-3.0557790	2.3351610
H	-0.2803900	-2.6359510	1.8461300
H	-1.1312380	-1.6283540	3.0236890
C	-3.3138280	0.2428250	2.3963640
H	-4.2847240	-0.2277480	2.6015710
H	-2.6603150	0.0488050	3.2510320
H	-3.4740020	1.3221930	2.3351760
C	-4.0200890	1.2470310	-0.5662630
H	-5.0292610	0.8184450	-0.6073320
H	-4.0227020	2.0416350	0.1845390
H	-3.8082850	1.7041710	-1.5363760
C	-2.6797450	-0.7653820	-2.6752210
H	-3.5906160	-1.3302530	-2.9148810
H	-2.8059780	0.2488250	-3.0626390
H	-1.8492090	-1.2269520	-3.2156960

Cp*Rh(CO)-Cyclooctane 1,1-Migration (5)

Final Energy = -927.607686421

C	-2.7927710	-0.3706000	-0.7087800
C	-1.8843600	-1.4527910	-0.6861300
C	-1.3405890	-1.5816220	0.6685800
C	-1.9130750	-0.5812820	1.4865600
C	-2.7087950	0.2665330	0.6032190
Rh	-0.7426290	0.4793950	-0.1689280
C	-0.4976810	2.3188880	-0.1241860
O	-0.3562050	3.4590310	-0.0962810
C	3.9284190	1.4700630	-0.5279730
C	3.7720500	1.1767220	0.9879260
C	2.2784020	-1.2297650	-1.4256910
C	4.2044360	-0.2366450	1.4411680
C	3.4933850	-1.7189830	-0.5996310
C	3.4050460	-1.4564680	0.9275480
H	4.6943330	0.8104550	-0.9476840
H	5.2572440	-0.3782040	1.1590750
H	2.5373390	-1.2463460	-2.4922370

H	4.4167020	-1.2787830	-0.9880160
H	4.3112550	2.4883380	-0.6576800
H	1.4664330	-1.9547500	-1.2968700
H	4.1777360	-0.2584470	2.5377740
H	3.5849390	-2.7971230	-0.7734060
C	2.6222660	1.3741540	-1.3524890
H	2.8691230	1.3894170	-2.4219610
H	2.0331140	2.2776670	-1.1594940
C	1.7217160	0.1585470	-1.0617320
H	1.4724250	0.1641040	0.0156200
H	0.7941810	0.3030640	-1.6653960
H	4.3921170	1.8877670	1.5452660
H	3.7978470	-2.3339290	1.4535880
H	2.3543770	-1.3710620	1.2350320
H	2.7392550	1.3726160	1.3041530
C	-0.4332410	-2.6995040	1.1203540
H	0.0663180	-2.4501560	2.0601640
H	-1.0045080	-3.6233310	1.2783280
H	0.3413170	-2.9190370	0.3794820
C	-1.7677790	-0.4131390	2.9766030
H	-1.7797450	0.6424880	3.2595490
H	-2.5920450	-0.9098630	3.5057790
H	-0.8305140	-0.8443310	3.3376550
C	-3.5964680	1.3970420	1.0675930
H	-3.7887270	2.1073300	0.2591530
H	-4.5630300	1.0113050	1.4150570
H	-3.1369370	1.9467820	1.8932010
C	-3.6954980	0.0480270	-1.8396540
H	-3.2867040	-0.2515170	-2.8081310
H	-4.6866150	-0.4135450	-1.7358660
H	-3.8338810	1.1319930	-1.8571250
C	-1.6125500	-2.4208200	-1.8115660
H	-2.2443980	-3.3134360	-1.7174370
H	-1.8163430	-1.9666460	-2.7847890
H	-0.5721200	-2.7579670	-1.8110840

Cp*Rh(CO)-Cyclooctane 1,2-Migration (1)

Final Energy = -927.5976820950

C	2.4341280	-0.4001530	1.4048000
C	1.5312100	-1.4157000	1.0207110
C	1.6984990	-1.6832170	-0.4097200
C	2.7048280	-0.8354640	-0.9209250
C	3.0667570	0.0717230	0.1703700
Rh	1.0321490	0.5058910	-0.1443740
C	1.0249460	2.3373330	-0.4657340
O	1.0099620	3.4693330	-0.6607310

C	-2.6687480	-1.3478710	-0.0323490
C	-2.1134200	-0.2302050	-0.9505330
C	-5.4836350	0.2537290	0.5687970
C	-2.1431190	1.2015240	-0.3637420
C	-4.3388380	1.1664310	1.0714500
C	-3.5084700	1.8519470	-0.0448600
H	-2.5710370	-1.0374410	1.0128010
H	-1.5462960	1.2031350	0.5636340
H	-5.8652870	-0.3366780	1.4121510
H	-3.6682230	0.6095970	1.7330300
H	-2.0398960	-2.2390320	-0.1363540
H	-6.3116750	0.8985860	0.2471080
H	-1.6250280	1.8601470	-1.0709780
H	-4.7954190	1.9392310	1.6998420
C	-4.1197330	-1.7956140	-0.3360640
H	-4.4722140	-2.4294850	0.4881750
H	-4.0911910	-2.4379270	-1.2258450
C	-5.1559550	-0.6886550	-0.6041660
H	-4.8369800	-0.0953080	-1.4686840
H	-6.0892660	-1.1768640	-0.9104970
H	-1.0590040	-0.4574290	-1.1866440
H	-3.2962320	2.8832190	0.2578180
H	-4.1040180	1.9271070	-0.9635740
H	-2.6287410	-0.2484100	-1.9194890
C	0.9797140	-2.7778170	-1.1589990
H	0.9982060	-2.6007600	-2.2374310
H	1.4481530	-3.7519480	-0.9688270
H	-0.0665910	-2.8545240	-0.8496250
C	3.3199030	-0.8536700	-2.2956260
H	3.5874500	0.1540050	-2.6234630
H	4.2342790	-1.4619290	-2.3042180
H	2.6319630	-1.2729840	-3.0343290
C	4.1907730	1.0776490	0.1132550
H	4.0506970	1.8694890	0.8537280
H	5.1528230	0.5906420	0.3165150
H	4.2519090	1.5466790	-0.8722240
C	2.7279220	0.0953400	2.7963930
H	1.8743980	-0.0589660	3.4615760
H	3.5881940	-0.4367530	3.2241120
H	2.9630640	1.1626550	2.7972490
C	0.6205850	-2.2004200	1.9325260
H	-0.3474140	-2.3963060	1.4626640
H	1.0660490	-3.1712010	2.1853920
H	0.4368240	-1.6616410	2.8655860

Cp*Rh(CO)-Cyclooctane 1,2-Migration (2)

Final Energy = -927.5981145050

C	2.1588850	-0.3853020	1.5189460
C	1.4834180	-1.4806670	0.9384310
C	1.9177500	-1.6216020	-0.4540830
C	2.8693610	-0.6173180	-0.7424280
C	2.9174070	0.2479640	0.4367110
Rh	0.9284760	0.4375940	-0.2128490
C	0.7247940	2.2691290	-0.4596570
O	0.5900160	3.3991990	-0.6168550
C	-1.9992800	-0.7435790	-0.5010120
C	-2.1931520	0.6143200	-1.2297910
C	-5.0548940	-0.7254820	0.7265320
C	-2.7090520	1.7765820	-0.3527710
C	-4.3568560	0.5463730	1.2666900
C	-4.1379790	1.6766450	0.2259850
H	-1.8448340	-0.5610030	0.5678420
H	-2.0083260	1.9078310	0.4830850
H	-4.9734090	-1.5215280	1.4784690
H	-3.3972250	0.2890310	1.7259260
H	-1.0770020	-1.2140450	-0.8693650
H	-6.1260320	-0.5057990	0.6292650
H	-2.6458080	2.6962860	-0.9470200
H	-4.9789270	0.9297770	2.0832720
C	-3.1286750	-1.7829610	-0.7124590
H	-2.9981210	-2.5997040	0.0100320
H	-2.9948390	-2.2272210	-1.7071170
C	-4.5766430	-1.2633120	-0.6351410
H	-4.7272530	-0.4958750	-1.4026140
H	-5.2379750	-2.0923860	-0.9158180
H	-1.2266550	0.9317480	-1.6517540
H	-4.3477370	2.6387240	0.7067190
H	-4.8679030	1.5848360	-0.5885270
H	-2.8459870	0.4799080	-2.1018470
C	1.4953110	-2.7466860	-1.3670080
H	2.0885770	-3.6490840	-1.1709270
H	0.4440880	-3.0114280	-1.2193050
H	1.6302100	-2.4771090	-2.4178260
C	3.7017850	-0.4694470	-1.9885930
H	3.8824120	0.5822740	-2.2244690
H	4.6778830	-0.9570700	-1.8634790
H	3.2082190	-0.9251010	-2.8509700
C	3.8876110	1.3892810	0.6227490
H	3.5147190	2.1111740	1.3539760
H	4.8557870	1.0157780	0.9793320
H	4.0567200	1.9201140	-0.3177480

C	2.1479680	0.0516420	2.9604460
H	1.2283040	-0.2562650	3.4643750
H	2.9935820	-0.3886090	3.5055700
H	2.2267570	1.1383250	3.0463210
C	0.5376500	-2.4314320	1.6295830
H	-0.3063990	-2.6956470	0.9846880
H	1.0496100	-3.3642360	1.8981760
H	0.1335660	-1.9939080	2.5460350

Cp*Rh(CO)-Cyclooctane 1,2-Migration (3)

Final Energy = -927.5983475010

C	-2.2703910	-1.1261520	-1.0180240
C	-1.2315000	-1.7118460	-0.2556940
C	-1.4151060	-1.3664680	1.1571050
C	-2.5371340	-0.5233360	1.2694940
C	-2.9971980	-0.2549570	-0.0988590
Rh	-1.0545520	0.5608940	-0.0924730
C	-1.3263910	2.3574110	-0.4864920
O	-1.4844960	3.4679250	-0.7338220
C	2.0197190	0.4644790	0.7038370
C	2.0929290	1.0090130	-0.7512540
C	5.1975980	-0.3823990	0.7362790
C	2.6821610	0.0345600	-1.7945620
C	4.5395760	-1.1913190	-0.4082790
C	4.1682390	-0.3716400	-1.6720190
H	2.0047450	-0.6291110	0.6762410
H	2.0729210	-0.8802390	-1.7806500
H	5.2290000	-1.0069570	1.6388250
H	3.6505280	-1.7154520	-0.0432280
H	1.0677890	0.7682550	1.1684820
H	6.2428720	-0.1965680	0.4572240
H	2.5365800	0.4812180	-2.7857500
H	5.2476240	-1.9784810	-0.6909700
C	3.1377490	0.9648110	1.6507040
H	3.1170930	0.3659740	2.5703830
H	2.8907010	1.9921000	1.9469910
C	4.5704090	0.9806500	1.0850740
H	4.6073220	1.6347770	0.2068470
H	5.2134570	1.4596790	1.8336030
H	1.0804830	1.2541390	-1.1082470
H	4.4006230	-0.9731170	-2.5582220
H	4.8054050	0.5191160	-1.7417260
H	2.6369870	1.9614850	-0.7673840
C	-0.5639240	-1.9014000	2.2811300
H	-0.6796330	-1.3005870	3.1868500
H	-0.8417530	-2.9350240	2.5239450

H	0.4971400	-1.9023940	2.0137960
C	-3.1820590	-0.0061240	2.5286120
H	-3.5820590	1.0008100	2.3853000
H	-4.0138700	-0.6554080	2.8325550
H	-2.4678960	0.0329640	3.3550930
C	-4.2608420	0.4957960	-0.4429360
H	-4.2285720	0.8729980	-1.4683900
H	-5.1353680	-0.1604980	-0.3503540
H	-4.4086600	1.3489690	0.2243150
C	-2.5916330	-1.3571490	-2.4711420
H	-1.7034820	-1.6645800	-3.0294820
H	-3.3472600	-2.1465420	-2.5817670
H	-2.9842500	-0.4517650	-2.9409160
C	-0.1772330	-2.6667240	-0.7592960
H	0.7833650	-2.5015350	-0.2610500
H	-0.4698450	-3.7069960	-0.5671420
H	-0.0209920	-2.5541220	-1.8353880

Cp*Rh(CO)-Cyclooctane 1,2-Migration (4)

Final Energy = -927.5980338440

C	-2.8531680	-0.0127120	1.0754320
C	-1.9522140	1.0520570	1.3042400
C	-1.6548140	1.7074630	0.0276030
C	-2.3585650	1.0449280	-1.0004100
C	-2.9957450	-0.1187830	-0.3774260
Rh	-0.9489180	-0.4871320	-0.0720900
C	-0.6745590	-2.1450160	-0.8699100
O	-0.4953360	-3.1697690	-1.3570780
C	2.0647880	0.5238230	0.5765940
C	2.2076790	-1.0190650	0.4568300
C	5.0423700	1.0925360	-0.6809330
C	3.4811850	-1.6186980	1.0956110
C	5.2576520	0.2434910	0.5960450
C	4.8497320	-1.2493450	0.4794390
H	2.6519560	0.8750020	1.4308460
H	3.4952960	-1.3364930	2.1575890
H	5.1653560	2.1533330	-0.4253250
H	4.7358790	0.6948960	1.4457640
H	1.0243000	0.7762270	0.8314870
H	5.8503840	0.8522580	-1.3840710
H	3.3842120	-2.7108900	1.0701460
H	6.3238910	0.3017870	0.8421510
C	2.4263160	1.3216080	-0.6988620
H	2.4841990	2.3887270	-0.4460770
H	1.5910820	1.2151100	-1.4038920
C	3.7124790	0.9029590	-1.4354170

H	3.6230820	-0.1406700	-1.7568440
H	3.7688200	1.4905540	-2.3599400
H	1.3573230	-1.4947010	0.9661150
H	5.5996590	-1.8570280	0.9985510
H	4.8835640	-1.5675080	-0.5701620
H	2.1437460	-1.3195430	-0.5961230
C	-1.4564120	1.5386260	2.6443220
H	-0.4155220	1.8716450	2.5912300
H	-2.0546340	2.3894810	2.9946710
H	-1.5174260	0.7505110	3.3991810
C	-0.8141820	2.9523370	-0.1136610
H	-0.4575450	3.0765760	-1.1394960
H	-1.3938800	3.8450240	0.1538460
H	0.0613750	2.9235870	0.5420220
C	-2.4760670	1.4480600	-2.4467010
H	-2.5267880	0.5736620	-3.1004010
H	-3.3854450	2.0414530	-2.6111420
H	-1.6211560	2.0521550	-2.7614840
C	-3.9547160	-1.0482080	-1.0808760
H	-4.0132410	-2.0144860	-0.5732200
H	-4.9627940	-0.6153590	-1.1023240
H	-3.6437310	-1.2290490	-2.1131180
C	-3.5591690	-0.8605530	2.1005540
H	-2.9902530	-0.9148070	3.0322830
H	-4.5480390	-0.4438360	2.3343900
H	-3.7052020	-1.8815850	1.7391620

Cp*Rh(CO)-Cyclooctane 1,2-Migration (5)

Final Energy = -927.5985666550

C	2.4977690	-0.5631620	1.2764130
C	1.7630050	-1.5892100	0.6457320
C	1.9400700	-1.4798000	-0.8050210
C	2.7886600	-0.3844040	-1.0798070
C	3.0230380	0.2827490	0.2024010
Rh	0.9409960	0.4525340	-0.0570880
C	0.6468090	2.2861510	0.0007430
O	0.4644790	3.4202250	0.0257340
C	-4.1919220	1.5084010	0.5764680
C	-5.2400350	0.8142920	-0.3329900
C	-1.9149300	-0.8134380	0.0157540
C	-5.5042010	-0.6774540	-0.0265330
C	-3.1238440	-1.5219160	0.6718910
C	-4.3596540	-1.6913510	-0.2515760
H	-4.1372120	0.9769100	1.5316740
H	-5.8284090	-0.7574450	1.0205230
H	-1.1823420	-0.5760780	0.8075380

H	-3.4204850	-0.9969040	1.5846120
H	-4.5457600	2.5159240	0.8214230
H	-1.4301860	-1.5311760	-0.6589570
H	-6.3588340	-0.9988450	-0.6350800
H	-2.7806230	-2.5108200	0.9967310
C	-2.7767840	1.6667290	-0.0325060
H	-2.0775350	1.9496330	0.7643770
H	-2.7996650	2.5131230	-0.7303720
C	-2.2100210	0.4597180	-0.8024510
H	-2.8800840	0.2074230	-1.6324030
H	-1.2691630	0.7778630	-1.2837170
H	-6.1988450	1.3320500	-0.2158190
H	-4.7838500	-2.6879380	-0.0843080
H	-4.0470970	-1.6736460	-1.3035360
H	-4.9639910	0.9364450	-1.3880380
C	1.3919770	-2.4675060	-1.8053380
H	2.0229300	-3.3644200	-1.8529240
H	0.3833390	-2.7946120	-1.5354900
H	1.3472310	-2.0341340	-2.8078290
C	3.3761000	0.0170370	-2.4072480
H	3.4930940	1.1013410	-2.4779070
H	4.3670970	-0.4357190	-2.5454460
H	2.7422710	-0.3045880	-3.2376270
C	3.9755270	1.4358270	0.4072190
H	3.7238790	2.0016570	1.3079890
H	5.0045490	1.0700530	0.5138190
H	3.9490320	2.1251640	-0.4407050
C	2.7343530	-0.3643140	2.7506630
H	1.9347700	-0.8104830	3.3475380
H	3.6813740	-0.8277850	3.0580020
H	2.7863290	0.6975960	3.0038770
C	0.9902390	-2.6950330	1.3209330
H	1.5720340	-3.6254040	1.3331020
H	0.7472500	-2.4368780	2.3548130
H	0.0513200	-2.9040180	0.7987260

Cp*Rh(CO)-Cyclooctane 1,2-Migration (6)

Final Energy = -927.5987482290

C	-2.6332220	0.0930700	1.3028200
C	-1.8803960	1.2729260	1.0899920
C	-1.9604720	1.6481550	-0.3247520
C	-2.7225080	0.6766870	-1.0036850
C	-3.0294370	-0.3719070	-0.0235030
Rh	-0.9221640	-0.4063690	-0.1117580
C	-0.5175420	-2.1349680	-0.6701360
O	-0.2627750	-3.2020030	-1.0112650

C	2.1470260	-0.2065090	0.7877000
C	2.7829840	-1.5077580	0.2347600
C	4.4551680	1.7328070	-0.4881540
C	4.2815540	-1.7019780	0.5569140
C	5.1937390	0.7520740	0.4569290
C	5.3009180	-0.7107350	-0.0494910
H	2.7305760	0.1529730	1.6407770
H	4.4004390	-1.6873500	1.6494750
H	4.2374330	2.6588220	0.0603110
H	4.7311110	0.7554830	1.4486690
H	1.1553560	-0.4458560	1.2062780
H	5.1498250	2.0108360	-1.2912360
H	4.5624940	-2.7119740	0.2336960
H	6.2033670	1.1520320	0.6036280
C	1.9655880	0.9310640	-0.2494470
H	1.6705220	1.8491850	0.2759400
H	1.1239390	0.6720400	-0.9173260
C	3.1666520	1.2278990	-1.1665340
H	3.3932330	0.3348960	-1.7591700
H	2.8514890	1.9899350	-1.8895190
H	2.2512270	-2.3642320	0.6633850
H	6.2971460	-1.0926300	0.2009490
H	5.2388820	-0.7349360	-1.1448670
H	2.6216840	-1.5722910	-0.8488630
C	-1.1945900	2.1064260	2.1447830
H	-0.2261830	2.4769970	1.7930700
H	-1.8028170	2.9806490	2.4094930
H	-1.0216310	1.5276730	3.0556600
C	-1.3706010	2.9103770	-0.9018490
H	-1.2858900	2.8475050	-1.9897610
H	-1.9958250	3.7797600	-0.6612550
H	-0.3720710	3.1052670	-0.4983880
C	-3.1764540	0.6955960	-2.4396350
H	-3.1923030	-0.3113050	-2.8643190
H	-4.1912340	1.1076160	-2.5195850
H	-2.5161280	1.3085960	-3.0583320
C	-3.9392280	-1.5470420	-0.2877110
H	-3.7549690	-2.3559770	0.4239670
H	-4.9909150	-1.2477090	-0.1959250
H	-3.7895160	-1.9449900	-1.2948190
C	-2.9791620	-0.5588010	2.6156680
H	-2.2421120	-0.3159520	3.3856430
H	-3.9609480	-0.2196610	2.9724750
H	-3.0166770	-1.6470670	2.5211640

Cp*Rh(CO)-Cyclooctane 1,3-Migration (1)

Final Energy = -927.5989069630

C	-2.4973360	-0.9539120	-1.0166000
C	-1.3490880	-1.6733830	-0.6299630
C	-1.1761990	-1.5398080	0.8189480
C	-2.2367730	-0.7623090	1.3422750
C	-2.9775100	-0.2632840	0.1855180
Rh	-1.0520160	0.5524150	-0.0830420
C	-1.3480930	2.3813440	-0.2504950
O	-1.5105620	3.5141500	-0.3494790
C	3.2403970	1.4247500	1.1847240
C	3.6260950	0.0314410	1.7473590
C	3.0840280	0.3413680	-1.9202060
C	4.8277060	-0.6573260	1.0614370
C	4.5310830	0.0786870	-1.4355940
C	4.6900860	-1.0820070	-0.4183910
H	4.1099790	1.8748540	0.6959960
H	5.6954740	0.0120370	1.1433930
H	3.0542150	1.2990220	-2.4554190
H	4.9609580	0.9911890	-1.0116580
H	2.9926650	2.0914360	2.0179790
H	2.8301180	-0.4305570	-2.6580970
H	5.0781580	-1.5522700	1.6448270
H	5.1295090	-0.1432860	-2.3262440
C	2.0252590	1.4307000	0.2273990
H	1.9496850	2.4128970	-0.2554630
H	1.1200620	1.3280110	0.8525540
C	1.9784360	0.3259510	-0.8479980
H	1.9630610	-0.6540990	-0.3587010
H	1.0161210	0.4114790	-1.3848960
H	3.8896010	0.1433290	2.8051420
H	5.5971580	-1.6434020	-0.6695140
H	3.8611050	-1.7933470	-0.5274250
H	2.7522150	-0.6331270	1.7271100
C	-0.4655990	-2.5165410	-1.5150400
H	-0.6787950	-3.5841770	-1.3771590
H	-0.6188790	-2.2761880	-2.5701580
H	0.5940270	-2.3628270	-1.2873720
C	-0.0996000	-2.2405430	1.6107630
H	0.0555870	-1.7601770	2.5804580
H	-0.3666620	-3.2896270	1.7918700
H	0.8557320	-2.2367210	1.0759940
C	-2.5662530	-0.5076420	2.7895790
H	-2.9813600	0.4931890	2.9333270
H	-3.3067460	-1.2325540	3.1535130
H	-1.6769200	-0.5941360	3.4195320

C	-4.2618050	0.5262070	0.2621440
H	-4.4267590	1.1025280	-0.6519890
H	-5.1190090	-0.1453720	0.3971950
H	-4.2454350	1.2258680	1.1018560
C	-3.1434020	-0.9022680	-2.3761910
H	-2.4234600	-1.1235790	-3.1682050
H	-3.9576290	-1.6357550	-2.4467390
H	-3.5671830	0.0849550	-2.5769920

Cp*Rh(CO)-Cyclooctane 1,4-Migration (1)

Final Energy = -927.5999091340

C	2.2824600	-0.4788050	1.3326830
C	1.3880060	-1.4994870	0.9466380
C	1.4347910	-1.6301030	-0.5112760
C	2.3908690	-0.7255220	-1.0310270
C	2.8160420	0.1003990	0.0943780
Rh	0.7494320	0.5058630	-0.0270650
C	0.6655420	2.3607410	-0.0946300
O	0.5851950	3.5059950	-0.1416440
C	-2.7396490	-1.6284830	0.0367160
C	-2.8323500	-1.1948860	-1.4494670
C	-3.7615150	1.2713900	1.1698340
C	-2.1215960	0.1277150	-1.8097020
C	-2.4854970	1.5634760	0.3423080
C	-2.6386010	1.4446400	-1.1943930
H	-1.8497460	-1.1781980	0.4903360
H	-1.0476580	0.0292420	-1.5469020
H	-3.4812810	1.1594030	2.2252160
H	-1.6607230	0.9137280	0.6814300
H	-2.5766300	-2.7122450	0.0803350
H	-4.3993550	2.1631620	1.1166110
H	-2.1352820	0.2341200	-2.9016090
H	-2.1642120	2.5797360	0.5925860
C	-3.9895740	-1.3270010	0.8974510
H	-3.7397160	-1.4939480	1.9533120
H	-4.7598630	-2.0669010	0.6437620
C	-4.6212530	0.0680460	0.7402270
H	-4.9466430	0.2040630	-0.2972770
H	-5.5390500	0.0854910	1.3408050
H	-2.3771560	-1.9746610	-2.0708710
H	-2.0699030	2.2549440	-1.6643340
H	-3.6858540	1.6031890	-1.4804000
H	-3.8846670	-1.1437750	-1.7575630
C	0.6676150	-2.6665160	-1.2958370
H	1.1853440	-3.6339340	-1.2738120
H	-0.3325250	-2.8204700	-0.8807600

H	0.5549900	-2.3698720	-2.3422100
C	2.8959270	-0.6321290	-2.4471740
H	3.1449240	0.3980400	-2.7144150
H	3.8013770	-1.2397310	-2.5787170
H	2.1486140	-0.9902700	-3.1602830
C	3.9115690	1.1373680	0.0385280
H	3.8056280	1.8691030	0.8436920
H	4.8952850	0.6622520	0.1418460
H	3.8959210	1.6780940	-0.9113080
C	2.6708710	-0.0786220	2.7318250
H	1.8786980	-0.3164670	3.4464600
H	3.5797980	-0.6077820	3.0480040
H	2.8704900	0.9938550	2.7981570
C	0.6087520	-2.4042630	1.8690880
H	1.1781530	-3.3180010	2.0836470
H	0.3936230	-1.9128280	2.8216820
H	-0.3430190	-2.7089020	1.4266410

Cp*Rh(CO)-Cyclooctane 1,4-Migration (2)

Final Energy = -927.5987860180

C	2.3111420	0.4553670	-1.2540790
C	1.7104560	1.5269220	-0.5560690
C	1.8444680	1.2944360	0.8847360
C	2.5164300	0.0696660	1.0854790
C	2.6861400	-0.5295270	-0.2411220
Rh	0.5917370	-0.4174980	-0.0286560
C	0.0687240	-2.1934990	-0.1727010
O	-0.2503400	-3.2950290	-0.2448390
C	-4.2710700	-0.3591130	-1.0263490
C	-3.4352530	-1.5038260	-0.3978930
C	-2.4681070	1.9999140	0.3791420
C	-3.2228690	-1.4270520	1.1312550
C	-3.0698040	1.1615430	1.5330740
C	-2.4385240	-0.2381990	1.7300200
H	-4.9327480	0.0712890	-0.2684290
H	-4.2123800	-1.4440660	1.6098690
H	-3.1136570	2.8690990	0.1970700
H	-4.1503790	1.0538970	1.3998160
H	-4.9336010	-0.7806910	-1.7906040
H	-1.5054140	2.3992830	0.7250140
H	-2.7167030	-2.3492210	1.4423720
H	-2.9412740	1.7437750	2.4523540
C	-3.4406290	0.7510510	-1.7140800
H	-4.1002270	1.5965960	-1.9510840
H	-3.0847080	0.3593660	-2.6754170
C	-2.2101310	1.2780990	-0.9539720

H	-1.5026110	0.4416860	-0.8045650
H	-1.6779170	1.9715810	-1.6153790
H	-3.9437310	-2.4552540	-0.5900020
H	-2.3436430	-0.4347770	2.8039300
H	-1.3960490	-0.2434330	1.3587320
H	-2.4686320	-1.5817290	-0.9097840
C	1.4339530	2.2797530	1.9508610
H	1.3306980	1.7919920	2.9234320
H	2.1812070	3.0774800	2.0512510
H	0.4789880	2.7574610	1.7132570
C	3.0029870	-0.5126050	2.3866730
H	2.9470590	-1.6040750	2.3795530
H	4.0491070	-0.2329950	2.5696400
H	2.4078320	-0.1531490	3.2301170
C	3.4684800	-1.7906730	-0.5174700
H	3.1695560	-2.2408200	-1.4676680
H	4.5425610	-1.5722630	-0.5693380
H	3.3137420	-2.5334120	0.2695070
C	2.5539840	0.3405130	-2.7362220
H	1.8303780	0.9310510	-3.3042350
H	3.5585300	0.7010220	-2.9954630
H	2.4753370	-0.6964460	-3.0725480
C	1.1445080	2.7873290	-1.1622250
H	1.8948560	3.5883970	-1.1589440
H	0.8311390	2.6259480	-2.1970170
H	0.2779360	3.1494420	-0.6015670