Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

London Dispersion Effects in the Coordination and Activation of Alkanes in σ-Complexes: A Local Energy Decomposition Study

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1. Comparison of calculated and experimentally determined geometrical and spectroscopic parameters

Table S1. Comparison of computed and experimental TM-C distances as well as symmetric (ν_1) and antisymmetric (ν_2) C-O stretching vibrations. The experimental values are in parentheses. The distances and frequencies are in the unit of Å and cm^{-1}, respectively.

Systems	TM-C	ν_1 (CO)	ν_2 (CO)
[CpMn(CO)$_2$(C$_2$H$_6$)]	2.520	1967.3 (1967)[1]	1917.5(1902)[1]
[CpMn(CO)$_2$(n-C$_7$H$_{16}$)] (I)	2.514	1966.4 (1962±2)[2]	1916.7 (1894±2)[2]
[CpMn(CO)$_2$(n-C$_7$H$_{16}$)] (II)	2.671	1962.9 (1962±2)[2]	1912.5 (1894±2)[2]
[CpRe(CO)$_2$(CH$_4$)]	2.616	1959.4 (1963)[3]	1908 (1902)[3]
[CpRe(CO)$_2$(n-C$_5$H$_{12}$)] (I)	2.632	1954.9 (1952)[4]	1903.9 (1887)[4]
[CpRe(CO)$_2$(n-C$_5$H$_{12}$)] (II)	2.681	1953.9 (1952)[4]	1903.8 (1887)[4]
[CpRe(CO)$_2$(n-C$_7$H$_{16}$)] (I)	2.633	1954.8 (1954)[5]	1904.8 (1890)[5]
[CpRe(CO)$_2$(n-C$_7$H$_{16}$)] (II)	2.702	1952.0 (1954)[5]	1902.2 (1890)[5]
[(HEB)Re(CO)$_2$(n-C$_5$H$_{12}$)]$^+$ (I)	2.707	2001.3	1963.5
[(HEB)Re(CO)$_2$(n-C$_5$H$_{12}$)]$^+$ (II)	2.873	1995.9	1958.8
[(PONOP)Rh(CH$_4$)]$^+$	2.384	N/A	N/A
[(PONOP)Rh(C$_2$H$_6$)]$^+$	2.428	N/A	N/A
[(dcpe)Rh(norbornane)]$^+$	2.407 (2.389)[6] 2.416 (2.400)[6]	N/A	N/A
[(dippe)Rh(norbornane)]$^+$	2.405 2.412	N/A	N/A
[(dibpe)Rh(norbornane)]$^+$	2.416 (2.494±10)[7] 2.423 (2.480±11)[7]	N/A	N/A
[(dcpe)Rh(n-C$_5$H$_{12}$]$^+$	2.513 (2.522)[8] 2.491 (2.513)[8]	N/A	N/A

2. Basis set study

Table S2. Basis set study on two representative systems. All values are in kJ/mol.

Systems	Def2-TZVPP	Def2-QZVPPD
[CpMn(CO)$_2$(C$_2$H$_6$)]	-57.6	-60.2
[CpRe(CO)$_2$(CH$_4$)]	-70.0	-69.3

3. Dispersion from strong pairs, weak pairs and perturbative triples correlation energy.

Table S3. Strong pairs (E^{C-SP}_{disp}), weak pairs (E^{C-WP}_{disp}) and perturbative triples ($E^{C-(T)}_{disp}$) dispersion energy contributions for studied complexes. All values in kJ/mol.

	E^{C-SP}_{disp}	E^{C-WP}_{disp}	$E^{C-(T)}_{disp}$	$E^{C-CCSD}_{disp}/E_{disp}$
[CpMn(CO)$_2$(C$_2$H$_6$)]	-39.7	-2.1	-6.9	86%
[CpMn(CO)$_2$(n-C$_7$H$_{16}$)] (I)	-40.1	-4.1	-7.0	86%
[CpMn(CO)$_2$(n-C$_7$H$_{16}$)] (II)	-52.7	-6.2	-9.7	86%
[CpRe(CO)$_2$(CH$_4$)]	-39.5	-1.2	-6.0	87%
[CpRe(CO)$_2$(n-C$_5$H$_{12}$)] (I)	-45.0	-3.9	-7.1	87%
[CpRe(CO)$_2$(n-C$_5$H$_{12}$)] (II)	-54.6	-5.0	-9.2	87%
[CpRe(CO)$_2$(n-C$_7$H$_{16}$)] (I)	-45.0	-4.0	-7.1	87%
[CpRe(CO)$_2$(n-C$_7$H$_{16}$)] (II)	-64.2	-6.3	-10.6	87%
[(HEB)Re(CO)$_2$(n-C$_5$H$_{12}$)]$^+$ (I)	-57.0	-8.2	-9.3	88%
[(HEB)Re(CO)$_2$(n-C$_5$H$_{12}$)]$^+$ (II)	-60.8	-8.8	-10.1	87%
[(PONOP)Rh(CH$_4$)]$^+$	-55.8	-3.2	-8.3	88%
[(PONOP)Rh(C$_2$H$_6$)]$^+$	-62.3	-5.5	-9.5	88%
[(dcpe)Rh(norbornane)]$^+$	-84.1	-14.0	-13.2	88%
[(dippe)Rh(norbornane)]$^+$	-80.1	-10.5	-12.4	88%
[(dibpe)Rh(norbornane)]$^+$	-84.7	-12.2	-13.2	88%
[(dcpe)Rh(n-C$_5$H$_{12}$]$^+$	-78.2	-11.5	-12.3	88%

4. Binding energy, enthalpy, and Gibbs free energy.

Table S4. Comparison of binding energy (ΔE), enthalpy (ΔH), and Gibbs free energy (ΔG). The energies are in kJ/mol.

	ΔE	ΔH	ΔG	Temperature (with corresponding references to related exp. work)
[CpMn(CO)$_2$(C$_2$H$_6$)]	-57.6	-54.8	-6.9	298K[3]
[CpMn(CO)$_2$(n-C$_7$H$_{16}$)] (I)	-61.1	-57.1	-5.2	298K[3]
[CpMn(CO)$_2$(n-C$_7$H$_{16}$)] (II)	-63.1	-60.3	-5.3	298K[3]
[CpRe(CO)$_2$(CH$_4$)]	-70.0	-59.8	-24.8	298K[3]
[CpRe(CO)$_2$(n-C$_5$H$_{12}$)] (I)	-82.7	-72.2	-29.7	298K[4]
[CpRe(CO)$_2$(n-C$_5$H$_{12}$)] (II)	-91.2	-80.2	-36.8	298K[4]
[CpRe(CO)$_2$(n-C$_7$H$_{16}$)] (I)	-83.9	-72.3	-29.8	298K[3]
[CpRe(CO)$_2$(n-C$_7$H$_{16}$)] (II)	-94.8	-83.9	-37.3	298K[3]
[(HEB)Re(CO)$_2$(n-C$_5$H$_{12}$)]$^+$ (I)	-104.3	-94.6	-66.6	178K[9]
[(HEB)Re(CO)$_2$(n-C$_5$H$_{12}$)]$^+$ (II)	-100.2	-92.2	-62.9	178K[9]
[(PONOP)Rh(CH$_4$)]$^+$	-85.6	-81.8	-38.6	263K[10]
[(PONOP)Rh(C$_2$H$_6$)]$^+$	-88.5	-86.6	-63.6	123K[11]
[(dcpe)Rh(norbornane)]$^+$	-127.8	-114.3	-67.7	298K[6]
[(dippe)Rh(norbornane)]$^+$	-127.0	-115.4	-75.4	253K[6]
[(dibpe)Rh(norbornane)]$^+$	-93.5	-88.6	-35.1	298K[7]
[(dcpe)Rh(n-C$_5$H$_{12}$]$^+$	-113.0	-104.9	-82.7	150K[8]

5. Orbital relaxation energy, frozen HF interaction energy, and HF interaction energy.

Table S5. Orbital relaxation energy ($\Delta E_{orb.relax}$), frozen Hartree-Fock interaction energy ($\Delta E_{int}^{HF,0}$), and HF interaction energy (ΔE_{int}^{HF}) for studied complexes. The unit is in kJ/mol.

	$\Delta E_{orb.relax}$	$\Delta E_{int}^{HF,0}$	ΔE_{int}^{HF}
[CpMn(CO)$_2$(C$_2$H$_6$)]	-54.7	72.6	17.9
[CpMn(CO)$_2$(n-C$_7$H$_{16}$)] (I)	-55.2	73.4	18.2
[CpMn(CO)$_2$(n-C$_7$H$_{16}$)] (II)	-51.3	84.0	32.7
[CpRe(CO)$_2$(CH$_4$)]	-135.2	112.5	-22.7
[CpRe(CO)$_2$(n-C$_5$H$_{12}$)] (I)	-144.5	118.1	-26.4
[CpRe(CO)$_2$(n-C$_5$H$_{12}$)] (II)	-141.7	123.4	-18.3
[CpRe(CO)$_2$(n-C$_7$H$_{16}$)] (I)	-144.6	118.2	-26.4
[CpRe(CO)$_2$(n-C$_7$H$_{16}$)] (II)	-142.8	132.6	-10.2
[(HEB)Re(CO)$_2$(n-C$_5$H$_{12}$)]$^+$ (I)	-160.8	130.7	-30.1
[(HEB)Re(CO)$_2$(n-C$_5$H$_{12}$)]$^+$ (II)	-141.9	122.4	-19.5
[(PONOP)Rh(CH$_4$)]$^+$	-93.1	98.1	5.0
[(PONOP)Rh(C$_2$H$_6$)]$^+$	-92.5	102.7	10.2
[(dcpe)Rh(norbornane)]$^+$	-164.9	148.8	-16.1
[(dippe)Rh(norbornane)]$^+$	-168.1	145.2	-22.9
[(dibpe)Rh(norbornane)]$^+$	-161.7	150.3	-11.4
[(dcpe)Rh(n-C$_5$H$_{12}$]$^+$	-125.2	122.3	-2.9

6. References

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7. XYZ coordinates

All coordinates are given in Å.

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[$CpMn(CO)_2(C_2H_6)$]

C	-4.44506	-0.03277	0.26810
C	-4.08049	-0.85522	-0.83646
C	-3.22503	-1.90208	-0.34954
C	-3.06842	-1.70241	1.04855
C	-3.81706	-0.55990	1.44668
H	-3.90305	-0.16607	2.44925
H	-2.43693	-2.29418	1.69935
H	-2.78614	-2.69521	-0.93824
H	-4.39822	-0.71783	-1.86049
H	-5.08509	0.83737	0.22433
Mn	-2.36671	0.03508	-0.01418
C	-2.40412	1.79108	0.30068
O	-2.51940	2.93471	0.49509
C	-1.68909	0.26868	-1.65048
O	-1.32565	0.40797	-2.74933
C	-0.07123	-0.53707	0.85372
C	1.14145	0.28316	0.41682
H	-0.93149	0.18983	1.03586
H	-0.29257	-1.34209	0.15345
H	0.05814	-0.97661	1.84828
H	1.00228	0.67831	-0.59279
H	2.04241	-0.33965	0.41918
H	1.31137	1.12853	1.09074

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[$CpMn(CO)_2(n\text{-}C_7H_{16})$] (I)

C	-4.30202	-0.04555	0.22442
C	-3.90734	-0.88742	-0.85481
C	-3.05117	-1.91448	-0.32849
C	-2.92422	-1.68336	1.06749
C	-3.69220	-0.54041	1.42614
H	-3.80222	-0.12624	2.41812
H	-2.29933	-2.25413	1.74289
H	-2.59217	-2.71507	-0.89119
H	-4.20624	-0.77551	-1.88758
H	-4.94981	0.81671	0.14941
Mn	-2.21930	0.03855	-0.01828
C	-2.28195	1.80167	0.24778
O	-2.41275	2.94909	0.40747
C	-1.50357	0.23612	-1.64289
O	-1.11287	0.34929	-2.73557
C	0.05576	-0.48426	0.91581
C	1.27653	0.33776	0.50160
C	2.56062	-0.49932	0.49507
C	3.79923	0.30908	0.09368
C	5.08580	-0.52301	0.08573
C	6.32739	0.28399	-0.31021
C	7.60810	-0.55647	-0.31328
H	-0.81382	0.23933	1.06418
H	-0.13491	-1.30010	0.21784
H	0.16627	-0.91298	1.91821
H	1.39530	1.18879	1.18447
H	1.10589	0.75913	-0.49569
H	2.43776	-1.34498	-0.19641
H	2.71848	-0.93507	1.49217
H	3.91830	1.15610	0.78409
H	3.64004	0.74388	-0.90292
H	4.96729	-1.36877	-0.60680
H	5.24144	-0.96137	1.08216
H	6.44331	1.12917	0.38188
H	6.17081	0.72050	-1.30590
H	8.47947	0.04242	-0.59881
H	7.80173	-0.97950	0.67951
H	7.52761	-1.39085	-1.01986

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[$CpMn(CO)_2(n\text{-}C_7H_{16})$] (II)

C	-3.97168	0.17449	-0.33796
C	-3.491672	-1.12449	-0.00231
C	-3.50194	-1.25264	1.42740
C	-3.99191	-0.02412	1.95294
C	-4.28795	0.86011	0.88454
H	-4.67935	1.86329	0.97387
H	-4.08885	0.21532	3.00415
H	-3.21075	-2.12439	1.99521
H	-3.17512	-1.88193	-0.70580
H	-4.08329	0.57004	-1.33769
Mn	-2.20370	0.33227	0.78070
C	-1.71546	1.73628	-0.20396
O	-1.46337	2.63051	-0.90899
C	-0.82856	-0.64179	0.20095
O	0.00923	-1.31970	-0.24540
H	-0.30968	-1.49860	2.60966
H	0.26594	0.69475	4.66753
H	1.02070	0.61050	3.07914
C	-0.08789	-1.16747	3.63064
C	0.10988	0.35383	3.63381
C	-1.19549	-1.64222	4.57682
C	-1.06748	1.15044	3.05557
C	-0.96010	2.66392	3.27190
H	-2.17112	-1.23081	4.29588
H	-0.11268	3.05550	2.69375
H	-2.009182	0.78451	3.46513
H	-1.004722	0.99457	1.93243
H	-0.719989	2.83600	4.33078
C	-2.232756	3.43447	2.91206
H	0.858005	-1.64389	3.91584
H	-1.283431	-2.73363	4.56111
H	-0.989899	-1.33671	5.60966
H	-2.49725	3.21780	1.87052
C	-2.083576	4.94546	3.10721
H	-3.062075	3.05998	3.52856
H	-1.280805	5.34154	2.47505
H	-1.839613	5.18841	4.14820
H	-3.006734	5.47327	2.84618

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[$CpRe(CO)_2(CH_4)$]

C	-1.90104	-1.21704	-0.23337
C	-1.56394	-0.47124	-1.42178
C	-1.63938	0.92646	-1.10276
C	-2.02239	1.05158	0.28108
C	-2.14718	-0.27030	0.80323
H	-1.96383	-2.29253	-0.14878
H	-1.34917	-0.88687	-2.39582
H	-1.48588	1.74094	-1.79637
H	-2.19203	1.97282	0.81926
H	-2.38909	-0.51544	1.83001
Re	0.03380	0.01805	0.05093
C	1.17869	1.51963	-0.26918
O	1.79208	2.47998	-0.53317
C	1.32191	-1.14004	-0.77170
O	2.03301	-1.86629	-1.34972
C	0.98286	-0.70761	2.37828
H	2.04450	-0.91112	2.51838
H	0.51577	-0.36995	3.30422
H	0.97458	0.23725	1.72202
H	0.48826	-1.60627	2.01448

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[$CpRe(CO)_2(n\text{-}C_5H_{12})$] (I)

C	-4.46463	-0.12110	0.22162
C	-4.04623	-0.94060	-0.87986
C	-3.23056	-2.00842	-0.35445
C	-3.13403	-1.81280	1.05377
C	-3.91155	-0.67695	1.43080
H	-4.06405	-0.30844	2.43482
H	-2.55793	-2.42869	1.73308
H	-2.78231	-2.81070	-0.92293
H	-4.33874	-0.81051	-1.91193
H	-5.12295	0.73363	0.15767
Re	-2.25459	0.06030	-0.00431
C	-2.28573	1.94921	0.30847
O	-2.41945	3.09516	0.50242
C	-1.42081	0.35728	-1.70388
O	-0.99391	0.49487	-2.78478
C	0.15487	-0.43421	0.93360
C	1.36998	0.37687	0.48298
C	2.65689	-0.45514	0.51279
C	3.88944	0.33865	0.06397
C	5.17382	-0.49523	0.09209
H	6.03818	0.09339	-0.23266
H	-0.71033	0.32056	1.08127
H	-0.03361	-1.27625	0.26666
H	0.26149	-0.82286	1.95167
H	1.48316	1.25742	1.12785
H	1.19312	0.75113	-0.53133
H	2.53534	-1.33457	-0.13562
H	2.82276	-0.83988	1.52947
H	4.00603	1.21834	0.71103
H	3.71924	0.72157	-0.95085
H	5.09141	-1.36476	-0.57032
H	5.37983	-0.86517	1.10337

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[$CpRe(CO)_2(n\text{-}C_5H_{12})$] (II)

C	-4.04056	0.11605	-0.40447
C	-3.71233	-1.16467	0.15264
C	-3.81373	-1.06801	1.58742
C	-4.17935	0.27758	1.89258
C	-4.35062	1.00954	0.68412
H	-4.65702	2.04203	0.59865
H	-4.30524	0.68151	2.88887
H	-3.66074	-1.86889	2.29642
H	-3.47712	-2.05662	-0.41036
H	-4.09745	0.35090	-1.45773
Re	-2.14321	0.30160	0.75453
C	-1.36783	1.50768	-0.51378
O	-0.99120	2.23230	-1.35195
C	-0.73212	-0.95357	0.44936
O	0.05071	-1.79423	0.22568
H	0.52852	0.54065	4.44387
H	1.25736	0.97885	2.88817
H	0.39489	-0.55955	3.05436
C	0.39727	0.48973	3.35680
C	-0.90560	1.18525	2.96236
C	-0.97664	2.65784	3.38921
H	-0.15094	3.20536	2.91488
H	-1.76406	0.63909	3.35994
H	-0.88051	1.26190	1.80942
H	-0.80109	2.70414	4.47308
C	-2.30416	3.33694	3.04898
H	-2.50606	3.19469	1.97850
C	-2.31164	4.82971	3.38978
H	-3.11661	2.83039	3.58781
H	-1.52997	5.35952	2.83386
H	-2.13071	4.99265	4.45864
H	-3.27290	5.28938	3.13782

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[$CpRe(CO)_2(n\text{-}C_7H_{16})$] (I)

C	-4.47459	-0.11570	0.22221
C	-4.05877	-0.93591	-0.87969
C	-3.24564	-2.00599	-0.35496
C	-3.14800	-1.81106	1.05326
C	-3.92244	-0.67327	1.43096
H	-4.07347	-0.30465	2.43516
H	-2.57321	-2.42860	1.73218
H	-2.79970	-2.80921	-0.92393
H	-4.35149	-0.80484	-1.91157
H	-5.13060	0.74084	0.15873
Re	-2.26413	0.06006	-0.00458
C	-2.29020	1.94899	0.30831
O	-2.42086	3.09530	0.50243
C	-1.42965	0.35449	-1.70422
O	-1.00227	0.49050	-2.78515
C	0.14362	-0.44111	0.93443
C	1.36171	0.36579	0.48454
C	2.64663	-0.46943	0.51974
C	3.88147	0.32047	0.07214
C	5.17029	-0.50744	0.10484
C	6.40730	0.27948	-0.34254
C	7.69055	-0.55613	-0.30436
H	-0.71946	0.31634	1.08092
H	-0.04698	-1.28305	0.26791
H	0.24796	-0.82989	1.95270
H	1.47566	1.24774	1.12735
H	1.18818	0.73787	-0.53113
H	2.52395	-1.35009	-0.12649
H	2.80831	-0.85156	1.53790
H	3.99971	1.20348	0.71585
H	3.71764	0.70050	-0.94576
H	5.05093	-1.39114	-0.53838
H	5.33219	-0.88840	1.12361
H	6.52390	1.16295	0.29975
H	6.24434	0.65812	-1.36062
H	8.55844	0.02806	-0.62833
H	7.89078	-0.92111	0.70992
H	7.60916	-1.42971	-0.96173

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[$CpRe(CO)_2(n\text{-}C_7H_{16})$] (II)

C	-4.10163	0.15705	-0.30229
C	-3.62339	-1.16454	-0.01082
C	-3.64426	-1.34373	1.41938
C	-4.11076	-0.12119	1.98742
C	-4.42228	0.80019	0.94812
H	-4.82562	1.79457	1.07352
H	-4.21083	0.07801	3.04724
H	-3.37316	-2.23996	1.95797
H	-3.34409	-1.90998	-0.74173
H	-4.24617	0.57353	-1.28887
Re	-2.15969	0.31840	0.78015
C	-1.57948	1.79578	-0.28867
O	-1.32506	2.68928	-1.00051
C	-0.66898	-0.71330	0.17111
O	0.16241	-1.41695	-0.25798
H	-0.09769	-1.43357	2.62165
H	0.20767	0.73494	4.76266
H	1.09017	0.71062	3.23812
C	0.00546	-1.11512	3.66517
C	0.14851	0.41050	3.71385
C	-1.17847	-1.64296	4.48108
C	-1.005803	1.18807	3.06336
C	-0.937276	2.70372	3.29103
H	-2.130896	-1.26701	4.09180
H	-0.079202	3.11502	2.74353
H	-1.964153	0.80501	3.41857
H	-0.827432	1.04737	1.93212
H	-0.734374	2.86815	4.35860
C	-2.211676	3.45353	2.89810
H	0.933569	-1.56280	4.04078
H	-1.220504	-2.73655	4.44785
H	-1.101589	-1.34049	5.53234
H	-2.443687	3.23478	1.84890
C	-2.092562	4.96627	3.10228
H	-3.051793	3.06215	3.48922
H	-1.282454	5.37801	2.49002
H	-1.878695	5.20989	4.14969
H	-3.018442	5.47819	2.82030

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[(HEB)Re$(CO)_2$(n-C_5H_{12})]$^+$ (I)

C	0.77638	1.52885	1.03323
C	1.77281	1.30643	0.01422
C	2.29008	-0.01115	-0.23338
C	1.75950	-1.12398	0.51326
H	-2.44833	1.15239	-0.52032
H	-1.76259	-0.60395	-0.25471
O	-0.35389	1.75510	-3.02028
Re	0.02417	-0.05299	-0.53652
C	-0.26294	1.06030	-2.09803
C	-3.72681	-0.53283	-1.06142
C	-0.09605	-1.59806	-1.69539
C	-2.65462	0.13478	-0.19557
H	-2.89254	0.13684	0.87036
C	0.25392	0.40669	1.74711
O	-0.09621	-2.55093	-2.35467
C	0.74583	-0.92487	1.50802
C	-0.78795	0.62771	2.82078
H	-1.41542	1.48273	2.55929
H	-1.44834	-0.24057	2.88170
C	0.32265	2.94244	1.36442
H	1.16199	3.62092	1.19673
H	0.10837	2.99607	2.43472
C	2.33871	2.48476	-0.74751
H	1.56456	3.24405	-0.87983
H	2.63100	2.16695	-1.75046
C	3.43415	-0.21308	-1.21671
H	4.06947	0.67513	-1.18453
H	4.05539	-1.03523	-0.85345
C	2.31107	-2.51069	0.26863
H	2.61910	-2.60534	-0.77481
H	1.52673	-3.25434	0.42567
C	0.23015	-2.09898	2.32626
H	1.04225	-2.81887	2.44989
H	-0.00773	-1.74669	3.33287
C	-0.12520	0.87008	4.19246
H	0.49032	0.01716	4.49226
H	0.51949	1.75325	4.17038
H	-0.89326	1.02423	4.95473
C	-0.99432	-2.81460	1.73469
H	-0.77954	-3.19925	0.73326
H	-1.28755	-3.65474	2.37078
H	-1.84864	-2.13480	1.65759
C	3.50589	-2.80226	1.19718
H	4.31771	-2.08629	1.03849
H	3.21540	-2.74543	2.25041
H	3.89214	-3.80596	1.00206
C	3.02644	-0.48965	-2.67135
H	2.41137	0.32115	-3.07133
H	3.91985	-0.58376	-3.29524
H	2.45347	-1.41668	-2.75420
C	3.55111	3.09443	-0.01680
H	3.93947	3.94245	-0.58667
H	3.28043	3.44905	0.98203

H	4.35640	2.36335	0.09969
C	-0.89635	3.44398	0.57698
H	-1.77780	2.83009	0.78478
H	-1.13011	4.47475	0.85821
H	-0.71053	3.41640	-0.50065
C	-3.45343	-0.41145	-2.56255
H	-2.47044	-0.84753	-2.78830
H	-3.39122	0.65267	-2.82529
C	-4.51297	-1.09519	-3.44058
C	-4.54319	-2.62062	-3.29369
H	-4.30883	-0.83809	-4.48618
H	-5.50115	-0.67789	-3.20678
H	-3.55978	-3.05362	-3.51210
H	-5.26456	-3.06291	-3.98695
H	-4.83111	-2.92991	-2.28302
H	-4.68013	-0.04331	-0.82099
H	-3.82878	-1.58295	-0.76779

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[(HEB)Re$(CO)_2$(n-C_5H_{12})]$^+$ (II)

C	1.04889	1.59369	1.08806
C	1.94991	1.28852	0.00583
C	2.36280	-0.06532	-0.24593
C	1.79775	-1.12918	0.54243
H	-2.63424	1.39245	-0.72155
H	-1.79718	-0.11460	-0.08206
O	-0.22307	1.85062	-2.91645
Re	0.08733	0.05238	-0.42151
C	-0.15720	1.16111	-1.98691
C	-3.07684	-0.38680	-1.90192
C	-0.19591	-1.50939	-1.52298
C	-2.76851	0.31809	-0.58727
C	-3.82471	0.03746	0.48960
C	0.52690	0.52374	1.87585
O	-0.27840	-2.47854	-2.15343
C	0.87685	-0.84337	1.60432
C	-0.29805	0.84206	3.10121
H	-0.88697	1.74608	2.94046
H	-1.00442	0.03602	3.30545
C	0.68875	3.03543	1.40822
H	1.51134	3.68356	1.10029
H	0.61523	3.14522	2.49323
C	2.53789	2.41210	-0.81962
H	1.80083	3.21073	-0.93255
H	2.75622	2.05294	-1.82731
C	3.43065	-0.35918	-1.28992
H	4.12468	0.48456	-1.30881
H	4.01499	-1.21619	-0.94612
C	2.22261	-2.55580	0.27407
H	2.47024	-2.67338	-0.78278
H	1.38829	-3.23349	0.46963
C	0.32246	-1.96323	2.47040
H	1.02918	-2.79487	2.47182
H	0.27393	-1.61487	3.50553
C	0.63110	1.03464	4.31807
H	1.21600	0.13167	4.51612
H	1.33296	1.85730	4.15335
H	0.03672	1.26163	5.20696
C	-1.06037	-2.47198	2.03479
H	-1.02153	-2.87966	1.02008
H	-1.41109	-3.25741	2.71068
H	-1.79489	-1.66061	2.04260
C	3.43392	-2.94460	1.14324
H	4.29155	-2.29544	0.94301
H	3.20110	-2.86656	2.20935
H	3.72870	-3.97555	0.93124
C	2.92547	-0.62899	-2.71496
H	2.34974	0.21757	-3.09900
H	3.77510	-0.79736	-3.38283
H	2.28426	-1.51327	-2.74943
C	3.82076	2.96804	-0.17184
H	4.22642	3.77666	-0.78530
H	3.62468	3.36314	0.82926

H	4.58733	2.19336	-0.07693
C	-0.61445	3.51953	0.75437
H	-1.45506	2.88230	1.04549
H	-0.83808	4.54591	1.05950
H	-0.53540	3.49446	-0.33662
H	-2.36304	-0.14507	-2.69084
H	-4.06857	-0.06583	-2.23793
H	-3.10339	-1.47235	-1.77299
H	-4.79696	0.24119	0.01985
C	-3.68630	0.87671	1.75718
H	-3.82205	-1.03228	0.73342
H	-3.76351	1.94003	1.49520
H	-2.68327	0.72974	2.17163
C	-4.73453	0.52544	2.81671
H	-5.74793	0.68556	2.43428
H	-4.61314	1.14273	3.71186
H	-4.65266	-0.52536	3.11641

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[(PONOP)Rh(CH_4)]$^+$

Rh	-0.00001	-0.52124	-0.04069
P	2.25350	-0.18685	-0.00605
P	-2.25350	-0.18676	-0.00603
C	1.16628	2.20050	-0.02089
C	-1.16618	2.20055	-0.02088
C	1.20553	3.58816	-0.00256
C	-1.20538	3.58821	-0.00255
C	0.00009	4.28307	0.00629
H	2.16645	4.08670	0.00498
H	-2.16627	4.08679	0.00500
H	0.00011	5.36775	0.02144
O	-2.32253	1.50931	-0.03376
O	2.32260	1.50922	-0.03379
C	-3.25197	-0.54159	-1.54524
C	-3.14644	-0.53655	1.59616
C	3.25193	-0.54175	-1.54528
C	3.14645	-0.53673	1.59611
N	0.00003	1.49156	-0.03005
C	-0.00006	-2.89911	-0.21316
H	-0.90063	-3.50631	-0.14896
H	-0.00006	-2.35141	-1.17636
H	0.90049	-3.50634	-0.14898
H	-0.00004	-2.24163	0.71873
C	2.37443	0.26632	2.66594
H	2.52119	1.34289	2.54682
H	1.30045	0.04966	2.62155
H	2.74620	-0.02290	3.65510
C	4.62743	-0.13151	1.60813
H	5.00764	-0.23396	2.63119
H	5.23102	-0.77821	0.96626
H	4.76795	0.90793	1.29963
C	2.99514	-2.03875	1.90924
H	3.46802	-2.67619	1.15782
H	3.47739	-2.24337	2.87144
H	1.94134	-2.31901	1.99696
C	-2.99447	-2.03839	1.90981
H	-1.94054	-2.31814	1.99772
H	-3.47670	-2.24291	2.87205
H	-3.46699	-2.67632	1.15858
C	-2.37489	0.26721	2.66578
H	-1.30080	0.05101	2.62157
H	-2.52211	1.34368	2.54627
H	-2.74663	-0.02183	3.65501
C	-4.62760	-0.13199	1.60789
H	-5.23085	-0.77918	0.96620
H	-5.00786	-0.23424	2.63096
H	-4.76856	0.90728	1.29901
C	-3.62574	-2.03438	-1.56816
H	-4.37620	-2.27770	-0.81127
H	-4.05010	-2.27688	-2.54865
H	-2.75216	-2.67772	-1.41828
C	-2.28890	-0.23251	-2.71305
H	-1.98918	0.82025	-2.71802

H	-1.38278	-0.84474	-2.66106
H	-2.80176	-0.44345	-3.65830
C	-4.50853	0.33366	-1.69612
H	-4.93143	0.15205	-2.69102
H	-5.27572	0.09340	-0.95957
H	-4.26865	1.39689	-1.62073
C	3.62576	-2.03453	-1.56804
H	4.05012	-2.27710	-2.54851
H	4.37624	-2.27773	-0.81113
H	2.75222	-2.67788	-1.41809
C	2.28879	-0.23283	-2.71307
H	1.38270	-0.84510	-2.66098
H	1.98901	0.81991	-2.71813
H	2.80162	-0.44384	-3.65832
C	4.50843	0.33355	-1.69629
H	5.27567	0.09340	-0.95976
H	4.93129	0.15188	-2.69120
H	4.26850	1.39678	-1.62099

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[(PONOP)Rh(C_2H_6)]$^+$

Rh	-0.01725	-0.51198	-0.03879
P	2.239821	-0.18577	-0.01542
P	-2.27134	-0.15962	0.001632
C	1.163803	2.205939	-0.02831
C	-1.16633	2.22142	-0.01117
C	1.213252	3.593101	-0.00834
C	-1.19625	3.609719	0.00883
C	0.013103	4.296917	0.009358
H	2.178184	4.083876	-0.00574
H	-2.15424	4.113698	0.024663
H	0.020694	5.381557	0.025841
O	-2.32546	1.53917	-0.01198
O	2.315861	1.508599	-0.04781
C	-3.2699	-0.46176	-1.5533
C	-3.17931	-0.48422	1.602446
C	3.251099	-0.53853	-1.55069
C	3.133421	-0.53136	1.587828
N	-0.00622	1.503329	-0.0319
C	0.126416	-2.92656	-0.24964
C	-0.84533	-4.09059	-0.04956
H	-0.04267	-2.41594	-1.2153
H	1.162053	-3.26130	-0.21967
H	0.005978	-2.23089	0.657504
C	2.358659	0.27039	2.656522
H	2.499823	1.347434	2.534473
H	1.28579	0.048131	2.612975
H	2.732971	-0.01410	3.646137
C	4.612412	-0.11900	1.598121
H	4.997132	-0.22903	2.618742
H	5.217757	-0.75538	0.947495
H	4.745171	0.924319	1.299413
C	2.987902	-2.03311	1.904488
H	3.464944	-2.67063	1.155606
H	3.469603	-2.23327	2.86794
H	1.934845	-2.31663	1.990968
C	-3.08334	-1.98806	1.919175
H	-2.04024	-2.31346	1.976066
H	-3.54578	-2.16920	2.89579
H	-3.60675	-2.60548	1.184533
C	-2.37764	0.29134	2.671394
H	-1.31175	0.038073	2.624591
H	-2.48727	1.372368	2.55362
H	-2.75791	0.014065	3.660778
C	-4.64430	-0.02534	1.614300
H	-5.27146	-0.65505	0.978338
H	-5.02589	-0.10628	2.638815
H	-4.74784	1.015989	1.297953
C	-3.64892	-1.94845	-1.6451
H	-4.36162	-2.23921	-0.86826
H	-4.12251	-2.13149	-2.61601
H	-2.76954	-2.59590	-1.58014
C	-2.29900	-0.10858	-2.70231
H	-2.01584	0.948348	-2.67795

H	-1.38384	-0.70840	-2.6544
H	-2.79830	-0.30342	-3.65826
C	-4.52501	0.420279	-1.67589
H	-4.92831	0.29557	-2.68758
H	-5.30529	0.134462	-0.96991
H	-4.29108	1.477914	-1.5344
C	3.697202	-2.01110	-1.55522
H	4.153607	-2.23558	-2.52567
H	4.443169	-2.21409	-0.78227
H	2.854871	-2.69721	-1.42217
C	2.277489	-0.28983	-2.7237
H	1.404500	-0.94773	-2.6679
H	1.923072	0.745832	-2.73852
H	2.80269	-0.48194	-3.66625
C	4.470356	0.386921	-1.7144
H	5.236339	0.206285	-0.95963
H	4.914893	0.188627	-2.69666
H	4.183963	1.440318	-1.6795
H	-0.71713	-4.82214	-0.85288
H	-1.88386	-3.75712	-0.05385
H	-0.65584	-4.59533	0.902039

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[(dcpe)Rh(norbornane)]$^{+}$

P	-1.54392	0.22189	-0.83901
P	1.42061	0.54285	-0.81975
C	-0.79017	-0.59409	2.95433
C	0.73299	-0.25698	3.02620
C	1.34196	-1.51066	3.70116
C	1.34979	-2.65130	2.66740
C	-0.16743	-2.97155	2.48683
C	-0.85423	-2.03360	3.50546
C	0.19335	-1.94564	4.63569
C	-2.37245	-1.35257	-1.35935
C	-1.33386	-2.37645	-1.84849
C	-1.99120	-3.70325	-2.25042
C	-2.82258	-4.27932	-1.09898
C	-3.87267	-3.26740	-0.62753
C	-3.22319	-1.93778	-0.21758
C	-2.93473	1.34965	-0.36252
C	-2.40536	2.69637	0.16184
C	-3.55706	3.59046	0.63991
C	-4.59025	3.80394	-0.47306
C	-5.11642	2.46370	-0.99954
C	-3.97213	1.55793	-1.48292
C	-0.83829	0.94348	-2.39778
C	0.65398	0.61087	-2.50946
C	2.81700	-0.66888	-0.95652
C	2.29035	-2.09740	-1.18049
C	3.43982	-3.11284	-1.16754
C	4.49937	-2.75657	-2.21747
C	5.01741	-1.32785	-2.01526
C	3.87281	-0.30097	-2.01665
C	2.23994	2.18801	-0.59337
C	3.05814	2.22237	0.71008
C	3.72994	3.58903	0.90665
C	2.69818	4.72258	0.88453
C	1.88100	4.69370	-0.41210
C	1.20868	3.32902	-0.61689
Rh	-0.03280	0.01044	0.75087
H	-1.36266	0.11419	3.55740
H	0.90240	0.66190	3.59049
H	2.30805	-1.31444	4.16962
H	1.89575	-3.51576	3.05498
H	1.82478	-2.34629	1.72981
H	-0.38727	-4.01906	2.70882
H	-0.50664	-2.76330	1.46469
H	-1.86160	-2.33772	3.79525
H	0.38432	-2.90800	5.11875
H	-0.05618	-1.20243	5.39961
H	-3.03399	-1.08703	-2.19687
H	-0.76863	-1.96892	-2.69486
H	-0.61457	-2.54718	-1.03679
H	-1.21742	-4.41481	-2.55989
H	-2.63939	-3.53881	-3.12207
H	-3.30711	-5.21099	-1.40957
H	-2.15715	-4.52974	-0.26050

H	-4.59067	-3.08186	-1.43794
H	-4.44386	-3.66946	0.21656
H	-2.57407	-2.10658	0.65326
H	-3.99669	-1.22550	0.08956
H	-3.42543	0.83477	0.47621
H	-1.86163	3.21178	-0.64129
H	-1.68254	2.51458	0.96713
H	-4.04364	3.11860	1.50490
H	-3.15879	4.55164	0.98356
H	-4.12388	4.36036	-1.29829
H	-5.42058	4.41736	-0.10743
H	-5.82466	2.62432	-1.81975
H	-5.66599	1.94773	-0.20020
H	-4.37649	0.59756	-1.82015
H	-3.48215	2.02453	-2.34813
H	-1.40036	0.59160	-3.26862
H	-0.98318	2.02575	-2.32675
H	0.79236	-0.37890	-2.95452
H	1.18518	1.33254	-3.13823
H	3.29409	-0.63947	0.03452
H	1.77891	-2.14973	-2.15088
H	1.54087	-2.33513	-0.41667
H	3.04518	-4.11931	-1.34622
H	3.90032	-3.12253	-0.16966
H	5.33092	-3.46797	-2.17469
H	4.05779	-2.84435	-3.22007
H	5.74063	-1.06790	-2.79596
H	5.54863	-1.26491	-1.05547
H	3.40009	-0.28277	-3.00810
H	4.27624	0.70004	-1.83239
H	2.92202	2.31025	-1.44737
H	3.81428	1.42898	0.71252
H	2.37884	2.02726	1.55209
H	4.46479	3.74710	0.10546
H	4.28478	3.59222	1.85138
H	3.19719	5.69099	0.99616
H	2.02039	4.61249	1.74297
H	2.54176	4.90284	-1.26453
H	1.11749	5.47968	-0.40222
H	0.65937	3.32588	-1.56578
H	0.47643	3.14765	0.18056
H	1.32060	-0.09042	2.05462
H	-1.34002	-0.58061	1.94639

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[(dippe)Rh(norbornane)]$^{+}$

C	-0.81968	-2.16967	2.14399
C	0.60167	-2.59952	1.76566
C	2.94646	-1.87628	0.15905
C	-2.65080	0.09146	1.64362
C	-1.83569	1.08958	2.47978
C	2.52569	-2.79278	-1.00118
C	1.98826	-0.17066	2.45241
C	-2.59811	-2.23748	-0.18622
C	-3.38611	-1.47481	-1.25878
C	2.25361	1.30294	2.12003
C	-0.62965	1.10045	-2.36537
C	0.92910	1.11444	-2.29388
C	-0.99019	2.59507	-2.51654
C	-0.69406	3.29644	-1.17465
C	0.86659	3.32767	-1.12550
C	1.27435	2.61630	-2.43045
C	0.17297	3.08344	-3.40578
P	-1.50658	-1.09721	0.79120
P	1.43916	-1.15483	0.96726
Rh	0.06165	-0.11528	-0.40925
H	-1.47527	-3.02779	2.32129
H	-0.80864	-1.57226	3.06141
H	1.16896	-2.94996	2.63405
H	0.57539	-3.40953	1.03287
H	3.43888	-2.47679	0.93595
C	3.92153	-0.79560	-0.32886
C	-3.73986	-0.60239	2.47558
H	-3.12474	0.64398	0.82171
C	3.15299	-0.82073	3.21446
H	1.09458	-0.20600	3.09148
H	-3.30046	-2.66570	0.54151
C	-1.76586	-3.36962	-0.80625
H	-0.97171	0.49201	-3.20463
H	-1.23677	0.70702	-1.47318
H	1.35898	0.50458	-3.09053
H	1.45180	0.74182	-1.34171
H	-1.99984	2.75326	-2.89964
H	-1.11413	4.30542	-1.16368
H	-1.12435	2.74529	-0.33055
H	1.26676	2.81645	-0.24515
H	1.24299	4.35392	-1.11559
H	2.30701	2.78929	-2.73839
H	0.17015	4.16686	-3.55401
H	0.21294	2.58682	-4.38042
H	-1.05129	1.55740	1.87593
H	-1.36109	0.59710	3.33581
H	-2.49268	1.87139	2.87384
H	-4.37872	-1.24781	1.86691
H	-4.37909	0.15399	2.94298
H	-3.30291	-1.20612	3.27803
H	-4.07263	-2.15979	-1.76655
H	-2.70911	-1.06212	-2.01366
H	-3.98021	-0.65712	-0.83977

H	-2.40890	-4.00904	-1.41978
H	-1.30260	-4.00204	-0.04312
H	-0.97426	-2.95789	-1.44230
H	3.11941	1.42259	1.46250
H	2.45189	1.86261	3.04011
H	1.38367	1.74384	1.62439
H	4.08405	-0.76607	2.64326
H	2.96057	-1.87084	3.45541
H	3.31192	-0.28872	4.15827
H	3.41630	-3.22543	-1.46867
H	1.97759	-2.22263	-1.75944
H	1.88705	-3.61702	-0.67235
H	4.78289	-1.27243	-0.80752
H	4.29441	-0.17003	0.48527
H	3.44887	-0.14504	-1.07225

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[(dibpe)Rh(norbornane)]$^{+}$

C	-0.82261	-2.06499	2.21223
C	0.54017	-2.57007	1.73692
C	2.82959	-1.93059	0.04982
C	-2.81309	-0.01441	1.76733
C	-2.25794	0.98334	2.80434
C	2.48834	-2.97380	-1.03360
C	3.77392	-3.69555	-1.46424
C	-3.39596	1.46932	3.71335
C	1.78224	-2.34452	-2.23846
C	-1.55069	2.15969	2.12775
C	2.11653	-0.22188	2.33769
C	-2.49372	-2.23894	-0.13744
C	-2.79534	-1.82439	-1.58924
C	2.42639	1.26323	2.07378
C	3.55833	1.45102	1.05846
C	-3.75619	-0.63283	-1.66490
C	2.74742	1.97304	3.39493
C	-3.34769	-3.02461	-2.36927
C	-0.60158	1.30636	-2.28613
C	0.95290	1.27670	-2.15476
C	-0.90308	2.79684	-2.58612
C	-0.70135	3.60153	-1.28996
C	0.84149	3.52705	-1.06534
C	1.34583	2.76146	-2.30777
C	0.34567	3.19852	-3.39967
P	-1.54568	-1.00970	0.86794
P	1.39581	-1.15156	0.91199
Rh	0.00322	0.02148	-0.32239
H	-1.50733	-2.88165	2.46361
H	-0.71241	-1.43904	3.10310
H	1.14820	-2.97119	2.55494
H	0.41861	-3.36001	0.98924
H	3.43696	-2.39320	0.84005
H	3.43519	-1.12669	-0.38419
H	-3.47101	-0.74655	2.25600
H	-3.42176	0.51603	1.02665
H	-1.52678	0.45961	3.43567
H	1.81722	-3.72327	-0.59300
H	3.55312	-4.45909	-2.21658
H	4.26062	-4.18519	-0.61432
H	4.48608	-2.98639	-1.90196
H	-3.87180	0.63450	4.23844
H	-4.16462	1.98455	3.12586
H	-3.01751	2.17204	4.46233
H	1.50213	-3.10995	-2.96862
H	2.44564	-1.62802	-2.73815
H	0.87193	-1.80791	-1.92584
H	-1.07347	2.81093	2.86655
H	-2.27118	2.76212	1.56212
H	-0.77841	1.79944	1.42903
H	3.01134	-0.75583	2.68566
H	1.36748	-0.29310	3.13636
H	-3.41902	-2.48803	0.40016

H	-1.87077	-3.14219	-0.14518
H	-1.83580	-1.52891	-2.03925
H	1.51148	1.70469	1.65437
H	3.76818	2.51430	0.90750
H	4.48098	0.97118	1.40487
H	3.30262	1.02437	0.08176
H	-3.96256	-0.36783	-2.70652
H	-3.34572	0.25578	-1.17182
H	-4.71202	-0.87159	-1.18427
H	2.92755	3.03953	3.22634
H	3.64602	1.55003	3.85891
H	1.92083	1.87622	4.10715
H	-3.53239	-2.75553	-3.41417
H	-4.29582	-3.36656	-1.93828
H	-2.64535	-3.86480	-2.35334
H	-0.94505	0.63606	-3.07509
H	-1.22846	1.03411	-1.36716
H	1.39238	0.64371	-2.92684
H	1.42337	0.91183	-1.17554
H	-1.87127	2.94446	-3.06772
H	-1.03121	4.63447	-1.43021
H	-1.26619	3.18130	-0.45445
H	1.09780	2.99835	-0.14069
H	1.28787	4.52327	-1.01336
H	2.40526	2.90197	-2.52910
H	0.38352	4.27073	-3.61110
H	0.45778	2.64258	-4.33597

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[(dcpe)Rh(n-C_5H_{12}]$^+$

C	15.84310	14.26486	15.41038
C	14.43966	14.54014	14.86638
C	14.07213	16.01544	14.67853
C	12.64063	16.12730	14.14131
C	12.12800	17.55514	13.93704
C	12.42671	10.80724	16.30861
C	13.71849	11.26974	17.00578
C	13.82205	10.69037	18.42401
C	12.59370	11.05644	19.26454
C	11.30445	10.59516	18.57593
C	11.19547	11.16792	17.15589
C	13.78520	10.83891	13.71188
C	13.84016	11.32449	12.25218
C	15.12720	10.85188	11.56323
C	15.26449	9.32644	11.63395
C	15.20315	8.83683	13.08506
C	13.91843	9.30467	13.78782
C	10.83793	10.64395	13.83190
C	9.59239	11.52891	13.94738
C	8.75002	14.19184	14.81852
C	8.88348	13.89831	16.32287
C	7.78160	14.60276	17.12673
C	7.78102	16.11344	16.86794
C	7.65543	16.41105	15.36975
C	8.76247	15.71048	14.56898
C	9.73571	13.82327	12.07662
C	10.66555	13.06497	11.11270
C	10.48437	13.55698	9.67090
C	9.02198	13.43739	9.22541
C	8.09067	14.18216	10.18880
C	8.26490	13.69473	11.63672
Rh	12.14219	13.68174	14.43231
P	10.06019	13.32182	13.83458
P	12.29388	11.50203	14.59460
H	16.02353	13.19169	15.51807
H	16.59780	14.67144	14.72991
H	15.97802	14.73325	16.39008
H	14.77104	16.49209	13.98042
H	14.15881	16.54957	15.63232
H	11.11445	17.56074	13.52762
H	12.77995	18.08884	13.23831
H	12.11964	18.10453	14.88339
H	12.46099	9.71491	16.18359
H	14.59836	10.98079	16.42011
H	13.71103	12.36717	17.06323
H	14.73816	11.05502	18.90168
H	13.90955	9.59712	18.36013
H	12.56131	12.14632	19.40361
H	12.67100	10.61097	20.26196
H	11.28968	9.49778	18.52603
H	10.42781	10.89801	19.15949
H	11.11504	12.26146	17.19724
H	10.28261	10.79509	16.67699

H	14.63601	11.28711	14.24596
H	13.75896	12.41803	12.22448
H	12.97357	10.93164	11.70350
H	15.13234	11.19047	10.52134
H	15.99097	11.32001	12.05581
H	16.20288	9.00795	11.16779
H	14.45069	8.86259	11.05906
H	16.07121	9.22253	13.63745
H	15.26159	7.74362	13.12504
H	13.04885	8.84151	13.30220
H	13.92468	8.96761	14.82936
H	11.09319	10.48055	12.78044
H	10.68603	9.66315	14.29372
H	8.84867	11.28604	13.18213
H	9.11471	11.39402	14.92181
H	7.79349	13.78116	14.46074
H	9.87207	14.24471	16.65556
H	8.84774	12.82008	16.51017
H	6.80587	14.18342	16.84518
H	7.91939	14.39593	18.19382
H	6.96552	16.59295	17.41957
H	8.71838	16.54617	17.24565
H	7.69817	17.49046	15.18653
H	6.67739	16.06528	15.00779
H	8.65005	15.93155	13.50219
H	9.73702	16.10855	14.88110
H	10.01569	14.88687	12.04557
H	11.70431	13.18080	11.44150
H	10.43121	11.99183	11.15592
H	11.13794	12.98682	9.00115
H	10.80168	14.60725	9.60866
H	8.90182	13.82617	8.20864
H	8.73858	12.37587	9.19478
H	8.30713	15.25862	10.14732
H	7.04529	14.05669	9.88610
H	7.60795	14.26535	12.30082
H	7.95481	12.64307	11.70230
H	12.57274	15.58264	13.17826
H	14.32820	14.01816	13.89328
H	13.72006	14.08858	15.61428
H	11.93916	15.64292	14.88754