Understanding the Differences Between Iron and Palladium in Cross-Coupling Reactions

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Table S6. Geometry parameters (in Å, degrees) of singlet ^{1}Fe(CO)4, computed at ZORA-OPBE/TZ2P, ZORA-BLYP/TZ2P, ZORA-M06L/TZ2P, and from the literature.

Table S7. Geometry parameters (in Å, degrees) of triplet ^{3}Fe(CO)4, computed at ZORA-OPBE/TZ2P, ZORA-BLYP/TZ2P, ZORA-M06L/TZ2P, and from the literature.

Fig. S1 Geometry and electronic energy (in kcal mol^{-1}) relative to reactants for the S_N2 reaction of anionic singlet $^{1}Fe(CO)_4^{-2}$ with $H_3C–X$ bonds (X = H, Cl, CH_3), computed at ZORA-OPBE/TZ2P.

Table S8. Cartesian coordinates (in Å), ADF total bonding energies (in kcal mol^{-1}) and in parentheses, imaginary frequency of transition state structure (in cm^{-1}) of all stationary points in this study, computed at ZORA-OPBE/TZ2P.

Table S1. Electronic and, in parentheses, Gibbs free energies (in kcal mol^{-1}) relative to reactants for the oxidative insertion of iron model catalysts into $H_3C–X$ bonds (X = H, Cl, CH_3), computed at ZORA-OPBE/TZ2P.

		RC	**TS**	**P**
$^1Fe(CO)_4$	C–H	-1.3 (-0.8)	10.4 (10.3)	0.8 (2.3)
	C–Cl	-9.0 (-7.2)	25.5 (27.6)	-15.1 (-11.3)
	C–C	0.1 (0.2)	48.0 (50.3)	10.2 (12.4)
$^3Fe(CO)_4$	C–H	0 (0.1)	64.4 (62.3)	45.2 (49.0)
	C–Cl	0 (0.2)	43.3 (45.2)	29.4 (30.8)
	C–C	-0.1 (-0.4)	76.9 (75.8)	51.1 (49.2)
$^1Fe(CO)_4^{-2}$	C–H	-2.4 (-2.3)	74.1 (69.8)	66.3 (62.4)

Table S2. Electronic energy with small frozen core and, in parentheses, electronic energy with no frozen core (in kcal mol^{-1}) for the oxidative insertion of iron model catalysts into $H_3C–X$ bonds (X = H, Cl, CH_3), computed at ZORA-OPBE/TZ2P.

		RC	**TS**	**P**
$^1Fe(CO)_4$	C–H	-1.3 (-1.6)	10.4 (9.9)	0.8 (1.4)
	C–Cl	-9.0 (-9.5)	25.5 (24.9)	-15.1 (-15.8)
	C–C	0.1 (0.2)	48.0 (47.5)	10.2 (9.8)
$^3Fe(CO)_4$	C–H	0 (0)	64.4 (64.6)	45.2 (46.4)
	C–Cl	0 (0)	43.3 (43.4)	29.4 (29.6)
	C–C	-0.1 (0.2)	76.9 (76.9)	51.1 (50.9)
$^1Fe(CO)_4^{-2}$	C–H	-2.4 (-2.1)	74.1 (73.9)	66.3 (66.4)

Table S3. Electronic energy (in kcal mol^{-1}) in gas phase and, in parentheses, electronic energy in solution (THF) relative to reactants for the oxidative insertion of iron model catalysts into $H_3C–X$ bonds (X = H, Cl, CH_3), computed at ZORA-OPBE/TZ2P.

		RC	**TS**	**P**
$^1Fe(CO)_4$	C–H	-1.3 (-0.25)	10.4 (11.2)	0.8 (3.15)
	C–Cl	-9.0 (-7.8)	25.5 (28.1)	-15.1 (-13.8)
	C–C	0.1 (0.2)	48.0 (49.1)	10.2 (12.3)
$^3Fe(CO)_4$	C–H	0 (1.2)	64.4 (64.3)	45.2 (48.6)
	C–Cl	0 (0.3)	43.3 (43.4)	29.4 (30.3)
	C–C	-0.1 (-0.7)	76.9 (77.1)	51.1 (51.3)
$^1Fe(CO)_4^{-2}$	C–H	-2.4 (-1.3)	74.1 (81.4)	66.3 (69.4)

Table S4. Electronic energies (in kcal mol^{-1}) relative to reactants for the oxidative insertion of $^1Fe(CO)_4$ into $H_3C–X$ bonds (X = H, Cl, CH_3) in the gas phase, computed at ZORA-OPBE/TZ2P, ZORA-BP86/TZ2P//ZORA-OPBE/TZ2P, ZORA-BLYP/TZ2P//ZORA-OPBE/TZ2P, ZORA-B3LYP/TZ2P//ZORA-OPBE/TZ2P, and ZORA-M06L/TZ2P//ZORA-OPBE/TZ2P.

	Method [a]	**RC**	**TS**	**P**
C–H	OPBE	-1.3	10.4	0.8
	BP86	-1.8	10.9	0.4
	BLYP	-1.5	14.5	3.4
	B3LYP	-2.2	14.4	2.3
	M06-L	-5.3	9.6	-1.1
C–Cl	OPBE	-9.0	25.5	-15.1
	BP86	-10.0	20.4	-20.6
	BLYP	-9.1	20.4	-19.5
	B3LYP	-10.2	23.4	-22.2
	M06-L	-8.2	22.8	-24.3
C–C	OPBE	0.1	48.0	10.2
	BP86	-1.1	41.7	3.2
	BLYP	-0.7	47.9	9.3
	B3LYP	-1.0	50.9	9.8
	M06-L	-1.2	45.9	5.9

[a] Indicates the DFT functional used to calculate the energy.

Table S5. Geometry parameters (in Å, degrees) of anionic singlet $^1Fe(CO)_4^{-2}$, computed at ZORA-OPBE/TZ2P, ZORA-BLYP/TZ2P, ZORA-M06L/TZ2P, and from the literature.

Method	**Fe – C**	**Fe - C**	**C – O**	**C - O**	**<(Fe – C – O)**	**<(Fe – C – O)**	**<(C – Fe – C)**	**<(C – Fe – C)**
OPBE[a]	1.727	1.727	1.200	1.200	179.8	179.8	109.7	109.7
BLYP[a]	1.771	1.771	1.206	1.206	179.9	179.9	109.6	109.6
M06-L[a]	1.747	1.747	1.194	1.194	179.9	179.9	109.6	109.6
Exp[b]	1.742	1.742	1.175	1.172	-	-	109.1	108.6
Exp[c]	1.738	1.745	1.175	1.162	-	-	109.5	109.6

[a] This work: computed using ZORA for reletivistic effects and the TZ2P basis set.
[b] R. G. Teller, R. G. Finke, J. P. Collman, H. B. Chin, R. Bau, *J. Am. Chem. Soc.* **1977**, *99*, 1104-1111.
Experimental results from X-ray crystal structures.
[c] H. B. Chin, R. Bau. J. Am. Chem. Soc. 1976, 98, 2434-2439.
Experimental results from X-ray crystal structures.

Table S6. Geometry parameters (in Å, degrees) of singlet $^1Fe(CO)_4$, computed at ZORA-OPBE/TZ2P, ZORA-BLYP/TZ2P, ZORA-M06L/TZ2P, and from the literature.

Method	**Fe – C**	**Fe - C**	**C – O**	**C - O**	**<(Fe – C – O)**	**<(Fe – C – O)**	**<(C – Fe – C)**	**<(C – Fe – C)**
OPBE[a]	1.777	1.732	1.151	1.158	178.2	170.5	181,7	126.6
BLYP[a]	1.806	1.806	1.157	1.157	170.3	170.3	141.5	141.8
M06-L[a]	1.808	1.773	1.144	1.149	172.1	170.5	154.4	129.6
Exp[b]	1.78	1.74	-	-	-	-	177.4	135.3
BP86[c]	1.803	1.770	1.153	1.153	-	-	159.8	130.2
M06-L[d]	1.823	1.777	1.144	1.151	-	-	168.3	127.8

[a] This work: computed using ZORA for reletivistic effects and the TZ2P basis set.
[b] H. Ihee, J. M. Cao, A. H. Zewail, *Angew. Chem. Int. Ed.* **2001**, *40*, 1532-1536.
Experimental results from ultrafast electron diffraction.
[c] A. Krapp, K. K. Pandey, G. Frenking, *J. Am. Chem. Soc.* **2007**, *129*, 7596-7610.
Computational results using ZORA for reletivistic effects and the TZ2P basis set.
[d] Z. Sun, H. F. Schaefer III, Y. Xie, Y. Liu, R. Zhong, *J. Comput. Chem.* **2014**, *35*, 998-1009.
Computational results using cc-pVTZ basis set.

Table S7. Geometry parameters (in Å, degrees) of triplet $^3Fe(CO)_4$, computed at ZORA-OPBE/TZ2P, ZORA-BLYP/TZ2P, ZORA-M06L/TZ2P, and from the literature.

Method	**Fe – C**	**Fe - C**	**C – O**	**C - O**	**<(Fe – C – O)**	**<(Fe – C – O)**	**<(C – Fe – C)**	**<(C – Fe – C)**
OPBE[a]	1.810	1.761	1.151	1.153	175.8	178.8	154.5	96
BLYP[a]	1.863	1.827	1.153	1.155	178.7	179.5	146.3	98.5
M06-L[a]	1.855	1.826	1.142	1.145	179.6	179.9	144.7	98.3
Exp[b]	-	-	-	-	-	-	145	120
BP86[c]	1.803	1.770	1.153	1.153	-	-	159.8	130.2
M06-L[d]	1.869	1.840	1.143	1.146	-	-	146.4	97.4

[a] This work: computed using ZORA for reletivistic effects and the TZ2P basis set.
[b] H. Ihee, J. M. Cao, A. H. Zewail, *Angew. Chem. Int. Ed.* **2001**, *40*, 1532-1536. Experimental results from ultrafast electron diffraction.
[c] A. Krapp, K. K. Pandey, G. Frenking, *J. Am. Chem. Soc.* **2007**, *129*, 7596-7610. Computational results using ZORA for reletivistic effects and the TZ2P basis set.
[d] Z. Sun, H. F. Schaefer III, Y. Xie, Y. Liu, R. Zhong, *J. Comput. Chem.* **2014**, *35*, 998-1009. Computational results using cc-pVTZ basis set.

Fig. S1 Geometry and electronic energy (in kcal mol^{-1}) relative to reactants for the S_N2 reaction of anionic singlet $^1Fe(CO)_4^{-2}$ with $H_3C–X$ bonds (where X = H, Cl, CH_3), computed at ZORA-OPBE/TZ2P.

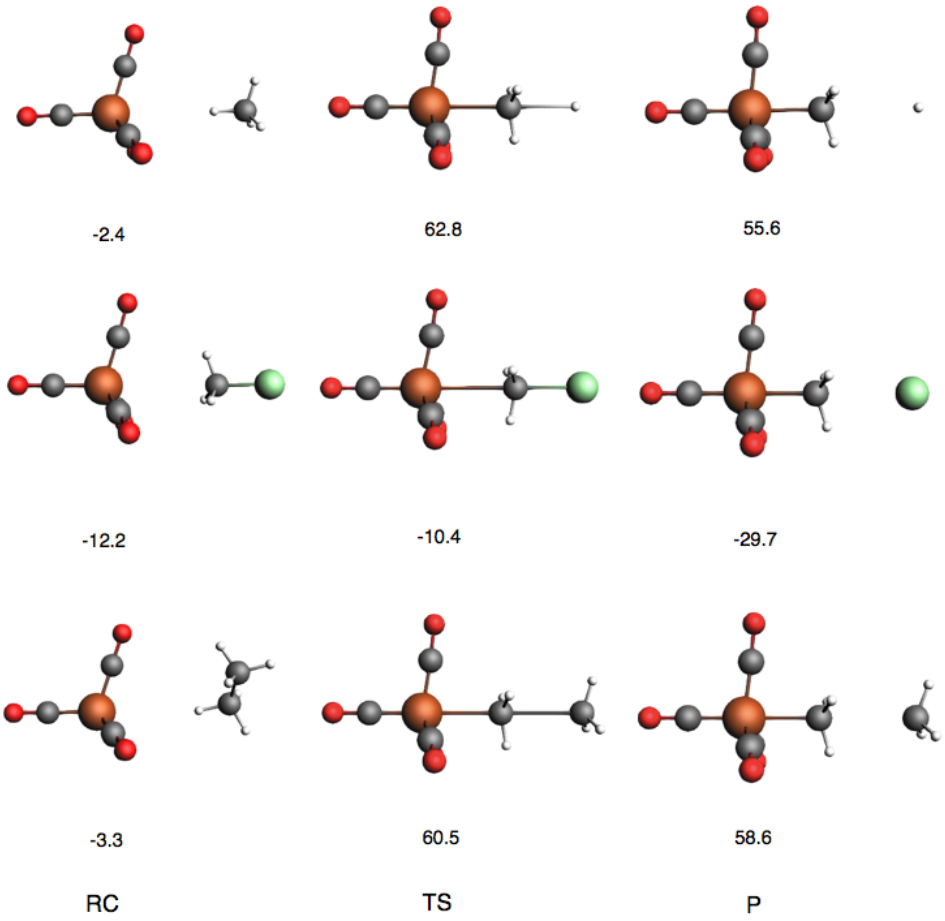

Table S8. Cartesian coordinates (in Å), ADF total bonding energies (in kcal mol^{-1}) and in parentheses, imaginary frequency of transition state structure (in cm^{-1}) of all stationary points in this study, computed at ZORA-OPBE/TZ2P.

RC: Pd+CH_4				-557.93	TS: Pd+CH_4				-548.86 (-638.52)	P: Pd+CH_4				-552.12
C	0.00000000	0.00000000	-1.93543615		C	-1.74196777	-2.22087997	0.00000000		C	-2.10134690	-2.41901732	0.18620613	
Pd	0.00000000	0.00000000	0.32205542		Pd	-2.13750904	-0.23784341	0.00000000		Pd	-2.73145901	-0.57025833	0.41934115	
H	-0.96181082	0.00000000	-1.33610429		H	-2.80956968	-2.49954731	0.00000000		H	-3.88639130	-1.04648079	-0.43099501	
H	0.00000000	-0.90063254	-2.55201285		H	-1.26528821	-2.62993236	0.89567676		H	-2.78392696	-3.12497645	0.66994616	
H	0.00000000	0.90063254	-2.55201285		H	-1.26528821	-2.62993236	-0.89567676		H	-1.97386865	-2.66955518	-0.87144525	
H	0.96181082	0.00000000	-1.33610429		H	-0.75509932	-0.88569836	0.00000000		H	-1.12556673	-2.41201402	0.69858365	
RC: Pd+CH_3Cl				-524.16	TS: Pd+CH_3Cl				-512.77 (-194.99)	P: Pd+CH_3Cl				-541.55
C	-1.47287227	-3.56288223	0.26327334		C	-2.17528160	-2.70744274	0.04185559		C	-2.24128754	-2.72324886	0.02797073	
Pd	-2.82627779	-0.34245554	0.45624055		Pd	-2.81199527	-0.48996192	0.39801798		Pd	-2.21746210	-0.87254938	0.63669530	
H	-1.57461503	-3.54757927	-0.82290172		H	-3.03828060	-2.14811751	-0.44447729		Cl	-0.32812332	-1.03352457	1.74551410	
H	-2.37930991	-3.94569640	0.73456493		H	-2.57511176	-3.48805558	0.68792144		H	-1.34236976	-2.94908132	-0.55095966	
H	-0.59964137	-4.14645722	0.56552918		H	-1.56169511	-3.12338103	-0.75763162		H	-3.14585457	-2.70484419	-0.60465481	
Cl	-1.20791067	-1.87762182	0.82999800		Cl	-0.93457054	-1.80746229	1.11087980		H	-2.35050906	-3.39492647	0.88372619	
RC: Pd+C_2H_6				-936.92	TS: Pd+C_2H_6				-913.48 (-480.74)	P: Pd+C_2H_6				-934.44
C	-0.88946600	-2.04338800	-0.17463600		C	0.70009173	0.65754447	-1.57799445		C	1.44496927	0.00000000	-1.98027211	
H	-2.49303200	-3.37733700	0.43314500		H	-0.20436740	-1.36376803	-0.91184594		H	-1.40855357	-0.90094754	-1.35980537	
H	-1.23793300	-2.00135900	-1.25408600		H	1.22041679	1.28476466	-2.36320542		H	2.35940354	0.00000000	-2.59580903	
H	-0.08816400	-2.78887200	-0.15842300		H	1.47760465	0.10735848	-1.04752662		H	1.40855357	-0.90094754	-1.35980537	
H	-0.40987200	-1.07999400	0.18635900		H	0.20436740	1.36376803	-0.91184594		H	1.40855357	0.90094754	-1.35980537	
H	-1.72154400	-2.51878800	1.77520600		H	-1.47760465	-0.10735848	-1.04752662		H	-1.40855357	0.90094754	-1.35980537	
C	-2.05029400	-2.41930700	0.73315900		C	-0.70009173	-0.65754447	-1.57799445		C	-1.44496927	0.00000000	-1.98027211	
H	-2.84402800	-1.66562800	0.70730000		H	-1.22041679	-1.28476466	-2.36320542		H	-2.35940354	0.00000000	-2.59580903	
Pd	-0.64978700	-0.18374000	-1.50171800		Pd	0.00000000	0.00000000	-3.39592210		Pd	0.00000000	0.00000000	-3.31857216	
RC: $Pd(CO)_2$+ CH_4				-1329.61	TS: $Pd(CO)_2$+ CH_4				-1296.17 (-542.12)	P: $Pd(CO)_2$+ CH_4				-1297.91
Pd	-0.06414951	-2.44190500	1.79987105		Pd	0.29344087	-3.40955739	1.17923774		Pd	0.02532863	-2.30155893	1.95129640	
H	2.50988985	-7.35497188	-0.25450190		H	-1.61529078	-3.27886712	-0.58090923		C	1.56954094	-1.72674987	2.94150840	
H	0.94140707	-6.51790215	-0.09782246		H	0.35365903	-4.68173609	0.27044156		C	-1.41905751	-1.06129709	2.41841636	
C	-1.85275106	-1.81378783	1.62990427		C	-0.49795146	-1.83188013	2.07464044		O	2.55914852	-1.50099073	3.47022442	
C	1.94529528	-6.45940250	-0.52651035		C	-1.35176932	-4.13143809	0.05415290		O	-2.29199261	-0.36623478	2.66362953	
H	1.87202436	-6.39201982	-1.61454559		H	-1.30483947	-5.02385777	-0.57157505		H	0.96480554	-3.43413170	1.39982931	
C	1.58542910	-2.11550416	2.69199056		C	2.12156276	-3.51852731	1.78019728		C	-1.23322298	-3.37235891	0.68304309	
H	2.45913377	-5.57308254	-0.14137475		H	-2.12722996	-4.28315103	0.81257110		H	-0.76158454	-4.22944304	0.20427162	
O	-2.87858188	-1.29892266	1.65930362		O	-0.93770215	-0.92497230	2.61691378		H	-1.59080701	-2.68049396	-0.08811253	
O	2.48393881	-1.76824590	3.31675104		O	3.21453376	-3.67518078	2.08730242		H	-2.08788925	-3.71655134	1.27651445	
RC: $Pd(CO)_2$+ CH_3Cl				-1292.30	TS: $Pd(CO)_2$+ CH_3Cl				-1257.35 (-287.64)	P: $Pd(CO)_2$+ CH_3Cl				-1287.03
Pd	0.20762769	-2.17082175	3.45685133		Pd	0.09340518	-3.40057459	1.33616957		Pd	-0.06557000	-2.36175000	1.97496900	
H	-1.96339015	1.00868608	1.78909139		O	-2.47799499	-3.82055043	-0.34278022		C	1.47139900	-1.93311300	3.28758400	
H	-2.87381105	1.82609219	0.48098263		O	0.67086432	-1.18500901	3.42582258		C	-1.01001800	-0.69873700	1.90206300	
C	-1.25531376	-3.27950337	2.94676826		C	-1.52373170	-3.71131258	0.28594105		O	2.35767000	-1.81288700	3.99473200	
C	-2.51130688	1.91041479	1.50779981		C	0.47886335	-2.04302150	2.68773539		O	-1.59562200	0.28656400	1.83970400	
H	-1.87020167	2.78876919	1.61002360		Cl	1.79684075	-4.98498591	1.01151774		Cl	0.90205200	-4.50890400	1.88015000	
C	1.42952685	-0.86482051	2.80934747		C	1.65123748	-3.06102446	-0.20645330		C	-1.51668900	-3.09251400	0.60904700	
Cl	-3.90095569	2.09114745	2.58784157		H	2.65656415	-2.82493719	0.12690288		H	-0.92324900	-3.41743600	-0.24956100	
O	-2.11244291	-3.86990338	2.46292836		H	1.00886289	-2.16895922	-0.27920806		H	-2.27125900	-2.35535900	0.32396600	
O	2.07066594	-0.09551138	2.24721489		H	1.61701657	-3.67501512	-1.10052938		H	-1.95968700	-3.94371400	1.13269400	
RC: $Pd(CO)_2$+ +C_2H_6				-1709.10	TS: $Pd(CO)_2$+ +C_2H_6				-1655.09 (-452.83)	P: $Pd(CO)_2$+ +C_2H_6				-1676.17
Pd	-0.57878086	-2.82371036	1.31950782		Pd	0.07341342	-3.28415047	1.22376583		Pd	0.11506207	-3.22483377	1.18544393	
O	-3.05617499	-3.63780186	-0.24253754		O	-2.65800856	-3.41021992	-0.18534767		O	-2.70867942	-3.66055704	0.06241640	
O	0.12855578	-0.50430888	3.15302006		O	-0.14008205	-0.93411461	3.20988952		O	-0.17841338	-0.84934519	3.10760237	
C	-2.06469166	-3.43560307	0.30034990		C	-1.68988159	-3.54957793	0.41954986		C	-1.66875111	-3.46473053	0.49665295	
C	-0.02035174	-1.42367619	2.48135918		C	0.04189081	-1.72793607	2.39837514		C	-0.11144807	-1.73352519	2.38497870	
H	4.81671409	-7.24622468	1.36478756		H	1.97792841	-5.52541075	1.45458490		C	2.12915259	-3.22598774	1.73243590	
C	3.37849241	-5.78123859	0.64709165		C	2.13831009	-3.46725921	0.63355276		C	0.68991604	-4.83729516	-0.00703551	
H	3.56083128	-5.06099426	1.45334440		H	2.81723182	-3.38898705	1.48317521		H	2.67310990	-2.71490586	0.92996631	
H	2.49734990	-6.36592884	0.92701118		H	1.96516206	-2.47130769	0.19046166		H	2.48113566	-4.25733028	1.80647597	
H	3.13041336	-5.20889843	-0.25457171		H	2.56395305	-4.09921054	-0.14447344		H	2.32321673	-2.70980285	2.67681289	
C	4.58434996	-6.68428184	0.45279307		C	1.03265356	-5.19942006	1.02311526		H	1.69359164	-4.65841346	-0.39870130	
H	4.41443297	-7.41413060	-0.34726515		H	0.22903779	-5.51731315	1.71148837		H	0.00535001	-5.02513655	-0.83899231	
H	5.47819385	-6.10842777	0.18615746		H	0.88185066	-5.64382216	0.03894981		H	0.70756156	-5.71842681	0.64459109	

RC: $Pd(PH_3)_2$+ CH_4 -1339.52

Pd	0.04601830	-2.17968359	1.98078367
H	3.04935852	-1.34955766	2.90448089
H	-2.25553764	-2.82680773	-0.13477425
P	-2.03178194	-2.35516281	1.18972535
H	-2.98230774	-3.22812389	1.79285356
H	-2.93808350	-1.25937367	1.07843852
P	2.20359375	-2.42092099	2.49040646
H	2.62874432	-3.30612896	3.52252855
H	3.11567765	-2.92003506	1.51784092
C	-0.17876482	-7.63492444	0.86100690
H	-0.96466219	-8.03168755	1.50879408
H	-0.46352749	-7.77611312	-0.18482110
H	-0.04343704	-6.56937885	1.06222047
H	0.75633303	-8.16557151	1.05757931

TS: $Pd(PH_3)_2$+ CH_4 -1308.79 (-587.74)

Pd	0.14041712	-2.99250931	1.74548279
H	2.34356608	-1.95764203	3.82935674
H	-2.95603752	-2.02833049	0.97709791
P	-1.69462983	-1.59697923	1.48815767
H	-2.25560925	-0.90947861	2.60391396
H	-1.63163215	-0.43534195	0.66414927
P	1.74789922	-1.63669753	2.57652182
H	2.98646166	-1.51906151	1.88391945
H	1.65009088	-0.23945252	2.85905753
C	-0.55760979	-4.88285714	1.08981960
H	0.03561137	-5.80026809	1.08459367
H	-0.87785051	-4.68275084	0.06071308
H	-1.43364795	-5.05225318	1.72660068
H	0.99341583	-4.30166428	1.71775803

P: $Pd(PH_3)_2$+ CH_4 -1311.18

Pd	0.15847936	-2.33035879	1.57912196
H	1.52238550	0.24518024	3.15660713
H	-2.21628662	-0.73479864	0.10615410
P	-1.68592078	-0.99178859	1.40052549
H	-2.90946495	-1.44552465	1.96647672
H	-1.80601672	0.34991450	1.86903830
P	1.68478871	-1.09180346	2.68082581
H	2.22278754	-1.59940069	3.89482808
H	2.94002138	-0.85785127	2.05611669
H	1.28582037	-3.43474265	1.57241926
C	-0.79769670	-3.87753728	0.56085952
H	-0.25263271	-4.08239478	-0.36675903
H	-1.83769914	-3.63832494	0.30955190
H	-0.78732127	-4.78478333	1.17328578

RC: $Pd(PH_3)_2$+ CH_3Cl -1302.27

C	3.39463592	1.62145001	0.25637816
Cl	3.83065213	3.21367138	-0.38198811
Pd	-1.22822534	-0.61556209	0.05606666
H	2.30723846	1.52388909	0.24990551
H	3.84554256	0.85449122	-0.37726890
H	3.77544516	1.53732085	1.27661011
P	-0.80206013	-0.47017285	-2.12927737
P	-1.77580393	-0.29893513	2.19519817
H	-1.57511035	0.97040364	2.80777217
H	-1.81923691	-0.70632779	-3.09838547
H	-3.12112424	-0.44009661	2.64177744
H	-1.21727002	-1.04130417	3.27720280
H	-0.37498258	0.76382895	-2.69636949
H	0.18094802	-1.25499649	-2.80114727

TS: $Pd(PH_3)_2$+ CH_3Cl -1271.14 (-364.82)

Pd	0.08805989	-2.99629170	1.85901762
H	2.73257805	-2.30878568	3.81988686
H	-1.41596857	-0.32043439	0.66326354
P	-1.62285286	-1.68040974	1.03918255
H	-2.40654213	-1.97818175	-0.11760734
H	-2.75312452	-1.37871435	1.85548273
P	1.66955674	-1.80766544	3.00189027
H	2.52856524	-0.97832415	2.22364005
H	1.34404767	-0.76813692	3.92413852
C	0.29666168	-5.06236222	2.69171151
H	1.32784901	-5.31868036	2.92069548
H	-0.34529285	-5.93212602	2.58137260
H	-0.15364876	-4.37100803	3.43909941
Cl	0.38553501	-4.94900827	0.55955361

P: $Pd(PH_3)_2$+ CH_3Cl -1309.76

Pd	-0.04902266	-2.39283936	1.69211277
H	1.70817573	0.14576356	2.99410678
H	-1.62357836	-0.69640822	-0.39334794
P	-1.39146549	-0.83001254	1.00069659
H	-2.75052381	-0.86589242	1.40877646
H	-1.15911321	0.54718105	1.27489373
P	1.62165107	-1.26881885	2.81917210
H	1.82767774	-1.62382693	4.17488513
H	2.94646029	-1.46806442	2.35930493
Cl	1.23245250	-4.23769250	2.31985006
C	-1.40586688	-3.64033214	0.74846575
H	-0.79867758	-4.20631115	0.03629264
H	-2.25875991	-3.18927123	0.22853059
H	-1.76663589	-4.29792989	1.54472788

RC: $Pd(PH_3)_2$+ C_2H_6 -1718.93

Pd	0.00000000	0.00000000	-1.15018261
C	-0.23797370	0.72135286	4.29930754
C	0.23797370	-0.72135286	4.29930754
H	0.11749259	1.26007901	3.41346394
H	-1.33268182	0.78228736	4.30239499
H	0.12215960	1.26396554	5.18128127
H	-0.11749259	-1.26007901	3.41346394
H	1.33268182	-0.78228736	4.30239499
H	-0.12215960	-1.26396554	5.18128127
P	-1.82347349	1.25832773	-0.89583284
P	1.82347349	-1.25832773	-0.89583284
H	1.76777675	-2.47707469	-0.16119136
H	-2.57631227	1.80916731	-1.97502850
H	2.57631227	-1.80916731	-1.97502850
H	2.96309159	-0.75206817	-0.20801902
H	-2.96309159	0.75206817	-0.20801902
H	-1.76777675	2.47707469	-0.16119136

TS: $Pd(PH_3)_2$+ C_2H_6 -1666.99 (-446.72)

Pd	0.00513108	-2.97517596	1.76589892
H	2.16587900	-0.45395078	1.52675469
H	-1.93854727	-0.62402673	0.74366435
P	-1.72998976	-1.46468249	1.87707474
H	-3.12179517	-1.76918203	2.02272969
H	-1.79627345	-0.37752686	2.80176662
P	1.93308592	-1.75371163	2.07253628
H	2.23087358	-1.33996676	3.40487355
H	3.27322119	-2.18454535	1.80876910
C	-0.82948679	-4.88514642	2.22901358
C	0.57829346	-4.76630417	0.75493440
H	0.87313622	-4.03435265	-0.02278811
H	-0.03860530	-5.51785644	0.26043317
H	1.46723746	-5.23219913	1.18418867
H	-0.33259305	-5.82528190	2.47233963
H	-1.76544676	-5.07974156	1.70226832
H	-1.03573801	-4.37624316	3.19107997

P: $Pd(PH_3)_2$+ C_2H_6 -1688.89

Pd	0.02031695	-2.52480198	1.96738709
H	1.56518650	-0.20191873	3.74153899
H	-2.39458930	-0.66166249	1.00256823
P	-1.67423405	-1.04319883	2.16770896
H	-2.81766978	-1.42062926	2.92548554
H	-1.57761919	0.27231846	2.71146912
P	1.68516945	-1.44035091	3.04323853
H	2.38701138	-2.11793001	4.07789442
H	2.84276619	-1.06979555	2.30397087
C	1.37305133	-4.08373651	1.65599777
C	-1.30271708	-3.74139899	0.90641420
H	-1.07688281	-3.60996414	-0.15878806
H	-2.36259560	-3.50733985	1.06745082
H	-1.13597553	-4.78750521	1.17829400
H	1.24625538	-4.47668890	0.64311351
H	1.12787572	-4.87257536	2.37722479
H	2.42640396	-3.80700786	1.78983268

RC: $Pd(PH_3)_2CH_3Cl$ + $MgCH_3Cl$ -1890.91

H	0.04681000	-2.73421600	3.70857300
Pd	-0.57754500	-4.31546600	1.07736500
H	-2.32976000	-1.99809100	-0.55322000
H	-1.98297100	-2.37104700	3.17482000
C	0.24684000	-5.36985200	2.64977000
P	-1.61314800	-3.21363400	-0.70358000
H	-0.84098800	-2.81768300	-1.82315200
H	-2.61250000	-3.92761900	-1.40631600
P	-0.75874000	-2.71538200	2.54651000
H	-0.42894500	-1.41090300	2.09997900
H	1.28110000	-5.03763900	2.78330700
H	0.21757800	-6.40945500	2.31735200
H	-0.31008100	-5.25742700	3.58465600
Cl	-0.01831300	-6.06716700	-0.42618800
Mg	2.15530000	-5.32556600	-1.49363300
Cl	2.28070800	-6.38938900	-3.47054000
C	3.23133200	-3.82222700	-0.46968600
H	3.41953400	-4.03194200	0.59380100
H	2.77601700	-2.82151600	-0.51524300
H	4.22101800	-3.73180400	-0.94313200

TS: $Pd(PH_3)_2CH_3Cl$ + $MgCH_3Cl$ -1886.06 (-94.38)

H	0.22494600	-2.72581500	3.58882500
Pd	-0.29940700	-4.21042600	0.90140200
H	-1.44811900	-1.49780700	-0.54645500
H	-1.63823500	-3.76112400	3.67626000
C	0.64143600	-5.40866700	2.31212800
P	-1.43854200	-2.91355200	-0.64104700
H	-1.14590600	-2.99491200	-2.02329200
H	-2.84120200	-3.08501800	-0.74798300
P	-0.80877700	-3.13715500	2.71248300
H	-1.50101200	-1.89872400	2.65223000
H	1.69966500	-5.13483300	2.28155600
H	0.47008000	-6.41624800	1.92567500
H	0.28661300	-5.36953500	3.34784800
Cl	-0.62730100	-6.16752400	-0.66582700
Mg	1.52001900	-5.41478600	-1.34603700
Cl	2.68181300	-6.50607700	-2.91541600
C	2.12040400	-3.57954400	-0.39790800
H	3.11723200	-3.89191600	-0.04501700
H	1.75015600	-2.89321600	0.37379900
H	2.28830300	-2.95114000	-1.28798400

P: $Pd(PH_3)_2CH_3Cl$ + $MgCH_3Cl$ -1907.77

Pd	-0.06374500	0.94031200	0.16194700
C	-1.41350600	1.16880700	1.72486200
H	-0.78581900	-1.93248500	-1.27298700
Cl	3.26808000	-0.10425800	1.23700100
H	0.45638800	3.24660100	1.64372800
H	2.58971900	1.59018700	-1.63581400
Mg	1.70061100	1.20550500	2.21488100
Cl	1.46287500	1.97959000	4.29617300
C	0.66992100	2.84782800	0.64321800
H	1.71641900	3.05830600	0.38130100
P	1.43437000	0.77828800	-1.59361400
H	0.05531800	3.44073600	-0.04734800
H	2.04637800	-0.45741000	-1.90264200
P	-1.00623900	-1.10596000	-0.14036500
H	-2.41756000	-1.22571300	-0.10753400
H	-0.71470800	-2.08125700	0.84291900
H	0.95888900	1.07013200	-2.90212600
H	-1.74177600	0.23004400	2.18491100
H	-2.27416900	1.63527600	1.22667700
H	-1.07062900	1.83338200	2.52100700

RC: $^1Fe(CO)_4 + CH_4$ -2211.23

Fe	0.35780891	0.03825438	0.48752113
O	-1.43802173	-1.12505914	-1.45217119
C	-0.66267593	-0.72030439	-0.69282048
O	-0.42629797	2.40938870	1.94586288
O	1.31561351	1.80643037	-1.63395533
O	-1.02975892	-1.52409692	2.53166218
C	-0.45657654	-0.92268086	1.73313339
C	0.96585099	1.09867994	-0.79455246
C	-0.03387049	1.46193516	1.40712795
C	2.63288174	-0.90589212	1.00999077
H	3.49023136	-0.75012839	0.35348151
H	2.76932847	-1.78794449	1.63748323
H	2.49816316	-0.02749979	1.64450324
H	1.77347037	-1.16072056	0.32248459

TS: $^1Fe(CO)_4 + CH_4$ -2199.50 (-751.90)

Fe	0.34088938	0.01304017	0.46047141
O	-1.75076143	-0.80080398	-1.37625394
C	-0.92335517	-0.47287970	-0.64254083
O	-0.49825553	2.41831727	1.90230645
O	1.69917876	1.48348141	-1.65721901
O	-0.63146929	-1.83766027	2.49088409
C	-0.26352657	-1.09418265	1.69324896
C	1.14917883	0.91693750	-0.82001466
C	-0.16094089	1.47030656	1.33983353
C	2.30114584	-0.40453727	1.22610154
H	3.11113121	-0.34009600	0.49583177
H	2.39620583	-1.34546235	1.77286522
H	2.39720271	0.42297797	1.93088228
H	1.34784361	-1.05951162	0.16991896

P: $^1Fe(CO)_4 + CH_4$ -2208.92

Fe	0.29982211	-0.00309893	0.42404388
O	-2.07990493	-0.37020876	-1.20397145
C	-1.13897130	-0.22101296	-0.55807796
O	-0.56545804	2.40898995	1.83351285
O	2.02676697	1.02740617	-1.66830284
O	-0.22973443	-2.13374035	2.32203604
C	-0.05907275	-1.26273353	1.59062569
C	1.31518802	0.66254168	-0.84171635
C	-0.23953997	1.45977257	1.27227726
C	2.07286263	0.15490377	1.54879572
H	2.55967332	1.11154984	1.34507853
H	2.73999583	-0.66394612	1.27566563
H	1.84296859	0.10398148	2.61564658
H	0.91467813	-1.22524559	-0.19518736

RC: $^1Fe(CO)_4 + CH_3Cl$ -2181.41

Fe	-0.01936064	-0.15862999	-0.26387674
O	-0.05035324	-0.34955885	-3.14878138
C	-0.02973485	-0.20042048	-2.00013474
O	-0.28789361	-2.56497274	1.31632131
O	-2.93782201	-0.03451368	-0.35282162
O	2.85057573	-0.69917106	-0.37188667
C	1.72388824	-0.45826832	-0.31687186
C	-1.78551936	-0.05560673	-0.30540754
C	-0.17602063	-1.56121316	0.74657031
C	0.23109620	1.97471388	2.43450193
H	0.35118661	3.01126695	2.75725060
H	1.06653635	1.35913434	2.76977676
H	-0.72146230	1.56535314	2.77266635
Cl	0.22986139	1.98869686	0.64936339

TS: $^1Fe(CO)_4 + CH_3Cl$ -2146.98 (-495.43)

Fe	-0.01429889	-0.11269874	-0.13857699
O	-0.06852218	-0.49641017	-3.02548199
C	-0.03596406	-0.25567690	-1.89807899
O	-0.33404494	-2.82228609	0.79166232
O	-2.91481956	0.23119949	0.08394145
O	2.88603516	-0.46463908	0.07135333
C	1.74573416	-0.31735114	0.00222885
C	-1.77238968	0.10424892	0.00992306
C	-0.20459094	-1.72268538	0.45468050
C	0.14161184	1.15746084	2.12213979
H	-0.69828766	1.77643887	2.42327756
H	1.11104070	1.54760304	2.41749445
H	0.01015151	0.11363674	2.37992803
Cl	0.26296998	2.19488517	0.21572376

P: $^1Fe(CO)_4 + CH_3Cl$ -2187.36

Fe	0.33093818	-0.02881487	0.42087429
O	-2.07971223	-0.36596849	-1.20104467
C	-1.13011226	-0.24308374	-0.57146966
O	-0.55415038	2.34501538	1.79235124
O	1.95097857	1.38156260	-1.56368296
O	-0.38352240	-1.88404422	2.56541825
C	-0.13022520	-1.15219512	1.72318340
C	1.29477969	0.84115422	-0.79786029
C	-0.20994704	1.39624218	1.23977484
C	2.06989184	0.18331183	1.57217398
H	2.56501440	1.13675228	1.37234080
H	2.69916884	-0.65242942	1.26316322
H	1.84822299	0.12773522	2.64077392
Cl	1.18469389	-1.91172218	-0.58711381

RC: $^1Fe(CO)_4 + C_2H_6$ -2589.31

Fe	-0.04757578	0.12197323	0.39976386
O	-2.05325228	-0.66088348	-1.51528489
C	-1.18535077	-0.43464220	-0.78187352
O	-0.50757653	2.43697079	2.05278637
O	1.13340471	1.87593406	-1.62519506
O	-1.41089828	-1.51241064	2.40975412
C	-0.85371760	-0.88414754	1.62202266
C	0.68936189	1.17380734	-0.82802158
C	-0.22338940	1.49467208	1.44152169
C	4.12323181	-2.01965385	0.77444093
H	4.37797617	-2.91775412	0.19959108
H	4.77527639	-1.99747048	1.65551947
H	4.37806942	-1.15095074	0.15590036
C	2.65555387	-2.01310953	1.17107700
H	2.40526372	-1.11480739	1.74956176
H	2.40111484	-2.88039174	1.79176817
H	2.00501656	-2.04441900	0.28792820

TS: $^1Fe(CO)_4 + C_2H_6$ -2541.36 (-621.71)

Fe	-0.00983488	0.17516124	-0.08517160
O	0.03977797	-2.41684263	-1.37533315
C	0.01829803	-1.35001954	-0.92516537
O	0.04963446	-0.44037329	2.74791143
O	-2.93023373	0.06562753	-0.15108061
O	2.90979022	0.22306481	-0.22321677
C	1.75732761	0.21116134	-0.17200543
C	-1.77794365	0.11633342	-0.12703553
C	0.02439530	-0.13155813	1.63377413
C	-0.06802213	2.44617394	0.15844692
H	-0.93305138	2.39110789	0.81850167
H	-0.14124653	3.38285705	-0.39280861
H	0.85534800	2.47551268	0.73584725
C	-0.06928757	1.74877952	-1.70370198
H	0.80092663	2.35803051	-1.94793869
H	-0.99272043	2.27761731	-1.93855186
H	-0.03075773	0.85424487	-2.32574463

P: $^1Fe(CO)_4 + C_2H_6$ -2578.97

Fe	0.32945709	-0.05469896	0.40141263
O	-2.07842475	-0.38647333	-1.19443617
C	-1.12452707	-0.25479792	-0.56346469
O	-0.57921349	2.34363627	1.77100097
O	2.02402957	1.20595415	-1.59763694
O	-0.25456433	-1.99979697	2.48286431
C	-0.05513131	-1.21808069	1.66329281
C	1.32854932	0.72875454	-0.81588334
C	-0.22171034	1.39346745	1.22810678
C	2.09186231	0.13861601	1.53626919
H	2.57838291	1.09609337	1.33285040
H	2.76410824	-0.67845192	1.26900014
H	1.86838686	0.09567192	2.60540678
C	1.04552014	-1.78562933	-0.55873600
H	2.04297912	-2.00467554	-0.17386477
H	1.09431879	-1.63433301	-1.64021001
H	0.38366888	-2.63432263	-0.36763315

RC: $^3Fe(CO)_4 + CH_4$ -2209.92

Fe	-0.36045477	1.44503040	0.16561190
O	-3.17435394	0.64507153	-0.28145876
C	-2.06402726	0.91102334	-0.13247043
O	-0.58652907	4.18147068	-0.81257591
O	2.59203816	1.25639209	0.09505895
O	-0.62352327	2.18700225	2.97180180
C	-0.51794937	1.87568685	1.86598424
C	1.44091545	1.28204284	0.09760814
C	-0.49501590	3.09258423	-0.44267807
C	0.08789916	-2.02503152	-1.45483739
H	1.09851479	-2.42498358	-1.33572680
H	0.03270865	-1.44422535	-2.37938684
H	-0.62678416	-2.85125118	-1.50053478
H	-0.15228133	-1.38180499	-0.60419182

TS: $^3Fe(CO)_4 + CH_4$ -2145.49 (-489.73)

Fe	0.09287166	-0.24812821	-0.06899336
O	-2.62942112	-0.79307697	-1.28455203
C	-1.91994720	-0.71776795	-0.37157109
O	-0.52744035	2.51399774	-0.93888924
O	3.00176103	0.06150096	-0.40835124
O	0.11474714	0.40050811	2.76521106
C	0.08113471	0.10208173	1.64192049
C	1.86912714	-0.05348660	-0.23431332
C	-0.34185369	1.40834172	-0.68014349
C	0.32374573	-2.18734255	-0.71232717
H	1.28589253	-2.63674876	-0.45812314
H	0.28222911	-1.98112995	-1.79171821
H	-0.48699516	-2.86696593	-0.43884361
H	0.08642487	-1.23453928	1.11729754

P: $^3Fe(CO)_4 + CH_4$ -2164.77

Fe	0.53713843	-0.17975285	0.34830057
O	-2.11315200	0.15966216	-0.90648861
C	-1.06587002	-0.34682487	-0.64845705
O	-0.67984279	2.09690269	1.68883136
O	1.85470168	1.37033110	-1.78468262
O	-0.16380112	-2.15566814	2.43210369
C	0.10806910	-1.44473225	1.56702666
C	1.34687047	0.70277584	-0.99430482
C	-0.21052383	1.19252145	1.15308522
C	2.11558875	0.37391197	1.55797932
H	2.52266296	1.36170125	1.33335893
H	2.83618817	-0.40099241	1.26398976
H	1.89843995	0.29313169	2.62497843
H	-0.77273924	-1.32203771	-1.16249410

RC: $^3Fe(CO)_4$ +CH_3Cl -2172.42

Fe	-0.34069632	-1.67506325	-1.37061419
O	-0.47406155	-2.87492200	-4.02375744
C	-0.42144317	-2.38517732	-2.98054481
O	-0.63829501	-4.20028798	0.05399342
O	-3.16247606	-0.80021143	-1.19110892
O	2.60771639	-1.49123154	-1.19658068
C	1.45762776	-1.51070099	-1.24755242
C	-2.04988181	-1.09147154	-1.24570993
C	-0.52031123	-3.19276841	-0.49559636
C	-0.60104435	2.51967017	1.60368051
H	-1.47193556	2.82564098	2.18763196
H	0.31527905	2.71717560	2.16441144
H	-0.66868477	1.45759474	1.35493272
Cl	-0.56405741	3.45515372	0.10244891

TS: $^3Fe(CO)_4$ +CH_3Cl -2129.10 (-916.88)

Fe	-0.05221000	-0.23784249	-0.00622311
O	-0.14607620	-0.44530647	-2.91364074
C	-0.10720695	-0.34765992	-1.76725107
O	-0.46082747	-3.08660011	0.48799131
O	-2.95594626	0.30805302	0.03917483
O	2.88446525	-0.55418660	-0.09168333
C	1.75458150	-0.35642512	-0.00743569
C	-1.81453089	0.17052988	0.07233063
C	-0.29767048	-1.95444520	0.33843918
C	0.18794200	1.10724840	1.84668837
H	-0.64572735	1.66329919	2.26519501
H	1.16427197	1.39597302	2.22453683
H	0.03111061	0.01852790	2.02368846
Cl	0.34673782	2.44391468	0.13213788

P: $^3Fe(CO)_4$ +CH_3Cl -2142.99

Fe	-0.06045095	-0.33650518	0.25899106
O	-0.04300957	0.20371117	-2.45874560
C	0.04897961	0.67541623	-1.37204356
O	-0.48334251	-3.27620888	-0.01057861
O	-2.90223955	0.31461856	0.54804831
O	2.85913470	-0.51481196	0.41035723
C	1.71479310	-0.43893406	0.33025335
C	-1.78805708	0.06521306	0.41412643
C	-0.32165081	-2.14311884	0.07930987
C	0.08738189	0.35356021	2.17316838
H	0.22580141	1.43702679	2.08907176
H	0.94392087	-0.08725285	2.69046601
H	-0.82453783	0.14204165	2.73836349
Cl	0.30969799	2.45304879	-1.15536523

RC: $^3Fe(CO)_4$ + C_2H_6 -2589.38

Fe	-0.59072821	0.25245306	1.45241591
O	-3.36548156	0.79878767	2.35461986
C	-2.30123265	0.58644968	1.96058766
O	0.76496120	2.19334485	3.16564208
O	1.63347738	-0.19525209	-0.46218390
O	-0.06439036	-2.02463590	3.20853907
C	-0.28158435	-1.13616559	2.49999958
C	0.73748872	-0.01310671	0.24092336
C	0.22931159	1.43667713	2.47420375
C	-2.89789190	1.94557280	-2.18945346
H	-2.14871603	2.06650860	-1.39283177
H	-3.80576939	2.47993853	-1.87159775
H	-2.51222058	2.45684560	-3.08416333
C	-3.18417143	0.47822938	-2.46642581
H	-3.56770668	-0.03182338	-1.57021995
H	-2.27703234	-0.05536940	-2.78740173
H	-3.93580970	0.35637379	-3.26045371

TS: $^3Fe(CO)_4$ + C_2H_6 -2512.46 (-1317.7)

Fe	-0.04136211	-0.16090204	-0.22890819
O	-0.20957964	-0.87958140	-3.05326855
C	-0.14121423	-0.58592087	-1.93892560
O	-0.41525712	-2.88147552	0.75281234
O	-2.92757937	0.40142484	-0.02945085
O	2.89178524	-0.43996362	-0.15478421
C	1.75278531	-0.26193398	-0.14971060
C	-1.78552452	0.25021603	-0.07309207
C	-0.26652571	-1.80262801	0.37057845
C	0.17209802	0.89948577	2.50014276
H	0.31922761	1.85875619	2.99379841
H	1.00608708	0.20587278	2.58097933
H	-0.81796333	0.46537014	2.62056380
H	1.24077310	2.22449752	0.82079858
C	0.26646136	1.86015994	0.49050440
H	-0.55018281	2.48299791	0.85967168
H	0.25978308	1.98041451	-0.61757049

P: $^3Fe(CO)_4$ + C_2H_6 -2538.23

Fe	-0.53238367	-1.81860822	-1.26600307
O	-0.08612307	-0.69001082	-3.90662522
C	-0.26477948	-1.14495502	-2.86266356
O	-0.84282299	-4.59700849	-2.10279719
O	-3.39359593	-1.20976549	-1.12071905
O	2.29234496	-2.03467013	-0.52353996
C	1.17648430	-1.97478895	-0.79851145
C	-2.27438015	-1.47433683	-1.16157109
C	-0.72203363	-3.50135787	-1.76552450
C	-0.65621501	-3.93234701	2.96495923
H	-1.55006977	-3.38295202	2.69189497
H	0.16829784	-4.00900554	2.26527585
H	-0.58509244	-4.40259182	3.93921808
H	0.59632573	0.42459440	-0.34756403
C	-0.38369545	-0.04345257	-0.22439488
H	-0.52912288	-0.30407897	0.83106820
H	-1.14966928	0.67553990	-0.52606716

RC: $^1Fe(PH_3)_4$ + CH_3Cl -2158.16

P	-0.80375100	0.45387400	-2.21997000
P	-2.33868000	0.36057100	1.08215400
H	-1.45736400	-0.74994700	-2.64997500
P	0.52325200	0.12795800	0.37936100
H	1.48977600	-0.45742100	-0.49854700
H	0.47876100	0.01358900	-2.68250600
H	-3.09739600	3.63341600	-0.73791200
P	-2.80448700	2.28037800	-1.10973300
H	-2.98792700	2.50718800	-2.51091900
H	-4.13203500	1.80343500	-0.89183200
H	-1.12315300	1.14652800	-3.43358700
H	-2.64327800	0.86805700	2.39866200
H	-3.71698600	0.08321600	0.81272000
H	-2.05856100	-0.94730800	1.59096000
H	1.49968900	0.69998200	1.25915300
H	0.33534100	-1.05484100	1.15623700
C	-0.23667100	4.01191400	1.63766700
Cl	-0.01087700	3.22878900	0.02500500
H	0.33816000	4.94131700	1.63448900
H	0.13060300	3.32545200	2.40248900
H	-1.30151100	4.20923600	1.77282500

TS: $^1Fe(PH_3)_4$ + CH_3Cl -2132.67 (-453.36)

Fe	-0.19999100	0.51819900	0.31491100
P	-1.54918900	-0.97429200	0.80668200
P	0.92658500	-0.09182600	-1.34398700
H	-2.56311800	-1.43201700	-0.09313200
P	-1.61505800	1.40879700	-0.99317700
H	-2.25908200	0.61996000	-1.98667700
H	-2.47096900	-0.85709200	1.91266800
H	1.13422000	-0.35999900	3.03087600
P	1.25830600	-0.33379300	1.60101200
H	1.59463200	-1.71075400	1.47905200
H	2.59813100	0.15744500	1.61582400
H	-1.14473700	-2.29479300	1.18083000
H	1.96649200	0.68080400	-1.97546300
H	1.72497800	-1.27958700	-1.32648600
H	0.31841200	-0.42291500	-2.59647300
H	-2.81738500	2.04949600	-0.54093600
H	-1.23893700	2.47951700	-1.85871500
Cl	0.50056100	2.69078100	0.99338400
C	-1.02166600	2.09593000	2.28056000
H	-0.76272800	1.25000800	2.91186800
H	-1.99187100	1.99200600	1.80198900
H	-0.94022500	3.03799800	2.82003400

P: $^1Fe(PH_3)_4$ + CH_3Cl -2191.42

Fe	-0.59157902	0.25582855	0.45813640
P	0.83842754	-1.14415962	-0.09902335
P	-2.30397809	-0.80935438	-0.23311807
Cl	-2.11569916	1.88516911	1.11776584
P	-0.75972736	-0.36472944	2.48672131
H	0.09321656	-1.36232815	3.04549222
H	1.69637477	-1.73062237	0.87726443
H	-0.12881374	2.85991644	-1.05606240
P	-0.40424292	1.48676814	-1.26733223
H	0.60079006	1.25882890	-2.25383865
H	-1.48224116	1.65903498	-2.17877592
H	1.61436710	0.86413283	1.93993007
C	1.02692677	1.35403347	1.14924363
H	0.60605542	2.27608831	1.56564178
H	1.75813305	1.63593006	0.37709519
H	-0.55032894	0.61820700	3.48464782
H	-1.97577205	-0.88951974	3.00428730
H	0.51278586	-2.37348579	-0.75005351
H	1.88528162	-0.78715939	-0.99899407
H	-3.17038514	-0.24073174	-1.20938267
H	-2.20403945	-2.08625409	-0.86490849
H	-3.34520472	-1.18160906	0.66387136

RC: $^{1}Fe(PH_3)_4CH_3Cl + MgClCH_3$ -2769.08

Fe	0.22311800	-2.16102900	-0.87487900
P	1.46079000	-3.82768700	-0.90393800
P	-1.24953700	-2.91655300	-2.23418200
Cl	-1.08636300	-0.17112800	-0.82471400
P	-0.79084200	-2.81495600	0.90379600
H	-0.17840100	-3.78750800	1.73872800
H	1.79162100	-4.48957800	0.31188200
H	1.79676600	0.20212000	-2.02970700
P	1.36255100	-1.10860400	-2.34846900
H	2.62032400	-1.60803800	-2.78824700
H	0.84567200	-0.81373200	-3.64039400
H	1.71068900	-1.96127600	1.40117200
C	1.62588900	-1.41343600	0.45186000
H	1.30835400	-0.39389500	0.69418300
H	2.65107000	-1.35275900	0.05753800
H	-1.06486200	-1.83424400	1.88933800
H	-2.07821800	-3.41963900	0.86580300
H	1.13999200	-5.00927000	-1.63761900
H	2.79880400	-3.71637600	-1.37898800
H	-1.51652800	-2.27215100	-3.47539300
H	-1.14429500	-4.22970000	-2.77859100
H	-2.61462000	-3.03447800	-1.84802500
H	-2.25047700	4.19131300	0.71899300
Mg	-1.71611600	1.54332000	0.91665100
Cl	-1.86202500	0.56030300	2.95480700
C	-1.97663900	3.41098600	-0.00547000
H	-1.06601500	3.75723000	-0.51600100
H	-2.76879600	3.39512400	-0.76809100

TS: $^{1}Fe(PH_3)_4CH_3Cl + MgClCH_3$ -2747.17 (-76.54)

Fe	0.64818700	-2.15582100	-0.93225400
P	1.66597700	-3.67093800	-1.87797000
P	-1.17887300	-2.24085200	-2.09376800
Cl	-2.30671500	-1.23342100	0.93769500
P	-0.10920800	-3.47677000	0.61018100
H	0.64486400	-4.66679100	0.81372600
H	1.80255500	-4.94820000	-1.26516600
H	2.51287800	0.20967400	-1.78059800
P	1.54273100	-0.70074000	-2.26970200
H	2.32199800	-1.19807300	-3.35498700
H	0.78305400	0.21188300	-3.04409000
H	2.45483800	-2.73592500	0.99918400
C	2.22251800	-1.92195600	0.29887600
H	1.88192700	-1.05959000	0.89493000
H	3.17239400	-1.63749700	-0.17280100
H	-0.10104600	-3.02333700	1.94812600
H	-1.39317100	-4.06981100	0.57513000
H	1.27171100	-4.14515400	-3.16421900
H	3.04220900	-3.49112400	-2.19130600
H	-1.93931400	-1.07281100	-2.35697500
H	-1.08887500	-2.66779400	-3.45167600
H	-2.26715900	-3.07791500	-1.73946200
H	0.70642300	1.81567000	0.45904300
Mg	-1.94084900	1.11175700	1.11875400
Cl	-3.32675300	2.44224400	2.28971800
C	-0.18598200	1.44055500	-0.06078000
H	0.02615300	0.40163000	-0.38796500
H	-0.31758700	2.05758200	-0.96093300

P: $^{1}Fe(PH_3)_4CH_3Cl + MgClCH_3$ -2779.67

Fe	0.14317700	0.33831600	0.36281800
P	0.20185000	-1.76178400	0.49668600
P	2.24617600	0.58436500	0.27804800
Cl	-0.53977300	5.64742100	2.16217200
P	-0.21781900	0.35309800	-1.72378800
H	-0.64669200	-0.82388500	-2.39906300
H	-0.39733100	-2.57586600	-0.50930200
H	-1.04886700	1.53221000	2.91771300
P	-0.07012200	0.61523000	2.45191300
H	-0.45183300	-0.46622800	3.29451200
H	0.98753400	1.08779600	3.28297300
H	-2.34994300	-0.50782100	-0.36391200
C	-1.92819300	0.09806200	0.45250300
H	-2.42113000	1.07730300	0.40304500
H	-2.28742400	-0.38862700	1.37204000
H	-1.23419400	1.20479800	-2.23088900
H	0.77714600	0.72134300	-2.67609000
H	1.42182900	-2.50066200	0.55652500
H	-0.41647500	-2.43751100	1.58970400
H	2.93238500	1.42165100	1.20825000
H	3.14954300	-0.51195500	0.40962000
H	2.88910000	1.13682200	-0.87037400
C	0.00242200	2.43113000	0.23343500
H	0.50734700	2.91424300	1.08552200
H	-1.08146300	2.63687900	0.26609500
H	0.43516700	2.80124300	-0.70962900
Mg	-0.41049000	4.84484300	0.09438300
Cl	-0.43457200	5.41420800	-2.05400200

RC: $^{1}Fe(PH_3)_4 + C_2H_6$ -2569.22

Fe	-0.22673700	0.30274100	0.28184800
P	-1.33735100	-1.44900000	0.63656700
P	0.87892500	-0.46395000	-1.33607000
C	0.85196400	2.06306700	-0.02781000
P	-1.67780600	1.31826800	-0.84341100
H	-3.03574300	0.88401900	-0.91144400
H	-2.76401000	-1.45320100	0.56068800
H	1.53139800	1.07106300	2.64424000
P	1.22669600	-0.00301200	1.76444200
H	1.08318000	-0.98921200	2.78605500
H	2.58254300	-0.32213100	1.45292300
H	-2.38582700	1.13237700	1.73313000
C	-1.29517800	1.11099100	1.88287700
H	-0.97302000	2.14696100	2.04755500
H	-1.15643000	0.57511600	2.83469500
H	-1.97524300	2.66642100	-0.50507200
H	-1.53562200	1.54995300	-2.24459500
H	-1.17681300	-2.64781200	-0.12482300
H	-1.29533200	-2.10902100	1.90298200
H	2.30628700	-0.51450400	-1.30059600
H	0.72757800	-1.79678000	-1.82943100
H	0.82564700	0.14511500	-2.62730500
H	1.94211100	1.94918200	0.07718100
H	0.53544900	2.81549100	0.70551700
H	0.71455600	2.50774000	-1.02570900

TS: $^{1}Fe(PH_3)_4 + C_2H_6$ -2522.4 (-675.54)

Fe	-0.31137500	0.43737000	0.27140400
P	-1.52387700	-1.03885900	1.11043800
P	0.80802100	-0.50465800	-1.22067400
H	-1.22659600	3.27307700	1.52112500
P	-1.78024600	0.87070100	-1.19244500
H	-2.22609800	-0.14806000	-2.07905800
H	-1.00721400	-2.18636600	1.79346400
H	1.16292100	0.36960100	3.02145600
P	1.23179000	-0.02969600	1.64718800
H	1.57169300	-1.38669500	1.90422500
H	2.58581400	0.41597600	1.47911900
H	-1.99034000	1.72518900	1.42536400
C	0.35265200	2.58839500	0.32412800
H	1.11183700	2.08693000	-0.28759200
C	-1.00860100	2.19964000	1.52584900
H	-3.09157400	1.33978600	-0.84266600
H	-1.58649500	1.86184200	-2.20790300
H	-2.51494300	-0.78285000	2.13060900
H	-2.43644400	-1.81848600	0.32978700
H	0.20687400	-1.13574100	-2.35663400
H	1.82657700	0.13307800	-2.02734800
H	1.65248400	-1.62612200	-0.93937900
H	0.90749200	3.13153500	1.09507500
H	-0.59327700	1.96585700	2.50782500
H	-0.15468700	3.31234700	-0.31572700

P: $^{1}Fe(PH_3)_4$ -2779.67

Fe	-0.14723100	0.33717600	0.27365000
P	-1.62410600	-0.92102100	0.98472200
P	1.09114200	0.13744700	-1.37373300
H	-1.85757900	-2.15943800	0.29884100
P	-1.55659700	1.49536800	-0.78076900
H	-2.97372100	1.33644600	-0.66771600
H	-3.01840300	-0.58808600	1.04442100
H	1.92169900	0.46503800	2.43841000
P	1.27258900	-0.49179200	1.59097100
H	0.95811300	-1.41593900	2.63684700
H	2.47293000	-1.16044800	1.19873600
H	-1.61640900	-1.54152600	2.27921200
H	2.10476800	1.07171900	-1.80596700
H	1.97717400	-0.97670900	-1.49676300
H	0.54845500	0.02133400	-2.69019000
H	-1.54253900	2.89053900	-0.45185900
H	-1.57153100	1.69212800	-2.19621600

RC: $Fe^{-II}(CO)_4 + CH_4$ -2215.96

Fe	0.04042068	-0.07953660	0.37040726
O	2.37030492	-1.33120920	-0.88240770
C	1.41436381	-0.81835428	-0.36870604
O	0.13855524	-0.56349707	3.25349800
O	-2.43317279	-1.22958468	-0.69200069
O	0.09008608	2.81045283	-0.08364265
C	0.06926760	1.62398981	0.09514918
C	-1.41770164	-0.75702815	-0.26092077
C	0.09695582	-0.36713753	2.07044411
C	-0.33665626	0.65816461	-4.41288564
H	0.22743267	-0.11469563	-4.94613322
H	0.08059650	1.64353315	-4.64780814
H	-1.38655628	0.62349983	-4.72112994
H	-0.26569813	0.47793505	-3.33480499

TS: $Fe^{-II}(CO)_4 + CH_4$ -2139.72 (-706.37)

Fe	-0.41896107	-0.05366525	-0.27208325
O	3.42770515	0.00534708	0.15242348
C	2.69430736	-0.20745744	-0.72903278
O	0.33264914	-1.85234246	1.91943673
O	-3.28757926	0.24640986	0.09796473
O	0.58058624	2.61177397	0.34381717
C	0.22616011	1.49964068	0.07392336
C	-2.11519753	0.09061470	-0.12596591
C	0.05394322	-1.14074240	0.99646090
C	-0.14353484	-1.21236011	-2.06707934
H	-0.39535932	-2.20503997	-1.66542393
H	0.89784314	-1.24492364	-2.42567600
H	-0.79969914	-1.05527350	-2.93940496
H	-0.22820453	0.26771951	-1.74033853

P: $Fe^{-II}(CO)_4 + CH_4$ -2147.21

Fe	-0.41460779	-0.00117577	-0.30304795
O	3.58658255	-0.08127604	0.14206203
C	2.88534152	-0.48661978	-0.68956496
O	0.40068555	-1.76910153	1.85472799
O	-3.28854077	0.09075564	0.07422721
O	0.41252570	2.69910704	0.44248609
C	0.09480343	1.57586001	0.12757707
C	-2.11144084	0.05658435	-0.15991349
C	0.14118800	-1.07661157	0.91101207
C	-0.37216638	-1.25934774	-1.95872124
H	-0.89489995	-2.21217186	-1.76379176
H	0.66751865	-1.50444408	-2.23595467
H	-0.85618324	-0.80694594	-2.84358237
H	0.32591873	1.12830829	-1.18410179

RC(S_N2): $Fe^{-II}(CO)_4 + CH_4$ -2215.98

Fe	0.02909300	-0.06980300	0.35290900
O	2.32309900	-1.35374200	-0.93980700
C	1.38269900	-0.82254200	-0.41766900
O	0.18714800	-0.57491400	3.22978300
O	-2.47324900	-1.24676800	-0.61124800
O	0.05095800	2.82676300	-0.08719000
C	0.04359100	1.63947900	0.08428300
C	-1.44653100	-0.75999200	-0.22666500
C	0.12567700	-0.36537800	2.05061400
C	-0.17640800	0.65121900	-4.31380500
H	0.63462500	0.09617200	-4.79661500
H	-0.05976500	1.72032500	-4.52007200
H	-1.13867800	0.30685500	-4.70701000
H	-0.14070000	0.48184500	-3.23213800

TS(S_N2): $Fe^{-II}(CO)_4 + CH_4$ -2150.98 (-577.92)

Fe	-0.11798500	0.23002300	-1.62465600
O	2.33858800	-1.18957500	-2.33510500
C	1.33617300	-0.60342200	-2.09661100
O	-0.00193300	-0.25201200	1.23061200
O	-2.68210100	-1.08888900	-2.11533400
O	-0.04819100	3.15151200	-1.50321700
C	-0.07875700	1.97068600	-1.60337800
C	-1.64048100	-0.54333000	-1.96503300
C	-0.04923000	-0.05470900	0.06122000
C	-0.23482000	0.65691000	-4.15714600
H	-0.27702600	-0.36288900	-4.50929900
H	-0.33532300	1.01859700	-6.29818600
H	-1.14660700	1.23366200	-4.19953900
H	0.69481100	1.18929100	-4.29175300

P(S_N2): $Fe^{-II}(CO)_4 + CH_4$ -2157.9

Fe	-0.09130800	0.21024500	-1.48933300
O	2.37809100	-1.24140700	-2.05085900
C	1.37981100	-0.64931000	-1.85161800
O	-0.08033900	-0.30786900	1.36415800
O	-2.64939000	-1.09845200	-2.00357000
O	-0.01034900	3.11759800	-1.24171000
C	-0.04260100	1.94733600	-1.36978800
C	-1.61535000	-0.56417400	-1.82394000
C	-0.08474500	-0.09768400	0.20250300
C	-0.09790900	0.61015800	-3.66150600
H	-0.12987000	-0.33627100	-4.19897200
H	-0.10953200	1.15583900	-6.61153300
H	-0.97371600	1.20602700	-3.91348200
H	0.80653300	1.15450600	-3.92841000

RC(S_N2): $Fe^{-II}(CO)_4 + CH_3Cl$ -2188.28

Fe	-0.10969400	0.17719700	-1.30864600
O	2.22571900	-1.17021900	-2.45511400
C	1.26653100	-0.61002800	-2.00732800
O	0.03659900	-0.29212400	1.56681000
O	-2.63427000	-1.03935200	-2.16077200
O	-0.06591800	3.08695500	-1.65187400
C	-0.08323100	1.89519000	-1.53420900
C	-1.59873400	-0.53325400	-1.83586500
C	-0.02137000	-0.09789800	0.38818200
C	-0.26217100	0.82895500	-5.16028800
H	0.63236600	0.24330400	-4.95901900
Cl	-0.33268000	1.15013000	-6.97347700
H	-1.15882100	0.27864900	-4.88260200
H	-0.22178000	1.78957400	-4.65113200

TS(S_N2): $Fe^{-II}(CO)_4 + CH_3Cl$ -2186.46 (-247.24)

Fe	-0.10841300	0.20201700	-1.46635300
O	2.32388200	-1.19373500	-2.30689500
C	1.32744600	-0.61399300	-2.01292400
O	-0.00286700	-0.27188800	1.39307300
O	-2.66006300	-1.09012800	-2.09019100
O	-0.04965700	3.12899400	-1.49929500
C	-0.07508200	1.94009800	-1.53512400
C	-1.61857700	-0.55308400	-1.88472300
C	-0.04492700	-0.07723700	0.22003800
C	-0.25101000	0.71934100	-4.49599000
H	-0.26930300	-0.36075700	-4.50258100
Cl	-0.35363700	1.08526300	-6.65014700
H	-1.15192300	1.23138900	-4.19075800
H	0.69238800	1.20068400	-4.28277000

P(S_N2): $Fe^{-II}(CO)_4 + CH_3Cl$ -2205.75

Fe	0.03474500	-0.60306800	1.53756300
O	2.49520900	-2.05818400	0.95524400
C	1.50062100	-1.46711400	1.17244900
O	0.05594300	-1.07007600	4.40121000
O	-2.52250200	-1.90790900	1.01977200
O	0.12171200	2.30868300	1.69197000
C	0.08696000	1.13472600	1.61184400
C	-1.48903200	-1.37764100	1.21095800
C	0.04764600	-0.88086600	3.23627800
C	0.01639200	-0.24133800	-0.63738900
Cl	-0.01108200	0.24866100	-3.59718200
H	0.92247800	0.29463700	-0.90338000
H	-0.86107800	0.35066100	-0.87941400
H	-0.02061400	-1.20127300	-1.14352800

RC(S_N2): $Fe^{-II}(CO)_4 + C_2H_6$ -2596.31

Fe	-0.01239400	-0.06893600	0.32298200
O	2.24975400	-1.22773800	-1.13183500
C	1.32107200	-0.75388200	-0.53793600
O	0.37451700	-0.49982400	3.19152100
O	-2.51044600	-1.37169900	-0.47805200
O	-0.14384800	2.81320800	-0.17848400
C	-0.09261700	1.63138500	0.02303200
C	-1.48699900	-0.83526000	-0.15627200
C	0.21683700	-0.32436900	2.01589400
C	-0.33065100	0.81213300	-4.25873200
H	-0.18928700	-0.05446700	-4.91906000
C	0.81691600	1.80056000	-4.38266400
H	-1.29101100	1.27669800	-4.52044500
H	-0.40864300	0.44286900	-3.22945200
H	1.76655100	1.32675400	-4.10786900
H	0.67683300	2.64256700	-3.69557400
H	0.91853300	2.20194500	-5.40272800

TS(S_N2): $Fe^{-II}(CO)_4 + C_2H_6$ -2532.42 (-313.36)

Fe	-0.11344800	0.21830000	-1.56415800
O	2.35169200	-1.18082300	-2.28601800
C	1.34582000	-0.60380400	-2.03837100
O	-0.00605100	-0.25308000	1.29388100
O	-2.66419500	-1.11494500	-2.08518600
O	-0.06230600	3.14148900	-1.47723900
C	-0.08527800	1.95875600	-1.55812400
C	-1.62751300	-0.56445400	-1.91762900
C	-0.04950900	-0.06050600	0.12351600
C	-0.23147400	0.64408000	-4.10165600
H	-0.26694400	-0.37742500	-4.44884100
C	-0.37190700	1.09111800	-6.74210800
H	-1.14691900	1.21465100	-4.14037800
H	0.69552500	1.18161400	-4.23247400
H	0.48448100	0.60346000	-7.23889000
H	-0.34412800	2.18046900	-6.91688900
H	-1.32041800	0.66944200	-7.11693000

P(S_N2): $Fe^{-II}(CO)_4 + C_2H_6$ -2534.49

Fe	-0.11396900	0.21695500	-1.54842000
O	2.35939600	-1.19727000	-2.19629500
C	1.35497000	-0.61810700	-1.97144000
O	0.00102100	-0.25943200	1.30928800
O	-2.66759200	-1.13349600	-1.98639700
O	-0.06186300	3.13290300	-1.37060300
C	-0.08475600	1.95718600	-1.48004100
C	-1.63431000	-0.57964600	-1.84445900
C	-0.04551800	-0.06565300	0.14307200
C	-0.21766200	0.59830600	-3.82175300
H	-0.25525400	-0.37205500	-4.30792500
C	-0.39120700	1.08870500	-6.77640000
H	-1.11743100	1.17652100	-4.00964700
H	0.67768100	1.14923700	-4.09451800
H	0.44117700	0.61776700	-7.34144000
H	-0.38692900	2.17502600	-7.00803100
H	-1.34350300	0.66430700	-7.15874400

CH_4 -554.09

C	0.00000000	0.00000000	0.00000000
H	0.63276400	-0.63276400	0.63276400
H	-0.63276400	-0.63276400	-0.63276400
H	-0.63276400	0.63276400	0.63276400
H	0.63276400	0.63276400	-0.63276400

CH_3Cl -516.57

C	0.00000000	0.00000000	-2.00508000
Cl	0.00000000	0.00000000	-0.23687800
H	-0.51699900	-0.89546800	-2.35691600
H	-0.51699900	0.89546800	-2.35691600
H	1.03399700	0.00000000	-2.35691600

C_2H_6 -933.49

C	0.00000000	0.00000000	-0.76004500
C	0.00000000	0.00000000	0.76004500
H	-0.00001600	-1.02019200	-1.16239400
H	-0.88350400	0.51011000	-1.16239400
H	0.88352000	0.51008200	-1.16239400
H	0.88352000	-0.51008200	1.16239400
H	-0.88350400	-0.51011000	1.16239400
H	-0.00001600	1.02019200	1.16239400

$Pd(CO)_2$ -775.51

Pd	0.00000000	0.00000000	-0.99564909
C	1.81458968	0.00000000	-0.41703934
C	-1.81458968	0.00000000	-0.41703934
O	2.84077579	0.00000000	0.09746426
O	-2.84077579	0.00000000	0.09746426

$Pd(PH_3)_2$ -785.19

Pd	0.00000000	0.00000000	0.00000000
H	0.66596013	1.01127603	2.98138684
H	0.66596013	-1.01127603	-2.98138684
P	0.00000000	0.00000000	-2.23097113
H	-1.20877080	-0.07110037	-2.98138684
H	0.54281067	1.08237640	-2.98138684
P	0.00000000	0.00000000	2.23097113
H	-1.20877080	0.07110037	2.98138684
H	0.54281067	-1.08237640	2.98138684

$^1Fe(CO)_4$ -1655.71

Fe	0.00000000	0.00000000	0.00266480
O	-2.92700731	0.00000000	0.08271546
C	-1.77694389	0.00000000	0.02975038
O	0.00000000	2.48259819	1.46467953
O	2.92700731	0.00000000	0.08271546
O	0.00000000	-2.48259819	1.46467953
C	0.00000000	-1.54757822	0.78082679
C	1.77694389	0.00000000	0.02975038
C	0.00000000	1.54757822	0.78082679

$^{3}Fe(CO)_4$ -1655.73

Fe	0.00000000	0.00000000	0.03357252
O	-2.90411507	0.00000000	-0.53617704
C	-1.76533556	0.00000000	-0.36612355
O	0.00000000	2.14900907	2.00272278
O	2.90411507	0.00000000	-0.53617704
O	0.00000000	-2.14900907	2.00272278
C	0.00000000	-1.30861404	1.21243264
C	1.76533556	0.00000000	-0.36612355
C	0.00000000	1.30861404	1.21243264

$Fe^{-II}(CO)_4$ -1659.49

Fe	0.00000000	0.00000000	0.41153541
O	-2.38251414	0.00000000	-1.28917807
C	-1.40641172	0.00000000	-0.59007386
O	0.00000000	2.38249942	2.11227250
O	2.38251414	0.00000000	-1.28917807
O	0.00000000	-2.38249942	2.11227250
C	0.00000000	-1.40640662	1.41315507
C	1.40641172	0.00000000	-0.59007386
C	0.00000000	1.40640662	1.41315507

$Fe(PH_3)_4$ -1636.72

Fe	-0.14723100	0.33717600	0.27365000
P	-1.62410600	-0.92102100	0.98472200
P	1.09114200	0.13744700	-1.37373300
H	-1.85757900	-2.15943800	0.29884100
P	-1.55659700	1.49536800	-0.78076900
H	-2.97372100	1.33644600	-0.66771600
H	-3.01840300	-0.58808600	1.04442100
H	1.92169900	0.46503800	2.43841000
P	1.27258900	-0.49179200	1.59097100
H	0.95811300	-1.41593900	2.63684700
H	2.47293000	-1.16044800	1.19873600
H	-1.61640900	-1.54152600	2.27921200
H	2.10476800	1.07171900	-1.80596700
H	1.97717400	-0.97670900	-1.49676300
H	0.54845500	0.02133400	-2.69019000
H	-1.54253900	2.89053900	-0.45185900
H	-1.57153100	1.69212800	-2.19621600

$MgClCH_3$ -566.84

C	0.00000000	0.00000000	1.59904100
H	0.50919900	0.88195900	1.18772500
H	-1.01839800	0.00000000	1.18772500
H	0.50919900	-0.88195900	1.18772500
Mg	0.00000000	0.00000000	3.67342100
Cl	0.00000000	0.00000000	5.87635300

$MgCl_2$ -201.89

Cl	-2.17781600	0.00000000	-5.36323700
Mg	0.00000000	0.00000000	-5.35707500
Cl	2.17781600	0.00000000	-5.36323700