Design of Transition Metal Complexes containing a P-E radical motif

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Supporting Information

Table S1. TPSS-D3/def2-TZVP + COSMO computed imaginary frequency (ImF), zero-point energies (ZPE), gas-phase enthalpic (Hc) and Gibbs free-energy (Gc) corrections; the COSMO-RS computed solvation enthalpic (Hsol) and Gibbs free-energy (Gsol) corrections in THF solution; TPSS-D3/def2-QZVP and PW6B95-D3/def2-QZVP single-point energies (TPSS-D3 and PW6B95-D3); the total PW6B95-D3 free energies G_P; the relative electronic energies (ΔE_T and ΔE_P) and Gibbs free-energies (ΔG_T and ΔG_P) at the TPSS-D3 and PW6B95-D3 levels.

Reactions in THF solution	Im cm^{-1}	ZPE kcal /mol	Hc kcal /mol	Gc kcal /mol	Hsol kcal /mol	Gsol kcal /mol	TPSS-D3 E_h	PW6B95-D3 E_h	G_P E_h	ΔE_T kcal /mol	ΔE_P kcal /mol	*ΔG_P kcal /mol*	ΔG_T kcal /mol
Oxidation potentials increase in the order: $TO^\bullet$ < Ph_3C^+ < TO^+ < $Ar_3N^{\bullet+}$ < NO^+ in THF solution (T = TEMP, Ar = *p*-C_6H_4Br)													
TO^-	0	160.512	168.399	138.591	-59.320	-54.280	-484.05326	-484.55442	-484.41705	0.00	0.00	*0.00*	0.00
$TO^\bullet$	0	162.359	170.357	140.227	-11.745	-8.190	-484.04614	-484.54639	-484.33296	4.47	5.04	*52.76*	52.20
$Ph_3C^\bullet$	0	173.175	182.680	148.778	-19.946	-14.265	-733.52607	-734.33363	-734.11626	0.00	0.00	*0.00*	0.00
Ph_3C^+	0	173.379	183.155	149.119	-54.424	-45.749	-733.31208	-734.11522	-733.94748	134.28	137.05	*105.91*	103.14
$TO^\bullet$	0	162.359	170.357	140.227	-11.745	-8.190	-484.04614	-484.54639	-484.33296	0.00	0.00	*0.00*	0.00
TO^+	0	162.717	170.852	140.436	-54.773	-47.381	-483.80092	-484.29361	-484.14231	153.88	158.62	*119.64*	114.90
Ar_3N	0	152.720	165.632	123.288	-28.878	-20.031	-8470.75507	-8475.24141	-8475.07385	0.00	0.00	*0.00*	0.00
$Ar_3N^{\bullet+}$	0	154.621	167.045	125.901	-68.658	-53.100	-8470.51268	-8474.98883	-8474.86980	152.10	158.50	*128.04*	121.64
$NO^\bullet$	0	2.719	4.793	-9.417	-1.411	0.521	-129.97359	-130.09903	-130.11019	0.00	0.00	*0.00*	0.00
NO^+	0	3.448	5.521	-8.590	-90.282	-77.401	-129.62405	-129.74954	-129.88356	219.34	219.31	*142.21*	142.25
*$Fe(CO)_4PPh_2O^\bullet$ (**1a$^\bullet$**) radical complex formation and P-to-O 1,2-Fe-shift* (T = TEMP)													
1aT	0	297.612	319.903	260.484	-25.777	-18.800	-3006.69024	-3009.00205	-3008.61389	-20.65	-18.31	*0.37*	-1.96
1a$^\bullet$ + T$^\bullet$	0	296.173	318.388	243.798	-32.205	-22.691	-3006.65733	-3008.97287	-3008.61449	0.00	0.00	*0.00*	0.00
1a$^\bullet$	0	136.532	151.486	105.485	-21.478	-15.385	-2597.87546	-2599.76296	-2599.61636	0.00	0.00	*0.00*	0.00
1ae_ts	0	136.119	151.125	104.942	-20.955	-14.759	-2597.84441	-2599.73531	-2599.58858	19.49	17.35	*17.43*	19.57
1ae$^\bullet$	0	136.357	151.173	105.646	-20.385	-14.407	-2597.84439	-2599.73788	-2599.58947	19.50	15.74	*16.88*	20.63
1a$^-$	0	136.244	151.049	105.181	-58.379	-51.549	-2597.98965	-2599.86677	-2599.77829	-71.66	-65.14	*-101.61*	-108.13
*$Fe(CO)_4PPh_2S^\bullet$ (**1b$^\bullet$**) radical complex formation and P-to-S 1,2-Fe-shift*													
1bT	0	296.174	318.874	258.645	-27.013	-19.668	-3329.70390	-3332.23852	-3331.85467	-41.73	-38.31	*-20.70*	-24.12
1b$^\bullet$ + T$^\bullet$	0	295.059	317.597	242.193	-32.670	-22.718	-3329.63739	-3332.17746	-3331.82169	0.00	0.00	*0.00*	0.00
1b$^\bullet$	0	135.418	150.695	103.880	-21.943	-15.412	-2920.85552	-2922.96756	-2922.82356	0.00	0.00	*0.00*	0.00

1be_ts	0	135.167	150.471	103.644	-21.287	-14.895	-2920.83815	-2922.95451	-2922.81006	10.90	8.19	*8.47*	11.18
1be•	0	135.563	150.701	104.395	-21.191	-14.911	-2920.83758	-2922.95654	-2922.81093	11.26	6.91	*7.93*	12.27
1b⁻	0	135.190	150.265	103.880	-58.709	-51.401	-2920.96327	-2923.06767	-2922.98103	-67.62	-62.82	*-98.81*	-103.60
*$Fe(CO)_4PPh_2NMe^•$ (**1c•**) radical complex formation and P-to-N 1,2-Fe-shift*													
1cT	0	323.403	346.362	285.969	-26.959	-19.806	-3026.14163	-3028.47683	-3028.04967	-40.97	-46.73	*-26.79*	-21.03
1c• + T•	0	320.328	343.723	266.847	-32.143	-22.514	-3026.07634	-3028.40237	-3028.00698	0.00	0.00	*0.00*	0.00
1c•	0	160.687	176.821	128.534	-21.416	-15.208	-2617.29446	-2619.19246	-2619.00885	0.00	0.00	*0.00*	0.00
1ce_ts	0	160.708	176.799	128.616	-20.331	-14.309	-2617.27675	-2619.18777	-2619.00260	11.11	2.94	*3.92*	12.10
1ce•	0	160.827	176.870	128.798	-20.276	-14.275	-2617.27704	-2619.18863	-2619.00312	10.93	2.40	*3.60*	12.13
1c⁻	0	160.162	176.206	128.019	-57.235	-50.211	-2617.39701	-2619.29405	-2619.16704	-64.35	-63.75	*-99.26*	-99.87
*$Fe(CO)_4PPh_2PMe^•$ (**1d•**) radical complex formation and P-to-P 1,2-Fe-shift*													
1dT	0	319.877	343.726	281.467	-28.063	-20.636	-3312.81305	-3315.35777	-3314.93910	-60.94	-64.19	*-46.05*	-42.79
1d• + T•	0	318.148	342.056	264.056	-33.318	-23.260	-3312.71594	-3315.25547	-3314.86572	0.00	0.00	*0.00*	0.00
1d•	0	158.507	175.154	125.743	-22.591	-15.954	-2903.93407	-2906.04557	-2905.86760	0.00	0.00	*0.00*	0.00
1de_ts	0	158.965	175.351	126.579	-22.091	-15.525	-2903.91962	-2906.04022	-2905.86023	9.07	3.35	*4.62*	10.33
1de•	0	158.689	175.174	126.213	-21.229	-14.965	-2903.93097	-2906.04771	-2905.86742	1.94	-1.35	*0.11*	3.40
1d⁻	0	157.922	174.449	125.317	-58.331	-50.826	-2904.02097	-2906.13099	-2906.00927	-54.53	-53.60	*-88.90*	-89.83
*$Fe(CO)_4P(NMeCH_2CH_2NMe)O^•$ (**2a•**) radical complex formation and P-to-O 1,2-Fe-shift*													
2aT	0	275.605	296.108	240.102	-21.005	-15.301	-2811.22510	-2813.30017	-2812.93892	-22.33	-18.73	*-0.25*	-3.84
2a• + T•	0	273.993	294.478	223.605	-27.205	-19.179	-2811.18952	-2813.27032	-2812.93853	0.00	0.00	*0.00*	0.00
2a•	0	114.352	127.576	85.292	-16.478	-11.873	-2402.40765	-2404.06041	-2403.94040	0.00	0.00	*0.00*	0.00
2ae_ts	70i	114.771	127.218	86.552	-17.736	-12.699	-2402.38058	-2404.03067	-2403.90997	16.99	18.66	*19.10*	17.42
2ae•	0	113.984	126.928	85.445	-15.292	-10.600	-2402.38271	-2404.03770	-2403.91542	15.65	14.25	*15.68*	17.07
2aec• (CO in ring)	0	114.739	127.719	85.786	-18.844	-13.642	-2402.38171	-2404.03771	-2403.91973	16.28	14.25	*12.97*	15.00
2a⁻	0	113.872	126.884	84.928	-54.202	-48.836	-2402.51540	-2404.15938	-2404.09885	-67.62	-62.10	*-99.43*	-104.94
*$Fe(CO)_4P(NMeCH_2CH_2NMe)S^•$ (**2b•**) radical complex formation and P-to-S 1,2-Fe-shift*													
2bT	0	273.986	295.012	237.824	-22.312	-16.319	-3134.23031	-3136.52964	-3136.17364	-47.46	-42.97	*-25.39*	-29.88
2b• + T•	0	272.641	293.490	221.708	-28.312	-19.675	-3134.15468	-3136.46116	-3136.13318	0.00	0.00	*0.00*	0.00
2b•	0	113.000	126.588	83.395	-17.585	-12.369	-2725.37280	-2727.25125	-2727.13505	0.00	0.00	*0.00*	0.00

2be_ts	0	113.032	126.523	83.564	-16.323	-11.266	-2725.35601	-2727.23465	-2727.11643	10.54	10.42	*11.69*	11.81
2be•	0	112.612	126.116	83.187	-16.330	-11.233	-2725.36812	-2727.24718	-2727.12950	2.94	2.56	*3.48*	3.87
2b⁻	0	112.747	126.061	83.425	-54.872	-48.914	-2725.48327	-2727.35374	-2727.29573	-69.32	-64.31	*-100.83*	-105.84
*$Fe(CO)_4P(NMeCH_2CH_2NMe)NMe^•$ (**2c•**) radical complex formation and P-to-N 1,2-Fe-shift*													
2cT	0	301.088	322.512	264.857	-20.885	-15.194	-2830.66950	-2832.76875	-2832.36787	-42.85	-47.83	*-27.38*	-22.40
2c• + T•	0	297.757	319.501	246.090	-26.896	-18.765	-2830.60122	-2832.69253	-2832.32424	0.00	0.00	*0.00*	0.00
2c•	0	138.116	152.599	107.777	-16.169	-11.459	-2421.81935	-2423.48263	-2423.32612	0.00	0.00	*0.00*	0.00
2ce_ts	0	138.378	152.608	108.440	-14.560	-10.037	-2421.77875	-2423.44042	-2423.28059	25.48	26.49	*28.57*	27.56
2ce•	0	138.503	152.430	109.138	-14.710	-10.093	-2421.81307	-2423.48427	-2423.32342	3.94	-1.03	*1.69*	6.67
2c⁻	0	137.783	152.061	107.687	-52.716	-47.142	-2421.92132	-2423.58450	-2423.48500	-63.99	-63.92	*-99.70*	-99.76
*$Fe(CO)_4P(NMeCH_2CH_2NMe)PMe^•$ (**2d•**) radical complex formation and P-to-P 1,2-Fe-shift*													
2dT	0	297.473	319.653	260.459	-22.815	-16.732	-3117.33130	-3119.63879	-3119.24737	-60.87	-63.26	*-47.11*	-44.71
2d• + T•	0	295.732	317.920	243.513	-25.664	-17.831	-3117.23430	-3119.53797	-3119.17230	0.00	0.00	*0.00*	0.00
2d•	0	136.091	151.018	105.200	-14.937	-10.525	-2708.45243	-2710.32807	-2710.17418	0.00	0.00	*0.00*	0.00
2de_ts	0	136.234	150.969	105.767	-15.666	-10.762	-2708.43180	-2710.30583	-2710.15142	12.94	13.95	*14.28*	13.27
2de•	0	136.118	151.001	105.325	-17.061	-11.814	-2708.44920	-2710.32721	-2710.17518	2.03	0.54	*-0.63*	0.86
2d⁻	0	135.189	150.143	104.143	-54.513	-48.330	-2708.54140	-2710.41767	-2710.32571	-55.83	-56.23	*-95.09*	-94.69
*$W(CO)_5PPh_2O^•$ (3**a•**) radical complex formation and P-to-O 1,2-W-shift*													
3aT	0	301.567	325.724	262.349	-26.610	-19.340	-1923.44404	-1925.27106	-1924.88079	-32.99	-36.37	*-18.86*	-15.47
3a• + T•	0	300.710	324.589	246.412	-32.553	-22.809	-1923.39147	-1925.21310	-1924.85074	0.00	0.00	*0.00*	0.00
3a•	0	141.069	157.687	108.099	-21.826	-15.503	-1514.60960	-1516.00319	-1515.85262	0.00	0.00	*0.00*	0.00
3aa•	0	141.684	158.063	108.987	-21.718	-15.381	-1514.60795	-1516.00151	-1515.84933	1.04	1.06	*2.07*	2.05
3a-	0	139.978	156.771	106.507	-56.210	-49.280	-1514.73566	-1516.13306	-1516.03885	-79.11	-81.49	*-116.86*	-114.48
3ae_ts	197i	141.234	157.167	109.000	-22.273	-15.644	-1514.60536	-1515.99943	-1515.84764	2.66	2.36	*3.12*	3.42
3ae•	0	141.380	157.757	108.609	-22.688	-15.980	-1514.60593	-1515.99739	-1515.84677	2.30	3.64	*3.67*	2.34
3ac• (CO in ring)	0	142.250	158.164	110.174	-23.203	-16.491	-1514.58646	-1515.98159	-1515.82929	14.52	13.55	*14.64*	15.60
*$W(CO)_5PPh_2S^•$ (**3b•**) radical complex formation and P-to-S 1,2-W-shift*													
3bT	0	300.131	324.765	260.379	-27.079	-19.703	-2246.45327	-2248.50489	-2248.11834	-47.55	-48.98	*-32.95*	-31.52
3b• + T•	0	300.190	324.159	245.764	-33.114	-23.006	-2246.37750	-2248.42683	-2248.06582	0.00	0.00	*0.00*	0.00

3b•	0	140.549	157.257	107.451	-22.387	-15.700	-1837.59562	-1839.21693	-1839.06770	0.00	0.00	*0.00*	0.00
3be_ts	225i	140.413	156.680	107.714	-22.317	-15.714	-1837.59231	-1839.21411	-1839.06449	2.08	1.77	*2.02*	2.32
3be•	0	140.284	157.035	106.845	-22.605	-15.881	-1837.59050	-1839.21061	-1839.06264	3.22	3.96	*3.18*	2.43
3bc• (CO in ring)	0	140.489	156.864	107.931	-23.256	-16.399	-1837.56117	-1839.17881	-1839.02993	21.62	23.92	*23.70*	21.40
3b⁻	0	138.938	155.999	105.068	-57.377	-49.851	-1837.71203	-1839.33572	-1839.24471	-73.05	-74.54	*-111.08*	-109.58
*$W(CO)_5PPh_2NMe^•$ (**3c•**) radical complex formation and P-to-N 1,2-W-shift*													
3cT	0	327.468	352.355	287.878	-26.709	-19.615	-1942.89261	-1944.74495	-1944.31443	-42.73	-48.54	*-28.65*	-22.84
3c• + T•	0	324.726	349.804	269.362	-32.648	-22.876	-1942.82452	-1944.66760	-1944.26878	0.00	0.00	*0.00*	0.00
3c•	0	165.085	182.902	131.049	-21.921	-15.570	-1534.04264	-1535.45769	-1535.27065	0.00	0.00	*0.00*	0.00
3ce_ts	325i	165.651	182.822	132.286	-21.635	-15.255	-1534.03079	-1535.44487	-1535.25536	7.43	8.04	*9.59*	8.99
3ce•	0	166.119	183.482	132.606	-22.326	-15.794	-1534.04125	-1535.45390	-1535.26474	0.87	2.38	*3.71*	2.20
3cc_ts	239i	165.769	182.680	132.849	-23.690	-16.968	-1534.01841	-1535.43025	-1535.24257	15.20	17.22	*17.62*	15.61
3cc• (CO in ring)	0	167.518	184.507	134.475	-25.113	-18.127	-1534.04309	-1535.46030	-1535.27188	-0.28	-1.64	*-0.77*	0.59
3c⁻	0	163.696	181.725	129.226	-55.244	-48.157	-1534.14112	-1535.55725	-1535.42505	-61.80	-62.47	*-96.88*	-96.21
*$W(CO)_5PPh_2PMe^•$ (**3d•**) radical complex formation and P-to-P 1,2-W-shift*													
3dT	0	324.067	349.813	283.350	-28.170	-20.720	-2229.55551	-2231.61489	-2231.19335	-55.66	-57.35	*-40.84*	-39.15
3d• + T•	0	323.225	348.506	267.654	-33.578	-23.422	-2229.46682	-2231.52350	-2231.12826	0.00	0.00	*0.00*	0.00
3d•	0	163.584	181.604	129.341	-22.851	-16.116	-1820.68494	-1822.31359	-1822.13014	0.00	0.00	*0.00*	0.00
3da•	0	163.093	181.337	128.550	-23.605	-16.799	-1820.68043	-1822.30952	-1822.12842	2.83	2.55	*1.08*	1.36
3de_ts	0	163.182	181.425	128.608	-22.475	-15.847	-1820.66699	-1822.29519	-1822.11248	11.26	11.55	*11.08*	10.80
3de•	0	163.787	181.747	129.569	-23.375	-16.522	-1820.68249	-1822.31131	-1822.12815	1.54	1.43	*1.25*	1.36
3dc• (CO in ring)	0	163.660	181.359	129.889	-25.391	-18.079	-1820.64891	-1822.27324	-1822.09205	22.61	25.32	*23.90*	21.20
3d⁻	0	161.519	180.088	126.165	-57.093	-49.456	-1820.77257	-1822.40225	-1822.27700	-54.99	-55.64	*-92.15*	-91.51
*$W(CO)_5PHPhO^•$ (**4a•**) radical complex formation, P-to-O 1,2-W-shift (**4ae•**) and P-to-O 1,2-H-shift (**4ap•**)*													
4aT	0	250.911	272.037	214.259	-22.202	-15.792	-1692.22753	-1693.79680	-1693.47751	-35.39	-38.54	*-21.90*	-18.75
4a• + T•	0	250.147	270.769	199.026	-28.144	-19.092	-1692.17113	-1693.73538	-1693.44261	0.00	0.00	*0.00*	0.00
4a•	0	90.506	103.867	60.713	-17.417	-11.786	-1283.38926	-1284.52547	-1284.44449	0.00	0.00	*0.00*	0.00
4ae_ts	161i	89.816	102.810	60.367	-18.051	-12.013	-1283.38453	-1284.52189	-1284.44182	2.96	2.25	*1.67*	2.39
4ae•	0	90.173	103.494	60.521	-16.515	-11.216	-1283.38727	-1284.52247	-1284.44089	1.24	1.88	*2.26*	1.62
4ap_ts	1445i	88.304	101.513	58.724	-19.892	-12.228	-1283.33594	-1284.47157	-1284.39446	33.45	33.82	*31.39*	31.02

4ap•	0	91.598	104.931	61.947	-29.999	-16.590	-1283.40013	-1284.54299	-1284.46770	-6.82	-11.00	*-14.57*	-10.39
4ac_ts	215i	89.908	102.871	60.631	-17.970	-12.239	-1283.36115	-1284.49962	-1284.41949	17.64	16.22	*15.68*	17.10
4ac• (CO in ring)	0	91.269	104.084	62.135	-20.188	-13.426	-1283.36494	-1284.50312	-1284.42248	15.26	14.03	*13.81*	15.04
4a⁻	0	89.136	102.870	58.405	-52.297	-46.416	-1283.51666	-1284.65577	-1284.63365	-79.95	-81.76	*-118.70*	-116.88
*$W(CO)_5PHPhS^•$ (**4b•**) radical complex formation, P-to-S 1,2-W-shift (**4be•**) and 1,2-H-shift (**4bp•**)*													
4bT	0	249.199	270.799	211.779	-23.694	-17.013	-2015.24020	-2017.03549	-2016.72210	-51.29	-52.82	*-38.12*	-36.59
4b• + T•	0	249.206	270.046	197.752	-29.510	-19.571	-2015.15846	-2016.95131	-2016.66134	0.00	0.00	*0.00*	0.00
4b•	0	89.565	103.144	59.439	-18.783	-12.265	-1606.37659	-1607.74141	-1607.66322	0.00	0.00	*0.00*	0.00
4be_ts	0	89.623	103.193	59.472	-19.439	-12.597	-1606.37130	-1607.73695	-1607.65924	3.32	2.80	*2.50*	3.02
4be•	0	89.339	102.940	59.297	-16.827	-11.376	-1606.37573	-1607.74056	-1607.66118	0.54	0.53	*1.28*	1.29
4bp_ts	982i	87.206	100.677	57.198	-18.755	-12.116	-1606.33538	-1607.69868	-1607.62383	25.86	26.81	*24.72*	23.77
4bp•	0	88.987	102.667	58.847	-21.264	-13.147	-1606.37447	-1607.74024	-1607.66440	1.33	0.73	*-0.74*	-0.14
4bc• (CO in ring)	0	89.664	102.938	60.012	-20.322	-13.370	-1606.34128	-1607.70259	-1607.62525	22.16	24.36	*23.83*	21.63
4b⁻	0	88.242	102.217	57.240	-52.861	-46.465	-1606.49518	-1607.86176	-1607.84158	-74.42	-75.53	*-111.92*	-110.81
*$W(CO)_5PHPhNMe^•$ (**4c•**) radical complex formation, P-to-N 1,2-W-shift (**4ce•**) and 1,2-H-shift (**4cp•**)*													
4cT	0	276.056	298.144	238.754	-22.653	-16.312	-1711.68265	-1713.27754	-1712.92004	-49.78	-54.94	*-36.66*	-31.50
4c• + T•	0	274.143	295.939	221.895	-28.887	-19.623	-1711.60332	-1713.18998	-1712.86162	0.00	0.00	*0.00*	0.00
4c•	0	114.502	129.037	83.582	-18.160	-12.317	-1302.82145	-1303.98008	-1303.86350	0.00	0.00	*0.00*	0.00
4ce_ts	0	114.413	129.047	83.432	-16.946	-11.505	-1302.81024	-1303.96860	-1303.85097	7.04	7.20	*7.86*	7.70
4ce•	0	115.044	129.393	84.350	-17.740	-12.126	-1302.82712	-1303.98385	-1303.86574	-3.56	-2.37	*-1.41*	-2.60
4cp_ts	1608i	112.866	127.286	82.060	-19.177	-12.840	-1302.77088	-1303.92808	-1303.81476	31.73	32.63	*30.58*	29.69
4cp•	0	116.888	131.408	86.044	-22.006	-14.009	-1302.85128	-1304.01510	-1303.89730	-18.72	-21.98	*-21.21*	-17.95
4c⁻	0	113.088	127.944	81.621	-51.237	-45.169	-1302.92355	-1304.08334	-1304.02224	-64.07	-64.80	*-99.61*	-98.88
*$W(CO)_5PHPhPMe^•$ (**4d•**) radical complex formation, P-to-P 1,2-W-shift (**4ce•**) and 1,2-H-shift (**4cp•**)*													
4dT	0	272.748	295.574	234.245	-24.242	-17.437	-1998.35008	-2000.15547	-1999.80695	-63.25	-66.18	*-50.86*	-47.93
4d• + T•	0	272.334	294.531	219.612	-29.501	-20.015	-1998.24929	-2000.05001	-1999.72591	0.00	0.00	*0.00*	0.00
4d•	0	112.693	127.629	81.299	-18.774	-12.709	-1589.46741	-1590.84010	-1590.72779	0.00	0.00	*0.00*	0.00
4de_ts	167i	111.509	126.230	80.490	-18.432	-12.453	-1589.44844	-1590.82107	-1590.70964	11.91	11.94	*11.39*	11.35
4de•	0	112.699	127.568	81.344	-18.801	-12.773	-1589.46685	-1590.83939	-1590.72710	0.35	0.45	*0.43*	0.33
4dp_ts	1163i	110.345	125.282	78.848	-18.917	-12.991	-1589.42407	-1590.79482	-1590.68686	27.20	28.41	*25.68*	24.46

4dp•	0	112.624	127.552	81.233	-18.469	-12.561	-1589.47133	-1590.84386	-1590.73141	-2.46	-2.35	*-2.27*	-2.38
4d⁻	0	111.113	126.478	78.954	-53.582	-46.811	-1589.55188	-1590.92493	-1590.87069	-53.00	-53.23	*-89.67*	-89.45
*$W(CO)_5$PHPhNH• (**4ch•**) radical complex formation, P-to-N 1,2-W-shift (**4che•**) and 1,2-H-shift (**4chp•**)*													
4chT	0	258.458	279.716	221.787	-24.799	-17.194	-1672.35612	-1673.91281	-1673.58376	-56.99	-63.05	*-46.42*	-40.36
4ch• + T•	0	256.990	277.666	205.944	-30.397	-19.872	-1672.26530	-1673.81233	-1673.50978	0.00	0.00	*0.00*	0.00
4ch•	0	97.349	110.764	67.631	-19.670	-12.566	-1263.48343	-1264.60242	-1264.51166	0.00	0.00	*0.00*	0.00
4che_ts	141i	97.043	110.176	67.594	-19.154	-12.335	-1263.47628	-1264.59655	-1264.50548	4.48	3.68	*3.88*	4.68
4che•	0	97.593	111.003	67.721	-20.355	-12.807	-1263.49205	-1264.61012	-1264.51959	-5.41	-4.83	*-4.98*	-5.56
4chp_ts	1547i	95.360	108.740	65.656	-22.960	-13.991	-1263.43664	-1264.55514	-1264.46979	29.36	29.67	*26.27*	25.96
4chp•	0	99.209	112.776	69.388	-25.030	-14.936	-1263.51814	-1264.64316	-1264.55337	-21.79	-25.56	*-26.18*	-22.40
4chc_ts	263i	97.303	110.198	68.120	-22.529	-14.386	-1263.45862	-1264.57608	-1264.48744	15.57	16.53	*15.20*	14.24
4chc• (CO in ring)	0	99.043	111.937	69.840	-26.259	-16.360	-1263.48240	-1264.60385	-1264.51561	0.65	-0.90	*-2.48*	-0.94
4ch-	0	95.662	109.740	64.833	-51.424	-45.648	-1263.59308	-1264.71446	-1264.68087	-68.81	-70.30	*-106.18*	-104.69
*$W(CO)_5$PHPhPH• (**4dh•**) radical complex formation, P-to-P 1,2-W-shift (**4dhe•**) and 1,2-H-shift (**4dhp•**)*													
4dhT	0	254.665	276.595	216.905	-23.759	-16.961	-1959.00255	-1960.76485	-1960.44321	-65.85	-67.84	*-52.58*	-50.59
4dh• + T•	0	254.011	275.147	202.360	-29.730	-19.566	-1958.89761	-1960.65673	-1960.35941	0.00	0.00	*0.00*	0.00
4dh•	0	94.370	108.245	64.047	-19.003	-12.260	-1550.11574	-1551.44682	-1551.36129	0.00	0.00	*0.00*	0.00
4dhe_ts	0	93.798	107.812	63.342	-17.757	-11.831	-1550.10090	-1551.43256	-1551.34746	9.31	8.95	*8.67*	9.03
4dhe•	0	94.515	108.304	64.364	-17.214	-11.612	-1550.11747	-1551.44943	-1551.36236	-1.09	-1.64	*-0.67*	-0.12
4dhp_ts	937i	92.310	106.095	62.015	-17.953	-12.048	-1550.08032	-1551.40997	-1551.32733	22.22	23.13	*21.31*	20.41
4dhp•	0	94.141	108.157	63.650	-17.699	-11.901	-1550.12045	-1551.45178	-1551.36630	-2.96	-3.11	*-3.15*	-3.00
4dhc_ts	0	94.433	108.260	64.167	-17.706	-11.784	-1550.11466	-1551.44577	-1551.35928	0.68	0.66	*1.26*	1.27
4dhc• (CO in ring)	0	94.605	108.096	64.825	-21.021	-13.811	-1550.08011	-1551.40669	-1551.32238	22.36	25.19	*24.41*	21.59
4dh⁻	0	92.765	107.145	61.509	-54.099	-47.387	-1550.21475	-1551.54737	-1551.52186	-62.13	-63.09	*-100.76*	-99.79

Table S2. TPSS-D3/def2-TZVP + COSMO optimized Cartesian coordinates (in Å) in THF solution. Each structure is labeled by a specific name (See **Table S1**), followed by the number of atoms, the total energy (in hartrees), and the detailed atomic coordinates (in double-column text list). For simplicity, T = TEMP and Pc = cyclic $PNMeCH_2CH_2NMe$ five-ring are used in molecule formula.

1ae_ts : P-to-O 1,2-Fe-shift of $[Fe(CO)_4]PPh_2O^{\bullet}$
33
Energy = -2597.761473466

P	-0.1249353	0.5149449	0.1281275
Fe	-0.3578221	-1.9468245	-0.2811570
C	0.7671887	-3.3897011	-0.4419892
O	1.3984244	-4.3438959	-0.5543612
C	-0.3450053	-1.5046585	-2.0572920
O	-0.3153362	-1.2458351	-3.1745235
C	-0.5678497	-2.0587995	1.5349901
O	-0.6703672	-2.1257702	2.6755104
C	-1.9577824	-2.6872229	-0.4992579
O	-2.9869955	-3.1900898	-0.6444247
O	1.0859468	-0.5088552	0.0434449
C	0.1297652	1.4758888	1.6568816
C	-0.6922875	2.5691850	1.9726658
C	1.1165338	1.0644407	2.5640554
C	-0.5056157	3.2604225	3.1671882
H	-1.4680808	2.8886557	1.2817500
C	1.2936443	1.7564776	3.7631707
H	1.7441036	0.2136018	2.3166678
C	0.4849504	2.8530620	4.0671697
H	-1.1374717	4.1125468	3.4015821
H	2.0656553	1.4390906	4.4588577
H	0.6236656	3.3896186	5.0014151
C	0.0979181	1.7256734	-1.2174819
C	1.3302852	1.7977389	-1.8817027
C	-0.9625768	2.5466443	-1.6253110
C	1.5047267	2.7035667	-2.9273604
H	2.1400393	1.1419535	-1.5750015
C	-0.7804384	3.4570765	-2.6658063
H	-1.9317606	2.4684133	-1.1388656
C	0.4522330	3.5351099	-3.3187518
H	2.4616983	2.7589082	-3.4390419
H	-1.6034650	4.0944966	-2.9764227
H	0.5901271	4.2377482	-4.1356866

1ae$^{\bullet}$: $PPh_2O[Fe(CO)_4]^{\bullet}$ complex
33
Energy = -2597.761085704

P	-4.5440911	2.4354225	0.6479584
Fe	-4.0506504	-0.7669866	0.0548903
C	-2.2482302	-0.5608413	0.3212872
O	-1.1096838	-0.4981583	0.4638852
C	-4.0904223	-0.2191186	-1.7156542
O	-4.0980994	-0.0316998	-2.8457270
C	-4.4619498	-1.4164531	1.7330687
O	-4.6920032	-1.8256435	2.7776117
C	-4.0007979	-2.4492250	-0.5595307
O	-3.9636280	-3.5333899	-0.9490626
O	-4.8685288	0.8679780	0.6885853
C	-3.1113703	2.6332716	1.7737850
C	-2.3188295	3.7928827	1.7264933
C	-2.8530225	1.6788349	2.7662390
C	-1.2724747	3.9708621	2.6288422
H	-2.5106363	4.5502267	0.9702228
C	-1.8016954	1.8544993	3.6675061
H	-3.4813984	0.7963416	2.8303635
C	-1.0069350	2.9991489	3.5992446
H	-0.6584603	4.8656578	2.5727263
H	-1.6062134	1.0989955	4.4237447
H	-0.1887859	3.1385290	4.3001307
C	-3.7482162	2.7586933	-0.9768992
C	-2.3928840	2.5049704	-1.2491802
C	-4.5768362	3.2059871	-2.0180265
C	-1.8866294	2.6743518	-2.5364274
H	-1.7334560	2.1826378	-0.4495669
C	-4.0707303	3.3776937	-3.3060645
H	-5.6250037	3.4124854	-1.8134417
C	-2.7254895	3.1077124	-3.5665775
H	-0.8386608	2.4701813	-2.7376444
H	-4.7221249	3.7211801	-4.1047038
H	-2.3293292	3.2395377	-4.5695334

1aT : $[Fe(CO)_4]PPh_2OT$ complex
61
Energy = -3006.580123413

P	0.4906732	0.4847869	-0.2413181
Fe	0.5614658	-1.0945891	-1.7861084
C	-0.9175064	-2.0931635	-1.9309004
O	-1.8610512	-2.7547798	-2.0454000
C	1.2588833	-2.2361661	-0.5895469
O	1.7278366	-2.9948542	0.1434974
C	-0.0563060	0.0685940	-3.0058837
O	-0.4294246	0.7899097	-3.8264642
C	2.0111617	-1.3187001	-2.7935546
O	2.9498287	-1.4747009	-3.4592617
O	-0.8545468	0.7096495	0.6952862
C	0.7727096	2.1984795	-0.8239859
C	0.1260103	3.2897375	-0.2289653
C	1.7154473	2.4268042	-1.8345832
C	0.4062974	4.5876719	-0.6548760

H	-0.5968968	3.1202928	0.5611937
C	2.0026468	3.7255868	-2.2512975
H	2.2218865	1.5837237	-2.2970407
C	1.3446779	4.8088163	-1.6652769
H	-0.1080825	5.4271598	-0.1955278
H	2.7341704	3.8904630	-3.0371314
H	1.5614448	5.8207337	-1.9952210
C	1.7823947	0.4136319	1.0560231
C	1.5221934	0.8265599	2.3694913
C	3.0781966	0.0125521	0.7066545
C	2.5407628	0.8175987	3.3217758
H	0.5237560	1.1484304	2.6434689
C	4.0978674	0.0147248	1.6572250
H	3.2862818	-0.3047265	-0.3117719
C	3.8298672	0.4128944	2.9684424
H	2.3272740	1.1289907	4.3405018
H	5.0984336	-0.3004497	1.3755324
H	4.6215928	0.4062981	3.7120759
C	-2.2011946	-0.9618289	1.7441069
C	-3.4643750	-1.8254793	1.5393026
C	-4.6886913	-1.0086325	1.1372802
C	-4.3688147	-0.2385281	-0.1402989
C	-3.1411950	0.6866487	0.0031931
H	-5.5441393	-1.6729862	0.9703980
H	-3.2518228	-2.5616867	0.7539697
H	-3.6385525	-2.3782525	2.4696318
H	-4.1660439	-0.9532278	-0.9478057
H	-5.2140609	0.3836300	-0.4564103
H	-4.9776455	-0.3217014	1.9417610
N	-2.0210130	-0.1884435	0.4743507
C	-2.3091314	-0.1204202	3.0314351
H	-1.5467417	0.6613757	3.0468903
H	-3.2874728	0.3479428	3.1488856
H	-2.1453949	-0.7737560	3.8947590
C	-1.0037160	-1.9099267	1.8698906
H	-0.9158193	-2.5206689	0.9690744
H	-0.0692978	-1.3648153	2.0272305
H	-1.1548948	-2.5734162	2.7275993
C	-2.7673840	1.1857270	-1.3966492
H	-1.9030819	1.8547162	-1.3715413
H	-2.5463137	0.3376413	-2.0478833
H	-3.6103081	1.7406782	-1.8210544
C	-3.4642982	1.9011528	0.8960634
H	-2.5484319	2.4175455	1.1913906
H	-4.0139346	1.6279755	1.7979663
H	-4.0830768	2.6026360	0.3268446

1a⁻ : $[Fe(CO)_4]PPh_2O^-$ anion complex

33

Energy = -2597.958500712

P	-2.3300568	0.7449500	0.0023601
Fe	-4.0969690	-0.7157359	-0.1029778
C	-5.4028209	-1.9225575	-0.2117200
O	-6.2513001	-2.7140615	-0.2842992
C	-3.4356907	-1.1212679	-1.7056117
O	-3.0196700	-1.4013297	-2.7584177
C	-3.3650684	-1.4420651	1.3502797
O	-2.9157878	-1.9393629	2.3034831
C	-5.2296018	0.6330232	0.1296752
O	-6.0106008	1.4863618	0.2864812
O	-0.9435479	0.1238370	-0.0284579
C	-2.4658552	1.7617279	1.5285058
C	-3.2788560	2.8994913	1.6172396
C	-1.7274909	1.3624728	2.6504242
C	-3.3596915	3.6193999	2.8091705
H	-3.8433662	3.2287867	0.7499389
C	-1.8099040	2.0803478	3.8443519
H	-1.0826970	0.4917738	2.5725770
C	-2.6281477	3.2095273	3.9272740
H	-3.9897365	4.5035798	2.8652058
H	-1.2322388	1.7617861	4.7085097
H	-2.6913386	3.7710257	4.8557552
C	-2.4261697	2.0543330	-1.2899069
C	-1.3559246	2.9618974	-1.3549724
C	-3.4742719	2.1766379	-2.2060992
C	-1.3428316	3.9750073	-2.3110607
H	-0.5322811	2.8630588	-0.6525885
C	-3.4632530	3.1914477	-3.1669893
H	-4.2971074	1.4691615	-2.1682950
C	-2.4000498	4.0930727	-3.2197645
H	-0.5101508	4.6727210	-2.3505666
H	-4.2842919	3.2747971	-3.8744178
H	-2.3904987	4.8827204	-3.9665413

1a• : $[Fe(CO)_4]PPh_2O^•$

33

Energy = -2597.795855365

P	-2.3162188	0.8297979	0.0613478
Fe	-3.9403374	-0.7915399	-0.1547620
C	-4.7838254	-2.3918971	-0.3603158
O	-5.3316282	-3.3931458	-0.4915787
C	-3.6333133	-0.6334461	-1.9494551
O	-3.4759483	-0.5487035	-3.0835414
C	-3.6437991	-1.0802995	1.6266809
O	-3.5041804	-1.2687168	2.7501164
C	-5.3858750	0.2676409	0.0104063
O	-6.3168451	0.9353886	0.1360564
O	-1.0151986	0.0491803	0.0776566
C	-2.5160253	1.8084402	1.5858685
C	-3.5243072	2.7711089	1.7338380
C	-1.6378464	1.5519613	2.6466462

C	-3.6540270	3.4668520	2.9339528
H	-4.2029808	2.9878685	0.9143333
C	-1.7684260	2.2546045	3.8453024
H	-0.8581018	0.8066108	2.5212507
C	-2.7767537	3.2086925	3.9913548
H	-4.4359064	4.2128301	3.0437812
H	-1.0823448	2.0561767	4.6638861
H	-2.8790074	3.7532665	4.9256806
C	-2.3363143	2.0767925	-1.2678149
C	-1.0958566	2.4697322	-1.7898835
C	-3.5116623	2.6509902	-1.7684454
C	-1.0356936	3.4382995	-2.7916704
H	-0.1891504	2.0058310	-1.4127534
C	-3.4476209	3.6214090	-2.7671460
H	-4.4819154	2.3366210	-1.3958327
C	-2.2095540	4.0171732	-3.2785904
H	-0.0720967	3.7379870	-3.1938789
H	-4.3632739	4.0605888	-3.1523561
H	-2.1612327	4.7684703	-4.0615891

1be_ts : P-to-S 1,2-Fe-shift of $[Fe(CO)_4]PPh_2S^{\bullet}$
33
Energy = -2920.747479697

P	-0.0218423	0.5108500	0.2543812
S	1.6473510	-0.7095160	0.1455985
C	0.1745470	1.5857466	1.7168501
C	0.0134940	1.6654449	-1.1567684
C	-0.5591129	2.7834328	1.7782581
C	0.9375138	1.1856990	2.8229468
C	1.1460783	2.4417923	-1.4424253
C	-1.1265091	1.7732870	-1.9624562
C	-0.5100633	3.5747522	2.9232537
H	-1.1554406	3.0999413	0.9265890
C	0.9793904	1.9816297	3.9679378
H	1.5074090	0.2621240	2.7744456
C	1.1316769	3.3195093	-2.5231245
H	2.0334449	2.3523813	-0.8220428
C	-1.1372758	2.6535457	-3.0464926
H	-2.0019959	1.1682920	-1.7408674
C	0.2572976	3.1755494	4.0220694
H	-1.0690808	4.5056941	2.9576094
H	1.5819458	1.6701151	4.8166479
C	-0.0096259	3.4256436	-3.3256785
H	2.0095856	3.9203807	-2.7431731
H	-2.0227557	2.7331364	-3.6703644
H	0.2928632	3.7941296	4.9141857
H	-0.0156938	4.1096694	-4.1695331
Fe	-0.2629844	-2.0525084	-0.3530160
C	0.4145325	-3.7209553	-0.6443771
C	0.0203524	-1.5288179	-2.0790679
C	-0.3727173	-2.2718452	1.4601565
C	-2.0218357	-2.2648970	-0.5961640
O	0.7813155	-4.7949831	-0.8387388
O	0.2427970	-1.2473665	-3.1703162
O	-0.4058350	-2.4169680	2.5984837
O	-3.1535101	-2.4186461	-0.7573566

1be$^{\bullet}$: $PPh_2S[Fe(CO)_4]^{\bullet}$ radical complex
33
Energy = -2920.747011393

P	-4.5721254	2.7382455	0.6348261
Fe	-3.9548252	-0.9122715	0.0765640
C	-2.2274335	-0.4207442	0.3925944
O	-1.1202028	-0.1712030	0.5747829
C	-4.1226446	-0.2572883	-1.6321262
O	-4.2661079	0.0699969	-2.7205393
C	-4.3148284	-1.4937345	1.7697994
O	-4.5169412	-1.8525340	2.8413151
C	-3.6070411	-2.5727993	-0.5259371
O	-3.3859809	-3.6389302	-0.8994209
S	-5.3920834	0.8037456	0.7201920
C	-3.1292923	2.6914791	1.7665613
C	-2.1541674	3.6992959	1.6637998
C	-3.0373123	1.7688782	2.8168037
C	-1.0937994	3.7517523	2.5667320
H	-2.2172560	4.4381505	0.8693643
C	-1.9773517	1.8254308	3.7219430
H	-3.8018301	1.0053990	2.9210716
C	-0.9979456	2.8112184	3.5957578
H	-0.3400890	4.5275839	2.4645375
H	-1.9166083	1.0955192	4.5245547
H	-0.1686520	2.8513080	4.2960666
C	-3.7908910	2.8884465	-1.0158464
C	-2.4562995	2.5586513	-1.2969431
C	-4.6135500	3.3451506	-2.0580919
C	-1.9602701	2.6723227	-2.5950906
H	-1.8023032	2.2248179	-0.4993390
C	-4.1184760	3.4509066	-3.3564588
H	-5.6467636	3.6105718	-1.8472417
C	-2.7901252	3.1139300	-3.6274149
H	-0.9255906	2.4125012	-2.8007995
H	-4.7662490	3.8010455	-4.1550677
H	-2.4022302	3.1997235	-4.6384040

1bT : $[Fe(CO)_4]PPh_2ST$ complex
61
Energy = -3329.586351941

P	0.8365092	0.1158984	0.2713925
Fe	0.6647140	-2.0030271	-0.4582428
C	0.5620903	-3.6765765	-1.0612578
O	0.4956478	-4.7619080	-1.4535120
C	0.5352879	-2.5718704	1.2359972

O	0.4846977	-2.9979204	2.3130451
C	-0.7412418	-1.5744563	-1.4870220
O	-1.6278331	-1.3924992	-2.2138785
C	2.3411525	-1.8310953	-1.0489529
O	3.4378862	-1.7658388	-1.4236825
S	-0.8091903	1.1239402	1.2482572
C	1.4305408	1.3119224	-0.9727095
C	1.7634470	2.6164013	-0.5712882
C	1.4877474	0.9730817	-2.3278137
C	2.1584910	3.5588479	-1.5151725
H	1.7068503	2.8914028	0.4778672
C	1.8791649	1.9220817	-3.2735650
H	1.2228833	-0.0321002	-2.6402855
C	2.2163650	3.2131802	-2.8694825
H	2.4176943	4.5644366	-1.1970567
H	1.9190591	1.6499297	-4.3241335
H	2.5224554	3.9513901	-3.6050959
C	2.0355687	0.3166461	1.6356999
C	1.6559433	0.0805685	2.9653134
C	3.3778912	0.6052337	1.3439199
C	2.6019102	0.1495515	3.9872689
H	0.6235181	-0.1554678	3.1995690
C	4.3206676	0.6628314	2.3681437
H	3.6852224	0.7833882	0.3187170
C	3.9344996	0.4403645	3.6918807
H	2.2957748	-0.0264361	5.0142404
H	5.3572956	0.8837171	2.1312616
H	4.6702322	0.4917490	4.4891520
C	-3.2004398	-0.1020755	1.3408649
C	-4.3906252	-0.5647686	0.4803012
C	-5.0618301	0.5678873	-0.2864110
C	-4.0258721	1.2114762	-1.1995986
C	-2.8089495	1.7781972	-0.4441159
H	-5.8957940	0.1771830	-0.8805342
H	-4.0244010	-1.3117087	-0.2353514
H	-5.0998907	-1.0688226	1.1471135
H	-3.6660710	0.4609296	-1.9136544
H	-4.4623585	2.0336003	-1.7787798
H	-5.4860475	1.3071075	0.4042316
N	-2.2545693	0.6924726	0.4585295
C	-3.6840619	0.6905785	2.5705139
H	-2.8269786	1.1029445	3.1144783
H	-4.3556243	1.5101176	2.3091332
H	-4.2207893	0.0164563	3.2466531
C	-2.4802708	-1.3581763	1.8358320
H	-3.2047023	-2.0013311	2.3464382
H	-2.0461664	-1.9057868	0.9966336
H	-1.6842278	-1.1148499	2.5435369
C	-1.7466634	2.1366117	-1.4865951
H	-0.8952124	2.6502993	-1.0352706
H	-1.3883300	1.2415982	-1.9992568
H	-2.1943008	2.8059927	-2.2287105
C	-3.1838516	3.0639655	0.3174276
H	-2.3429086	3.3937358	0.9370009
H	-4.0587514	2.9361838	0.9572196
H	-3.4064519	3.8580944	-0.4034390

1b⁻ : $[Fe(CO)_4]PPh_2S^-$ anion complex

33

Energy = -2920.921731961

P	-2.3203392	0.7439965	-0.0204335
S	-0.5018697	-0.0863313	-0.1313598
C	-2.4103120	1.7448919	1.5233037
C	-2.4246434	2.0670496	-1.2969925
C	-3.1975557	2.9021171	1.5965956
C	-1.7142204	1.3191470	2.6606118
C	-1.4345585	3.0628222	-1.2967785
C	-3.4277113	2.1046628	-2.2684722
C	-3.2861850	3.6201431	2.7893196
H	-3.7344679	3.2486288	0.7191929
C	-1.8101163	2.0324491	3.8555094
H	-1.0866322	0.4349419	2.5903713
C	-1.4585349	4.0817545	-2.2447774
H	-0.6436087	3.0246940	-0.5526332
C	-3.4463282	3.1213576	-3.2280735
H	-4.1941848	1.3359073	-2.2711657
C	-2.5958855	3.1856122	3.9233756
H	-3.8920229	4.5216595	2.8317707
H	-1.2649177	1.6921743	4.7322132
C	-2.4659475	4.1126364	-3.2161973
H	-0.6907014	4.8509523	-2.2314889
H	-4.2296776	3.1368618	-3.9812991
H	-2.6651461	3.7458438	4.8520957
H	-2.4815869	4.9054060	-3.9594068
Fe	-4.1257581	-0.6832636	-0.0897882
C	-5.4917535	-1.8188830	-0.1698824
C	-3.4857510	-1.2028984	-1.6729491
C	-3.4360224	-1.4244176	1.3816533
C	-5.2121289	0.7133061	0.0959246
O	-6.3823445	-2.5628701	-0.2248055
O	-3.0934172	-1.5617495	-2.7086207
O	-3.0221929	-1.9312141	2.3437215
O	-5.9607446	1.5991778	0.2180110

1b• : $[Fe(CO)_4]PPh_2S^•$ radical complex

33

Energy = -2920.765636915

P	-2.4468109	0.8312615	0.0448622
S	-0.9151993	-0.4510689	-0.0177853
C	-2.4957384	1.8145872	1.5783328
C	-2.3867136	2.0911872	-1.2688857

C	-3.4070992	2.8747771	1.6929466
C	-1.6645142	1.4874664	2.6548914
C	-1.1427035	2.6035919	-1.6610342
C	-3.5588898	2.5790571	-1.8587963
C	-3.4813161	3.6011341	2.8791955
H	-4.0518655	3.1371882	0.8590741
C	-1.7401950	2.2217152	3.8388454
H	-0.9643799	0.6628511	2.5554247
C	-1.0774315	3.6015159	-2.6311592
H	-0.2337528	2.2094939	-1.2149307
C	-3.4889219	3.5806074	-2.8272009
H	-4.5252709	2.1740039	-1.5742674
C	-2.6477459	3.2758898	3.9531238
H	-4.1865005	4.4226841	2.9646176
H	-1.0883153	1.9698200	4.6702814
C	-2.2493174	4.0925070	-3.2131536
H	-0.1113147	3.9929612	-2.9360830
H	-4.4010073	3.9531665	-3.2839036
H	-2.7048836	3.8464413	4.8755569
H	-2.1948219	4.8666727	-3.9729231
Fe	-4.0199568	-0.7817172	-0.1501081
C	-4.6890590	-2.4496620	-0.3408635
C	-3.6879650	-0.6963641	-1.9432395
C	-3.7486225	-1.0742143	1.6325050
C	-5.5259888	0.2006600	-0.0328778
O	-5.1169846	-3.5106490	-0.4648792
O	-3.5191323	-0.6595850	-3.0796558
O	-3.6306227	-1.2670375	2.7591784
O	-6.4842263	0.8356235	0.0614568

1ce_ts : 1,2-Fe-shift of $[Fe(CO)_4]PPh_2NMe^{\bullet}$
37
Energy = -2617.190555351

P	-0.3539935	0.4484105	0.2089974
Fe	-0.0851532	-2.1902055	0.0041147
C	1.1921006	-3.4779487	0.1228385
O	1.9727193	-4.3222473	0.2009284
C	0.1242059	-1.9347225	-1.7905736
O	0.3357568	-1.8413103	-2.9174886
C	-0.3839855	-2.0376036	1.8122766
O	-0.5061910	-1.9229945	2.9475119
C	-1.5442283	-3.1995837	-0.2503600
O	-2.4896598	-3.8395271	-0.4229094
C	-0.0528285	1.8905628	1.2954362
C	-0.7832842	3.0791910	1.1316765
C	0.8352656	1.7741816	2.3752133
C	-0.6063997	4.1400581	2.0178383
H	-1.4787073	3.1781053	0.3021922
C	1.0129544	2.8399829	3.2575189
H	1.3870153	0.8476602	2.5084245
C	0.2931344	4.0243644	3.0821130
H	-1.1682056	5.0595406	1.8772536
H	1.7142207	2.7461077	4.0823640
H	0.4298372	4.8526873	3.7715334
C	-0.4916946	1.2215904	-1.4444893
C	0.4504903	2.1588320	-1.9000790
C	-1.5343281	0.8303175	-2.2959556
C	0.3569351	2.6785568	-3.1899136
H	1.2487504	2.4868410	-1.2402995
C	-1.6324213	1.3568939	-3.5840335
H	-2.2685077	0.1100390	-1.9432038
C	-0.6839799	2.2777673	-4.0327631
H	1.0930867	3.3979820	-3.5379015
H	-2.4467168	1.0513947	-4.2349242
H	-0.7566781	2.6872222	-5.0364065
N	0.9951483	-0.5069426	0.3365627
C	2.3027013	-0.2375715	-0.2493529
H	2.7478435	0.6466960	0.2265051
H	2.9628228	-1.0911355	-0.0673279
H	2.2633498	-0.0587213	-1.3350541

1ce$^{\bullet}$: $PPh_2NMe[Fe(CO)_4]^{\bullet}$ radical complex
37
Energy = -2617.190851996

P	-0.1843471	0.3924298	0.2782519
Fe	0.3678583	-2.2267149	-0.0310535
C	1.7896917	-3.3452721	0.1397623
O	2.6755277	-4.0734554	0.2528056
C	0.6188540	-1.8866340	-1.8052926
O	0.8579432	-1.7158865	-2.9172287
C	-0.0773410	-2.1499859	1.7526335
O	-0.2958740	-2.0870536	2.8775168
C	-0.9250976	-3.4148259	-0.3898878
O	-1.7633800	-4.1711934	-0.6311862
C	0.0429556	1.8708409	1.3342223
C	-0.7321184	3.0267696	1.1451745
C	0.9263069	1.8092220	2.4227436
C	-0.6035735	4.1092083	2.0139976
H	-1.4250568	3.0841451	0.3099205
C	1.0574867	2.8966073	3.2860406
H	1.5117135	0.9070589	2.5777608
C	0.2932020	4.0487338	3.0847335
H	-1.2005159	5.0029784	1.8536228
H	1.7558923	2.8446295	4.1169843
H	0.3932489	4.8941987	3.7595072
C	-0.4276248	1.1253475	-1.3836770
C	0.4188637	2.1286136	-1.8834215
C	-1.4487039	0.6219398	-2.2018376
C	0.2529167	2.6046379	-3.1828307
H	1.2007143	2.5405099	-1.2517251
C	-1.6198276	1.1045146	-3.4995552
H	-2.1068998	-0.1528914	-1.8160914

C	-0.7661563	2.0932258	-3.9918035
H	0.9162016	3.3757324	-3.5651608
H	-2.4168990	0.7114610	-4.1243669
H	-0.8954207	2.4687247	-5.0030247
N	1.2388806	-0.4508652	0.3796063
C	2.5327703	-0.0197066	-0.1343125
H	2.7805067	0.9705146	0.2703584
H	3.3059247	-0.7241678	0.1893620
H	2.5631668	0.0432868	-1.2330773

1cT : $[Fe(CO)_4]PPh_2NmeT$ complex

65

Energy = -3026.030590323

P	-0.6315727	0.1929008	0.2281986
Fe	-0.5103601	-1.7964194	-0.8467644
C	-0.4504475	-3.3670223	-1.6784345
O	-0.4103011	-4.3888613	-2.2186456
C	0.9804565	-1.3427298	-1.7276192
O	1.9144823	-1.1798750	-2.3987840
C	-0.5681414	-2.6415041	0.7334857
O	-0.6479615	-3.2566814	1.7128622
C	-2.1245233	-1.4665395	-1.5377614
O	-3.1810585	-1.3399506	-2.0027216
N	0.7500808	0.8898950	0.9784517
C	-1.7936042	0.0237165	1.6329478
C	-3.1721676	-0.0049353	1.3757961
C	-1.3398653	-0.2190727	2.9351932
C	-4.0760508	-0.2662830	2.4035798
H	-3.5408947	0.1788195	0.3716385
C	-2.2449433	-0.4769009	3.9637350
H	-0.2755085	-0.2004314	3.1438150
C	-3.6151448	-0.5032854	3.7006503
H	-5.1411346	-0.2821680	2.1911842
H	-1.8780585	-0.6574233	4.9699533
H	-4.3205192	-0.7066989	4.5011424
C	-1.4451812	1.5015878	-0.7702534
C	-2.0780871	2.5924129	-0.1524295
C	-1.3700291	1.4664155	-2.1694015
C	-2.6145243	3.6257924	-0.9196762
H	-2.1726516	2.6263595	0.9281289
C	-1.9065282	2.4979343	-2.9360141
H	-0.8922753	0.6208216	-2.6550393
C	-2.5274352	3.5822219	-2.3124842
H	-3.1059871	4.4609191	-0.4287415
H	-1.8437237	2.4535459	-4.0194382
H	-2.9493719	4.3857546	-2.9093944
C	2.7028946	1.7481010	-0.3116320
C	3.9442902	1.1584349	-1.0138871
C	4.9172610	0.5154422	-0.0323948
C	4.1851018	-0.6030957	0.6964216
C	2.9113979	-0.1516517	1.4429391
H	5.7830471	0.1086862	-0.5681206
H	3.6134468	0.4054998	-1.7357663
H	4.4238354	1.9696524	-1.5744341
H	3.8866427	-1.3596269	-0.0404546
H	4.8367940	-1.0973233	1.4264778
H	5.3053919	1.2566944	0.6769151
N	2.0586093	0.6318266	0.4767059
C	3.1680938	3.0146239	0.4582875
H	3.9250472	2.7995230	1.2130146
H	3.6214269	3.6922682	-0.2742265
H	2.3493019	3.5521141	0.9342802
C	1.7233720	2.2031263	-1.3938980
H	1.3690447	1.3530442	-1.9791520
H	0.8595692	2.7256370	-0.9767642
H	2.2371804	2.8951228	-2.0692253
C	2.1774385	-1.4375779	1.8288274
H	1.8961981	-1.9945781	0.9338002
H	2.8447467	-2.0556687	2.4389158
H	1.2772836	-1.2373949	2.4117426
C	3.2759234	0.5770900	2.7555584
H	2.3761474	0.8203359	3.3282160
H	3.8491242	1.4921668	2.6006102
H	3.8811442	-0.0965244	3.3725081
C	0.4963922	2.1331410	1.7361780
H	1.3304215	2.3153919	2.4109037
H	0.3607884	3.0019720	1.0814247
H	-0.4106456	2.0103371	2.3312724

1c⁻ : $[Fe(CO)_4]PPh_2NMe^-$ anion complex

37

Energy = -2617.358310583

P	0.4811268	0.5655875	0.0440327
C	0.8098681	2.1413995	-0.8773545
C	1.9493340	0.4719915	1.1295510
N	-0.7312882	0.7236072	1.0740896
C	0.5328295	3.3328745	-0.1894791
C	1.2838120	2.2142476	-2.1909630
C	1.8277320	-0.1900071	2.3584726
C	3.1923351	0.9962256	0.7554819
C	-2.0972449	0.6137904	0.5902630
C	0.7421876	4.5698400	-0.7969772
H	0.1407131	3.2678988	0.8226556
C	1.4950280	3.4522441	-2.8029306
H	1.4757178	1.2962715	-2.7381539
C	2.9332688	-0.3278583	3.1975684
H	0.8537168	-0.5768043	2.6418706
C	4.2990801	0.8569066	1.5940670
H	3.2947979	1.5178814	-0.1915493
H	-2.4224422	1.4740939	-0.0233034
H	-2.2592810	-0.2913605	-0.0237036

H	-2.7795743	0.5538348	1.4488544
C	1.2274832	4.6322871	-2.1070866
H	0.5236546	5.4857376	-0.2531469
H	1.8636255	3.4944147	-3.8249149
C	4.1732829	0.1930561	2.8163604
H	2.8286792	-0.8406244	4.1505997
H	5.2590994	1.2695937	1.2945204
H	1.3879337	5.5957660	-2.5841476
H	5.0352543	0.0851498	3.4697078
Fe	0.4462331	-1.2321956	-1.4348496
C	0.3403378	-2.6166671	-2.5436279
C	-0.0075247	-2.1813134	0.0055098
C	-0.7873621	-0.3018391	-2.3168633
C	2.1779210	-0.9746363	-1.7321591
O	0.2721620	-3.5202499	-3.2746182
O	-0.3028301	-2.8357116	0.9235394
O	-1.5830911	0.2885563	-2.9353178
O	3.3174049	-0.8584107	-1.9629012

1c• : $[Fe(CO)_4]PPh_2NMe^•$ radical complex
37
Energy = -2617.210637749

P	0.6359088	0.4533323	-0.1027265
C	0.8200343	2.0866567	-0.8808307
C	1.9530255	0.3995921	1.1419233
N	-0.7589058	0.3542633	0.7868208
C	0.8131501	3.2178950	-0.0465859
C	0.9306191	2.2473593	-2.2658561
C	1.7158293	-0.1461175	2.4099675
C	3.2331434	0.8616719	0.8056143
C	-1.9905870	0.9679610	0.3317534
C	0.9105389	4.4915949	-0.5990337
H	0.7373012	3.0963164	1.0305970
C	1.0345098	3.5258489	-2.8156773
H	0.9437205	1.3738548	-2.9097204
C	2.7566433	-0.2236970	3.3352614
H	0.7210104	-0.4953898	2.6644049
C	4.2682952	0.7801675	1.7346964
H	3.4184850	1.2911946	-0.1745724
H	-1.8743868	1.6955994	-0.4810674
H	-2.6917460	0.1844089	0.0130087
H	-2.4542534	1.4636198	1.1945478
C	1.0224477	4.6461431	-1.9844405
H	0.9030843	5.3632492	0.0486299
H	1.1244008	3.6446252	-3.8912449
C	4.0316790	0.2358695	2.9995460
H	2.5699802	-0.6424109	4.3198806
H	5.2570749	1.1451766	1.4730711
H	1.1021160	5.6407810	-2.4132439
H	4.8396270	0.1733242	3.7227208
Fe	0.5554674	-1.3260111	-1.4726738
C	0.3814738	-2.7766038	-2.5090714
C	0.5220287	-2.3569215	0.0075265
C	-0.8100915	-0.5429023	-2.3430258
C	2.2063844	-0.9408487	-2.0341088
O	0.2743593	-3.7095966	-3.1803337
O	0.5106749	-3.0536493	0.9309030
O	-1.6966919	-0.0710606	-2.9217887
O	3.2776302	-0.7097186	-2.4117752

1de_ts : 1,2-Fe-shift of $[Fe(CO)_4]PPh_2PMe^•$
37
Energy = -2903.827471961

P	-0.1808392	0.5552779	0.1952993
Fe	-0.1716337	-2.1961693	0.3344218
C	0.7237594	-3.7674561	0.3523572
O	1.2938588	-4.7709409	0.3639274
C	-0.0501614	-2.0283548	-1.4690291
O	0.0611759	-2.0560095	-2.6177738
C	-0.1470865	-1.9977925	2.1461885
O	-0.1083748	-1.9173587	3.2946717
C	-1.9007017	-2.6842268	0.2802997
O	-3.0095803	-3.0007920	0.2329340
C	-0.0519523	2.0855885	1.1972556
C	-0.2728545	3.3622959	0.6596553
C	0.1992674	1.9573710	2.5741901
C	-0.2316778	4.4879648	1.4846930
H	-0.4808092	3.4795512	-0.3991533
C	0.2478525	3.0844434	3.3907777
H	0.3714779	0.9743306	3.0049260
C	0.0298096	4.3547859	2.8490629
H	-0.4001547	5.4716903	1.0550207
H	0.4502511	2.9713692	4.4522180
H	0.0620471	5.2328629	3.4875065
C	-0.4256173	1.1087011	-1.5194594
C	0.5610999	1.8012953	-2.2398284
C	-1.6565830	0.8305212	-2.1318583
C	0.3168498	2.2066772	-3.5507956
H	1.5119070	2.0328378	-1.7700603
C	-1.8975908	1.2366542	-3.4439284
H	-2.4209710	0.2937312	-1.5767458
C	-0.9108103	1.9224363	-4.1543696
H	1.0839385	2.7435869	-4.1013955
H	-2.8533482	1.0169558	-3.9106344
H	-1.0974313	2.2363991	-5.1773299
P	1.6345058	-0.6197053	0.4744127
C	2.6105064	-0.5709841	-1.1137591
H	3.3188077	0.2606975	-1.0429860
H	3.1802006	-1.5043227	-1.1715470
H	2.0092555	-0.4595543	-2.0174557

1de• : $PPh_2PMe[Fe(CO)_4]^•$ radical complex

37
Energy = -2903.838195493

P	1.3681311	0.3569674	1.5603588
Fe	-1.8752212	-0.7377651	-0.3685271
C	-0.4106548	-1.2447771	-1.3213919
O	0.4457942	-1.5682281	-2.0228827
C	-2.0497262	1.0352837	-0.5834391
O	-2.2065344	2.1733378	-0.6911430
C	-2.8733164	-1.3213828	-1.7438946
O	-3.5208681	-1.6828044	-2.6281217
C	-3.2235637	-1.1596057	0.7575236
O	-4.1096192	-1.4247613	1.4496839
C	2.3474873	-0.8784571	0.6333746
C	3.4767975	-0.4775617	-0.1000072
C	2.0853225	-2.2507192	0.7735142
C	4.3001812	-1.4259982	-0.7051182
H	3.7121611	0.5779752	-0.2013666
C	2.9109008	-3.1960914	0.1677603
H	1.2225709	-2.5792782	1.3479924
C	4.0180345	-2.7878277	-0.5784764
H	5.1641764	-1.0985797	-1.2767472
H	2.6842174	-4.2531995	0.2747696
H	4.6578370	-3.5248036	-1.0552107
C	1.2007223	1.7856468	0.4244352
C	1.2923747	1.7128808	-0.9745972
C	0.9070483	3.0213284	1.0247458
C	1.0943995	2.8512093	-1.7517198
H	1.5253363	0.7692236	-1.4546510
C	0.6938101	4.1563626	0.2427187
H	0.8481891	3.0900143	2.1083493
C	0.7883844	4.0736288	-1.1471194
H	1.1709084	2.7834053	-2.8333112
H	0.4619350	5.1044316	0.7195444
H	0.6276813	4.9573027	-1.7579054
P	-0.6548754	-0.5281816	1.5052012
C	-1.4523759	0.5216371	2.8024442
H	-2.4570755	0.1473429	3.0125097
H	-0.8518684	0.4815726	3.7150592
H	-1.5273272	1.5619381	2.4681093

1dT : $[Fe(CO)_4]PPh_2PMeT$ complex
65
Energy = -3312.694343693

P	-0.9205136	-0.0202310	-0.2515613
Fe	-0.8161489	-1.1434593	1.7193820
C	0.6323428	-0.2265643	2.2273133
O	1.5560879	0.3318954	2.6582927
C	-0.6630408	-2.6677032	0.7928817
O	-0.5853832	-3.6879670	0.2453101
C	-0.8005312	-2.0242180	3.2642495
O	-0.7939508	-2.5956774	4.2703436
C	-2.4655305	-0.5336837	2.0293319
O	-3.5417812	-0.1588211	2.2542745
P	0.8944208	-0.3735628	-1.5723374
C	-1.4549548	1.7211189	-0.1223008
C	-1.8734293	2.4276066	-1.2632071
C	-1.3737704	2.3934641	1.1039370
C	-2.1936473	3.7803217	-1.1740933
H	-1.9674897	1.9162489	-2.2150788
C	-1.6952084	3.7471780	1.1901238
H	-1.0649680	1.8478768	1.9903429
C	-2.1005565	4.4449744	0.0514779
H	-2.5197057	4.3147925	-2.0617638
H	-1.6322138	4.2548790	2.1482588
H	-2.3514342	5.4996467	0.1186739
C	-2.2022364	-0.7480534	-1.3450252
C	-1.9145622	-1.8357071	-2.1841905
C	-3.5229010	-0.2755402	-1.2746936
C	-2.9203958	-2.4183377	-2.9548778
H	-0.9040492	-2.2282891	-2.2329828
C	-4.5264084	-0.8668452	-2.0392850
H	-3.7679542	0.5542425	-0.6202682
C	-4.2280117	-1.9363996	-2.8864520
H	-2.6793254	-3.2536834	-3.6060426
H	-5.5433278	-0.4909490	-1.9712498
H	-5.0109496	-2.3939144	-3.4843898
C	3.3301464	-1.0758410	-0.7240609
C	4.3936469	-0.7956264	0.3535314
C	5.0410246	0.5761390	0.2434085
C	3.9383814	1.6149622	0.3812624
C	2.8508851	1.5050330	-0.7078938
H	5.7865000	0.7070800	1.0361308
H	3.9154239	-0.8806189	1.3377323
H	5.1389747	-1.5962798	0.2832897
H	3.4626445	1.4957040	1.3612773
H	4.3394622	2.6342586	0.3324726
H	5.5711373	0.6855457	-0.7108749
N	2.3387528	0.0849900	-0.8120126
C	3.9872461	-1.3356847	-2.0918777
H	3.2106663	-1.5013839	-2.8479315
H	4.6165052	-0.5053106	-2.4191229
H	4.6105996	-2.2355164	-2.0398088
C	2.6149817	-2.3630323	-0.2810956
H	2.0088047	-2.1749144	0.6092931
H	1.9713500	-2.7758124	-1.0602439
H	3.3786874	-3.1098448	-0.0358956
C	1.7120426	2.4222570	-0.2610826
H	0.9057736	2.4956065	-0.9911623
H	1.2938439	2.0737824	0.6842625
H	2.1105698	3.4303325	-0.1066512
C	3.4297135	2.0235169	-2.0414710
H	2.7073907	1.9428559	-2.8542802

H	4.3323922	1.4827921	-2.3332944
H	3.6953453	3.0803888	-1.9266390
C	0.4903490	0.7568645	-2.9798906
H	1.2332104	0.5831130	-3.7645736
H	-0.4823806	0.4240656	-3.3582290
H	0.4377542	1.8244148	-2.7586682

1d⁻ : $[Fe(CO)_4]PPh_2PMe^-$ anion complex
37
Energy = -2903.975270991

P	0.5232667	0.6034041	0.1272442
C	0.8395951	2.1528566	-0.8433792
C	2.0386677	0.4951457	1.1584288
P	-0.9820943	0.8627751	1.5996132
C	0.5339529	3.3848706	-0.2497890
C	1.3807025	2.1391927	-2.1343808
C	2.0825455	-0.4720568	2.1745949
C	3.1570808	1.3103520	0.9470490
C	-2.4937803	0.6567644	0.4953479
C	0.7789840	4.5794786	-0.9260810
H	0.0869097	3.3804653	0.7428652
C	1.6223066	3.3338533	-2.8153165
H	1.5990078	1.1887802	-2.6108445
C	3.2196801	-0.6119802	2.9681175
H	1.2135839	-1.1018736	2.3410496
C	4.2967131	1.1669142	1.7410784
H	3.1389271	2.0587680	0.1612304
H	-2.6275144	1.4766255	-0.2189855
H	-2.4536191	-0.2874029	-0.0607426
H	-3.3697326	0.6325009	1.1542233
C	1.3248397	4.5572956	-2.2124433
H	0.5367959	5.5279153	-0.4529136
H	2.0385963	3.3072892	-3.8191726
C	4.3318661	0.2073277	2.7535335
H	3.2392470	-1.3625264	3.7541208
H	5.1568823	1.8083274	1.5675179
H	1.5075275	5.4870923	-2.7449832
H	5.2195921	0.0961125	3.3705474
Fe	0.3852116	-1.2125213	-1.3293352
C	0.2891050	-2.5598267	-2.4786568
C	-0.2026031	-2.1922906	0.0466585
C	-0.7848813	-0.2406231	-2.2589558
C	2.1485061	-1.0644923	-1.5208741
O	0.2319579	-3.4381830	-3.2387030
O	-0.5824215	-2.8873171	0.8990117
O	-1.5360781	0.3717089	-2.9074573
O	3.3046544	-1.0091443	-1.6661210

1d• : $[Fe(CO)_4]PPh_2PMe^•$ radical complex
37
Energy = -2903.843078068

P	0.6534814	0.4384527	-0.0158256
C	0.8176325	2.0625338	-0.8239603
C	2.0370180	0.3915969	1.1718952
P	-1.0901161	0.5991166	1.3133487
C	0.8683780	3.2162425	-0.0228397
C	0.8552325	2.1821050	-2.2165096
C	1.9149436	-0.3240642	2.3713778
C	3.2520413	1.0169909	0.8593555
C	-2.3448465	1.2271898	0.1070992
C	0.9579958	4.4718077	-0.6158414
H	0.8425884	3.1260841	1.0597698
C	0.9461362	3.4440468	-2.8069509
H	0.8250095	1.2893827	-2.8328158
C	2.9945163	-0.4069990	3.2491249
H	0.9791957	-0.8134909	2.6252964
C	4.3293526	0.9287886	1.7398228
H	3.3554475	1.5739778	-0.0664673
H	-1.9340261	1.9881702	-0.5627368
H	-2.7502002	0.4054137	-0.4908622
H	-3.1604662	1.6614441	0.6926239
C	0.9970804	4.5869490	-2.0093477
H	0.9962767	5.3605690	0.0069526
H	0.9778741	3.5306817	-3.8888526
C	4.2030967	0.2181946	2.9350250
H	2.8895792	-0.9583884	4.1787393
H	5.2671478	1.4166898	1.4910032
H	1.0697544	5.5678364	-2.4697725
H	5.0428179	0.1534669	3.6206522
Fe	0.5787570	-1.3700013	-1.3739642
C	0.5714910	-2.8028547	-2.4373825
C	0.4049885	-2.4052025	0.0821735
C	-0.8353865	-0.7014882	-2.2473363
C	2.2327477	-0.9249123	-1.8836459
O	0.5737326	-3.7290093	-3.1278211
O	0.3057184	-3.1150251	0.9938620
O	-1.7374544	-0.3105722	-2.8652228
O	3.3064452	-0.6501455	-2.2268702

2aec• : $PcO[Fe(CO)_4]^•$ radical with CO in ring
27
Energy = -2402.308304082

N	3.8796459	-0.7305673	1.5522905
C	4.5331763	-0.6938906	0.2324395
C	4.6083903	-2.1566908	-0.2243782
H	5.5292048	-0.2528087	0.3314364
H	3.9476386	-0.0878832	-0.4722601
H	4.5469431	-2.2374015	-1.3131912
H	5.5354043	-2.6363224	0.1158503
N	3.4461123	-2.8173838	0.3963752
C	3.7045221	0.5231413	2.2857947
H	3.1886256	0.3177183	3.2277309

H	4.6864816	0.9483895	2.5128643
H	3.1210152	1.2523626	1.7090028
C	3.1172114	-4.1968733	0.0477081
H	2.2698290	-4.5309120	0.6514173
H	2.8451319	-4.2635102	-1.0106163
H	3.9685451	-4.8593841	0.2439540
P	2.8344384	-2.0081353	1.6872955
Fe	0.9760274	-1.9641195	3.6674839
C	1.2827574	-2.3836939	5.4308398
O	1.3982921	-2.6243989	6.5524934
C	1.0099546	-1.5173152	1.7644167
O	0.3256024	-1.0725028	0.8795835
C	-0.4646869	-2.9935988	3.4087118
O	-1.4403303	-3.5909721	3.2286695
C	0.1261947	-0.4395591	3.9851039
O	-0.4758648	0.5365812	4.1570121
O	2.8030819	-2.6879170	3.0712547

2ae_ts : P-to-O 1,2-Fe-shift of $[Fe(CO)_4]PcO^{\bullet}$

27

Energy = -2402.308477915

N	2.0815301	0.3660482	1.1566769
C	3.5163516	0.5911205	0.9003579
C	3.6543722	0.5877328	-0.6252171
H	4.1146690	-0.2074667	1.3581728
H	3.8170587	1.5510027	1.3286801
H	3.4786174	1.5878241	-1.0446174
H	4.6421585	0.2405174	-0.9412967
N	2.6304237	-0.3610733	-1.0912211
C	1.5568075	0.5231935	2.5068920
H	0.4724837	0.3797477	2.4827285
H	1.9956406	-0.2103582	3.1938086
H	1.7712319	1.5333013	2.8700146
C	2.5312665	-0.6467619	-2.5226669
H	1.7493584	-1.3922711	-2.6847478
H	2.2965953	0.2570043	-3.0990813
H	3.4838047	-1.0576724	-2.8690084
P	1.3133114	-0.3966112	-0.0851408
Fe	-1.1972111	-0.3312081	0.1691371
C	-1.6058990	-1.2143490	1.7308613
O	-1.8943933	-1.7288076	2.7213177
C	-0.1589328	0.6821795	-0.9503869
O	0.0908000	1.5632521	-1.7169430
C	-2.3765348	-1.0193435	-1.0036568
O	-3.1628814	-1.3820949	-1.7681740
C	-2.0753920	1.1260397	0.6477507
O	-2.6834876	2.0693022	0.9328376
O	0.6204990	-1.7431557	0.0295592

2ae$^{\bullet}$: $PcO[Fe(CO)_4]^{\bullet}$ radical with N in ring

27

Energy = -2402.306292750

N	2.2140651	-1.5092997	0.2882614
C	3.0777144	-0.8900292	1.2957733
C	1.5512227	-2.7631413	0.6226393
P	1.5517966	-0.4429170	-0.8694189
C	3.7108497	0.2830834	0.5594293
H	3.8316756	-1.6086963	1.6349362
H	2.5172804	-0.5477106	2.1806117
H	2.2970578	-3.5206933	0.8903786
H	0.8482818	-2.6566650	1.4622027
H	0.9913276	-3.1173245	-0.2483416
N	2.6332173	0.8128853	-0.2918456
O	0.1185321	0.0997847	-0.4143270
H	4.0619288	1.0696079	1.2369060
H	4.5568746	-0.0479422	-0.0590123
C	3.0389644	1.8711494	-1.2222369
H	3.3782499	2.7411756	-0.6501200
H	3.8568589	1.5389294	-1.8746958
H	2.1844339	2.1617159	-1.8378926
Fe	-0.3671898	1.1626246	1.1184673
C	-2.0773717	0.6293222	0.7261280
C	1.3524488	1.9571956	1.2530312
C	-0.9830280	2.6167646	1.9617436
C	-0.1720096	0.0971230	2.5841014
O	-3.1496997	0.2835276	0.5115890
O	2.1353320	2.6833193	1.7050149
O	-1.3754001	3.5541567	2.5090222
O	-0.0731351	-0.5641126	3.5220655

2aT : $[Fe(CO)_4]PcOT$ complex

55

Energy = -2811.122444815

N	2.5634725	0.2080632	0.3404766
C	3.5267031	-0.2465694	-0.6731935
C	2.6743848	-0.9320659	-1.7405453
H	4.2520880	-0.9441100	-0.2359858
H	4.0598772	0.6180374	-1.0767451
H	2.3098241	-0.2055623	-2.4827517
H	3.2329914	-1.7160534	-2.2640814
N	1.5430688	-1.5224224	-1.0160681
C	2.7558458	1.5006162	0.9804475
H	1.8565350	1.7670516	1.5375018
H	3.6099700	1.4931746	1.6675338
H	2.9252286	2.2652927	0.2129207
C	0.4970460	-2.1097677	-1.8444537
H	-0.3123156	-2.4918020	-1.2231231
H	0.0818015	-1.3688135	-2.5427268
H	0.9109732	-2.9444825	-2.4205563
P	1.2584530	-0.8105363	0.4745642
Fe	-0.7216225	0.0832856	0.9424230
C	-0.1133215	0.5211748	2.5621913

O	0.2420220	0.7948864	3.6339787
C	-2.2964472	0.8781743	1.2306949
O	-3.3139391	1.3948695	1.4160152
C	-1.4498050	-1.5462993	0.8920959
O	-1.9511147	-2.5942720	0.8957121
C	-0.4440382	1.0674938	-0.5254693
O	-0.2540447	1.7031581	-1.4794779
O	1.4107797	-1.9481790	1.6496324
C	3.2379687	-2.3332877	3.1453555
C	2.3594900	-4.1613864	1.5757368
C	4.5069875	-3.1844872	3.3603357
C	3.6584571	-4.9509878	1.8469190
C	4.2508527	-4.6810341	3.2252361
H	4.9053234	-2.9333373	4.3502954
H	5.2558838	-2.8782407	2.6180881
H	3.4270842	-6.0139703	1.7120153
H	4.3927325	-4.6754372	1.0784608
H	5.1866879	-5.2377903	3.3498712
H	3.5708254	-5.0286137	4.0121531
N	2.7025510	-2.7119813	1.7895363
C	2.2549332	-2.4851482	4.3245931
H	2.6347880	-1.9016505	5.1700070
H	1.2724180	-2.0925236	4.0545999
H	2.1442141	-3.5174960	4.6584403
C	3.6716163	-0.8665160	3.0848942
H	4.2976199	-0.6874240	2.2074951
H	2.8075706	-0.2005443	3.0541728
H	4.2474164	-0.6294297	3.9857246
C	1.1860854	-4.7041655	2.4168754
H	0.8460858	-5.6450341	1.9711003
H	1.4595051	-4.9082117	3.4525999
H	0.3512181	-3.9997715	2.4034860
C	2.0037257	-4.3627501	0.0991986
H	1.0126902	-3.9656469	-0.1236897
H	2.7364009	-3.8748769	-0.5474249
H	1.9927490	-5.4372320	-0.1139102

2a^{-} : [Fe(CO)$_4$]PcO^{-} anion complex
27
Energy = -2402.493068467

N	2.1650947	0.8680597	0.1129164
C	3.0957255	0.4799169	-0.9483026
C	2.3046278	-0.5038046	-1.8008330
H	4.0038028	-0.0016276	-0.5429379
H	3.4011704	1.3633210	-1.5218112
H	1.6264889	0.0334393	-2.4830860
H	2.9642425	-1.1434736	-2.4008160
N	1.5688560	-1.3177981	-0.8327957
C	2.7107758	1.7509397	1.1350783
H	1.9299475	2.0109595	1.8525214
H	3.5484331	1.2926552	1.6862150
H	3.0673466	2.6748061	0.6640063
C	0.6596633	-2.3073816	-1.3919071
H	0.2701528	-2.9459663	-0.5965889
H	-0.1925978	-1.8506203	-1.9209395
H	1.2108775	-2.9397736	-2.0980940
P	1.1874366	-0.4566459	0.6030642
Fe	-1.0222415	0.1774380	0.7649471
C	-0.5448889	1.0727494	2.2227352
O	-0.2979899	1.6539397	3.2057612
C	-0.7963888	0.8630891	-0.8619959
O	-0.6662202	1.3182415	-1.9291163
C	-1.3837703	-1.5391605	1.0509116
O	-1.6673148	-2.6505408	1.2706733
C	-2.7267163	0.6814386	0.8401909
O	-3.8413653	1.0134836	0.8869963
O	1.6882771	-1.1774720	1.8332938

2a$^{\bullet}$: [Fe(CO)$_4$]PcO$^{\bullet}$ radical complex
27
Energy = -2402.336354476

N	2.1477959	0.8349291	0.1980465
C	2.9618968	0.6607610	-1.0109941
C	2.2558555	-0.4180577	-1.8368322
H	3.9761024	0.3389264	-0.7300773
H	3.0373504	1.6059261	-1.5577791
H	1.5186973	0.0249496	-2.5212727
H	2.9727679	-0.9903718	-2.4352152
N	1.6248182	-1.2990161	-0.8531738
C	2.6375958	1.7691502	1.2041227
H	1.9877419	1.7472403	2.0807446
H	3.6562706	1.5059157	1.5209607
H	2.6444113	2.7861648	0.7983362
C	0.9062088	-2.4745653	-1.3305442
H	0.5306046	-3.0391477	-0.4734184
H	0.0621309	-2.2136113	-1.9857454
H	1.5930997	-3.1174787	-1.8907399
P	1.2145247	-0.5226786	0.5833615
Fe	-0.9223363	0.3492313	0.7188396
C	-0.4330784	0.6825117	2.4453567
O	-0.2017848	0.8753088	3.5554654
C	-0.9278656	0.4187390	-1.0980405
O	-0.9808229	0.4437592	-2.2481129
C	-1.6522876	-1.2791654	0.9526174
O	-2.1095980	-2.3265080	1.0999528
C	-2.4245876	1.3669564	0.8548490
O	-3.3813856	1.9998087	0.9469446
O	1.5692989	-1.3094650	1.8124351

2be_ts : P-to-S 1,2-Fe-shift of [Fe(CO)$_4$]PcS$^{\bullet}$
27
Energy = -2725.272294898

N	2.0282321	0.3408584	1.4106722
C	3.4313278	-0.0939359	1.4765845
C	3.9718179	0.1975596	0.0819278
H	3.5071794	-1.1659262	1.7148171
H	3.9513380	0.4796947	2.2494046
H	4.2259373	1.2639339	-0.0262252
H	4.8604849	-0.4005125	-0.1477417
N	2.8771630	-0.1944744	-0.8112369
C	1.2856656	0.4679682	2.6540275
H	0.3202923	0.9374152	2.4516398
H	1.1125349	-0.5030011	3.1386690
H	1.8462996	1.1102381	3.3412926
C	3.0733832	-0.0146549	-2.2469148
H	2.1799599	-0.3554466	-2.7769148
H	3.2709477	1.0339258	-2.5148108
H	3.9218985	-0.6256195	-2.5721236
P	1.3369040	0.0988824	-0.1098935
Fe	-1.4263173	0.0663713	-0.1823341
C	-1.5487696	-0.6581230	1.4728445
O	-1.6584037	-1.1692238	2.4991534
C	-0.9862139	0.5917463	-1.8706864
O	-0.7132616	0.8864452	-2.9480010
C	-2.9994973	-0.6627624	-0.6931190
O	-4.0375444	-1.0585088	-1.0046378
C	-1.8211174	1.7244561	0.3594793
O	-2.1084623	2.7882635	0.7062531
S	0.2548487	-1.6457574	-0.4562237

2be• : PcS[Fe(CO)$_4$]• radical complex

27

Energy = -2725.284811699

N	2.0285065	-1.4960827	-0.1751908
C	2.6030869	-1.0335939	1.0844788
C	1.1231309	-2.6399661	-0.1101413
P	1.6765208	-0.1722752	-1.1954249
C	3.5401838	0.0983770	0.6887470
H	3.1110538	-1.8505443	1.6050830
H	1.7927692	-0.6437935	1.7410747
H	1.6679459	-3.5062775	0.2775609
H	0.2629959	-2.4398184	0.5432512
H	0.7542016	-2.8686587	-1.1127113
N	2.8595668	0.7747620	-0.4241209
S	-0.2537276	0.5681205	-0.5302199
H	3.7091835	0.7936043	1.5198785
H	4.5136255	-0.2937987	0.3582414
C	3.6164270	1.7828837	-1.1594158
H	3.8399745	2.6325064	-0.5050992
H	4.5627922	1.3748754	-1.5435204
H	3.0206180	2.1450768	-2.0006404
Fe	-0.1221277	1.1277746	1.7031552
C	-1.1909971	-0.3351227	1.8576025
C	1.1095290	2.3964181	1.2112951
C	-1.4596322	2.3285632	1.9201787
C	0.5031321	1.0238142	3.3821328
O	-1.9021204	-1.2344576	1.9562830
O	1.7651687	3.3084317	0.9666584
O	-2.3148011	3.0855866	2.0683262
O	0.8932716	0.9674289	4.4669485

2bT : [Fe(CO)$_4$]PcST complex

55

Energy = -3134.120363150

P	1.0949025	-0.6117818	0.3720105
S	0.9917286	-2.0053291	1.9921996
Fe	-0.8812091	0.4050041	0.5873732
N	2.4420514	0.3679409	0.3062257
C	3.4642116	-0.1182092	-0.6299502
C	2.6708947	-0.8364134	-1.7181091
H	4.1704875	-0.7982830	-0.1355871
H	4.0170001	0.7364346	-1.0298632
H	2.3157564	-0.1246907	-2.4785463
H	3.2640090	-1.6131431	-2.2118778
N	1.5402633	-1.4559376	-1.0148064
C	2.6828163	1.5763061	1.0794951
H	1.7529459	1.8908316	1.5552647
H	3.4457902	1.4288705	1.8521677
H	3.0121369	2.3736699	0.4034615
C	0.5588942	-2.1593039	-1.8330490
H	-0.1770801	-2.6454278	-1.1926042
H	0.0368031	-1.4785500	-2.5204859
H	1.0685948	-2.9328634	-2.4156778
C	-0.4524058	0.8523862	2.2665934
O	-0.2296245	1.1747349	3.3604434
C	-2.4233984	1.3072312	0.6789876
O	-3.4160986	1.8974954	0.7306976
C	-1.7355093	-1.1548080	0.3820937
O	-2.3509113	-2.1323996	0.2603677
C	-0.3478435	1.3639495	-0.8211435
O	0.0015289	1.9904391	-1.7355152
C	3.3084829	-2.4818241	3.2862330
C	2.3163873	-4.3501844	1.7523056
C	4.6508756	-3.2338156	3.2143430
C	3.7126851	-5.0004541	1.7627134
C	4.4923205	-4.7398614	3.0458073
H	5.2146751	-2.9910740	4.1226462
H	5.2191548	-2.8397588	2.3610510
H	3.5776170	-6.0746503	1.5900010
H	4.2825717	-4.6010068	0.9131059
H	5.4765888	-5.2192129	2.9937876
H	3.9751097	-5.1752055	3.9096375
N	2.4688458	-2.8831183	2.0917820
C	2.6127545	-2.7300534	4.6392858

H	3.1978136	-2.2634531	5.4393788
H	1.6156677	-2.2771794	4.6393423
H	2.5123686	-3.7917321	4.8717362
C	3.6180415	-0.9865111	3.1745492
H	4.0680538	-0.7678175	2.2028807
H	2.7158425	-0.3811653	3.2936469
H	4.3256222	-0.7071337	3.9621764
C	1.3561272	-5.1003833	2.6968079
H	1.1554504	-6.0986350	2.2926244
H	1.7621670	-5.2203679	3.7028539
H	0.4027833	-4.5656442	2.7678258
C	1.7691919	-4.4651708	0.3265086
H	0.7307813	-4.1291778	0.2737445
H	2.3684977	-3.8632475	-0.3599594
H	1.8050854	-5.5149476	0.0161949

2b^{-} : [Fe(CO)$_4$]PcS anion complex

27

Energy = -2725.450158536

N	2.1420587	0.8892375	0.0835556
C	3.1046374	0.4705390	-0.9411697
C	2.6695351	1.7764420	1.1128153
P	1.1819394	-0.4530771	0.5764707
C	2.3154276	-0.4932110	-1.8171139
H	3.9808181	-0.0356990	-0.5002320
H	3.4496813	1.3478705	-1.4996178
H	1.8567980	2.1079468	1.7625512
H	3.4343373	1.2866579	1.7366321
H	3.1093993	2.6558219	0.6294014
N	1.5555149	-1.2971698	-0.8623501
S	1.9164992	-1.4258011	2.1613060
H	1.6605314	0.0590879	-2.5101605
H	2.9755859	-1.1436322	-2.4042546
C	0.6806476	-2.3292795	-1.3887348
H	0.3438304	-2.9741664	-0.5735914
H	-0.2059463	-1.9187359	-1.8993316
H	1.2425549	-2.9442519	-2.1011429
Fe	-1.0199682	0.1824799	0.7709856
C	-0.5526704	1.0436884	2.2584169
C	-0.8008961	0.8857304	-0.8512537
C	-1.4256228	-1.5346189	1.0167863
C	-2.7153065	0.7177850	0.8518225
O	-0.3196352	1.6063859	3.2531623
O	-0.6765317	1.3463033	-1.9156656
O	-1.7443225	-2.6406963	1.2023863
O	-3.8220144	1.0716683	0.9028973

2b$^{\bullet}$: [Fe(CO)$_4$]PcS$^{\bullet}$ radical complex

27

Energy = -2725.291630915

N	2.1295332	0.8524606	0.1972841
C	2.9608150	0.6755521	-1.0030557
C	2.6722758	1.7128847	1.2435406
P	1.2025751	-0.5259232	0.5576320
C	2.2267037	-0.3519544	-1.8633379
H	3.9564706	0.3052815	-0.7161683
H	3.0779040	1.6334169	-1.5188768
H	2.0008878	1.7246627	2.1033556
H	3.6562747	1.3562875	1.5778743
H	2.7719910	2.7331935	0.8605599
N	1.6113809	-1.2651966	-0.9002013
S	1.6970545	-1.6266770	2.1163076
H	1.4831274	0.1316511	-2.5130501
H	2.9229317	-0.9100314	-2.4979229
C	0.9529949	-2.4751311	-1.3708553
H	0.6432388	-3.0676980	-0.5056824
H	0.0734213	-2.2626142	-1.9958305
H	1.6624717	-3.0666151	-1.9588044
Fe	-0.9369970	0.3541917	0.7101489
C	-0.4555711	0.8097567	2.4168639
C	-0.9910980	0.3288756	-1.1072282
C	-1.6623526	-1.2642034	1.0422721
C	-2.4480505	1.3647123	0.8058894
O	-0.2584687	1.1023244	3.5114784
O	-1.0825914	0.2937017	-2.2545340
O	-2.1210447	-2.2999434	1.2470007
O	-3.4089958	1.9943405	0.8699116

2ce_ts : 1,2-Fe-shift of [Fe(CO)$_4$]PcNMe$^{\bullet}$

31

Energy = -2421.699777690

N	2.3890059	0.8593942	0.0841848
C	3.3386645	-0.0247630	-0.5906019
C	2.6487107	-1.3843976	-0.6355221
H	4.2826189	-0.0771090	-0.0280648
H	3.5527706	0.3581179	-1.5948225
H	1.9607416	-1.4526923	-1.4959673
H	3.3656409	-2.2091613	-0.6954130
N	1.9144168	-1.4439264	0.6297908
C	2.6793434	2.2839093	0.0915609
H	1.8349652	2.8149427	0.5314263
H	3.5900294	2.4962914	0.6690350
H	2.8267336	2.6374330	-0.9360335
C	1.1876328	-2.6722328	0.9047812
H	0.6815972	-2.5886726	1.8694269
H	0.4391976	-2.9008394	0.1301313
H	1.8993119	-3.5029401	0.9571869
P	1.1845809	0.1087640	0.9768260
Fe	-1.0307691	0.0840016	-0.2251246
C	-0.1096464	0.9174419	-1.5422310
O	0.4374335	1.4591564	-2.4013045
C	-1.5062797	-0.9530835	1.1808525

O	-1.8905007	-1.6116625	2.0503785
C	-2.5576921	1.0381731	-0.3602163
O	-3.5529838	1.6107386	-0.4881223
C	-1.2925955	-1.3015413	-1.3072021
O	-1.4806180	-2.1953918	-2.0208575
N	0.0210282	1.3512934	1.0267593
C	-0.6312380	1.7659213	2.2714785
H	0.0453512	2.4214290	2.8344403
H	-1.5335549	2.3298307	2.0138473
H	-0.9284643	0.9347915	2.9248257

2ce• : PcNMe[Fe(CO)$_4$]• radical complex

31

Energy = -2421.733886154

N	2.1081390	-1.3843559	-0.2173123
C	2.7429276	-1.0765177	1.0590295
C	1.1419387	-2.4781530	-0.2174315
P	1.7178683	0.0543020	-1.0988139
C	3.7004402	0.0526777	0.7164521
H	3.2527262	-1.9565869	1.4645582
H	1.9940183	-0.7330854	1.8043274
H	1.6431656	-3.4119284	0.0590150
H	0.3178895	-2.3034955	0.4912315
H	0.7193690	-2.5882125	-1.2206152
N	2.9354743	0.9123724	-0.2040393
H	4.0099824	0.6269517	1.5970369
H	4.5996076	-0.3361478	0.2177022
C	3.7037101	1.9566993	-0.8804733
H	4.0659000	2.6791687	-0.1407877
H	4.5673374	1.5366093	-1.4139250
H	3.0607997	2.4778674	-1.5935889
Fe	0.0604484	1.1832605	1.4321789
C	-1.2377164	-0.0780899	1.4716879
C	1.6928236	2.1201554	1.4277972
C	-0.9975778	2.6455598	1.3041896
C	0.2086741	1.1202474	3.2148354
O	-2.0784260	-0.8663766	1.5102644
O	2.4636865	2.9319303	1.7238794
O	-1.6806243	3.5735677	1.2454034
O	0.3063371	1.0789247	4.3664993
N	0.3045929	0.7287676	-0.4665424
C	-0.8470769	0.7347837	-1.3829417
H	-0.5170372	0.5279627	-2.4086752
H	-1.6006630	-0.0180323	-1.1149644
H	-1.3336798	1.7164881	-1.3672940

2cT : [Fe(CO)$_4$]PcNMeT complex

59

Energy = -2830.564117340

P	1.1360225	-0.9042923	0.5015877
Fe	-0.7314209	0.3703706	0.5871764
N	2.5615566	-0.0313159	0.5009041
N	1.4871411	-1.6091264	-0.9931933
N	1.1666597	-2.0921474	1.7288816
C	-0.3664564	0.6970740	2.2998188
C	-2.1067716	1.5081032	0.6222428
C	-1.7928146	-1.0099087	0.1945615
C	0.0258919	1.2556516	-0.7709824
C	3.5185695	-0.5072838	-0.5092769
C	2.7534784	1.3036685	1.0509889
C	2.6638848	-1.0456728	-1.6545175
C	0.4666780	-2.1956715	-1.8474258
N	2.3912472	-2.7920357	1.9532426
C	-0.0807845	-2.5845029	2.3437280
O	-0.1660659	0.9187284	3.4246380
O	-2.9946224	2.2489325	0.6495509
O	-2.5340893	-1.8747426	-0.0396348
O	0.5027773	1.8378669	-1.6559632
H	4.1536770	-1.2978013	-0.0892896
H	4.1489092	0.3260161	-0.8289962
H	1.9255954	1.5552756	1.7125237
H	3.6838875	1.3556968	1.6280704
H	2.7949315	2.0517893	0.2484883
H	2.3811498	-0.2447901	-2.3552305
H	3.1854471	-1.8301742	-2.2165129
H	-0.3019234	-2.6769229	-1.2420088
H	-0.0144571	-1.4419163	-2.4884171
H	0.9218127	-2.9621636	-2.4844814
C	2.4154394	-4.2502389	1.5501909
C	3.0789887	-2.4227158	3.2494301
H	-0.5436309	-3.3893996	1.7603728
H	0.1375958	-2.9521095	3.3440733
H	-0.7908650	-1.7622291	2.4210168
C	3.8980328	-4.6722293	1.4942906
C	1.6582375	-5.2636407	2.4525796
C	1.8459231	-4.4044933	0.1398213
C	4.5259872	-2.9540306	3.1595794
C	2.4029754	-2.9071510	4.5567011
C	3.1921201	-0.9020726	3.3700463
C	4.6280346	-4.4331709	2.8113762
H	3.9374612	-5.7298565	1.2063586
H	4.3874695	-4.0929889	0.7002863
H	1.6597948	-6.2301371	1.9362454
H	2.1378263	-5.4169090	3.4194795
H	0.6190881	-4.9828781	2.6225971
H	0.7817204	-4.1578634	0.1015591
H	2.3767580	-3.7651227	-0.5648549
H	1.9585148	-5.4500485	-0.1646050
H	5.0232924	-2.7354841	4.1120677
H	5.0407529	-2.3758612	2.3809220
H	3.0600341	-2.6518509	5.3958519
H	1.4549267	-2.3875037	4.7215314

H	2.2219097	-3.9800981	4.5914503
H	3.7928364	-0.4990736	2.5563513
H	2.2122395	-0.4205009	3.3666933
H	3.6849745	-0.6675090	4.3196975
H	5.6806280	-4.7263063	2.7204926
H	4.1985076	-5.0501382	3.6101949

2c⁻ : $[Fe(CO)_4]PcNMe^-$ anion complex

31

Energy = -2421.891679309

N	2.5792696	0.5251763	0.0710891
C	3.3482200	0.4888431	-1.1712161
C	3.3157899	0.9789013	1.2419361
P	1.5803170	-0.8751960	0.2595146
C	2.4374353	-0.2207300	-2.1675447
H	4.2915115	-0.0745696	-1.0478511
H	3.5966902	1.5063087	-1.4982501
H	2.6642104	0.9608212	2.1179202
H	4.1936281	0.3458100	1.4550908
H	3.6568584	2.0097318	1.0857596
N	1.8198593	-1.2868034	-1.3858911
N	2.2028032	-2.0179969	1.1593853
H	1.6941693	0.4768479	-2.5844806
H	3.0091656	-0.6522906	-2.9992528
C	0.8745076	-2.1487090	-2.0739023
C	1.6555395	-2.4960919	2.4095810
H	0.5915979	-2.9727589	-1.4144515
H	-0.0417756	-1.6176415	-2.3809927
H	1.3513081	-2.5692413	-2.9676480
H	2.2459121	-2.1489423	3.2742836
H	0.6151173	-2.1725139	2.5795642
H	1.6623447	-3.5968773	2.4352480
Fe	-0.6025185	-0.2055583	0.7691712
C	0.0341937	0.3337971	2.3347893
C	-2.2661471	0.2988379	1.1287003
C	-1.0495766	-1.9165507	0.5799377
C	-0.4414956	0.8762548	-0.6319627
O	0.3895011	0.7036885	3.3867585
O	-3.3572572	0.6342186	1.3635121
O	-1.3924167	-3.0299043	0.4833143
O	-0.3829949	1.6123053	-1.5374009

2c• : $[Fe(CO)_4]PcNMe^•$ radical complex

31

Energy = -2421.742413046

N	2.5284607	0.6186986	0.0661635
C	3.5231595	0.1773157	-0.9272327
C	2.9898550	1.5262308	1.1138614
P	1.4132868	-0.6096491	0.3536876
C	2.7160776	-0.6478996	-1.9212341
H	4.3223659	-0.4219125	-0.4650850
H	3.9712411	1.0569270	-1.3982902
H	2.1329429	1.8917562	1.6815312
H	3.6975035	1.0468161	1.8036167
H	3.4793602	2.3809600	0.6373929
N	1.7445465	-1.3938467	-1.1029642
N	1.9313923	-1.4886318	1.6676849
H	2.1960971	0.0061133	-2.6368390
H	3.3463538	-1.3501096	-2.4764271
C	0.7508593	-2.1737250	-1.8391459
C	2.0028729	-2.9319034	1.6507928
H	0.1667921	-2.7870568	-1.1531259
H	0.0674043	-1.5346512	-2.4163562
H	1.2757663	-2.8422616	-2.5285782
H	2.6980983	-3.2698483	2.4256977
H	1.0159197	-3.3600928	1.8900965
H	2.3037650	-3.3262808	0.6694538
Fe	-0.6546912	-0.0088617	0.9028188
C	-0.0183752	0.6569639	2.4479508
C	-2.3084810	0.5565408	1.3106528
C	-1.1914613	-1.7150829	0.8432355
C	-0.6124565	0.9421412	-0.6103196
O	0.3147358	1.0853134	3.4724323
O	-3.3714304	0.9271928	1.5677994
O	-1.5723388	-2.8123553	0.8429633
O	-0.5838548	1.5503662	-1.5975223

2de_ts : 1,2-Fe-shift of $[Fe(CO)_4]PcPMe^•$

31

Energy = -2708.346055296

N	2.2634376	-0.0313454	1.2374555
C	3.2636675	0.7597544	0.5111371
C	2.8822835	0.6511660	-0.9644312
H	4.2615561	0.3392604	0.7001204
H	3.2560461	1.8007381	0.8546745
H	2.1851486	1.4549612	-1.2534567
H	3.7569039	0.6989744	-1.6203918
N	2.2349293	-0.6591374	-1.0813754
C	2.3576652	-0.0479034	2.6882498
H	1.6995344	-0.8188505	3.0913092
H	3.3929390	-0.2644224	2.9831143
H	2.0655671	0.9202717	3.1152129
C	1.7954491	-1.0530586	-2.4123111
H	1.3248616	-2.0379239	-2.3636825
H	1.0810920	-0.3390226	-2.8478713
H	2.6685198	-1.1140082	-3.0699009
P	1.2289611	-0.9580818	0.2915943
Fe	-0.9655822	0.4291226	-0.2983496
C	-0.1326373	1.6833964	0.6867370
O	0.3773688	2.5007488	1.3252602
C	-0.6715826	1.3640869	-1.7924292
O	-0.5210440	1.9913266	-2.7539108

C	-1.2501204	-1.0816498	-1.2308509
O	-1.4849649	-2.0326089	-1.8479843
C	-2.6732853	0.8340723	0.0927023
O	-3.7711660	1.0911950	0.3450629
P	-0.7250989	-0.8763487	1.6730814
C	-1.4526029	-2.5546132	1.3391592
H	-1.4062697	-3.1224102	2.2741881
H	-2.4982204	-2.4734203	1.0268940
H	-0.8918858	-3.0970402	0.5711220

2de• : PcPMe[Fe(CO)$_4$]• radical complex

31

Energy = -2708.364342998

N	2.0977996	-1.6477169	-0.0659018
C	2.7073421	-1.1417864	1.1735311
C	1.1880207	-2.7853497	0.0418305
P	1.7895922	-0.3801623	-1.1419232
C	3.6069196	0.0219965	0.7479644
H	3.2677348	-1.9392377	1.6700072
H	1.9147302	-0.7794285	1.8507888
H	1.7309287	-3.6363353	0.4647574
H	0.3242503	-2.5645726	0.6813522
H	0.8287429	-3.0563320	-0.9534918
N	2.9946208	0.5722467	-0.4699652
H	3.6609297	0.7857237	1.5331492
H	4.6277190	-0.3145446	0.5183702
C	3.7201912	1.5977984	-1.2090861
H	3.7898128	2.5172750	-0.6192071
H	4.7350211	1.2529013	-1.4524834
H	3.1929586	1.8180572	-2.1401972
Fe	-0.2758359	1.1659194	1.6826433
C	-0.9181480	-0.4809060	2.0715755
C	0.8338655	2.3928538	1.0011415
C	-1.7878466	2.1201871	1.7216768
C	0.3826171	1.3730472	3.3351629
O	-1.3708949	-1.5105865	2.3408858
O	1.5198004	3.2385186	0.6036074
O	-2.7630110	2.7429236	1.7406700
O	0.8171912	1.5124096	4.3992435
P	-0.3152851	0.4121773	-0.4959996
C	-0.2980586	1.8289599	-1.7189181
H	-0.2869944	1.4006365	-2.7267147
H	-1.2299047	2.3884390	-1.5901547
H	0.5402459	2.5222030	-1.6156310

2dT : [Fe(CO)$_4$]PcNMeT complex

59

Energy = -3117.219316383

P	1.0591264	-0.6339558	0.3971981
Fe	-0.8935368	0.5032009	0.2829880
N	2.4161295	0.3602050	0.4427661
N	1.6394119	-1.4540913	-0.9829738
P	0.7710925	-2.4895794	1.6303101
C	-0.6807928	1.0503167	1.9665943
C	-2.3939482	1.4567608	0.0928373
C	-1.7798314	-1.0273298	0.0032209
C	-0.1088002	1.3746644	-1.0616414
C	3.4911936	-0.0787412	-0.4531743
C	2.6035001	1.5431184	1.2650895
C	2.7647383	-0.7536413	-1.6117270
C	0.7066817	-2.1299280	-1.8789117
N	2.2694797	-3.1790472	2.0602162
C	-0.1527932	-1.9371185	3.1350343
O	-0.5961200	1.4334768	3.0632048
O	-3.3598334	2.0815105	-0.0344630
O	-2.4426051	-1.9624418	-0.1939830
O	0.3956273	1.9579226	-1.9320365
H	4.1804830	-0.7756943	0.0449235
H	4.0578160	0.7971018	-0.7832315
H	1.6390797	1.8711234	1.6546622
H	3.2837988	1.3662267	2.1077288
H	3.0149058	2.3481062	0.6450678
H	2.4194974	-0.0069020	-2.3423817
H	3.3999480	-1.4819741	-2.1268094
H	0.0051478	-2.7235382	-1.2895488
H	0.1408931	-1.4206486	-2.5012194
H	1.2691733	-2.8060797	-2.5303079
C	2.4416940	-4.6021979	1.5514296
C	3.1152762	-2.6995365	3.2135554
H	-0.4182401	-2.8425009	3.6900112
H	0.3496139	-1.2383389	3.8052796
H	-1.0777502	-1.4804805	2.7732148
C	3.9350025	-4.9774057	1.5003816
C	1.6513063	-5.6024005	2.4162415
C	1.9322168	-4.7160178	0.1045290
C	4.5742799	-3.1678631	3.0338356
C	2.5963552	-3.1869146	4.5841194
C	3.1646194	-1.1701324	3.2093033
C	4.6980485	-4.6626367	2.7783201
H	3.9941398	-6.0434865	1.2520639
H	4.3971267	-4.4244981	0.6711527
H	1.6799360	-6.5964834	1.9556131
H	2.0488056	-5.6875772	3.4298075
H	0.6040182	-5.2852319	2.4803891
H	0.8425721	-4.6713169	0.0440409
H	2.3498316	-3.9106225	-0.5051034
H	2.2596070	-5.6807126	-0.2998458
H	5.1299077	-2.8660082	3.9294933
H	5.0087700	-2.6278006	2.1817352
H	3.1991798	-2.7312999	5.3777375
H	1.5556521	-2.9027411	4.7431197
H	2.6722701	-4.2708303	4.6887678

H	3.5994201	-0.8189164	2.2729699
H	2.1832449	-0.7070690	3.3307972
H	3.7965036	-0.8337009	4.0375138
H	5.7518111	-4.9435980	2.6690432
H	4.3028024	-5.2396103	3.6233217

2d⁻ : $[Fe(CO)_4]PcNMe^-$ anion complex

31

Energy = -2708.504719307

N	2.4141091	0.3937748	0.2008553
C	3.2285647	0.0693090	-0.9660227
C	3.0953186	1.0366262	1.3108407
P	1.1631577	-0.7548127	0.5049164
C	2.2860716	-0.6820287	-1.9010620
H	4.0905844	-0.5653111	-0.6945847
H	3.6102708	0.9882700	-1.4288213
H	2.3998818	1.1630837	2.1424187
H	3.9534016	0.4457867	1.6724871
H	3.4594367	2.0246213	1.0018812
N	1.4824094	-1.5084118	-1.0059236
P	1.4437529	-2.0974566	2.0904721
H	1.6702839	0.0206390	-2.4847373
H	2.8372025	-1.3224894	-2.6006395
C	0.4893524	-2.3802786	-1.6066474
C	3.1345564	-2.7822376	1.5781057
H	0.0628243	-3.0171141	-0.8270611
H	-0.3277619	-1.8226435	-2.0934709
H	0.9738564	-3.0191108	-2.3544717
H	3.3172863	-3.6973548	2.1539682
H	3.1485145	-3.0334070	0.5119905
H	3.9531378	-2.0834104	1.7850018
Fe	-0.8844410	0.2730057	0.7485583
C	-0.2931689	0.8667944	2.3210758
C	-2.4621118	1.0778240	0.9031747
C	-1.6202413	-1.3534454	0.6973391
C	-0.4670900	1.1727763	-0.7262955
O	0.0102018	1.3112509	3.3575722
O	-3.4925182	1.6104573	0.9995143
O	-2.1879386	-2.3726112	0.6704929
O	-0.2131366	1.7870713	-1.6862153

2d• : $[Fe(CO)_4]PcPMe^•$ radical complex

31

Energy = -2708.369548417

N	2.4235575	0.3587353	0.1983928
C	3.3232860	-0.0703220	-0.8782214
C	2.9611202	1.2207411	1.2432458
P	1.1286645	-0.7010340	0.4334811
C	2.4205811	-0.8139841	-1.8568737
H	4.1283581	-0.7183987	-0.5031232
H	3.7762919	0.8143054	-1.3374638
H	2.1534740	1.5406330	1.9037679
H	3.7324430	0.7176200	1.8433062
H	3.4017760	2.1082751	0.7782903
N	1.4434432	-1.5201486	-1.0132310
P	1.5383817	-2.1306445	2.0667009
H	1.9180750	-0.1105996	-2.5368375
H	2.9792897	-1.5418168	-2.4535278
C	0.4127795	-2.2988937	-1.6955123
C	3.1671006	-2.7996547	1.4893350
H	-0.1407149	-2.8974343	-0.9698905
H	-0.2939840	-1.6614935	-2.2457293
H	0.8995821	-2.9806630	-2.3992841
H	3.4019322	-3.6979770	2.0677663
H	3.1340389	-3.0453990	0.4237845
H	3.9622227	-2.0631578	1.6603333
Fe	-0.8516015	0.2550648	0.8012058
C	-0.2995976	0.7427484	2.4288534
C	-2.4196125	1.1036635	0.9964567
C	-1.6298248	-1.3528159	0.7819744
C	-0.5053922	1.1734744	-0.6953591
O	-0.0018181	1.0711344	3.5033336
O	-3.4274102	1.6567851	1.1152198
O	-2.1817491	-2.3749479	0.7928382
O	-0.2789256	1.7653716	-1.6685208

3aa• : higher $[W(CO)_5]PPh_2O^•$ radical complex

35

Energy = -1514.544602916

P	0.6376233	1.3298833	-0.0386598
O	2.0949351	0.8547317	-0.2154122
C	0.4423268	2.2903683	1.4876083
C	0.0860863	2.3662456	-1.4151932
C	-0.4168820	3.3909155	1.6049897
C	1.1952642	1.8720604	2.5964635
C	1.0412424	2.7743353	-2.3573583
C	-1.2621089	2.7151213	-1.5894372
C	-0.5224296	4.0633534	2.8226140
H	-0.9871643	3.7367380	0.7493519
C	1.0922937	2.5528744	3.8062614
H	1.8679335	1.0246309	2.4994672
C	0.6502347	3.5421369	-3.4535400
H	2.0794851	2.4850844	-2.2262375
C	-1.6446348	3.4853717	-2.6856990
H	-2.0143760	2.3841054	-0.8800948
C	0.2288860	3.6458067	3.9224530
H	-1.1862307	4.9186987	2.9078854
H	1.6839528	2.2312140	4.6581444
C	-0.6896002	3.8996621	-3.6176277
H	1.3925387	3.8597753	-4.1799532
H	-2.6881575	3.7560834	-2.8158318
H	0.1453397	4.1731105	4.8682361

H	-0.9916193	4.4952191	-4.4741319
W	0.0580093	-1.1567339	-0.1012309
C	-0.7704814	-2.9965464	-0.1526628
C	0.5789757	-1.1805681	-2.1039519
C	-0.4058007	-1.0052146	1.8978704
C	-1.8285960	-0.5297307	-0.6542611
C	1.8964513	-1.9923670	0.4313287
O	-1.3018975	-4.0264211	-0.1771728
O	0.8655008	-1.1747964	-3.2196847
O	-0.6738589	-0.9207947	3.0168185
O	-2.8993354	-0.2414400	-0.9695479
O	2.8833127	-2.5043424	0.7239701

3ac• : $[W(CO)_5]PPh_2O^•$ with CO in ring
35
Energy = -1514.525254902

P	-2.5349847	1.0492968	0.1306206
C	-2.6724699	2.0130549	1.6467385
C	-2.6098002	2.2738260	-1.1926279
O	-0.9584267	0.4816344	0.0522934
C	-1.8437135	3.1295362	1.8516888
C	-3.6088257	1.6478406	2.6223513
C	-1.8271683	2.1118419	-2.3451501
C	-3.5267989	3.3329237	-1.1109719
C	-1.9457907	3.8574907	3.0330384
H	-1.1241944	3.4212602	1.0922803
C	-3.7181767	2.3912306	3.7971444
H	-4.2523840	0.7885624	2.4602836
C	-1.9516389	3.0149997	-3.3990080
H	-1.1161088	1.2945811	-2.4104765
C	-3.6538028	4.2247205	-2.1740933
H	-4.1307383	3.4648508	-0.2177369
C	-2.8842618	3.4906911	4.0033589
H	-1.2985747	4.7137335	3.1967997
H	-4.4494759	2.1107471	4.5485578
C	-2.8657431	4.0678589	-3.3166466
H	-1.3345041	2.8960787	-4.2844267
H	-4.3623591	5.0447540	-2.1072977
H	-2.9653549	4.0664487	4.9205787
H	-2.9621401	4.7675555	-4.1415455
W	-3.3971692	-1.3108347	-0.1407664
C	-3.8840482	-3.2933619	-0.4165529
C	-3.4301956	-1.0094393	-2.1737005
C	-3.2110780	-1.6732301	1.8721205
C	-5.2523147	-0.5115071	0.0816983
C	-1.2140152	-0.9146622	-0.1387401
O	-4.1856115	-4.3983135	-0.5689097
O	-3.4420426	-0.8456052	-3.3171808
O	-3.0870287	-1.8975534	2.9992530
O	-6.2664006	0.0293224	0.2193900
O	-0.2675164	-1.6523167	-0.2674778

3ae_ts : P-to-O 1,2-W-shift of $[W(CO)_5]PPh_2O^•$
35
Energy = -1514.541365852

P	0.2365715	1.2728180	0.0430706
O	1.4966251	0.3646360	0.1751435
C	0.1605786	2.4542923	1.4028341
C	0.2202037	2.1694839	-1.5211373
C	-0.5472365	3.6635831	1.3142993
C	0.7887958	2.0958256	2.6074147
C	1.3924070	2.2064397	-2.2916506
C	-0.9625909	2.7461496	-2.0103432
C	-0.6122728	4.5090806	2.4192110
H	-1.0277965	3.9535199	0.3853719
C	0.7233331	2.9509957	3.7046174
H	1.3396593	1.1621300	2.6681726
C	1.3841559	2.8462640	-3.5295680
H	2.2952969	1.7330709	-1.9180966
C	-0.9591577	3.3892379	-3.2464751
H	-1.8847259	2.6797050	-1.4393920
C	0.0199433	4.1549497	3.6143509
H	-1.1514198	5.4488601	2.3451274
H	1.2220455	2.6782694	4.6299675
C	0.2128923	3.4411190	-4.0052844
H	2.2927163	2.8799132	-4.1237172
H	-1.8733741	3.8383971	-3.6227267
H	-0.0332297	4.8179560	4.4727877
H	0.2102223	3.9355889	-4.9721804
W	-0.0672451	-1.3496953	0.0775592
C	-0.9871654	-3.1271423	0.0521974
C	0.5625166	-1.5661446	-1.8817482
C	-0.6753613	-1.0919146	2.0317756
C	-1.8828525	-0.6897105	-0.6514988
C	1.5918698	-2.4420125	0.7380141
O	-1.5009036	-4.1718749	0.0385644
O	0.9013146	-1.6965801	-2.9750839
O	-1.0384635	-0.9737365	3.1206406
O	-2.9171905	-0.3921572	-1.0677608
O	2.4279193	-3.1631782	1.0680354

3ae• : $PPh_2O[W(CO)_5]^•$ radical complex
35
Energy = -1514.542089110

P	-1.6241892	-0.9812711	-0.8290195
C	-2.7227338	-1.7842123	0.3529499
C	-2.2603243	0.6974617	-1.0946332
O	-0.2162780	-0.9229284	-0.1699114
C	-2.2109117	-2.3524547	1.5294736
C	-4.0920516	-1.8935629	0.0564205
C	-3.0207461	1.3597415	-0.1177201
C	-1.9018441	1.3649706	-2.2762866

C	-3.0714044	-2.9989198	2.4149131
H	-1.1501555	-2.2731631	1.7451448
C	-4.9447587	-2.5372057	0.9492433
H	-4.4878871	-1.4676837	-0.8618743
C	-3.3991659	2.6850784	-0.3194301
H	-3.3016423	0.8448911	0.7956771
C	-2.2797356	2.6920370	-2.4683140
H	-1.3304140	0.8449389	-3.0400672
C	-4.4358549	-3.0911447	2.1278712
H	-2.6780612	-3.4275431	3.3320436
H	-6.0047336	-2.6105533	0.7249779
C	-3.0265290	3.3513349	-1.4897155
H	-3.9785392	3.2009782	0.4405607
H	-1.9963342	3.2091976	-3.3799937
H	-5.1024503	-3.5965572	2.8204192
H	-3.3217812	4.3855859	-1.6399084
W	1.5428358	0.2875210	-0.0555327
C	3.2114041	1.3672001	0.1586812
C	0.5185438	2.0687340	0.1817737
C	2.7375513	-1.3834919	-0.2756146
C	1.6161803	0.6770544	-2.0799098
C	1.5582552	-0.0252552	1.9916373
O	4.1815676	2.0028393	0.2799427
O	0.0681355	3.1227742	0.3254580
O	3.4718176	-2.2684943	-0.3854764
O	1.7063084	0.9397817	-3.2019161
O	1.6241753	-0.1635651	3.1357597

3aT : $[W(CO)_5]PPh_2OT$ complex

63

Energy = -1923.351944388

P	0.3637455	0.7915531	0.0335315
O	-1.2040581	1.2909157	0.2210713
C	0.9019057	2.0167002	-1.2205655
C	1.0820556	1.5372913	1.5478622
N	-2.2869719	0.2916471	0.1115882
C	0.2703696	3.2686327	-1.2929764
C	1.9629384	1.7393281	-2.0888969
C	2.2955581	1.0694631	2.0648160
C	0.4440523	2.6162263	2.1791858
C	-3.0956036	0.6850984	-1.0886631
C	-2.9526226	0.2530232	1.4551868
C	0.6869009	4.2137387	-2.2270890
H	-0.5537349	3.4973853	-0.6262398
C	2.3860712	2.6900941	-3.0185522
H	2.4592512	0.7762453	-2.0453246
C	2.8616736	1.6613425	3.1940237
H	2.7999375	0.2353424	1.5897935
C	1.0054037	3.2015313	3.3120076
H	-0.4972512	2.9881454	1.7907805
C	-4.2931098	-0.2868052	-1.1369146
C	-2.2196593	0.4330151	-2.3217487
C	-3.5709634	2.1505337	-1.1172489
C	-4.1561941	-0.7019770	1.3125423
C	-3.3990941	1.6178596	2.0157986
C	-1.9510162	-0.3730467	2.4331728
C	1.7472056	3.9277454	-3.0917081
H	0.1842557	5.1753136	-2.2803153
H	3.2094042	2.4589553	-3.6879789
C	2.2163102	2.7267838	3.8222066
H	3.8020840	1.2841234	3.5851190
H	0.4962789	4.0293107	3.7974911
C	-5.0882826	-0.3178410	0.1659108
H	-3.9143258	-1.2930742	-1.3502480
H	-4.9238401	0.0117134	-1.9820534
H	-1.3684125	1.1187674	-2.3572686
H	-1.8481264	-0.5939132	-2.3187337
H	-2.8147716	0.5861874	-3.2276849
H	-2.7450456	2.8263450	-0.8853112
H	-4.3889114	2.3446698	-0.4222810
H	-3.9269813	2.3819752	-2.1265364
H	-3.7766741	-1.7160124	1.1426207
H	-4.6859852	-0.7070621	2.2720919
H	-2.6060551	2.3597228	1.9032400
H	-4.3026758	1.9969060	1.5363534
H	-3.6100902	1.5044401	3.0842105
H	-1.5963390	-1.3328034	2.0509366
H	-1.0912308	0.2812425	2.6013285
H	-2.4417175	-0.5414467	3.3971373
H	2.0706891	4.6662313	-3.8195113
H	2.6516071	3.1832614	4.7063995
H	-5.9040056	-1.0453940	0.0880820
H	-5.5546196	0.6561381	0.3568182
W	0.9576498	-1.6384441	-0.4119774
C	1.0876776	-1.9589453	1.6186424
C	2.9521236	-1.1742115	-0.4903729
C	-0.9845851	-2.3581868	-0.3958874
C	0.7999160	-1.3292677	-2.4414731
C	1.5161826	-3.5577445	-0.7496602
O	1.1668649	-2.1689540	2.7525897
O	4.0946205	-0.9845701	-0.5520306
O	-1.9933391	-2.9203531	-0.4234364
O	0.7194984	-1.1896782	-3.5864101
O	1.8461498	-4.6510376	-0.9406315

3a⁻ : $[W(CO)_5]PPh_2O^-$ anion complex

35

Energy = -1514.717778749

P	-1.8053423	1.3022845	0.5318951
O	-0.3609220	1.4767187	0.9983027
C	-2.8952709	1.4977340	2.0118512
C	-2.2939972	2.8075512	-0.4192431

C	-4.2867089	1.6417894	1.9330924
C	-2.2899422	1.4381849	3.2721376
C	-1.4832723	3.9442697	-0.3039225
C	-3.4233060	2.8617536	-1.2441229
C	-5.0577196	1.7249854	3.0913470
H	-4.7724710	1.6950101	0.9630523
C	-3.0603831	1.5164652	4.4350050
H	-1.2094509	1.3324359	3.3204099
C	-1.8052542	5.1172676	-0.9882801
H	-0.5968962	3.8866603	0.3226816
C	-3.7533647	4.0350207	-1.9232132
H	-4.0404345	1.9764003	-1.3703853
C	-4.4461536	1.6587091	4.3477343
H	-6.1362101	1.8416904	3.0171559
H	-2.5785452	1.4663004	5.4086002
C	-2.9445610	5.1670507	-1.7959825
H	-1.1669099	5.9925822	-0.8943051
H	-4.6336498	4.0633254	-2.5604899
H	-5.0482102	1.7184860	5.2507609
H	-3.1949457	6.0789718	-2.3318205
W	-2.3655859	-0.9252290	-0.6751790
C	-2.6494404	-2.7151713	-1.5530348
C	-2.1284062	0.0344745	-2.4745989
C	-2.5595382	-1.6952848	1.2204900
C	-4.3835272	-0.5774422	-0.7258700
C	-0.3293085	-1.2380174	-0.5943566
O	-2.8120702	-3.7549876	-2.0607909
O	-1.9834599	0.5901132	-3.4826658
O	-2.6650884	-2.1056350	2.2993409
O	-5.5338629	-0.4119407	-0.7658411
O	0.8129033	-1.4149492	-0.5498810

3a• : $[W(CO)_5]PPh_2O^•$ radical complex
35
Energy = -1514.546146922

P	-2.0568147	1.4039434	0.5816801
O	-0.5657902	1.2745891	0.9287189
C	-3.0809289	1.5642569	2.0710451
C	-2.4195841	2.8504577	-0.4444478
C	-4.3566893	2.1444146	2.0426240
C	-2.5832920	1.0258782	3.2671760
C	-1.5126959	3.9198856	-0.4415438
C	-3.5699045	2.9100904	-1.2435594
C	-5.1271820	2.1839532	3.2038793
H	-4.7443381	2.5749570	1.1246866
C	-3.3555939	1.0760184	4.4256895
H	-1.5912789	0.5848538	3.2845403
C	-1.7683107	5.0458631	-1.2228938
H	-0.6141781	3.8618124	0.1655448
C	-3.8241414	4.0415954	-2.0157416
H	-4.2600677	2.0712558	-1.2750061
C	-4.6291267	1.6501236	4.3943722
H	-6.1137509	2.6373160	3.1796537
H	-2.9637305	0.6679139	5.3527300
C	-2.9239545	5.1098182	-2.0049035
H	-1.0638511	5.8725011	-1.2223850
H	-4.7167384	4.0854580	-2.6324776
H	-5.2311450	1.6847140	5.2976901
H	-3.1196861	5.9885749	-2.6123022
W	-2.0583086	-0.8823661	-0.5512878
C	-2.5275279	-2.5867698	-1.5315254
C	-2.0378530	0.1253988	-2.3479536
C	-2.0011350	-1.8192274	1.2880196
C	-4.0973821	-0.6611915	-0.3152258
C	-0.0073420	-1.2029482	-0.7851600
O	-2.8520844	-3.5420656	-2.0999527
O	-2.0128063	0.6802660	-3.3585567
O	-1.9705969	-2.3463704	2.3128147
O	-5.2361718	-0.5532467	-0.1736095
O	1.1126756	-1.4141457	-0.9324588

3bc• : $[W(CO)_5]PPh_2S^•$ with a CO in ring
35
Energy = -1837.490510998

P	-2.3647089	1.0651145	0.1584827
C	-2.6054538	2.0425535	1.6659594
C	-2.5421066	2.2829421	-1.1785821
S	-0.3492553	0.4098489	0.1235864
C	-1.8502450	3.2073951	1.8792286
C	-3.5470472	1.6375783	2.6187795
C	-1.7956036	2.1689725	-2.3586433
C	-3.5301544	3.2735766	-1.0697599
C	-2.0319621	3.9474963	3.0434819
H	-1.1257476	3.5313179	1.1372636
C	-3.7335469	2.3890836	3.7798327
H	-4.1362747	0.7417893	2.4508758
C	-2.0268151	3.0477099	-3.4152588
H	-1.0311496	1.4026641	-2.4448564
C	-3.7609837	4.1440850	-2.1336823
H	-4.1112816	3.3687838	-0.1573287
C	-2.9742284	3.5393967	3.9935727
H	-1.4415711	4.8433226	3.2105148
H	-4.4690175	2.0746723	4.5139575
C	-3.0093086	4.0341425	-3.3054327
H	-1.4378926	2.9621773	-4.3235322
H	-4.5243012	4.9112060	-2.0438898
H	-3.1156765	4.1215511	4.8993147
H	-3.1872021	4.7175761	-4.1304341
W	-3.3299604	-1.2868342	-0.1454721
C	-4.0523241	-3.1782957	-0.4380356
C	-3.3001625	-0.9863635	-2.1789111
C	-3.2053015	-1.6825184	1.8670842

C -5.1103942 -0.3317156 0.0278246
C -1.1156586 -1.2598688 -0.1424689
O -4.5020084 -4.2322968 -0.6002646
O -3.2776783 -0.8312920 -3.3235280
O -3.1104138 -1.9340986 2.9914810
O -6.0818429 0.2921756 0.1290716
O -0.4475783 -2.2558317 -0.2953444

3be_ts : P-to-S 1,2-W-shift of $[W(CO)_5]PPh_2S^{\bullet}$
35
Energy = -1837.519659941
P -1.3070356 -0.0990545 0.6346581
C -2.0130923 -1.7531328 0.3970864
C -2.6031866 1.0962327 0.1942232
S -0.5492311 0.1983689 2.4728213
C -2.4077787 -2.5222090 1.4984654
C -2.1213399 -2.2806449 -0.8988201
C -2.5001593 2.4092121 0.6768191
C -3.6708082 0.7429951 -0.6425490
C -2.9264248 -3.8014785 1.3010633
H -2.3033242 -2.1184591 2.5013950
C -2.6266811 -3.5652326 -1.0885164
H -1.7900032 -1.7021850 -1.7563636
C -3.4509801 3.3601028 0.3160815
H -1.6896417 2.6716200 1.3499523
C -4.6100864 1.7056164 -1.0134823
H -3.7732446 -0.2753953 -1.0030764
C -3.0391464 -4.3223629 0.0103393
H -3.2351385 -4.3940472 2.1572240
H -2.7041174 -3.9708984 -2.0927550
C -4.5024688 3.0127497 -0.5367388
H -3.3705557 4.3730439 0.6992445
H -5.4350042 1.4265527 -1.6624204
H -3.4334461 -5.3231847 -0.1387555
H -5.2398867 3.7574755 -0.8213465
W 1.1237552 0.2614302 -0.0927520
C 2.8390566 0.3988056 -1.1446446
C 0.3233667 0.1523900 -1.9928006
C 2.3666229 0.4625255 1.5752727
C 1.2966484 -1.7927873 0.0424368
C 0.8565922 2.3043408 -0.1114700
O 3.7793382 0.4617900 -1.8232472
O -0.0253162 0.1193250 -3.0923612
O 3.1464781 0.5903916 2.4113645
O 1.3852962 -2.9381364 0.1284318
O 0.7217809 3.4497730 -0.1232631

3be$^{\bullet}$: $PPh_2S[W(CO)_5]^{\bullet}$ radical complex
35
Energy = -1837.517676280
P -1.5522508 1.0401448 -0.6442798
C -2.2527745 -0.6432280 -0.6908519
C -2.8902608 2.0745315 0.0345502
S -0.0911775 1.0562390 0.8303292
C -2.8319988 -1.2208623 0.4509331
C -2.2132940 -1.3607755 -1.8929122
C -2.5835336 3.2721361 0.7003534
C -4.2336382 1.7445598 -0.2072817
C -3.3685481 -2.5027410 0.3822252
H -2.8581328 -0.6650385 1.3835436
C -2.7495154 -2.6483991 -1.9542517
H -1.7679693 -0.9121844 -2.7759694
C -3.6057471 4.1073879 1.1453992
H -1.5466554 3.5419749 0.8805185
C -5.2517606 2.5888722 0.2347740
H -4.4835095 0.8260852 -0.7293515
C -3.3269169 -3.2173165 -0.8193589
H -3.8134300 -2.9493347 1.2667262
H -2.7160256 -3.2032462 -2.8871453
C -4.9419628 3.7685900 0.9141261
H -3.3587737 5.0245643 1.6722780
H -6.2881729 2.3206200 0.0508968
H -3.7425606 -4.2195854 -0.8670223
H -5.7369427 4.4230226 1.2595143
W 1.6866946 -0.6044221 0.2829778
C 3.2572398 -1.8204284 -0.0862622
C 1.3024045 -0.4985668 -1.7418777
C 2.0646938 -0.7157646 2.3147450
C 0.5028197 -2.3073753 0.3601786
C 3.0019676 0.9904239 0.1744162
O 4.1629217 -2.5132935 -0.3028584
O 1.1158796 -0.4579919 -2.8799541
O 2.2953188 -0.7883609 3.4414169
O -0.0595846 -3.3122853 0.3907124
O 3.7661312 1.8507821 0.1095784

3bT : $[W(CO)_5]PPh_2ST$ complex
63
Energy = -2246.353554066
P 0.4939817 1.0469882 0.0258316
S -1.5015166 1.8137480 -0.1761500
C 1.3086196 2.2069708 -1.1437847
C 1.0776326 1.7218267 1.6348606
N -2.5850665 0.5003603 0.0107167
C 2.4780507 2.8911903 -0.7846750
C 0.8081710 2.3431427 -2.4470582
C 2.1310839 1.1033670 2.3173432
C 0.5271278 2.9014574 2.1581772
C -3.5081053 0.3785838 -1.1892633
C -3.1453083 0.3733782 1.4124611
C 3.1374674 3.6917754 -1.7178075
H 2.8749490 2.7994943 0.2209577

C	1.4662545	3.1472376	-3.3744947
H	-0.1009881	1.8239511	-2.7298484
C	2.6200001	1.6432014	3.5081812
H	2.5811576	0.2019240	1.9167351
C	1.0104402	3.4363705	3.3498220
H	-0.2895893	3.3925378	1.6379400
C	-4.4281037	-0.8410394	-0.9883883
C	-2.6522426	0.1162399	-2.4340502
C	-4.3514601	1.6454215	-1.4339002
C	-4.0673118	-0.8591677	1.4602389
C	-3.8940998	1.6297172	1.8941752
C	-1.9680017	0.1150546	2.3585937
C	2.6342545	3.8229161	-3.0125977
H	4.0441694	4.2154721	-1.4290248
H	1.0661479	3.2471941	-4.3793005
C	2.0573240	2.8076477	4.0294432
H	3.4372839	1.1499762	4.0258823
H	0.5696387	4.3456520	3.7483247
C	-5.1278725	-0.8590193	0.3655909
H	-3.8287432	-1.7517412	-1.0903556
H	-5.1544813	-0.8348232	-1.8093402
H	-2.0885358	1.0043765	-2.7292583
H	-1.9514173	-0.7012324	-2.2514401
H	-3.3084484	-0.1615419	-3.2652852
H	-3.7073460	2.5288676	-1.5003334
H	-5.0894599	1.8133333	-0.6469017
H	-4.8865414	1.5454559	-2.3845242
H	-3.4501157	-1.7595930	1.3585915
H	-4.5238766	-0.8869119	2.4564275
H	-3.2707527	2.5189227	1.7538663
H	-4.8398128	1.7804258	1.3695233
H	-4.1122499	1.5323608	2.9632270
H	-1.3421890	-0.6958145	1.9741157
H	-1.3485403	1.0062989	2.4851110
H	-2.3514250	-0.1728365	3.3430482
H	3.1472872	4.4499285	-3.7359929
H	2.4316222	3.2250869	4.9596813
H	-5.7551516	-1.7537070	0.4498493
H	-5.7956268	0.0047593	0.4712904
W	1.0859108	-1.3830363	-0.4823900
C	1.2266516	-1.8817746	1.5106252
C	3.0191100	-0.6836883	-0.5606100
C	-0.7835649	-2.2575861	-0.4071551
C	0.8515480	-0.9954225	-2.4921790
C	1.8028382	-3.2087552	-0.9473683
O	1.2737485	-2.2249326	2.6139863
O	4.1169356	-0.3245536	-0.6187448
O	-1.7451465	-2.8971776	-0.3590067
O	0.7275234	-0.8332472	-3.6297265
O	2.2382488	-4.2508349	-1.2168533

3b^{-} : $[W(CO)_5]PPh_2S^-$ anion complex

35

Energy = -1837.685095582

P	-1.7544636	1.3414072	0.5349306
S	0.1524994	1.5669046	1.1464891
C	-2.8548798	1.5293213	2.0134227
C	-2.2542044	2.8436490	-0.4220046
C	-4.2145010	1.8403157	1.8715262
C	-2.3460302	1.2812229	3.2923814
C	-1.5653755	4.0486478	-0.2383045
C	-3.3316589	2.8086152	-1.3147804
C	-5.0469743	1.9033270	2.9880291
H	-4.6260463	2.0432742	0.8875180
C	-3.1806082	1.3364396	4.4105599
H	-1.2879547	1.0535615	3.3947532
C	-1.9563447	5.1987107	-0.9236264
H	-0.7143470	4.0616305	0.4388030
C	-3.7266024	3.9582618	-2.0010208
H	-3.8586315	1.8740564	-1.4838563
C	-4.5331725	1.6476849	4.2627136
H	-6.0974216	2.1537688	2.8636378
H	-2.7716930	1.1392628	5.3984790
C	-3.0398556	5.1575964	-1.8057976
H	-1.4119129	6.1277858	-0.7738798
H	-4.5629802	3.9137298	-2.6937034
H	-5.1830708	1.6941987	5.1326141
H	-3.3399710	6.0522619	-2.3449396
W	-2.3285881	-0.9114969	-0.6263127
C	-2.7070688	-2.7032788	-1.4531509
C	-2.1605478	-0.0347121	-2.4761298
C	-2.4171415	-1.6822454	1.2799491
C	-4.3447021	-0.5454822	-0.5716529
C	-0.3031193	-1.3110595	-0.6822666
O	-2.9361617	-3.7428684	-1.9341237
O	-2.0462487	0.4514279	-3.5226099
O	-2.4576393	-2.1125183	2.3540363
O	-5.4943964	-0.3809403	-0.5551145
O	0.8205086	-1.5748819	-0.7366950

3b$^{\bullet}$: $[W(CO)_5]PPh_2S^{\bullet}$ radical complex

35

Energy = -1837.523255181

P	-2.0395455	1.3894178	0.5274457
S	-0.0711370	1.1712395	0.8784103
C	-2.9994632	1.5852672	2.0616645
C	-2.4273796	2.8673813	-0.4554827
C	-4.2868579	2.1395725	2.0125645
C	-2.4901211	1.1063374	3.2750453
C	-1.7161053	4.0551881	-0.2350323
C	-3.4516437	2.8343027	-1.4095408
C	-5.0564381	2.2101330	3.1728080

H	-4.6839749	2.5226748	1.0772713
C	-3.2633951	1.1847221	4.4319910
H	-1.4890720	0.6862422	3.3067326
C	-2.0334796	5.1986554	-0.9645214
H	-0.9136787	4.0772046	0.4970255
C	-3.7696022	3.9831858	-2.1337852
H	-3.9963412	1.9128933	-1.5927899
C	-4.5472201	1.7327906	4.3824449
H	-6.0518989	2.6422381	3.1318083
H	-2.8615015	0.8203418	5.3728392
C	-3.0606809	5.1645020	-1.9118540
H	-1.4777090	6.1162685	-0.7956660
H	-4.5639048	3.9522302	-2.8734274
H	-5.1481164	1.7917441	5.2851911
H	-3.3035985	6.0573328	-2.4803583
W	-2.0893874	-0.9108099	-0.5750405
C	-2.5846524	-2.6473921	-1.4870286
C	-1.8956310	0.0377491	-2.3944923
C	-2.1641641	-1.7642632	1.3024602
C	-4.1352706	-0.6298403	-0.5074837
C	-0.0953706	-1.5077876	-0.7483943
O	-2.9391336	-3.6170465	-2.0135947
O	-1.7626988	0.5632717	-3.4123760
O	-2.1954825	-2.2396555	2.3519158
O	-5.2837283	-0.5329889	-0.4793577
O	0.9670793	-1.9255246	-0.8875179

3cc_ts : N-C cyclization of $[W(CO)_5]PPh_2NMe^{\bullet}$
39
Energy = -1533.954602938

P	0.2090399	1.0618234	0.0036682
C	-0.0345911	2.2119410	1.3801933
C	-0.0038727	2.0789369	-1.4830336
N	1.8444399	0.5393108	-0.0386994
C	0.4520706	3.5277486	1.3113090
C	-0.6846381	1.7709145	2.5404826
C	0.9479567	2.0567878	-2.5091201
C	-1.1840415	2.8212712	-1.6364864
C	2.8150743	0.9204152	0.9873913
C	0.3050128	4.3806179	2.4020716
H	0.9382720	3.8801937	0.4062325
C	-0.8345563	2.6298716	3.6286450
H	-1.0796641	0.7602587	2.5799156
C	0.7254440	2.7873618	-3.6767695
H	1.8563384	1.4751215	-2.3860062
C	-1.4014044	3.5458297	-2.8063345
H	-1.9266271	2.8385883	-0.8428725
H	2.4587491	0.7317148	2.0078440
H	3.7300001	0.3499816	0.8083195
H	3.0316201	1.9901924	0.8915061
C	-0.3365389	3.9320773	3.5605712
H	0.6866907	5.3958580	2.3487782
H	-1.3440765	2.2859059	4.5236344
C	-0.4466456	3.5302645	-3.8270418
H	1.4690631	2.7751525	-4.4683006
H	-2.3143470	4.1227567	-2.9211101
H	-0.4543045	4.6019867	4.4072421
H	-0.6179420	4.0964034	-4.7379631
W	-0.2327227	-1.3883445	0.0583024
C	-0.0881679	-3.4121432	-0.0595267
C	-0.6435858	-1.2337926	-1.9565152
C	0.1711580	-1.5665547	2.0661423
C	-2.2372371	-1.5100295	0.4768708
C	1.8733844	-1.1734337	-0.4248942
O	0.0291399	-4.5622158	-0.1383509
O	-0.8734599	-1.1437782	-3.0843477
O	0.3925573	-1.7037199	3.1942723
O	-3.3708379	-1.5752376	0.7092379
O	2.9526771	-1.5765201	-0.6929077

3ce_ts : 1,2-W-shift of $[W(CO)_5]PPh_2NMe^{\bullet}$
39
Energy = -1533.963091910

P	0.1085283	1.2947044	-0.2273837
C	-0.2176552	2.7643909	0.7816579
C	0.3145195	1.8460537	-1.9346226
N	1.3931770	0.4147086	0.2590653
C	0.1775351	4.0464620	0.3661126
C	-0.8119867	2.5992328	2.0426658
C	1.4291576	1.4169664	-2.6692965
C	-0.6881842	2.6055975	-2.5603483
C	2.3885040	0.8486529	1.2396933
C	-0.0165912	5.1416102	1.2063578
H	0.6394537	4.1836499	-0.6065182
C	-0.9957350	3.6958318	2.8819981
H	-1.1352562	1.6128533	2.3616508
C	1.5530063	1.7720011	-4.0117779
H	2.1837753	0.8112455	-2.1760283
C	-0.5549324	2.9597161	-3.9001926
H	-1.5626217	2.9245468	-1.9987061
H	3.0089736	-0.0092108	1.5151970
H	3.0381887	1.6176998	0.8036982
H	1.9408255	1.2561910	2.1574669
C	-0.6004233	4.9685416	2.4636814
H	0.2933587	6.1304196	0.8807916
H	-1.4553859	3.5592391	3.8561169
C	0.5649630	2.5436278	-4.6278151
H	2.4218460	1.4471067	-4.5771828
H	-1.3256216	3.5564126	-4.3795070
H	-0.7507951	5.8246657	3.1147686
H	0.6630608	2.8170799	-5.6743769
W	-0.1651416	-1.2279773	0.6036167

C	-1.0508940	-3.0057643	0.9416296
C	-0.2917089	-1.5834413	-1.4320085
C	-0.0407764	-0.9077448	2.6371706
C	-2.1147871	-0.5585202	0.6925780
C	1.5651346	-2.4055607	0.6926246
O	-1.5159159	-4.0517925	1.1639853
O	-0.3845653	-1.8102280	-2.5585737
O	-0.0045182	-0.7856896	3.7858843
O	-3.2333397	-0.2773117	0.7748614
O	2.4125056	-3.1829831	0.7868782

3ce• : $PPh_2NMe[W(CO)_5]^{\bullet}$ radical complex
39
Energy = -1533.974862187

P	-1.5490081	-0.5782738	-0.6202361
C	-2.9194560	-1.5395703	0.1179637
C	-2.1528240	1.1434483	-0.5443028
N	-0.2815570	-0.5874370	0.5228323
C	-4.0083598	-0.9628362	0.7887995
C	-2.8644787	-2.9366720	-0.0246671
C	-2.0255658	1.9259063	0.6137346
C	-2.7553728	1.6883233	-1.6855393
C	-0.3694682	-1.4479165	1.7072082
C	-5.0103880	-1.7719200	1.3246923
H	-4.0707074	0.1160898	0.8933589
C	-3.8611167	-3.7433736	0.5208602
H	-2.0364595	-3.3902360	-0.5648378
C	-2.4966287	3.2366370	0.6256375
H	-1.5491782	1.5088895	1.4955399
C	-3.2353946	2.9977900	-1.6665357
H	-2.8388838	1.0908406	-2.5898383
H	-1.3784794	-1.4437692	2.1318809
H	-0.1133686	-2.4861824	1.4565327
H	0.3460441	-1.0948603	2.4532276
C	-4.9364202	-3.1607874	1.1964743
H	-5.8488996	-1.3176552	1.8447550
H	-3.8048905	-4.8225240	0.4110541
C	-3.1019616	3.7739568	-0.5136978
H	-2.3926338	3.8397256	1.5232075
H	-3.6992251	3.4160095	-2.5551790
H	-5.7188906	-3.7873079	1.6148816
H	-3.4633881	4.7981760	-0.5038902
W	1.5841520	0.4006710	-0.0191893
C	3.3896043	1.2041251	-0.4829663
C	0.7815660	2.0379665	-0.9945957
C	2.6676310	-1.1153595	0.8664176
C	1.5754352	-0.5789856	-1.8413910
C	1.5645834	1.4172013	1.7776206
O	4.4284085	1.6510118	-0.7422529
O	0.4747148	2.9886332	-1.5756351
O	3.3580065	-1.9175257	1.3328353
O	1.5971127	-1.1038338	-2.8691897
O	1.5721079	2.0050659	2.7727810

3cT : $[W(CO)_5]PPh_2NMeT$ complex
67
Energy = -1942.798756865

P	0.0392015	1.0396228	-0.0234675
C	0.5964682	2.1291963	-1.4060069
C	0.7740788	1.9643411	1.3917017
N	-2.5586504	0.2505113	0.1024658
C	0.8471591	3.4966894	-1.2118687
C	0.7537922	1.5973250	-2.6926183
C	0.0049789	2.4505956	2.4536047
C	2.1652693	2.1474576	1.4312641
C	-3.3537018	0.1718445	-1.1720877
C	-3.2218723	-0.0343413	1.4260040
C	1.2417552	4.3059169	-2.2758855
H	0.7448284	3.9310752	-0.2223736
C	1.1486929	2.4033928	-3.7589726
H	0.5687759	0.5439310	-2.8611750
C	0.6090687	3.0848677	3.5410895
H	-1.0731128	2.3394671	2.4288526
C	2.7704654	2.7764681	2.5157853
H	2.7803049	1.8108194	0.6039405
C	-4.0966488	-1.1771882	-1.1701909
C	-2.3595316	0.1740158	-2.3338587
C	-4.3991096	1.2894071	-1.4362788
C	-4.1124651	-1.2914514	1.2926455
C	-4.0433797	1.1368627	2.0079379
C	-2.1371242	-0.3942144	2.4512611
C	1.3951288	3.7615382	-3.5526249
H	1.4333323	5.3616946	-2.1059806
H	1.2702711	1.9688785	-4.7470682
C	1.9935887	3.2422720	3.5798496
H	-0.0066206	3.4562509	4.3554575
H	3.8489285	2.9058885	2.5290263
C	-4.9959123	-1.3243241	0.0520932
H	-3.3594679	-1.9878861	-1.1762660
H	-4.6715589	-1.2443486	-2.1008613
H	-1.8644338	1.1431033	-2.4413900
H	-1.5976282	-0.5939303	-2.1771286
H	-2.8880571	-0.0376285	-3.2690376
H	-5.0844559	1.4381826	-0.6004581
H	-4.9971563	0.9926868	-2.3054169
H	-3.9325830	2.2454000	-1.6745168
H	-3.4583784	-2.1687690	1.2654824
H	-4.7094138	-1.3639227	2.2091528
H	-3.4074569	2.0049545	2.2039024
H	-4.8649360	1.4456487	1.3573925
H	-4.4737673	0.8245437	2.9657288
H	-2.6173245	-0.6686835	3.3967973

H	-1.5488094	-1.2447768	2.1036215
H	-1.4577051	0.4348374	2.6461228
H	1.7096694	4.3911948	-4.3799745
H	2.4652276	3.7302945	4.4278536
H	-5.5430038	-2.2735029	0.0132472
H	-5.7477194	-0.5262248	0.0777647
W	1.0472032	-1.3425880	-0.1242033
C	2.8250671	-0.4333977	-0.5994199
C	0.7887222	-1.7198736	-2.1290712
C	1.3123268	-1.1183674	1.9124526
C	-0.6491776	-2.4850070	0.1259853
C	2.0767251	-3.0655214	-0.0111525
O	3.8483692	-0.0007043	-0.9271791
O	0.6710732	-2.0235476	-3.2397540
O	1.4718913	-1.0439409	3.0535733
O	-1.5082387	-3.2563731	0.1958179
O	2.6896878	-4.0499461	0.0720371
N	-1.6375114	1.3283935	0.1756483
C	-2.0823297	2.7191327	-0.0505493
H	-1.4250968	3.3971956	0.5010757
H	-2.0487486	3.0004781	-1.1100317
H	-3.0959599	2.8404073	0.3239036

3c$^-$: [W(CO)$_5$]PPh$_2$NMe$^-$ anion complex

39

Energy = -1534.117410267

P	-1.9170225	1.1918280	0.1177586
C	-2.5207759	2.2120087	1.5489571
C	-2.3081899	2.3171208	-1.2679516
N	-0.3037869	1.1370787	0.1225560
C	-2.2534577	3.5911527	1.5720164
C	-3.0958500	1.6278325	2.6822821
C	-1.3338131	2.5975498	-2.2297383
C	-3.5941018	2.8531944	-1.4163592
C	0.3218052	0.1982865	1.0355663
C	-2.5760908	4.3634403	2.6858058
H	-1.7940053	4.0587038	0.7046647
C	-3.4115790	2.3943649	3.8070881
H	-3.3071520	0.5627492	2.6815093
C	-1.6407729	3.4026755	-3.3296530
H	-0.3437130	2.1752198	-2.0846030
C	-3.9015389	3.6576893	-2.5114401
H	-4.3550006	2.6392723	-0.6693760
H	-0.1257765	-0.8148715	0.9949294
H	1.3848724	0.0910988	0.7791981
H	0.2752294	0.5108742	2.0966390
C	-3.1576123	3.7660546	3.8100338
H	-2.3762062	5.4324132	2.6805944
H	-3.8600195	1.9207020	4.6769872
C	-2.9243289	3.9328147	-3.4736727
H	-0.8776179	3.6171000	-4.0741382
H	-4.9019370	4.0694414	-2.6182126
H	-3.4092057	4.3676860	4.6796327
H	-3.1647573	4.5571416	-4.3304815
W	-3.2670914	-1.0415384	-0.1783214
C	-4.2796825	-2.7509261	-0.4544202
C	-3.7780691	-0.4007463	-2.0629432
C	-2.6643664	-1.6843703	1.6774753
C	-4.9285715	-0.0924047	0.5612231
C	-1.5574616	-1.8333788	-1.0034022
O	-4.8798156	-3.7435207	-0.6060904
O	-4.0634092	-0.0797085	-3.1402939
O	-2.3297418	-2.0851690	2.7165081
O	-5.8772009	0.4564931	0.9459458
O	-0.6094468	-2.2717534	-1.5068087

3c$^\bullet$: [W(CO)$_5$]PPh$_2$NMe$^\bullet$ radical complex

39

Energy = -1533.976791765

P	-2.1371392	1.1897532	0.0793659
C	-2.5269866	2.1875707	1.5544432
C	-2.3964377	2.3246261	-1.3138931
N	-0.4973234	0.8730961	0.0379028
C	-2.1176808	3.5307518	1.5986041
C	-3.1455599	1.6179565	2.6734206
C	-1.4297793	2.4789168	-2.3135009
C	-3.6303592	2.9810474	-1.4244776
C	0.1807912	0.4378892	1.2423029
C	-2.3332582	4.2885174	2.7468500
H	-1.6396302	3.9797667	0.7328158
C	-3.3581145	2.3786200	3.8235799
H	-3.4680990	0.5823905	2.6424461
C	-1.6965433	3.2952772	-3.4137883
H	-0.4802097	1.9622208	-2.2213808
C	-3.8896526	3.7957345	-2.5239956
H	-4.3847955	2.8583463	-0.6513648
H	0.3953807	-0.6380555	1.1642534
H	1.1551654	0.9409171	1.2798922
H	-0.3610109	0.6254988	2.1782492
C	-2.9533672	3.7133964	3.8601601
H	-2.0200644	5.3281083	2.7736559
H	-3.8418906	1.9302556	4.6862107
C	-2.9229215	3.9530878	-3.5208746
H	-0.9433532	3.4174192	-4.1869849
H	-4.8449391	4.3061852	-2.6038463
H	-3.1221901	4.3073942	4.7535955
H	-3.1269196	4.5868762	-4.3790388
W	-3.2520344	-1.0754136	-0.2463174
C	-4.2387258	-2.8200244	-0.5239569
C	-3.7960628	-0.4581908	-2.1386475
C	-2.6402526	-1.6971798	1.6165538
C	-4.9806725	-0.2544083	0.5154370

C	-1.5256662	-1.8755054	-1.0576325
O	-4.8201939	-3.8123752	-0.6752633
O	-4.0944369	-0.1268246	-3.2028046
O	-2.2862441	-2.0720482	2.6525370
O	-5.9592039	0.2055955	0.9236330
O	-0.5768794	-2.3435905	-1.5186757

3dc• : $[W(CO)_5]PPh_2PMe^•$ with a CO in ring

39

Energy = -1820.578219880

P	-2.5122733	1.0928656	0.3118358
C	-2.8743810	2.0869458	1.7893399
C	-2.4968342	2.2650652	-1.0820194
P	-0.4748841	0.3123459	0.6416461
C	-2.0776263	3.1970476	2.1161035
C	-3.9152896	1.7077938	2.6446383
C	-1.9469005	1.8537304	-2.3064882
C	-3.0859523	3.5329722	-0.9833569
C	0.7907995	1.2490235	-0.3256887
C	-2.3275820	3.9173607	3.2809135
H	-1.2657845	3.4983701	1.4593924
C	-4.1649127	2.4338532	3.8103757
H	-4.5240196	0.8428505	2.4036731
C	-1.9721124	2.7029276	-3.4090693
H	-1.5089772	0.8637974	-2.4013500
C	-3.1151946	4.3774844	-2.0939967
H	-3.5267283	3.8586829	-0.0469840
H	1.1020212	2.1111047	0.2719379
H	1.6545769	0.5896984	-0.4566514
H	0.4267257	1.5845652	-1.2987607
C	-3.3729050	3.5369816	4.1284956
H	-1.7064621	4.7726176	3.5298510
H	-4.9751020	2.1346618	4.4684913
C	-2.5557425	3.9683085	-3.3047800
H	-1.5414098	2.3749824	-4.3501658
H	-3.5781995	5.3562925	-2.0094173
H	-3.5655158	4.0999547	5.0369777
H	-2.5781309	4.6291516	-4.1661935
W	-3.3619331	-1.2838852	-0.0892676
C	-3.8635160	-3.2226704	-0.4043456
C	-3.7174575	-0.9099085	-2.0791266
C	-2.9993598	-1.7407811	1.8819241
C	-5.2156101	-0.6345455	0.3346776
C	-1.1250585	-1.0922149	-0.3891049
O	-4.1814558	-4.3276562	-0.5700792
O	-3.9488898	-0.7262499	-3.1979910
O	-2.8057116	-2.0116820	2.9905566
O	-6.2771881	-0.2208906	0.5717523
O	-0.5222837	-1.8773522	-1.0882799

3de_ts : 1,2-W-shift of $[W(CO)_5]PPh_2PMe^•$

39

Energy = -1820.593059405

P	-1.3574398	0.0653952	0.0358255
C	-2.9028897	-0.8599032	-0.2501736
C	-1.8292585	1.8105419	0.2007264
P	-0.4033608	-0.5437264	1.8759000
C	-4.1074489	-0.4393421	0.3345133
C	-2.8762164	-2.0180675	-1.0390374
C	-1.5481710	2.5629039	1.3488727
C	-2.4286535	2.4322757	-0.9077168
C	-0.8759621	-2.3522923	1.8782703
C	-5.2703561	-1.1795187	0.1315412
H	-4.1312007	0.4593137	0.9435289
C	-4.0421642	-2.7597065	-1.2297612
H	-1.9513175	-2.3303601	-1.5143020
C	-1.8662821	3.9206388	1.3878049
H	-1.0926377	2.0841285	2.2110596
C	-2.7600368	3.7838120	-0.8562316
H	-2.6388289	1.8559411	-1.8049681
H	-1.8268668	-2.4678780	2.4073778
H	-0.9677998	-2.7818679	0.8786309
H	-0.1014321	-2.8963270	2.4267519
C	-5.2389226	-2.3408160	-0.6462928
H	-6.2020226	-0.8514545	0.5836986
H	-4.0169563	-3.6565584	-1.8416935
C	-2.4745656	4.5317204	0.2899771
H	-1.6467408	4.4979518	2.2813133
H	-3.2322315	4.2557128	-1.7129672
H	-6.1481910	-2.9142751	-0.8008935
H	-2.7253776	5.5878771	0.3255144
W	1.4497937	-0.3442767	-0.1568301
C	3.2782628	-0.3533061	-0.9691425
C	0.9190790	0.7958363	-1.8074957
C	2.3272903	-1.4845866	1.3331848
C	0.9592666	-2.0816747	-1.1493783
C	1.8686422	1.4054361	0.8550068
O	4.3622348	-0.3747878	-1.3953249
O	0.7093710	1.4152990	-2.7587771
O	2.8831130	-2.1068356	2.1306252
O	0.7062748	-3.0526251	-1.7240870
O	2.0951895	2.3854576	1.4198851

3de• : $PPh_2PMe[W(CO)_5]^•$ radical complex

39

Energy = -1820.609027661

P	-2.0632805	-0.3715943	-0.9190943
C	-3.4033890	-1.3232788	-0.1034909
C	-2.2669397	1.3470219	-0.3296839
P	-0.2878573	-0.9751770	0.1855433
C	-4.1055000	-0.8601721	1.0183207
C	-3.7323229	-2.5726401	-0.6532822

C	-1.8525578	1.7934077	0.9351883
C	-2.8394370	2.2643577	-1.2240613
C	-0.2883982	-2.8102131	0.0260800
C	-5.1123103	-1.6402778	1.5853586
H	-3.8671086	0.1100068	1.4433094
C	-4.7301125	-3.3570093	-0.0740872
H	-3.2100108	-2.9270827	-1.5384528
C	-2.0002011	3.1321191	1.2936070
H	-1.4115156	1.0903626	1.6362981
C	-2.9996475	3.6002154	-0.8582160
H	-3.1484138	1.9315885	-2.2115408
H	-1.2421668	-3.2272724	0.3600703
H	-0.1065012	-3.1095674	-1.0116222
H	0.5176832	-3.2028794	0.6516620
C	-5.4222725	-2.8914577	1.0453538
H	-5.6534374	-1.2724510	2.4526853
H	-4.9729281	-4.3245676	-0.5039292
C	-2.5742650	4.0367983	0.3979599
H	-1.6670226	3.4676477	2.2713863
H	-3.4436316	4.3017811	-1.5584787
H	-6.2059029	-3.4969699	1.4914473
H	-2.6865408	5.0804066	0.6774900
W	1.8650672	0.2520756	-0.1786828
C	3.6574068	1.1144539	-0.5687314
C	0.9521244	1.7063881	-1.3273688
C	2.7979110	-1.1786082	0.9710877
C	2.0724657	-0.9557464	-1.8385720
C	1.5948571	1.4537375	1.4822482
O	4.6880880	1.5896407	-0.8100416
O	0.4919237	2.5382115	-1.9818206
O	3.3309342	-1.9794835	1.6121547
O	2.1698872	-1.6408787	-2.7629331
O	1.4533876	2.1333954	2.4049098

3dT : $[W(CO)_5]PPh_2PmeT$ complex
67
Energy = -2229.454791265

P	-0.0975664	0.8655810	-0.0124639
C	-0.8289966	0.9259789	-1.6835173
C	0.3380458	2.5815370	0.4435483
N	-3.0877540	-0.2488796	1.1815874
C	-1.5853260	-0.1914831	-2.0728694
C	-0.5828106	1.9414466	-2.6150346
C	1.4292935	2.8147153	1.2918837
C	-0.5007203	3.6582244	0.1044338
C	-4.4273611	0.0814649	0.5290767
C	-2.9289454	-1.6068858	1.8277632
C	-2.1009946	-0.2832127	-3.3627926
H	-1.7685071	-0.9883508	-1.3574330
C	-1.0996880	1.8459809	-3.9079471
H	0.0247523	2.7979183	-2.3406727
C	1.7021490	4.0969096	1.7647409
H	2.0557495	1.9826687	1.5969711
C	-0.2183864	4.9430276	0.5663176
H	-1.3739258	3.4879129	-0.5163490
C	-4.8800961	-1.0952293	-0.3568699
C	-4.3346129	1.3079893	-0.3989831
C	-5.4904286	0.4178861	1.5949798
C	-3.4231841	-2.6968831	0.8550962
C	-3.6800032	-1.7135978	3.1726416
C	-1.4496770	-1.8925513	2.1166995
C	-1.8617018	0.7388221	-4.2843635
H	-2.6877459	-1.1513725	-3.6497257
H	-0.8994015	2.6379672	-4.6241793
C	0.8835073	5.1661304	1.3949762
H	2.5523848	4.2601316	2.4206436
H	-0.8657841	5.7690521	0.2856968
C	-4.8351541	-2.4485472	0.3405538
H	-4.2290974	-1.1241918	-1.2401295
H	-5.8931251	-0.8715733	-0.7116987
H	-4.2153405	2.2422390	0.1536023
H	-3.5119725	1.2154207	-1.1125396
H	-5.2748763	1.3566663	-0.9604943
H	-5.0974990	1.1717488	2.2848934
H	-5.8086496	-0.4500401	2.1732594
H	-6.3760570	0.8314477	1.0999198
H	-2.7291235	-2.7415909	0.0052817
H	-3.3572375	-3.6607322	1.3737710
H	-4.7615075	-1.7912648	3.0569489
H	-3.3368055	-2.6154133	3.6920657
H	-3.4600042	-0.8496502	3.8057369
H	-1.1296441	-1.4757353	3.0720207
H	-1.3027660	-2.9755318	2.1649980
H	-0.8052814	-1.4983340	1.3281473
H	-2.2600996	0.6682863	-5.2923122
H	1.0986849	6.1675134	1.7567650
H	-5.1259524	-3.2404191	-0.3591710
H	-5.5562639	-2.4805389	1.1665846
W	1.8925066	-0.8131384	-0.1709823
C	1.9618548	-1.0201522	1.8767508
C	3.2988702	0.6900652	-0.1539112
C	0.6516747	-2.4336787	-0.4259216
C	1.8287242	-0.5739668	-2.2170632
C	3.4327353	-2.0885043	-0.3598285
O	2.0338642	-1.1514410	3.0250526
O	4.1462213	1.4753992	-0.2179453
O	0.0283134	-3.3848554	-0.6451307
O	1.8246535	-0.4542924	-3.3657096
O	4.3287168	-2.8229627	-0.4652566
P	-2.0240497	1.0625274	1.2677807
C	-1.1870471	1.0711866	2.9256417
H	-1.9354855	0.8422798	3.6896250

H -0.3394311 0.3950911 3.0367691
H -0.8416588 2.0975251 3.0799265

3d⁻ : $[W(CO)_5]PPh_2PMe^-$ anion complex
39
Energy = -1820.742062504
P -2.1004779 0.8548574 0.2028678
C -2.5703514 1.9153948 1.6333140
C -2.2649061 2.0573866 -1.1921829
P -0.0957984 0.2179269 0.4749113
C -2.2547987 3.2833443 1.6663055
C -3.1345278 1.3341647 2.7783326
C -1.2849408 2.0948318 -2.1881684
C -3.4000415 2.8709689 -1.3222709
C 0.7298643 1.8871133 0.7989495
C -2.5073336 4.0466978 2.8080023
H -1.8172909 3.7545621 0.7915239
C -3.3938318 2.0946392 3.9159853
H -3.3714912 0.2746675 2.7732662
C -1.4311284 2.9311541 -3.2967411
H -0.4145076 1.4492402 -2.0745775
C -3.5460975 3.7097133 -2.4256037
H -4.1724443 2.8439802 -0.5574588
H 0.3272483 2.3827518 1.6907778
H 1.7970639 1.6970029 0.9663096
H 0.6370531 2.5773940 -0.0486221
C -3.0806247 3.4576676 3.9358743
H -2.2548214 5.1042452 2.8141943
H -3.8443844 1.6260218 4.7872855
C -2.5605167 3.7430180 -3.4171367
H -0.6610133 2.9520927 -4.0641378
H -4.4307743 4.3351088 -2.5164309
H -3.2829713 4.0531204 4.8221777
H -2.6753036 4.3967611 -4.2778840
W -3.6185177 -1.1815062 -0.2419951
C -4.7552193 -2.8031935 -0.5768268
C -4.2691786 -0.3396417 -1.9993108
C -2.8952916 -2.0087275 1.5020304
C -5.1782331 -0.2675940 0.7276614
C -2.0548254 -2.0211150 -1.2970117
O -5.4210523 -3.7456928 -0.7626999
O -4.6444448 0.1084632 -2.9999288
O -2.5050637 -2.5062613 2.4727920
O -6.0791904 0.2504916 1.2439069
O -1.2270971 -2.5274515 -1.9280153

3d• : $[W(CO)_5]PPh_2PMe^{\bullet}$ radical complex
39
Energy = -1820.611693603
P -1.0645730 0.0122648 -0.5190752
C -1.8509242 1.6033117 -0.0883194
C -2.2112815 -1.2370870 0.1631792
P -1.4472708 -0.1459176 -2.6817268
C -1.8026220 2.6852529 -0.9762824
C -2.4023572 1.7797112 1.1886573
C -3.5925996 -1.0956546 -0.0543680
C -1.7323424 -2.3641064 0.8387778
C -0.8222713 -1.8747610 -2.9032129
C -2.3100809 3.9272831 -0.5951579
H -1.3653311 2.5623993 -1.9639605
C -2.9074006 3.0228074 1.5654696
H -2.4403106 0.9464252 1.8844548
C -4.4754442 -2.0666472 0.4095068
H -3.9707171 -0.2228721 -0.5791381
C -2.6197706 -3.3385560 1.2993525
H -0.6673581 -2.4759592 1.0115187
H 0.2642383 -1.9094103 -2.7705253
H -1.2851612 -2.5666918 -2.1918375
H -1.0603105 -2.1913555 -3.9221522
C -2.8632942 4.0981008 0.6748015
H -2.2722778 4.7596263 -1.2917951
H -3.3354924 3.1513637 2.5554023
C -3.9901685 -3.1906495 1.0858527
H -5.5420657 -1.9493809 0.2417330
H -2.2392489 -4.2080401 1.8270636
H -3.2577927 5.0657568 0.9707187
H -4.6810214 -3.9474205 1.4457223
W 1.3989146 -0.0500795 0.1533576
C 3.3212061 -0.0351920 0.7732297
C 1.2870195 1.9798464 0.5062364
C 1.5675524 -2.0653521 -0.2235892
C 2.0037878 0.3496424 -1.7771476
C 0.7735239 -0.3908772 2.0868675
O 4.4219029 -0.0296771 1.1422775
O 1.2509891 3.1155986 0.7081499
O 1.7068089 -3.1944284 -0.4379146
O 2.3655009 0.5820248 -2.8502565
O 0.4253559 -0.5586123 3.1762824

4ac_ts : O-C cyclization of $[W(CO)_5]PHPhO^{\bullet}$
25
Energy = -1283.310249473
P 0.7492932 1.1114822 -1.0286393
C 0.2300360 2.7560928 -0.4999170
H 0.6491796 1.2450252 -2.4313634
O 2.2733625 0.8576890 -0.6333111
C 0.7613663 3.3120448 0.6719892
C -0.7664977 3.4393712 -1.2120246
C 0.3006854 4.5478801 1.1231334
H 1.5386672 2.7842678 1.2168189
C -1.2309292 4.6695149 -0.7490942
H -1.1736972 3.0165673 -2.1273906

C	-0.6976120	5.2239029	0.4173068
H	0.7207718	4.9835463	2.0247891
H	-2.0007470	5.1989951	-1.3024877
H	-1.0567090	6.1850568	0.7731933
W	-0.1158440	-0.9707362	0.0991507
C	-0.2982326	-2.7565042	1.1508220
C	0.1882656	-1.9738576	-1.6695701
C	-0.3244765	0.1029661	1.8389170
C	-2.0035519	-0.3843861	-0.4947598
C	2.0497659	-0.6507584	0.2315842
O	-0.4029073	-3.7464945	1.7292173
O	0.3736746	-2.5122786	-2.6730589
O	-0.4337438	0.7193519	2.8080364
O	-3.0049102	0.0476355	-0.8662143
O	3.0728547	-1.0655419	0.6302394

4ac• : $[W(CO)_5]PHPhO^{\bullet}$ with a CO in ring

25

Energy = -1283.315553675

P	-2.4416244	0.9545548	0.2465369
C	-2.6454772	1.9994504	1.6909500
H	-2.2874163	1.9262695	-0.7593864
O	-0.9010061	0.2890035	0.2988067
C	-2.0853876	3.2885466	1.7112739
C	-3.3660533	1.5313376	2.8000658
C	-2.2307388	4.0880825	2.8419072
H	-1.5392839	3.6596676	0.8485113
C	-3.5113790	2.3375388	3.9264597
H	-3.8174381	0.5445040	2.7746580
C	-2.9410114	3.6123614	3.9477177
H	-1.7954065	5.0824604	2.8596201
H	-4.0717471	1.9758521	4.7829127
H	-3.0567613	4.2409357	4.8256573
W	-3.4284072	-1.3141766	-0.1955065
C	-3.9651163	-3.2548282	-0.6332302
C	-3.3909639	-0.8257222	-2.1955846
C	-3.3197043	-1.8736212	1.7749620
C	-5.2564817	-0.4806013	0.1263938
C	-1.2248535	-1.0628436	-0.0381504
O	-4.2879465	-4.3350264	-0.8821828
O	-3.3575608	-0.5491401	-3.3161543
O	-3.2416072	-2.2165814	2.8762110
O	-6.2511659	0.0635865	0.3536392
O	-0.3209980	-1.8491018	-0.1801868

4ae_ts : 1,2-W-shift of $[W(CO)_5]PHPhO^{\bullet}$

25

Energy = -1283.332139260

P	1.3351787	-0.9771443	-0.7695579
O	0.6743063	-1.8451900	0.3427708
H	1.4975431	-1.6882062	-1.9839168
C	-1.5307751	-1.0042792	1.9513707
W	-0.9267900	-0.1087982	0.1534751
O	-1.9947007	-1.3963018	2.9300707
C	-2.5258154	1.0579430	0.4591010
C	-0.7956914	1.0354883	-1.5625787
C	0.2228803	1.2288068	1.2215162
C	-2.0500926	-1.4804876	-0.9147202
O	-3.4542670	1.7354115	0.6410913
O	-0.8017533	1.7134646	-2.4947683
O	0.8413788	1.9999311	1.8156851
O	-2.6959104	-2.2263217	-1.5089324
C	3.0054631	-0.4514189	-0.3810250
C	3.8699271	-0.0480318	-1.4121550
C	3.4139523	-0.3639821	0.9587424
C	5.1410612	0.4273881	-1.0996788
H	3.5561819	-0.1170003	-2.4509332
C	4.6908585	0.1041477	1.2603059
H	2.7396647	-0.6787651	1.7498670
C	5.5520593	0.5033528	0.2346197
H	5.8136062	0.7319858	-1.8959484
H	5.0149210	0.1574014	2.2953659
H	6.5451401	0.8716529	0.4742640

4ae• : $PHPhO[W(CO)_5]^{\bullet}$ radical complex

25

Energy = -1283.333655113

P	2.2875885	-1.2807730	-1.8706729
O	0.8142611	-1.8707117	-1.8265274
H	2.9651255	-2.1331577	-0.9601760
C	-1.6593994	-2.7428561	-0.5511997
W	-1.1805988	-1.2469831	-1.9105466
O	-1.9954107	-3.5555716	0.1927658
C	-3.1356715	-0.7557557	-1.9414693
C	-0.8468243	0.2844847	-3.2572690
C	-0.9885820	0.1772564	-0.4130059
C	-1.5827221	-2.6124461	-3.4171764
O	-4.2609210	-0.4631317	-1.9598855
O	-0.7328674	1.1622442	-3.9979001
O	-1.0137434	0.9934964	0.4005288
O	-1.8859980	-3.3517185	-4.2479347
C	2.2915778	0.2678169	-0.9199390
C	2.0339314	1.4799893	-1.5801294
C	2.4998065	0.2638454	0.4690740
C	1.9555426	2.6683495	-0.8567170
H	1.8990778	1.4909750	-2.6582225
C	2.4307678	1.4566573	1.1869074
H	2.7032551	-0.6702442	0.9856312
C	2.1524784	2.6557539	0.5259118
H	1.7480718	3.6027451	-1.3696248
H	2.5859733	1.4497871	2.2618312
H	2.0940809	3.5824236	1.0893419

4ap_ts : P-to-O 1,2-H-shift of $[W(CO)_5]PHPhO^{\bullet}$
25
Energy = -1283.283254378

P	1.1329821	-1.1595857	-0.2204905
O	1.3598754	-2.7000953	0.2456824
H	1.2580087	-2.4143624	-1.1042612
C	-1.2472580	-1.1504271	1.8251519
W	-0.9769465	0.0450110	0.1600462
O	-1.3949976	-1.8251624	2.7473867
C	-2.7205873	1.0242115	0.5769057
C	-0.7000256	1.2051191	-1.5252314
C	0.0415688	1.4314562	1.2996101
C	-1.9793045	-1.3733589	-0.9627389
O	-3.7017516	1.5814237	0.8265213
O	-0.5474614	1.8529275	-2.4680535
O	0.6061119	2.2040967	1.9437415
O	-2.5362466	-2.1697966	-1.5827713
C	2.7381746	-0.3530896	-0.2222509
C	2.8322671	1.0127151	-0.5435083
C	3.9015389	-1.0802082	0.0880689
C	4.0736142	1.6411337	-0.5581377
H	1.9362448	1.5788844	-0.7798178
C	5.1375823	-0.4404870	0.0855427
H	3.8232872	-2.1346998	0.3332217
C	5.2260260	0.9166090	-0.2404034
H	4.1433689	2.6946014	-0.8106496
H	6.0345024	-0.9994310	0.3353665
H	6.1933477	1.4101499	-0.2455081

4ap$^{\bullet}$: $[W(CO)_5]PPhOH^{\bullet}$ radical complex
25
Energy = -1283.349385262

P	0.2145937	-0.6867840	-0.8774933
O	0.3557164	-2.3120597	-1.0557009
H	1.2611182	-2.6025333	-1.2718717
C	-2.5323971	-1.7253323	0.2363448
W	-2.0931379	0.1413349	-0.5337589
O	-2.7731924	-2.7679144	0.6658979
C	-3.9924958	0.7428788	-0.1313413
C	-1.6414507	1.9975447	-1.3157558
C	-1.4932401	0.7935723	1.3283446
C	-2.6435954	-0.5307139	-2.4087650
O	-5.0748540	1.0686116	0.1227772
O	-1.3968604	3.0401052	-1.7488082
O	-1.1479779	1.1533305	2.3690117
O	-2.9563010	-0.9038885	-3.4552440
C	1.6052852	-0.1667643	0.1224779
C	1.7806114	1.2177756	0.3287821
C	2.5333661	-1.0665364	0.6810111
C	2.8513816	1.6859681	1.0803418
H	1.0728827	1.9215125	-0.1020280
C	3.6032268	-0.5880259	1.4335746
H	2.4064077	-2.1378313	0.5545833
C	3.7674554	0.7850580	1.6347314
H	2.9747454	2.7536645	1.2351273
H	4.3067824	-1.2902990	1.8712092
H	4.6029815	1.1523585	2.2229139

4aT : $[W(CO)_5]PHPhOT$ complex
53
Energy = -1692.147389106

P	0.2023796	0.7691239	-0.0825104
O	-1.3650519	1.2909807	-0.1348410
C	0.9845499	2.0749664	-1.0660387
H	0.5934623	1.2444132	1.1911335
N	-2.4083286	0.2429111	-0.0278396
C	1.4631156	3.2328848	-0.4355798
C	1.1229171	1.9390609	-2.4552782
C	-3.2737556	0.4187000	-1.2386209
C	-3.0227953	0.3828783	1.3318841
C	2.0729741	4.2391017	-1.1847424
H	1.3623058	3.3433461	0.6407705
C	1.7235311	2.9486822	-3.2027503
H	0.7665644	1.0420682	-2.9508025
C	-4.4234071	-0.5995269	-1.0943551
C	-2.4264113	0.0227984	-2.4538620
C	-3.8124773	1.8449465	-1.4648376
C	-4.1795317	-0.6368051	1.3827867
C	-3.5064332	1.7987953	1.7003347
C	-1.9583374	-0.0453211	2.3517834
C	2.2013304	4.0983855	-2.5675770
H	2.4470217	5.1302637	-0.6893063
H	1.8270556	2.8370783	-4.2779509
C	-5.1690101	-0.4704319	0.2317992
H	-4.0025936	-1.6091228	-1.1726127
H	-5.0983085	-0.4584022	-1.9464278
H	-1.6251530	0.7456908	-2.6297796
H	-1.9868750	-0.9656321	-2.3034359
H	-3.0593967	-0.0057283	-3.3465193
H	-3.0093057	2.5778117	-1.3554584
H	-4.6220734	2.1050898	-0.7814837
H	-4.2021875	1.9131586	-2.4860350
H	-3.7524435	-1.6461723	1.3466802
H	-4.6752666	-0.5244996	2.3538442
H	-2.7453086	2.5400953	1.4440830
H	-4.4405580	2.0692349	1.2057348
H	-3.6767515	1.8408912	2.7813877
H	-1.5188242	-1.0046965	2.0664563
H	-1.1628148	0.7009457	2.4407378
H	-2.4217056	-0.1525955	3.3377407
H	2.6771802	4.8814045	-3.1508318

H	-5.9501174	-1.2361656	0.2973841
H	-5.6754109	0.5001984	0.2964485
W	0.9699588	-1.6006578	-0.4539750
C	1.2524308	-1.6793990	1.5841067
C	2.8331392	-0.7644689	-0.6997923
C	-0.8875571	-2.4893020	-0.2385798
C	0.7012434	-1.5548645	-2.4940839
C	1.7909496	-3.4441114	-0.6228058
O	1.4187856	-1.7231178	2.7270165
O	3.8852640	-0.3079122	-0.8469571
O	-1.8736026	-3.0799249	-0.1281656
O	0.5749386	-1.5743350	-3.6443698
O	2.2771294	-4.4940667	-0.7089205

4a⁻ : $[W(CO)_5]PHPhO^-$ anion complex
25
Energy = -1283.512227813

P	0.2794791	-0.8463467	-1.1473908
O	0.4298480	-2.3495484	-1.3702293
H	0.7121645	-0.1312772	-2.3112489
C	-2.2248959	-1.7225318	0.5674343
W	-2.0200321	0.0683412	-0.4255378
O	-2.3027331	-2.7349435	1.1250060
C	-3.8641317	0.7173205	0.0751245
C	-1.5518795	1.7761869	-1.4545287
C	-1.2088175	0.8748906	1.2808437
C	-2.7101426	-0.7990811	-2.1562649
O	-4.9337337	1.0943923	0.3549359
O	-1.2356022	2.7256869	-2.0448523
O	-0.7482622	1.3237749	2.2455491
O	-3.0858320	-1.2938034	-3.1358584
C	1.6029974	-0.2463106	-0.0216978
C	1.9587586	1.1083203	0.0338120
C	2.2285891	-1.1519651	0.8419866
C	2.9260515	1.5494839	0.9348338
H	1.4755003	1.8220624	-0.6309704
C	3.1940766	-0.7106392	1.7507390
H	1.9547353	-2.2025997	0.7863985
C	3.5447140	0.6397757	1.7990852
H	3.1996252	2.6011843	0.9655916
H	3.6738522	-1.4213125	2.4193738
H	4.2967215	0.9839714	2.5042278

4a• : $[W(CO)_5]PHPhO^•$ radical complex
25
Energy = -1283.337727908

P	0.4177320	-0.2242866	-1.2732163
O	0.2893244	-1.6598476	-1.8050107
H	0.8273782	0.7004493	-2.2650341
C	-1.8978015	-1.8310176	0.6019292
W	-2.0114433	-0.1103621	-0.5525002
O	-1.8240887	-2.7823906	1.2461061
C	-3.8258338	0.4609967	0.1505953
C	-2.0298859	1.5539052	-1.7669858
C	-1.2203291	0.9059110	1.0624079
C	-2.8107157	-1.1833272	-2.1501035
O	-4.8372442	0.8424553	0.5623092
O	-2.0186858	2.4763958	-2.4584460
O	-0.7809353	1.4588148	1.9718307
O	-3.2703069	-1.7694651	-3.0257966
C	1.6941589	0.0076408	-0.0219679
C	2.4076676	1.2126870	0.0247377
C	1.9122126	-0.9803570	0.9488446
C	3.3401454	1.4261918	1.0396942
H	2.2416121	1.9774855	-0.7301781
C	2.8518170	-0.7644597	1.9537578
H	1.3571612	-1.9134134	0.9063151
C	3.5617413	0.4392186	2.0021353
H	3.8964799	2.3580893	1.0742488
H	3.0307156	-1.5323014	2.7004974
H	4.2901754	0.6060187	2.7901914

4bc• : $[W(CO)_5]PHPhS^•$ with a CO in ring
25
Energy = -1606.282126807

P	-2.2743356	0.9470005	0.3031971
C	-2.5931395	2.0133640	1.7237780
H	-2.1538159	1.9202614	-0.7067023
S	-0.3136507	0.1469111	0.4191272
C	-2.3024241	3.3848600	1.6528422
C	-3.1401634	1.4733636	2.8965201
C	-2.5506202	4.2035959	2.7528755
H	-1.8865603	3.8077182	0.7425763
C	-3.3826473	2.2961724	3.9935862
H	-3.3807209	0.4165219	2.9470715
C	-3.0872922	3.6598856	3.9223072
H	-2.3273841	5.2646611	2.6961959
H	-3.8082707	1.8763693	4.8998400
H	-3.2813737	4.3006367	4.7773143
W	-3.3771537	-1.2946506	-0.1957358
C	-4.1709256	-3.1171282	-0.6781792
C	-3.3295944	-0.7424297	-2.1801790
C	-3.2970946	-1.9407240	1.7495868
C	-5.1158154	-0.3223821	0.1906988
C	-1.1626055	-1.4203355	-0.1008773
O	-4.6556880	-4.1306055	-0.9534022
O	-3.2900891	-0.4327639	-3.2921034
O	-3.2408144	-2.3383642	2.8341408
O	-6.0623355	0.2883402	0.4583634
O	-0.5510218	-2.4277696	-0.3669408

4be_ts : 1,2-W-shift of $[W(CO)_5]PHPhS^•$

25
Energy = -1606.310513681
P 1.3842647 0.1146578 -1.1572313
S 0.4578879 -1.5349232 -1.8521440
H 1.7870477 0.9633666 -2.2081328
C 0.0543248 0.3237019 1.6777396
W -0.9549222 0.3734388 -0.1211579
O 0.5799931 0.3206106 2.7042050
C -2.5575654 1.0762294 0.8680875
C -2.0118043 0.4176202 -1.9078292
C -0.5428724 2.3821613 -0.4130347
C -1.6987880 -1.5182354 0.3479487
O -3.4462540 1.5419235 1.4549284
O -2.6236684 0.4476704 -2.8820722
O -0.3895849 3.5188417 -0.5223872
O -2.1985338 -2.5117056 0.6434298
C 2.9427075 -0.1863912 -0.3059596
C 4.0865905 0.5290687 -0.6883786
C 3.0060546 -1.1056422 0.7513800
C 5.2889896 0.3223092 -0.0120719
H 4.0408234 1.2348106 -1.5135168
C 4.2105836 -1.3093150 1.4177470
H 2.1220735 -1.6703033 1.0335530
C 5.3509378 -0.5929195 1.0401245
H 6.1761760 0.8718457 -0.3121457
H 4.2617828 -2.0256677 2.2320964
H 6.2886082 -0.7532161 1.5639467

4be• : PHPhS[W(CO)$_5$]• radical complex
25
Energy = -1606.314058655
P 1.3873382 -0.5029271 -2.0888194
S -0.3488249 -1.6243220 -1.6869937
H 2.2402889 -1.6095605 -2.3179245
C -2.7036573 -2.1249900 0.3523917
W -2.0120966 -0.3266157 -0.4023256
O -3.1137473 -3.1142502 0.7774319
C -3.5090630 0.6515381 0.5581387
C -1.3440849 1.4770030 -1.1569229
C -0.8408231 -0.0053398 1.2865013
C -3.3124807 -0.5887857 -1.9949479
O -4.3645672 1.2139359 1.1006799
O -1.0048953 2.4991878 -1.5689543
O -0.2878529 0.2041465 2.2734099
O -4.0648166 -0.7236602 -2.8559106
C 2.0339367 0.0342672 -0.4673157
C 2.0516764 1.4052622 -0.1732721
C 2.5315807 -0.8835886 0.4722700
C 2.5524106 1.8538089 1.0495851
H 1.6837050 2.1196975 -0.9036377
C 3.0369887 -0.4300695 1.6880165
H 2.5173615 -1.9470437 0.2516686
C 3.0453400 0.9375690 1.9786891
H 2.5611770 2.9166790 1.2722899
H 3.4196844 -1.1432629 2.4123618
H 3.4364723 1.2863524 2.9299515

4bH : aa
26
Energy = -1606.942944541
P -0.1282335 0.6470301 -0.4513145
S -2.1311313 0.7059948 -1.1750682
C 0.7500673 1.9843789 -1.3084287
H -0.3645474 1.2935370 0.7774094
C 0.9833913 3.2063724 -0.6638644
C 1.2307185 1.7792421 -2.6097036
C 1.6975378 4.2122794 -1.3161707
H 0.6115717 3.3708822 0.3438939
C 1.9329288 2.7894424 -3.2605248
H 1.0543086 0.8323600 -3.1125817
C 2.1698208 4.0056791 -2.6129884
H 1.8815857 5.1559647 -0.8112773
H 2.3009616 2.6280780 -4.2693013
H 2.7237151 4.7901753 -3.1201022
W 0.9838297 -1.6093922 -0.3625781
C 1.3663185 -1.2669539 1.6348288
C 2.7764080 -0.7152516 -0.8539358
C -0.8116445 -2.4854962 0.1494873
C 0.5780556 -1.9078894 -2.3586211
C 1.9156514 -3.4067717 -0.2574645
O 1.5729391 -1.0638517 2.7525043
O 3.7848998 -0.2218654 -1.1221377
O -1.8123996 -2.9840094 0.4385256
O 0.3497715 -2.0767227 -3.4798434
O 2.4507428 -4.4328142 -0.1954521
H -2.0451503 -0.4699837 -1.8226929

4bp_ts : 1,2-H-shift of [W(CO)$_5$]PHPhS•
25
Energy = -1606.274033852
P 1.1871068 -0.9438109 -0.2007593
S 1.5166048 -2.9832428 0.1169917
H 1.3950250 -2.0993407 -1.2645944
C -1.3120376 -1.1281310 1.6929296
W -1.0267595 0.1296536 0.0766640
O -1.4588415 -1.8419820 2.5852234
C -2.8508827 0.9718905 0.3935893
C -0.7304704 1.3528272 -1.5603505
C -0.1799695 1.5516203 1.3085918
C -1.8545150 -1.3201181 -1.1439370
O -3.8857558 1.4526209 0.5848522
O -0.5758350 2.0371416 -2.4767019

O	0.2863940	2.3459633	2.0032219
O	-2.3127960	-2.1333569	-1.8201028
C	2.7675407	-0.0798244	-0.1288276
C	2.7659547	1.3026025	-0.3928428
C	3.9751116	-0.7284114	0.1767369
C	3.9564626	2.0218412	-0.3533072
H	1.8349942	1.8094312	-0.6285800
C	5.1609503	-0.0003816	0.2185459
H	3.9725944	-1.7943464	0.3824777
C	5.1553270	1.3723899	-0.0463783
H	3.9491436	3.0875268	-0.5601649
H	6.0918388	-0.5039972	0.4617549
H	6.0831263	1.9355890	-0.0116064

4bp• : $[W(CO)_5]PPhSH^•$ radical complex
25
Energy = -1606.314019229

P	0.1996712	-0.6423856	-0.8787636
S	0.3742555	-2.6797957	-1.3271305
H	1.6651926	-2.6668482	-1.7244243
C	-2.5560438	-1.6422511	0.3560750
W	-2.1118606	0.1859111	-0.5001044
O	-2.8036818	-2.6606179	0.8369377
C	-4.0129855	0.7931492	-0.1227709
C	-1.6840328	2.0234711	-1.3472680
C	-1.5090262	0.9044680	1.3363908
C	-2.6619038	-0.5652665	-2.3442068
O	-5.0980022	1.1267913	0.1079474
O	-1.4597546	3.0550459	-1.8131719
O	-1.1698833	1.2988129	2.3662912
O	-2.9700462	-0.9874263	-3.3727550
C	1.6036148	-0.1698819	0.1394152
C	1.7431353	1.2077117	0.4112726
C	2.5594716	-1.0697248	0.6440866
C	2.8081034	1.6677989	1.1769091
H	1.0137222	1.9115461	0.0187133
C	3.6217747	-0.5996186	1.4120838
H	2.4541784	-2.1342040	0.4603946
C	3.7515666	0.7658828	1.6796570
H	2.9043568	2.7297840	1.3821336
H	4.3471770	-1.3035439	1.8094639
H	4.5820522	1.1262236	2.2791856

4bT : $[W(CO)_5]PHPhST$ complex
53
Energy = -2015.152378248

P	0.0077678	-0.1584723	0.3580733
S	-1.5397662	0.3996719	-0.9883076
C	0.0932970	1.0974505	1.6534884
H	-0.5820023	-1.2043427	1.0954233
N	-2.8952086	0.8577732	-0.0483062
C	0.9481885	2.1999794	1.5187634
C	-0.7607140	1.0106486	2.7632435
C	-3.9668818	-0.2079990	0.0298942
C	-3.2792440	2.3124577	-0.2338174
C	0.9469795	3.2060361	2.4808360
H	1.6072588	2.2717761	0.6588930
C	-0.7565658	2.0189184	3.7266020
H	-1.4267990	0.1602225	2.8690672
C	-5.0638985	0.2714996	0.9982386
C	-3.3476217	-1.4767667	0.6301976
C	-4.5657771	-0.5686221	-1.3431690
C	-4.4186119	2.6433750	0.7479954
C	-3.6892023	2.6403762	-1.6828649
C	-2.0845011	3.1966128	0.1415809
C	0.0932828	3.1175004	3.5842322
H	1.6101301	4.0587189	2.3716983
H	-1.4187295	1.9485797	4.5845426
C	-5.5858283	1.6664165	0.6758864
H	-4.6476696	0.2758619	2.0144652
H	-5.8694329	-0.4716641	0.9783192
H	-2.6015613	-1.9158348	-0.0386765
H	-2.8822147	-1.2581727	1.5957661
H	-4.1383338	-2.2174206	0.7879395
H	-5.1646070	0.2413719	-1.7635771
H	-5.2113716	-1.4474393	-1.2400935
H	-3.7663288	-0.8145434	-2.0503253
H	-4.0064917	2.6292956	1.7656521
H	-4.7438820	3.6694589	0.5408625
H	-2.9020915	2.3287230	-2.3782512
H	-4.6216414	2.1542331	-1.9758282
H	-3.8239208	3.7222881	-1.7877511
H	-1.7676004	3.0000171	1.1677287
H	-1.2358814	3.0350898	-0.5279346
H	-2.3885562	4.2456490	0.0618438
H	0.0933549	3.9036261	4.3335812
H	-6.3618508	1.9529696	1.3946770
H	-6.0517659	1.6882633	-0.3168248
W	1.9946504	-0.7375211	-1.0735053
C	2.0156776	-2.5852973	-0.1656727
C	3.2748281	-0.0308239	0.3773877
C	0.7484699	-1.4989149	-2.5342381
C	1.8779055	1.1308660	-1.9361098
C	3.5906848	-1.2215894	-2.2233480
O	2.0083038	-3.6182743	0.3526623
O	4.0079052	0.3497134	1.1857408
O	0.0935666	-1.9543218	-3.3700426
O	1.8092848	2.1796909	-2.4179266
O	4.5064511	-1.5013067	-2.8782186

4b⁻ : $[W(CO)_5]PHPhS^-$ anion complex
25

Energy = -1606.480855353

P	0.3157467	-0.8124151	-1.1845658
S	0.5469577	-2.7695193	-1.5878820
H	0.7444862	-0.0689094	-2.3158583
C	-2.2571034	-1.7770032	0.4867422
W	-1.9995210	0.0462501	-0.4420184
O	-2.3901514	-2.7970333	1.0155501
C	-3.8381867	0.6799527	0.0792555
C	-1.5662813	1.8128078	-1.3845462
C	-1.2003050	0.7825835	1.3020466
C	-2.6915340	-0.7444252	-2.2119611
O	-4.9043072	1.0546785	0.3738772
O	-1.2878167	2.8050595	-1.9195617
O	-0.7499245	1.1953970	2.2865956
O	-3.0740151	-1.1915717	-3.2097363
C	1.6259489	-0.2361605	-0.0291864
C	1.9695264	1.1223790	0.0113288
C	2.2332209	-1.1237738	0.8628544
C	2.9110912	1.5841459	0.9295426
H	1.4984999	1.8213695	-0.6769244
C	3.1686084	-0.6595028	1.7907349
H	1.9717466	-2.1781148	0.8095006
C	3.5103728	0.6935800	1.8257395
H	3.1778533	2.6377243	0.9475952
H	3.6343672	-1.3564399	2.4830278
H	4.2417710	1.0539724	2.5442112

4b• : $[W(CO)_5]PHPhS^{\bullet}$ radical complex

25

Energy = -1606.315867167

P	1.3280507	0.0710887	-1.3347383
S	0.5317109	-1.5155165	-2.2781537
H	1.7940343	1.0403301	-2.2473748
C	0.3711362	0.8102483	1.5261975
W	-0.8521111	0.5227182	-0.1141547
O	1.0381375	0.9684043	2.4517428
C	-2.3852054	1.1879437	1.0331031
C	-2.1465105	0.2410938	-1.7182414
C	-0.5785933	2.4541355	-0.7847554
C	-1.1317027	-1.4246466	0.5521216
O	-3.2231723	1.6144355	1.7087760
O	-2.8978278	0.1119765	-2.5802813
O	-0.4252740	3.5318524	-1.1645912
O	-1.3004784	-2.4913810	0.9510387
C	2.8271075	-0.2792187	-0.3878258
C	3.8818805	0.6423477	-0.4033728
C	2.8980184	-1.4203296	0.4223122
C	5.0069031	0.4187406	0.3913812
H	3.8289413	1.5258377	-1.0344954
C	4.0254895	-1.6391273	1.2090496
H	2.0785227	-2.1341867	0.4235430
C	5.0786462	-0.7191114	1.1964314
H	5.8266533	1.1307569	0.3762833
H	4.0845730	-2.5262683	1.8324208
H	5.9559226	-0.8921864	1.8127083

4c0 : aa

25

Energy = -1262.865173586

P	0.0888160	-1.1088819	-0.3231346
C	-2.9601340	-1.6384697	0.3071758
W	-2.0721406	0.0565927	-0.4729786
O	-3.4510689	-2.5905075	0.7333036
C	-3.8965177	0.9675458	-0.6091058
C	-1.1754238	1.7311714	-1.2821521
C	-1.8418237	0.8123234	1.4346758
C	-2.3026410	-0.7363404	-2.3670530
O	-4.9274374	1.4835407	-0.6836809
O	-0.6819524	2.6668492	-1.7428802
O	-1.7231143	1.2295671	2.5036363
O	-2.4311435	-1.1904604	-3.4189846
C	1.5842527	-0.3650876	0.3373065
C	1.5584827	0.9722880	0.7640618
C	2.7771460	-1.1053909	0.4336823
C	2.7079420	1.5660446	1.2802833
H	0.6403632	1.5467699	0.6911596
C	3.9206550	-0.5076146	0.9512357
H	2.7875193	-2.1382196	0.1017628
C	3.8882165	0.8263910	1.3743201
H	2.6829570	2.6005703	1.6077168
H	4.8409996	-1.0789691	1.0270661
H	4.7849070	1.2877027	1.7776482
N	0.4793430	-2.5811492	-0.7329880
H	-0.3187197	-3.0915767	-1.1212219

4ce_ts : 1,2-W-shift of $[W(CO)_5]PHPhNMe^{\bullet}$

29

Energy = -1302.754695877

P	1.3649120	-0.6394275	-0.9264871
H	1.5344217	-1.2653569	-2.1902520
C	-1.9306222	-0.9943950	1.5207331
W	-1.0167351	0.1192104	0.0023759
O	-2.5752861	-1.4740706	2.3488413
C	-2.6324698	1.2769251	0.3529194
C	-0.7072826	1.5749232	-1.4325287
C	0.0622291	1.1832319	1.4117179
C	-2.0461126	-0.9531858	-1.4284551
O	-3.5961055	1.8911355	0.5826104
O	-0.6397601	2.4292613	-2.2062911
O	0.6500268	1.7923438	2.1940629
O	-2.6500957	-1.5146799	-2.2363045
C	3.0612326	-0.3119477	-0.3981572

C	3.9908613	0.2263163	-1.3028878
C	3.4147129	-0.4980602	0.9462115
C	5.2738467	0.5478611	-0.8662583
H	3.7174349	0.3809522	-2.3440324
C	4.7005573	-0.1721682	1.3745426
H	2.6820801	-0.9071604	1.6360865
C	5.6300651	0.3508381	0.4718611
H	5.9968999	0.9516714	-1.5690654
H	4.9784353	-0.3283753	2.4129631
H	6.6304507	0.6057347	0.8091666
N	0.5280714	-1.5379873	0.1380169
C	0.2838079	-2.9769778	0.0360051
H	-0.3703052	-3.2871374	0.8563385
H	-0.1996391	-3.2600060	-0.9107500
H	1.2284646	-3.5271973	0.1219329

4ce• : $W(CO)_5$]PHPhNMe• radical complex
29
Energy = -1302.772221315

P	2.0875288	-0.8706881	-0.6690826
H	1.7859024	-1.2828652	0.6497990
C	-1.6508372	1.7663013	-0.1302446
W	-1.2139998	-0.2494152	-0.0054100
O	-1.9498651	2.8810188	-0.1735985
C	-3.0144199	-0.5014968	0.8959980
C	-0.9105945	-2.2858169	0.1819538
C	-2.1419527	-0.5179595	-1.8352093
C	-0.3738362	-0.0045040	1.8651500
O	-4.0471556	-0.6414708	1.4101068
O	-0.8025595	-3.4274155	0.3198357
O	-2.7096069	-0.6734193	-2.8283896
O	0.0593694	0.1236621	2.9282990
C	3.4091577	0.3519421	-0.3302934
C	4.6203833	0.2596946	-1.0283485
C	3.2208288	1.3903341	0.5968759
C	5.6374829	1.1877358	-0.7951047
H	4.7655082	-0.5378568	-1.7521881
C	4.2346289	2.3173591	0.8240120
H	2.2808595	1.4697090	1.1361057
C	5.4441973	2.2153567	0.1286295
H	6.5757057	1.1098795	-1.3366384
H	4.0862398	3.1175162	1.5435320
H	6.2336794	2.9394304	0.3081808
N	0.6988004	0.0815175	-0.9535580
C	0.8715206	1.0613274	-2.0373504
H	0.0018203	1.0438785	-2.6996894
H	0.9533623	2.0662804	-1.6046834
H	1.7762674	0.8711401	-2.6261281

4chc_ts : N-C cyclization $[W(CO)_5]$PHPhNH•
26
Energy = -1263.409972840

P	-0.8926111	0.6584690	-1.2359853
C	-0.3364991	0.3154548	-2.9170719
H	-1.7618097	1.7476325	-1.4416719
N	-1.9764968	-0.5888340	-0.7230053
C	-1.2166277	0.4803277	-3.9998083
C	0.9730217	-0.1316862	-3.1413025
C	-0.7892401	0.1795807	-5.2909712
H	-2.2283246	0.8391394	-3.8312444
C	1.3954899	-0.4286330	-4.4361205
H	1.6579559	-0.2332263	-2.3051026
C	0.5143477	-0.2760971	-5.5084963
H	-1.4702508	0.3040645	-6.1274983
H	2.4113080	-0.7710299	-4.6082219
H	0.8451483	-0.5051826	-6.5172159
W	0.2094932	0.1244699	0.9283660
C	0.6206379	-0.6521890	2.7645554
C	-0.8528008	1.6968553	1.7272293
C	1.2831380	-1.4339075	0.1238482
C	1.9245897	1.2453663	1.0590636
C	-1.6482515	-1.0076326	0.9360303
O	0.8137894	-1.1170748	3.8058286
O	-1.4478328	2.5838871	2.1661771
O	1.9016872	-2.3162224	-0.2969455
O	2.8884452	1.8777017	1.1640857
O	-2.4440319	-1.7342843	1.4203528
H	-1.8599594	-1.4575752	-1.2593555

4chc• : $[W(CO)_5]$PHPhNH• with a CO in ring
26
Energy = -1263.436572948

P	-2.4689059	1.0161042	0.2160313
C	-2.6567692	2.0541899	1.6777816
H	-2.3859569	2.0086360	-0.7796284
N	-0.9209903	0.2804119	0.2116170
C	-2.2523453	3.3985706	1.6422197
C	-3.2048699	1.5206641	2.8534749
C	-2.3766728	4.1919708	2.7811860
H	-1.8436024	3.8205773	0.7280134
C	-3.3247996	2.3176553	3.9895585
H	-3.5437052	0.4898505	2.8745079
C	-2.9087279	3.6509047	3.9540847
H	-2.0629734	5.2310728	2.7523688
H	-3.7498856	1.9028588	4.8984184
H	-3.0078475	4.2718889	4.8395150
W	-3.4307437	-1.2929846	-0.2425522
C	-4.0235783	-3.1932993	-0.7017917
C	-3.4040492	-0.7856815	-2.2338946
C	-3.2813601	-1.8860204	1.7119596
C	-5.2585120	-0.4996619	0.0928912
C	-1.1894452	-1.0355420	-0.1203261

O -4.3876311 -4.2609312 -0.9668290
O -3.3743124 -0.5032499 -3.3557921
O -3.1797845 -2.2548759 2.8055127
O -6.2742800 0.0110438 0.3232758
O -0.3421088 -1.8968570 -0.3184004
H 0.0178818 0.6758111 0.2905150

4che_ts : 1,2-W-shift of $[W(CO)_5]PHPhNH^{\bullet}$
26
Energy = -1263.421354208
P 1.2089239 -0.8546123 -0.9736002
H 1.3811261 -1.5644924 -2.1890615
C -1.8819097 -1.0505848 1.7222795
W -1.0917158 0.0135456 0.1018094
O -2.4348348 -1.5267144 2.6137779
C -2.6335043 1.2413530 0.5343000
C -0.8109657 1.3987686 -1.4092468
C 0.1274309 1.0859832 1.3824306
C -2.2465888 -1.0845570 -1.2050964
O -3.5442185 1.9054400 0.8176258
O -0.7475022 2.2157043 -2.2214573
O 0.7925081 1.7063898 2.0905266
O -2.8971936 -1.6876166 -1.9428701
C 2.8978364 -0.4688697 -0.4589131
C 3.7685204 0.1965938 -1.3374025
C 3.2994629 -0.7380207 0.8569896
C 5.0426844 0.5586567 -0.9072434
H 3.4552923 0.4220413 -2.3542562
C 4.5742085 -0.3654399 1.2816841
H 2.6099786 -1.2443566 1.5261490
C 5.4465804 0.2809689 0.4030872
H 5.7207123 1.0603726 -1.5916883
H 4.8878111 -0.5823921 2.2989456
H 6.4386797 0.5705527 0.7371241
N 0.4355308 -1.7267977 0.1851415
H 0.0930044 -2.6424989 -0.1030959

4che$^{\bullet}$: $PHPhNH[W(CO)_5]^{\bullet}$ radical complex
26
Energy = -1263.440193777
P 2.1605517 -0.8518884 -0.9305539
H 1.9526874 -1.4988107 0.3125098
C -1.4013707 1.7819134 0.0605226
W -1.1468186 -0.2715207 0.0282113
O -1.5886929 2.9196451 0.1009807
C -2.8757793 -0.4145336 1.0871421
C -1.0078487 -2.3379479 0.0558723
C -2.2387110 -0.3046319 -1.7301449
C -0.1298002 -0.2619058 1.8288488
O -3.8631757 -0.4897761 1.6943110
O -0.9775151 -3.4901573 0.1062677
O -2.8910232 -0.3227260 -2.6815395
O 0.3982223 -0.2675543 2.8550895
C 3.4025203 0.4077915 -0.4493875
C 4.7518713 0.1796731 -0.7552154
C 3.0295904 1.5934809 0.2023413
C 5.7202497 1.1148209 -0.3883884
H 5.0426298 -0.7274865 -1.2790816
C 3.9983619 2.5318242 0.5533321
H 1.9833894 1.7738115 0.4328008
C 5.3440960 2.2923255 0.2614856
H 6.7650601 0.9299949 -0.6208008
H 3.7056982 3.4480673 1.0584582
H 6.0973079 3.0246335 0.5374947
N 0.6978272 -0.0149187 -1.0263642
H 0.7283825 0.6581213 -1.7949101

4chp_ts : P/N 1,2-H-shift $[W(CO)_5]PHPhNH^{\bullet}$
26
Energy = -1263.386481788
P 1.1676257 -1.1291210 -0.3914075
H 1.2387433 -2.2068688 -1.4736481
C -1.3693513 -1.3157716 1.4807556
W -0.9512131 0.0991805 0.0353083
O -1.6037058 -2.1094486 2.2838223
C -2.6960788 1.0509924 0.4536652
C -0.5285153 1.4861719 -1.4299611
C 0.0093721 1.2607844 1.4418497
C -1.8906804 -1.1002898 -1.3593257
O -3.6900899 1.5897058 0.7049036
O -0.3004730 2.2675292 -2.2501677
O 0.5404833 1.9078943 2.2371640
O -2.4149332 -1.7744751 -2.1352964
C 2.7983621 -0.3908900 -0.1635477
C 2.9186973 1.0044468 -0.2951154
C 3.9429627 -1.1549168 0.1192344
C 4.1586669 1.6203111 -0.1552904
H 2.0383253 1.6038802 -0.5059779
C 5.1797514 -0.5325104 0.2693562
H 3.8775641 -2.2334073 0.2315113
C 5.2915080 0.8533448 0.1288876
H 4.2406818 2.6975271 -0.2628559
H 6.0575767 -1.1302741 0.4957590
H 6.2583648 1.3341417 0.2432286
N 1.1834157 -2.8320049 -0.1463219
H 2.1482697 -3.1872379 -0.0742184

4chp$^{\bullet}$: $[W(CO)_5]PPhNH_2^{\bullet}$ radical complex
26
Energy = -1263.468519983
P 1.2095522 -0.9657569 -0.7504495
H 0.5324695 -3.1766056 -0.6240209

C	-1.1174485	-1.4079161	1.3521335
W	-0.9310565	0.1127305	-0.0281280
O	-1.2146930	-2.2610418	2.1244289
C	-2.6396137	0.9456477	0.6719995
C	-0.7223432	1.6312635	-1.4113004
C	0.1756978	1.2118902	1.3221714
C	-1.9869939	-1.0062292	-1.4008946
O	-3.6128364	1.4110941	1.0991021
O	-0.6136739	2.4889050	-2.1780136
O	0.8017355	1.8211793	2.0766097
O	-2.5834922	-1.6304259	-2.1697165
C	2.8104659	-0.3010144	-0.2935747
C	3.0508013	1.0585729	-0.5785205
C	3.8293176	-1.0642465	0.3071521
C	4.2745502	1.6389430	-0.2666156
H	2.2723986	1.6559874	-1.0469114
C	5.0542477	-0.4751505	0.6141535
H	3.6541938	-2.1050758	0.5601641
C	5.2827775	0.8732955	0.3290085
H	4.4455602	2.6881102	-0.4889152
H	5.8302344	-1.0701088	1.0875097
H	6.2388812	1.3269922	0.5724033
N	1.3765572	-2.6257833	-0.5021308
H	2.1880405	-3.0965629	-0.8953326

4chT : $[W(CO)_5]$PHPhNHT complex

54

Energy = -1672.277542049

P	0.0056824	1.0389745	0.7990642
N	-1.5964358	1.3855988	0.3933507
C	0.8336277	2.6182739	0.4432322
H	0.1089176	1.1120292	2.2134969
N	-2.5362054	0.3701452	0.1059861
C	1.6190140	3.2271808	1.4309589
C	0.7701970	3.1882927	-0.8363693
C	-3.2454040	0.6777682	-1.1865527
C	-3.3481528	-0.0203392	1.3122130
C	2.3385580	4.3869342	1.1406959
H	1.6680520	2.7940522	2.4268050
C	1.4799077	4.3526513	-1.1204982
H	0.1653310	2.7214235	-1.6071769
C	-4.2260912	-0.4697530	-1.4866350
C	-2.1909773	0.6974761	-2.2992436
C	-3.9759648	2.0367393	-1.1944865
C	-4.3131137	-1.1451538	0.8975689
C	-4.1239158	1.1426970	1.9654270
C	-2.3796040	-0.5918896	2.3571328
C	2.2689190	4.9511265	-0.1338981
H	2.9458339	4.8523268	1.9116393
H	1.4216280	4.7917876	-2.1121121
C	-5.1578758	-0.7865379	-0.3211589
H	-3.6417057	-1.3665657	-1.7255671
H	-4.7923124	-0.1993878	-2.3855739
H	-1.5027839	1.5364924	-2.1782976
H	-1.6163879	-0.2313944	-2.2959231
H	-2.6885599	0.7996030	-3.2692478
H	-4.3063263	2.2586539	-2.2148495
H	-3.3041887	2.8446571	-0.8855079
H	-4.8559720	2.0485654	-0.5486466
H	-3.7196332	-2.0390174	0.6687860
H	-4.9436778	-1.3828685	1.7623887
H	-4.9727117	1.4754156	1.3656868
H	-4.5072048	0.8134401	2.9370131
H	-3.4730776	2.0042387	2.1524530
H	-1.7205058	-1.3341205	1.8986038
H	-1.7695976	0.1889148	2.8211041
H	-2.9520235	-1.0777715	3.1539336
H	2.8255367	5.8562344	-0.3590454
H	-5.8149476	-1.6238575	-0.5826343
H	-5.8105021	0.0677993	-0.1021755
W	1.1663618	-1.0071152	-0.1118079
C	1.1086870	-1.7890109	1.7902254
C	2.9226441	-0.0415126	0.3453307
C	-0.5532842	-2.0568009	-0.5786086
C	1.2188907	-0.1562529	-1.9868521
C	2.2402038	-2.5928611	-0.7649307
O	1.0787884	-2.2132947	2.8657609
O	3.9223032	0.4837662	0.5958564
O	-1.4479481	-2.7350081	-0.8512338
O	1.2766559	0.3178881	-3.0401356
O	2.8656275	-3.4990532	-1.1336217
H	-1.9775622	2.2520320	0.7787802

4ch$^-$: $[W(CO)_5]$PHPhNH$^-$ anion complex

26

Energy = -1263.588442779

P	0.3649561	-0.6401056	-1.3193477
H	0.7870693	0.2779200	-2.3324812
C	-2.0673461	-1.7555031	0.4245721
W	-1.9813632	0.0762427	-0.5031258
O	-2.0864581	-2.7892399	0.9503237
C	-3.8424168	0.5925835	0.0698095
C	-1.6389004	1.8575772	-1.4595275
C	-1.1758543	0.8540158	1.2204644
C	-2.6816855	-0.7431887	-2.2533107
O	-4.9235367	0.8964439	0.3927776
O	-1.3956705	2.8533255	-2.0046719
O	-0.7220943	1.2876017	2.1946399
O	-3.0750042	-1.2078649	-3.2410362
C	1.6417450	-0.1391465	-0.0962254
C	2.0395420	1.1986466	0.0297156
C	2.1777073	-1.0943584	0.7735874

C	2.9501336	1.5773552	1.0147392
H	1.6305031	1.9478099	-0.6465592
C	3.0910461	-0.7179728	1.7611777
H	1.8746844	-2.1320775	0.6533022
C	3.4772259	0.6184367	1.8861081
H	3.2521988	2.6180064	1.1039548
H	3.5034720	-1.4673412	2.4326493
H	4.1877924	0.9125487	2.6542039
N	0.6432932	-2.1632907	-1.7877173
H	-0.2284496	-2.6907560	-1.7360815

4ch• : $[W(CO)_5]PHPhNH^{\bullet}$ radical complex
26
Energy = -1263.432582703

P	0.4172739	-0.3689539	-1.2881496
H	0.8431065	0.4129791	-2.3889149
C	-2.0326227	-1.8769389	0.4485631
W	-1.9801290	-0.0467328	-0.5244704
O	-2.0728206	-2.8857546	1.0048403
C	-3.8385496	0.4407275	0.1192631
C	-1.8776324	1.7592243	-1.5103468
C	-1.1950853	0.7887672	1.1919863
C	-2.7428317	-0.9036374	-2.2389909
O	-4.8931128	0.7510979	0.4854144
O	-1.8065505	2.7662274	-2.0706185
O	-0.7562372	1.2517723	2.1525443
O	-3.1815500	-1.3790258	-3.1959310
C	1.6997683	-0.0346071	-0.0636794
C	2.3263161	1.2178924	-0.0485669
C	1.9918408	-0.9809908	0.9272724
C	3.2494981	1.5193800	0.9525520
H	2.0996076	1.9542478	-0.8158595
C	2.9197389	-0.6746764	1.9208815
H	1.5016437	-1.9498087	0.9105829
C	3.5460782	0.5744393	1.9365684
H	3.7381420	2.4891138	0.9604823
H	3.1534870	-1.4107621	2.6844312
H	4.2656641	0.8102640	2.7151018
N	0.4392527	-1.9903613	-1.5929766
H	-0.0117065	-2.2062150	-2.4900391

4cp_ts : P/N 1,2-H-shift of $[W(CO)_5]PHPhNH^{\bullet}$
29
Energy = -1302.716888217

P	1.1279422	-0.9749990	-0.3800691
H	1.4254316	-2.2262270	-1.2359691
C	-1.8911688	-1.7573779	0.3394965
W	-1.0836925	0.1096055	-0.0234435
O	-2.3479637	-2.7969818	0.5417219
C	-2.8631194	1.0055611	0.3624742
C	-0.2352063	1.9415195	-0.4252344
C	-0.5956182	0.2699889	1.9718383
C	-1.5840448	-0.0795603	-2.0216077
O	-3.8730878	1.5212033	0.6017667
O	0.2368865	2.9703670	-0.6569603
O	-0.3276459	0.3569614	3.0928737
O	-1.8724126	-0.1858302	-3.1338178
C	2.6879248	-0.0662373	-0.2212359
C	2.8174281	0.9521717	0.7365074
C	3.7824520	-0.3806396	-1.0456242
C	4.0232327	1.6367482	0.8746820
H	1.9759227	1.2078897	1.3731756
C	4.9852028	0.3089831	-0.9062220
H	3.6848626	-1.1522945	-1.8047068
C	5.1071591	1.3158821	0.0545722
H	4.1158917	2.4203806	1.6204823
H	5.8244152	0.0650972	-1.5508892
H	6.0444519	1.8542399	0.1596686
N	1.3180144	-2.6230961	0.1242630
C	2.5748855	-3.0811626	0.7192614
H	2.6353828	-4.1683138	0.6257857
H	3.4724761	-2.6266473	0.2828631
H	2.5571939	-2.8165346	1.7861468

4cp• : $[W(CO)_5]PPhNH_2^{\bullet}$ radical complex
29
Energy = -1302.798375882

P	1.0639649	-0.9906266	-0.7021225
N	1.2802386	-2.6193223	-0.3440802
C	2.6746222	-0.2810399	-0.3226840
C	3.6378239	-0.9119879	0.4852834
C	2.9638112	0.9839693	-0.8700683
C	4.8602496	-0.2892650	0.7325027
H	3.4218598	-1.8720161	0.9443513
C	4.1827059	1.6022144	-0.6132156
H	2.2288249	1.4782119	-1.5009233
C	5.1373426	0.9661335	0.1867902
H	5.5934338	-0.7816458	1.3651621
H	4.3917990	2.5788482	-1.0398640
H	6.0898447	1.4483284	0.3856063
W	-1.0149993	0.2096093	0.0749807
C	-1.1168736	-1.1039957	1.6601492
C	-2.2345012	-1.0035870	-1.0603377
C	0.2369806	1.4158612	1.1839375
C	-0.8746333	1.5404241	-1.4961321
C	-2.6223832	1.1957275	0.8019384
O	-1.1614126	-1.8306283	2.5574260
O	-2.9293493	-1.6719110	-1.6994284
O	0.9385754	2.0879096	1.8075750
O	-0.8007210	2.2971295	-2.3665470
O	-3.5385306	1.7543889	1.2455285
C	0.2032554	-3.6085743	-0.3994564

H	-0.7323665	-3.1330661	-0.1004990
H	0.0818594	-4.0258594	-1.4060121
H	0.4245385	-4.4189805	0.3001031
H	2.2051288	-2.9985989	-0.5304043

4cT : $[W(CO)_5]$PHPhNHT complex
57
Energy = -1711.600623368

P	-0.0507664	1.0832858	0.7675512
N	-1.6692607	1.5465309	0.5322960
C	0.8916517	2.5872746	0.3473566
H	0.1317784	1.1826141	2.1752308
N	-2.6257901	0.5594089	0.1994155
C	1.6042350	3.2710373	1.3406111
C	0.9693761	3.0288258	-0.9814282
C	-3.2940372	0.8162551	-1.1210916
C	-3.4055688	-0.0092810	1.3504653
C	2.3882732	4.3772170	1.0103483
H	1.5458702	2.9372865	2.3734547
C	1.7408971	4.1413823	-1.3078902
H	0.4265532	2.5023529	-1.7595792
C	-4.0823373	-0.4511828	-1.5093435
C	-2.1961667	1.0151074	-2.1723582
C	-4.2234927	2.0500832	-1.1818922
C	-4.1461455	-1.2582966	0.8335856
C	-4.4333826	0.9258947	2.0361802
C	-2.3988255	-0.4585064	2.4146792
C	2.4554242	4.8150440	-0.3128610
H	2.9402051	4.8988058	1.7870215
H	1.7918546	4.4795772	-2.3387777
C	-4.9944608	-0.9657165	-0.4004396
H	-3.3634099	-1.2372384	-1.7644723
H	-4.6532520	-0.2230003	-2.4168976
H	-1.6791824	1.9671705	-2.0320871
H	-1.4663975	0.2040004	-2.1120045
H	-2.6457787	1.0123469	-3.1708368
H	-4.6404239	2.1222263	-2.1928374
H	-3.6699010	2.9733436	-0.9925106
H	-5.0589933	1.9905997	-0.4816745
H	-3.4045136	-2.0246262	0.5830278
H	-4.7605305	-1.6486180	1.6533006
H	-5.1902861	1.3015383	1.3457528
H	-4.9501592	0.3510386	2.8130670
H	-3.9552154	1.7766382	2.5234681
H	-1.6339173	-1.0977363	1.9643744
H	-1.9109450	0.3920984	2.9019687
H	-2.9185356	-1.0304826	3.1898644
H	3.0624007	5.6782364	-0.5702486
H	-5.5065864	-1.8770387	-0.7304044
H	-5.7760065	-0.2317011	-0.1674281
W	1.0739870	-1.0084894	-0.1298893
C	0.9896832	-1.7696746	1.7811658
C	2.8261740	-0.0361600	0.3393374
C	-0.6099940	-2.0812034	-0.6471310
C	1.1882198	-0.2390399	-2.0364080
C	2.1734001	-2.5987495	-0.7144894
O	0.9597077	-2.1963805	2.8553363
O	3.8290475	0.4821329	0.5882766
O	-1.4805614	-2.7717406	-0.9647247
O	1.2880524	0.1622711	-3.1167887
O	2.8155982	-3.5091263	-1.0420912
C	-2.0564321	2.8081270	1.2024016
H	-1.9509189	2.7400396	2.2950375
H	-1.4146087	3.6166696	0.8415478
H	-3.0888375	3.0434877	0.9588149

4c$^-$: $[W(CO)_5]$PHPhNH$^-$ anion complex
29
Energy = -1302.912924301

P	0.4060449	-0.4977557	-1.3985899
H	0.7514894	0.5197009	-2.3614128
C	-2.2478310	-1.8144418	0.1027064
W	-1.9867828	0.1162856	-0.5582249
O	-2.3849724	-2.8909204	0.5138195
C	-3.8272681	0.6512252	0.0456408
C	-1.5379945	2.0088107	-1.2008673
C	-1.1671493	0.5592443	1.2729454
C	-2.6611078	-0.3779405	-2.4354655
O	-4.8979815	0.9744127	0.3864982
O	-1.2462395	3.0729574	-1.5645672
O	-0.7054664	0.8015904	2.3089131
O	-3.0362548	-0.6400917	-3.5033258
C	1.6652669	-0.0246454	-0.1616219
C	1.9739778	1.3223058	0.0685635
C	2.2698486	-1.0099399	0.6253070
C	2.8686909	1.6798432	1.0761939
H	1.5101587	2.0939215	-0.5429411
C	3.1687741	-0.6535264	1.6330680
H	2.0253444	-2.0491810	0.4228039
C	3.4673583	0.6911803	1.8634463
H	3.1013993	2.7277466	1.2481491
H	3.6361561	-1.4253688	2.2398423
H	4.1645290	0.9691852	2.6496247
N	0.7986185	-1.9870629	-1.8565220
C	-0.1891862	-2.8153523	-2.5220880
H	0.0514792	-3.8763431	-2.3623225
H	-1.2170385	-2.6565452	-2.1443721
H	-0.2343985	-2.6576351	-3.6159500

4c$^\bullet$: $[W(CO)_5]$PHPhNH$^\bullet$ radical complex
29
Energy = -1302.767801792

P	0.3080452	-0.3440625	-1.2680478
H	0.7011242	0.4737619	-2.3583323
C	-2.0091964	-1.8447747	0.4968445
W	-2.0525974	0.0041923	-0.4240653
O	-1.9856499	-2.8749474	1.0177384
C	-3.9052051	0.4000963	0.2944792
C	-2.0093591	1.8290234	-1.3760346
C	-1.2363862	0.8456836	1.2747504
C	-2.8624120	-0.8436533	-2.1175552
O	-4.9621176	0.6411036	0.7057423
O	-1.9658508	2.8481711	-1.9188526
O	-0.7840653	1.3157996	2.2264346
O	-3.3356746	-1.3173258	-3.0600702
C	1.6277987	-0.0252112	-0.0721889
C	2.3316641	1.1837414	-0.1260805
C	1.8747686	-0.9383017	0.9616716
C	3.2832809	1.4765356	0.8517110
H	2.1425032	1.8931830	-0.9277948
C	2.8330385	-0.6433584	1.9290865
H	1.3267908	-1.8751364	1.0002747
C	3.5345204	0.5643462	1.8776987
H	3.8300700	2.4137577	0.8068993
H	3.0306079	-1.3547751	2.7255175
H	4.2771441	0.7926701	2.6365905
N	0.4809889	-1.9418973	-1.7114483
C	0.0813406	-2.3528782	-3.0441045
H	-0.7720768	-3.0407877	-2.9693489
H	-0.1717505	-1.5357226	-3.7319992
H	0.9081203	-2.9375739	-3.4702651

4de_ts : 1,2-W-shift of $[W(CO)_5]PHPhPH^{\bullet}$
29
Energy = -1589.386409459

P	1.3594992	0.5486244	-1.1810557
H	1.6838471	1.2823883	-2.3494368
C	-0.5072183	-1.6691801	1.1690797
W	-0.9384592	0.1285117	0.2502432
O	-0.2848507	-2.6761354	1.6867557
C	-2.3638638	0.4425970	1.6246359
C	-1.4128997	1.9289947	-0.6573038
C	0.3402226	1.0464415	1.6044600
C	-2.4454145	-0.7594402	-0.8562895
O	-3.2144966	0.5877311	2.4063832
O	-1.7063048	2.9403290	-1.1303334
O	0.9792761	1.5726094	2.4083922
O	-3.3197073	-1.2611174	-1.4178047
C	2.9626716	0.1805045	-0.4302498
C	4.0548009	1.0280200	-0.6706861
C	3.1026657	-0.9026765	0.4494718
C	5.2772558	0.7797992	-0.0470818
H	3.9539965	1.8721622	-1.3472471
C	4.3262621	-1.1425005	1.0703471
H	2.2621053	-1.5648225	0.6364192
C	5.4155000	-0.3025916	0.8245518
H	6.1217289	1.4334204	-0.2448536
H	4.4299512	-1.9877342	1.7442921
H	6.3680597	-0.4916878	1.3103253
P	0.3403065	-1.2559636	-1.7703720
C	-0.4519454	-0.5944233	-3.3353528
H	-1.3017714	-1.2395391	-3.5759642
H	-0.8110638	0.4332753	-3.2363742
H	0.2745124	-0.6534435	-4.1517264

4de$^{\bullet}$: $PHPhPH[W(CO)_5]^{\bullet}$ radical complex
29
Energy = -1589.404720464

P	2.2735624	-0.8308370	-0.1631713
H	2.0478803	-0.9820969	1.2265602
C	-2.3917259	1.7235885	-0.1278218
W	-1.7150370	-0.2090238	0.1358317
O	-2.7761249	2.8021189	-0.2780047
C	-3.6043939	-0.8503004	0.5162946
C	-1.0202202	-2.1336707	0.4013426
C	-1.9947655	-0.5528838	-1.8785759
C	-1.3631982	0.1473142	2.1413468
O	-4.6833643	-1.2261312	0.7133257
O	-0.6366631	-3.2119929	0.5540993
O	-2.1324138	-0.7387652	-3.0097036
O	-1.1628920	0.3400491	3.2618043
C	3.6908031	0.3280242	-0.1211881
C	4.4924586	0.4294114	-1.2681224
C	3.9910343	1.1159600	1.0013792
C	5.5719442	1.3140567	-1.2965007
H	4.2752542	-0.1880836	-2.1360253
C	5.0793859	1.9858813	0.9747228
H	3.3720549	1.0490873	1.8915753
C	5.8679829	2.0901024	-0.1750975
H	6.1848629	1.3885149	-2.1901099
H	5.3088670	2.5881503	1.8491963
H	6.7125276	2.7728299	-0.1937181
P	0.5931634	0.5320736	-0.4538509
C	0.9409347	1.2788188	-2.1000371
H	0.8339228	0.5278248	-2.8903668
H	0.2186136	2.0808002	-2.2735917
H	1.9539615	1.6903544	-2.1290314

4dhc_ts : P/C cyclization of $[W(CO)_5]PHPhPH^{\bullet}$
26
Energy = -1550.055237093

P	0.8612621	1.2016875	-0.8797039
C	0.1416147	2.8107475	-0.4152311
H	0.8613154	1.2550742	-2.2909880

P 2.9547141 1.2644162 -0.3038242
C 0.9260321 3.9732252 -0.3999135
C -1.2172597 2.8894513 -0.0825356
C 0.3549427 5.1969919 -0.0539878
H 1.9804733 3.9215037 -0.6585541
C -1.7870986 4.1165307 0.2537406
H -1.8287500 1.9925473 -0.0803549
C -1.0014235 5.2703125 0.2710241
H 0.9696989 6.0920996 -0.0389925
H -2.8412928 4.1689323 0.5081819
H -1.4442313 6.2246451 0.5404691
W -0.0334300 -0.9452347 0.1404895
C -0.8733441 -2.6455398 0.8457155
C 0.7588358 -1.9244428 -1.4885624
C -0.7117473 0.1217924 1.7681609
C -1.7879586 -0.6231722 -0.8914465
C 1.6505291 -1.4354337 1.2444098
O -1.3810995 -3.6131769 1.2332445
O 1.2222401 -2.4571322 -2.4030274
O -1.0705515 0.7160891 2.6909632
O -2.7835410 -0.4816682 -1.4603211
O 2.5302341 -1.7847187 1.9051317
H 3.2501157 0.2497425 -1.2569033

4dhc• : $[W(CO)_5]PHPhPH^•$ with a CO in ring
26
Energy = -1550.023134653
P -2.2544764 0.9637096 0.4686117
C -2.6950676 2.0760818 1.8250844
H -1.9472506 1.8825477 -0.5533878
P -0.3357634 -0.0412020 0.9166642
C -2.3582882 3.4369401 1.7781779
C -3.3796166 1.5639074 2.9362379
C -2.7004440 4.2733932 2.8394735
H -1.8343365 3.8399246 0.9158483
C -3.7123081 2.4030262 3.9976214
H -3.6548849 0.5135703 2.9653402
C -3.3735485 3.7572803 3.9494618
H -2.4422062 5.3273970 2.7991792
H -4.2422480 2.0030580 4.8567479
H -3.6394645 4.4117966 4.7742006
W -3.3667538 -1.2501682 -0.1180649
C -4.1157962 -3.0591683 -0.6621218
C -3.4972443 -0.5976168 -2.0697622
C -3.1947215 -1.9894983 1.7891241
C -5.1087575 -0.3641592 0.3798520
C -1.1304613 -1.3699829 -0.1638059
O -4.5743537 -4.0789019 -0.9715376
O -3.5751540 -0.2329163 -3.1637283
O -3.1027653 -2.4306939 2.8557562
O -6.0737521 0.1929031 0.7053663
O -0.5791426 -2.2394029 -0.8004448
H 0.5527937 0.5652036 -0.0112808

4dhe_ts : P/P 1,2-W-shift of $[W(CO)_5]PHPhPH^•$
26
Energy = -1550.041481091
P 1.3954862 0.2242910 -1.4494216
H 1.8232764 0.6143899 -2.7439887
C -0.5943615 -1.4978810 1.4432651
W -1.0659773 -0.0115700 0.0941717
O -0.3414391 -2.3283518 2.2036165
C -2.5187137 0.6145595 1.3206448
C -1.5495783 1.4715318 -1.2670903
C 0.1872452 1.2540916 1.1532864
C -2.5096746 -1.2134661 -0.7821849
O -3.3856311 0.9336300 2.0267037
O -1.8451896 2.3086719 -2.0042170
O 0.8219296 1.9753527 1.7925054
O -3.3420220 -1.8718543 -1.2314129
C 2.9494194 0.0545416 -0.5440283
C 4.0458701 0.8506716 -0.9115829
C 3.0489293 -0.7961415 0.5665923
C 5.2333322 0.7764131 -0.1848001
H 3.9755535 1.5173556 -1.7669130
C 4.2369103 -0.8608855 1.2908139
H 2.2056265 -1.4177160 0.8553068
C 5.3309356 -0.0757760 0.9173246
H 6.0820779 1.3854563 -0.4817675
H 4.3105654 -1.5283592 2.1443042
H 6.2560385 -0.1290935 1.4833860
P 0.3845677 -1.6759248 -1.5522500
H -0.2539875 -1.2875590 -2.7628168

4dhe• : $PHPhPH[W(CO)_5]^•$ radical complex
26
Energy = -1550.057638045
P 1.7767883 0.4808542 -2.0329003
H 2.4992722 -0.5169088 -2.7352246
C -1.0259018 -0.5590308 1.0654994
W -2.0360140 0.1396613 -0.6012054
O -0.5163566 -0.9540200 2.0213096
C -3.5777099 0.7619930 0.5634136
C -3.0436884 0.7977932 -2.2730694
C -1.1545556 1.9897305 -0.3403028
C -2.9310128 -1.7113907 -0.8405061
O -4.4602959 1.1395418 1.2127279
O -3.6050111 1.1565895 -3.2158780
O -0.6723412 3.0273029 -0.1923708
O -3.4459286 -2.7366988 -0.9608629
C 2.2306755 0.0503837 -0.3149359
C 2.2361219 1.0752613 0.6428286

C	2.5717616	-1.2559894	0.0705287
C	2.5685950	0.7965580	1.9690666
H	1.9864090	2.0907822	0.3489279
C	2.9129272	-1.5275540	1.3935308
H	2.5646667	-2.0565182	-0.6637511
C	2.9087375	-0.5030948	2.3444246
H	2.5661489	1.5951000	2.7051508
H	3.1751517	-2.5404975	1.6851834
H	3.1699998	-0.7199868	3.3760416
P	-0.1835066	-0.4631732	-2.1535949
H	-0.4044819	-0.3415295	-3.5473454

4dhp_ts : P/P 1,2-H-shift of $[W(CO)_5]PHPhPH^{\bullet}$
26
Energy = -1550.020612558

P	1.1935707	-0.9378985	-0.2760019
H	1.2368033	-1.9597694	-1.5071025
C	-1.3287998	-1.1297888	1.6622354
W	-1.0281077	0.1471224	0.0665104
O	-1.4961651	-1.8463984	2.5507799
C	-2.8318965	1.0018706	0.4118558
C	-0.7332370	1.4064761	-1.5415407
C	-0.1360203	1.5224768	1.3175385
C	-1.8920570	-1.2436248	-1.1905260
O	-3.8632890	1.4898820	0.6166674
O	-0.5835675	2.1153586	-2.4410564
O	0.3597542	2.2925024	2.0203829
O	-2.3798150	-2.0162792	-1.8959735
C	2.7852628	-0.1118525	-0.0906917
C	2.8457632	1.2549852	-0.4234934
C	3.9347647	-0.7554463	0.3964865
C	4.0377098	1.9579449	-0.2816160
H	1.9586381	1.7598492	-0.7940532
C	5.1232589	-0.0429307	0.5407216
H	3.8960785	-1.8028170	0.6781920
C	5.1795895	1.3106122	0.1995034
H	4.0765117	3.0100662	-0.5468594
H	6.0055881	-0.5452890	0.9261125
H	6.1087441	1.8611236	0.3120833
P	1.3710316	-3.1232975	-0.2751513
H	2.7577428	-3.1088296	-0.5877215

4dhp$^{\bullet}$: $[W(CO)_5]PPhPH_2^{\bullet}$ radical complex
26
Energy = -1550.060741740

P	-0.0466633	-1.0749130	-0.0224327
C	-3.2041028	-1.5375431	0.3267749
W	-2.1897326	0.1406798	-0.3270643
O	-3.7733533	-2.4752715	0.6830288
C	-3.9421461	1.1074880	-0.6792680
C	-1.1451866	1.7912025	-0.9946979
C	-2.1506050	0.9084612	1.5920289
C	-2.2586684	-0.6290578	-2.2443625
O	-4.9373007	1.6615671	-0.8920469
O	-0.5629573	2.7119088	-1.3749604
O	-2.1477581	1.3470336	2.6596972
O	-2.3057687	-1.0588139	-3.3135883
C	1.5253453	-0.3235501	0.4064390
C	1.5054074	0.9427735	1.0307121
C	2.7682482	-0.9426796	0.1667308
C	2.6909912	1.5684908	1.3973875
H	0.5547364	1.4295972	1.2258247
C	3.9511970	-0.3078216	0.5328471
H	2.8068505	-1.9149886	-0.3133767
C	3.9189883	0.9468598	1.1488454
H	2.6592208	2.5419545	1.8774759
H	4.9026102	-0.7929527	0.3351540
H	4.8447534	1.4377228	1.4335255
P	0.2042825	-3.0446518	-0.9420452
H	1.1341957	-2.6667120	-1.9487286
H	1.2033347	-3.5371407	-0.0626633

4dhT : $[W(CO)_5]PHPhPHT$ complex
54
Energy = -1958.915745644

P	-0.1634274	1.1240336	-0.7198769
P	2.0132774	1.7390541	-0.4555737
C	-0.8824828	2.7338722	-0.2635539
H	-0.1814592	1.2771426	-2.1227500
N	2.9260813	0.3604237	-0.0424383
C	-0.8908109	3.7989177	-1.1771366
C	-1.3646125	2.9392687	1.0377974
C	3.3521321	0.1388000	1.3891471
C	3.7541217	-0.1477900	-1.2021592
C	-1.3877663	5.0456216	-0.7953475
H	-0.5183542	3.6495123	-2.1867173
C	-1.8568326	4.1860697	1.4159441
H	-1.3618306	2.1207810	1.7512830
C	3.9909424	-1.2561509	1.5460759
C	2.1190405	0.1549276	2.3057043
C	4.3407150	1.2280456	1.8498698
C	4.3316618	-1.5350401	-0.8791211
C	4.8866292	0.8311567	-1.5695232
C	2.8176869	-0.3069412	-2.4119762
C	-1.8710150	5.2409780	0.4994313
H	-1.3987679	5.8623458	-1.5113971
H	-2.2346740	4.3335568	2.4234946
C	5.0243443	-1.5857809	0.4767912
H	3.1953955	-2.0094590	1.5078617
H	4.4295446	-1.2978316	2.5496457
H	1.7038157	1.1556042	2.4511596
H	1.3396418	-0.4904365	1.8944069

H	2.4062650	-0.2267776	3.2906786
H	3.9129153	2.2254199	1.7004108
H	5.2853917	1.1765472	1.3028363
H	4.5562914	1.1081978	2.9173545
H	3.5153452	-2.2672917	-0.8859739
H	5.0177705	-1.8020159	-1.6910428
H	5.6326122	0.9060770	-0.7745763
H	5.3918887	0.4925469	-2.4808012
H	4.4774592	1.8305959	-1.7530892
H	1.9682926	-0.9477320	-2.1534662
H	2.4403620	0.6593735	-2.7672561
H	3.3655833	-0.7691308	-3.2397810
H	-2.2608839	6.2110116	0.7937714
H	5.4383534	-2.5849283	0.6524759
H	5.8663593	-0.8835033	0.5133304
W	-1.4174843	-0.9946472	-0.0473652
C	-1.4663426	-1.4006108	-2.0644462
C	-3.1188472	0.1559172	-0.2211847
C	0.2368823	-2.2137635	0.1099940
C	-1.3442617	-0.5714310	1.9655794
C	-2.5703531	-2.6062239	0.3237442
O	-1.4811301	-1.6188986	-3.1995183
O	-4.0813132	0.7871997	-0.3196149
O	1.1023238	-2.9774520	0.1914885
O	-1.3303535	-0.3569803	3.1031122
O	-3.2493591	-3.5274773	0.5231243
H	1.7530787	2.2443468	0.8360161

4dh$^-$: [W(CO)$_5$]PHPhPH$^-$ anion complex
26
Energy = -1550.201250132

P	0.3021433	-0.4652037	-1.3919219
H	0.7061781	0.5343038	-2.3173945
C	-1.9162570	-1.7343857	0.5674701
W	-2.0435066	0.0457747	-0.4627432
O	-1.8462905	-2.7240421	1.1645584
C	-3.8815008	0.4246460	0.2616693
C	-2.0095243	1.7992440	-1.5264205
C	-1.1829654	1.0132102	1.1330326
C	-2.8494735	-0.9300624	-2.0905742
O	-4.9488251	0.6482971	0.6797746
O	-1.9620218	2.7881343	-2.1312576
O	-0.7020880	1.5626840	2.0324857
O	-3.3345261	-1.4622556	-2.9971989
C	1.5933689	-0.1129593	-0.1335118
C	2.2704529	1.1129780	-0.1250583
C	1.8643097	-1.0494773	0.8720791
C	3.2019557	1.4000267	0.8746064
H	2.0676409	1.8460287	-0.9032919
C	2.7893927	-0.7609628	1.8739778
H	1.3518392	-2.0088927	0.8488561
C	3.4617098	0.4651993	1.8785810
H	3.7259070	2.3525379	0.8672503
H	2.9909168	-1.4940465	2.6510711
H	4.1868264	0.6874954	2.6569123
P	0.4453730	-2.4218822	-2.2042855
H	1.8294157	-2.3012308	-2.5519811

4dh$^\bullet$: [W(CO)$_5$]PHPhPH$^\bullet$ anion complex
26
Energy = -1550.056632392

P	0.4126580	-0.2280381	-1.2713121
H	0.8332430	0.6650829	-2.2788483
C	-1.8747089	-1.8974311	0.4638773
W	-2.0066982	-0.0857095	-0.5145894
O	-1.8181058	-2.9045448	1.0280639
C	-3.9154403	0.1371040	0.1178751
C	-2.0965571	1.7210506	-1.5020343
C	-1.3511925	0.8743872	1.1906448
C	-2.6821341	-1.0277165	-2.2207693
O	-5.0066570	0.2812465	0.4830150
O	-2.1317550	2.7312460	-2.0605830
O	-0.9967634	1.4163446	2.1458990
O	-3.0881694	-1.5436763	-3.1715172
C	1.6999287	0.0398024	-0.0192631
C	2.6672892	1.0375804	-0.1940558
C	1.7023060	-0.7371419	1.1478017
C	3.6266856	1.2570931	0.7952924
H	2.6715399	1.6415289	-1.0973115
C	2.6700990	-0.5224424	2.1260458
H	0.9502776	-1.5086294	1.2925412
C	3.6305776	0.4776705	1.9529902
H	4.3713005	2.0356997	0.6581349
H	2.6711230	-1.1307739	3.0255173
H	4.3792319	0.6492794	2.7207360
P	0.7908397	-2.2249196	-2.0708529
H	0.0015331	-1.9389334	-3.2206120

4dp_ts : P/P 1,2-H-shift of [W(CO)$_5$]PHPhPMe$^\bullet$
29
Energy = -1589.362444366

P	1.1513769	-0.7734830	-0.1927283
H	1.6022371	-2.0606696	-1.0977303
C	-1.9252224	-1.7965220	0.1777953
W	-1.1793433	0.1136646	-0.0506170
O	-2.3521888	-2.8614376	0.3087042
C	-3.0317623	0.8987350	0.1597930
C	-0.3968871	2.0041088	-0.2988572
C	-0.8960139	0.2382743	1.9884407
C	-1.4439060	-0.0333705	-2.0962497
O	-4.0899116	1.3554781	0.2945790
O	0.0436462	3.0618544	-0.4415068

O	-0.7317465	0.3031977	3.1300718
O	-1.5985104	-0.1124467	-3.2372039
C	2.6245057	0.2789051	-0.1086091
C	2.8191899	1.0840979	1.0248716
C	3.5510661	0.3252145	-1.1612695
C	3.9302976	1.9219326	1.1026649
H	2.1041240	1.0557442	1.8423990
C	4.6626030	1.1626157	-1.0745570
H	3.3974639	-0.2850799	-2.0466572
C	4.8533929	1.9609045	0.0552350
H	4.0749491	2.5429088	1.9818100
H	5.3754138	1.1956480	-1.8933194
H	5.7178247	2.6152598	0.1179446
P	1.7180798	-2.8387011	0.3669753
C	3.5455414	-2.6640270	0.6410594
H	3.9287382	-3.6690191	0.8428264
H	4.0603057	-2.2572136	-0.2322428
H	3.7433031	-2.0216938	1.5041257

4dp• : $[W(CO)_5]$PPhPHMe• radical complex

29

Energy = -1589.409126648

P	0.3287732	1.2455268	0.3834865
P	-1.2661857	2.0736900	-0.8470267
C	1.3803276	2.6312965	0.8339279
C	2.4578981	2.3912779	1.7120551
C	1.1573713	3.9467143	0.3800974
C	3.2844219	3.4324100	2.1196987
H	2.6400757	1.3826680	2.0724366
C	1.9910569	4.9837241	0.7874807
H	0.3497463	4.1534803	-0.3171039
C	3.0544984	4.7327749	1.6597001
H	4.1102307	3.2312746	2.7957300
H	1.8145955	5.9899947	0.4187929
H	3.7023513	5.5448162	1.9758485
W	1.2135858	-1.0502333	-0.0318518
C	3.0862994	-0.2379197	-0.3337895
C	0.7631996	-0.7870892	-2.0315458
C	1.6636686	-1.3320733	1.9658685
C	-0.6843435	-1.8026773	0.2609903
C	1.9363428	-2.8967136	-0.4610688
O	4.1311636	0.2187622	-0.5102535
O	0.5114224	-0.6466489	-3.1487293
O	1.9205034	-1.5053693	3.0780085
O	-1.7504455	-2.2185862	0.4164895
O	2.3574194	-3.9459408	-0.7186493
C	-2.3986436	2.8705281	0.3990017
H	-2.6286297	2.2088051	1.2355742
H	-1.9256757	3.7823855	0.7716007
H	-3.3200893	3.1454773	-0.1234735
H	-1.9073552	0.8166656	-0.9629496

4dT : $[W(CO)_5]$PHPhPMeT complex

57

Energy = -1998.260393963

P	0.1564616	0.9785957	0.9150135
P	-1.6760964	1.9491419	0.0794071
C	1.2287742	2.4550447	0.9154015
H	-0.0169559	0.8654141	2.3140580
N	-2.8795454	0.7670270	-0.1395977
C	1.7779276	2.9331567	2.1130002
C	1.5348970	3.1029732	-0.2906712
C	-3.5023957	0.8381042	-1.5294434
C	-3.6284162	0.0944498	0.9851176
C	2.6283935	4.0388884	2.1034897
H	1.5430622	2.4392607	3.0520736
C	2.3794846	4.2113683	-0.2948071
H	1.1082796	2.7455499	-1.2229018
C	-4.2399711	-0.4725909	-1.8654714
C	-2.4019198	0.9846985	-2.5967733
C	-4.4544455	2.0429735	-1.6409110
C	-4.3120588	-1.1934997	0.4840744
C	-4.6983860	1.0067235	1.6221138
C	-2.6288377	-0.3354831	2.0652095
C	2.9303246	4.6797260	0.9006164
H	3.0527853	4.3992654	3.0362370
H	2.6099377	4.7086499	-1.2323593
C	-5.1590613	-0.9734415	-0.7613814
H	-3.4910882	-1.2458432	-2.0730055
H	-4.7926998	-0.2988190	-2.7959719
H	-1.9377527	1.9727273	-2.5898927
H	-1.6240012	0.2309726	-2.4456727
H	-2.8552156	0.8235081	-3.5813761
H	-4.8122780	2.1442676	-2.6718076
H	-3.9216868	2.9629099	-1.3726106
H	-5.3241665	1.9450278	-0.9870261
H	-3.5397933	-1.9386334	0.2604550
H	-4.9141826	-1.5845082	1.3126148
H	-5.5073648	1.2326754	0.9244253
H	-5.1352606	0.4957603	2.4875274
H	-4.2721279	1.9497884	1.9646856
H	-1.8180703	-0.9224959	1.6206685
H	-2.2028564	0.5115687	2.6071275
H	-3.1446970	-0.9653782	2.7969097
H	3.5921047	5.5409616	0.8938692
H	-5.6355362	-1.9121164	-1.0662858
H	-5.9672185	-0.2578528	-0.5661532
W	1.2275156	-1.0536820	-0.1788851
C	3.0366841	-0.2231265	0.3601625
C	1.2947564	-0.0493399	-1.9740762
C	1.0798149	-1.9782814	1.6540530
C	-0.5137019	-1.9779191	-0.7690922

C	2.2286478	-2.6232414	-0.9586603
O	4.0619469	0.2235338	0.6495059
O	1.3355584	0.5079961	-2.9873184
O	0.9769564	-2.4774914	2.6922105
O	-1.4308731	-2.5836173	-1.1312453
O	2.8152832	-3.5245667	-1.3985233
C	-2.0505861	3.0392631	1.5346536
H	-2.2023301	2.5309088	2.4896791
H	-1.1901580	3.7108523	1.6263555
H	-2.9310932	3.6441546	1.2975567

4d⁻ : $[W(CO)_5]PHPhPMe^-$ anion complex

29

Energy = -1589.535081523

P	0.4902864	-0.3996713	-1.3898875
H	0.7997841	0.6792446	-2.2693481
C	-2.0409046	-1.9014379	0.1370519
W	-1.9221246	0.0474074	-0.5178761
O	-2.0960426	-2.9879247	0.5351279
C	-3.7674812	0.4690647	0.1494040
C	-1.6194032	1.9697198	-1.1622265
C	-1.1183845	0.5676168	1.3025207
C	-2.6770570	-0.4426037	-2.3678657
O	-4.8415226	0.7266446	0.5302527
O	-1.4096810	3.0509968	-1.5264481
O	-0.6828690	0.8744434	2.3312094
O	-3.1239200	-0.6846234	-3.4106373
C	1.7146820	0.0576341	-0.1029829
C	2.2603758	1.3474966	-0.0618324
C	2.0566680	-0.8596529	0.8991993
C	3.1293331	1.7159003	0.9663189
H	2.0024695	2.0655282	-0.8371723
C	2.9245387	-0.4912748	1.9264359
H	1.6409305	-1.8635084	0.8535572
C	3.4628907	0.7978178	1.9644479
H	3.5487269	2.7186211	0.9852189
H	3.1818451	-1.2111015	2.6993297
H	4.1401741	1.0839034	2.7647880
P	1.1586738	-2.2903326	-2.1232434
C	-0.4345353	-2.9345615	-2.8956683
H	-0.2819199	-4.0047004	-3.0807154
H	-1.2897115	-2.8287350	-2.2197837
H	-0.6863570	-2.4602521	-3.8499236

4d• : $[W(CO)_5]PHPhPMe^•$ radical complex

29

Energy = -1589.405695218

P	1.1154962	0.7102689	0.8023678
H	1.2824375	0.7776343	2.2003908
C	-0.6363283	-0.1661240	-1.9406767
W	-1.1386867	-0.2003843	0.0534488
O	-0.3895355	-0.1552983	-3.0717465
C	-2.9326831	-0.9970448	-0.4277804
C	-1.6577925	-0.2108121	2.0486610
C	-0.3536147	-2.0986948	0.2346343
C	-1.9221981	1.6987637	-0.1368945
O	-3.9595085	-1.4672698	-0.6933446
O	-1.9458275	-0.2109195	3.1670857
O	0.0775200	-3.1657580	0.3315516
O	-2.3848593	2.7507994	-0.2568214
C	2.6500027	-0.1574252	0.3394004
C	3.7857093	-0.0628178	1.1591953
C	2.7189240	-0.8776822	-0.8595413
C	4.9701130	-0.6930489	0.7832737
H	3.7399975	0.4971664	2.0892308
C	3.9100878	-1.4971679	-1.2375602
H	1.8396785	-0.9646196	-1.4897307
C	5.0351216	-1.4070717	-0.4165429
H	5.8427465	-0.6260870	1.4263808
H	3.9555066	-2.0551518	-2.1679728
H	5.9602906	-1.8956144	-0.7076857
P	1.5170276	2.8230436	0.3307230
C	1.6546576	2.6402889	-1.5059277
H	2.3880585	1.8750242	-1.7825264
H	0.6849491	2.3704237	-1.9380935
H	1.9665578	3.6025730	-1.9202641

Ar_3N : $(p\text{-}BrC_6H_4)_3N$ amine

34

Energy = -8470.563310441

N	-0.0004318	-0.0008500	0.0008093
C	-0.0002127	1.4158389	-0.0014067
C	-0.8307674	2.1240386	-0.8822483
C	0.8311160	2.1265998	0.8766322
C	-0.8387814	3.5160000	-0.8829287
H	-1.4721863	1.5841512	-1.5711329
C	0.8415707	3.5185403	0.8709367
H	1.4715575	1.5887432	1.5680111
C	0.0022665	4.2011806	-0.0078228
H	-1.4807201	4.0562483	-1.5699131
H	1.4839671	4.0608112	1.5558949
C	-1.2158386	-0.7091369	-0.1671789
C	-1.2534084	-1.8816847	-0.9358779
C	-2.3957785	-0.2453505	0.4326384
C	-2.4440701	-2.5844196	-1.0974476
H	-0.3481698	-2.2447456	-1.4113603
C	-3.5940324	-0.9329381	0.2625926
H	-2.3764450	0.6565792	1.0356270
C	-3.6058576	-2.1003367	-0.4987086
H	-2.4660654	-3.4872320	-1.6977478
H	-4.5012975	-0.5699007	0.7326205
C	1.2148767	-0.7089906	0.1700890

C	2.3947584	-0.2466581	-0.4309663
C	1.2523951	-1.8800006	0.9411236
C	3.5930017	-0.9338925	-0.2594692
H	2.3753180	0.6536519	-1.0363637
C	2.4430074	-2.5825211	1.1040103
H	0.3470822	-2.2422553	1.4170741
C	3.6049047	-2.0994462	0.5046620
H	4.5001035	-0.5723033	-0.7309283
H	2.4647440	-3.4847124	1.7052494
Br	0.0047439	6.1152452	-0.0129883
Br	-5.2483326	-3.0564966	-0.7261279
Br	5.2476881	-3.0543198	0.7353014

$Ar_3N^{\bullet+}$: $(p\text{-}BrC_6H_4)_3N^{\bullet+}$ radical cation
34
Energy = -8470.367610204

N	-0.0001621	-0.0008143	0.0003797
C	0.0001150	1.4084813	-0.0019346
C	-0.8647173	2.1063800	-0.8653081
C	0.8654776	2.1088663	0.8588864
C	-0.8623640	3.4916769	-0.8704046
H	-1.5048215	1.5617028	-1.5505505
C	0.8642871	3.4941800	0.8588237
H	1.5054243	1.5662038	1.5458775
C	0.0013704	4.1765904	-0.0071882
H	-1.5094124	4.0361551	-1.5479944
H	1.5115878	4.0406429	1.5345726
C	-1.2092920	-0.7055224	-0.1663928
C	-1.2257248	-1.8993072	-0.9112581
C	-2.3925552	-0.2101141	0.4120995
C	-2.4149359	-2.5896148	-1.0795947
H	-0.3177504	-2.2582908	-1.3830823
C	-3.5810280	-0.9031031	0.2498061
H	-2.3675257	0.6922354	1.0130364
C	-3.5847226	-2.0874406	-0.4968333
H	-2.4401598	-3.4974194	-1.6708163
H	-4.4918989	-0.5402091	0.7111582
C	1.2087876	-0.7053926	0.1690054
C	2.3920795	-0.2119947	-0.4111363
C	1.2249834	-1.8971377	0.9171373
C	3.5803219	-0.9050287	-0.2473561
H	2.3672196	0.6887116	-1.0145389
C	2.4139596	-2.5875162	1.0868925
H	0.3170074	-2.2544726	1.3902127
C	3.5837590	-2.0874101	0.5023711
H	4.4912038	-0.5437131	-0.7099229
H	2.4389995	-3.4937663	1.6805049
Br	0.0025163	6.0677656	-0.0110738
Br	-5.2080418	-3.0308585	-0.7235950
Br	5.2067185	-3.0310284	0.7308722

$NO^{\bullet}$: $NO^{\bullet}$ radical
2
Energy = -129.9680916564

N	0.0219978	0.0000000	0.0000000
O	1.1780022	0.0000000	0.0000000

NO^{+} : cation
2
Energy = -129.7291079400

N	0.0681067	0.0000000	0.0000000
O	1.1318933	0.0000000	0.0000000

$Ph_3C^{\bullet}$: trityl radical
34
Energy = -733.4910215845

C	-0.0000313	0.0008206	-0.0000345
C	-0.0000715	1.4581175	-0.0022430
C	-0.9216257	2.1913181	-0.7866825
C	0.9215357	2.1938009	0.7798059
C	-0.9170347	3.5817766	-0.7913036
H	-1.6263198	1.6525736	-1.4129156
C	0.9179157	3.5842732	0.7788616
H	1.6252695	1.6570982	1.4088651
C	0.0006893	4.2892660	-0.0076339
H	-1.6264447	4.1187712	-1.4153035
H	1.6279014	4.1232598	1.4004854
H	0.0010776	5.3755130	-0.0097962
C	-1.2504290	-0.7285598	-0.1703508
C	-1.2871267	-1.9767775	-0.8354601
C	-2.4731998	-0.2154313	0.3228533
C	-2.4813195	-2.6695937	-1.0008229
H	-0.3668325	-2.3837707	-1.2433885
C	-3.6642130	-0.9150261	0.1631487
H	-2.4708874	0.7303630	0.8562242
C	-3.6783638	-2.1460624	-0.5010234
H	-2.4822810	-3.6191133	-1.5294421
H	-4.5862708	-0.5039164	0.5653565
H	-4.6098508	-2.6904598	-0.6270893
C	1.2503123	-0.7281562	0.1723600
C	2.4731334	-0.2165498	-0.3222995
C	1.2868648	-1.9745502	0.8408716
C	3.6641301	-0.9156369	-0.1602680
H	2.4708252	0.7274357	-0.8588600
C	2.4809967	-2.6669346	1.0083785
H	0.3664904	-2.3803461	1.2497979
C	3.6782369	-2.1445005	0.5079126
H	4.5861589	-0.5060017	-0.5640432
H	2.4817608	-3.6152275	1.5391903
H	4.6099368	-2.6878112	0.6370614

Ph_3C^{+} : trityl carbocation

34
Energy = -733.3236523814

C	0.0004352	0.0002639	-0.0001375
C	0.0005369	1.4432770	-0.0025635
C	-0.9298040	2.1621420	-0.7946745
C	0.9308437	2.1647831	0.7872311
C	-0.9165434	3.5482431	-0.8037333
H	-1.6122595	1.6175585	-1.4382137
C	0.9170705	3.5508751	0.7922927
H	1.6136336	1.6223209	1.4322125
C	0.0002425	4.2439890	-0.0068668
H	-1.6107850	4.0922903	-1.4355487
H	1.6109514	4.0970410	1.4226791
H	0.0002218	5.3296866	-0.0085940
C	-1.2376229	-0.7212686	-0.1711405
C	-1.2552046	-1.9731986	-0.8359093
C	-2.4553994	-0.1894672	0.3225307
C	-2.4492057	-2.6553521	-1.0105354
H	-0.3355968	-2.3634137	-1.2583966
C	-3.6394440	-0.8934187	0.1676926
H	-2.4424324	0.7444852	0.8739408
C	-3.6399631	-2.1216913	-0.5037533
H	-2.4608222	-3.5979266	-1.5477502
H	-4.5630131	-0.4958842	0.5752660
H	-4.5711644	-2.6649116	-0.6321985
C	1.2378980	-0.7215677	0.1730606
C	2.4561180	-0.1920765	-0.3220682
C	1.2545243	-1.9715955	0.8414229
C	3.6396168	-0.8964558	-0.1651139
H	2.4438791	0.7400960	-0.8764863
C	2.4479566	-2.6542733	1.0178508
H	0.3346559	-2.3597125	1.2652460
C	3.6391842	-2.1227589	0.5099423
H	4.5635280	-0.5007808	-0.5737206
H	2.4587911	-3.5954300	1.5575525
H	4.5701062	-2.6659061	0.6406973

TOH : TEMP-OH
30
Energy = -484.6280094845

O	0.0029487	-2.0724761	0.0780636
C	-1.2871126	-0.0717481	-0.0500409
C	1.2896709	-0.0695833	-0.0496051
C	-1.2454340	1.3819080	-0.5608577
C	1.2458211	1.3839830	-0.5605105
C	-0.0005209	2.1369712	-0.0973463
H	-2.1621489	1.8840906	-0.2291416
H	-1.2617950	1.3617463	-1.6586138
H	2.1616436	1.8875671	-0.2284723
H	1.2624799	1.3640506	-1.6582854
H	-0.0012578	3.1522926	-0.5108741
H	-0.0008338	2.2440684	0.9943753
N	0.0018575	-0.7049147	-0.4586952
C	-1.5995267	-0.1232244	1.4597729
H	-2.6576042	0.1149050	1.6155111
H	-1.4128220	-1.1275650	1.8487267
H	-1.0090234	0.5915140	2.0362569
C	-2.3961790	-0.8238533	-0.8022877
H	-2.1627676	-0.8628391	-1.8712697
H	-2.5005789	-1.8453313	-0.4252373
H	-3.3525304	-0.3068282	-0.6673268
C	1.6020094	-0.1202497	1.4602671
H	2.6597462	0.1195454	1.6158178
H	1.0105117	0.5938670	2.0364999
H	1.4168830	-1.1247431	1.8495410
C	2.4000196	-0.8202644	-0.8013091
H	2.5077490	-1.8405686	-0.4220231
H	2.1650894	-0.8625909	-1.8697732
H	3.3551214	-0.3002852	-0.6688804
H	0.0045799	-2.6080002	-0.7314997

TO^- : $TEMPO^-$ anion
29
Energy = -484.0919742077

O	0.0012594	-2.0699897	0.1511810
C	-1.2704896	-0.0687689	-0.0339116
C	1.2706908	-0.0674813	-0.0345073
C	-1.2429607	1.3707976	-0.5753273
C	1.2423369	1.3734475	-0.5734807
C	-0.0016067	2.1402910	-0.1261834
H	-2.1630208	1.8870135	-0.2671828
H	-1.2468502	1.3221098	-1.6738944
H	2.1608195	1.8902754	-0.2618025
H	1.2493054	1.3276748	-1.6723717
H	-0.0021751	3.1535811	-0.5500226
H	-0.0026941	2.2571597	0.9656806
N	0.0002349	-0.7643059	-0.4121295
C	-1.5708584	-0.1034696	1.4807944
H	-2.6473390	-0.0080386	1.6720698
H	-1.2199909	-1.0790228	1.8395600
H	-1.0578488	0.6917987	2.0300209
C	-2.3800448	-0.8458829	-0.7588370
H	-2.1990557	-0.8201751	-1.8398082
H	-2.3494037	-1.8872647	-0.4270446
H	-3.3666425	-0.4131989	-0.5470205
C	1.5721762	-0.1019573	1.4801171
H	2.6487624	-0.0051277	1.6702334
H	1.0588956	0.6931375	2.0293784
H	1.2226740	-1.0777085	1.8395354
C	2.3800009	-0.8441027	-0.7596248
H	2.3497456	-1.8853870	-0.4275563
H	2.1973758	-0.8190896	-1.8399559

H	3.3667115	-0.4111443	-0.5490082

TO• : TEMPO• radical

29

Energy = -484.0199119877

O	-0.0000187	-2.0361975	0.0574260
C	-1.3291976	-0.0714412	0.0006091
C	1.3292100	-0.0714144	0.0005786
C	-1.2411880	1.3616711	-0.5498131
C	1.2410581	1.3615027	-0.5502511
C	0.0000793	2.1127316	-0.0735264
H	-2.1594067	1.8854539	-0.2603649
H	-1.2270215	1.3164314	-1.6468545
H	2.1594986	1.8853130	-0.2615724
H	1.2262571	1.3158857	-1.6472692
H	0.0000224	3.1298091	-0.4805849
H	0.0003203	2.2101640	1.0190137
N	0.0000284	-0.7626786	-0.1463354
C	-1.7345874	-0.0808549	1.4872560
H	-2.7696298	0.2637886	1.5820791
H	-1.6643951	-1.0988031	1.8806371
H	-1.0993534	0.5742849	2.0890289
C	-2.3519721	-0.8736140	-0.8135684
H	-2.0421442	-0.9365897	-1.8616079
H	-2.4600187	-1.8846952	-0.4160335
H	-3.3204807	-0.3653174	-0.7646838
C	1.7345211	-0.0804133	1.4872681
H	2.7694008	0.2646973	1.5821406
H	1.0990044	0.5745623	2.0889256
H	1.6647012	-1.0983037	1.8808572
C	2.3521247	-0.8737272	-0.8132630
H	2.4599471	-1.8848063	-0.4156861
H	2.0425751	-0.9367328	-1.8613829
H	3.3206735	-0.3655354	-0.7641205

TO+ : TEMPO+ cation

29

Energy = -483.8301363958

O	-0.0001829	-1.8491069	-0.7574866
C	-1.3441694	-0.0795407	-0.0083877
C	1.3442110	-0.0799357	-0.0084567
C	-1.2487656	1.3660811	-0.5654675
C	1.2491925	1.3655258	-0.5658815
C	0.0004365	2.1115498	-0.1125730
H	-2.1622914	1.8709001	-0.2368238
H	-1.2768516	1.3109680	-1.6593431
H	2.1631053	1.8701308	-0.2380376
H	1.2763486	1.3099999	-1.6597054
H	0.0006933	3.1101194	-0.5609394
H	0.0005960	2.2592488	0.9722616
N	-0.0000406	-0.7516295	-0.2720003
C	-1.5982109	-0.0919982	1.5190458
H	-2.6522442	0.1688278	1.6441171
H	-1.4350665	-1.0873954	1.9377649
H	-0.9962314	0.6391693	2.0544531
C	-2.4172132	-0.8909128	-0.7228766
H	-2.1961528	-0.9934037	-1.7881988
H	-2.5343252	-1.8845960	-0.2848567
H	-3.3584512	-0.3473527	-0.6095510
C	1.5978221	-0.0920833	1.5192168
H	2.6519895	0.1681100	1.6444467
H	0.9961205	0.6396844	2.0541266
H	1.4338876	-1.0872252	1.9381963
C	2.4171413	-0.8917570	-0.7225674
H	2.5338157	-1.8854711	-0.2845149
H	2.1962954	-0.9942030	-1.7879945
H	3.3585499	-0.3485331	-0.6090642

T• : TEMP• radical

28

Energy = -408.7570084419

C	-1.2675407	-0.0685821	-0.0160759
C	1.2678109	-0.0686132	-0.0167972
C	-1.2408437	1.3855892	-0.5416563
C	1.2396525	1.3829818	-0.5484785
C	0.0014761	2.1454697	-0.0814705
H	-2.1609326	1.8906563	-0.2237354
H	-1.2515658	1.3587324	-1.6399609
H	2.1627862	1.8881701	-0.2397540
H	1.2416785	1.3512044	-1.6467013
H	0.0011603	3.1594789	-0.4974092
H	0.0047256	2.2538783	1.0106722
N	0.0001330	-0.7904117	-0.1338767
C	-1.6842592	-0.0882690	1.4789501
H	-2.7295019	0.2306658	1.5574230
H	-1.5929270	-1.1001169	1.8844821
H	-1.0701695	0.5856608	2.0807817
C	-2.3014329	-0.8854379	-0.8114099
H	-2.0108782	-0.9394904	-1.8657644
H	-2.3662686	-1.9043493	-0.4162277
H	-3.2897005	-0.4158183	-0.7454093
C	1.6829837	-0.0815788	1.4786960
H	2.7279229	0.2384499	1.5569612
H	1.0678599	0.5944170	2.0770001
H	1.5919654	-1.0917078	1.8885155
C	2.3030368	-0.8884053	-0.8069909
H	2.3681699	-1.9052730	-0.4066255
H	2.0137978	-0.9481438	-1.8614572
H	3.2908883	-0.4177887	-0.7422052