

Carbonyl Migration from Phosphorus to the Metal in Binuclear Phosphaketonyl Metal Carbonyl Complexes to Give Bridging Diphosphido Complexes

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Supporting Information

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Table S60 to S62. Harmonic vibrational frequencies(cm^{-1}) and IR intensities (km/mol) of $\text{Mn}(\text{CO})_3(\text{PCO})$.

Complete Gaussian 09 reference (Reference 21)

Table S1. Coordinates of Mn₂(CO)₈(PCO)₂ **28-1S(C_{2h})**.

	B3LYP			BP86		
Mn	0.000000	0.000000	1.933878	0.000000	0.000000	1.914742
Mn	0.000000	0.000000	-1.933878	0.000000	0.000000	-1.914742
C	-1.348197	2.343273	0.000000	-1.342794	2.301075	0.000000
C	1.348197	-2.343273	0.000000	1.342794	-2.301075	0.000000
C	0.001445	-1.340051	-3.176134	0.000908	-1.320205	-3.151178
C	1.867065	-0.004238	-1.875708	1.848906	-0.007798	-1.885450
C	-0.001445	1.340051	-3.176134	-0.000908	1.320205	-3.151178
C	1.867065	-0.004238	1.875708	1.848906	-0.007798	1.885450
C	0.001445	-1.340051	3.176134	0.000908	-1.320205	3.151178
C	-1.867065	0.004238	-1.875708	-1.848906	0.007798	-1.885450
C	-1.867065	0.004238	1.875708	-1.848906	0.007798	1.885450
C	-0.001445	1.340051	3.176134	-0.000908	1.320205	3.151178
O	0.000000	-2.191074	-3.958435	0.000000	-2.170323	-3.957646
O	3.020234	-0.008560	-1.864478	3.017200	-0.010863	-1.918363
O	0.000000	2.191074	-3.958435	0.000000	2.170323	-3.957646
O	3.020234	-0.008560	1.864478	3.017200	-0.010863	1.918363
O	0.000000	2.191074	3.958435	0.000000	2.170323	3.957646
O	-3.020234	0.008560	1.864478	-3.017200	0.010863	1.918363
O	0.000000	-2.191074	3.958435	0.000000	-2.170323	3.957646
O	-3.020234	0.008560	-1.864478	-3.017200	0.010863	-1.918363
P	0.178082	1.620175	0.000000	0.199956	1.576881	0.000000
O	-2.354764	2.935268	0.000000	-2.343871	2.924385	0.000000
O	2.354764	-2.935268	0.000000	2.343871	-2.924385	0.000000
P	-0.178082	-1.620175	0.000000	-0.199956	-1.576881	0.000000

Table S2. Coordinates of Mn₂(CO)₈(PCO)₂ **28-2S(C_{2v})**.

	B3LYP			BP86		
Mn	0.000000	1.930003	0.218737	0.000000	1.907237	0.220222
Mn	0.000000	-1.930003	0.218737	0.000000	-1.907237	0.220222
C	-2.382908	0.000000	-1.062507	-2.335657	0.000000	-1.087561
C	2.382908	0.000000	-1.062507	2.335657	0.000000	-1.087561
C	1.339386	3.171840	0.175575	1.318173	3.144743	0.185224
C	0.000000	1.794768	-1.643852	0.000000	1.805076	-1.625238
C	-1.339386	3.171840	0.175575	-1.318173	3.144743	0.185224
C	0.000000	1.950749	2.087348	0.000000	1.942609	2.070047
C	1.339386	-3.171840	0.175575	1.318173	-3.144743	0.185224
C	0.000000	-1.950749	2.087348	0.000000	-1.942609	2.070047
C	-1.339386	-3.171840	0.175575	-1.318173	-3.144743	0.185224
C	0.000000	-1.794768	-1.643852	0.000000	-1.805076	-1.625238
O	0.000000	1.990461	3.239819	0.000000	2.015061	3.236460
O	2.189664	-3.954415	0.145083	2.166189	-3.953067	0.159112
O	0.000000	-1.990461	3.239819	0.000000	-2.015061	3.236460
O	-2.189664	-3.954415	0.145083	-2.166189	-3.953067	0.159112
O	-2.189664	3.954415	0.145083	-2.166189	3.953067	0.159112
O	0.000000	-1.739996	-2.795803	0.000000	-1.794607	-2.794063
O	0.000000	1.739996	-2.795803	0.000000	1.794607	-2.794063
O	2.189664	3.954415	0.145083	2.166189	3.953067	0.159112
P	1.625484	0.000000	0.446836	1.589530	0.000000	0.444350
O	2.998408	0.000000	-2.054655	2.975685	0.000000	-2.077743
P	-1.625484	0.000000	0.446836	-1.589530	0.000000	0.444350
O	-2.998408	0.000000	-2.054655	-2.975685	0.000000	-2.077743

Table S3. Coordinates of Mn₂(CO)₈(PCO)₂ **28-3S(C₁)**.

	B3LYP			BP86		
Mn	-2.189350	-0.028726	0.004160	-2.147440	-0.035030	0.008526
Mn	2.251303	-0.172727	-0.025159	2.212763	-0.174362	-0.040411
C	-0.015266	-1.760365	-1.070729	-0.040409	-1.592070	-1.234749
C	0.136993	2.280546	0.649738	0.124390	2.242629	0.649944
C	-2.915257	1.560319	0.508144	-2.896750	1.470048	0.656496
C	-1.649119	0.630694	-1.662402	-1.670005	0.779140	-1.585594
C	-3.782207	-0.610766	-0.667959	-3.732389	-0.562318	-0.677357
C	-2.522231	-0.796604	1.681393	-2.450459	-0.933871	1.600519
C	3.196998	0.841740	1.159475	3.133013	0.656047	1.260562
C	2.147759	-1.574363	1.233777	2.055366	-1.675308	1.051438
C	3.764889	-0.896517	-0.769468	3.722147	-0.854077	-0.781145
C	2.238147	1.229812	-1.285318	2.340639	1.342126	-1.110666
O	-2.729169	-1.268326	2.712129	-2.659773	-1.493219	2.604166
O	3.787298	1.485537	1.916331	3.737866	1.191404	2.110050
O	2.122813	-2.418775	2.013666	2.025544	-2.602307	1.757629
O	4.721465	-1.344707	-1.234019	4.709976	-1.279145	-1.242395
O	1.041388	-1.258566	-1.394150	1.006896	-1.042007	-1.552774
O	-4.797012	-0.963860	-1.095117	-4.771063	-0.876798	-1.119503
O	2.249784	2.087685	-2.050504	2.476897	2.293970	-1.769362
O	-1.311255	1.038512	-2.686151	-1.387422	1.302154	-2.590712
O	-3.400124	2.563701	0.821186	-3.424998	2.434127	1.066614
P	-1.404440	-2.450445	-0.606064	-1.406965	-2.365656	-0.780919
P	0.063161	0.632079	0.991384	0.063998	0.582673	1.015302
O	0.185579	3.439404	0.507290	0.160850	3.415002	0.524373

Table S4. Coordinates of Mn₂(CO)₇(PCO)₂ **27-1S(C_s)**.

	B3LYP			BP86		
Mn	-0.066768	-2.375450	0.000000	-0.068353	-2.328141	0.000000
Mn	-0.091553	2.346125	0.000000	-0.090911	2.313851	0.000000
C	-1.827614	-2.817678	0.000000	-1.814809	-2.779254	0.000000
C	-0.039564	-2.339357	1.866154	-0.066565	-2.312341	1.849418
C	-0.039564	-2.339357	-1.866154	-0.066565	-2.312341	-1.849418
C	0.643802	-4.050057	0.000000	0.654763	-3.986324	0.000000
C	1.235322	2.474059	-1.324291	1.217783	2.464099	-1.312141
C	-1.371787	1.980982	-1.325485	-1.357548	1.941645	-1.310570
C	-1.371787	1.980982	1.325485	-1.357548	1.941645	1.310570
C	-0.434742	4.155951	0.000000	-0.455839	4.106009	0.000000
C	1.235322	2.474059	1.324291	1.217783	2.464099	1.312141
O	1.113169	-5.110099	0.000000	1.130813	-5.059144	0.000000
O	-0.028178	-2.328865	-3.022449	-0.083885	-2.330362	-3.020393
O	-0.028178	-2.328865	3.022449	-0.083885	-2.330362	3.020393
O	2.048898	2.548994	2.132380	2.037590	2.567313	2.131942
O	-0.643907	5.290117	0.000000	-0.681723	5.251949	0.000000
O	2.048898	2.548994	-2.132380	2.037590	2.567313	-2.131942
O	-2.153363	1.743449	-2.134114	-2.152740	1.707619	-2.127732
O	-2.952896	-3.103443	0.000000	-2.948976	-3.090122	0.000000
O	-2.153363	1.743449	2.134114	-2.152740	1.707619	2.127732
P	0.388464	-0.064149	0.000000	0.439445	-0.066069	0.000000
P	2.129739	-1.030133	0.000000	2.182990	-1.049983	0.000000

Table S5. Coordinates of Mn₂(CO)₇(PCO)₂ **27-2S(C_s)**.

	B3LYP			BP86		
Mn	0.042236	2.897688	0.000000	0.034803	2.913897	0.000000
Mn	-0.098066	-2.708396	0.000000	-0.087108	-2.728485	0.000000
C	1.020178	4.439121	0.000000	1.094606	4.384280	0.000000
C	0.049515	2.898541	1.862201	0.031976	2.957218	1.846304
C	0.049515	2.898541	-1.862201	0.031976	2.957218	-1.846304
C	-1.681970	3.499398	0.000000	-1.659372	3.566533	0.000000
C	0.977804	-3.477610	-1.326970	0.988177	-3.477496	-1.314459
C	0.977804	-3.477610	1.326970	0.988177	-3.477496	1.314459
C	-1.007753	-1.746785	1.326445	-1.009371	-1.799394	1.315857
C	-1.300395	-4.093746	0.000000	-1.254602	-4.126324	0.000000
C	-1.007753	-1.746785	-1.326445	-1.009371	-1.799394	-1.315857
O	-2.785846	3.850058	0.000000	-2.763213	3.963359	0.000000
O	0.049492	2.923052	-3.017254	0.023506	3.023753	-3.014384
O	0.049492	2.923052	3.017254	0.023506	3.023753	3.014384
O	-1.566633	-1.161020	-2.144091	-1.596138	-1.231114	-2.146682
O	-2.061255	-4.962219	0.000000	-2.008523	-5.020208	0.000000
O	1.644988	-3.941899	-2.141955	1.662168	-3.950126	-2.139707
O	1.644988	-3.941899	2.141955	1.662168	-3.950126	2.139707
O	1.666729	5.399674	0.000000	1.801896	5.319891	0.000000
O	-1.566633	-1.161020	2.144091	-1.596138	-1.231114	2.146682
P	0.757452	0.908992	0.000000	0.673753	0.905605	0.000000
P	1.664647	-0.863188	0.000000	1.620954	-0.860989	0.000000

Table S6. Coordinates of Mn₂(CO)₇(PCO)₂ **27-3S(C_s)**.

	B3LYP			BP86		
Mn	0.014006	0.207370	1.337007	0.021285	0.194364	1.320820
Mn	0.014006	0.207370	-1.337007	0.021285	0.194364	-1.320820
C	1.759506	-2.164572	0.000000	1.633508	-2.200853	0.000000
C	-2.810242	-0.799790	0.000000	-2.830479	-0.693337	0.000000
C	1.598583	-0.075582	-2.194141	1.575764	-0.135038	-2.181795
C	-0.885229	-0.677028	-2.667369	-0.887091	-0.632418	-2.654644
C	-0.885229	-0.677028	2.667369	-0.887091	-0.632418	2.654644
C	-0.274346	1.807361	2.171071	-0.195378	1.792616	2.142600
C	1.164452	1.306926	0.000000	1.216610	1.221433	0.000000
C	1.598583	-0.075582	2.194141	1.575764	-0.135038	2.181795
C	-0.274346	1.807361	-2.171071	-0.195378	1.792616	-2.142600
O	-0.447744	2.805595	2.728032	-0.321666	2.810780	2.709165
O	-1.450533	-1.234529	3.505504	-1.459229	-1.157902	3.530192
O	2.588642	-0.248790	2.766805	2.566732	-0.328219	2.777926
O	-1.450533	-1.234529	-3.505504	-1.459229	-1.157902	-3.530192
O	2.588642	-0.248790	-2.766805	2.566732	-0.328219	-2.777926
O	-0.447744	2.805595	-2.728032	-0.321666	2.810780	-2.709165
O	2.007075	2.110629	0.000000	2.111320	1.993973	0.000000
P	-2.010361	0.697770	0.000000	-1.939574	0.771076	0.000000
O	-3.486276	-1.748931	0.000000	-3.596765	-1.587844	0.000000
P	0.084501	-1.847416	0.000000	-0.045829	-1.827200	0.000000
O	2.878122	-2.485776	0.000000	2.748700	-2.573159	0.000000

Table S7. Coordinates of Mn₂(CO)₇(PCO)₂ **27-4S(C_{2v})**.

	B3LYP			BP86		
Mn	0.000000	1.340925	-0.043638	0.000000	1.324547	-0.056577
Mn	0.000000	-1.340925	-0.043638	0.000000	-1.324547	-0.056577
C	2.902231	0.000000	-0.478775	2.859095	0.000000	-0.454619
C	-2.902231	0.000000	-0.478775	-2.859095	0.000000	-0.454619
C	0.000000	-2.686523	-1.291172	0.000000	-2.668792	-1.274720
C	-1.328774	-2.178167	0.881920	-1.307426	-2.161612	0.865759
C	1.328774	-2.178167	0.881920	1.307426	-2.161612	0.865759
C	0.000000	0.000000	1.540534	0.000000	0.000000	1.511259
C	-1.328774	2.178167	0.881920	-1.307426	2.161612	0.865759
C	1.328774	2.178167	0.881920	1.307426	2.161612	0.865759
C	0.000000	2.686523	-1.291172	0.000000	2.668792	-1.274720
O	2.154771	2.738978	1.466340	2.127758	2.744304	1.468153
O	2.154771	-2.738978	1.466340	2.127758	-2.744304	1.468153
O	0.000000	0.000000	2.705176	0.000000	0.000000	2.693742
O	-2.154771	-2.738978	1.466340	-2.127758	-2.744304	1.468153
O	0.000000	-3.534653	-2.073771	0.000000	-3.550931	-2.043543
O	-2.154771	2.738978	1.466340	-2.127758	2.744304	1.468153
O	0.000000	3.534653	-2.073771	0.000000	3.550931	-2.043543
P	-1.521567	0.000000	-1.471184	-1.484430	0.000000	-1.479859
O	-3.906460	0.000000	0.110219	-3.871480	0.000000	0.143549
P	1.521567	0.000000	-1.471184	1.484430	0.000000	-1.479859
O	3.906460	0.000000	0.110219	3.871480	0.000000	0.143549

Table S8. Coordinates of Mn₂(CO)₇(PCO)₂ **27-5S(C₁)**.

	B3LYP			BP86		
Mn	-1.837890	-0.045903	0.086506	-1.826956	-0.034278	0.092727
C	0.345171	-2.531150	-0.930457	0.336909	-2.501817	-0.994999
C	0.007294	2.709707	-0.349977	0.058298	2.648170	-0.402980
C	3.156712	1.506549	0.313691	3.142659	1.474410	0.310350
C	3.233477	-0.836741	-0.960050	3.212314	-0.846844	-0.906293
C	-2.235503	0.987563	-1.418177	-2.251513	0.989779	-1.386608
C	-3.063508	0.871701	1.088069	-3.032486	0.873434	1.093786
C	2.278231	-0.681251	1.420190	2.263916	-0.658923	1.395160
C	-1.332132	-1.089053	1.553320	-1.348896	-1.084808	1.540677
C	-3.015891	-1.333567	-0.448645	-3.010373	-1.296130	-0.429758
O	3.901240	2.349825	0.585776	3.920198	2.308095	0.592248
O	4.034674	-1.483939	-1.488513	4.043789	-1.512107	-1.402564
O	-2.502010	1.618775	-2.345499	-2.564388	1.622553	-2.317718
O	-3.757135	-2.150387	-0.795581	-3.781251	-2.110325	-0.770980
O	-1.047532	-1.748777	2.454839	-1.100071	-1.768825	2.453913
O	-3.831597	1.453446	1.725979	-3.813492	1.455632	1.743977
O	2.453656	-1.250945	2.414343	2.466909	-1.228161	2.405439
P	0.101334	-0.884365	-1.220811	0.100312	-0.821974	-1.167495
O	0.517492	-3.675587	-0.785625	0.511428	-3.664892	-0.939410
O	-0.011316	3.620605	-1.082609	0.084727	3.558357	-1.155065
P	0.048848	1.490229	0.812061	0.054420	1.455235	0.807136
Mn	1.975666	0.182917	-0.124163	1.959406	0.179671	-0.124301

Table S9. Coordinates of Mn₂(CO)₇(PCO)₂ **27-6S(C_s)**.

	B3LYP			BP86		
Mn	-0.461522	1.927839	0.000000	-0.464098	1.891264	0.000000
Mn	-0.106695	-1.840763	0.000000	-0.097315	-1.821695	0.000000
C	0.434519	0.285981	2.592509	0.401220	0.317315	2.564546
C	0.434519	0.285981	-2.592509	0.401220	0.317315	-2.564546
C	-0.683350	3.151240	-1.330726	-0.673948	3.109728	-1.305497
C	-1.899158	-2.372727	0.000000	-1.849566	-2.412860	0.000000
C	-0.683350	3.151240	1.330726	-0.673948	3.109728	1.305497
C	0.269932	-3.017154	1.345164	0.299727	-2.982926	1.326846
C	1.310392	2.207906	0.000000	1.268175	2.208740	0.000000
C	1.656569	-1.215090	0.000000	1.645669	-1.192832	0.000000
C	0.269932	-3.017154	-1.345164	0.299727	-2.982926	-1.326846
O	-2.997904	-2.721410	0.000000	-2.942275	-2.826300	0.000000
O	-0.829468	3.924788	-2.179658	-0.813511	3.913619	-2.150888
O	2.755538	-0.867857	0.000000	2.765694	-0.863051	0.000000
O	2.456540	2.380531	0.000000	2.424391	2.430141	0.000000
O	0.509997	-3.756574	2.200975	0.560729	-3.739834	2.182660
O	-0.829468	3.924788	2.179658	-0.813511	3.913619	2.150888
O	0.509997	-3.756574	-2.200975	0.560729	-3.739834	-2.182660
P	-0.850016	0.020599	-1.533111	-0.876879	0.009594	-1.487880
O	1.277750	0.463891	-3.379343	1.230878	0.519898	-3.376261
P	-0.850016	0.020599	1.533111	-0.876879	0.009594	1.487880
O	1.277750	0.463891	3.379343	1.230878	0.519898	3.376261

Table S10. Coordinates of Mn₂(CO)₇(PCO)₂ **27-7S(C_s)**.

	B3LYP			BP86		
Mn	-0.188946	-1.462243	0.000000	-0.174229	-1.410694	0.000000
Mn	-0.307597	1.588158	0.000000	-0.314161	1.504563	0.000000
C	1.174323	0.299640	2.477081	1.168791	0.320475	2.452838
C	1.174323	0.299640	-2.477081	1.168791	0.320475	-2.452838
C	-0.411719	3.386174	0.000000	-0.446744	3.281698	0.000000
C	1.677821	-1.353644	0.000000	1.672493	-1.284255	0.000000
C	1.530917	1.848518	0.000000	1.496708	1.835138	0.000000
C	-0.141132	-2.712379	1.327219	-0.100505	-2.659128	1.308398
C	-2.160808	1.660334	0.000000	-2.145184	1.607450	0.000000
C	-2.062328	-1.517262	0.000000	-2.026531	-1.523336	0.000000
C	-0.141132	-2.712379	-1.327219	-0.100505	-2.659128	-1.308398
O	-3.306972	1.822648	0.000000	-3.303260	1.808512	0.000000
O	-0.476961	4.545505	0.000000	-0.539023	4.455713	0.000000
O	-3.210669	-1.605344	0.000000	-3.184286	-1.669141	0.000000
O	-0.107726	-3.518470	2.154308	-0.048829	-3.494347	2.126884
O	-0.107726	-3.518470	-2.154308	-0.048829	-3.494347	-2.126884
O	2.658566	2.109520	0.000000	2.621296	2.174380	0.000000
O	2.830202	-1.339563	0.000000	2.840567	-1.284877	0.000000
P	-0.444301	0.281091	-1.933300	-0.470908	0.259313	-1.909754
O	2.229455	0.328808	-2.967993	2.219500	0.404400	-2.973979
P	-0.444301	0.281091	1.933300	-0.470908	0.259313	1.909754
O	2.229455	0.328808	2.967993	2.219500	0.404400	2.973979

Table S11. Coordinates of Mn₂(CO)₇(PCO)₂ **27-8S(C_s)**.

	B3LYP			BP86		
Mn	0.000000	0.000000	-1.448070	0.000000	0.000000	-1.395469
C	-0.495681	2.811756	0.224897	0.000000	2.834396	0.230861
C	0.495681	-2.811756	0.224897	0.000000	-2.834396	0.230861
C	-1.411054	-1.193229	1.772848	-1.577546	-0.915444	1.743273
C	0.000000	0.000000	3.408159	0.000000	0.000000	3.306922
C	-1.456468	-1.176237	-1.421944	-1.608730	-0.920172	-1.383908
C	0.838620	-1.029125	-2.698894	0.658106	-1.130204	-2.647041
C	1.411054	1.193229	1.772848	1.577546	0.915444	1.743273
C	1.456468	1.176237	-1.421944	1.608730	0.920172	-1.383908
C	-0.838620	1.029125	-2.698894	-0.658106	1.130204	-2.647041
O	-2.273170	-1.936314	1.983825	-2.563492	-1.493861	2.015544
O	0.000000	0.000000	4.569318	0.000000	0.000000	4.484541
O	-2.354461	-1.896925	-1.458423	-2.624966	-1.490790	-1.451138
O	-1.361079	1.670929	-3.505194	-1.070603	1.836631	-3.484266
O	2.354461	1.896925	-1.458423	2.624966	1.490790	-1.451138
O	1.361079	-1.670929	-3.505194	1.070603	-1.836631	-3.484266
O	2.273170	1.936314	1.983825	2.563492	1.493861	2.015544
P	-1.387898	1.357963	0.306170	-1.146923	1.542480	0.289960
O	0.000000	3.864428	0.186977	0.651728	3.813007	0.234517
O	0.000000	-3.864428	0.186977	-0.651728	-3.813007	0.234517
P	1.387898	-1.357963	0.306170	1.146923	-1.542480	0.289960
Mn	0.000000	0.000000	1.607012	0.000000	0.000000	1.524695

Table S12. Coordinates of Mn₂(CO)₆(PCO)₂ **26-1S(C₂)**.

	B3LYP			BP86		
Mn	0.001786	1.404295	-0.026992	-0.002556	1.382145	-0.033976
Mn	-0.001786	-1.404295	-0.026992	0.002556	-1.382145	-0.033976
C	-0.615279	3.026808	-0.533547	-0.583168	2.995254	-0.584946
C	1.693122	2.000125	-0.502116	1.687959	1.984741	-0.445264
C	0.551931	1.659639	1.701439	0.523529	1.619616	1.691822
C	1.677098	-1.045151	0.699038	1.687959	-1.090773	0.670423
C	0.615279	-3.026808	-0.533547	0.583168	-2.995254	-0.584946
C	-0.551931	-1.659639	1.701439	-0.523529	-1.619616	1.691822
C	-1.693122	-2.000125	-0.502116	-1.687959	-1.984741	-0.445264
C	-1.677098	1.045151	0.699038	-1.687959	1.090773	0.670423
O	-2.722692	0.932719	1.179732	-2.751770	1.013972	1.151118
O	0.879193	1.832202	2.797022	0.841160	1.791273	2.805727
O	-1.022136	4.063136	-0.849992	-0.970035	4.047175	-0.928600
O	2.722692	2.489956	-0.704189	2.732727	2.491646	-0.612157
O	1.022136	-4.063136	-0.849992	0.970035	-4.047175	-0.928600
O	-2.722692	-2.489956	-0.704189	-2.732727	-2.491646	-0.612157
O	-0.879193	-1.832202	2.797022	-0.841160	-1.791273	2.805727
O	2.722692	-0.932719	1.179732	2.751770	-1.013972	1.151118
P	-1.004099	0.173477	-1.792977	-1.027209	0.114332	-1.764769
P	1.004099	-0.173477	-1.792977	1.027209	-0.114332	-1.764769

Table S13. Coordinates of Mn₂(CO)₆(PCO)₂ **26-2S(C_s)**.

	B3LYP			BP86		
Mn	0.092223	-1.384553	0.000000	0.104657	-1.361228	0.000000
Mn	-0.069508	1.441656	0.000000	-0.055990	1.416178	0.000000
C	-1.395121	-2.461492	0.000000	-1.395271	-2.393644	0.000000
C	-0.061111	-1.419743	1.866821	-0.063699	-1.399631	1.847667
C	1.272727	-2.769543	0.000000	1.235057	-2.763311	0.000000
C	0.932023	2.993706	0.000000	0.888857	2.982701	0.000000
C	-0.794732	2.090321	1.546492	-0.731784	2.050611	1.566719
C	-0.794732	2.090321	-1.546492	-0.731784	2.050611	-1.566719
C	-1.624546	0.398675	0.000000	-1.647947	0.449955	0.000000
C	-0.061111	-1.419743	-1.866821	-0.063699	-1.399631	-1.847667
O	-0.259881	-1.539558	-2.997388	-0.276309	-1.533806	-2.990397
O	2.031460	-3.638368	0.000000	1.968316	-3.674656	0.000000
O	-2.314043	-3.155554	0.000000	-2.338109	-3.081189	0.000000
O	-0.259881	-1.539558	2.997388	-0.276309	-1.533806	2.990397
O	-1.246808	2.523905	2.521082	-1.165573	2.491830	2.562715
O	-2.768057	0.156891	0.000000	-2.806132	0.220780	0.000000
O	-1.246808	2.523905	-2.521082	-1.165573	2.491830	-2.562715
O	1.521117	3.987474	0.000000	1.438008	4.016152	0.000000
P	1.697831	0.233478	-1.037087	1.693947	0.199440	-1.050313
P	1.697831	0.233478	1.037087	1.693947	0.199440	1.050313

Table S14. Coordinates of Mn₂(CO)₆(PCO)₂ **26-3S(C_s)**.

	B3LYP			BP86		
Mn	-0.005413	-0.060593	2.201585	-0.005407	-0.060594	2.201584
Mn	-0.005413	-0.060593	-2.201585	-0.005407	-0.060594	-2.201584
C	0.335547	-1.334366	3.452708	0.335548	-1.334362	3.452712
C	-1.849395	-0.183798	2.566754	-1.849388	-0.183805	2.566746
C	0.148428	1.379373	3.312923	0.148406	1.379376	3.312920
C	-1.849395	-0.183798	-2.566754	-1.849388	-0.183805	-2.566746
C	0.335547	-1.334366	-3.452708	0.335548	-1.334362	-3.452712
C	0.148428	1.379373	-3.312923	0.148406	1.379376	-3.312920
C	1.820345	0.025988	-1.814837	1.820336	0.026029	-1.814845
C	1.820345	0.025988	1.814837	1.820336	0.026029	1.814845
O	2.955208	0.075859	1.616798	2.955223	0.075862	1.616801
O	0.233921	2.308702	3.995545	0.233876	2.308707	3.995542
O	0.550764	-2.156429	4.238910	0.550764	-2.156425	4.238916
O	-2.969595	-0.261342	2.824065	-2.969586	-0.261362	2.824054
O	0.550764	-2.156429	-4.238910	0.550764	-2.156425	-4.238916
O	2.955208	0.075859	-1.616798	2.955223	0.075862	-1.616801
O	0.233921	2.308702	-3.995545	0.233876	2.308707	-3.995542
O	-2.969595	-0.261342	-2.824065	-2.969586	-0.261362	-2.824054
P	-0.733429	1.170580	0.000000	-0.733433	1.170567	0.000000
P	-0.434118	-0.842939	0.000000	-0.434097	-0.842947	0.000000

Table S15. Coordinates of Mn₂(CO)₆(PCO)₂ **26-1T**(C_{2v}).

	B3LYP			BP86		
Mn	0.000000	2.056960	0.038497	0.000000	2.042381	-0.050676
Mn	0.000000	-2.056960	0.038497	0.000000	-2.042381	-0.050676
C	1.420342	3.179757	-0.252519	-1.420811	3.137123	0.254628
C	0.000000	2.578056	1.848871	0.000000	2.647500	-1.812730
C	-1.420342	3.179757	-0.252519	1.420811	3.137123	0.254628
C	0.000000	-2.578056	1.848871	0.000000	-2.647500	-1.812730
C	1.420342	-3.179757	-0.252519	-1.420811	-3.137123	0.254628
C	-1.420342	-3.179757	-0.252519	1.420811	-3.137123	0.254628
C	0.000000	-1.676689	-1.791336	0.000000	-1.686415	1.767585
C	0.000000	1.676689	-1.791336	0.000000	1.686415	1.767585
O	0.000000	1.527740	-2.935021	0.000000	1.566741	2.929418
O	-2.334871	3.863506	-0.434459	2.346359	3.826629	0.455233
O	2.334871	3.863506	-0.434459	-2.346359	3.826629	0.455233
O	0.000000	2.933512	2.944618	0.000000	3.090106	-2.892831
O	2.334871	-3.863506	-0.434459	-2.346359	-3.826629	0.455233
O	0.000000	-1.527740	-2.935021	0.000000	-1.566741	2.929418
O	-2.334871	-3.863506	-0.434459	2.346359	-3.826629	0.455233
O	0.000000	-2.933512	2.944618	0.000000	-3.090106	-2.892831
P	-1.102738	0.000000	0.573145	1.095096	0.000000	-0.606279
P	1.102738	0.000000	0.573145	-1.095096	0.000000	-0.606279

Table S16. Coordinates of Mn₂(CO)₆(PCO)₂ **26-4S(C₂)**.

	B3LYP			BP86		
Mn	-0.183500	3.057074	0.000000	0.692287	-2.951528	0.000000
Mn	0.183500	-3.057074	0.000000	-0.692287	2.951528	0.000000
C	-0.044274	4.217292	1.403647	0.701153	-4.097572	1.403903
C	-2.044540	3.255007	0.000000	2.548223	-2.938802	0.000000
C	-0.044274	4.217292	-1.403647	0.701153	-4.097572	-1.403903
C	-1.666253	-2.830936	0.000000	1.150869	3.005937	0.000000
C	0.044274	-4.217292	1.403647	-0.701153	4.097572	1.403903
C	0.044274	-4.217292	-1.403647	-0.701153	4.097572	-1.403903
C	2.044540	-3.255007	0.000000	-2.548223	2.938802	0.000000
C	1.666253	2.830936	0.000000	-1.150869	-3.005937	0.000000
O	2.814161	2.715889	0.000000	-2.317347	-3.079870	0.000000
O	0.044274	4.926523	-2.312960	0.701153	-4.815506	-2.329986
O	0.044274	4.926523	2.312960	0.701153	-4.815506	2.329986
O	-3.187580	3.409652	0.000000	3.715770	-2.982266	0.000000
O	-0.044274	-4.926523	2.312960	-0.701153	4.815506	2.329986
O	3.187580	-3.409652	0.000000	-3.715770	2.982266	0.000000
O	-0.044274	-4.926523	-2.312960	-0.701153	4.815506	-2.329986
O	-2.814161	-2.715889	0.000000	2.317347	3.079870	0.000000
P	-0.396022	0.910575	0.000000	0.600902	-0.806782	0.000000
P	0.396022	-0.910575	0.000000	-0.600902	0.806782	0.000000

Table S17. Coordinates of Mn₂(CO)₆(PCO)₂ **26-2T(C₂)**.

	B3LYP			BP86		
Mn	0.040854	2.039444	0.059919	-0.014312	2.011892	0.061048
Mn	-0.040854	-2.039444	0.059919	0.014312	-2.011892	0.061048
C	0.777874	3.650698	-0.442965	0.587708	3.646210	-0.473058
C	-0.469164	2.815320	1.692728	-0.460667	2.772934	1.695681
C	-1.624054	2.278926	-0.687181	-1.692953	2.174679	-0.628643
C	-0.783985	-1.320588	-1.494022	-0.736355	-1.339312	-1.490304
C	-0.777874	-3.650698	-0.442965	-0.587708	-3.646210	-0.473058
C	1.624054	-2.278926	-0.687181	1.692953	-2.174679	-0.628643
C	0.469164	-2.815320	1.692728	0.460667	-2.772934	1.695681
C	0.783985	1.320588	-1.494022	0.736355	1.339312	-1.490304
O	1.287887	0.954568	-2.466064	1.257190	1.009121	-2.483977
O	-2.657938	2.460666	-1.173811	-2.758602	2.318491	-1.093725
O	1.221707	4.668498	-0.765261	0.946895	4.704680	-0.824336
O	-0.783985	3.313962	2.683824	-0.736355	3.287391	2.708074
O	-1.221707	-4.668498	-0.765261	-0.946895	-4.704680	-0.824336
O	0.783985	-3.313962	2.683824	0.736355	-3.287391	2.708074
O	2.657938	-2.460666	-1.173811	2.758602	-2.318491	-1.093725
O	-1.287887	-0.954568	-2.466064	-1.257190	-1.009121	-2.483977
P	1.009608	0.084015	1.190744	1.020850	0.116075	1.160230
P	-1.009608	-0.084015	1.190744	-1.020850	-0.116075	1.160230

Table S18. Coordinates of Mn₂(CO)₆(PCO)₂ **26-5S(C₂)**.

	B3LYP			BP86		
Mn	0.000000	0.000000	-1.334545	0.000000	0.000000	-1.297915
Mn	0.000000	0.000000	1.481495	0.000000	0.000000	1.462479
C	2.042240	0.441523	-1.236642	1.978998	0.264691	-1.324573
C	-2.042240	-0.441523	-1.236642	-1.978998	-0.264691	-1.324573
C	0.000000	-1.275667	-2.617564	0.000000	-1.293077	-2.555676
C	0.000000	1.275667	-2.617564	0.000000	1.293077	-2.555676
C	0.792298	1.696716	1.407332	0.966882	1.581351	1.375056
C	-1.187859	0.562035	2.754989	-1.080375	0.713125	2.744183
C	-0.792298	-1.696716	1.407332	-0.966882	-1.581351	1.375056
C	1.187859	-0.562035	2.754989	1.080375	-0.713125	2.744183
P	-1.686111	0.889635	-0.120430	-1.589489	1.027980	-0.068403
P	1.686111	-0.889635	-0.120430	1.589489	-1.027980	-0.068403
O	-1.915504	0.914039	3.580404	-1.744521	1.164718	3.594715
O	-0.028963	-2.108402	-3.418226	-0.059496	-2.137012	-3.364239
O	-1.280444	-2.739927	1.386133	-1.570890	-2.579782	1.355025
O	1.915504	-0.914039	3.580404	1.744521	-1.164718	3.594715
O	1.280444	2.739927	1.386133	1.570890	2.579782	1.355025
O	-2.810217	-1.159844	-1.783202	-2.878354	-0.814892	-1.893619
O	0.028963	2.108402	-3.418226	0.059496	2.137012	-3.364239
O	2.810217	1.159844	-1.783202	2.878354	0.814892	-1.893619

Table S19. Coordinates of Mn₂(CO)₆(PCO)₂ **26-6S(C₁)**.

	B3LYP			BP86		
Mn	-1.383611	-0.339639	-0.246818	-1.325258	-0.291610	-0.119038
Mn	1.408790	-0.113199	-0.011116	1.378223	-0.106796	-0.010824
C	-0.363454	2.531689	-0.724378	-0.292402	2.490673	-0.738394
C	-1.469456	-0.871708	1.756472	-1.806225	-0.469673	1.702530
C	2.559814	-1.076902	1.033640	2.565673	-1.023535	1.016635
C	2.746120	0.977874	-0.614998	2.738317	0.799042	-0.813417
C	1.025897	1.019764	1.428592	1.170532	1.151223	1.337306
C	1.642628	-1.308042	-1.433773	1.396522	-1.483363	-1.255193
C	-2.744319	0.765045	0.211473	-2.812091	0.737388	-0.237356
C	-2.540359	-1.231375	-1.280879	-2.213568	-1.507387	-1.060336
O	0.827735	1.714911	2.326539	1.087766	1.921838	2.211405
O	3.601532	1.661162	-0.983362	3.629516	1.371669	-1.309994
O	3.320300	-1.658130	1.680884	3.374778	-1.585521	1.648122
O	-2.094709	-0.581072	2.720206	-2.545938	-0.290068	2.624941
O	1.807648	-2.050109	-2.300026	1.442818	-2.366033	-2.017776
O	-3.265072	-1.837420	-1.955663	-2.791743	-2.339496	-1.660071
O	-3.616855	1.454837	0.533296	-3.792980	1.378925	-0.281316
O	-0.534607	3.569692	-0.227041	-0.458702	3.563725	-0.288012
P	-0.144901	1.090650	-1.602775	-0.134204	1.006310	-1.601693
P	-0.264330	-1.871189	0.924962	-0.223715	-1.502734	1.342861

Table S20. Coordinates of Mn₂(CO)₆(PCO)₂ **26-7S(C_s)**.

	B3LYP			BP86		
Mn	0.055312	-1.448314	0.000000	0.057220	-1.360861	0.000000
Mn	0.298002	1.590435	0.000000	0.319899	1.524737	0.000000
C	0.412166	0.100696	2.887286	0.469001	0.093648	2.883430
C	0.412166	0.100696	-2.887286	0.469001	0.093648	-2.883430
C	1.005804	-2.972726	0.000000	0.914772	-2.908642	0.000000
C	-1.053233	-2.060397	1.304287	-1.058947	-1.950756	1.279786
C	-1.053233	-2.060397	-1.304287	-1.058947	-1.950756	-1.279786
C	-1.458997	1.219126	0.000000	-1.408427	1.129807	0.000000
C	0.058330	2.808438	1.333216	0.015836	2.717197	1.317727
C	0.058330	2.808438	-1.333216	0.015836	2.717197	-1.317727
O	1.653779	-3.933272	0.000000	1.504875	-3.926144	0.000000
O	-0.167587	0.184173	-3.891858	-0.095202	0.161070	-3.911242
O	-0.167587	0.184173	3.891858	-0.095202	0.161070	3.911242
O	-0.087241	3.590706	-2.173642	-0.189192	3.512143	-2.156526
O	-0.087241	3.590706	2.173642	-0.189192	3.512143	2.156526
O	-2.601148	1.010961	0.000000	-2.573906	0.956521	0.000000
O	-1.775109	-2.463372	2.115953	-1.805707	-2.369735	2.084899
O	-1.775109	-2.463372	-2.115953	-1.805707	-2.369735	-2.084899
P	1.364570	-0.027396	1.486533	1.413904	-0.028121	1.461937
P	1.364570	-0.027396	-1.486533	1.413904	-0.028121	-1.461937

Table S21. Coordinates of Mn₂(CO)₅(PCO)₂ **25-1S(C_s)**.

	B3LYP			BP86		
Mn	-0.008756	1.362095	0.000000	0.003157	-1.338760	0.000000
Mn	-0.045354	-1.349917	0.000000	0.040618	1.333101	0.000000
C	-0.678759	2.551138	1.251578	0.688903	-2.504623	1.249097
C	-0.678759	2.551138	-1.251578	0.688903	-2.504623	-1.249097
C	1.694901	1.972496	0.000000	-1.673618	-1.999093	0.000000
C	1.833284	-1.233633	0.000000	-1.821625	1.189548	0.000000
C	-0.043734	-2.630176	1.321582	0.043142	2.623983	1.301554
C	-1.920857	-1.270018	0.000000	1.897077	1.214564	0.000000
C	-0.043734	-2.630176	-1.321582	0.043142	2.623983	-1.301554
P	-0.092762	0.195714	1.795117	0.077420	-0.171583	1.819702
P	-0.092762	0.195714	-1.795117	0.077420	-0.171583	-1.819702
O	-0.043340	-3.450797	2.134807	0.045235	3.472110	2.106692
O	-3.072682	-1.221995	0.000000	3.063011	1.147973	0.000000
O	-0.043340	-3.450797	-2.134807	0.045235	3.472110	-2.106692
O	2.786889	2.354630	0.000000	-2.761833	-2.434361	0.000000
O	2.984024	-1.174811	0.000000	-2.986745	1.125570	0.000000
O	-1.108179	3.344353	1.977600	1.134265	-3.302543	1.984242
O	-1.108179	3.344353	-1.977600	1.134265	-3.302543	-1.984242

Table S22. Coordinates of Mn₂(CO)₅(PCO)₂ **25-2S(C_s)**.

	B3LYP			BP86		
Mn	-0.001656	-1.267224	0.000000	-0.023711	-1.261227	0.000000
Mn	-0.291108	1.637711	0.000000	-0.316117	1.606215	0.000000
C	0.137935	-1.287522	1.866904	0.129728	-1.300652	1.845994
C	0.137935	-1.287522	-1.866904	0.129728	-1.300652	-1.845994
C	-0.750911	-2.921550	0.000000	-0.663517	-2.940944	0.000000
C	1.741083	-1.864739	0.000000	1.740819	-1.721634	0.000000
C	1.458148	1.224054	0.000000	1.439493	1.323075	0.000000
C	0.032536	2.698763	-1.449497	-0.030692	2.656991	-1.451563
C	0.032536	2.698763	1.449497	-0.030692	2.656991	1.451563
P	-1.737422	0.140346	1.059799	-1.701010	0.093848	1.085309
P	-1.737422	0.140346	-1.059799	-1.701010	0.093848	-1.085309
O	0.357419	-1.397007	2.994850	0.366865	-1.436147	2.984443
O	-1.263541	-3.954733	0.000000	-1.104514	-4.024778	0.000000
O	0.357419	-1.397007	-2.994850	0.366865	-1.436147	-2.984443
O	2.827566	-2.243612	0.000000	2.865893	-2.029569	0.000000
O	0.221088	3.390989	-2.361207	0.145489	3.358844	-2.377527
O	0.221088	3.390989	2.361207	0.145489	3.358844	2.377527
O	2.617234	1.081130	0.000000	2.618516	1.249055	0.000000

Table S23. Coordinates of Mn₂(CO)₅(PCO)₂ **25-1T(C₁)**.

	B3LYP			BP86		
Mn	1.210592	-0.042291	-0.004345	1.221556	-0.030138	-0.013344
Mn	-1.501464	-0.130848	-0.076301	-1.476787	-0.151313	-0.130282
C	1.265109	-1.790343	0.649133	1.305022	-1.823586	0.445338
C	1.105113	1.805642	-0.252204	1.100847	1.818641	-0.025191
C	2.748355	-0.218984	-0.965999	2.815758	-0.052699	-0.869724
C	2.028927	0.389045	1.573458	1.886002	0.224072	1.658624
C	-0.967069	0.258820	1.666447	-1.138350	0.171216	1.634810
C	-2.225856	1.580594	-0.227673	-2.348787	1.447527	-0.241836
C	-3.068538	-1.125223	0.240788	-2.952527	-1.208697	0.131733
P	-0.244587	-1.525790	-1.459131	-0.122700	-1.360894	-1.596165
P	-0.253713	0.443464	-2.033616	-0.152496	0.693170	-1.948106
O	1.367428	-2.824498	1.155060	1.437334	-2.916024	0.846251
O	3.721001	-0.333486	-1.577602	3.849348	-0.069804	-1.418309
O	1.105848	2.960260	-0.294512	1.101118	2.984269	0.083387
O	2.549945	0.663029	2.565637	2.335985	0.390750	2.724274
O	-2.688439	2.642019	-0.255328	-2.932606	2.465711	-0.265007
O	-4.020223	-1.757375	0.404740	-3.900327	-1.880929	0.288217
O	-0.856807	0.545809	2.789961	-1.078236	0.412690	2.785210

Table S24. Coordinates of Mn₂(CO)₅(PCO)₂ **25-3S(C_s)**.

	B3LYP			BP86		
Mn	-0.266413	0.026182	1.309708	-0.246303	0.037729	1.292307
Mn	-0.266413	0.026182	-1.309708	-0.246303	0.037729	-1.292307
C	-1.538170	-0.612787	-2.443689	-1.533895	-0.574862	-2.408279
C	2.637375	-0.018034	0.000000	2.575422	-0.045796	0.000000
C	0.974872	-0.919350	2.251185	0.947854	-0.929155	2.238178
C	0.974872	-0.919350	-2.251185	0.947854	-0.929155	-2.238178
C	-0.261549	1.560591	-2.311312	-0.214344	1.534340	-2.317549
C	-1.538170	-0.612787	2.443689	-1.533895	-0.574862	2.408279
C	-0.261549	1.560591	2.311312	-0.214344	1.534340	2.317549
O	-2.293282	-0.988680	-3.237843	-2.311301	-0.937224	-3.210035
O	1.731878	-1.589846	-2.815139	1.681263	-1.627750	-2.831754
O	1.731878	-1.589846	2.815139	1.681263	-1.627750	2.831754
O	-0.327444	2.544076	-2.916177	-0.267876	2.513737	-2.960355
O	-2.293282	-0.988680	3.237843	-2.311301	-0.937224	3.210035
O	-0.327444	2.544076	2.916177	-0.267876	2.513737	2.960355
O	3.572203	-0.701861	0.000000	3.478940	-0.791634	0.000000
P	-1.824402	-0.834203	0.000000	-1.818943	-0.841647	0.000000
P	1.360303	1.142453	0.000000	1.352434	1.186801	0.000000

Table S25. Coordinates of Mn(CO)₅(PCO) **15-1S(C_s)**.

	B3LYP			BP86		
Mn	0.177856	-0.475291	0.000000	-0.181568	-0.465198	0.000000
C	0.180551	-0.279507	1.868522	1.666708	-0.311763	0.000000
C	-1.686760	-0.280026	0.000000	-0.185095	-0.243347	1.845530
C	0.048738	-2.299777	0.000000	-0.059656	-2.274935	0.000000
C	2.050589	-0.543607	0.000000	-0.185095	-0.243347	-1.845530
C	0.180551	-0.279507	-1.868522	-2.033724	-0.563411	0.000000
C	-1.028928	2.545473	0.000000	1.048459	2.524872	0.000000
O	0.180551	-0.141819	-3.010579	-3.196232	-0.648023	0.000000
O	-0.035277	-3.451967	0.000000	0.021888	-3.442571	0.000000
O	0.180551	-0.141819	3.010579	2.830684	-0.258205	0.000000
O	3.200351	-0.589710	0.000000	-0.185095	-0.093285	-3.001132
O	-2.833102	-0.185219	0.000000	-0.185095	-0.093285	3.001132
O	-2.118206	2.992787	0.000000	2.144191	2.987947	0.000000
P	0.565748	2.056398	0.000000	-0.560874	2.045396	0.000000

Table S26. Coordinates of Mn(CO)₅(PCO) **15-2S(C_s)**.

	B3LYP			BP86		
Mn	-0.303204	-0.501584	0.000000	0.316126	-0.505330	0.000000
C	-0.297961	-0.355083	1.891677	2.182130	-0.406823	0.000000
C	-2.197228	-0.422848	0.000000	0.310713	-0.368351	1.865172
C	-0.321241	-2.342931	0.000000	0.379261	-2.320567	0.000000
C	1.600476	-0.495338	0.000000	0.310713	-0.368351	-1.865172
C	-0.297961	-0.355083	-1.891677	-1.550303	-0.539644	0.000000
C	0.626809	2.308183	0.000000	-0.703199	2.334494	0.000000
O	-0.297961	-0.231462	-3.031112	-2.710325	-0.586865	0.000000
O	-0.325166	-3.497415	0.000000	0.406002	-3.490685	0.000000
O	-0.297961	-0.231462	3.031112	3.344034	-0.372665	0.000000
O	2.743815	-0.556526	0.000000	0.310713	-0.281244	-3.024078
O	-3.342556	-0.372189	0.000000	0.310713	-0.281244	3.024078
P	1.878558	3.273927	0.000000	-1.962076	3.321337	0.000000
O	-0.389622	1.565217	0.000000	0.332876	1.616284	0.000000

Table S27. Coordinates of Mn(CO)₄(PCO) **14-1S(C_s)**.

	B3LYP			BP86		
Mn	0.232751	-0.286362	0.000000	0.229968	-0.266512	0.000000
C	-1.632707	-0.244646	0.000000	-1.617402	-0.241938	0.000000
C	0.233362	-1.522345	1.336284	0.227693	-1.494432	1.313006
C	0.233362	-1.522345	-1.336284	0.227693	-1.494432	-1.313006
C	2.101184	-0.243364	0.000000	2.078771	-0.253601	0.000000
C	-1.194989	2.490919	0.000000	-1.189426	2.476798	0.000000
O	-2.785616	-0.274324	0.000000	-2.784827	-0.305950	0.000000
O	0.233362	-2.263948	-2.223856	0.227693	-2.258895	-2.202616
O	0.233362	-2.263948	2.223856	0.227693	-2.258895	2.202616
O	3.253959	-0.254981	0.000000	3.246554	-0.303350	0.000000
O	-2.282673	2.917718	0.000000	-2.284723	2.916501	0.000000
P	0.434719	2.035040	0.000000	0.455180	2.026210	0.000000

Table S28. Coordinates of Mn(CO)₄(PCO) **14-2S(C_s)**.

	B3LYP			BP86		
Mn	0.266441	-0.431157	0.000000	0.261706	-0.415391	0.000000
C	2.172997	-0.387553	0.000000	2.137641	-0.438325	0.000000
C	0.268263	-1.688813	1.316448	0.265867	-1.656319	1.298534
C	0.268263	-1.688813	-1.316448	0.265867	-1.656319	-1.298534
C	-1.627174	-0.411666	0.000000	-1.598727	-0.455399	0.000000
O	0.268263	-2.443627	-2.192627	0.265867	-2.435618	-2.175479
O	0.268263	-2.443627	2.192627	0.265867	-2.435618	2.175479
O	3.320128	-0.395340	0.000000	3.297633	-0.540423	0.000000
O	-2.774075	-0.447062	0.000000	-2.759409	-0.554912	0.000000
C	-0.472247	2.441240	0.000000	-0.474995	2.476449	0.000000
P	-1.445525	3.681329	0.000000	-1.412577	3.768544	0.000000
O	0.337578	1.476233	0.000000	0.314055	1.496081	0.000000

Table S29. Coordinates of Mn(CO)₃(PCO) **13-1S(C_s)**.

	B3LYP			BP86		
Mn	-0.054569	-0.035802	0.000000	-0.084123	-0.028132	0.000000
C	1.743666	0.139223	0.000000	1.692369	0.071786	0.000000
C	-0.041438	-1.293540	1.318207	-0.094997	-1.279536	1.287352
C	-0.041438	-1.293540	-1.318207	-0.094997	-1.279536	-1.287352
O	-0.041438	-2.045155	2.196769	-0.094997	-2.050400	2.172321
O	-0.041438	-2.045155	-2.196769	-0.094997	-2.050400	-2.172321
O	2.896398	0.245090	0.000000	2.866134	0.114962	0.000000
C	-1.536407	1.334686	0.000000	-1.469692	1.413695	0.000000
P	-0.252377	2.363694	0.000000	-0.075656	2.330932	0.000000
O	-2.263076	0.360055	0.000000	-2.295913	0.508448	0.000000

Table S30. Coordinates of Mn(CO)₃(PCO) **13-2S(C_{3v})**.

	B3LYP			BP86		
Mn	0.000000	0.000000	0.466896	0.000000	0.000000	0.457128
C	0.000000	1.493461	1.484923	0.000000	1.450241	1.483079
C	-1.293375	-0.746730	1.484923	-1.255945	-0.725120	1.483079
C	1.293375	-0.746730	1.484923	1.255945	-0.725120	1.483079
O	-2.143380	-1.237481	2.098196	-2.104297	-1.214916	2.133439
O	2.143380	-1.237481	2.098196	2.104297	-1.214916	2.133439
O	0.000000	2.474962	2.098196	0.000000	2.429833	2.133439
O	0.000000	0.000000	-1.335699	0.000000	0.000000	-1.345280
C	0.000000	0.000000	-2.596304	0.000000	0.000000	-2.606705
P	0.000000	0.000000	-4.166287	0.000000	0.000000	-4.194914

Table S31. Coordinates of Mn(CO)₃(PCO) **13-1T(C_s)**.

	B3LYP			BP86		
Mn	0.000000	0.551883	0.000000	0.000000	0.533139	0.000000
C	1.678889	1.391268	0.000000	1.635006	1.406741	0.000000
C	0.165798	-2.625779	0.000000	0.178128	-2.614576	0.000000
C	-1.583809	-0.448560	0.000000	-1.570314	-0.448646	0.000000
C	-0.970354	2.225934	0.000000	-0.947529	2.162020	0.000000
O	-2.579492	-1.035985	0.000000	-2.589901	-1.026964	0.000000
O	-1.557398	3.214824	0.000000	-1.538702	3.168908	0.000000
O	2.713161	1.907331	0.000000	2.661423	1.972742	0.000000
P	1.344362	-1.426856	0.000000	1.347887	-1.386096	0.000000
O	-0.564844	-3.542595	0.000000	-0.531576	-3.560970	0.000000

Table S32. Harmonic vibrational frequencies(cm^{-1}) and IR intensities (KM/Mole) of $\text{Mn}_2(\text{CO})_8(\text{PCO})_2$ **28-1S**(C_{2h}).

B3LYP	BP86
18(0), 44(0), 49(0), 54(0), 58(0), 66(1), 66(1), 70(0), 76(0), 76(0), 80(0), 81(0), 89(0), 92(0), 95(0), 101(1), 107(0), 107(0), 110(0), 119(0), 135(0), 140(0), 192(0), 214(0), 228(0), 253(2), 399(6), 402(0), 415(0), 416(0), 417(0), 419(4), 449(0), 450(0), 463(12), 464(0), 464(0), 471(11), 474(52), 476(0), 482(8), 482(0), 500(0), 502(11), 551(6), 554(0), 575(0), 577(1), 630(0), 638(160), 643(0), 644(135), 669(313), 677(0), 704(31), 704(0), 2019(683), 2024(0), 2060(0), 2061(0), 2064(1836), 2072(808), 2080(0), 2087(2930), 2121(1439), 2155(0)	11(0), 41(0), 45(0), 51(0), 55(0), 64(1), 65(1), 67(0), 71(0), 73(0), 78(0), 79(0), 86(0), 89(0), 91(0), 97(1), 103(0), 103(0), 107(0), 115(0), 130(0), 139(0), 204(1), 226(0), 243(0), 267(2), 415(2), 416(0), 420(0), 424(0), 428(2), 430(0), 449(0), 450(4), 454(0), 457(0), 468(0), 473(20), 488(0), 488(0), 491(0), 491(5), 492(0), 496(36), 539(7), 542(0), 564(0), 566(1), 634(0), 639(145), 641(0), 646(142), 671(281), 677(0), 681(0), 681(11), 1952(111), 1962(0), 1968(0), 1973(0), 1976(1699), 1986(631), 1994(0), 1997(2817), 2039(1248), 2068(0)

Table S33. Harmonic vibrational frequencies(cm^{-1}) and IR intensities (KM/Mole) of $\text{Mn}_2(\text{CO})_8(\text{PCO})_2$ **28-2S**(C_{2v}).

B3LYP	BP86
23(0), 44(0), 48(0), 54(0), 60(0), 63(0), 65(1), 70(0), 76(0), 78(0), 79(0), 81(0), 88(0), 92(0), 95(0), 100(1), 107(0), 108(0), 110(0), 119(0), 134(0), 141(0), 192(0), 214(0), 226(0), 252(2), 400(6), 402(1), 414(0), 416(1), 416(0), 419(4), 449(0), 450(0), 462(13), 464(0), 464(0), 470(10), 473(47), 476(0), 480(4), 484(13), 497(0), 502(9), 551(5), 555(0), 575(0), 576(0), 631(0), 639(152), 641(3), 643(143), 669(310), 677(0), 703(27), 706(3), 2021(155), 2023(463), 2060(2), 2061(0), 2064(2010), 2072(809), 2079(239), 2087(2506), 2121(1437), 2155(23)	23(0), 41(0), 44(0), 51(0), 59(0), 60(0), 63(1), 68(0), 72(0), 77(0), 77(0), 79(0), 84(0), 90(0), 91(0), 99(1), 103(0), 104(0), 107(0), 115(0), 129(0), 139(0), 202(1), 226(0), 239(0), 264(1), 415(0), 416(0), 419(4), 423(0), 428(1), 429(1), 449(3), 450(0), 454(0), 458(1), 469(0), 469(18), 487(0), 488(0), 491(3), 491(0), 492(0), 495(38), 539(7), 543(0), 563(0), 565(0), 636(0), 638(2), 639(139), 644(146), 671(280), 678(0), 679(11), 683(0), 1956(0), 1958(11), 1967(0), 1973(0), 1981(2058), 1986(631), 1991(1001), 1998(1498), 2039(1246), 2068(17)

Table S34. Harmonic vibrational frequencies(cm^{-1}) and IR intensities (KM/Mole) of $\text{Mn}_2(\text{CO})_8(\text{PCO})_2$ **28-3S(C₁)**.

B3LYP	BP86
14(0), 37(0), 46(0), 50(0), 60(0), 68(0), 70(0), 76(1), 79(0), 83(0), 85(0), 89(0), 91(0), 97(0), 99(0), 104(0), 105(0), 114(0), 124(0), 125(0), 141(1), 170(1), 189(0), 209(0), 245(2), 275(15), 382(2), 396(3), 399(1), 405(5), 412(0), 413(3), 432(23), 449(0), 452(12), 452(24), 453(7), 467(5), 470(1), 472(2), 473(5), 483(2), 499(2), 510(9), 551(8), 558(4), 571(1), 573(2), 622(23), 629(119), 641(52), 644(75), 666(282), 672(13), 713(5), 835(7), 1828(821), 2022(149), 2057(614), 2068(964), 2074(1004), 2076(556), 2090(557), 2099(1885), 2132(867), 2162(158)	13(0), 37(0), 45(0), 50(0), 57(0), 65(0), 68(0), 76(0), 76(0), 80(0), 84(0), 87(0), 90(0), 95(1), 97(0), 101(0), 104(0), 112(0), 121(0), 124(0), 140(0), 179(1), 199(1), 223(0), 250(6), 278(3), 401(0), 409(2), 412(0), 415(1), 416(0), 425(2), 438(4), 446(1), 453(2), 455(2), 459(19), 466(1), 475(16), 476(16), 480(3), 492(1), 496(1), 498(1), 542(3), 548(2), 560(0), 564(4), 631(17), 635(111), 642(56), 644(66), 669(259), 678(33), 690(0), 801(5), 1775(429), 1957(14), 1974(48), 1979(801), 1981(854), 1989(743), 1997(1094), 2002(1302), 2047(968), 2073(141)

Table S35. Harmonic vibrational frequencies(cm^{-1}) and IR intensities (KM/Mole) of $\text{Mn}_2(\text{CO})_7(\text{PCO})_2$ **27-1S(C_s)**.

B3LYP	BP86
7(0), 23(0), 28(0), 49(0), 60(0), 65(0), 67(0), 73(0), 84(0), 85(0), 90(0), 95(0), 95(0), 97(0), 106(1), 107(1), 108(1), 116(0), 135(1), 162(0), 165(0), 218(9), 341(8), 362(0), 388(12), 397(0), 402(3), 409(0), 411(1), 412(0), 430(10), 441(5), 447(18), 447(21), 455(10), 473(3), 473(34), 484(7), 501(0), 537(11), 546(0), 548(2), 557(0), 581(0), 633(67), 644(69), 656(84), 658(130), 664(519), 669(86), 678(51), 2034(775), 2049(1119), 2054(596), 2091(829), 2103(897), 2107(1447), 2109(1682), 2121(11), 2173(342)	8(0), 23(0), 28(0), 47(0), 55(0), 60(0), 61(0), 67(0), 80(0), 81(0), 86(0), 90(0), 91(0), 93(0), 102(1), 102(1), 104(1), 111(0), 135(0), 159(0), 163(1), 213(9), 347(28), 368(0), 405(0), 406(0), 410(0), 416(4), 423(0), 428(2), 434(6), 434(1), 465(13), 465(12), 470(3), 481(0), 483(1), 488(22), 492(2), 522(7), 532(0), 534(2), 545(0), 564(0), 625(65), 643(27), 651(68), 659(120), 664(290), 668(328), 675(31), 1956(630), 1961(973), 1975(436), 2006(648), 2015(988), 2016(1334), 2030(1262), 2035(0), 2090(310)

Table S36. Harmonic vibrational frequencies(cm^{-1}) and IR intensities (KM/Mole) of $\text{Mn}_2(\text{CO})_7(\text{PCO})_2$ **27-2S(C_s)**.

B3LYP	BP86
7(0), 10(0), 26(0), 43(0), 44(0), 58(0), 69(0), 70(0), 78(0), 80(0), 90(0), 91(0), 96(0), 100(0), 101(0), 103(0), 112(2), 121(1), 124(1), 180(2), 180(0), 244(8), 306(5), 365(0), 390(0), 392(19), 403(0), 410(1), 412(0), 413(4), 424(0), 429(2), 451(13), 453(8), 454(21), 462(7), 481(11), 495(25), 498(1), 512(10), 550(0), 552(1), 560(1), 575(0), 627(87), 641(61), 656(164), 661(127), 663(186), 669(367), 698(129), 2049(1002), 2064(982), 2066(608), 2082(792), 2094(945), 2096(1648), 2109(40), 2114(2263), 2164(278)	7(0), 16(0), 25(0), 39(0), 43(0), 54(0), 63(0), 65(0), 73(0), 76(0), 86(0), 88(0), 93(0), 97(0), 97(0), 99(0), 108(2), 116(1), 119(0), 174(0), 178(2), 245(15), 314(0), 369(0), 391(0), 406(2), 407(0), 418(3), 419(4), 427(0), 431(0), 435(2), 453(5), 468(12), 471(12), 477(1), 481(1), 491(4), 501(1), 504(11), 537(0), 539(1), 547(1), 559(0), 621(82), 638(37), 646(77), 662(118), 664(127), 670(480), 689(94), 1967(909), 1979(863), 1985(398), 1998(701), 2006(951), 2007(1505), 2026(17), 2038(1628), 2083(269)

Table S37. Harmonic vibrational frequencies(cm^{-1}) and IR intensities (KM/Mole) of $\text{Mn}_2(\text{CO})_7(\text{PCO})_2$ **27-3S(C_s)**.

B3LYP	BP86
30(14), 39(0), 50(1), 55(0), 65(0), 67(0), 71(24), 73(0), 86(6), 89(0), 90(0), 92(0), 96(0), 97(0), 109(0), 114(0), 129(0), 137(0), 160(37), 183(0), 216(0), 234(1), 245(3), 266(6), 318(64), 356(0), 419(3), 450(4), 450(1), 451(5), 452(1), 454(24), 469(18), 476(6), 480(0), 481(6), 483(0), 499(1), 505(3), 517(21), 517(22), 527(0), 554(18), 602(0), 604(71), 620(76), 640(6), 653(233), 665(25), 672(15), 690(21), 1986(449), 2026(160), 2030(517), 2054(5), 2067(2013), 2068(0), 2076(1876), 2101(2297), 2137(83)	38(0), 43(0), 48(0), 51(0), 62(0), 64(0), 70(0), 80(0), 86(0), 87(0), 90(0), 94(0), 95(0), 105(4), 109(6), 110(0), 126(0), 130(0), 188(48), 192(0), 225(1), 244(0), 262(0), 285(1), 342(89), 376(0), 418(2), 438(9), 443(1), 453(1), 457(1), 459(0), 460(0), 469(46), 472(2), 479(0), 489(1), 502(7), 502(0), 515(12), 519(10), 538(0), 550(10), 600(0), 601(77), 620(74), 638(0), 648(221), 651(13), 662(16), 667(7), 1888(333), 1954(0), 1961(259), 1968(3), 1980(6), 1984(1685), 1992(1785), 2018(1974), 2050(62)

Table S38. Harmonic vibrational frequencies(cm^{-1}) and IR intensities (KM/Mole) of $\text{Mn}_2(\text{CO})_7(\text{PCO})_2$ **27-4S(C_{2v})**.

B3LYP	BP86
40(0), 47(0), 51(0), 58(8), 66(22), 71(0), 71(0), 76(0), 79(0), 90(4), 90(0), 92(1), 97(0), 97(0), 110(0), 115(0), 128(0), 137(0), 168(42), 183(1), 212(0), 232(1), 237(4), 268(3), 319(68), 357(0), 421(4), 449(8), 451(29), 451(0), 453(0), 453(0), 473(0), 478(6), 478(6), 481(5), 485(0), 498(9), 507(0), 516(20), 516(20), 530(0), 557(9), 605(0), 606(73), 619(74), 639(4), 655(236), 667(17), 682(36), 690(8), 1984(341), 2023(260), 2029(59), 2051(0), 2067(26), 2072(2809), 2076(1279), 2102(2272), 2139(138)	40(0), 41(0), 48(0), 56(0), 69(0), 69(0), 73(0), 74(0), 83(0), 88(0), 91(1), 95(0), 97(0), 106(4), 109(0), 111(3), 124(0), 133(0), 193(1), 200(45), 217(0), 241(0), 252(0), 285(0), 346(100), 377(0), 421(3), 431(0), 451(0), 454(2), 454(0), 459(0), 460(0), 467(4), 468(35), 478(3), 492(1), 502(9), 504(0), 514(12), 520(8), 541(0), 553(3), 602(75), 604(0), 619(72), 637(0), 650(222), 663(13), 666(12), 672(12), 1885(282), 1949(3), 1965(0), 1966(270), 1979(0), 1988(875), 1996(2406), 2017(1986), 2051(92)

Table S39. Harmonic vibrational frequencies(cm^{-1}) and IR intensities (KM/Mole) of $\text{Mn}_2(\text{CO})_7(\text{PCO})_2$ **27-5S(C₁)**.

B3LYP	BP86
20(0), 30(0), 38(0), 48(1), 49(0), 57(1), 66(0), 71(0), 74(0), 79(0), 81(0), 86(0), 92(0), 95(0), 99(0), 103(0), 110(0), 114(0), 125(0), 144(0), 190(2), 218(1), 232(1), 268(10), 400(3), 402(0), 413(0), 418(2), 425(2), 446(0), 450(0), 456(1), 464(3), 466(6), 468(24), 476(7), 476(2), 495(13), 502(13), 505(8), 510(16), 551(3), 575(1), 611(35), 617(13), 634(81), 643(71), 672(189), 677(22), 698(11), 713(15), 2019(393), 2031(82), 2039(449), 2051(888), 2063(1378), 2078(709), 2079(1764), 2103(1608), 2145(175)	22(0), 30(0), 35(0), 43(1), 46(0), 56(1), 64(0), 68(0), 71(0), 75(0), 80(0), 84(0), 89(0), 93(0), 96(0), 100(0), 107(0), 111(0), 122(0), 143(0), 197(1), 229(2), 244(1), 286(3), 409(1), 412(1), 420(1), 423(1), 428(1), 435(2), 448(1), 450(1), 460(3), 467(2), 482(9), 488(9), 491(6), 492(2), 494(13), 516(14), 536(5), 539(3), 564(1), 612(30), 618(14), 636(77), 642(68), 668(4), 674(162), 683(26), 691(6), 1945(154), 1946(376), 1959(265), 1970(12), 1980(1406), 1990(1992), 1994(522), 2014(1309), 2061(230)

Table S40. Harmonic vibrational frequencies(cm^{-1}) and IR intensities (KM/Mole) of $\text{Mn}_2(\text{CO})_7(\text{PCO})_2$ **27-6S(C_s)**.

B3LYP	BP86
25(0), 31(0), 37(0), 50(0), 51(0), 58(0), 60(1), 71(0), 72(0), 81(0), 81(0), 82(0), 90(0), 96(0), 98(0), 106(0), 110(0), 114(0), 120(0), 145(0), 183(2), 223(1), 232(1), 259(9), 398(3), 398(0), 412(0), 416(2), 423(2), 446(0), 455(0), 458(0), 463(3), 464(33), 470(2), 476(4), 477(6), 494(1), 502(18), 504(4), 507(18), 551(1), 575(0), 616(38), 621(7), 634(78), 640(72), 672(182), 678(23), 712(23), 715(1), 2027(172), 2029(30), 2040(469), 2050(800), 2063(1868), 2076(1022), 2079(951), 2102(1715), 2146(219)	25(0), 32(0), 33(0), 46(0), 46(0), 57(0), 60(1), 66(0), 67(0), 77(0), 79(0), 79(0), 88(0), 93(0), 94(0), 101(0), 108(0), 110(0), 114(0), 144(0), 186(0), 234(1), 244(2), 272(1), 408(0), 412(0), 419(2), 426(0), 427(2), 429(0), 443(2), 450(1), 463(2), 469(0), 477(17), 488(6), 489(14), 492(1), 502(4), 517(8), 538(3), 540(1), 565(0), 616(32), 623(9), 637(71), 640(69), 674(147), 684(29), 691(9), 695(2), 1943(332), 1946(164), 1968(1), 1971(56), 1986(1359), 1986(2176), 1992(284), 2016(1423), 2062(238)

Table S41. Harmonic vibrational frequencies(cm^{-1}) and IR intensities (KM/Mole) of $\text{Mn}_2(\text{CO})_7(\text{PCO})_2$ **27-7S(C_s)**.

B3LYP	BP86
34(0), 47(0), 48(0), 55(0), 60(0), 70(0), 73(1), 76(0), 81(0), 83(0), 93(0), 93(0), 96(0), 104(0), 105(0), 108(1), 112(0), 118(0), 132(0), 137(0), 176(0), 199(0), 256(1), 310(2), 397(3), 406(0), 410(1), 412(0), 415(0), 418(3), 447(0), 459(0), 462(12), 469(13), 477(5), 479(7), 486(27), 487(1), 494(0), 497(47), 503(11), 551(1), 577(0), 598(9), 624(25), 632(104), 640(68), 649(81), 668(133), 671(29), 675(2), 2020(16), 2033(701), 2034(718), 2039(733), 2068(931), 2080(278), 2085(1949), 2096(1683), 2150(161)	36(0), 45(0), 46(0), 51(0), 55(0), 64(0), 68(1), 71(0), 78(0), 82(0), 91(0), 94(0), 95(0), 102(0), 104(0), 108(1), 109(0), 118(0), 126(1), 155(0), 194(1), 212(6), 285(1), 328(0), 409(0), 415(0), 416(1), 422(0), 423(1), 433(0), 438(1), 439(3), 444(2), 465(1), 466(0), 481(1), 487(14), 490(5), 491(1), 518(43), 527(7), 536(1), 561(0), 602(8), 607(30), 629(37), 635(108), 643(35), 644(11), 656(98), 668(89), 1930(310), 1946(360), 1959(283), 1963(426), 1987(949), 1990(1270), 1996(714), 2009(1614), 2063(194)

Table S42. Harmonic vibrational frequencies(cm^{-1}) and IR intensities (KM/Mole) of $\text{Mn}_2(\text{CO})_7(\text{PCO})_2$ **27-8S** (C_s).

B3LYP	BP86
34(0), 46(0), 48(0), 57(0), 64(0), 67(0), 74(0), 76(1), 82(0), 84(0), 90(0), 94(0), 94(0), 104(0), 105(0), 107(1), 113(0), 116(0), 132(0), 137(0), 178(1), 201(0), 256(1), 309(2), 396(2), 404(0), 411(1), 413(0), 415(0), 419(3), 447(0), 460(3), 462(12), 469(11), 477(7), 479(8), 487(26), 487(0), 494(1), 499(40), 503(10), 551(1), 577(0), 599(8), 625(24), 632(106), 640(70), 648(74), 668(136), 671(29), 674(5), 2021(456), 2028(0), 2034(797), 2041(876), 2068(863), 2080(194), 2088(2437), 2095(1433), 2150(143)	35(0), 43(0), 45(0), 53(0), 58(0), 60(1), 66(0), 70(1), 80(0), 82(0), 89(0), 95(0), 95(0), 103(0), 103(0), 107(1), 108(0), 116(0), 126(1), 157(0), 196(2), 213(6), 285(1), 328(0), 411(1), 414(1), 417(0), 424(0), 426(1), 427(1), 438(1), 441(2), 446(1), 462(0), 467(1), 481(0), 486(14), 491(2), 491(5), 518(43), 527(5), 537(1), 561(0), 602(11), 608(28), 629(41), 636(122), 636(9), 647(20), 655(92), 667(97), 1929(392), 1946(321), 1961(445), 1961(243), 1985(727), 1994(72), 1996(2293), 2007(1468), 2064(185)

Table S43. Harmonic vibrational frequencies(cm^{-1}) and IR intensities (KM/Mole) of $\text{Mn}_2(\text{CO})_6(\text{PCO})_2$ **26-1S** (C_2).

B3LYP	BP86
21(1), 32(0), 48(0), 65(0), 71(0), 76(0), 82(0), 100(0), 101(0), 105(0), 110(0), 111(0), 114(0), 119(0), 121(1), 149(1), 165(0), 198(0), 235(1), 279(0), 283(3), 392(9), 397(0), 415(7), 415(1), 422(0), 426(1), 434(0), 437(1), 462(1), 469(9), 490(13), 493(1), 497(5), 505(9), 518(5), 524(26), 579(18), 584(1), 612(3), 623(104), 625(73), 632(6), 638(113), 658(414), 675(41), 2044(25), 2048(130), 2056(980), 2063(1148), 2065(21), 2070(1194), 2085(2873), 2141(407)	21(0), 26(1), 48(0), 59(0), 65(0), 70(1), 81(0), 96(0), 98(0), 99(0), 105(0), 108(0), 108(0), 114(0), 116(0), 140(1), 175(0), 205(0), 255(3), 287(0), 293(2), 393(0), 395(3), 415(1), 420(0), 432(6), 432(1), 435(2), 437(1), 456(0), 470(2), 498(1), 499(3), 500(0), 503(0), 526(3), 528(8), 561(6), 566(1), 584(1), 615(122), 620(5), 621(16), 635(121), 648(381), 665(28), 1964(20), 1968(247), 1973(1028), 1983(1025), 1988(4), 1994(886), 2015(1979), 2060(323)

Table S44. Harmonic vibrational frequencies(cm^{-1}) and IR intensities (KM/Mole) of $\text{Mn}_2(\text{CO})_6(\text{PCO})_2$ **26-2S(C_s)**.

B3LYP	BP86
26(0), 45(0), 53(0), 58(0), 73(0), 80(0), 89(0), 90(0), 99(0), 104(0), 109(0), 112(0), 119(0), 135(0), 137(1), 159(1), 180(2), 231(0), 241(0), 282(0), 297(1), 399(6), 407(6), 407(0), 412(0), 423(1), 431(1), 439(4), 447(1), 449(0), 470(13), 472(5), 480(9), 483(17), 495(14), 509(38), 528(4), 579(0), 580(21), 586(1), 619(83), 626(3), 632(103), 637(129), 660(325), 676(45), 1975(389), 2044(513), 2062(336), 2074(1607), 2082(357), 2091(483), 2100(2218), 2148(446)	22(0), 43(0), 48(0), 52(0), 71(0), 76(0), 84(0), 88(0), 96(1), 101(0), 106(0), 107(1), 115(0), 131(0), 131(0), 147(3), 182(1), 227(0), 255(1), 293(0), 298(1), 399(16), 406(0), 410(0), 421(3), 424(0), 426(1), 438(1), 443(1), 455(1), 485(1), 492(2), 494(0), 496(11), 502(4), 511(4), 519(24), 557(12), 561(0), 565(0), 615(8), 622(9), 628(166), 632(113), 650(338), 667(15), 1918(280), 1967(101), 1981(194), 1983(1738), 1992(523), 2003(297), 2023(1888), 2063(322)

Table S45. Harmonic vibrational frequencies(cm^{-1}) and IR intensities (KM/Mole) of $\text{Mn}_2(\text{CO})_6(\text{PCO})_2$ **26-3S(C_s)**.

B3LYP	BP86
26(0), 30(0), 43(0), 43(0), 70(0), 71(0), 78(0), 78(0), 84(0), 90(0), 90(0), 100(0), 105(1), 109(0), 112(0), 113(1), 119(0), 152(0), 187(0), 203(37), 326(16), 389(14), 391(0), 393(3), 401(1), 415(1), 419(17), 420(2), 423(4), 458(0), 462(2), 463(0), 468(59), 476(0), 477(19), 537(7), 540(1), 573(1), 575(3), 599(8), 625(0), 627(20), 631(129), 633(112), 670(355), 676(11), 2054(240), 2057(1765), 2062(228), 2075(823), 2079(166), 2086(2339), 2113(2165), 2151(19)	21(0), 29(0), 41(0), 46(0), 64(0), 72(0), 74(0), 75(0), 80(0), 87(0), 87(0), 96(1), 101(1), 104(0), 109(0), 112(0), 142(0), 158(0), 198(0), 200(9), 352(0), 391(0), 401(5), 416(10), 418(2), 419(1), 420(4), 423(0), 428(1), 474(2), 476(1), 481(2), 486(40), 489(0), 491(8), 522(8), 527(3), 559(1), 561(3), 580(4), 618(8), 625(123), 631(14), 642(108), 670(298), 675(12), 1969(372), 1972(33), 1973(1382), 1990(405), 1991(2109), 1994(225), 2034(1941), 2065(26)

Table S46. Harmonic vibrational frequencies(cm^{-1}) and IR intensities (KM/Mole) of $\text{Mn}_2(\text{CO})_6(\text{PCO})_2$ **26-1T**(C_{2v}).

B3LYP	BP86
6(0), 32(0), 43(0), 50(0), 51(0), 60(1), 72(0), 74(0), 87(0), 90(0), 91(0), 98(1), 101(0), 104(0), 110(0), 119(1), 155(0), 170(0), 209(0), 253(0), 298(5), 384(0), 387(45), 389(6), 404(0), 408(0), 411(0), 415(2), 417(10), 425(0), 438(21), 451(0), 467(0), 468(24), 476(0), 493(48), 507(1), 528(2), 566(0), 568(0), 608(19), 613(121), 617(0), 619(131), 654(407), 664(23), 2058(0), 2059(1963), 2062(283), 2078(988), 2083(109), 2089(2289), 2105(2328), 2150(34)	7(0), 14(0), 39(0), 48(0), 49(0), 54(1), 69(0), 72(0), 81(0), 88(0), 88(0), 91(0), 98(0), 100(0), 107(0), 112(0), 148(0), 167(0), 208(0), 258(0), 319(8), 388(0), 403(1), 407(1), 414(2), 416(0), 417(2), 418(17), 424(2), 428(0), 451(4), 467(1), 480(0), 482(9), 490(1), 493(0), 500(28), 519(2), 550(0), 552(0), 598(17), 611(123), 614(107), 621(0), 650(354), 658(25), 1973(0), 1974(1755), 1977(160), 1992(427), 1994(1194), 2000(896), 2025(2229), 2064(42)

Table S47. Harmonic vibrational frequencies(cm^{-1}) and IR intensities (KM/Mole) of $\text{Mn}_2(\text{CO})_6(\text{PCO})_2$ **26-4S**(C_2).

B3LYP	BP86
-6(0), 11(0), 18(0), 26(0), 48(0), 66(0), 70(0), 74(0), 76(0), 78(0), 91(0), 91(0), 101(1), 104(0), 109(2), 123(0), 148(0), 158(0), 185(0), 250(0), 334(70), 378(0), 392(0), 406(13), 406(0), 409(1), 415(0), 421(6), 422(0), 445(1), 454(0), 476(20), 476(0), 484(0), 485(55), 523(10), 523(0), 572(0), 573(0), 623(0), 625(166), 626(166), 631(0), 645(0), 666(544), 680(0), 2058(0), 2060(2125), 2073(0), 2074(1420), 2077(0), 2079(2763), 2110(3671), 2146(0)	0(0), 14(0), 16(0), 23(0), 48(0), 62(0), 65(0), 71(0), 74(0), 74(0), 88(0), 88(0), 97(0), 100(0), 104(1), 115(0), 137(0), 156(0), 182(0), 270(0), 353(10), 379(0), 392(0), 401(1), 408(0), 421(4), 425(0), 430(6), 431(0), 446(11), 464(0), 487(6), 489(0), 497(0), 498(26), 511(0), 513(1), 556(0), 557(0), 603(0), 618(151), 619(0), 630(142), 634(0), 662(450), 669(0), 1973(0), 1974(1917), 1983(0), 1989(2335), 1990(889), 1992(0), 2033(2879), 2061(0)

Table S48. Harmonic vibrational frequencies(cm^{-1}) and IR intensities (KM/Mole) of $\text{Mn}_2(\text{CO})_6(\text{PCO})_2$ **26-2T(C₂)**.

B3LYP	BP86
27(0), 29(0), 37(0), 52(1), 65(0), 77(0), 77(0), 83(0), 84(0), 92(2), 98(1), 99(2), 107(0), 109(2), 111(1), 117(0), 133(0), 173(0), 205(16), 222(0), 254(12), 371(1), 371(7), 390(0), 391(17), 396(7), 396(1), 408(7), 410(7), 419(53), 431(1), 456(11), 457(0), 463(21), 470(41), 501(2), 501(13), 555(2), 559(5), 605(31), 607(45), 607(15), 621(110), 622(18), 634(161), 642(43), 2048(569), 2054(40), 2057(1699), 2064(0), 2064(1495), 2071(2118), 2106(1712), 2139(112)	28(0), 28(0), 36(0), 54(0), 62(0), 74(0), 77(0), 80(0), 81(0), 89(1), 95(0), 97(1), 102(0), 106(0), 109(2), 112(0), 131(0), 174(0), 207(11), 231(0), 267(7), 374(0), 375(3), 386(0), 391(0), 412(1), 415(1), 420(2), 420(8), 445(36), 457(0), 469(1), 470(1), 475(12), 478(21), 499(1), 499(7), 542(1), 546(5), 582(2), 603(24), 604(46), 621(39), 623(92), 632(154), 640(27), 1959(352), 1971(1307), 1972(215), 1977(64), 1982(1594), 1982(1284), 2019(1650), 2053(79)

Table S49. Harmonic vibrational frequencies(cm^{-1}) and IR intensities (KM/Mole) of $\text{Mn}_2(\text{CO})_6(\text{PCO})_2$ **26-5S(C₂)**.

B3LYP	BP86
21(0), 49(2), 53(0), 60(0), 66(1), 80(0), 89(0), 91(0), 96(0), 98(0), 102(0), 111(4), 114(0), 115(1), 120(2), 168(0), 184(4), 198(9), 230(0), 233(18), 319(8), 325(0), 395(4), 405(14), 410(29), 417(0), 417(5), 422(2), 447(0), 463(11), 469(26), 475(24), 477(0), 483(6), 507(13), 520(6), 539(26), 551(1), 561(4), 568(1), 615(22), 619(19), 632(71), 639(69), 646(82), 664(159), 1874(1173), 1894(157), 2068(253), 2071(693), 2083(805), 2084(1690), 2095(1604), 2142(183)	26(0), 49(0), 50(0), 63(0), 72(0), 80(0), 85(0), 87(0), 93(0), 99(0), 100(0), 112(0), 112(0), 115(0), 126(0), 174(0), 211(4), 221(0), 267(2), 295(6), 333(4), 350(0), 397(17), 411(6), 419(6), 421(1), 423(0), 427(2), 439(1), 457(0), 468(0), 481(15), 482(12), 488(6), 489(0), 515(8), 531(1), 534(1), 550(1), 562(21), 566(14), 594(20), 630(65), 632(61), 642(161), 658(101), 1803(902), 1824(128), 1985(68), 1992(567), 1994(1665), 1999(594), 2019(1376), 2059(185)

Table S50. Harmonic vibrational frequencies(cm^{-1}) and IR intensities (KM/Mole) of $\text{Mn}_2(\text{CO})_6(\text{PCO})_2$ **26-6S(C₁)**.

B3LYP	BP86
18(0), 44(1), 51(0), 59(1), 62(1), 69(0), 78(0), 83(0), 88(0), 91(0), 94(0), 100(0), 106(0), 109(0), 120(1), 125(1), 151(0), 179(7), 204(8), 215(0), 291(4), 326(8), 398(4), 408(5), 414(7), 416(4), 418(16), 429(0), 444(0), 464(20), 468(19), 475(3), 478(6), 486(12), 493(5), 500(15), 535(22), 546(2), 553(9), 570(0), 616(28), 629(78), 637(77), 658(29), 663(168), 686(7), 1883(608), 2030(152), 2038(940), 2069(662), 2074(1263), 2080(448), 2084(2259), 2141(286)	15(0), 31(1), 47(0), 56(0), 62(0), 71(0), 75(0), 83(1), 87(0), 92(0), 94(0), 99(0), 101(0), 107(0), 119(0), 127(0), 166(0), 193(8), 233(1), 253(1), 310(3), 328(5), 395(0), 404(6), 414(1), 418(1), 423(0), 427(1), 434(4), 439(1), 459(4), 480(6), 482(16), 492(2), 493(2), 505(7), 517(3), 531(6), 549(9), 553(9), 595(36), 624(72), 628(92), 641(66), 651(7), 656(119), 1826(564), 1951(296), 1961(301), 1988(945), 1989(1094), 1996(218), 2001(1892), 2056(280)

Table S51. Harmonic vibrational frequencies(cm^{-1}) and IR intensities (KM/Mole) of $\text{Mn}_2(\text{CO})_6(\text{PCO})_2$ **26-7S(C_s)**.

B3LYP	BP86
24(0), 33(0), 34(0), 55(0), 59(0), 61(1), 65(0), 75(0), 81(0), 86(0), 90(0), 100(1), 101(1), 107(0), 110(0), 111(0), 121(0), 149(0), 210(0), 221(9), 245(7), 260(2), 402(2), 406(0), 423(3), 428(0), 451(0), 453(0), 470(2), 472(1), 475(6), 487(0), 489(0), 502(5), 507(21), 510(14), 513(17), 514(15), 604(35), 613(28), 617(9), 619(10), 669(81), 681(52), 683(33), 690(2), 2026(268), 2027(0), 2038(503), 2044(8), 2050(508), 2071(3099), 2087(1998), 2126(304)	23(0), 33(0), 37(0), 52(0), 54(0), 57(1), 61(1), 74(0), 80(0), 85(0), 91(0), 98(0), 101(0), 103(0), 107(0), 112(0), 132(0), 147(0), 219(0), 238(4), 253(1), 279(1), 411(1), 411(1), 419(1), 433(0), 442(3), 448(0), 459(3), 459(0), 468(5), 473(3), 498(7), 507(2), 516(14), 524(3), 532(4), 534(3), 597(30), 612(27), 615(6), 619(16), 663(58), 664(14), 672(14), 683(45), 1935(211), 1943(126), 1953(836), 1954(27), 1980(13), 1999(1752), 2000(2342), 2039(219)

Table S52. Harmonic vibrational frequencies(cm^{-1}) and IR intensities (KM/Mole) of $\text{Mn}_2(\text{CO})_5(\text{PCO})_2$ **25-1S(C_s)**.

B3LYP	BP86
31(0), 51(0), 59(0), 72(0), 83(0), 84(0), 87(0), 100(0), 101(0), 103(0), 115(0), 119(0), 125(0), 133(0), 157(1), 197(1), 254(0), 286(15), 390(5), 398(5), 401(0), 406(0), 410(12), 422(0), 424(4), 439(2), 455(6), 460(53), 473(1), 480(20), 487(1), 495(2), 534(12), 547(0), 558(0), 568(14), 593(87), 613(61), 629(227), 634(67), 660(85), 2055(443), 2057(337), 2073(670), 2078(1971), 2084(382), 2088(2017), 2140(145)	25(0), 50(0), 53(0), 68(0), 78(0), 79(0), 84(0), 96(0), 97(0), 99(0), 109(0), 114(0), 118(0), 126(0), 157(0), 196(0), 259(0), 286(19), 389(2), 392(0), 403(0), 410(4), 417(4), 419(0), 421(0), 432(2), 448(2), 471(26), 474(2), 480(0), 489(13), 499(2), 527(2), 530(0), 539(0), 560(15), 589(118), 604(61), 623(170), 624(61), 651(73), 1971(184), 1971(393), 1992(1678), 1994(538), 2000(297), 2004(1858), 2055(153)

Table S53. Harmonic vibrational frequencies(cm^{-1}) and IR intensities (KM/Mole) of $\text{Mn}_2(\text{CO})_5(\text{PCO})_2$ **25-2S(C_s)**.

B3LYP	BP86
9(0), 29(0), 43(1), 57(1), 75(0), 79(0), 90(0), 91(0), 99(0), 102(0), 107(1), 122(1), 132(2), 135(1), 152(0), 223(3), 225(0), 284(0), 288(1), 392(1), 398(3), 402(0), 412(3), 412(1), 424(1), 446(1), 457(8), 466(5), 474(21), 484(11), 500(34), 500(26), 524(2), 538(2), 573(7), 573(0), 599(67), 609(1), 627(77), 645(78), 664(166), 1983(343), 2029(727), 2066(1516), 2073(1343), 2084(938), 2093(393), 2145(784)	13(0), 26(0), 41(1), 55(1), 73(0), 74(0), 87(0), 89(0), 93(0), 95(0), 103(0), 116(0), 127(0), 132(2), 158(1), 240(0), 240(0), 289(0), 292(0), 394(1), 400(0), 411(0), 414(0), 422(2), 429(2), 444(0), 461(3), 471(3), 489(6), 491(12), 493(9), 502(12), 508(1), 521(3), 559(0), 574(11), 605(66), 605(0), 621(74), 636(79), 662(146), 1921(245), 1943(551), 1976(1225), 1981(617), 1992(1489), 2002(289), 2056(639)

Table S54. Harmonic vibrational frequencies(cm^{-1}) and IR intensities (KM/Mole) of $\text{Mn}_2(\text{CO})_5(\text{PCO})_2$ **25-1T(C₁)**.

B3LYP	BP86
24(0), 39(0), 47(0), 61(0), 68(1), 78(0), 84(0), 89(0), 91(0), 100(0), 102(0), 112(0), 128(0), 140(1), 156(1), 196(1), 215(0), 272(3), 276(2), 338(2), 350(15), 374(11), 388(8), 406(3), 407(3), 423(1), 426(1), 455(9), 465(10), 469(11), 475(10), 495(11), 505(22), 513(44), 521(9), 535(17), 575(5), 599(7), 608(75), 629(66), 662(204), 1988(404), 2038(345), 2063(1381), 2066(1523), 2078(1674), 2079(588), 2135(617)	20(0), 30(0), 36(0), 55(0), 65(0), 73(0), 78(0), 85(0), 88(0), 99(0), 103(0), 109(0), 123(0), 133(0), 156(0), 201(0), 237(1), 277(1), 286(0), 359(0), 364(1), 396(1), 402(1), 408(0), 422(2), 425(14), 430(1), 470(5), 479(3), 482(1), 485(2), 504(3), 505(4), 543(24), 555(11), 556(17), 558(11), 587(28), 602(72), 615(60), 653(170), 1930(272), 1949(433), 1975(1196), 1976(1275), 1988(1264), 1995(249), 2049(630)

Table S55. Harmonic vibrational frequencies(cm^{-1}) and IR intensities (KM/Mole) of $\text{Mn}_2(\text{CO})_5(\text{PCO})_2$ **25-3S(C_s)**.

B3LYP	BP86
19(0), 22(0), 61(1), 66(0), 73(0), 73(0), 80(0), 94(0), 98(0), 101(0), 109(0), 110(0), 117(0), 141(0), 147(0), 190(0), 255(1), 292(1), 296(3), 396(0), 402(1), 406(3), 438(6), 446(0), 448(1), 454(6), 456(4), 470(0), 471(2), 495(3), 522(53), 523(1), 531(17), 537(8), 581(15), 602(65), 608(2), 616(90), 633(7), 643(233), 660(1), 2035(178), 2046(1), 2051(103), 2056(1266), 2071(2143), 2083(2541), 2125(102)	8(0), 19(0), 54(1), 62(0), 68(0), 70(0), 77(0), 92(0), 95(0), 97(0), 104(0), 105(0), 114(0), 133(0), 140(1), 193(0), 258(3), 308(0), 309(0), 389(0), 397(1), 412(0), 435(1), 446(0), 448(1), 453(1), 455(0), 458(6), 465(5), 481(0), 531(1), 533(10), 536(0), 537(14), 581(22), 593(66), 603(8), 614(77), 630(5), 633(181), 654(1), 1952(473), 1957(0), 1965(37), 1968(1058), 1992(1429), 2000(2055), 2035(90)

Table S56. Harmonic vibrational frequencies(cm^{-1}) and IR intensities (KM/Mole) of $\text{Mn}(\text{CO})_5(\text{PCO})$ **15-1S(C_s)**.

B3LYP	BP86
10(0), 65(0), 71(0), 73(0), 91(0), 95(0), 97(0), 100(0), 114(1), 114(1), 122(0), 238(0), 365(0), 389(2), 400(0), 405(1), 416(1), 441(22), 452(24), 456(0), 469(3), 499(6), 510(4), 546(0), 559(0), 564(0), 661(126), 662(125), 671(233), 754(11), 1992(842), 2079(762), 2098(1434), 2101(1334), 2114(22), 2172(150)	16(0), 58(0), 64(0), 68(0), 86(1), 92(0), 94(0), 94(0), 109(1), 110(1), 118(0), 243(0), 371(0), 396(0), 414(0), 419(0), 427(0), 433(0), 459(13), 470(10), 480(8), 487(9), 489(1), 531(0), 548(0), 555(0), 664(119), 664(115), 675(212), 736(6), 1936(589), 1994(670), 2007(1352), 2008(1217), 2028(10), 2089(115)

Table S57. Harmonic vibrational frequencies(cm^{-1}) and IR intensities (KM/Mole) of $\text{Mn}(\text{CO})_5(\text{PCO})$ **15-2S(C_s)**.

B3LYP	BP86
6(0), 54(1), 69(0), 78(0), 86(0), 92(0), 93(0), 95(0), 106(1), 134(2), 137(2), 310(20), 347(0), 366(2), 374(0), 389(5), 403(34), 405(29), 409(1), 447(2), 449(0), 508(7), 533(1), 541(0), 544(1), 552(5), 646(109), 652(101), 655(152), 870(21), 1708(576), 2083(798), 2127(1266), 2128(1165), 2147(64), 2195(141)	14(0), 52(0), 62(0), 75(0), 81(0), 88(0), 91(0), 91(0), 99(1), 127(1), 128(1), 264(3), 357(0), 395(1), 402(0), 404(0), 409(2), 417(6), 436(20), 440(21), 472(1), 494(25), 512(1), 533(0), 535(0), 542(3), 652(106), 658(103), 663(192), 832(1), 1641(72), 1993(634), 2022(1238), 2024(1135), 2047(24), 2097(312)

Table S58. Harmonic vibrational frequencies(cm^{-1}) and IR intensities (KM/Mole) of $\text{Mn}(\text{CO})_4(\text{PCO})$ **14-1S**(C_s).

B3LYP	BP86
28(0), 58(0), 75(0), 89(0), 92(0), 93(1), 103(0), 115(0), 119(0), 287(22), 378(0), 394(1), 401(2), 420(6), 459(0), 475(0), 479(10), 482(30), 512(12), 554(5), 568(0), 615(52), 633(78), 681(100), 703(28), 2016(890), 2059(1033), 2074(520), 2079(1710), 2146(215)	29(0), 58(0), 70(0), 86(0), 86(0), 89(0), 100(0), 109(0), 114(0), 300(9), 379(0), 398(0), 425(1), 430(2), 456(0), 479(1), 482(2), 497(3), 504(31), 546(5), 558(0), 625(46), 630(75), 684(89), 686(5), 1951(386), 1969(910), 1981(1071), 1988(1119), 2058(163)

Table S59. Harmonic vibrational frequencies(cm^{-1}) and IR intensities (KM/Mole) of $\text{Mn}(\text{CO})_4(\text{PCO})$ **14-2S**(C_s).

B3LYP	BP86
21(1), 50(0), 77(0), 79(0), 88(0), 96(0), 105(0), 121(4), 157(1), 334(39), 354(0), 366(5), 389(0), 394(40), 419(5), 459(2), 465(3), 470(5), 511(16), 547(0), 565(0), 602(52), 628(55), 677(71), 904(47), 1683(168), 2059(1043), 2084(652), 2114(1303), 2166(379)	23(0), 46(0), 73(0), 75(0), 87(0), 94(1), 103(0), 125(2), 156(0), 321(13), 361(0), 393(0), 403(5), 416(1), 436(30), 446(2), 473(6), 489(2), 498(20), 540(3), 558(0), 624(43), 627(52), 685(70), 874(21), 1651(35), 1968(919), 1989(372), 1999(1280), 2068(429)

Table S60. Harmonic vibrational frequencies(cm^{-1}) and IR intensities (KM/Mole) of $\text{Mn}(\text{CO})_3(\text{PCO})$ **13-1S**(C_s).

B3LYP	BP86
39(0), 86(0), 86(0), 102(0), 108(0), 112(1), 227(0), 255(9), 387(0), 429(0), 439(2), 442(1), 449(2), 488(24), 523(26), 571(2), 609(21), 615(48), 687(49), 803(0), 1782(318), 2056(857), 2060(1033), 2119(651)	38(0), 85(0), 85(0), 100(0), 107(0), 107(1), 222(1), 266(2), 395(1), 412(1), 436(0), 451(4), 474(3), 518(11), 533(9), 557(0), 614(21), 624(49), 692(41), 767(1), 1742(266), 1962(907), 1964(715), 2027(492)

Table S61. Harmonic vibrational frequencies(cm^{-1}) and IR intensities (KM/Mole) of $\text{Mn}(\text{CO})_3(\text{PCO})$ **13-2S**(C_{3v}).

B3LYP	BP86
23(0), 23(0), 91(0), 91(0), 102(0), 161(3), 161(3), 324(49), 382(0), 393(0), 393(0), 471(0), 471(0), 480(13), 500(24), 500(24), 623(21), 623(21), 689(26), 971(167), 1708(298), 2053(1037), 2053(1038), 2116(913)	26(0), 26(0), 91(0), 91(0), 102(0), 162(2), 162(2), 327(21), 394(0), 395(1), 395(1), 469(1), 469(1), 512(31), 524(10), 524(10), 631(19), 631(19), 695(17), 941(97), 1669(69), 1951(885), 1951(885), 2021(675)

Table S62. Harmonic vibrational frequencies(cm^{-1}) and IR intensities (KM/Mole) of $\text{Mn}(\text{CO})_3(\text{PCO})$ **13-1T(C_s)**.

B3LYP	BP86
36(0), 50(0), 56(1), 92(0), 97(2), 104(0), 116(0), 265(20), 317(1), 341(0), 395(2), 399(5), 413(2), 467(58), 473(0), 504(6), 534(41), 562(7), 608(76), 724(28), 2000(607), 2045(2318), 2081(571), 2141(433)	34(0), 49(0), 55(1), 83(0), 93(2), 95(0), 110(0), 281(13), 329(1), 336(0), 401(1), 423(3), 438(4), 446(0), 484(27), 488(4), 542(55), 563(4), 611(46), 698(20), 1934(537), 1958(1900), 1982(878), 2039(250)

Complete Gaussian 09 reference (Reference 21)

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