

Manganese Carbonyl Fluorides: Are They Viable Molecules?

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Supporting Information

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Tables S7 to S12. Coordinates of $\text{Mn}_2(\text{CO})_n\text{F}_2$ ($n = 8, 7, 6$).

Tables S13 to S18 Harmonic vibrational frequencies (cm^{-1}) and IR intensities (km/mol) of $\text{Mn}(\text{CO})_n\text{F}$ ($n = 5, 4, 3$).

Tables S19 to S24 Harmonic vibrational frequencies (cm^{-1}) and IR intensities (km/mol) of $\text{Mn}_2(\text{CO})_n\text{F}_2$ ($n = 8, 7, 6$).

Complete Gaussian 03 reference (Reference 24)

Table S1 Coordinates of Mn(CO)₅F **15-1S** (C_{4v})

B3LYP/DZP				BP86/DZP		
Mn	0.000000	0.000000	0.037214	0.000000	0.000000	0.060220
C	0.000000	1.884706	0.191839	0.000000	1.861388	0.188142
C	0.000000	0.000000	-1.801901	0.000000	0.000000	-1.757289
C	0.000000	-1.884706	0.191839	0.000000	-1.861388	0.188142
C	1.884706	0.000000	0.191839	1.861388	0.000000	0.188142
C	-1.884706	0.000000	0.191839	-1.861388	0.000000	0.188142
F	0.000000	0.000000	1.992575	0.000000	0.000000	2.023917
O	3.021648	0.000000	0.344258	3.017412	0.000000	0.304661
O	0.000000	0.000000	-2.959063	0.000000	0.000000	-2.930198
O	0.000000	-3.021648	0.344258	0.000000	-3.017412	0.304661
O	-3.021648	0.000000	0.344258	-3.017412	0.000000	0.304661
O	0.000000	3.021648	0.344258	0.000000	3.017412	0.304661

Table S2 Coordinates of Mn(CO)₄F **14-1S** (C_{2v})

B3LYP/DZP				BP86/DZP		
Mn	0.000000	0.000000	0.297870	0.000000	0.000000	0.339612
F	0.000000	0.000000	2.131658	0.000000	0.000000	2.166363
C	0.000000	1.901057	0.409049	0.000000	1.876299	0.385078
C	-1.297095	0.000000	-0.976134	-1.261226	0.000000	-0.931270
C	0.000000	-1.901057	0.409049	0.000000	-1.876299	0.385078
C	1.297095	0.000000	-0.976134	1.261226	0.000000	-0.931270
O	2.181078	0.000000	-1.723655	2.143731	0.000000	-1.705753
O	-2.181078	0.000000	-1.723655	-2.143731	0.000000	-1.705753
O	0.000000	3.045132	0.484490	0.000000	3.038696	0.366174
O	0.000000	-3.045132	0.484490	0.000000	-3.038696	0.366174

Table S3 Coordinates of Mn(CO)₄F **14-2T** (C_{4v})

B3LYP/DZP				BP86/DZP		
Mn	0.000000	0.000000	0.328195	0.000000	0.000000	0.400265
C	0.000000	1.807535	-0.295177	0.000000	1.738139	-0.276586
C	1.807535	0.000000	-0.295177	1.738139	0.000000	-0.276586
C	0.000000	-1.807535	-0.295177	0.000000	-1.738139	-0.276586
C	-1.807535	0.000000	-0.295177	-1.738139	0.000000	-0.276586
O	0.000000	2.906980	-0.638942	0.000000	2.816764	-0.726580
O	2.906980	0.000000	-0.638942	2.816764	0.000000	-0.726580
O	0.000000	-2.906980	-0.638942	0.000000	-2.816764	-0.726580
O	-2.906980	0.000000	-0.638942	-2.816764	0.000000	-0.726580
F	0.000000	0.000000	2.147278	0.000000	0.000000	2.209109

Table S4 Coordinates of Mn(CO)₃F **13-1S** (C_{3v})

B3LYP/DZP				BP86/DZP		
Mn	0.000000	0.000000	0.548870	0.000000	0.000000	0.567753
C	0.000000	1.484687	-0.477301	0.000000	1.434962	-0.469815
C	1.285777	-0.742343	-0.477301	1.242714	-0.717481	-0.469815
C	-1.285777	-0.742343	-0.477301	-1.242714	-0.717481	-0.469815
F	0.000000	0.000000	2.308358	0.000000	0.000000	2.317928
O	2.141626	-1.236468	-1.079398	2.097263	-1.210855	-1.108271
O	0.000000	2.472937	-1.079398	0.000000	2.421711	-1.108271
O	-2.141626	-1.236468	-1.079398	-2.097263	-1.210855	-1.108271

Table S5 Coordinates of Mn(CO)₃F **13-2T** (C_s)

B3LYP/DZP				BP86/DZP		
Mn	0.292294	-0.342280	0.000000	-0.282878	0.417026	0.000000
F	1.918821	-1.105555	0.000000	-1.719519	1.475685	0.000000
C	0.238062	0.462828	1.763528	-0.273436	-0.429288	1.671917
C	-1.568406	-0.213985	0.000000	1.495793	-0.006553	0.000000
C	0.238062	0.462828	-1.763528	-0.273436	-0.429288	-1.671917
O	0.238062	0.982390	2.789066	-0.273436	-1.052356	2.660658
O	0.238062	0.982390	-2.789066	-0.273436	-1.052356	-2.660658
O	-2.729005	-0.185158	0.000000	2.653634	-0.209790	0.000000

Table S6 Coordinates of Mn(CO)₃F **13-3T** (C_{2v})

B3LYP/DZP				BP86/DZP		
Mn	0.000000	0.000000	0.191784	0.000000	0.000000	0.229596
F	0.000000	0.000000	2.032908	0.000000	0.000000	2.059385
C	0.000000	1.904027	0.313967	0.000000	1.878659	0.286085
C	0.000000	0.000000	-1.735080	0.000000	0.000000	-1.657273
C	0.000000	-1.904027	0.313967	0.000000	-1.878659	0.286085
O	0.000000	3.050459	0.416042	0.000000	3.045464	0.302923
O	0.000000	-3.050459	0.416042	0.000000	-3.045464	0.302923
O	0.000000	0.000000	-2.888072	0.000000	0.000000	-2.826314

Table S7 Coordinates of $\text{Mn}_2(\text{CO})_8\text{F}_2$ **28-1S** (D_{2h})

B3LYP/DZP				BP86/DZP		
F	0.000000	0.000000	1.248186	0.000000	0.000000	1.252975
F	0.000000	0.000000	-1.248186	0.000000	0.000000	-1.252975
Mn	1.593016	0.000000	0.000000	1.582157	0.000000	0.000000
Mn	-1.593016	0.000000	0.000000	-1.582157	0.000000	0.000000
C	-2.835938	0.000000	-1.342675	-2.822484	0.000000	-1.305402
C	-2.835938	0.000000	1.342675	-2.822484	0.000000	1.305402
C	-1.616468	1.897941	0.000000	-1.653492	1.870334	0.000000
C	-1.616468	-1.897941	0.000000	-1.653492	-1.870334	0.000000
C	1.616468	1.897941	0.000000	1.653492	1.870334	0.000000
C	1.616468	-1.897941	0.000000	1.653492	-1.870334	0.000000
C	2.835938	0.000000	-1.342675	2.822484	0.000000	-1.305402
C	2.835938	0.000000	1.342675	2.822484	0.000000	1.305402
O	-1.703808	3.043597	0.000000	-1.809512	3.024481	0.000000
O	-3.596011	0.000000	-2.213276	-3.616318	0.000000	-2.167270
O	-3.596011	0.000000	2.213276	-3.616318	0.000000	2.167270
O	1.703808	3.043597	0.000000	1.809512	3.024481	0.000000
O	3.596011	0.000000	-2.213276	3.616318	0.000000	-2.167270
O	3.596011	0.000000	2.213276	3.616318	0.000000	2.167270
O	1.703808	-3.043597	0.000000	1.809512	-3.024481	0.000000
O	-1.703808	-3.043597	0.000000	-1.809512	-3.024481	0.000000

Table S8 Coordinates of $\text{Mn}_2(\text{CO})_7\text{F}_2$ **27-1S** (C_s)

B3LYP/DZP				BP86/DZP		
C	-1.493845	2.271466	0.000000	-1.431556	2.306403	0.000000
C	1.931038	-1.640975	0.000000	1.893636	-1.728902	0.000000
F	0.187926	0.113942	1.222055	0.232054	0.125056	1.220143
O	-2.593869	2.636476	0.000000	-2.532649	2.722234	0.000000
O	3.074278	-1.746517	0.000000	3.036014	-1.949890	0.000000
C	-0.074630	-2.746313	-1.336764	-0.103585	-2.722125	-1.299560
O	-0.143234	-3.507817	-2.202869	-0.194959	-3.512201	-2.159440
F	0.187926	0.113942	-1.222055	0.232054	0.125056	-1.220143
C	-0.074630	-2.746313	1.336764	-0.103585	-2.722125	1.299560
O	-0.143234	-3.507817	2.202869	-0.194959	-3.512201	2.159440
Mn	0.181890	1.643722	0.000000	0.193786	1.645324	0.000000
C	0.642354	2.814573	-1.321339	0.628584	2.823350	-1.276627
C	0.642354	2.814573	1.321339	0.628584	2.823350	1.276627
O	0.956910	3.534717	-2.169841	0.935306	3.586961	-2.113706
O	0.956910	3.534717	2.169841	0.935306	3.586961	2.113706
Mn	0.036929	-1.502078	0.000000	0.038004	-1.485682	0.000000
C	-1.856449	-1.311385	0.000000	-1.829373	-1.315534	0.000000
O	-3.001550	-1.234486	0.000000	-2.992552	-1.300433	0.000000

Table S9 Coordinates of $\text{Mn}_2(\text{CO})_7\text{F}_2$ **27-2S** (C_s)

B3LYP/DZP				BP86/DZP		
C	-0.141190	1.341872	1.898799	-0.117069	-1.374027	1.872273
F	1.131828	-0.250159	0.000000	-1.060005	0.477457	0.000000
O	-0.142070	1.417332	3.045042	-0.138134	-1.516044	3.027360
C	-1.488135	2.567102	0.000000	0.927575	-2.786068	0.000000
O	-2.360625	3.324900	0.000000	1.617883	-3.732396	0.000000
F	-1.415658	-0.266465	0.000000	1.462570	-0.017796	0.000000
C	1.193774	2.577780	0.000000	-1.626247	-2.282643	0.000000
O	2.057890	3.344936	0.000000	-2.620560	-2.902025	0.000000
Mn	-0.141226	1.328645	0.000000	-0.109977	-1.315118	0.000000
C	-0.141190	1.341872	-1.898799	-0.117069	-1.374027	-1.872273
O	-0.142070	1.417332	-3.045042	-0.138134	-1.516044	-3.027360
Mn	-0.132160	-1.787836	0.000000	0.472557	1.697438	0.000000
C	-0.141190	-1.898199	1.896029	0.482972	1.877380	1.857628
C	-0.141190	-1.898199	-1.896029	0.482972	1.877380	-1.857628
C	1.061822	-3.153135	0.000000	-0.406435	3.248273	0.000000
O	-0.118964	-2.069489	3.034673	0.482972	2.147462	2.995486
O	-0.118964	-2.069489	-3.034673	0.482972	2.147462	-2.995486
O	1.846416	-4.008667	0.000000	-0.992974	4.270016	0.000000

Table S10 Coordinates of $\text{Mn}_2(\text{CO})_7\text{F}_2$ **27-3T** (C_{2v})

B3LYP/DZP				BP86/DZP		
C	0.000000	1.897917	-1.413394	0.000000	1.870514	-1.440703
F	1.269880	0.000000	0.194557	1.272655	0.000000	0.212009
O	0.000000	3.043027	-1.508282	0.000000	3.022883	-1.608513
C	-1.344444	0.000000	-2.624909	-1.307838	0.000000	-2.597515
O	-2.217285	0.000000	-3.382837	-2.172016	0.000000	-3.388975
F	-1.269880	0.000000	0.194557	-1.272655	0.000000	0.212009
C	1.344444	0.000000	-2.624909	1.307838	0.000000	-2.597515
O	2.217285	0.000000	-3.382837	2.172016	0.000000	-3.388975
Mn	0.000000	0.000000	-1.386218	0.000000	0.000000	-1.361834
C	0.000000	-1.897917	-1.413394	0.000000	-1.870514	-1.440703
O	0.000000	-3.043027	-1.508282	0.000000	-3.022883	-1.608513
Mn	0.000000	0.000000	1.798407	0.000000	0.000000	1.783815
C	0.000000	1.899884	1.815224	0.000000	1.869304	1.846828
C	0.000000	-1.899884	1.815224	0.000000	-1.869304	1.846828
C	0.000000	0.000000	3.707300	0.000000	0.000000	3.647389
O	0.000000	3.050733	1.875013	0.000000	3.031896	1.966763
O	0.000000	-3.050733	1.875013	0.000000	-3.031896	1.966763
O	0.000000	0.000000	4.860502	0.000000	0.000000	4.817280

Table S11 Coordinates of $\text{Mn}_2(\text{CO})_6\text{F}_2$ **26-1S** (C_{2v})

B3LYP/DZP				BP86/DZP		
C	0.000000	1.996453	1.487974	0.000000	2.005991	1.436748
C	0.000000	-1.996453	1.487974	0.000000	-2.005991	1.436748
F	1.202170	0.000000	-0.392707	1.201084	0.000000	-0.452351
O	0.000000	-2.243922	2.618824	0.000000	-2.291678	2.577057
O	0.000000	2.243922	2.618824	0.000000	2.291678	2.577057
C	-1.319978	-2.766129	-0.584482	-1.275112	-2.763607	-0.548696
O	-2.166493	-3.517557	-0.818905	-2.111189	-3.559052	-0.759863
F	-1.202170	0.000000	-0.392707	-1.201084	0.000000	-0.452351
Mn	0.000000	-1.551248	-0.249112	0.000000	-1.541935	-0.256945
C	1.319978	-2.766129	-0.584482	1.275112	-2.763607	-0.548696
O	2.166493	-3.517557	-0.818905	2.111189	-3.559052	-0.759863
Mn	0.000000	1.551248	-0.249112	0.000000	1.541935	-0.256945
C	-1.319978	2.766129	-0.584482	-1.275112	2.763607	-0.548696
C	1.319978	2.766129	-0.584482	1.275112	2.763607	-0.548696
O	-2.166493	3.517557	-0.818905	-2.111189	3.559052	-0.759863
O	2.166493	3.517557	-0.818905	2.111189	3.559052	-0.759863

Table S12 Coordinates of $\text{Mn}_2(\text{CO})_6\text{F}_2$ **26-2T** (C_{2v})

B3LYP/DZP				BP86/DZP		
C	0.000000	1.337069	-2.578270	0.000000	1.299318	-2.548400
O	0.000000	2.202730	-3.343227	0.000000	2.158515	-3.344520
C	0.000000	-1.337069	-2.578270	0.000000	-1.299318	-2.548400
O	0.000000	-2.202730	-3.343227	0.000000	-2.158515	-3.344520
F	0.000000	1.234025	0.290743	0.000000	1.235662	0.311779
F	0.000000	-1.234025	0.290743	0.000000	-1.235662	0.311779
Mn	0.000000	0.000000	1.796183	0.000000	0.000000	1.810044
C	-1.900509	0.000000	-1.295864	-1.873003	0.000000	-1.329855
O	-3.048496	0.000000	-1.299616	-3.033124	0.000000	-1.420026
Mn	0.000000	0.000000	-1.328871	0.000000	0.000000	-1.303279
C	1.900509	0.000000	-1.295864	1.873003	0.000000	-1.329855
O	3.048496	0.000000	-1.299616	3.033124	0.000000	-1.420026
C	0.000000	1.226235	3.188613	0.000000	1.175023	3.194239
C	0.000000	-1.226235	3.188613	0.000000	-1.175023	3.194239
O	0.000000	-1.944846	4.099723	0.000000	-1.882453	4.134987
O	0.000000	1.944846	4.099723	0.000000	1.882453	4.134987

Table S13 Harmonic vibrational frequencies(cm^{-1}) and IR intensities (KM/Mole) of $\text{Mn}(\text{CO})_5\text{F}$ **15-1S** (C_{4v})

B3LYP/SDD	BP86/SDD
53(0), 81(0), 81(0), 94(0), 94(0), 94(0), 100(0), 141(2), 141(2), 351(0), 370(4), 381(0), 401(41), 401(41), 423(1), 423(1), 429(27), 521(0), 527(45), 547(0), 557(3), 557(3), 657(126), 657(126), 669(73), 2067(861), 2119(1367), 2119(1367), 2139(0), 2198(0)	44(0), 78(0), 78(0), 88(0), 88(0), 92(0), 94(0), 134(1), 134(1), 359(0), 403(7), 412(0), 420(3), 420(3), 430(28), 430(28), 447(19), 516(0), 521(28), 538(0), 552(2), 552(2), 666(123), 666(123), 676(74), 1981(740), 2023(1298), 2023(1298), 2050(0), 2112(0)

Table S14 Harmonic vibrational frequencies(cm^{-1}) and IR intensities (KM/Mole) of $\text{Mn}(\text{CO})_4\text{F}$ **14-1S** (C_{2v})

B3LYP/SDD	BP86/SDD
58(5), 72(0), 83(2), 86(0), 93(1), 106(0), 172(1), 343(0), 362(4), 372(59), 393(0), 434(13), 441(4), 476(4), 551(41), 560(0), 590(61), 596(47), 631(53), 705(5), 2053(1079), 2079(530), 2119(1386), 2182(3)	60(2), 68(0), 85(0), 85(4), 92(1), 105(0), 172(0), 349(0), 395(4), 402(46), 405(0), 445(12), 471(6), 499(1), 553(32), 556(0), 588(52), 620(34), 636(51), 716(5), 1966(916), 1987(418), 2010(1340), 2088(9)

Table S15 Harmonic vibrational frequencies(cm^{-1}) and IR intensities (KM/Mole) of $\text{Mn}(\text{CO})_4\text{F}$ **14-2T** (C_{4v})

B3LYP/SDD	BP86/SDD
-34(0), 78(1), 78(1), 89(0), 94(0), 113(3), 113(3), 267(0), 337(0), 357(2), 358(71), 358(71), 380(0), 380(0), 381(0), 498(68), 526(0), 555(25), 555(25), 650(41), 2055(1938), 2055(1938), 2085(0), 2155(83)	16(0), 83(0), 83(0), 92(0), 95(0), 114(3), 114(3), 314(0), 355(0), 376(1), 376(1), 411(1), 416(0), 422(31), 422(31), 519(0), 525(78), 570(35), 570(35), 675(13), 1967(1468), 1967(1468), 1986(0), 2058(109)

Table S16 Harmonic vibrational frequencies(cm^{-1}) and IR intensities (KM/Mole) of $\text{Mn}(\text{CO})_3\text{F}$ **13-1S** (C_{3v})

B3LYP/SDD	BP86/SDD
62(6), 62(6), 95(2), 95(2), 109(0), 386(0), 390(0), 390(0), 436(6), 494(19), 494(19), 624(101), 638(18), 638(18), 759(21), 2054(1069), 2054(1070), 2126(238)	69(4), 69(4), 96(2), 96(2), 110(0), 402(0), 402(0), 403(0), 485(2), 533(7), 533(7), 628(82), 652(16), 652(16), 771(22), 1958(898), 1958(898), 2034(177)

Table S17 Harmonic vibrational frequencies(cm^{-1}) and IR intensities (KM/Mole) of $\text{Mn}(\text{CO})_3\text{F}$ **13-2T** (C_s)

B3LYP/SDD	BP86/SDD
52(0), 77(3), 80(0), 89(18), 131(5), 289(6), 336(86), 341(9), 354(6), 379(2), 398(4), 441(15), 516(39), 570(6), 656(65), 2012(1092), 2070(1825), 2148(131)	60(0), 84(7), 85(1), 86(7), 131(3), 298(1), 385(5), 397(9), 397(57), 402(3), 410(2), 487(6), 538(44), 582(11), 675(49), 1940(765), 1954(1458), 2035(141)

Table S18 Harmonic vibrational frequencies(cm^{-1}) and IR intensities (KM/Mole) of $\text{Mn}(\text{CO})_3\text{F}$ **13-3T** (C_{2v})

B3LYP/SDD	BP86/SDD
58(3), 66(2), 79(0), 104(10), 158(1), 304(0), 351(0), 365(1), 377(114), 388(21), 425(6), 525(16), 547(6), 562(86), 638(10), 2069(2135), 2076(780), 2161(29)	56(2), 59(1), 76(0), 104(7), 158(1), 302(0), 357(0), 395(2), 401(74), 418(12), 430(20), 530(18), 557(4), 566(78), 646(5), 1970(1844), 1983(601), 2066(26)

Table S19 Harmonic vibrational frequencies(cm^{-1}) and IR intensities (KM/Mole) of $\text{Mn}_2(\text{CO})_8\text{F}_2$ **28-1S** (D_{2h})

B3LYP/SDD	BP86/SDD
28(0), 50(0), 52(0), 55(0), 69(0), 73(0), 80(0), 86(0), 87(0), 88(0), 90(0), 101(2), 102(0), 115(0), 117(0), 162(0), 177(0), 192(0), 330(40), 366(1), 368(0), 370(0), 375(0), 380(0), 386(100), 395(0), 401(0), 411(0), 413(121), 421(6), 459(10), 459(0), 461(0), 464(0), 477(2), 481(132), 553(19), 560(0), 579(0), 581(0), 619(0), 627(97), 638(0), 640(101), 688(44), 691(0), 2061(0), 2064(1950), 2081(0), 2082(1009), 2090(0), 2108(2472), 2160(248), 2178(0)	30(0), 37(0), 50(0), 54(0), 69(0), 76(0), 79(0), 83(0), 86(0), 87(0), 87(0), 100(2), 103(0), 115(0), 117(0), 161(0), 173(0), 191(0), 331(26), 373(0), 386(0), 397(0), 400(0), 401(2), 406(0), 411(0), 415(0), 415(34), 421(48), 435(141), 467(0), 472(0), 487(0), 490(0), 494(59), 495(3), 556(28), 560(0), 574(0), 576(0), 632(0), 639(82), 643(0), 643(97), 702(39), 706(0), 1974(0), 1977(1669), 1980(0), 1993(757), 2000(0), 2005(2273), 2072(316), 2089(0)

Table S20 Harmonic vibrational frequencies(cm^{-1}) and IR intensities (KM/Mole) of $\text{Mn}_2(\text{CO})_7\text{F}_2$ **27-1S** (C_s)

B3LYP/SDD	BP86/SDD
21(0), 32(0), 52(0), 71(0), 72(0), 76(0), 84(0), 87(0), 91(0), 93(1), 104(0), 112(0), 116(0), 136(0), 172(2), 203(1), 335(36), 365(1), 377(7), 379(56), 385(0), 398(1), 410(19), 415(75), 422(2), 434(3), 457(9), 463(0), 469(1), 470(13), 494(26), 509(7), 511(164), 555(13), 576(0), 620(40), 631(21), 636(1), 639(73), 685(19), 704(6), 2044(659), 2055(642), 2066(1291), 2090(599), 2106(1557), 2125(417), 2176(45)	20(0), 29(0), 52(0), 71(0), 72(0), 77(0), 85(0), 87(0), 90(0), 94(1), 105(0), 112(0), 117(0), 135(0), 170(1), 204(1), 334(22), 380(6), 391(1), 400(1), 410(0), 412(11), 416(38), 432(16), 442(11), 450(92), 467(1), 483(0), 490(1), 493(21), 518(68), 531(6), 541(22), 557(24), 573(0), 633(22), 640(30), 644(41), 651(25), 702(18), 720(5), 1952(519), 1961(684), 1978(954), 2001(461), 2004(1417), 2035(426), 2087(79)

Table S21 Harmonic vibrational frequencies(cm^{-1}) and IR intensities (KM/Mole) of $\text{Mn}_2(\text{CO})_7\text{F}_2$ **27-2S** (C_s)

B3LYP/SDD	BP86/SDD
32(0), 51(0), 52(0), 54(0), 72(0), 75(0), 84(0), 86(0), 87(0), 96(0), 97(2), 112(0), 117(0), 158(0), 176(0), 185(1), 336(36), 362(19), 366(1), 369(3), 372(5), 379(29), 385(99), 389(12), 397(53), 400(2), 416(5), 431(85), 460(6), 463(22), 468(25), 489(5), 502(49), 556(10), 579(0), 605(1), 621(25), 625(18), 626(42), 639(55), 687(25), 2042(812), 2060(566), 2063(1024), 2087(433), 2102(2162), 2143(187), 2174(43)	32(0), 37(0), 53(0), 55(0), 73(0), 79(0), 79(0), 85(0), 87(0), 97(0), 97(1), 114(0), 117(0), 163(0), 177(0), 178(2), 334(23), 367(3), 386(26), 393(1), 394(40), 402(10), 402(1), 407(1), 411(1), 413(7), 421(92), 444(79), 471(0), 489(6), 492(11), 505(3), 521(14), 555(14), 575(0), 622(0), 625(21), 632(19), 640(36), 644(51), 700(31), 1948(738), 1952(582), 1978(853), 2000(354), 2001(1711), 2042(284), 2085(86)

Table S22 Harmonic vibrational frequencies(cm^{-1}) and IR intensities (KM/Mole) of $\text{Mn}_2(\text{CO})_7\text{F}_2$ **27-3T** (C_{2v})

B3LYP/SDD	BP86/SDD
20(0), 29(0), 46(1), 52(0), 68(1), 72(0), 81(2), 82(0), 87(0), 91(0), 95(0), 105(0), 108(0), 151(0), 170(0), 171(4), 289(6), 329(37), 358(0), 361(46), 366(10), 366(5), 371(52), 373(22), 382(56), 386(53), 390(0), 394(81), 413(8), 458(5), 462(3), 468(1), 473(121), 527(8), 556(9), 575(6), 581(0), 613(14), 623(50), 640(49), 689(24), 2042(944), 2060(1003), 2069(1006), 2085(247), 2099(2112), 2145(255), 2172(32)	25(0), 32(0), 33(1), 52(0), 58(3), 73(0), 79(1), 80(0), 86(0), 87(0), 96(0), 107(0), 107(0), 152(0), 165(0), 170(3), 311(2), 332(31), 358(0), 368(1), 388(38), 390(12), 391(14), 394(0), 400(80), 402(52), 406(15), 412(2), 416(70), 470(0), 482(45), 492(1), 493(43), 518(11), 557(10), 576(0), 588(6), 627(10), 635(42), 643(47), 703(22), 1944(843), 1975(853), 1976(704), 1997(255), 1998(1844), 2050(262), 2084(73)

Table S23 Harmonic vibrational frequencies(cm^{-1}) and IR intensities (KM/Mole) of $\text{Mn}_2(\text{CO})_6\text{F}_2$ **26-1S** (C_{2v})

B3LYP/SDD	BP86/SDD
20(0), 30(0), 63(0), 75(0), 82(0), 84(0), 90(1), 93(0), 94(0), 100(0), 111(0), 120(0), 159(7), 220(1), 348(47), 371(0), 395(0), 396(0), 413(88), 426(5), 427(1), 440(0), 458(12), 466(0), 487(1), 491(16), 492(0), 493(16), 519(12), 520(239), 627(0), 633(23), 636(0), 637(36), 702(13), 703(1), 2047(178), 2057(0), 2059(1659), 2061(1928), 2123(807), 2139(17)	19(0), 25(0), 64(0), 76(0), 84(0), 86(0), 86(0), 94(0), 95(0), 100(0), 112(0), 121(0), 143(5), 221(2), 352(30), 365(0), 408(0), 412(0), 436(0), 440(0), 449(139), 456(0), 479(2), 481(0), 513(7), 520(97), 521(0), 535(8), 539(12), 539(70), 637(0), 645(20), 650(0), 653(29), 721(10), 721(4), 1955(159), 1963(0), 1965(1370), 1966(1614), 2035(676), 2048(16)

Table S24 Harmonic vibrational frequencies(cm^{-1}) and IR intensities (KM/Mole) of $\text{Mn}_2(\text{CO})_6\text{F}_2$ **26-2T** (C_{2v})

B3LYP/SDD	BP86/SDD
26(0), 28(0), 52(0), 71(0), 76(0), 84(0), 85(3), 87(0), 97(0), 105(1), 116(0), 124(0), 163(4), 195(0), 337(43), 365(1), 372(0), 380(62), 386(0), 391(20), 411(1), 414(89), 419(26), 430(15), 434(2), 459(5), 464(0), 470(31), 504(13), 516(132), 556(14), 576(0), 620(53), 637(31), 638(57), 685(19), 1973(1410), 2066(1014), 2089(1137), 2096(101), 2105(1397), 2176(62)	22(0), 27(0), 51(0), 69(0), 74(0), 85(3), 86(0), 87(0), 100(0), 101(1), 116(0), 122(0), 158(2), 193(0), 338(23), 387(0), 392(0), 393(4), 400(2), 411(9), 415(42), 427(54), 443(1), 447(74), 457(15), 467(1), 489(0), 492(24), 523(15), 525(48), 557(28), 573(0), 634(44), 644(55), 652(13), 701(23), 1904(957), 1978(865), 2000(877), 2002(1307), 2005(156), 2086(102)

Complete Gaussian 03 reference (Reference 24)

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