Binuclear Hexafluorocyclopentadiene Iron Carbonyls: Bis(dihapto) Versus Trihapto-monohapto Bonding in Iron-Iron Bonded Structures

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Supporting Information

Tables S1 to S6. Coordinates of $(C_5F_6)Fe(CO)_n$ (n = 4, 3, 2).

Tables S7 to S22. Coordinates of $(C_5F_6)Fe_2(CO)_n$ (n = 8, 7, 6, 5).

Tables S23 to S28 Harmonic vibrational frequencies (cm^{-1}) and IR intensities (km/mol) of $(C_5F_6)Fe(CO)_n$ (n = 4, 3, 2).

Tables S29 to S44 Harmonic vibrational frequencies (cm^{-1}) and IR intensities (km/mol) of $(C_5F_6)Fe_2(CO)_n$ (n = 8, 7, 6, 5).

Tables S45 to S46 Total energies (E and E_{ZPVE}, in Hartree), relative energies with and without ZPVE corrections (ΔE and ΔE_{ZPVE} in kcal/mol), ΔH and ΔG (in kcal/mol) at the standard condition, number of imaginary vibrational frequencies (Nimag), and the LUMO-HOMO gaps (in eV) for mononuclear $(C_5F_6)Fe(CO)_n$ (n = 4, 3, 2) structures.

Tables S47 to S50 Total energies (E and E_{ZPVE}, in Hartree), relative energies with and without ZPVE corrections (ΔE and ΔE_{ZPVE} in kcal/mol), ΔH and ΔG (in kcal/mol) at the standard condition, number of imaginary vibrational frequencies (Nimag), and the LUMO-HOMO gaps (in eV), and Fe-Fe bond distances (in Å) for binuclear $(C_5F_6)Fe_2(CO)_n$ (n= 8, 7, 6, 5) structures.

Table 51. The ν(CO) frequencies of the mononuclear $(C_5F_6)Fe(CO)_n$ (n = 4, 3, 2) and binuclear $(C_5F_6)Fe_2(CO)_n$ (n = 8, 7, 6, 5) derivatives (with the BP86 method). Infrared intensities are given in parentheses in km/mol.

Complete Gaussian 03 reference (Reference 28)

Table S1 Coordinates of $(C_5F_6)Fe(CO)_4$ **14-1S** (C_1)

	B3LYP/DZP			BP86/DZP		
C	0.469920	-0.824981	-0.668247	0.479754	-0.823560	-0.697217
C	0.335175	0.563768	-1.078900	0.348123	0.577787	-1.093753
C	1.552339	1.265629	-0.606420	1.554637	1.284422	-0.591057
C	2.408855	0.413347	-0.019821	2.418263	0.416572	-0.004718
Fe	-1.121105	0.037591	0.263127	-1.121648	0.030014	0.257054
C	-1.796503	-1.340129	1.263958	-1.785771	-1.345959	1.233960
C	-2.176135	-0.509213	-1.156744	-2.186059	-0.492729	-1.128351
C	-0.191784	0.611696	1.741449	-0.219579	0.580091	1.732083
C	-2.150670	1.542797	0.395511	-2.126307	1.529620	0.397672
O	-2.190828	-2.231653	1.876134	-2.193325	-2.248689	1.850246
O	-2.775326	2.509213	0.449058	-2.755815	2.510368	0.464907
O	-2.889688	-0.837040	-1.991198	-2.935216	-0.816178	-1.956114
O	0.308768	0.992681	2.701950	0.266994	0.955527	2.721229
C	1.852425	-0.995338	-0.005082	1.863270	-0.999509	-0.014934
F	3.502206	0.719685	0.675545	3.502714	0.722365	0.718569
F	1.676827	2.588332	-0.673898	1.672380	2.617045	-0.631764
F	-0.057383	0.864828	-2.354995	-0.055257	0.906858	-2.364003
F	0.202248	-1.800487	-1.586413	0.215256	-1.795184	-1.626821
F	2.619713	-1.872774	-0.707325	2.642774	-1.871962	-0.734154
F	1.801233	-1.478298	1.277852	1.802550	-1.506786	1.268431

Table S2 Coordinates of $(C_5F_6)Fe(CO)_3$ **13-1S** (C_s)

	B3LYP/DZP			BP86/DZP		
C	0.083521	-0.950067	1.119768	0.084618	-0.962763	1.126466
C	1.367121	-0.427179	0.706231	1.368653	-0.413596	0.714167
C	1.367121	-0.427179	-0.706231	1.368653	-0.413596	-0.714167
C	0.083521	-0.950067	-1.119768	0.084618	-0.962763	-1.126466
C	-2.012305	0.733203	0.000000	-1.993462	0.728288	0.000000
C	0.013430	1.984483	1.326530	0.006023	1.983754	1.300786
F	-0.178161	-1.222307	-2.408539	-0.194656	-1.219764	-2.418654
F	2.376874	-0.079870	-1.491404	2.391241	-0.078248	-1.501787
F	-0.178161	-1.222307	2.408539	-0.194656	-1.219764	2.418654
F	2.376874	-0.079870	1.491404	2.391241	-0.078248	1.501787
C	-0.404932	-1.864115	0.000000	-0.405016	-1.882715	0.000000
F	0.148039	-3.125099	0.000000	0.162860	-3.150831	0.000000
F	-1.746873	-2.065914	0.000000	-1.754357	-2.093145	0.000000
O	-3.163386	0.752395	0.000000	-3.159937	0.758993	0.000000
O	0.138651	2.747371	2.180604	0.121418	2.777938	2.150260
Fe	-0.198620	0.756917	0.000000	-0.192266	0.756879	0.000000
C	0.013430	1.984483	-1.326530	0.006023	1.983754	-1.300786
O	0.138651	2.747371	-2.180604	0.121418	2.777938	-2.150260

Table S3 Coordinates of $(C_5F_6)Fe(CO)_3$ **13-2S** (C_1)

	B3LYP/DZP			BP86/DZP		
C	0.465320	-0.630171	-0.816163	0.466597	-0.644448	-0.798916
C	0.292153	0.824581	-0.889713	0.302462	0.830595	-0.879247
C	1.403131	1.409203	-0.105956	1.427882	1.413184	-0.109584
C	2.229858	0.455898	0.355596	2.260318	0.445762	0.353496
C	-2.146851	-1.704656	0.174610	-2.179465	-1.656383	0.156885
C	-0.885579	0.106086	1.596998	-0.900266	0.110967	1.551955
O	-2.630393	-2.733189	0.352364	-2.702927	-2.677303	0.370236
O	-0.631729	0.239477	2.713768	-0.666693	0.244691	2.692367
C	1.771463	-0.924807	-0.068649	1.785601	-0.940285	-0.054233
F	3.207318	0.600419	1.247250	3.251712	0.593202	1.239603
F	1.453582	2.705765	0.189075	1.493159	2.719056	0.177120
F	0.008419	1.403088	-2.104100	-0.005189	1.409101	-2.096233
F	0.283769	-1.342216	-1.974501	0.275304	-1.365552	-1.957564
F	2.664701	-1.554228	-0.883370	2.671865	-1.587554	-0.883975
F	1.612621	-1.734954	1.023841	1.628773	-1.747244	1.052067
Fe	-1.292187	-0.086751	-0.108246	-1.292252	-0.080522	-0.120998
C	-2.576675	1.241368	-0.062141	-2.572676	1.220058	-0.065665
O	-3.337098	2.104921	-0.038238	-3.353474	2.086086	-0.007773

Table S4 Coordinates of $(C_5F_6)Fe(CO)_2$ **12-1S** (C_s)

	B3LYP/DZP			BP86/DZP	
C	-0.021252	0.914929	1.131113	0.042879	-0.932887	1.142273
C	-1.190409	0.205907	0.713039	1.198647	-0.186482	0.722240
C	-1.190409	0.205907	-0.713039	1.198647	-0.186482	-0.722240
C	-0.021252	0.914929	-1.131113	0.042879	-0.932887	-1.142273
Fe	0.479872	-0.721564	0.000000	-0.469279	0.707181	0.000000
C	0.595582	-1.952009	-1.332191	-0.611765	1.937304	-1.296197
C	0.595582	-1.952009	1.332191	-0.611765	1.937304	1.296197
F	0.244852	1.205018	-2.415380	-0.241692	-1.218396	-2.427828
F	-2.145043	-0.294436	-1.484691	2.164808	0.314527	-1.494267
F	0.244852	1.205018	2.415380	-0.241692	-1.218396	2.427828
F	-2.145043	-0.294436	1.484691	2.164808	0.314527	1.494267
C	0.460149	1.802629	0.000000	-0.456574	-1.807350	0.000000
F	-0.002684	3.096791	0.000000	-0.028758	-3.125673	0.000000
F	1.830203	1.914764	0.000000	-1.844339	-1.879648	0.000000
O	0.619445	-2.723469	-2.189919	-0.648416	2.747482	-2.141771
O	0.619445	-2.723469	2.189919	-0.648416	2.747482	2.141771

Table S5 Coordinates of $(C_5F_6)Fe(CO)_2$ **12-2T** (C_s)

	B3LYP/DZP			BP86/DZP	
C	-0.303717	-0.799785	1.146838	-0.252592	-0.805673	1.141921
C	-1.300698	0.115645	0.721147	-1.313734	0.078130	0.723214
C	-1.300698	0.115645	-0.721147	-1.313734	0.078130	-0.723214
C	-0.303717	-0.799785	-1.146838	-0.252592	-0.805673	-1.141921
Fe	0.546330	0.795915	0.000000	0.478784	0.796892	0.000000
C	2.386878	0.465566	0.000000	2.299742	0.589220	0.000000
C	0.192841	2.658039	0.000000	0.137434	2.609996	0.000000
O	3.523825	0.292054	0.000000	3.464744	0.506127	0.000000
O	-0.017128	3.789310	0.000000	-0.061599	3.761800	0.000000
C	-0.037095	-1.768497	0.000000	0.035221	-1.785839	0.000000
F	-0.145165	-1.175256	-2.426650	-0.042338	-1.140160	-2.430135
F	-2.150910	0.795192	-1.486683	-2.202919	0.701315	-1.504667
F	-2.150910	0.795192	1.486683	-2.202919	0.701315	1.504667
F	-0.145165	-1.175256	2.426650	-0.042338	-1.140160	2.430135
F	-0.876762	-2.863698	0.000000	-0.788205	-2.909283	0.000000
F	1.217700	-2.294583	0.000000	1.310720	-2.281064	0.000000

Table S6 Coordinates of $(C_5F_6)Fe(CO)_2$ **12-3S** (C_1)

	B3LYP/DZP			BP86/DZP		
C	0.037248	0.476963	-0.810219	0.023593	0.386878	-0.850277
C	-0.428192	-0.919663	-0.876818	-0.418566	-1.030955	-0.744537
C	-1.704632	-0.946891	-0.129626	-1.705372	-0.991486	-0.010146
C	-2.027252	0.267664	0.349326	-2.056234	0.279613	0.318996
Fe	1.390724	-0.714625	-0.142855	1.399536	-0.702845	-0.069531
C	2.919907	0.256186	0.136355	2.919516	0.259733	0.090348
C	0.974628	-0.782450	1.564758	1.021026	-0.538006	1.596534
O	3.805235	0.970875	0.328020	3.827962	0.988927	0.224619
O	0.706866	-0.850552	2.686151	0.788134	-0.447203	2.745453
C	-0.992815	1.305889	-0.026431	-1.032427	1.289817	-0.169057
F	-2.982512	0.555167	1.232945	-3.027983	0.651364	1.162445
F	-2.344791	-2.083711	0.134609	-2.332673	-2.105876	0.387060
F	-0.401477	-1.557176	-2.105671	-0.347829	-1.829134	-1.886170
F	0.485012	1.058035	-1.964703	0.474760	0.839747	-2.065684
F	-1.496991	2.311936	-0.794613	-1.550768	2.191773	-1.069169
F	-0.473575	1.901470	1.092631	-0.529497	2.030638	0.877747

Table S7 Coordinates of $(C_5F_6)Fe_2(CO)_8$ **28-1S** (C_2)

	B3LYP/DZP			BP86/DZP		
C	-0.301293	1.166694	0.753706	-0.335019	1.163847	0.750657
C	-0.202972	0.714407	-0.624146	-0.225855	0.710052	-0.635309
C	0.202972	-0.714407	-0.624146	0.225855	-0.710052	-0.635309
C	0.301293	-1.166694	0.753706	0.335019	-1.163847	0.750657
F	1.372381	-1.925538	1.137068	1.416098	-1.911868	1.139382
F	1.181387	-1.078473	-1.520415	1.196014	-1.062351	-1.549273
F	-1.372381	1.925538	1.137068	-1.416098	1.911868	1.139382
F	-1.181387	1.078473	-1.520415	-1.196014	1.062351	-1.549273
C	0.000000	0.000000	1.705111	0.000000	0.000000	1.709357
F	1.063270	0.229656	2.535028	1.066215	0.255778	2.543862
F	-1.063270	-0.229656	2.535028	-1.066215	-0.255778	2.543862
Fe	1.211915	2.135963	-0.216458	1.185068	2.156612	-0.215009
C	2.030097	2.359104	-1.833871	2.000693	2.382431	-1.814500
C	1.855529	3.253111	1.080564	1.795013	3.265515	1.080975
C	0.000000	3.443275	-0.698865	0.000000	3.450269	-0.700985
C	2.562473	0.954889	0.209369	2.547067	1.027655	0.208593
O	3.482817	0.310308	0.441310	3.504939	0.409716	0.443396
O	-0.692070	4.302446	-1.011564	-0.684636	4.332895	-1.024322
O	2.519486	2.481152	-2.869964	2.508202	2.518614	-2.856846
O	2.232531	3.947675	1.918582	2.168804	3.976067	1.927751
Fe	-1.211915	-2.135963	-0.216458	-1.185068	-2.156612	-0.215009
C	-1.855529	-3.253111	1.080564	-1.795013	-3.265515	1.080975
C	0.000000	-3.443275	-0.698865	0.000000	-3.450269	-0.700985
C	-2.030097	-2.359104	-1.833871	-2.000693	-2.382431	-1.814500
C	-2.562473	-0.954889	0.209369	-2.547067	-1.027655	0.208593
O	-2.232531	-3.947675	1.918582	-2.168804	-3.976067	1.927751
O	-2.519486	-2.481152	-2.869964	-2.508202	-2.518614	-2.856846
O	0.692070	-4.302446	-1.011564	0.684636	-4.332895	-1.024322
O	-3.482817	-0.310308	0.441310	-3.504939	-0.409716	0.443396

Table S8 Coordinates of $(C_5F_6)Fe_2(CO)_8$ **28-2S** (C_s)

	B3LYP/DZP			BP86/DZP	
C	1.239426	-0.408516	1.245646	1.289572	-0.357133	1.253865
C	0.782904	0.877508	0.770926	0.803105	0.924827	0.771445
C	0.782904	0.877508	-0.770926	0.803105	0.924827	-0.771445
C	1.239426	-0.408516	-1.245646	1.289572	-0.357133	-1.253865
F	2.390819	-0.489464	-1.989826	2.427936	-0.417337	-2.027260
F	1.410906	2.013742	-1.220307	1.376300	2.089959	-1.229841
F	2.390819	-0.489464	1.989826	2.427936	-0.417337	2.027260
F	1.410906	2.013742	1.220307	1.376300	2.089959	1.229841
C	1.299738	-1.354459	0.000000	1.389350	-1.307120	0.000000
F	2.458931	-2.043870	0.000000	2.595376	-1.935405	0.000000
F	0.293530	-2.291083	0.000000	0.429445	-2.301057	0.000000
Fe	-0.406864	0.101721	-2.307161	-0.408566	0.087989	-2.283649
Fe	-0.406864	0.101721	2.307161	-0.408566	0.087989	2.283649
C	0.633609	1.125963	-3.457105	0.506908	1.156040	-3.450294
C	-0.413224	-1.121998	-3.660405	-0.393917	-1.099755	-3.643928
C	-1.700282	1.393314	-2.373258	-1.757468	1.300694	-2.275526
C	-1.628794	-1.037528	-1.568654	-1.543761	-1.124490	-1.566778
C	-1.628794	-1.037528	1.568654	-1.543761	-1.124490	1.566778
C	-1.700282	1.393314	2.373258	-1.757468	1.300694	2.275526
C	0.633609	1.125963	3.457105	0.506908	1.156040	3.450294
C	-0.413224	-1.121998	3.660405	-0.393917	-1.099755	3.643928
O	1.186866	1.726034	-4.261695	0.988087	1.797318	-4.292645
O	-0.375259	-1.900137	-4.509649	-0.352804	-1.864057	-4.525779
O	-2.498506	2.224793	-2.366094	-2.614819	2.091989	-2.236005
O	-2.488624	-1.771320	-1.356137	-2.373188	-1.919872	-1.367152
O	-2.498506	2.224793	2.366094	-2.614819	2.091989	2.236005
O	-2.488624	-1.771320	1.356137	-2.373188	-1.919872	1.367152
O	-0.375259	-1.900137	4.509649	-0.352804	-1.864057	4.525779
O	1.186866	1.726034	4.261695	0.988087	1.797318	4.292645

Table S9 Coordinates of $(C_5F_6)Fe_2(CO)_7$ **27-1S** (C_1)

	B3LYP/DZP			BP86/DZP		
C	-1.752137	1.147186	0.521216	-1.768336	1.179143	0.505326
C	-1.983740	0.868054	-0.881536	-2.015462	0.827991	-0.878184
C	-0.712555	0.753737	-1.446109	-0.724264	0.668205	-1.448884
C	0.366609	1.360649	-0.581658	0.354568	1.343955	-0.624346
F	1.053051	2.336466	-1.313140	1.040596	2.290996	-1.396346
F	-0.505075	0.518748	-2.740675	-0.530250	0.406029	-2.750064
F	-2.777112	1.496065	1.329754	-2.777086	1.513005	1.341813
F	-3.147894	0.796583	-1.520099	-3.187937	0.778147	-1.520231
C	-0.521666	2.046183	0.507572	-0.522443	2.069307	0.461861
F	-0.851737	3.318873	0.114306	-0.851789	3.340917	0.026417
F	0.054081	2.199231	1.730062	0.070911	2.254767	1.680529
Fe	1.609698	-0.155599	0.040702	1.603612	-0.157540	0.055461
Fe	-1.146568	-0.780075	0.103455	-1.128499	-0.779507	0.098869
C	1.792536	-0.654596	-1.725814	1.928434	-0.559725	-1.700710
C	3.092072	0.874708	-0.068687	3.006683	0.954346	0.137843
C	2.270299	-1.805745	0.507810	2.393705	-1.735555	0.499014
C	1.518040	0.190175	1.848139	1.314724	0.059774	1.838435
C	-0.563152	-2.211310	-0.851167	-0.340249	-2.165348	-0.728582
C	-2.815527	-1.445752	0.118434	-2.700256	-1.573313	-0.128092
C	-0.839987	-1.325293	1.790571	-1.114193	-1.268648	1.829093
O	2.039799	-1.000701	-2.793194	2.280991	-0.840507	-2.774157
O	4.039409	1.524244	-0.125100	3.927800	1.664562	0.215146
O	2.689351	-2.841565	0.787464	2.929866	-2.735174	0.770818
O	1.644247	0.297224	2.985926	1.349930	0.109650	3.003620
O	-0.248323	-3.143854	-1.457102	0.045026	-3.127697	-1.277443
O	-0.752679	-1.708043	2.877382	-1.223451	-1.614357	2.940141
O	-3.858548	-1.934074	0.151807	-3.698961	-2.168017	-0.256661

Table S10 Coordinates of $(C_5F_6)Fe_2(CO)_7$ **27-2S** (C_1)

	B3LYP/DZP			BP86/DZP		
C	-1.047426	-0.938698	-0.616695	-1.045642	-0.931737	-0.620245
C	-0.672335	0.472515	-0.727911	-0.673222	0.501422	-0.700416
C	0.381070	0.755650	0.273432	0.377911	0.767156	0.314772
C	0.696875	-0.481553	0.969714	0.702038	-0.491263	0.988778
F	0.821051	-0.466699	2.329966	0.842369	-0.509626	2.350416
F	0.238172	1.912662	1.002748	0.247331	1.920999	1.055983
F	-1.252837	-1.653342	-1.770703	-1.247404	-1.626190	-1.793678
F	-0.546350	1.011048	-1.994855	-0.561027	1.078382	-1.957965
C	-0.190665	-1.621369	0.447515	-0.180759	-1.633874	0.438656
F	-0.923469	-2.161148	1.467050	-0.918075	-2.196834	1.454630
F	0.510992	-2.666077	-0.093124	0.530488	-2.671440	-0.126862
Fe	-2.591814	0.255558	-0.273971	-2.595168	0.251839	-0.282980
C	-2.506385	0.420731	1.484047	-2.532607	0.374483	1.441623
C	-4.011743	-0.923093	-0.178409	-4.008495	-0.904158	-0.226609
C	-3.253365	1.965862	-0.468786	-3.293169	1.930239	-0.426313
O	-3.622539	3.049747	-0.591262	-3.705879	3.020608	-0.492589
O	-2.485272	0.541241	2.629781	-2.544204	0.474713	2.608310
O	-4.867128	-1.690750	-0.113302	-4.888954	-1.667504	-0.156934
Fe	2.303505	0.169632	-0.114002	2.308143	0.176658	-0.111276
C	3.561208	-1.107815	0.246532	3.548259	-1.102772	0.215329
C	2.863576	1.105291	1.376802	2.906704	1.073386	1.356424
C	2.936709	1.531945	-1.151305	2.918800	1.546029	-1.123720
C	1.913449	-0.729035	-1.674434	1.933728	-0.681823	-1.669183
O	4.331519	-1.926734	0.497329	4.334831	-1.934456	0.441430
O	3.308259	2.411534	-1.796703	3.295989	2.443582	-1.767864
O	3.281953	1.689266	2.270500	3.371940	1.647447	2.254135
O	1.783487	-1.267494	-2.679524	1.823556	-1.207023	-2.702317

Table S11 Coordinates of $(C_5F_6)Fe_2(CO)_7$ **27-3S** (C_s)

	B3LYP/DZP			BP86/DZP		
C	-1.534638	-0.052861	1.196419	-1.535404	-0.048411	1.205086
C	-0.945550	-1.270312	0.767289	-0.936400	-1.281819	0.769710
C	-0.945550	-1.270312	-0.767289	-0.936400	-1.281819	-0.769710
C	-1.534638	-0.052861	-1.196419	-1.535404	-0.048411	-1.205086
F	-2.206831	0.035674	-2.364748	-2.222695	0.028955	-2.373022
F	-1.117040	-2.444364	-1.390182	-1.122298	-2.461261	-1.397147
F	-2.206831	0.035674	2.364748	-2.222695	0.028955	2.373022
F	-1.117040	-2.444364	1.390182	-1.122298	-2.461261	1.397147
C	-2.193515	0.631105	0.000000	-2.200315	0.636336	0.000000
F	-3.530418	0.332931	0.000000	-3.546062	0.320495	0.000000
F	-2.115336	1.986099	0.000000	-2.133337	2.001185	0.000000
Fe	0.555277	0.062621	-1.344483	0.551427	0.059969	-1.338961
C	0.482382	-0.647767	-3.011430	0.505458	-0.638376	-2.991189
C	0.264945	1.858465	-1.583627	0.262004	1.845219	-1.577795
C	2.335506	0.312165	-1.619635	2.310210	0.322415	-1.614363
C	2.335506	0.312165	1.619635	2.310210	0.322415	1.614363
C	0.482382	-0.647767	3.011430	0.505458	-0.638376	2.991189
C	0.264945	1.858465	1.583627	0.262004	1.845219	1.577795
O	0.483017	-1.081158	-4.078017	0.532219	-1.067265	-4.076753
O	0.115552	2.982230	-1.786945	0.118848	2.983392	-1.787762
O	3.457306	0.482926	-1.815170	3.440845	0.503193	-1.841552
O	3.457306	0.482926	1.815170	3.440845	0.503193	1.841552
O	0.115552	2.982230	1.786945	0.118848	2.983392	1.787762
O	0.483017	-1.081158	4.078017	0.532219	-1.067265	4.076753
Fe	0.555277	0.062621	1.344483	0.551427	0.059969	1.338961
C	1.276003	-1.217044	0.000000	1.296599	-1.213604	0.000000
O	1.893297	-2.224473	0.000000	1.916443	-2.233233	0.000000

Table S12 Coordinates of $(C_5F_6)Fe_2(CO)_7$ **27-4T** (C_1)

	B3LYP/DZP			BP86/DZP		
C	1.039648	0.899805	-0.655112	-0.972362	-1.153646	-0.522222
C	0.649091	-0.470533	-0.766634	-0.630603	0.182682	-0.910776
C	-0.397105	-0.762436	0.239867	0.338876	0.746168	0.064618
C	-0.679539	0.463915	0.967001	0.683477	-0.311405	1.018129
F	-0.780712	0.420300	2.329108	0.731337	-0.018000	2.353612
F	-0.289472	-1.943915	0.929496	0.124233	2.029848	0.506236
F	1.288583	1.640463	-1.771712	-1.241955	-2.106079	-1.460711
F	0.555493	-1.056738	-1.995338	-0.586547	0.546168	-2.223231
C	0.238155	1.581784	0.456403	-0.127681	-1.586549	0.689854
F	1.026091	2.053091	1.474047	-0.867814	-1.988208	1.774736
F	-0.427001	2.674307	-0.027632	0.651913	-2.673981	0.349931
Fe	2.636285	-0.176237	-0.015957	-2.604901	0.058691	-0.081061
C	2.452016	-1.108323	1.652208	-2.742880	0.475327	1.697575
C	4.036027	1.079739	0.183333	-4.307841	-0.498412	-0.467749
C	3.193459	-1.646665	-1.082921	-2.826994	1.764668	-0.656353
O	3.500903	-2.569722	-1.697219	-2.993745	2.869040	-1.002517
O	2.395015	-1.693185	2.640377	-2.878945	0.785523	2.816681
O	4.861670	1.875824	0.260017	-5.400410	-0.822095	-0.729931
Fe	-2.312752	-0.115543	-0.115439	2.318739	0.179935	-0.126775
C	-3.538709	1.179174	0.291833	3.579232	-0.937978	0.540793
C	-2.881009	-1.078158	1.355427	2.790622	1.407653	1.134781
C	-2.994007	-1.430392	-1.184300	2.969036	1.312964	-1.381164
C	-1.911114	0.816736	-1.652850	2.057337	-1.010316	-1.476893
O	-4.288383	2.007769	0.571360	4.374300	-1.665564	0.986689
O	-3.396862	-2.280136	-1.850237	3.372676	2.058095	-2.183372
O	-3.305033	-1.674769	2.237963	3.177240	2.186709	1.905844
O	-1.768583	1.378070	-2.643631	2.008678	-1.744073	-2.379015

Table S13 Coordinates of $(C_5F_6)Fe_2(CO)_6$ **26-1S** (C_1)

	B3LYP/DZP			BP86/DZP		
C	1.661318	-1.205523	0.330904	1.684940	-1.234134	0.267601
C	1.693399	-0.791993	-1.041702	1.668946	-0.744650	-1.082749
C	0.314996	-0.650205	-1.409194	0.247435	-0.571425	-1.393541
C	-0.582202	-1.407952	-0.478238	-0.595870	-1.442232	-0.481419
F	-1.369466	-2.373441	-1.077429	-1.376451	-2.399345	-1.096731
F	-0.051577	-0.422233	-2.683768	-0.132485	-0.343088	-2.676558
F	2.778767	-1.579346	0.987366	2.823871	-1.591215	0.899661
F	2.727682	-0.796241	-1.885470	2.664390	-0.745623	-1.984312
C	0.408606	-2.035264	0.540053	0.439188	-2.082195	0.498106
F	0.625257	-3.353466	0.247697	0.672066	-3.396648	0.151733
F	-0.041941	-2.017748	1.829263	0.029015	-2.106777	1.806754
Fe	-1.453555	0.280603	0.004574	-1.437202	0.267925	-0.005338
Fe	1.077543	0.769444	0.060502	1.067834	0.781031	0.048587
C	-2.842408	-0.021804	-1.118190	-2.870760	-0.003898	-1.018039
C	-2.386558	-0.438031	1.352208	-2.300141	-0.420126	1.365143
C	-1.918628	2.071441	0.296548	-1.891519	2.033369	0.234621
C	0.438184	1.044177	1.709380	0.420556	0.946854	1.711697
C	2.767215	1.312076	0.373958	2.733337	1.332243	0.395877
C	0.768942	2.318828	-0.821799	0.768977	2.383980	-0.709777
O	-3.698168	-0.191498	-1.864624	-3.805766	-0.159946	-1.698314
O	-2.960017	-0.900103	2.234859	-2.882627	-0.869972	2.271787
O	-2.264136	3.146130	0.508939	-2.271126	3.116730	0.439884
O	0.192850	1.253854	2.825318	0.197531	1.103642	2.853762
O	0.621400	3.306842	-1.404018	0.659365	3.433418	-1.216062
O	3.835652	1.685592	0.592715	3.808798	1.724215	0.629628

Table S14 Coordinates of $(C_5F_6)Fe_2(CO)_6$ **26-2T** (C_1)

	B3LYP/DZP			BP86/DZP		
C	-1.922969	-0.873330	-0.520578	-1.988391	-0.782458	-0.543528
C	-2.119238	-0.616538	0.892586	-2.213934	-0.385196	0.838143
C	-0.856361	-0.684336	1.476848	-0.971312	-0.562827	1.493134
C	0.162954	-1.305791	0.556276	0.022369	-1.293708	0.628912
F	0.825397	-2.345351	1.207801	0.674321	-2.306487	1.332038
F	-0.602448	-0.483415	2.762191	-0.758142	-0.341346	2.789247
F	-2.971309	-1.066047	-1.342238	-3.000753	-0.896035	-1.426435
F	-3.256831	-0.287933	1.487880	-3.358373	0.018402	1.393066
C	-0.755166	-1.862159	-0.573398	-0.900787	-1.869358	-0.498718
F	-1.163199	-3.140687	-0.313666	-1.413385	-3.101907	-0.148569
F	-0.169452	-1.910331	-1.803237	-0.288582	-2.054605	-1.708257
Fe	1.558544	0.135652	-0.073548	1.515347	0.095704	-0.079221
Fe	-0.907028	0.844437	-0.124650	-0.822865	0.853972	-0.137521
C	2.411988	0.020189	1.571356	2.364865	-0.048655	1.516208
C	2.469978	-1.170258	-1.011763	2.345802	-1.268891	-0.937950
C	2.648892	1.481723	-0.681361	2.714476	1.313222	-0.685482
C	-0.264142	1.066994	-1.815793	-0.048349	0.876351	-1.786856
C	-2.331044	1.972373	-0.354881	-2.051934	2.103192	-0.508358
C	-0.034370	2.078892	0.899644	0.097161	2.025387	0.900719
O	2.989140	-0.077802	2.563816	2.980310	-0.146943	2.504913
O	3.080742	-1.980562	-1.556188	2.951594	-2.124788	-1.452138
O	3.343378	2.320115	-1.063129	3.518299	2.071222	-1.067452
O	-0.004625	1.247319	-2.926600	0.214835	0.987505	-2.925071
O	0.383299	2.920016	1.573553	0.535558	2.865705	1.591138
O	-3.212180	2.692790	-0.525082	-2.815609	2.947781	-0.769121

Table S15 Coordinates of $(C_5F_6)Fe_2(CO)_6$ **26-3S** (C_2)

	B3LYP/DZP			BP86/DZP		
C	-0.764342	0.921155	0.706309	-0.759216	0.935687	0.713459
C	-0.479663	0.560774	-0.685496	-0.472838	0.569253	-0.696511
C	0.479663	-0.560774	-0.685496	0.472838	-0.569253	-0.696511
C	0.764342	-0.921155	0.706309	0.759216	-0.935687	0.713459
F	2.063402	-1.192008	1.053283	2.060163	-1.222669	1.060674
F	1.540342	-0.520458	-1.569958	1.531992	-0.557111	-1.591937
F	-2.063402	1.192008	1.053283	-2.060163	1.222669	1.060674
F	-1.540342	0.520458	-1.569958	-1.531992	0.557111	-1.591937
C	0.000000	0.000000	1.656263	0.000000	0.000000	1.668500
F	0.864631	0.665487	2.481726	0.879817	0.660903	2.496552
F	-0.864631	-0.665487	2.481726	-0.879817	-0.660903	2.496552
Fe	0.000000	2.447582	-0.299446	0.000000	2.453876	-0.301081
C	1.720433	2.246673	0.049600	1.682842	2.253743	0.044467
C	-0.168513	3.849194	0.892553	-0.154604	3.855644	0.860168
C	0.349080	3.139019	-1.973413	0.367879	3.170679	-1.937538
O	0.568708	3.529372	-3.034396	0.629116	3.596133	-2.993165
O	2.848253	2.147415	0.265391	2.830717	2.170118	0.262315
O	-0.276808	4.692916	1.668258	-0.226794	4.725994	1.634692
Fe	0.000000	-2.447582	-0.299446	0.000000	-2.453876	-0.301081
C	0.168513	-3.849194	0.892553	0.154604	-3.855644	0.860168
C	-0.349080	-3.139019	-1.973413	-0.367879	-3.170679	-1.937538
C	-1.720433	-2.246673	0.049600	-1.682842	-2.253743	0.044467
O	0.276808	-4.692916	1.668258	0.226794	-4.725994	1.634692
O	-0.568708	-3.529372	-3.034396	-0.629116	-3.596133	-2.993165
O	-2.848253	-2.147415	0.265391	-2.830717	-2.170118	0.262315

Table S16 Coordinates of $(C_5F_6)Fe_2(CO)_6$ **26-4S** (C_1)

	B3LYP/DZP			BP86/DZP		
C	-1.340752	-0.846650	0.231681	-1.340138	-0.819147	0.292821
C	-0.781299	-0.323888	-1.021582	-0.786320	-0.361677	-1.004378
C	0.301465	0.626514	-0.692263	0.296913	0.613112	-0.735892
C	0.424742	0.698115	0.755138	0.430755	0.769539	0.714478
F	0.534527	1.921177	1.353825	0.550694	2.024514	1.247875
F	0.330296	1.795339	-1.417248	0.337456	1.730124	-1.542295
F	-1.600596	-2.187594	0.338869	-1.612150	-2.153756	0.480015
F	-0.595311	-1.225792	-2.064438	-0.627634	-1.317572	-2.013978
C	-0.615261	-0.215052	1.422531	-0.604232	-0.115433	1.449047
F	-1.441967	0.511772	2.230557	-1.429741	0.657408	2.227788
F	-0.068695	-1.181427	2.223194	-0.042499	-1.045582	2.297920
Fe	-2.714720	-0.010045	-0.839223	-2.719257	-0.066524	-0.829701
C	-2.693019	1.645764	-0.234355	-2.749183	1.557932	-0.273610
C	-4.345794	-0.373263	-0.101766	-4.348365	-0.386726	-0.132530
O	-2.709134	2.741569	0.128531	-2.818843	2.680676	0.067317
O	-5.313388	-0.622743	0.477705	-5.351768	-0.593550	0.439481
Fe	2.125224	-0.080740	-0.074254	2.130877	-0.080467	-0.076241
C	3.175236	-0.379859	1.392292	3.170050	-0.292800	1.392527
C	2.797477	1.636421	-0.174405	2.833684	1.586910	-0.283304
C	2.964627	-0.452780	-1.650591	2.950284	-0.552842	-1.617478
C	1.625574	-1.852068	-0.016054	1.649842	-1.824481	0.090323
O	3.813624	-0.551978	2.335802	3.827289	-0.416815	2.348830
O	3.471543	-0.670498	-2.662873	3.466371	-0.844950	-2.623401
O	3.286129	2.671571	-0.243389	3.366101	2.611593	-0.419971
O	1.429302	-2.982971	0.002199	1.472474	-2.972053	0.178560

Table S17 Coordinates of $(C_5F_6)Fe_2(CO)_5$ **25-1S** (C_1)

	B3LYP/DZP			BP86/DZP		
C	-1.213936	1.430975	0.036030	-1.167499	1.489088	0.194144
C	-1.323561	0.715397	-1.201151	-1.308663	0.884847	-1.104341
C	0.020086	0.202626	-1.430330	0.043292	0.335535	-1.383109
C	1.038564	0.995145	-0.666627	1.081417	1.092370	-0.574755
F	2.067342	1.565066	-1.352038	2.113184	1.709722	-1.210459
F	0.327758	-0.353839	-2.620914	0.318497	-0.079432	-2.647181
F	-2.227389	2.177103	0.518280	-2.163092	2.190342	0.775260
F	-2.265113	0.829870	-2.142347	-2.226294	1.157699	-2.047699
C	0.190436	2.013920	0.145507	0.257424	2.031626	0.364855
F	0.259730	3.255476	-0.420917	0.331103	3.340071	-0.064792
F	0.618824	2.172447	1.431821	0.699173	2.040269	1.662714
Fe	1.275410	-0.654500	0.248914	1.233046	-0.656229	0.163824
Fe	-1.102843	-0.643170	0.198569	-1.102952	-0.633803	0.115464
C	2.604765	-1.262505	-0.795573	2.506182	-1.288263	-0.872024
C	2.493475	-0.217372	1.486112	2.478460	-0.413308	1.380129
C	-1.126374	-2.336680	-0.445685	-1.509026	-2.082479	-0.868037
C	-2.849431	-0.738592	0.673089	-2.693548	-0.692874	0.948385
C	-0.443914	-0.781454	1.877901	-0.228048	-1.297067	1.608186
O	3.433435	-1.689429	-1.470776	3.339606	-1.750458	-1.552579
O	3.254097	0.121767	2.281919	3.300371	-0.211232	2.189687
O	-1.159794	-3.406678	-0.879899	-1.786093	-3.010291	-1.521394
O	-0.303851	-0.866826	3.029398	-0.110258	-1.789587	2.674708
O	-3.956106	-0.809388	0.984961	-3.718067	-0.743940	1.505493

Table S18 Coordinates of $(C_5F_6)Fe_2(CO)_5$ **25-2S** (C_1)

	B3LYP/DZP			BP86/DZP		
C	1.702933	-0.916433	0.294634	-1.616414	1.007109	0.260219
C	1.510604	-0.695138	-1.106750	-1.453924	0.671644	-1.137732
C	0.076700	-0.730870	-1.323964	-0.004035	0.640334	-1.368418
C	-0.601739	-1.421963	-0.169600	0.698930	1.440274	-0.276718
F	-1.422929	-2.479332	-0.451687	1.541765	2.447395	-0.650892
F	-0.381821	-0.821487	-2.592723	0.434098	0.638369	-2.655415
F	2.922888	-1.117023	0.822304	-2.825719	1.269573	0.791223
F	2.414910	-0.768640	-2.080413	-2.365277	0.779831	-2.113531
C	0.554405	-1.805902	0.783622	-0.433245	1.905464	0.682850
F	0.888240	-3.125697	0.640321	-0.760610	3.228847	0.459879
F	0.259024	-1.640600	2.101443	-0.113361	1.814666	2.009590
Fe	-1.348906	0.398056	-0.076985	1.319376	-0.421521	-0.045406
Fe	0.920638	0.887647	-0.070635	-0.916242	-0.857892	-0.037008
C	-2.865904	-0.038360	-0.982311	2.901732	-0.195626	-0.875308
C	-2.198179	0.275502	1.493135	2.071753	-0.288259	1.550420
C	-1.414537	2.191274	-0.444937	1.228398	-2.214134	-0.314554
C	0.753873	1.263249	1.672464	-0.978273	-1.117066	1.721321
C	2.468997	1.777905	-0.433929	-2.414597	-1.777309	-0.448709
O	-3.814681	-0.290114	-1.581499	3.922479	-0.078375	-1.429895
O	-2.704267	0.184360	2.525132	2.559532	-0.205193	2.610939
O	-1.499007	3.320507	-0.676471	1.239719	-3.373656	-0.491425
O	0.750614	1.471587	2.809426	-1.088221	-1.253478	2.877451
O	3.403494	2.407556	-0.677745	-3.343700	-2.436545	-0.715213

Table S19 Coordinates of $(C_5F_6)Fe_2(CO)_5$ **25-3T**(C_1)

	B3LYP/DZP			BP86/DZP		
C	-1.638644	1.166346	0.189150	-1.655076	1.072008	0.238446
C	-1.619480	0.536531	-1.070181	-1.655508	0.397420	-1.024779
C	-0.217075	0.412248	-1.443172	-0.243823	0.404050	-1.456514
C	0.609966	1.400993	-0.663443	0.523929	1.472369	-0.716555
F	1.335161	2.304920	-1.401955	1.230019	2.387192	-1.457186
F	0.104382	0.094099	-2.719333	0.061343	0.085668	-2.742216
F	-2.766563	1.550677	0.806690	-2.785358	1.386532	0.903437
F	-2.648912	0.261946	-1.865280	-2.698798	0.150762	-1.833447
C	-0.407757	2.074443	0.289516	-0.501532	2.090434	0.272342
F	-0.720822	3.332287	-0.142499	-0.935859	3.318339	-0.185083
F	0.046543	2.222732	1.565089	-0.002918	2.312100	1.528027
C	2.166838	-1.962335	-0.541066	2.338806	-1.738033	-0.593392
C	3.019632	0.518967	0.512681	2.848604	0.659590	0.676056
C	0.839394	-0.735459	1.556855	0.714468	-0.786199	1.550255
C	-1.358355	-2.272899	-0.672589	-1.048933	-2.377426	-0.640881
C	-1.893502	-1.196067	1.653908	-1.879202	-1.332721	1.522957
O	2.573270	-3.007547	-0.807531	2.902241	-2.711181	-0.904842
O	3.926376	1.045141	0.986641	3.694072	1.187708	1.283588
O	1.106666	-0.920638	2.674791	1.062792	-0.988049	2.661061
O	-2.588820	-1.445108	2.538805	-2.603711	-1.666221	2.377124
O	-1.703042	-3.203277	-1.258198	-1.288161	-3.370010	-1.208972
Fe	-0.812227	-0.787827	0.265458	-0.740550	-0.830627	0.241937
Fe	1.517234	-0.262370	-0.193550	1.486545	-0.152151	-0.186286

Table S20 Coordinates of $(C_5F_6)Fe_2(CO)_5$ **25-4S** (C_1)

	B3LYP/DZP			BP86/DZP		
C	-2.029030	-0.657601	-0.137669	-2.017138	-0.605510	-0.167967
C	-1.759723	-0.206799	1.151212	-1.762197	-0.189613	1.161634
C	-0.355423	-0.445455	1.440606	-0.369986	-0.483066	1.465593
C	0.107690	-1.570785	0.537951	0.102607	-1.582119	0.535063
F	0.473798	-2.716182	1.213573	0.495393	-2.746781	1.170836
F	0.076433	-0.420689	2.729042	0.083796	-0.437083	2.747473
F	-3.222458	-0.597168	-0.732813	-3.224085	-0.553170	-0.758093
F	-2.587049	0.493350	1.921324	-2.599000	0.497599	1.951050
C	-1.079892	-1.818777	-0.430392	-1.088113	-1.801542	-0.450960
F	-1.709646	-2.994701	-0.135984	-1.752314	-2.970730	-0.147626
F	-0.722218	-1.900656	-1.738721	-0.718327	-1.901095	-1.762977
C	2.873585	0.946195	0.360449	2.857500	0.934444	0.360704
C	2.486681	-1.448505	-0.818410	2.468151	-1.414915	-0.782225
C	0.705704	0.566486	-1.228598	0.731050	0.570220	-1.243620
C	0.264945	2.583141	0.558866	0.249947	2.527423	0.591733
C	-1.643296	2.050931	-1.224899	-1.609380	2.035041	-1.223862
O	3.766977	1.663341	0.485488	3.791086	1.629331	0.475525
O	3.053673	-2.185356	-1.501316	3.067446	-2.153001	-1.466037
O	0.819746	0.828826	-2.374291	0.866514	0.838217	-2.397768
O	-2.256385	2.605008	-2.027222	-2.211395	2.621199	-2.035539
O	0.811137	3.523742	0.944837	0.779441	3.484749	1.009507
Fe	-0.685105	1.154550	0.025257	-0.684254	1.127365	0.013538
Fe	1.540168	-0.318129	0.175417	1.519310	-0.292934	0.180000

Table S21 Coordinates of $(C_5F_6)Fe_2(CO)_5$ **25-5S** (C_s)

	B3LYP/DZP			BP86/DZP		
C	1.416890	0.145327	1.225225	1.423963	0.163402	1.232367
C	1.017345	1.445304	0.705629	0.934650	1.440569	0.719802
C	1.017345	1.445304	-0.705629	0.934650	1.440569	-0.719802
C	1.416890	0.145327	-1.225225	1.423963	0.163402	-1.232367
F	2.178420	0.114353	-2.360414	2.175763	0.141671	-2.377458
F	0.836366	2.535127	-1.452017	0.772568	2.555271	-1.453229
F	2.178420	0.114353	2.360414	2.175763	0.141671	2.377458
F	0.836366	2.535127	1.452017	0.772568	2.555271	1.453229
C	2.058535	-0.549658	0.000000	2.082020	-0.521812	0.000000
F	3.407629	-0.320657	0.000000	3.435862	-0.257220	0.000000
F	1.905972	-1.897783	0.000000	1.957367	-1.881959	0.000000
C	-2.335933	0.565631	-1.541378	-2.311010	0.551404	-1.528051
C	-0.535757	-1.108136	-2.668493	-0.507526	-1.105287	-2.645375
C	-0.956624	-1.181427	0.000000	-0.977705	-1.222353	0.000000
C	-2.335933	0.565631	1.541378	-2.311010	0.551404	1.528051
C	-0.535757	-1.108136	2.668493	-0.507526	-1.105287	2.645375
O	-3.427217	0.876074	-1.750208	-3.406703	0.879388	-1.777621
O	-0.482739	-1.910037	-3.493338	-0.447422	-1.906091	-3.493400
O	-1.334267	-2.303415	0.000000	-1.353066	-2.356729	0.000000
O	-0.482739	-1.910037	3.493338	-0.447422	-1.906091	3.493400
O	-3.427217	0.876074	1.750208	-3.406703	0.879388	1.777621
Fe	-0.581099	0.097212	1.348311	-0.581256	0.074090	1.317431
Fe	-0.581099	0.097212	-1.348311	-0.581256	0.074090	-1.317431

Table S22 Coordinates of $(C_5F_6)Fe_2(CO)_5$ **25-6T** (C_1)

	B3LYP/DZP			BP86/DZP		
C	1.055112	-0.763181	0.677951	1.007881	-0.904122	0.578031
C	0.686944	0.636604	0.594178	0.671221	0.489702	0.793298
C	-0.346780	0.787194	-0.448972	-0.353769	0.902758	-0.186740
C	-0.641779	-0.535077	-1.004550	-0.650386	-0.258679	-1.066403
F	-0.805557	-0.644572	-2.363293	-0.782266	-0.025536	-2.418988
F	-0.262797	1.851916	-1.327005	-0.302962	2.161618	-0.763378
F	1.226378	-1.357259	1.892613	1.120380	-1.781224	1.618154
F	0.579014	1.376906	1.744395	0.675766	1.021453	2.055542
C	0.270399	-1.571488	-0.358583	0.275580	-1.416904	-0.675148
F	1.086557	-2.132257	-1.316323	1.176715	-1.646213	-1.720290
F	-0.392705	-2.614018	0.219154	-0.364919	-2.605247	-0.458874
Fe	2.571889	0.346684	-0.105070	2.509419	0.313083	-0.050418
C	3.088583	2.109138	-0.519391	3.355259	1.836763	-0.670050
C	3.853139	-1.016526	0.171084	3.769438	-0.887152	0.502304
O	3.374346	3.212604	-0.683863	3.904389	2.810349	-1.014357
O	4.576927	-1.885392	0.386116	4.536435	-1.679163	0.892270
Fe	-2.252247	0.280699	-0.188659	-2.272870	0.350026	-0.122338
C	-3.602504	-0.883369	-0.671931	-3.610527	-0.602085	-0.921301
C	-3.011517	1.852402	0.406635	-3.085729	1.671374	0.839684
C	-2.161739	-0.377108	1.449115	-2.234768	-0.704073	1.249977
O	-4.415000	-1.637672	-0.982504	-4.443542	-1.249127	-1.421071
O	-3.444638	2.849779	0.785966	-3.576607	2.510657	1.485889
O	-2.132620	-0.798062	2.521518	-2.260663	-1.408964	2.184802

Table S23 Harmonic vibrational frequencies(cm^{-1}) and IR intensities (KM/Mole) of $(C_5F_6)Fe(CO)_4$ **14-1S** (C_1)

B3LYP/DZP	BP86/DZP
41(0), 50(0), 63(0), 72(0), 90(0), 97(0), 102(0), 106(0), 111(0), 128(0), 149(1), 202(5), 207(1), 222(1), 249(0), 263(1), 287(1), 295(1), 350(11), 383(1), 397(4), 400(2), 417(4), 429(4), 435(2), 441(32), 455(11), 471(6), 477(11), 501(15), 532(5), 561(0), 601(67), 620(9), 631(85), 641(149), 664(26), 716(138), 755(17), 796(3), 968(181), 997(173), 1117(79), 1133(85), 1149(13), 1266(203), 1350(156), 1384(204), 1405(50), 1777(120), 2097(976), 2117(477), 2128(938), 2178(295)	38(0), 46(0), 61(0), 69(0), 87(0), 94(0), 98(0), 102(0), 106(0), 122(0), 143(0), 196(2), 199(0), 213(0), 239(0), 255(0), 278(1), 287(0), 340(10), 380(2), 392(0), 417(12), 419(9), 431(7), 437(0), 453(5), 459(0), 468(2), 474(4), 503(6), 516(11), 548(0), 595(15), 605(76), 631(34), 636(67), 643(139), 687(104), 719(44), 768(5), 934(176), 968(158), 1065(112), 1088(59), 1107(5), 1213(201), 1300(128), 1340(196), 1360(65), 1703(137), 2007(881), 2019(816), 2028(464), 2088(262)

Table S24 Harmonic vibrational frequencies(cm^{-1}) and IR intensities (KM/Mole) of $(C_5F_6)Fe(CO)_3$ **13-1S** (C_s)

B3LYP/DZP	BP86/DZP
38(0), 79(0), 85(0), 91(0), 92(0), 106(0), 132(0), 177(0), 193(2), 200(1), 203(1), 209(2), 235(0), 235(0), 288(1), 309(2), 333(2), 385(14), 432(4), 447(0), 447(4), 460(5), 474(34), 497(22), 509(6), 510(10), 527(1), 553(9), 595(66), 597(45), 624(21), 628(88), 695(1), 705(78), 794(0), 957(188), 993(200), 1072(204), 1112(18), 1174(22), 1316(313), 1372(56), 1486(73), 1514(173), 1606(233), 2098(762), 2103(788), 2148(663)	35(0), 77(0), 83(0), 89(0), 90(0), 102(0), 126(0), 168(0), 190(1), 194(1), 199(0), 205(1), 226(0), 228(0), 280(1), 302(3), 322(1), 384(8), 440(1), 442(8), 452(9), 468(5), 478(11), 494(11), 499(14), 505(3), 521(3), 538(12), 583(39), 598(46), 615(27), 628(88), 656(2), 682(86), 764(0), 922(187), 963(173), 1022(218), 1071(19), 1135(6), 1267(278), 1324(61), 1439(88), 1460(204), 1543(243), 2000(679), 2009(716), 2057(530)

Table S25 Harmonic vibrational frequencies(cm^{-1}) and IR intensities (KM/Mole) of $(C_5F_6)Fe(CO)_3$ **13-2S** (C_1)

B3LYP/DZP	BP86/DZP
36(0), 53(0), 64(0), 71(0), 87(0), 96(0), 98(0), 124(0), 143(0), 183(3), 196(5), 207(5), 242(2), 254(2), 268(1), 280(7), 351(3), 375(2), 401(3), 420(2), 431(5), 432(10), 440(2), 451(9), 473(6), 489(8), 519(5), 556(55), 574(33), 595(36), 624(27), 663(18), 728(116), 762(16), 808(2), 970(192), 992(192), 1116(59), 1127(117), 1151(15), 1273(174), 1346(177), 1361(108), 1392(152), 1776(113), 2093(652), 2099(955), 2149(556)	33(0), 50(0), 62(0), 70(0), 84(0), 93(0), 96(0), 119(0), 142(0), 176(3), 192(1), 198(5), 232(2), 245(2), 259(1), 272(7), 343(4), 369(2), 396(0), 415(4), 428(1), 442(1), 451(4), 453(2), 469(3), 494(3), 502(5), 570(43), 576(32), 600(34), 620(21), 634(21), 701(76), 727(30), 780(3), 934(190), 959(189), 1066(137), 1076(51), 1107(8), 1215(165), 1277(132), 1302(135), 1345(163), 1703(132), 1991(611), 1996(842), 2052(442)

Table S26 Harmonic vibrational frequencies(cm^{-1}) and IR intensities (KM/Mole) of $(C_5F_6)Fe(CO)_2$ **12-1S** (C_s)

B3LYP/DZP	BP86/DZP
46(0), 68(2), 82(0), 86(0), 107(1), 171(1), 186(4), 192(1), 197(3), 214(3), 237(0), 238(0), 280(2), 317(0), 335(2), 370(36), 442(12), 444(7), 446(4), 460(48), 509(2), 512(14), 519(26), 551(10), 564(9), 612(24), 623(24), 649(1), 670(68), 795(0), 956(206), 989(191), 1058(212), 1127(48), 1150(7), 1306(521), 1378(52), 1508(65), 1551(141), 1589(202), 2079(945), 2121(901)	50(0), 63(2), 80(0), 85(0), 101(0), 161(0), 181(2), 186(1), 196(1), 214(2), 229(0), 231(0), 272(1), 311(1), 328(0), 381(21), 426(8), 453(4), 472(0), 474(29), 487(7), 511(8), 523(28), 539(16), 577(10), 599(2), 601(1), 620(39), 646(62), 764(0), 920(213), 957(166), 1000(221), 1089(46), 1104(4), 1262(426), 1329(55), 1454(107), 1496(177), 1525(194), 1979(790), 2022(722)

Table S27 Harmonic vibrational frequencies(cm^{-1}) and IR intensities (KM/Mole) of $(C_5F_6)Fe(CO)_2$ **12-2T** (C_s)

B3LYP/DZP	BP86/DZP
45(0), 69(0), 70(0), 75(0), 121(0), 154(3), 173(3), 182(5), 184(3), 190(2), 235(0), 235(0), 268(0), 299(0), 303(8), 335(0), 356(34), 374(1), 394(17), 442(28), 449(17), 474(45), 488(36), 489(0), 503(1), 547(20), 607(7), 652(0), 668(19), 791(1), 946(141), 987(222), 1058(203), 1106(30), 1167(14), 1306(402), 1370(36), 1486(65), 1573(144), 1577(194), 2088(1176), 2133(774)	41(0), 67(0), 71(0), 72(0), 113(0), 159(0), 177(2), 183(3), 183(1), 203(0), 225(0), 227(0), 260(0), 294(0), 303(2), 334(0), 390(0), 395(36), 426(0), 433(14), 455(5), 479(1), 504(50), 514(14), 516(1), 535(53), 590(2), 614(2), 652(19), 761(1), 904(142), 955(184), 1006(223), 1062(33), 1126(0), 1257(317), 1321(53), 1428(108), 1483(214), 1516(244), 1980(978), 2022(721)

Table S28 Harmonic vibrational frequencies(cm^{-1}) and IR intensities (KM/Mole) of $(C_5F_6)Fe(CO)_2$ **12-3S** (C_1)

B3LYP/DZP	BP86/DZP
41(0), 57(0), 74(0), 88(0), 93(0), 124(0), 145(1), 172(12), 199(3), 204(5), 242(2), 254(2), 268(1), 290(10), 356(3), 387(2), 416(3), 435(2), 436(1), 450(7), 473(15), 500(2), 520(5), 546(12), 593(17), 624(11), 661(17), 718(85), 762(46), 811(14), 963(212), 992(170), 1111(39), 1124(123), 1150(23), 1272(151), 1332(134), 1346(133), 1390(202), 1771(111), 2071(882), 2116(732)	40(0), 54(0), 72(1), 87(0), 91(0), 118(0), 145(1), 169(10), 192(1), 197(3), 232(2), 245(2), 260(1), 280(8), 344(3), 375(1), 418(1), 422(1), 444(1), 456(1), 476(2), 500(7), 515(0), 564(12), 602(10), 619(11), 634(11), 686(49), 728(58), 781(9), 925(216), 958(162), 1066(78), 1068(96), 1108(11), 1216(139), 1261(139), 1294(126), 1343(199), 1698(126), 1962(745), 2011(556)

Table S29 Harmonic vibrational frequencies(cm^{-1}) and IR intensities (KM/Mole) of $Fe_2(C_5F_6)(CO)_8$ **28-1S** (C_2)

B3LYP/DZP	BP86/DZP
34(0), 38(0), 40(0), 50(0), 62(0), 63(1), 69(0), 81(0), 93(0), 97(0), 98(0), 101(0), 105(0), 111(0), 111(0), 115(0), 119(0), 133(1), 155(4), 156(0), 210(6), 218(0), 224(1), 234(1), 252(0), 277(0), 289(1), 299(0), 301(6), 382(0), 382(4), 397(2), 399(0), 403(41), 403(0), 416(1), 420(14), 426(6), 437(1), 438(28), 442(3), 448(84), 454(1), 457(1), 458(21), 469(0), 477(0), 501(45), 510(2), 562(0), 562(1), 576(139), 603(6), 607(186), 616(0), 629(34), 634(140), 638(338), 645(17), 723(3), 725(42), 751(17), 791(3), 942(147), 976(178), 1079(31), 1104(0), 1120(77), 1254(232), 1258(65), 1281(19), 1390(100), 1398(1), 2091(104), 2094(1765), 2113(861), 2117(13), 2123(132), 2129(1985), 2167(771), 2182(23)	33(0), 35(0), 38(0), 47(0), 59(0), 61(0), 65(0), 77(0), 89(0), 94(0), 95(0), 98(0), 100(0), 107(0), 107(0), 110(0), 115(0), 129(0), 150(2), 151(0), 203(3), 211(0), 217(0), 225(0), 243(0), 268(0), 279(0), 289(0), 294(1), 379(0), 382(14), 394(15), 397(0), 414(3), 423(1), 430(5), 433(29), 435(47), 436(0), 438(3), 443(1), 456(2), 457(0), 465(1), 469(0), 474(1), 475(7), 513(23), 515(1), 549(0), 549(3), 554(139), 595(5), 604(5), 608(184), 634(59), 638(123), 640(316), 647(19), 691(47), 703(0), 713(17), 763(1), 908(153), 950(146), 1043(32), 1067(0), 1070(75), 1202(212), 1210(50), 1244(34), 1345(96), 1352(0), 2005(82), 2008(1529), 2018(163), 2022(1017), 2026(5), 2026(1426), 2080(788), 2093(20)

Table S30 Harmonic vibrational frequencies(cm^{-1}) and IR intensities (KM/Mole) of $Fe_2(C_5F_6)(CO)_8$ **28-2S** (C_s)

B3LYP/DZP	BP86/DZP
-23(0), 28(0), 38(0), 52(0), 57(1), 58(0), 79(0), 81(0), 88(0), 94(0), 94(0), 106(0), 107(0), 108(0), 109(0), 115(0), 127(0), 153(1), 181(0), 187(0), 190(3), 196(8), 213(1), 225(2), 265(4), 276(3), 293(2), 307(0), 345(1), 356(5), 373(0), 387(5), 389(0), 396(11), 400(4), 409(58), 417(0), 425(52), 428(18), 432(3), 436(6), 438(0), 452(9), 458(9), 460(16), 490(2), 495(7), 515(12), 517(41), 558(131), 564(12), 567(10), 598(41), 604(48), 609(30), 632(79), 635(218), 639(133), 644(91), 670(14), 738(11), 773(22), 789(146), 929(128), 953(32), 1054(26), 1078(103), 1128(15), 1199(126), 1203(0), 1265(261), 1395(81), 1404(39), 2085(183), 2089(638), 2092(1513), 2112(239), 2116(42), 2126(1556), 2161(1095), 2179(89)	-22(0), 26(0), 35(0), 49(0), 54(0), 55(0), 78(0), 81(0), 83(0), 90(0), 91(0), 104(0), 104(0), 106(0), 107(0), 110(0), 123(0), 147(0), 175(0), 180(0), 183(0), 189(5), 205(0), 215(3), 255(4), 270(3), 286(1), 300(0), 334(2), 345(2), 360(0), 391(10), 392(0), 407(36), 415(1), 419(5), 424(2), 430(16), 431(3), 433(9), 440(3), 458(2), 462(2), 471(4), 475(1), 481(3), 483(8), 524(5), 526(20), 549(35), 551(81), 552(6), 580(22), 601(35), 603(84), 634(320), 636(14), 637(13), 645(172), 652(22), 700(8), 745(12), 759(127), 896(119), 927(46), 1010(12), 1044(82), 1084(15), 1157(0), 1162(153), 1208(224), 1348(116), 1359(26), 1994(478), 1999(282), 2006(1172), 2020(800), 2020(6), 2025(863), 2071(990), 2088(117)

Table S31 Harmonic vibrational frequencies(cm^{-1}) and IR intensities (KM/Mole) of $Fe_2(C_5F_6)(CO)_7$ **27-1S** (C_1)

B3LYP/DZP	BP86/DZP
33(0), 45(0), 55(0), 63(0), 77(0), 81(0), 90(0), 92(0), 97(0), 101(0), 111(0), 115(0), 122(0), 130(1), 135(2), 157(0), 171(1), 174(0), 180(3), 209(2), 210(0), 226(2), 240(2), 245(0), 267(2), 278(2), 299(2), 338(10), 389(13), 396(3), 400(1), 412(9), 416(1), 424(25), 429(1), 441(5), 445(1), 453(2), 460(8), 479(23), 486(5), 493(7), 501(27), 517(3), 520(20), 546(46), 564(1), 570(35), 586(31), 593(48), 602(46), 617(176), 625(29), 627(35), 641(127), 736(29), 777(34), 823(101), 933(138), 967(165), 1069(16), 1084(50), 1127(158), 1222(75), 1274(186), 1355(88), 1468(117), 1611(181), 2063(217), 2070(75), 2097(636), 2109(1356), 2111(681), 2117(1594), 2168(482)	14(0), 46(0), 55(0), 58(0), 75(0), 81(0), 87(0), 92(0), 94(0), 98(0), 109(0), 114(0), 116(0), 129(1), 137(1), 153(1), 166(1), 171(2), 182(1), 201(1), 206(0), 219(1), 230(1), 238(0), 257(2), 272(1), 291(3), 330(6), 380(2), 396(1), 406(3), 412(3), 422(2), 425(8), 431(5), 437(18), 456(5), 462(0), 473(1), 475(5), 493(1), 495(4), 510(6), 519(9), 524(15), 543(20), 548(1), 561(12), 581(47), 590(27), 593(56), 609(43), 610(134), 628(49), 635(142), 693(20), 745(35), 786(101), 902(136), 937(142), 1030(17), 1040(60), 1080(140), 1176(93), 1224(170), 1309(74), 1434(120), 1525(214), 1969(126), 1988(50), 2009(478), 2011(1292), 2021(184), 2032(1567), 2080(423)

Table S32 Harmonic vibrational frequencies(cm^{-1}) and IR intensities (KM/Mole) of $Fe_2(C_5F_6)(CO)_7$ **27-2S** (C_1)

B3LYP/DZP	BP86/DZP
32(0), 36(0), 41(0), 50(0), 63(0), 64(0), 69(0), 86(0), 88(0), 94(0), 98(0), 100(0), 107(0), 110(0), 113(0), 125(0), 149(2), 154(1), 186(5), 208(10), 219(2), 225(1), 246(8), 254(1), 280(0), 291(8), 297(2), 372(2), 383(2), 398(1), 402(17), 405(2), 418(6), 422(3), 426(4), 431(10), 438(8), 441(5), 445(3), 452(46), 458(11), 462(12), 473(3), 485(12), 506(19), 551(48), 562(4), 568(80), 588(45), 597(88), 607(100), 620(79), 632(76), 642(174), 725(19), 735(24), 753(15), 794(6), 948(157), 971(182), 1073(22), 1104(2), 1119(82), 1256(148), 1266(150), 1284(11), 1358(74), 1392(37), 2091(68), 2094(1736), 2095(596), 2114(550), 2125(1126), 2144(874), 2176(220)	30(0), 35(0), 38(0), 46(0), 59(0), 62(0), 68(0), 81(0), 85(0), 91(0), 96(0), 96(0), 103(0), 106(0), 109(0), 121(0), 146(1), 152(0), 177(4), 201(6), 211(1), 217(0), 237(9), 243(0), 270(0), 283(5), 288(2), 365(1), 382(6), 395(9), 401(1), 414(4), 423(8), 427(4), 436(8), 438(15), 440(4), 447(4), 454(2), 456(4), 462(0), 470(2), 475(4), 491(10), 515(11), 549(1), 557(15), 572(121), 584(63), 596(46), 609(125), 626(27), 638(69), 644(184), 696(37), 709(5), 717(12), 766(4), 913(166), 944(157), 1033(22), 1063(11), 1071(73), 1206(129), 1210(129), 1243(28), 1284(65), 1345(47), 1993(498), 1994(631), 2007(1005), 2020(882), 2026(533), 2050(712), 2087(269)

Table S33 Harmonic vibrational frequencies(cm^{-1}) and IR intensities (KM/Mole) of $Fe_2(C_5F_6)(CO)_7$ **27-3S** (C_s)

B3LYP/DZP	BP86/DZP
8(3), 46(0), 60(2), 70(0), 76(0), 81(0), 96(0), 97(0), 106(0), 106(1), 113(0), 114(0), 126(0), 127(0), 139(0), 169(0), 179(30), 195(7), 203(0), 212(9), 213(0), 223(0), 251(5), 252(0), 269(0), 270(2), 301(11), 302(37), 315(11), 374(5), 384(20), 392(0), 423(4), 425(8), 427(27), 437(1), 443(3), 444(19), 456(12), 464(17), 469(4), 478(1), 502(63), 515(22), 521(0), 540(51), 544(10), 571(167), 577(52), 596(24), 601(105), 605(90), 619(30), 643(181), 655(28), 734(28), 748(57), 782(1), 954(123), 983(132), 1107(57), 1122(0), 1148(85), 1303(330), 1310(10), 1320(111), 1504(169), 1513(83), 1892(466), 2084(0), 2090(9), 2101(813), 2109(1141), 2119(2007), 2157(491)	21(0), 46(0), 62(1), 66(0), 73(0), 79(0), 92(0), 93(0), 102(0), 102(0), 108(0), 109(0), 123(0), 123(0), 132(0), 164(0), 187(3), 193(3), 198(0), 211(0), 220(6), 220(0), 246(0), 251(5), 262(0), 262(2), 303(2), 303(6), 341(54), 380(1), 383(15), 390(2), 412(5), 423(1), 433(7), 436(28), 441(0), 456(7), 459(18), 476(1), 484(7), 490(3), 500(31), 516(11), 519(4), 532(6), 549(8), 564(154), 579(27), 583(45), 592(84), 597(79), 614(35), 636(199), 640(22), 707(25), 727(65), 750(1), 919(113), 952(125), 1053(78), 1074(0), 1101(58), 1247(302), 1256(14), 1267(105), 1426(239), 1432(86), 1835(378), 1993(83), 2002(8), 2006(647), 2021(1030), 2034(1526), 2067(424)

Table S34 Harmonic vibrational frequencies(cm^{-1}) and IR intensities (KM/Mole) of $Fe_2(C_5F_6)(CO)_7$ **27-4T** (C_1)

B3LYP/DZP	BP86/DZP
10(0), 35(0), 40(1), 48(0), 53(1), 61(1), 63(0), 65(0), 72(1), 86(0), 94(0), 98(0), 100(1), 106(1), 110(1), 119(3), 136(2), 148(5), 192(7), 204(6), 214(0), 228(2), 242(1), 256(0), 278(0), 291(3), 295(1), 297(3), 322(33), 344(7), 367(37), 377(21), 381(7), 384(10), 398(13), 399(0), 413(28), 420(18), 428(1), 435(1), 438(2), 444(90), 451(36), 457(11), 463(12), 472(23), 483(50), 506(19), 539(135), 562(0), 603(77), 613(7), 631(78), 641(179), 701(11), 719(57), 738(10), 790(5), 936(119), 978(179), 1088(42), 1107(18), 1115(72), 1254(262), 1266(70), 1298(29), 1396(56), 1456(58), 2085(793), 2090(436), 2094(1517), 2114(639), 2126(1130), 2138(962), 2176(237)	16(0), 33(0), 36(0), 44(0), 52(1), 62(0), 63(0), 69(1), 76(0), 82(0), 91(0), 92(0), 97(0), 104(0), 109(0), 112(2), 124(0), 147(2), 187(0), 195(2), 206(0), 219(0), 229(2), 246(0), 267(1), 284(0), 287(0), 310(1), 340(2), 370(28), 378(9), 388(0), 399(7), 419(2), 421(38), 425(16), 433(44), 436(0), 450(5), 456(26), 459(4), 464(7), 468(9), 473(6), 506(34), 512(38), 517(91), 529(20), 536(9), 549(0), 593(8), 605(82), 635(68), 642(173), 657(15), 678(9), 698(59), 761(4), 908(139), 950(128), 1054(45), 1060(64), 1077(25), 1202(243), 1218(51), 1264(41), 1343(57), 1422(51), 1971(889), 1984(574), 2009(857), 2019(1073), 2024(918), 2029(287), 2088(365)

Table S35 Harmonic vibrational frequencies(cm^{-1}) and IR intensities (KM/Mole) of $Fe_2(C_5F_6)(CO)_6$ **26-1S** (C_1)

B3LYP/DZP	BP86/DZP
30(0), 46(0), 55(0), 70(0), 79(0), 82(1), 85(0), 91(1), 100(0), 102(0), 105(0), 107(0), 112(0), 131(1), 142(2), 167(2), 185(3), 203(0), 214(1), 216(2), 234(2), 244(1), 264(1), 284(2), 312(3), 341(3), 363(16), 382(4), 404(7), 409(2), 415(9), 426(1), 441(7), 445(5), 452(5), 469(26), 476(6), 488(6), 496(18), 508(20), 525(26), 532(37), 543(41), 562(39), 576(56), 586(5), 607(44), 618(109), 629(17), 633(32), 709(16), 767(15), 836(107), 932(126), 975(120), 1086(73), 1091(18), 1128(102), 1235(188), 1276(181), 1347(134), 1447(101), 1532(256), 2037(571), 2069(257), 2108(674), 2115(1166), 2121(1163), 2162(609)	36(0), 45(0), 51(0), 68(0), 76(0), 80(0), 83(0), 90(0), 98(0), 100(1), 101(1), 107(0), 111(0), 132(1), 142(0), 166(1), 187(0), 193(2), 208(1), 213(1), 226(1), 238(0), 257(1), 278(2), 305(2), 327(1), 359(5), 394(3), 398(5), 409(16), 425(7), 426(5), 436(3), 454(6), 463(6), 478(3), 483(3), 490(6), 502(3), 511(5), 523(10), 536(49), 540(29), 567(72), 581(5), 588(14), 593(43), 610(96), 619(11), 639(50), 669(6), 735(16), 794(90), 900(119), 933(67), 1039(106), 1056(9), 1085(104), 1181(206), 1210(151), 1288(162), 1351(204), 1480(224), 1967(353), 1983(80), 2006(518), 2008(804), 2029(1540), 2065(444)

Table S36 Harmonic vibrational frequencies(cm^{-1}) and IR intensities (KM/Mole) of $Fe_2(C_5F_6)(CO)_6$ **26-2T** (C_1)

B3LYP/DZP	BP86/DZP
35(0), 46(0), 51(0), 60(0), 68(0), 82(0), 84(0), 86(0), 91(0), 92(0), 97(0), 105(0), 109(0), 113(1), 151(2), 157(0), 169(0), 191(1), 214(3), 224(2), 234(1), 240(0), 260(3), 273(0), 298(2), 333(3), 335(0), 343(4), 387(2), 394(3), 403(1), 409(14), 419(1), 423(6), 434(8), 449(33), 453(0), 463(4), 472(27), 482(9), 498(2), 503(26), 522(34), 545(24), 549(76), 563(19), 564(32), 575(53), 585(9), 617(9), 731(19), 764(59), 793(25), 936(107), 971(139), 1071(38), 1095(42), 1132(153), 1220(69), 1262(239), 1367(74), 1474(152), 1621(233), 2059(184), 2070(204), 2083(1367), 2085(636), 2113(1692), 2145(420)	37(0), 41(0), 47(0), 60(0), 72(0), 84(0), 85(0), 87(0), 88(0), 91(0), 96(0), 103(0), 111(1), 117(0), 145(3), 161(2), 172(0), 194(0), 205(2), 221(0), 228(1), 235(0), 250(2), 264(1), 288(2), 324(5), 331(12), 352(0), 393(3), 404(1), 409(40), 414(2), 426(2), 445(3), 447(9), 455(0), 462(1), 473(17), 476(31), 487(5), 489(5), 497(7), 527(24), 540(39), 548(79), 558(36), 562(44), 573(10), 587(49), 598(4), 678(5), 715(91), 756(7), 906(118), 933(126), 1032(34), 1046(82), 1088(117), 1182(98), 1219(213), 1330(78), 1433(162), 1543(274), 1956(283), 1972(5), 1985(793), 1990(866), 2016(1447), 2045(376)

Table S37 Harmonic vibrational frequencies(cm^{-1}) and IR intensities (KM/Mole) of $Fe_2(C_5F_6)(CO)_6$ **26-3S** (C_2)

B3LYP/DZP	BP86/DZP
32(0), 35(0), 40(0), 43(0), 66(0), 66(0), 71(1), 81(0), 87(0), 89(0), 95(0), 101(0), 104(0), 119(0), 142(3), 151(0), 180(3), 188(6), 207(17), 221(0), 244(1), 254(0), 255(13), 277(13), 283(0), 370(0), 372(4), 399(6), 405(0), 422(5), 423(0), 429(5), 431(1), 433(19), 435(4), 443(0), 447(0), 459(24), 461(0), 485(28), 486(2), 549(75), 554(4), 567(70), 574(71), 590(45), 594(4), 615(232), 618(9), 733(1), 738(38), 752(14), 799(8), 955(165), 965(192), 1069(14), 1101(1), 1119(91), 1264(76), 1269(212), 1289(4), 1347(127), 1364(2), 2091(10), 2092(102), 2094(1729), 2095(1306), 2137(1508), 2152(18)	31(0), 34(0), 38(0), 40(0), 63(0), 65(0), 71(0), 79(0), 84(0), 87(0), 93(0), 99(0), 102(0), 117(0), 141(1), 153(0), 172(2), 181(4), 203(11), 213(0), 236(1), 244(0), 245(13), 269(14), 273(0), 361(0), 368(3), 397(6), 405(0), 413(4), 424(5), 430(0), 434(2), 442(4), 448(0), 452(5), 454(2), 463(0), 468(2), 487(14), 494(3), 557(12), 569(1), 572(88), 580(62), 592(23), 606(184), 625(66), 628(1), 705(32), 709(2), 719(7), 772(5), 919(175), 935(177), 1025(12), 1058(1), 1071(95), 1205(55), 1214(190), 1244(7), 1270(147), 1289(0), 1991(111), 1992(256), 1994(955), 1995(1466), 2045(1215), 2056(13)

Table S38 Harmonic vibrational frequencies(cm^{-1}) and IR intensities (KM/Mole) of $Fe_2(C_5F_6)(CO)_6$ **26-4S** (C_1)

B3LYP/DZP	BP86/DZP
35(0), 40(0), 45(0), 54(0), 64(0), 71(0), 87(0), 89(0), 95(0), 99(0), 102(0), 107(0), 114(0), 125(1), 151(4), 152(1), 174(21), 208(7), 217(1), 225(0), 251(11), 255(0), 279(0), 293(7), 298(5), 380(1), 387(2), 399(1), 404(18), 413(0), 419(4), 430(1), 435(10), 439(12), 447(31), 451(32), 458(11), 464(2), 473(3), 497(15), 506(13), 546(12), 563(2), 576(146), 593(8), 606(94), 621(45), 633(78), 642(178), 722(17), 737(19), 748(28), 793(24), 942(177), 971(186), 1067(6), 1104(6), 1123(74), 1254(116), 1265(172), 1281(23), 1344(83), 1392(39), 2068(844), 2090(1006), 2108(1371), 2115(72), 2124(1150), 2174(308)	33(0), 38(0), 43(0), 51(0), 62(0), 69(0), 85(0), 88(0), 93(0), 96(0), 99(0), 104(0), 109(0), 122(0), 146(2), 155(0), 170(17), 201(3), 208(0), 216(0), 243(8), 245(2), 270(0), 284(4), 289(2), 373(1), 385(9), 394(9), 411(1), 424(8), 429(2), 435(13), 438(7), 446(12), 450(3), 461(2), 467(3), 475(5), 477(3), 508(6), 515(11), 549(1), 558(49), 570(65), 598(20), 609(105), 630(24), 637(60), 644(185), 697(41), 702(4), 716(23), 765(18), 906(188), 943(157), 1023(8), 1064(10), 1076(68), 1201(97), 1213(142), 1237(53), 1281(67), 1342(47), 1961(673), 2005(927), 2007(926), 2018(743), 2025(450), 2086(338)

Table S39 Harmonic vibrational frequencies(cm^{-1}) and IR intensities (KM/Mole) of $Fe_2(C_5F_6)(CO)_5$ **25-1S** (C_1)

B3LYP/DZP	BP86/DZP
29(0), 54(0), 59(0), 66(0), 79(0), 84(0), 90(0), 96(0), 99(0), 112(1), 116(1), 146(1), 163(2), 173(6), 198(3), 203(1), 212(1), 226(3), 237(1), 251(0), 267(1), 272(1), 325(2), 349(6), 365(3), 399(1), 415(3), 419(4), 430(2), 446(4), 456(2), 464(13), 476(12), 488(13), 499(4), 515(4), 524(58), 532(41), 557(43), 574(23), 582(18), 602(41), 612(131), 636(23), 645(10), 712(9), 763(17), 824(105), 933(106), 975(70), 1079(74), 1106(26), 1128(103), 1247(296), 1281(143), 1344(165), 1411(166), 1520(247), 2024(533), 2082(350), 2095(1029), 2113(1826), 2140(348)	26(0), 51(0), 57(0), 68(0), 73(0), 80(0), 85(0), 94(0), 98(0), 108(1), 115(1), 152(1), 171(1), 186(1), 192(0), 201(1), 206(1), 229(1), 233(2), 247(0), 260(1), 267(1), 320(1), 335(7), 347(2), 392(8), 407(8), 413(2), 435(0), 454(4), 460(1), 465(3), 484(3), 487(8), 500(0), 516(17), 523(37), 541(51), 556(38), 577(22), 579(4), 587(13), 600(71), 631(78), 652(6), 677(7), 731(16), 776(76), 900(101), 935(65), 1030(89), 1058(25), 1083(94), 1196(283), 1223(139), 1286(185), 1321(230), 1468(272), 1915(408), 1982(489), 2005(694), 2017(1547), 2044(345)

Table S40 Harmonic vibrational frequencies(cm^{-1}) and IR intensities (KM/Mole) of $Fe_2(C_5F_6)(CO)_5$ **25-2S** (C_1)

B3LYP/DZP	BP86/DZP
43(0), 49(2), 53(0), 71(0), 79(0), 81(0), 87(1), 94(0), 96(0), 97(0), 113(1), 124(3), 165(0), 180(1), 199(3), 201(0), 212(2), 227(0), 242(3), 246(1), 262(1), 275(2), 316(1), 351(2), 368(30), 396(1), 403(17), 412(0), 430(1), 437(8), 443(0), 449(16), 474(6), 478(3), 494(28), 501(16), 520(55), 528(14), 533(58), 555(65), 572(34), 581(27), 592(35), 619(39), 628(22), 723(7), 757(48), 800(73), 935(151), 962(97), 1081(74), 1097(25), 1135(112), 1249(207), 1267(206), 1335(156), 1419(134), 1526(232), 2066(580), 2070(189), 2095(1373), 2108(1552), 2144(493)	35(0), 42(0), 55(0), 69(0), 78(0), 78(0), 83(1), 89(0), 92(0), 95(0), 109(1), 120(1), 161(0), 185(0), 198(0), 202(2), 209(1), 222(0), 238(0), 246(1), 256(1), 265(2), 313(1), 339(1), 377(8), 394(3), 403(1), 410(12), 431(2), 438(5), 446(2), 464(4), 473(1), 482(2), 499(6), 502(4), 524(50), 528(17), 545(35), 564(76), 570(29), 589(4), 594(53), 604(13), 623(40), 690(3), 724(46), 760(66), 899(137), 929(66), 1031(76), 1054(33), 1091(87), 1202(257), 1206(180), 1276(181), 1342(170), 1457(273), 1967(437), 1985(204), 1997(990), 2015(1415), 2047(427)

Table S41 Harmonic vibrational frequencies(cm^{-1}) and IR intensities (KM/Mole) of $Fe_2(C_5F_6)(CO)_5$ **25-3T** (C_1)

B3LYP/DZP	BP86/DZP
43(0), 45(0), 53(0), 62(0), 73(0), 75(1), 79(0), 86(0), 91(0), 107(1), 127(0), 153(2), 163(3), 176(0), 189(2), 202(3), 211(2), 218(0), 232(3), 245(3), 259(2), 264(1), 308(4), 316(3), 333(2), 369(7), 376(5), 393(22), 406(13), 413(9), 420(5), 425(5), 443(18), 453(6), 458(9), 484(26), 495(3), 507(51), 524(53), 531(4), 534(20), 563(47), 569(3), 589(40), 620(5), 702(11), 761(27), 817(68), 942(120), 970(92), 1080(62), 1097(41), 1134(119), 1243(170), 1260(253), 1332(154), 1423(144), 1580(166), 1986(508), 2078(98), 2091(1309), 2108(1757), 2142(476)	31(0), 42(0), 47(0), 63(0), 73(0), 75(0), 75(0), 84(0), 92(0), 107(1), 121(0), 151(1), 161(0), 181(1), 190(1), 197(2), 206(1), 221(0), 234(1), 245(1), 246(2), 256(1), 305(2), 309(5), 331(1), 367(14), 389(13), 393(11), 400(5), 417(7), 430(10), 435(5), 450(2), 457(8), 475(9), 482(4), 497(18), 512(20), 520(53), 533(37), 543(29), 556(9), 567(15), 594(38), 607(27), 666(5), 726(26), 774(54), 903(114), 934(112), 1031(83), 1053(28), 1086(94), 1200(252), 1213(177), 1285(180), 1342(187), 1488(224), 1893(361), 1985(55), 1998(1207), 2012(1564), 2044(438)

Table S42 Harmonic vibrational frequencies(cm^{-1}) and IR intensities (KM/Mole) of $Fe_2(C_5F_6)(CO)_5$ **25-4S** (C_1)

B3LYP/DZP	BP86/DZP
36(0), 55(0), 59(0), 65(1), 74(2), 78(2), 82(2), 92(1), 98(1), 107(2), 119(6), 131(1), 148(3), 164(1), 184(2), 194(3), 212(4), 216(3), 239(0), 252(3), 260(12), 268(2), 304(2), 317(3), 375(19), 391(4), 398(11), 413(23), 421(21), 435(6), 441(12), 449(20), 463(11), 469(19), 489(13), 496(18), 508(18), 525(16), 551(25), 570(0), 583(12), 593(7), 610(68), 615(39), 638(50), 707(2), 767(10), 834(49), 944(129), 986(63), 1081(66), 1102(35), 1142(123), 1222(117), 1263(201), 1330(165), 1424(160), 1618(113), 1897(396), 2066(56), 2087(1402), 2095(2154), 2138(646)	34(0), 49(0), 56(0), 63(1), 73(1), 76(1), 82(1), 90(0), 98(1), 104(0), 119(2), 131(4), 140(1), 157(0), 179(1), 197(2), 207(3), 211(1), 231(0), 244(0), 254(3), 265(2), 296(2), 313(2), 369(9), 381(7), 384(11), 408(2), 430(9), 440(34), 443(5), 448(8), 464(6), 475(4), 481(16), 491(6), 503(11), 530(17), 545(12), 561(1), 579(5), 589(29), 593(14), 611(46), 630(60), 672(7), 737(14), 799(52), 910(109), 947(69), 1033(54), 1055(37), 1092(121), 1182(124), 1204(229), 1277(141), 1394(161), 1524(149), 1833(242), 1968(17), 1988(1091), 2002(1819), 2039(501)

Table S43 Harmonic vibrational frequencies(cm^{-1}) and IR intensities (KM/Mole) of $Fe_2(C_5F_6)(CO)_5$ **25-5S** (C_s)

B3LYP/DZP	BP86/DZP
-47(1), 47(0), 59(0), 66(1), 67(1), 79(0), 81(1), 89(0), 89(0), 105(0), 114(1), 121(3), 142(1), 166(0), 194(4), 211(0), 223(2), 231(3), 240(4), 252(1), 258(3), 274(8), 300(0), 313(6), 346(0), 390(7), 402(9), 413(25), 418(2), 420(0), 440(2), 445(2), 448(27), 457(42), 475(6), 497(16), 514(12), 535(10), 538(0), 557(25), 562(0), 584(23), 617(42), 623(68), 624(6), 739(16), 758(57), 796(1), 950(113), 974(130), 1072(1), 1089(65), 1142(161), 1257(301), 1270(3), 1381(161), 1438(88), 1551(180), 1884(342), 2063(152), 2090(1366), 2101(2061), 2140(591)	-33(1), 48(0), 54(0), 62(0), 64(1), 76(0), 78(1), 85(0), 86(0), 98(0), 110(1), 111(3), 155(1), 161(0), 200(3), 203(0), 217(0), 223(2), 236(2), 242(1), 247(2), 276(3), 293(0), 315(4), 365(3), 379(11), 399(8), 412(7), 412(6), 422(0), 437(3), 450(1), 455(3), 461(15), 478(19), 494(6), 504(8), 519(0), 527(16), 547(3), 552(30), 576(27), 602(4), 607(60), 613(37), 698(21), 724(51), 762(4), 916(107), 939(129), 1023(1), 1051(83), 1093(124), 1199(307), 1222(3), 1348(183), 1393(93), 1460(167), 1821(252), 1964(80), 1989(1193), 2010(1619), 2039(449)

Table S44 Harmonic vibrational frequencies(cm^{-1}) and IR intensities (KM/Mole) of $Fe_2(C_5F_6)(CO)_5$ **25-6T** (C_1)

B3LYP/DZP	BP86/DZP
5(0), 32(0), 37(0), 44(0), 56(0), 61(1), 67(1), 70(1), 78(0), 87(0), 96(0), 110(1), 121(5), 142(0), 181(6), 190(3), 206(9), 218(1), 245(5), 254(1), 262(4), 265(4), 281(1), 284(10), 369(4), 372(0), 385(1), 393(16), 406(11), 419(13), 422(3), 423(35), 432(9), 436(18), 446(4), 456(84), 464(12), 478(9), 489(7), 549(26), 560(142), 579(44), 596(61), 613(15), 712(14), 737(26), 744(25), 784(17), 943(124), 964(191), 1074(20), 1091(40), 1120(63), 1260(190), 1268(141), 1285(36), 1358(85), 1406(62), 2073(1143), 2092(1104), 2094(683), 2126(1467), 2148(201)	21(0), 27(0), 34(0), 38(0), 51(0), 55(1), 67(0), 74(0), 78(1), 84(0), 94(0), 107(1), 118(3), 144(1), 171(6), 185(5), 203(5), 208(0), 233(5), 241(1), 253(1), 268(0), 277(9), 322(1), 356(1), 363(9), 381(1), 394(3), 406(13), 413(5), 426(4), 438(5), 443(1), 454(4), 458(1), 472(3), 482(37), 487(5), 498(23), 528(78), 566(110), 580(67), 586(11), 622(27), 668(10), 681(47), 716(22), 762(6), 901(158), 940(163), 1020(60), 1039(8), 1080(28), 1212(59), 1214(224), 1258(76), 1275(53), 1389(66), 1964(1021), 1992(650), 1995(798), 2010(1624), 2052(361)

Table S45. Total energies (E and E_{ZPVE}, in Hartree), relative energies with and without ZPVE corrections (ΔE and ΔE_{ZPVE} in kcal/mol), ΔH and ΔG (in kcal/mol) at the standard condition, the LUMO-HOMO gaps (in eV), and number of imaginary vibrational frequencies (Nimag) for the $(C_5F_6)Fe(CO)_4$ and $(C_5F_6)Fe(CO)_3$ structures.

	14-1S(C_1)	**13-1S**(C_s)	**13-2S**(C_1)
B3LYP			
$-E$	2506.90577	2393.56112	2393.52102
$-E_{ZPVE}$	2506.82495	2393.48860	2393.44962
ΔE	0.0	0.0	25.2
ΔE_{ZPVE}	0.0	0.0	24.5
ΔH	0.0	0.0	24.8
ΔG	0.0	0.0	23.3
Nimag	none	none	none
LUMO-HOMO	5.0	5.6	3.1
BP86			
$-E$	2507.16515	2393.82034	2393.77049
$-E_{ZPVE}$	2507.08684	2393.75000	2393.70142
ΔE	0.0	0.0	31.3
ΔE_{ZPVE}	0.0	0.0	30.5
ΔH	0.0	0.0	30.9
ΔG	0.0	0.0	29.3
Nimag	none	none	none
LUMO-HOMO	3.2	3.7	1.3

Table S46. Total energies (E and E_{ZPVE}, in Hartree), relative energies with and without ZPVE corrections (ΔE and ΔE_{ZPVE} in kcal/mol), ΔH and ΔG (in kcal/mol) at the standard condition, the LUMO-HOMO gaps (in eV), spin expectation values (S^2), and number of imaginary vibrational frequencies (Nimag) for three $(C_5F_6)Fe(CO)_2$ structures.

	12-1S(C_s)	**12-2T**(C_s)	**12-3S**(C_1)
B3LYP			
$-E$	2280.16122	2280.16057	2280.12859
$-E_{ZPVE}$	2280.09804	2280.09913	2280.06576
ΔE	0.0	0.4	20.5
ΔE_{ZPVE}	0.0	-0.7	20.3
ΔH	0.0	-0.2	20.4
ΔG	0.0	-1.9	19.7
Nimag	none	none	none
S^2	0.00	2.11	0.00
LUMO-HOMO	3.5	(α)4.4	3.3
		(β)3.0	
BP86			
$-E$	2280.41320	2280.39229	2280.36973
$-E_{ZPVE}$	2280.35192	2280.33252	2280.30897
ΔE	0.0	13.1	27.3
ΔE_{ZPVE}	0.0	13.0	27.0
ΔH	0.0	12.5	27.1
ΔG	0.0	11.0	26.3
Nimag	none	none	none
S^2	0.00	2.03	0.00
LUMO-HOMO	1.8	(α)2.9	1.4
		(β)1.4	

Table S47. Total energies (E and E_{ZPVE}, in Hartree), relative energies with and without ZPVE corrections (ΔE and ΔE_{ZPVE} in kcal/mol), ΔH and ΔG (in kcal/mol) at the standard condition, the LUMO-HOMO gaps (in eV), and number of imaginary vibrational frequencies (Nimag) for two $(C_5F_6)Fe_2(CO)_8$ structures.

	28-1S(C_2)	**28-2S**(C_s)
B3LYP		
$-E$	4224.13944	4224.08009
$-E_{ZPVE}$	4224.02386	4224.96520
ΔE	0.0	37.2
ΔE_{ZPVE}	0.0	36.6
ΔH	0.0	36.3
ΔG	0.0	37.4
Nimag	none	23i
LUMO-HOMO	5.2	4.3
BP86		
$-E$	4224.65150	4224.59677
$-E_{ZPVE}$	4224.53902	4224.48500
ΔE	0.0	34.3
ΔE_{ZPVE}	0.0	33.9
ΔH	0.0	33.4
ΔG	0.0	34.5
Nimag	none	22i
LUMO-HOMO	3.4	2.6

Table S48. Total energies (E and E_{ZPVE}, in Hartree), relative energies with and without ZPVE corrections (ΔE and ΔE_{ZPVE} in kcal/mol), ΔH and ΔG (in kcal/mol) at the standard condition, the LUMO-HOMO gaps (in eV), spin expectation values (S^2), and number of imaginary vibrational frequencies (Nimag) for four $(C_5F_6)Fe_2(CO)_7$ structures.

	27-1S(C_1)	**27-2S**(C_1)	**27-3S**(C_s)	**27-4T**(C_1)
B3LYP				
$-E$	4110.76162	4110.75485	4110.72445	4110.75265
$-E_{ZPVE}$	4110.65419	4110.64872	4110.61762	4110.64881
ΔE	0.0	4.2	23.3	5.6
ΔE_{ZPVE}	0.0	3.4	22.9	3.4
ΔH	0.0	3.8	22.4	4.4
ΔG	0.0	1.9	24.4	-0.5
Nimag	none	none	none	none
S^2	0.00	0.00	0.00	2.09
LUMO-HOMO	3.8	3.2	4.1	(α)4.9
				(β)2.6
BP86				
$-E$	4111.27755	4111.25670	4111.25213	4111.24090
$-E_{ZPVE}$	4111.17315	4111.15351	4111.14814	4111.13917
ΔE	0.0	13.1	16.0	23.0
ΔE_{ZPVE}	0.0	12.3	15.7	21.3
ΔH	0.0	12.6	15.7	22.1
ΔG	0.0	11.1	16.2	18.3
Nimag	none	none	none	none
S^2	0.00	0.00	0.00	2.02
LUMO-HOMO	2.4	1.5	2.5	(α)2.7
				(β)1.0

Table S49. Total energies (E and E_{ZPVE}, in Hartree), relative energies with and without ZPVE corrections (ΔE and ΔE_{ZPVE} in kcal/mol), ΔH and ΔG (in kcal/mol) at the standard condition, the LUMO-HOMO gaps (in eV), spin expectation values (S^2), and number of imaginary vibrational frequencies (Nimag) for four $(C_5F_6)Fe_2(CO)_6$ structures.

	26-1S(C_1)	**26-2T**(C_1)	**26-3S**(C_2)	**26-4S**(C_1)
B3LYP				
$-E$	3997.39250	3997.39259	3997.37013	3997.36212
$-E_{ZPVE}$	3997.29464	3997.29635	3997.27351	3997.26454
ΔE	0.0	0.0	14.0	19.0
ΔE_{ZPVE}	0.0	-1.0	13.2	18.8
ΔH	0.0	-0.6	13.6	18.9
ΔG	0.0	-2.4	12.2	18.4
Nimag	none	none	none	none
S^2	0.00	2.08	0.00	0.00
LUMO-HOMO	2.8	(α)4.3	3.2	3.4
		(β)3.0		
BP86				
$-E$	3997.90144	3997.88688	3997.86185	3997.85608
$-E_{ZPVE}$	3997.80640	3997.79328	3997.76797	3997.76115
ΔE	0.0	9.1	24.8	28.5
ΔE_{ZPVE}	0.0	8.2	24.1	28.4
ΔH	0.0	8.6	24.4	28.4
ΔG	0.0	7.0	22.9	27.7
Nimag	none	none	none	none
S^2	0.00	2.02	0.00	0.00
LUMO-HOMO	1.3	(α)2.3	1.4	1.4
		(β)1.1		

Table S50. Total energies (E and E_{ZPVE}, in Hartree), relative energies with and without ZPVE corrections (ΔE and ΔE_{ZPVE} in kcal/mol), ΔH and ΔG (in kcal/mol) at the standard condition, the LUMO-HOMO gaps (in eV), spin expectation values (S^2), and number of imaginary vibrational frequencies (Nimag) for the six $(C_5F_6)Fe_2(CO)_5$ structures.

	25-1S(C_1)	**25-2S**(C_1)	**25-3T**(C_1)	**25-4S**(C_1)	**25-5S**(C_s)	**25-6T**(C_1)
B3LYP						
$-E$	3884.02356	3884.00756	3884.01961	3883.99459	3883.98821	3884.00302
$-E_{ZPVE}$	3883.93400	3883.91861	3883.93206	3883.90599	3883.90000	3883.91654
ΔE	0.0	10.0	2.5	18.2	22.2	12.9
ΔE_{ZPVE}	0.0	9.7	1.2	17.6	21.3	11.0
ΔH	0.0	9.8	1.7	17.8	21.1	11.9
ΔG	0.0	9.5	0.1	17.3	21.9	6.7
Nimag	none	none	none	none	1(47i)	none
S^2	0.00	0.00	2.10	0.00	0.00	2.11
LUMO-HOMO	3.5	3.1	(α)3.6 (β)3.3	2.3	2.4	(α)3.1 (β)2.6
BP86						
$-E$	3884.52699	3884.51377	3884.50768	3884.50067	3884.49755	3884.46313
$-E_{ZPVE}$	3884.44017	3884.42740	3884.42270	3884.41481	3884.41210	3884.37913
ΔE	0.0	8.3	12.1	16.5	18.5	40.1
ΔE_{ZPVE}	0.0	8.0	10.9	15.9	17.6	38.3
ΔH	0.0	8.2	11.4	16.2	17.4	39.2
ΔG	0.0	7.8	9.7	15.5	18.1	34.7
Nimag	none	none	none	none	1(33i)	none
S^2	0.00	0.00	2.04	0.00	0.00	2.04
LUMO-HOMO	1.7	1.4	(α)1.7 (β)1.2	0.9	0.9	(α)0.8 (β)0.7

Table S51. The *v*(CO) frequencies of the mononuclear $(C_5F_6)Fe(CO)_n$ (n = 4, 3, 2) and binuclear $(C_5F_6)Fe_2(CO)_n$ (n = 8, 7, 6, 5) derivatives (with the BP86 method). Infrared intensities are given in parentheses in km/mol.

Structures	ν (CO)
$(C_5F_6)Fe(CO)_4$ **(14-1S)**	2088(262), 2028(464), 2019(816), 2007(881)
$(C_5F_6)Fe(CO)_3$ **(13-1S)**	2057(530), 2009(716),2000(679)
$(C_5F_6)Fe(CO)_3$ **(13-2S)**	2052(442), 1996(842),1991(611)
$(C_5F_6)Fe(CO)_2$ **(12-1S)**	2022(722),1979(790)
$(C_5F_6)Fe(CO)_2$ **(12-2T)**	2022(721),1980(978)
$(C_5F_6)Fe(CO)_2$ **(12-3S)**	2011(556),1962(745)
$(C_5F_6)Fe_2(CO)_8$ **(28-1S)**	2093(20), 2080(788), 2026(1426), 2026(5), 2022(1017), 2018(163), 2008(1529), 2005(82)
$(C_5F_6)Fe_2(CO)_8$ **(28-2S)**	2088(117), 2071(990), 2025(863), 2020(800), 2020(6), 2006(1172), 1999(282), 1994(478)
$(C_5F_6)Fe_2(CO)_7$ **(27-1S)**	2080(423), 2032(1567), 2021(184), 2011(1292), 2009(478), 1988(50), 1969(126)
$(C_5F_6)Fe_2(CO)_7$ **(27-2S)**	2087(269), 2050(712),2026(533), 2020(882), 2007(1005), 1994(631), 1993(498)
$(C_5F_6)Fe_2(CO)_7$ **(27-3S)**	2067(424), 2034(1526), 2021(1030), 2006(647), 2002(8), 1993(83), **1835(378)**
$(C_5F_6)Fe_2(CO)_7$ **(27-4T)**	2088(365), 2029(287), 2024(918), 2019(1073), 2009(857), 1984(574), 1971(889)
$(C_5F_6)Fe_2(CO)_6$ **(26-1S)**	2065(444), 2029(1540), 2008(804), 2006(518), 1983(80), 1967(353)
$(C_5F_6)Fe_2(CO)_6$ **(26-2T)**	2045(376), 2016(1447), 1990(866), 1985(793), 1972(5), 1956(283)
$(C_5F_6)Fe_2(CO)_6$ **(26-3S)**	2055(428), 2021(1735), 2002(1152), 1993(533), 1986(130), 1964(3),
$(C_5F_6)Fe_2(CO)_6$ **(26-4S)**	2056(13), 2045(1215), 1995(1466), 1994(955), 1992(256), 1991(111)
$(C_5F_6)Fe_2(CO)_5$ **(25-1S)**	2044(345), 2017(1547), 2005(694), 1982(489), 1915(408)
$(C_5F_6)Fe_2(CO)_5$ **(25-2S)**	2047(427), 2015(1415), 1997(990), 1985(204), 1967(437)
$(C_5F_6)Fe_2(CO)_5$ **(25-3T)**	2044(438), 2012(1564), 1998(1207), 1985(55), **1893(361)**
$(C_5F_6)Fe_2(CO)_5$ **(25-4S)**	2039(501), 2002(1819), 1988(1091), 1968(17), **1833(242)**
$(C_5F_6)Fe_2(CO)_5$ **(25-5S)**	2039(449), 2010(1619), 1989(1193), 1964(80), **1821(252)**
$(C_5F_6)Fe_2(CO)_5$ **(25-6T)**	2052(361), 2010(1624), 1995(798), 1992(650), 1964(1021)

Bold face means bridging CO groups**.**

Complete Gaussian 03 reference (Reference 28)

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