The Hapticity of the Acenaphthylene Ligand in its Mononuclear, Binuclear, and Trinuclear Iron Carbonyl Complexes

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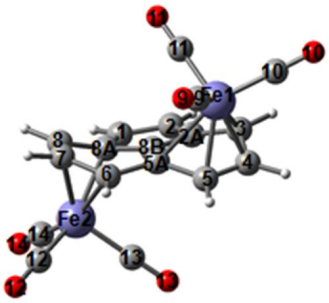
Supporting Information

Figures S1-S2: The higher energy optimized $C_{12}H_8Fe_2(CO)_n$ (n=6, 5, 4) , and $C_{12}H_8Fe_3(CO)_n$ (n=9, 8) structures.

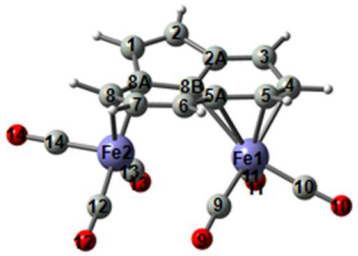
Tables S1-S30: Interatomic distances (iron-carbon distance, carbon-carbon distance, iron-carbonyl distance in Å) for $C_{12}H_8Fe(CO)_n$ (n = 4, 3, 2), $C_{12}H_8Fe_2(CO)_n$ (n = 8, 7, 6, 5, 4), and $C_{12}H_8Fe_3(CO)_n$ (n=9, 8) structures using the B3LYP, BP86 and M06-L methods.

Tables S31-S66: Theoretical Cartesian coordinates (in Å) for all of the $C_{12}H_8Fe(CO)_n$ (n=4, 3, 2), $C_{12}H_8Fe_2(CO)_n$ (n = 8, 7, 6, 5, 4), and $C_{12}H_8Fe_3(CO)_n$ (n = 9, 8) structures by the M06-L method.

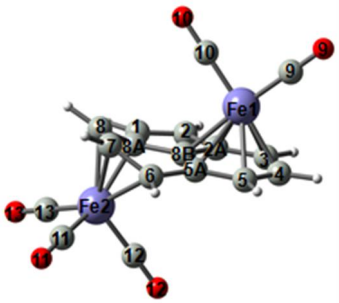
Tables S67-S78: Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses, in km/mol) for all of the $C_{12}H_8Fe(CO)_n$ (n = 4, 3, 2), $C_{12}H_8Fe_2(CO)_n$ (n = 8, 7, 6, 5, 4), and $C_{12}H_8Fe_3(CO)_n$ (n=9, 8) structures by the M06-L method.



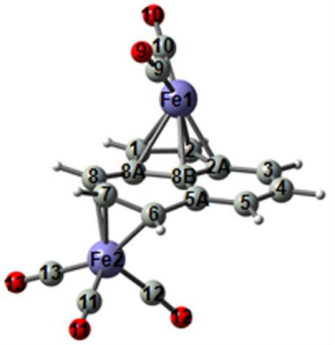
Fe26-3 (22.0 kcal/mol)
C_1 , η^4 , η^4



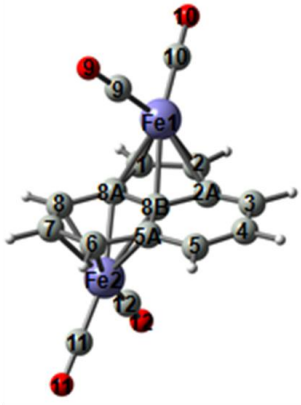
Fe26-4 (35.6 kcal/mol)
C_1 , η^4, η^2



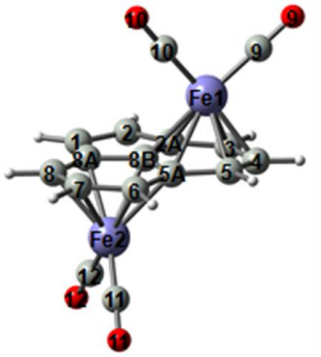
Fe25-4 (24.8 kcal/mol)
C_1 , η^6, η^4



Fe25-5 (29.8 kcal/mol)
C_1 , η^5 , η^3

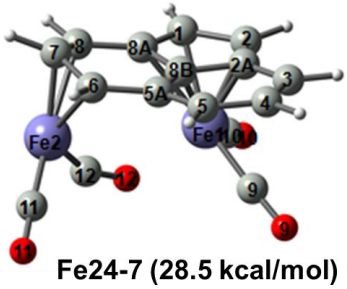


Fe24-4 (13.7 kcal/mol)
C_1, η^5, η^6



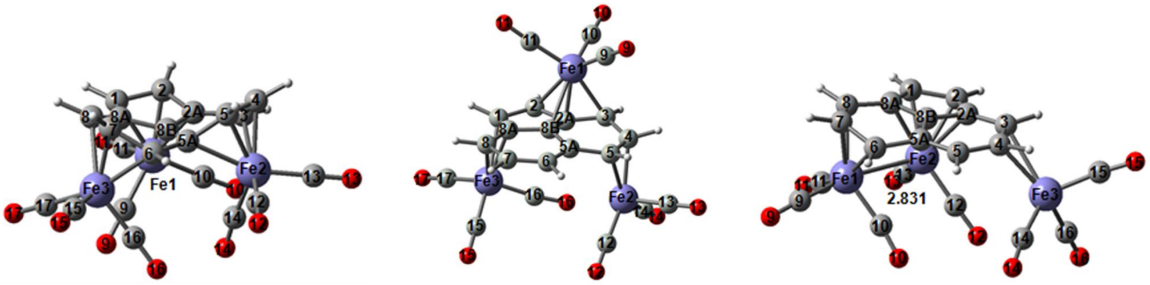
Fe24-5 (15.6 kcal/mol)
C_1 , η^6 , η^6

Fe24-6 (16.7 kcal/mol)
C_2 , η^6 , η^6



Fe24-7 (28.5 kcal/mol)
C_1 , η^5 , η^3

Figure S1. The higher energy optimized $C_{12}H_8Fe_2(CO)_n$ (n=6, 5, 4) structures.



Fe39-2 (18.7 kcal/mol)
C_1, η^4, η^3, η^3

Fe39-3 (32.6 kcal/mol)
C_1, η^4, η^3, η^2

Fe38-3 (30.2 kcal/mol)
C_1, η^5, η^3, η^2

Figure S2. The higher energy optimized $C_{12}H_8Fe_3(CO)_n$ (n=9, 8) structures.

Table S1. Iron-carbon distances (in Å) for $C_{12}H_8Fe(CO)_4$ structures using B3LYP, BP86, and M06-L methods.

	Fe14-1			Fe14-2		
	B3LYP	BP86	M06-L	B3LYP	BP86	M06-L
Fe-C1	2.185	2.181	2.158	3.085	3.045	3.018
Fe-C2	2.185	2.181	2.158	4.026	4.002	3.928
Fe-C2A	3.158	3.155	3.097	4.145	4.121	4.045
Fe-C3	4.206	4.216	4.120	5.333	5.325	5.213
Fe-C4	5.310	5.324	5.190	5.740	5.735	5.616
Fe-C5	5.584	5.599	5.454	5.187	5.178	5.083
Fe-C5A	4.842	4.853	4.731	3.945	3.921	3.869
Fe-C6	5.584	5.599	5.454	3.855	3.834	3.793
Fe-C7	5.310	5.324	5.190	3.151	3.122	3.115
Fe-C8	4.206	4.216	4.120	2.290	2.241	2.271
Fe-C8A	3.158	3.155	3.097	2.354	2.298	2.316
Fe-C8B	3.586	3.584	3.509	3.259	3.222	3.188

Table S2. Carbon-carbon distances (in Å) for $C_{12}H_8Fe(CO)_4$ structures using B3LYP, BP86, and M06-L methods.

	Fe14-1			Fe14-2		
	B3LYP	BP86	M06-L	B3LYP	BP86	M06-L
C1-C2	1.437	1.451	1.434	1.369	1.382	1.359
C2-C2A	1.490	1.491	1.473	1.471	1.472	1.453
C2A-C3	1.385	1.396	1.376	1.395	1.406	1.385
C3-C4	1.430	1.434	1.412	1.421	1.426	1.404
C4-C5	1.391	1.401	1.378	1.398	1.407	1.385
C5-C5A	1.429	1.435	1.415	1.422	1.428	1.409
C5A-C8B	1.406	1.416	1.399	1.399	1.408	1.390
C8B-C2A	1.419	1.426	1.409	1.414	1.422	1.404
C5A-C6	1.429	1.435	1.415	1.445	1.450	1.431
C6-C7	1.391	1.401	1.378	1.376	1.385	1.363
C7-C8	1.430	1.434	1.412	1.457	1.463	1.440
C8-C8A	1.385	1.396	1.376	1.417	1.435	1.413
C8A-C8B	1.419	1.426	1.409	1.444	1.453	1.431
C8A-C1	1.490	1.491	1.473	1.484	1.485	1.467

Table S3. Iron-carbonyl distances (in Å) for $C_{12}H_8Fe(CO)_4$ structures using B3LYP, BP86, and M06-L methods.

	Fe14-1			Fe14-2		
	B3LYP	BP86	M06-L	B3LYP	BP86	M06-L
Fe-C9	1.803	1.793	1.807	1.792	1.784	1.794
Fe-C10	1.821	1.802	1.818	1.830	1.811	1.829
Fe-C11	1.803	1.793	1.807	1.801	1.792	1.803
Fe-C12	1.832	1.812	1.833	1.821	1.805	1.820
C9-O9	1.159	1.173	1.148	1.161	1.174	1.151
C10-O10	1.154	1.170	1.144	1.152	1.167	1.143
C11-O11	1.159	1.173	1.148	1.159	1.172	1.149
C12-O12	1.151	1.167	1.142	1.155	1.171	1.146

Table S4. Iron-carbon distances (in Å) for $C_{12}H_8Fe(CO)_3$ structures using B3LYP, BP86, and M06-L methods.

	Fe13-1			Fe13-2		
	B3LYP	BP86	M06-L	B3LYP	BP86	M06-L
Fe-C1	2.048	2.059	2.041	3.428	3.433	3.350
Fe-C2	2.048	2.059	2.041	4.286	4.304	4.185
Fe-C2A	2.446	2.392	2.330	4.056	4.079	3.966
Fe-C3	3.527	3.489	3.396	5.073	5.102	4.957
Fe-C4	4.323	4.252	4.105	5.118	5.146	5.005
Fe-C5	4.380	4.284	4.112	4.241	4.263	4.154
Fe-C5A	3.620	3.517	3.365	2.965	2.975	2.909
Fe-C6	4.380	4.284	4.112	2.237	2.229	2.192
Fe-C7	4.323	4.252	4.105	2.081	2.070	2.057
Fe-C8	3.527	3.489	3.396	2.092	2.085	2.067
Fe-C8A	2.446	2.392	2.330	2.259	2.265	2.215
Fe-C8B	2.496	2.396	2.289	2.882	2.894	2.826

Table S5.Carbon-carbon distances (in Å) for $C_{12}H_8Fe(CO)_3$ structures using B3LYP, BP86, and M06-L methods.

	Fe13-1			Fe13-2			
	B3LYP	BP86	M06-L	B3LYP	BP86	M06-L	
C1-C2	1.462	1.472	1.454	1.375	1.388	1.363	1.375
C2-C2A	1.465	1.464	1.443	1.474	1.477	1.457	1.474
C2A-C3	1.397	1.409	1.392	1.411	1.420	1.400	1.411
C3-C4	1.418	1.421	1.398	1.408	1.415	1.391	1.408
C4-C5	1.399	1.410	1.388	1.418	1.425	1.404	1.418
C5-C5A	1.423	1.429	1.408	1.402	1.410	1.390	1.402
C5A-C8B	1.423	1.433	1.418	1.386	1.393	1.376	1.386
C8B-C2A	1.435	1.447	1.431	1.395	1.403	1.385	1.395
C5A-C6	1.423	1.429	1.408	1.484	1.488	1.470	1.484
C6-C7	1.399	1.410	1.388	1.436	1.449	1.430	1.436
C7-C8	1.418	1.421	1.398	1.426	1.434	1.414	1.426
C8-C8A	1.397	1.409	1.392	1.431	1.444	1.427	1.431
C8A-C8B	1.435	1.447	1.431	1.461	1.469	1.451	1.461
C8A-C1	1.465	1.464	1.443	1.473	1.473	1.455	1.473

Table S6. Iron-carbonyl distances (in Å) for $C_{12}H_8Fe(CO)_3$ structures using B3LYP, BP86, and M06-L methods.

	Fe13-1			Fe13-2		
	B3LYP	BP86	M06-L	B3LYP	BP86	M06-L
Fe-C9	1.826	1.810	1.828	1.791	1.770	1.789
Fe-C10	1.760	1.744	1.764	1.812	1.803	1.820
Fe-C11	1.826	1.810	1.828	1.800	1.780	1.799
C9-O9	1.156	1.172	1.146	1.158	1.175	1.149
C10-O10	1.159	1.176	1.149	1.155	1.170	1.145
C11-O11	1.156	1.172	1.146	1.158	1.174	1.148

Table S7. Iron-carbon distances (in Å) for $C_{12}H_8Fe(CO)_2$ structures using B3LYP, BP86, and M06-L methods.

	Fe12-1			Fe12-2		
	B3LYP	BP86	M06-L	B3LYP	BP86	M06-L
Fe-C1	2.052	2.055	2.028	3.853	3.859	3.761
Fe-C2	2.074	2.074	2.056	3.341	3.352	3.277
Fe-C2A	2.266	2.233	2.210	2.211	2.217	2.185
Fe-C3	3.342	3.328	3.271	2.140	2.125	2.100
Fe-C4	4.071	4.056	3.963	2.118	2.102	2.086
Fe-C5	4.068	4.049	3.940	2.137	2.125	2.101
Fe-C5A	3.278	3.253	3.158	2.261	2.237	2.206
Fe-C6	3.979	3.959	3.820	3.384	3.359	3.287
Fe-C7	3.864	3.844	3.686	4.154	4.134	4.034
Fe-C8	3.082	3.066	2.927	4.161	4.149	4.042
Fe-C8A	2.165	2.147	2.097	3.331	3.322	3.242
Fe-C8B	2.224	2.190	2.145	2.231	2.212	2.180

Table S8. Carbon-carbon distances (in Å) for $C_{12}H_8Fe(CO)_2$ structures using B3LYP, BP86, and M06-L methods.

	Fe12-1			Fe12-2		
	B3LYP	BP86	M06-L	B3LYP	BP86	M06-L
C1-C2	1.444	1.456	1.436	1.376	1.389	1.365
C2-C2A	1.452	1.455	1.435	1.469	1.468	1.451
C2A-C3	1.412	1.423	1.406	1.419	1.431	1.414
C3-C4	1.407	1.412	1.387	1.430	1.440	1.419
C4-C5	1.409	1.420	1.399	1.423	1.435	1.413
C5-C5A	1.414	1.420	1.398	1.443	1.450	1.433
C5A-C8B	1.424	1.433	1.418	1.411	1.422	1.405
C8B-C2A	1.432	1.445	1.427	1.431	1.442	1.424
C5A-C6	1.428	1.433	1.416	1.430	1.436	1.417
C6-C7	1.394	1.403	1.379	1.393	1.403	1.381
C7-C8	1.426	1.431	1.412	1.429	1.433	1.410
C8-C8A	1.405	1.416	1.397	1.389	1.400	1.379
C8A-C8B	1.434	1.442	1.427	1.428	1.437	1.421
C8A-C1	1.455	1.461	1.442	1.465	1.465	1.445

Table S9. Iron-carbonyl distances (in Å) for $C_{12}H_8Fe(CO)_2$ structures using B3LYP, BP86, and M06-L methods.

	Fe12-1			Fe12-2		
	B3LYP	BP86	M06-L	B3LYP	BP86	M06-L
Fe-C9	1.790	1.770	1.785	1.758	1.745	1.757
Fe-C10	1.752	1.737	1.751	1.776	1.760	1.775
C9-O9	1.162	1.179	1.153	1.166	1.181	1.156
C10-O10	1.165	1.182	1.155	1.163	1.178	1.153

Table S10. Iron-carbon distances (in Å) for $C_{12}H_8Fe_2(CO)_8$ structures using B3LYP, BP86, and M06-L methods.

	Fe28-1			Fe28-2			Fe28-3			Fe28-4		
	B3LYP	BP86	M06-L	B3LYP	BP86	M06-L	B3LYP	BP86	M06-L	B3LYP	BP86	M06-L
Fe1-C1	2.165	2.179	2.167	2.198	2.199	2.173	5.915	5.907	5.805	5.745	5.739	5.621
Fe1-C2	2.169	2.179	2.162	2.168	2.165	2.142	5.300	5.284	5.199	5.160	5.145	5.050
Fe1-C2A	3.138	3.150	3.064	3.145	3.146	3.077	3.925	3.898	3.850	3.844	3.828	3.758
Fe1-C8B	3.565	3.581	3.481	3.603	3.607	3.512	3.871	3.898	3.788	3.820	3.809	3.719
Fe1-C8A	3.138	3.145	3.129	3.205	3.206	3.141	5.202	5.189	5.103	5.065	5.063	4.948
Fe1-C3	4.173	4.198	4.039	4.194	4.208	4.101	3.257	3.225	3.204	3.165	3.138	3.109
Fe1-C4	5.268	5.303	5.063	5.314	5.335	5.180	2.318	2.269	2.296	2.243	2.215	2.219
Fe1-C5	5.541	5.579	5.303	5.614	5.638	5.467	2.327	2.268	2.284	2.248	2.227	2.212
Fe1-C5A	4.806	4.840	4.610	4.884	4.903	4.760	3.278	3.237	3.212	3.202	3.191	3.134
Fe1-C6	5.543	5.572	5.307	5.708	5.737	5.568	4.313	4.287	4.234	4.153	4.153	4.092
Fe1-C7	5.276	5.307	5.077	5.472	5.497	5.355	5.487	5.478	5.391	5.314	5.328	5.229
Fe1-C8	4.182	4.202	4.093	4.314	4.330	4.239	5.910	5.911	5.808	5.725	5.741	5.617
Fe2-C3	5.887	6.020	5.230	5.941	5.922	5.830	5.469	5.464	5.808	6.076	6.024	5.873
Fe2-C4	6.119	6.074	5.609	5.493	5.475	5.390	5.902	5.904	5.812	6.144	6.094	5.978
Fe2-C5	5.422	5.212	5.065	4.296	4.264	4.216	5.302	5.291	5.223	5.281	5.216	5.160
Fe2-C5A	4.190	3.958	3.862	3.315	3.264	3.259	4.000	3.970	3.943	4.028	3.936	3.921
Fe2-C6	3.771	3.308	3.776	2.327	2.261	2.308	3.885	3.854	3.834	3.356	3.256	3.313
Fe2-C7	2.929	2.434	3.103	2.318	2.256	2.316	3.157	3.116	3.127	2.510	2.370	2.498
Fe2-C8	2.459	2.362	2.294	3.262	3.215	3.222	2.306	2.243	2.293	2.504	2.352	2.433
Fe2-C8A	3.028	3.193	2.364	3.974	3.933	3.907	2.412	2.343	2.379	3.332	3.217	3.199
Fe2-C8B	3.819	3.846	3.209	3.974	3.929	3.905	3.333	3.290	3.277	3.953	3.853	3.809

Table S11. Carbon-carbon distances (in Å) for $C_{12}H_8Fe_2(CO)_8$ structures using B3LYP, BP86, and M06-L methods.

	Fe28-1			Fe28-2			Fe28-3			Fe28-4		
	B3LYP	BP86	M06-L	B3LYP	BP86	M06-L	B3LYP	BP86	M06-L	B3LYP	BP86	M06-L
C1-C2	1.439	1.452	1.430	1.438	1.451	1.436	1.368	1.381	1.358	1.373	1.387	1.362
C2-C2A	1.491	1.490	1.470	1.493	1.495	1.474	1.468	1.468	1.450	1.470	1.470	1.452
C2A-C3	1.384	1.392	1.382	1.391	1.401	1.381	1.379	1.391	1.371	1.370	1.382	1.362
C3-C4	1.431	1.440	1.404	1.422	1.426	1.405	1.445	1.450	1.427	1.461	1.464	1.441
C4-C5	1.390	1.397	1.384	1.398	1.408	1.384	1.425	1.444	1.421	1.427	1.443	1.424
C5-C5A	1.429	1.439	1.407	1.419	1.424	1.406	1.449	1.458	1.438	1.466	1.471	1.452
C5A-C8B	1.408	1.425	1.397	1.399	1.409	1.391	1.390	1.399	1.382	1.403	1.414	1.394
C8B-C2A	1.420	1.432	1.403	1.414	1.421	1.404	1.433	1.441	1.382	1.442	1.449	1.431
C5A-C6	1.428	1.421	1.429	1.455	1.464	1.440	1.436	1.442	1.423	1.405	1.410	1.395
C6-C7	1.391	1.421	1.364	1.420	1.440	1.412	1.381	1.390	1.369	1.418	1.432	1.403
C7-C8	1.440	1.451	1.437	1.454	1.460	1.436	1.448	1.456	1.431	1.431	1.447	1.419
C8-C8A	1.400	1.420	1.409	1.374	1.384	1.366	1.418	1.437	1.414	1.412	1.429	1.403
C8A-C8B	1.417	1.414	1.432	1.435	1.443	1.424	1.439	1.449	1.427	1.402	1.409	1.393
C8A-C1	1.487	1.484	1.481	1.484	1.485	1.467	1.482	1.483	1.464	1.472	1.472	1.454

Table S12. Iron-carbonyl distances (in Å) for $C_{12}H_8Fe_2(CO)_8$ structures using B3LYP, BP86, and M06-L methods.

	Fe28-1			Fe28-2			Fe28-3			Fe28-4		
	B3LYP	BP86	M06-L	B3LYP	BP86	M06-L	B3LYP	BP86	M06-L	B3LYP	BP86	M06-L
Fe1-C9	1.833	1.812	1.831	1.832	1.813	1.834	1.796	1.788	1.799	1.799	1.790	1.802
Fe1-C10	1.806	1.794	1.807	1.801	1.790	1.804	1.821	1.804	1.819	1.824	1.805	1.821
Fe1-C11	1.808	1.795	1.807	1.822	1.803	1.819	1.795	1.788	1.797	1.802	1.794	1.805
Fe1-C12	1.826	1.805	1.820	1.808	1.797	1.814	1.825	1.806	1.821	1.831	1.812	1.832
C9-O9	1.151	1.167	1.142	1.151	1.167	1.142	1.159	1.173	1.149	1.159	1.172	1.148
C10-O10	1.157	1.172	1.148	1.159	1.173	1.148	1.155	1.171	1.146	1.154	1.169	1.144
C11-O11	1.157	1.172	1.148	1.154	1.170	1.144	1.161	1.174	1.151	1.159	1.173	1.149
C12-O12	1.152	1.169	1.144	1.157	1.171	1.146	1.153	1.168	1.144	1.151	1.166	1.142
Fe2-C13	1.788	1.784	1.794	1.821	1.804	1.819	1.791	1.784	1.792	1.820	1.803	1.817
Fe2-C14	1.826	1.808	1.826	1.796	1.789	1.799	1.826	1.807	1.822	1.789	1.784	1.788
Fe2-C15	1.785	1.780	1.798	1.820	1.804	1.817	1.801	1.793	1.803	1.824	1.804	1.823
Fe2-C16	1.817	1.803	1.817	1.794	1.787	1.791	1.821	1.805	1.820	1.788	1.782	1.787
C13-O13	1.163	1.176	1.151	1.156	1.171	1.146	1.161	1.174	1.151	1.156	1.172	1.147
C14-O14	1.155	1.169	1.143	1.160	1.173	1.149	1.152	1.168	1.144	1.163	1.176	1.153
C15-O15	1.164	1.177	1.150	1.154	1.168	1.146	1.158	1.172	1.148	1.154	1.170	1.145
C16-O16	1.157	1.172	1.146	1.161	1.174	1.152	1.155	1.171	1.146	1.162	1.176	1.153

Table S13. Iron-carbon distances (in Å) for $C_{12}H_8Fe_2(CO)_7$ structures using B3LYP, BP86, and M06-L methods.

	Fe27-1		
	B3LYP	BP86	M06-L
Fe1-C1	2.058	2.052	2.038
Fe1-C2	2.070	2.093	2.062
Fe1-C2A	2.368	2.516	2.428
Fe1-C8B	2.346	2.331	2.251
Fe1-C8A	2.347	2.240	2.224
Fe1-C3	3.468	3.584	3.489
Fe1-C4	4.171	4.217	4.099
Fe1-C5	4.186	4.164	4.041
Fe1-C5A	3.432	3.370	3.271
Fe2-C5A	4.162	3.981	3.933
Fe2-C6	5.323	5.114	5.020
Fe2-C7	5.983	5.640	5.515
Fe2-C8	5.783	5.303	5.187
Fe2-C8A	4.770	4.226	4.152
Fe2-C8B	3.836	3.402	3.376

	Fe27-2			Fe27-3			Fe27-4		
	B3LYP	BP86	M06-L	B3LYP	BP86	M06-L	B3LYP	BP86	M06-L
Fe1-C1	2.199	2.187	2.179	3.402	3.400	3.338	5.995	5.883	5.776
Fe1-C2	2.169	2.156	2.149	4.248	4.255	4.164	5.332	5.255	5.188
Fe1-C2A	3.171	3.158	3.091	4.012	4.024	3.933	4.056	3.947	3.944
Fe1-C8B	3.647	3.632	3.525	2.859	2.869	2.803	4.126	3.936	3.914
Fe1-C8A	3.268	3.255	3.192	2.244	2.250	2.206	5.419	5.253	5.160
Fe1-C3	4.226	4.224	4.112	5.045	2.250	4.957	3.291	3.233	3.283
Fe1-C4	5.341	5.342	5.165	5.087	5.109	5.004	2.474	2.338	2.457
Fe1-C5	5.658	5.656	5.455	4.195	4.210	4.131	2.669	2.397	2.484
Fe1-C5A	4.925	4.916	4.744	2.942	2.952	2.893	3.585	3.332	3.334
Fe1-C6	5.656	5.644	5.450	2.225	2.232	2.193	4.637	4.383	4.311
Fe1-C7	5.652	5.654	5.532	2.079	2.071	2.058	5.954	5.724	5.638
Fe1-C8	4.564	4.565	4.515	2.085	2.077	2.063	6.307	6.111	6.017
Fe2-C3	5.240	3.692	5.185	2.394	2.289	2.352	5.159	5.226	5.108
Fe2-C4	5.242	5.268	5.198	2.416	2.318	2.394	5.220	5.288	5.163
Fe2-C5	4.303	4.323	4.279	3.335	3.271	3.286	4.310	4.355	4.261
Fe2-C5A	2.987	2.997	2.965	4.002	3.944	3.918	2.986	3.003	2.948
Fe2-C6	2.202	2.197	2.174	5.356	5.315	5.260	2.237	2.229	2.195
Fe2-C7	2.059	2.051	2.039	6.009	6.004	5.910	2.078	2.066	2.051
Fe2-C8	2.102	2.092	2.059	5.938	5.935	5.829	2.085	2.083	2.064
Fe2-C8A	2.313	2.314	2.219	5.123	5.082	5.001	2.254	2.278	2.229
Fe2-C8B	2.952	2.961	2.911	3.894	3.831	3.791	2.902	2.933	2.874

Table S14. Carbon-carbon distances (in Å) for $C_{12}H_8Fe_2(CO)_7$ structures using B3LYP, BP86, and M06-L methods.

	Fe27-1			**Fe27-2**			**Fe27-3**			**Fe27-4**		
	B3LYP	BP86	M06-L	B3LYP	BP86	M06-L	B3LYP	BP86	M06-L	B3LYP	BP86	M06-L
C1-C2	1.459	1.465	1.450	1.441	1.457	1.438	1.378	1.389	1.366	1.374	1.387	1.363
C2-C2A	1.449	1.472	1.450	1.492	1.495	1.479	1.468	1.471	1.451	1.473	1.474	1.455
C2A-C3	1.421	1.431	1.411	1.407	1.416	1.397	1.434	1.447	1.423	1.399	1.403	1.387
C3-C4	1.442	1.466	1.440	1.408	1.415	1.392	1.426	1.446	1.418	1.426	1.442	1.412
C4-C5	1.392	1.386	1.366	1.417	1.425	1.403	1.440	1.451	1.424	1.428	1.447	1.420
C5-C5A	1.428	1.449	1.429	1.401	1.408	1.390	1.387	1.394	1.377	1.413	1.433	1.408
C5A-C8B	1.428	1.432	1.418	1.389	1.397	1.377	1.401	1.411	1.391	1.377	1.378	1.363
C8B-C2A	1.437	1.459	1.439	1.393	1.402	1.384	1.384	1.391	1.375	1.406	1.420	1.398
C5A-C6	1.413	1.409	1.390	1.486	1.490	1.473	1.481	1.481	1.465	1.483	1.487	1.469
C6-C7	1.408	1.428	1.406	1.441	1.454	1.436	1.437	1.449	1.430	1.438	1.452	1.433
C7-C8	1.409	1.402	1.381	1.426	1.434	1.413	1.425	1.435	1.413	1.424	1.432	1.412
C8-C8A	1.405	1.430	1.410	1.428	1.441	1.431	1.433	1.445	1.428	1.435	1.446	1.430
C8A-C8B	1.436	1.444	1.428	1.461	1.467	1.449	1.460	1.467	1.448	1.460	1.468	1.448
C8A-C1	1.457	1.455	1.436	1.493	1.494	1.477	1.470	1.472	1.453	1.475	1.474	1.457

Table S15. Iron-carbonyl distances (in Å) for $C_{12}H_8Fe_2(CO)_7$ structures using B3LYP, BP86, and M06-L methods.

	Fe27-1			Fe27-3		
	B3LYP	BP86	M06-L	B3LYP	BP86	M06-L
Fe1-C9	1.823	1.796	1.818	1.794	1.772	1.791
Fe1-C10	1.826	1.808	1.827	1.812	1.801	1.819
Fe1-C11	1.772	1.755	1.772	1.803	1.782	1.802
C9-O9	1.154	1.172	1.146	1.157	1.174	1.148
C10-O10	1.154	1.172	1.146	1.154	1.170	1.144
C11-O11	1.156	1.174	1.148	1.156	1.173	1.147
Fe2-C12	1.789	1.805	1.819	1.790	1.785	1.790
Fe2-C13	1.815	1.784	1.791	1.819	1.803	1.817
Fe2-C14	1.784	1.800	1.813	1.789	1.784	1.789
Fe2-C15	1.818	1.782	1.788	1.821	1.804	1.819
C12-O12	1.163	1.171	1.146	1.162	1.175	1.153
C13-O13	1.158	1.176	1.153	1.157	1.172	1.147
C14-O14	1.165	1.173	1.148	1.162	1.175	1.153
C15-O15	1.157	1.176	1.153	1.154	1.169	1.146

	Fe27-2			Fe27-4		
	B3LYP	BP86	M06-L	B3LYP	BP86	M06-L
Fe1-C9	1.828	1.810	1.832	1.788	1.784	1.790
Fe1-C10	1.800	1.790	1.803	1.818	1.802	1.815
Fe1-C11	1.822	1.804	1.818	1.783	1.779	1.783
Fe1-C12	1.807	1.798	1.809	1.827	1.808	1.825
C9-O9	1.151	1.166	1.142	1.163	1.175	1.153
C10-O10	1.159	1.173	1.149	1.157	1.172	1.147
C11-O11	1.154	1.170	1.145	1.164	1.176	1.154
C12-O12	1.157	1.171	1.148	1.154	1.169	1.145
Fe2-C13	1.790	1.771	1.794	1.794	1.772	1.791
Fe2-C14	1.808	1.799	1.812	1.811	1.803	1.820
Fe2-C15	1.799	1.779	1.797	1.802	1.779	1.798
C13-O13	1.158	1.175	1.148	1.157	1.174	1.147
C14-O14	1.156	1.171	1.146	1.154	1.170	1.145
C15-O15	1.157	1.173	1.148	1.157	1.173	1.147

Table S16. Iron-carbon distances (in Å) for $C_{12}H_8Fe_2(CO)_6$ structures using B3LYP, BP86, and M06-L methods.

	Fe26-1			Fe26-2			Fe26-3			Fe26-4		
	B3LYP	BP86	M06-L	B3LYP	BP86	M06-L	B3LYP	BP86	M06-L	B3LYP	BP86	M06-L
Fe1-C1	4.789	4.687	4.657	2.094	2.127	2.082	4.303	4.278	4.191	4.630	4.593	4.576
Fe1-C2	4.046	3.934	3.931	1.971	2.031	2.040	3.464	3.438	3.383	4.374	4.368	4.366
Fe1-C2A	2.818	2.715	2.719	2.505	2.207	2.180	2.271	2.252	2.216	3.106	3.103	3.114
Fe1-C8B	3.200	3.138	3.102	2.961	2.395	2.239	2.837	2.814	2.749	2.479	2.418	2.426
Fe1-C8A	4.333	4.274	4.212	2.913	2.535	2.330	4.026	3.995	3.906	3.686	3.615	3.585
Fe1-C3	2.192	2.157	2.147	3.495	3.259	3.230	2.098	2.072	2.062	3.008	3.027	3.008
Fe1-C4	2.001	2.015	1.995	4.509	4.086	3.977	2.072	2.085	2.071	2.186	2.193	2.166
Fe1-C5	2.186	2.189	2.159	4.815	4.241	4.074	2.220	2.300	2.242	2.062	2.064	2.050
Fe1-C5A	2.963	2.954	2.897	4.175	3.574	3.400	2.910	2.947	2.887	2.232	2.180	2.169
Fe2-C5A	3.458	3.466	3.348	2.974	3.063	3.015	2.940	2.409	2.320	3.550	3.453	3.380
Fe2-C6	4.166	4.169	4.051	2.161	2.135	2.128	2.334	2.117	2.093	3.649	3.634	3.635
Fe2-C7	4.084	4.073	3.988	2.035	1.968	1.941	2.041	2.064	2.058	3.054	3.073	3.104
Fe2-C8	3.318	3.295	3.257	2.146	2.265	2.185	2.273	2.262	2.233	2.125	2.140	2.169
Fe2-C8A	2.244	2.216	2.196	2.421	2.992	3.048	3.057	3.010	2.956	2.052	2.038	2.024
Fe2-C8B	2.297	2.292	2.202	2.987	3.337	3.343	3.248	2.966	2.884	2.778	2.644	2.519

Table S17. Carbon-carbon distances (in Å) for $C_{12}H_8Fe_2(CO)_6$ structures using B3LYP, BP86, and M06-L methods.

	Fe26-1			Fe26-2			Fe26-3			Fe26-4		
	B3LYP	BP86	M06-L	B3LYP	BP86	M06-L	B3LYP	BP86	M06-L	B3LYP	BP86	M06-L
C1-C2	1.456	1.462	1.445	1.468	1.462	1.442	1.383	1.395	1.373	1.367	1.380	1.358
C2-C2A	1.448	1.457	1.436	1.482	1.457	1.434	1.470	1.476	1.455	1.456	1.455	1.440
C2A-C3	1.415	1.427	1.410	1.420	1.437	1.416	1.429	1.444	1.427	1.360	1.368	1.347
C3-C4	1.446	1.446	1.433	1.398	1.396	1.376	1.426	1.437	1.416	1.472	1.479	1.459
C4-C5	1.444	1.454	1.437	1.424	1.438	1.414	1.440	1.445	1.426	1.446	1.457	1.441
C5-C5A	1.459	1.466	1.443	1.396	1.401	1.384	1.474	1.468	1.457	1.424	1.431	1.414
C5A-C8B	1.427	1.432	1.420	1.396	1.429	1.423	1.403	1.442	1.426	1.428	1.451	1.434
C8B-C2A	1.449	1.455	1.437	1.402	1.440	1.431	1.454	1.453	1.437	1.476	1.490	1.469
C5A-C6	1.395	1.402	1.383	1.484	1.472	1.443	1.409	1.441	1.426	1.455	1.458	1.441
C6-C7	1.427	1.436	1.413	1.447	1.466	1.447	1.441	1.433	1.413	1.364	1.375	1.354
C7-C8	1.391	1.397	1.376	1.430	1.459	1.454	1.441	1.452	1.432	1.463	1.467	1.445
C8-C8A	1.425	1.436	1.416	1.415	1.419	1.419	1.451	1.477	1.461	1.441	1.453	1.434
C8A-C8B	1.427	1.440	1.426	1.460	1.450	1.423	1.373	1.370	1.351	1.464	1.461	1.438
C8A-C1	1.450	1.455	1.435	1.488	1.466	1.441	1.465	1.468	1.447	1.477	1.477	1.461

Table S18. Iron-carbonyl distances (in Å) for $C_{12}H_8Fe_2(CO)_6$ structures using B3LYP, BP86, and M06-L methods.

	Fe26-1			**Fe26-2**			**Fe26-3**			**Fe26-4**		
	B3LYP	BP86	M06-L	B3LYP	BP86	M06-L	B3LYP	BP86	M06-L	B3LYP	BP86	M06-L
Fe1-C9	1.774	1.764	1.764	1.816	1.782	1.807	1.794	1.772	1.788	1.821	1.814	1.835
Fe1-C10	1.787	1.772	1.772	1.755	1.766	1.789	1.805	1.780	1.799	1.774	1.756	1.770
Fe1-C11	1.808	1.799	1.799	1.828	1.799	1.822	1.816	1.801	1.817	1.813	1.803	1.813
C9-O9	1.163	1.178	1.178	1.158	1.169	1.142	1.156	1.174	1.148	1.158	1.173	1.147
C10-O10	1.163	1.178	1.178	1.160	1.174	1.146	1.155	1.172	1.147	1.159	1.174	1.149
C11-O11	1.162	1.177	1.177	1.156	1.168	1.142	1.153	1.170	1.145	1.156	1.170	1.147
Fe2-C12	1.812	1.789	1.789	1.785	1.756	1.778	1.787	1.777	1.794	1.828	1.810	1.824
Fe2-C13	1.823	1.807	1.807	1.802	1.794	1.798	1.816	1.802	1.816	1.816	1.790	1.805
Fe2-C14	1.781	1.764	1.764	1.801	1.776	1.783	1.765	1.767	1.786	1.755	1.737	1.754
C12-O12	1.154	1.171	1.171	1.159	1.179	1.154	1.164	1.177	1.152	1.157	1.173	1.150
C13-O13	1.153	1.170	1.170	1.158	1.177	1.157	1.162	1.173	1.149	1.157	1.175	1.149
C14-O14	1.156	1.173	1.173	1.158	1.178	1.154	1.164	1.177	1.151	1.160	1.178	1.152

Table S19. Iron-carbon distances (in Å) for $C_{12}H_8Fe_2(CO)_5$ structures using B3LYP, BP86, and M06-L methods.

	Fe25-1		
	B3LYP	BP86	M06-L
Fe1-C1	2.128	2.108	2.077
Fe1-C2	2.128	2.108	2.077
Fe1-C2A	2.151	2.158	2.121
Fe1-C8B	2.124	2.130	2.106
Fe1-C8A	2.151	2.158	2.121
Fe1-C3	3.189	3.202	3.134
Fe1-C4	3.773	3.800	3.728
Fe1-C5	3.681	3.714	3.659
Fe1-C5A	3.037	3.065	3.033
Fe2-C5	2.257	2.272	2.236
Fe2-C5A	2.082	2.071	2.070
Fe2-C6	2.257	2.272	2.236
Fe2-C7	3.225	3.220	3.163
Fe2-C8	3.748	3.723	3.666
Fe2-C8A	3.498	3.455	3.432
Fe2-C8B	2.761	2.710	2.707

	Fe25-2			Fe25-3			Fe25-4			Fe25-5		
	B3LYP	BP86	M06-L	B3LYP	BP86	M06-L	B3LYP	BP86	M06-L	B3LYP	BP86	M06-L
Fe1-C1	2.119	2.125	2.085	3.853	3.847	3.766	3.886	3.882	3.811	2.083	2.084	2.058
Fe1-C2	2.114	2.117	2.078	3.490	3.493	3.423	3.393	3.381	3.327	2.037	2.055	2.027
Fe1-C2A	2.232	2.232	2.179	2.379	2.396	2.368	2.223	2.209	2.183	2.167	2.166	2.135
Fe1-C8B	2.143	2.161	2.098	2.175	2.183	2.169	2.156	2.143	2.111	2.239	2.209	2.160
Fe1-C8A	2.129	2.172	2.106	3.209	3.218	3.178	3.321	3.310	3.254	2.335	2.265	2.255
Fe1-C3	3.302	3.304	3.216	2.251	2.235	2.200	2.168	2.159	2.137	3.163	3.204	3.140
Fe1-C4	3.951	3.963	3.841	2.143	2.121	2.105	2.106	2.102	2.080	3.937	3.970	3.882
Fe1-C5	3.874	3.901	3.767	2.172	2.146	2.124	2.174	2.166	2.145	4.058	4.063	3.974
Fe1-C5A	3.072	3.105	2.998	2.212	2.224	2.194	2.225	2.214	2.191	3.369	3.348	3.278
Fe2-C5A	2.983	2.952	2.926	3.382	3.345	3.354	2.953	2.963	2.911	2.990	2.995	2.935
Fe2-C6	2.215	2.221	2.180	3.563	3.551	3.532	2.219	2.219	2.182	2.192	2.187	2.157
Fe2-C7	2.073	2.062	2.050	3.047	3.049	3.023	2.077	2.068	2.054	2.030	2.038	2.026
Fe2-C8	2.190	2.129	2.159	2.171	2.199	2.178	2.096	2.094	2.078	2.216	2.171	2.160
Fe2-C8A	2.711	2.537	2.674	2.094	2.093	2.097	2.261	2.298	2.243	2.727	2.678	2.620
Fe2-C8B	3.079	2.968	3.031	2.675	2.633	2.643	2.880	2.900	2.838	3.139	3.110	3.041

Table S20. Carbon-carbon distances (in Å) for $C_{12}H_8Fe_2(CO)_5$ structures using B3LYP, BP86, and M06-L methods.

	Fe25-1		
	B3LYP	BP86	M06-L
C1-C2	1.433	1.445	1.424
C2-C2A	1.443	1.454	1.435
C2A-C3	1.449	1.448	1.433
C3-C4	1.370	1.384	1.358
C4-C5	1.462	1.461	1.444
C5-C5A	1.431	1.440	1.425
C5A-C8B	1.422	1.427	1.411
C8B-C2A	1.431	1.443	1.425
C5A-C6	1.431	1.440	1.425
C6-C7	1.462	1.461	1.444
C7-C8	1.370	1.384	1.358
C8-C8A	1.449	1.448	1.433
C8A-C8B	1.431	1.443	1.425
C8A-C1	1.443	1.454	1.435

	Fe25-2			Fe25-3			Fe25-4			Fe25-5		
	B3LYP	BP86	M06-L	B3LYP	BP86	M06-L	B3LYP	BP86	M06-L	B3LYP	BP86	M06-L
C1-C2	1.442	1.446	1.434	1.397	1.411	1.395	1.372	1.385	1.361	1.449	1.456	1.440
C2-C2A	1.453	1.462	1.439	1.436	1.434	1.409	1.473	1.474	1.456	1.454	1.461	1.440
C2A-C3	1.433	1.439	1.423	1.419	1.429	1.412	1.416	1.425	1.406	1.422	1.433	1.415
C3-C4	1.387	1.396	1.372	1.430	1.441	1.420	1.434	1.444	1.423	1.399	1.403	1.380
C4-C5	1.435	1.440	1.419	1.422	1.432	1.411	1.438	1.447	1.427	1.423	1.435	1.413
C5-C5A	1.387	1.397	1.377	1.426	1.441	1.424	1.411	1.421	1.402	1.396	1.400	1.380
C5A-C8B	1.419	1.425	1.411	1.423	1.434	1.415	1.403	1.414	1.396	1.417	1.423	1.408
C8B-C2A	1.419	1.430	1.416	1.439	1.452	1.438	1.414	1.427	1.410	1.422	1.433	1.417
C5A-C6	1.471	1.471	1.455	1.450	1.447	1.433	1.484	1.485	1.469	1.464	1.474	1.454
C6-C7	1.439	1.451	1.431	1.369	1.385	1.361	1.437	1.449	1.431	1.447	1.456	1.440
C7-C8	1.417	1.429	1.409	1.463	1.461	1.441	1.424	1.432	1.411	1.431	1.434	1.415
C8-C8A	1.448	1.454	1.437	1.438	1.443	1.428	1.430	1.440	1.424	1.419	1.441	1.421
C8A-C8B	1.448	1.457	1.439	1.429	1.434	1.418	1.463	1.466	1.450	1.450	1.457	1.442
C8A-C1	1.429	1.447	1.421	1.457	1.460	1.439	1.472	1.471	1.454	1.450	1.452	1.434

Table S21. Iron-carbonyl distances (in Å) for $C_{12}H_8Fe_2(CO)_5$ structures using B3LYP, BP86, and M06-L methods.

	Fe25-1		
	B3LYP	BP86	M06-L
Fe1-C9	1.770	1.756	1.770
Fe1-C10	1.770	1.756	1.770
C9-O9	1.160	1.177	1.152
C10-O10	1.160	1.177	1.152
Fe2-C11	1.792	1.780	1.793
Fe2-C12	1.792	1.780	1.793
Fe2-C13	1.782	1.766	1.780
C11-O11	1.159	1.175	1.150
C12-O12	1.159	1.175	1.150
C13-O13	1.159	1.176	1.151

	Fe25-2			Fe25-3			Fe25-4			Fe25-5		
	B3LYP	BP86	M06-L	B3LYP	BP86	M06-L	B3LYP	BP86	M06-L	B3LYP	BP86	M06-L
Fe1-C9	1.780	1.765	1.775	1.763	1.755	1.768	1.757	1.748	1.759	1.803	1.778	1.796
Fe1-C10	1.768	1.751	1.763	1.766	1.754	1.767	1.762	1.753	1.762	1.764	1.741	1.757
C9-O9	1.158	1.173	1.151	1.162	1.176	1.152	1.167	1.182	1.157	1.159	1.176	1.151
C10-O10	1.160	1.176	1.152	1.161	1.176	1.151	1.168	1.182	1.158	1.161	1.179	1.153
Fe2-C11	1.799	1.847	1.807	1.799	1.783	1.794	1.794	1.774	1.793	1.775	1.766	1.779
Fe2-C12	1.797	1.778	1.796	1.806	1.790	1.807	1.809	1.800	1.815	1.811	1.802	1.816
Fe2-C13	1.772	1.747	1.774	1.767	1.751	1.766	1.802	1.781	1.800	1.792	1.776	1.791
C11-O11	1.167	1.191	1.154	1.158	1.174	1.150	1.157	1.174	1.148	1.162	1.177	1.152
C12-O12	1.158	1.175	1.149	1.160	1.177	1.152	1.155	1.171	1.146	1.160	1.175	1.150
C13-O13	1.160	1.177	1.151	1.161	1.178	1.152	1.156	1.173	1.148	1.161	1.177	1.151

Table S22. Iron-carbon distances (in Å) for $C_{12}H_8Fe_2(CO)_4$ structures using B3LYP, BP86, and M06-L methods.

	Fe24-1			Fe24-2			Fe24-3		
	B3LYP	BP86	M06-L	B3LYP	BP86	M06-L	B3LYP	BP86	M06-L
Fe1-C1	2.138	2.109	2.090	2.143	2.116	2.077	2.146	2.129	2.094
Fe1-C2	2.056	2.057	2.012	2.129	2.102	2.064	2.155	2.128	2.094
Fe1-C2A	2.059	2.067	2.025	2.124	2.109	2.072	2.149	2.135	2.102
Fe1-C8B	2.130	2.106	2.082	2.108	2.096	2.067	2.125	2.124	2.087
Fe1-C8A	2.248	2.182	2.184	2.156	2.151	2.108	2.159	2.157	2.119
Fe1-C3	3.023	3.070	2.964	3.148	3.140	3.084	3.161	3.141	3.095
Fe1-C4	3.735	3.790	3.672	3.713	3.720	3.655	3.719	3.718	3.660
Fe1-C5	3.578	3.661	3.512	3.607	3.624	3.557	3.609	3.631	3.565
Fe1-C5A	3.035	3.036	2.966	2.966	2.981	2.931	3.019	3.043	2.979
Fe2-C3	2.229	2.180	2.187	3.681	3.665	3.610	3.591	3.590	3.556
Fe2-C4	2.082	2.083	2.058	3.186	3.183	3.130	3.090	3.093	3.064
Fe2-C5	2.230	2.297	2.202	2.255	2.266	2.221	2.149	2.163	2.143
Fe2-C5A	2.986	2.916	2.921	2.102	2.087	2.078	2.073	2.050	2.046
Fe2-C6	4.134	4.063	4.033	2.294	2.304	2.263	2.355	2.322	2.277
Fe2-C7	5.055	4.928	4.928	3.252	3.230	3.188	3.245	3.181	3.158
Fe2-C8	5.117	4.976	4.994	3.761	3.721	3.681	3.708	3.645	3.634
Fe2-C8A	4.222	4.118	4.132	3.503	3.460	3.433	3.435	3.390	3.383
Fe2-C8B	3.106	3.006	3.047	2.773	2.725	2.722	2.683	2.643	2.652

	Fe24-4			Fe24-5			Fe24-6			Fe24-7		
	B3LYP	BP86	M06-L	B3LYP	BP86	M06-L	B3LYP	BP86	M06-L	B3LYP	BP86	M06-L
Fe1-C1	2.065	2.063	2.045	3.933	3.935	3.877	3.895	3.895	3.830	2.128	2.141	2.109
Fe1-C2	2.070	2.073	2.052	3.390	3.376	3.341	3.365	3.359	3.313	2.037	2.038	2.021
Fe1-C2A	2.208	2.195	2.157	2.213	2.194	2.177	2.206	2.190	2.165	2.246	2.196	2.166
Fe1-C8B	2.223	2.184	2.129	2.232	2.220	2.187	2.219	2.198	2.160	2.316	2.285	2.216
Fe1-C8A	2.226	2.180	2.143	3.405	3.410	3.354	3.373	3.368	3.311	2.354	2.364	2.317
Fe1-C3	3.172	3.176	3.093	2.172	2.149	2.134	2.181	2.160	2.143	3.307	3.262	3.201
Fe1-C4	3.957	3.953	3.847	2.100	2.090	2.075	2.109	2.103	2.088	4.072	4.031	3.931
Fe1-C5	4.049	4.033	3.928	2.106	2.102	2.079	2.097	2.093	2.073	4.147	4.115	4.005
Fe1-C5A	3.308	3.275	3.192	2.280	2.271	2.243	2.257	2.240	2.206	3.430	3.405	3.319
Fe2-C3	4.184	4.189	4.125	4.176	4.172	4.100	4.171	4.175	4.103	5.440	5.475	5.415
Fe2-C4	4.157	4.151	4.098	4.168	4.156	4.093	4.163	4.163	4.093	5.230	5.263	5.195
Fe2-C5	3.368	3.349	3.317	3.458	3.444	3.402	3.447	3.440	3.390	4.155	4.175	4.117
Fe2-C5A	2.236	2.213	2.190	2.290	2.277	2.242	2.257	2.240	2.206	2.953	2.955	2.921
Fe2-C6	2.139	2.117	2.105	2.135	2.126	2.106	2.097	2.093	2.073	2.152	2.129	2.107
Fe2-C7	2.126	2.112	2.097	2.117	2.101	2.090	2.109	2.103	2.088	1.973	1.960	1.947
Fe2-C8	2.128	2.118	2.094	2.145	2.130	2.113	2.181	2.160	2.143	2.239	2.220	2.183
Fe2-C8A	2.232	2.246	2.211	2.215	2.223	2.191	2.206	2.190	2.165	2.988	2.983	2.947
Fe2-C8B	2.224	2.209	2.163	2.267	2.255	2.212	2.219	2.198	2.160	3.230	3.236	3.199

Table S23. Carbon-carbon distances (in Å) for $C_{12}H_8Fe_2(CO)_4$ structures using B3LYP, BP86, and M06-L methods.

	Fe24-1			Fe24-2			Fe24-3		
	B3LYP	BP86	M06-L	B3LYP	BP86	M06-L	B3LYP	BP86	M06-L
C1-C2	1.448	1.450	1.439	1.423	1.431	1.422	1.425	1.434	1.425
C2-C2A	1.437	1.455	1.432	1.441	1.455	1.440	1.432	1.448	1.432
C2A-C3	1.451	1.452	1.439	1.445	1.443	1.437	1.449	1.448	1.439
C3-C4	1.418	1.432	1.410	1.359	1.373	1.358	1.356	1.370	1.356
C4-C5	1.439	1.443	1.430	1.457	1.455	1.448	1.462	1.459	1.450
C5-C5A	1.466	1.451	1.448	1.425	1.435	1.426	1.441	1.448	1.436
C5A-C8B	1.423	1.436	1.415	1.423	1.427	1.419	1.416	1.421	1.415
C8B-C2A	1.447	1.452	1.438	1.427	1.439	1.427	1.428	1.437	1.427
C5A-C6	1.387	1.407	1.377	1.425	1.435	1.424	1.410	1.422	1.414
C6-C7	1.434	1.426	1.417	1.449	1.447	1.440	1.441	1.442	1.435
C7-C8	1.388	1.410	1.374	1.360	1.376	1.360	1.367	1.381	1.364
C8-C8A	1.431	1.428	1.418	1.439	1.436	1.430	1.435	1.438	1.431
C8A-C8B	1.423	1.437	1.420	1.426	1.437	1.425	1.428	1.440	1.428
C8A-C1	1.444	1.456	1.431	1.437	1.451	1.438	1.438	1.447	1.434

	Fe24-4			Fe24-5			Fe24-6			Fe24-7		
	B3LYP	BP86	M06-L	B3LYP	BP86	M06-L	B3LYP	BP86	M06-L	B3LYP	BP86	M06-L
C1-C2	1.441	1.454	1.434	1.375	1.389	1.366	1.375	1.388	1.365	1.463	1.467	1.450
C2-C2A	1.452	1.458	1.438	1.462	1.463	1.443	1.461	1.463	1.443	1.449	1.455	1.434
C2A-C3	1.403	1.414	1.395	1.415	1.427	1.409	1.412	1.425	1.407	1.426	1.436	1.418
C3-C4	1.424	1.428	1.408	1.429	1.439	1.417	1.430	1.441	1.418	1.391	1.398	1.374
C4-C5	1.394	1.405	1.381	1.436	1.447	1.427	1.432	1.442	1.422	1.427	1.435	1.414
C5-C5A	1.427	1.432	1.414	1.438	1.445	1.429	1.440	1.448	1.431	1.394	1.402	1.382
C5A-C8B	1.429	1.438	1.424	1.429	1.443	1.426	1.444	1.466	1.449	1.427	1.432	1.419
C8B-C2A	1.438	1.445	1.431	1.440	1.449	1.433	1.444	1.452	1.436	1.428	1.441	1.426
C5A-C6	1.440	1.450	1.430	1.444	1.450	1.433	1.440	1.448	1.431	1.464	1.470	1.450
C6-C7	1.424	1.438	1.416	1.423	1.436	1.415	1.432	1.442	1.422	1.428	1.444	1.426
C7-C8	1.426	1.434	1.415	1.427	1.435	1.413	1.430	1.441	1.418	1.443	1.455	1.441
C8-C8A	1.434	1.447	1.430	1.419	1.432	1.414	1.412	1.425	1.407	1.442	1.446	1.430
C8A-C8B	1.456	1.477	1.463	1.438	1.447	1.431	1.444	1.452	1.436	1.441	1.447	1.430
C8A-C1	1.450	1.452	1.432	1.463	1.462	1.444	1.461	1.463	1.443	1.428	1.439	1.420

Table S24. Iron-carbonyl distances (in Å) for $C_{12}H_8Fe_2(CO)_4$ structures using B3LYP, BP86, and M06-L methods.

	Fe24-1			Fe24-2			Fe24-3		
	B3LYP	BP86	M06-L	B3LYP	BP86	M06-L	B3LYP	BP86	M06-L
Fe1-C9	2.022	1.981	2.004	1.787	1.766	1.773	1.768	1.756	1.765
Fe1-C10	1.775	1.760	1.767	2.051	2.010	2.039	1.769	1.759	1.764
C9-O9	1.194	1.202	1.187	1.146	1.165	1.154	1.149	1.165	1.153
C10-O10	1.161	1.179	1.154	1.181	1.196	1.187	1.151	1.167	1.157
Fe2-C11	1.772	1.750	1.775	1.785	1.766	1.782	1.791	1.761	1.775
Fe2-C12	1.798	1.764	1.796	1.792	1.777	1.788	1.785	1.769	1.784
C11-O11	1.161	1.178	1.152	1.147	1.165	1.152	1.146	1.167	1.153
C12-O12	1.158	1.176	1.149	1.144	1.160	1.149	1.147	1.166	1.154

	Fe24-4			Fe24-5			Fe24-6			Fe24-7		
	B3LYP	BP86	M06-L	B3LYP	BP86	M06-L	B3LYP	BP86	M06-L	B3LYP	BP86	M06-L
Fe1-C9	1.785	1.767	1.778	1.751	1.735	1.747	1.754	1.737	1.752	1.797	1.766	1.788
Fe1-C10	1.752	1.737	1.753	1.776	1.761	1.773	1.776	1.759	1.771	1.774	1.747	1.770
C9-O9	1.163	1.179	1.154	1.165	1.181	1.156	1.164	1.180	1.155	1.155	1.175	1.148
C10-O10	1.164	1.181	1.155	1.163	1.179	1.154	1.163	1.179	1.154	1.157	1.176	1.149
Fe2-C11	1.758	1.741	1.754	1.761	1.747	1.759	1.776	1.759	1.771	1.766	1.753	1.766
Fe2-C12	1.775	1.761	1.774	1.776	1.760	1.774	1.754	1.737	1.752	1.695	1.700	1.703
C11-O11	1.164	1.180	1.155	1.165	1.180	1.155	1.163	1.179	1.154	1.165	1.182	1.156
C12-O12	1.163	1.178	1.153	1.162	1.178	1.153	1.164	1.180	1.155	1.204	1.214	1.191

Table S25. Iron-carbon distances (in Å) for $C_{12}H_8Fe_3(CO)_9$ structures using B3LYP, BP86, and M06-L methods.

	Fe39-1			Fe39-2			Fe39-3		
	B3LYP	BP86	M06-L	B3LYP	BP86	M06-L	B3LYP	BP86	M06-L
Fe1-C1	2.084	2.081	2.066	2.115	2.122	2.093	3.227	3.178	3.123
Fe1-C2	2.078	2.080	2.057	2.114	1.991	1.976	2.431	2.337	2.316
Fe1-C2A	2.314	2.302	2.261	2.922	2.224	2.191	1.978	1.977	1.963
Fe1-C8B	2.269	2.316	2.220	3.280	2.609	2.538	2.328	2.359	2.269
Fe1-C8A	2.242	2.256	2.212	2.990	2.724	2.667	3.134	3.129	3.034
Fe1-C3	3.501	3.498	3.422	4.014	3.384	3.318	2.195	2.246	2.208
Fe2-C3	2.172	2.159	2.135	3.055	2.202	2.174	3.052	3.035	3.004
Fe2-C4	1.958	1.978	1.954	2.289	2.055	2.042	2.113	2.132	2.107
Fe2-C5	2.177	2.172	2.138	2.042	2.066	2.050	2.125	2.137	2.111
Fe2-C5A	2.995	2.892	2.902	2.409	2.259	2.208	3.012	2.972	2.940
Fe3-C6	2.196	2.173	2.148	2.191	2.110	2.083	3.820	3.831	3.767
Fe3-C7	2.018	2.028	2.017	2.065	1.982	1.974	3.254	3.261	3.199
Fe3-C8	2.135	2.133	2.117	2.077	2.224	2.221	2.376	2.327	2.312
Fe3-C8A	2.862	2.843	2.792	2.233	2.815	2.789	2.128	2.075	2.089
Fe3-C1	4.055	4.040	3.983	3.509	4.120	4.063	2.275	2.217	2.221

Table S26. Carbon-carbon distances (in Å) for $C_{12}H_8Fe_3(CO)_9$ structures using B3LYP, BP86, and M06-L methods.

	Fe39-1			Fe39-2			Fe39-3		
	B3LYP	BP86	M06-L	B3LYP	BP86	M06-L	B3LYP	BP86	M06-L
C1-C2	1.457	1.461	1.446	1.437	1.476	1.461	1.470	1.492	1.472
C2-C2A	1.451	1.458	1.439	1.483	1.457	1.443	1.422	1.432	1.414
C2A-C3	1.448	1.461	1.440	1.398	1.490	1.474	1.420	1.425	1.411
C3-C4	1.462	1.471	1.455	1.426	1.454	1.436	1.487	1.483	1.467
C4-C5	1.452	1.449	1.441	1.447	1.429	1.408	1.447	1.456	1.441
C5-C5A	1.438	1.442	1.428	1.435	1.458	1.443	1.460	1.455	1.437
C5A-C8B	1.455	1.454	1.442	1.398	1.454	1.439	1.426	1.433	1.419
C8B-C2A	1.416	1.424	1.407	1.404	1.411	1.390	1.440	1.446	1.436
C5A-C6	1.424	1.444	1.421	1.496	1.501	1.487	1.406	1.422	1.401
C6-C7	1.436	1.441	1.421	1.442	1.466	1.448	1.411	1.410	1.390
C7-C8	1.453	1.460	1.443	1.420	1.449	1.430	1.418	1.435	1.410
C8-C8A	1.451	1.456	1.438	1.439	1.421	1.400	1.421	1.429	1.412
C8A-C8B	1.429	1.436	1.419	1.464	1.443	1.426	1.455	1.459	1.444
C8A-C1	1.431	1.445	1.422	1.501	1.472	1.451	1.431	1.443	1.424

Table S27. Iron-carbonyl distances (in Å) for $C_{12}H_8Fe_3(CO)_9$ structures using B3LYP, BP86, and M06-L methods.

	Fe39-1			Fe39-2			Fe39-3		
	B3LYP	BP86	M06-L	B3LYP	BP86	M06-L	B3LYP	BP86	M06-L
Fe1-C9	1.815	1.797	1.815	1.794	1.783	1.823	1.799	1.783	1.800
Fe1-C10	1.818	1.797	1.820	1.777	1.758	1.799	1.789	1.778	1.794
Fe1-C11	1.791	1.773	1.794	1.765	1.807	1.775	1.826	1.798	1.818
C9-O9	1.151	1.168	1.143	1.156	1.174	1.147	1.155	1.172	1.146
C10-O10	1.150	1.167	1.142	1.162	1.174	1.149	1.156	1.173	1.147
C11-O11	1.154	1.172	1.146	1.163	1.170	1.149	1.154	1.172	1.145
Fe2-C12	1.787	1.774	1.789	1.774	1.782	1.801	1.830	1.812	1.833
Fe2-C13	1.780	1.766	1.779	1.771	1.777	1.798	1.762	1.733	1.751
Fe2-C14	1.798	1.795	1.800	1.823	1.799	1.813	1.825	1.807	1.825
C12-O12	1.162	1.177	1.152	1.163	1.172	1.146	1.155	1.171	1.146
C13-O13	1.162	1.177	1.153	1.163	1.172	1.147	1.158	1.175	1.149
C14-O14	1.165	1.178	1.156	1.160	1.168	1.144	1.155	1.171	1.146
Fe3-C15	1.795	1.777	1.794	1.798	1.759	1.771	1.778	1.776	1.785
Fe3-C16	1.808	1.797	1.812	1.806	1.788	1.795	1.744	1.739	1.739
Fe3-C17	1.781	1.771	1.786	1.807	1.781	1.796	1.799	1.796	1.809
C15-O15	1.159	1.175	1.149	1.155	1.177	1.152	1.161	1.175	1.151
C16-O16	1.160	1.175	1.150	1.154	1.174	1.152	1.188	1.203	1.183
C17-O17	1.160	1.175	1.150	1.155	1.175	1.151	1.164	1.178	1.154

Table S28. Iron-carbon distances (in Å) for $C_{12}H_8Fe_3(CO)_8$ structures using B3LYP, BP86, and M06-L methods.

	Fe38-1			Fe38-2			Fe38-3		
	B3LYP	BP86	M06-L	B3LYP	BP86	M06-L	B3LYP	BP86	M06-L
Fe1-C5A	2.729	2.646	2.542	2.718	2.626	2.445	2.981	2.954	2.916
Fe1-C6	2.206	2.165	2.142	2.223	2.172	2.126	2.217	2.227	2.182
Fe1-C7	2.006	2.020	2.012	2.011	2.023	2.024	2.075	2.062	2.051
Fe1-C8	2.147	2.161	2.137	2.157	2.162	2.159	2.194	2.129	2.163
Fe2-C1	2.145	2.135	2.099	2.143	2.142	2.091	2.119	2.126	2.082
Fe2-C2	2.107	2.103	2.070	2.127	2.118	2.065	2.120	2.123	2.084
Fe2-C2A	2.193	2.209	2.165	2.204	2.219	2.114	2.216	2.218	2.167
Fe2-C8B	2.152	2.174	2.109	2.134	2.158	2.061	2.136	2.156	2.095
Fe2-C8A	2.253	2.254	2.201	2.236	2.234	2.171	2.126	2.171	2.103
Fe3-C3	2.149	2.132	2.113	2.137	2.115	2.144	2.640	2.453	2.478
Fe3-C4	2.107	2.091	2.087	2.094	2.088	2.072	2.183	2.082	2.152
Fe3-C5	2.306	2.301	2.287	2.288	2.302	2.235	3.212	3.187	3.207

Table S29. Carbon-carbon distances (in Å) for $C_{12}H_8Fe_3(CO)_8$ structures using B3LYP, BP86, and M06-L methods.

	Fe38-1			Fe38-2			Fe38-3		
	B3LYP	BP86	M06-L	B3LYP	BP86	M06-L	B3LYP	BP86	M06-L
C1-C2	1.459	1.465	1.450	1.445	1.451	1.446	1.442	1.445	1.434
C2-C2A	1.429	1.442	1.423	1.437	1.451	1.422	1.448	1.457	1.433
C2A-C3	1.447	1.449	1.436	1.445	1.450	1.440	1.441	1.450	1.433
C3-C4	1.429	1.441	1.423	1.416	1.429	1.412	1.396	1.415	1.388
C4-C5	1.422	1.433	1.411	1.440	1.448	1.424	1.442	1.445	1.424
C5-C5A	1.444	1.447	1.432	1.445	1.444	1.445	1.381	1.392	1.372
C5A-C8B	1.445	1.448	1.435	1.443	1.449	1.435	1.425	1.433	1.417
C8B-C2A	1.432	1.440	1.424	1.435	1.442	1.423	1.419	1.430	1.417
C5A-C6	1.414	1.433	1.413	1.412	1.431	1.414	1.470	1.468	1.452
C6-C7	1.439	1.440	1.420	1.438	1.439	1.416	1.438	1.450	1.430
C7-C8	1.449	1.457	1.440	1.450	1.458	1.438	1.416	1.428	1.408
C8-C8A	1.464	1.467	1.454	1.466	1.471	1.461	1.448	1.454	1.438
C8A-C8B	1.418	1.427	1.409	1.405	1.415	1.400	1.444	1.454	1.436
C8A-C1	1.424	1.435	1.415	1.438	1.447	1.422	1.430	1.447	1.421

Table S30.Iron-carbonyl distances (in Å) for $C_{12}H_8Fe_3(CO)_8$ structures using B3LYP, BP86, and M06-L methods.

	Fe38-1			**Fe38-2**			**Fe38-3**		
	B3LYP	BP86	M06-L	B3LYP	BP86	M06-L	B3LYP	BP86	M06-L
Fe1-C9	1.798	1.781	1.798	1.799	1.780	1.798	1.777	1.749	1.778
Fe1-C10	1.806	1.795	1.808	1.809	1.798	1.811	1.799	1.844	1.806
Fe1-C11	1.776	1.795	1.782	1.776	1.766	1.784	1.799	1.779	1.798
C9-O9	1.160	1.175	1.150	1.160	1.175	1.149	1.158	1.176	1.150
C10-O10	1.160	1.175	1.150	1.160	1.174	1.149	1.163	1.190	1.151
C11-O11	1.160	1.175	1.150	1.160	1.175	1.149	1.157	1.174	1.149
Fe2-C12	1.789	1.774	1.786	1.781	1.763	1.773	1.776	1.762	1.772
Fe2-C13	1.780	1.761	1.778	1.783	1.767	1.774	1.769	1.754	1.764
C12-O12	1.157	1.174	1.150	1.156	1.173	1.153	1.158	1.173	1.152
C13-O13	1.156	1.173	1.148	1.157	1.174	1.152	1.159	1.175	1.151
Fe3-C14	1.790	1.774	1.793	1.867	1.897	1.803	1.792	1.785	1.800
Fe3-C15	1.761	1.749	1.763	1.764	1.751	1.781	1.783	1.768	1.773
Fe3-C16	1.881	1.908	1.877	1.782	1.763	1.795	1.770	1.747	1.755
C14-O14	1.157	1.174	1.149	1.183	1.196	1.150	1.164	1.177	1.153
C15-O15	1.159	1.175	1.151	1.159	1.175	1.150	1.166	1.180	1.157
C16-O16	1.185	1.196	1.171	1.158	1.175	1.150	1.159	1.174	1.151

Table S31.The theoretical Cartesian coordinates (in Å) for the structure **Fe14-1** of $C_{12}H_8Fe(CO)_4$ using M06-L method.

Center Number	Atomic Number	Atomic Type	Coordinates(Angstroms)		
			x	y	z
1	6	0	-0.816734	1.114431	1.163447
2	6	0	-0.516856	1.850510	0.000000
3	6	0	-0.816734	1.114431	-1.163447
4	6	0	-0.556440	1.690634	-2.385033
5	1	0	-0.757372	1.171381	-3.314705
6	6	0	-0.005624	2.990919	-2.415391
7	6	0	0.296279	3.698171	-1.272196
8	6	0	0.050448	3.128844	0.000000
9	6	0	0.296279	3.698171	1.272196
10	6	0	-0.005624	2.990919	2.415391
11	1	0	0.190482	3.445161	3.379086
12	1	0	0.720095	4.692737	1.346043
13	1	0	0.190482	3.445161	-3.379086
14	1	0	0.720095	4.692737	-1.346043
15	6	0	-1.350711	-0.183261	-0.716913
16	6	0	-1.350711	-0.183261	0.716913
17	1	0	-2.076192	-0.721621	-1.311578
18	1	0	-2.076192	-0.721621	1.311578
19	6	0	-0.556440	1.690634	2.385033
20	1	0	-0.757372	1.171381	3.314705
21	26	0	0.109416	-1.601871	0.000000
22	6	0	1.432799	-0.333785	0.000000
23	6	0	0.808713	-2.322363	-1.502693
24	6	0	-1.223218	-2.837963	0.000000
25	6	0	0.808713	-2.322363	1.502693
26	8	0	2.300152	0.408442	0.000000
27	8	0	1.261750	-2.789667	-2.448584
28	8	0	-2.069114	-3.608443	0.000000
29	8	0	1.261750	-2.789667	2.448584

Table S32. The theoretical Cartesian coordinates (in Å) for the structure **Fe14-2** of $C_{12}H_8Fe(CO)_4$ using M06-L method.

Center Number	Atomic Number	Atomic Type	Coordinates(Angstroms)		
			x	y	z
1	6	0	-0.444572	0.491805	-1.050096
2	6	0	-1.686254	0.159896	-0.419857
3	6	0	-2.361342	1.332757	-0.046054
4	6	0	-3.613721	1.206266	0.531195
5	1	0	-4.185831	2.072898	0.840341
6	6	0	-4.158824	-0.078684	0.681617
7	6	0	-3.510156	-1.216995	0.233369
8	6	0	-2.240165	-1.114004	-0.367717
9	6	0	-1.482839	-2.159594	-0.985815
10	6	0	-0.309628	-1.879159	-1.620715
11	1	0	0.230909	-2.676871	-2.115514
12	1	0	-1.862658	-3.174287	-0.975636
13	1	0	-5.136671	-0.178704	1.136432
14	1	0	-3.987664	-2.185185	0.326279
15	6	0	-1.530714	2.442457	-0.482938
16	6	0	-0.420488	1.957325	-1.098216
17	1	0	-1.763156	3.487794	-0.342678
18	1	0	0.368955	2.549227	-1.537764
19	6	0	0.259443	-0.557809	-1.680852
20	1	0	1.003144	-0.362819	-2.442983
21	26	0	1.435579	-0.042797	0.192080
22	6	0	0.421292	-1.121053	1.265902
23	6	0	1.415937	1.222951	1.476130
24	6	0	2.492170	1.020340	-0.840135
25	6	0	2.743158	-1.269676	0.236323
26	8	0	-0.165412	-1.796641	1.976638
27	8	0	1.449215	2.012401	2.309665
28	8	0	3.179540	1.676941	-1.479372
29	8	0	3.607673	-2.022735	0.333645

Table S33. The theoretical Cartesian coordinates (in Å) for the structure **Fe13-1** of $C_{12}H_8Fe(CO)_3$ using M06-L method.

Center Number	Atomic Number	Atomic Type	Coordinates(Angstroms)		
			x	y	z
1	6	0	1.108021	-0.577396	1.181179
2	6	0	0.536241	-1.147389	0.000000
3	6	0	1.108021	-0.577396	-1.181179
4	6	0	0.817032	-1.168662	-2.406857
5	1	0	1.232359	-0.788642	-3.330305
6	6	0	-0.065105	-2.253667	-2.414137
7	6	0	-0.632320	-2.800159	-1.270879
8	6	0	-0.306140	-2.287994	0.000000
9	6	0	-0.632320	-2.800159	1.270879
10	6	0	-0.065105	-2.253667	2.414137
11	1	0	-0.308634	-2.705025	3.369087
12	1	0	-1.280816	-3.663374	1.352805
13	1	0	-0.308634	-2.705025	-3.369087
14	1	0	-1.280816	-3.663374	-1.352805
15	6	0	1.804037	0.602755	-0.727025
16	6	0	1.804037	0.602755	0.727025
17	1	0	2.397724	1.259240	-1.343695
18	1	0	2.397724	1.259240	1.343695
19	6	0	0.817032	-1.168662	2.406857
20	1	0	1.232359	-0.788642	3.330305
21	26	0	-0.045561	1.066451	0.000000
22	6	0	-1.225482	1.088711	-1.396386
23	6	0	0.249591	2.805222	0.000000
24	6	0	-1.225482	1.088711	1.396386
25	8	0	-1.955753	1.106235	-2.279076
26	8	0	0.480378	3.931261	0.000000
27	8	0	-1.955753	1.106235	2.279076

Table S34.The theoretical Cartesian coordinates (in Å) for the structure **Fe13-2** of $C_{12}H_8Fe(CO)_3$ using M06-L method.

Center Number	Atomic Number	Atomic Type	Coordinates(Angstroms)		
			x	y	z
1	6	0	-0.436789	1.107484	1.107484
2	6	0	-1.515093	0.186852	0.186852
3	6	0	-2.590939	0.856705	0.856705
4	6	0	-3.666191	0.075026	0.075026
5	1	0	-4.539563	0.516705	0.516705
6	6	0	-3.580168	-1.305928	-1.305928
7	6	0	-2.453505	-1.947897	-1.947897
8	6	0	-1.377194	-1.177616	-1.177616
9	6	0	-0.024576	-1.550180	-1.550180
10	6	0	0.701121	-0.684151	-0.684151
11	1	0	1.449692	-1.071737	-1.071737
12	1	0	0.254138	-2.597890	-2.597890
13	1	0	-4.406352	-1.917708	-1.917708
14	1	0	-2.422261	-3.029771	-3.029771
15	6	0	-2.200346	2.259464	2.259464
16	6	0	-0.940782	2.409542	2.409542
17	1	0	-2.814524	3.063431	3.063431
18	1	0	-0.408761	3.344057	3.344057
19	6	0	0.516744	0.711024	0.711024
20	1	0	1.083544	1.415272	1.415272
21	26	0	1.259302	-0.090309	-0.090309
22	6	0	2.693074	-1.158911	-1.158911
23	6	0	0.514212	-0.431042	-0.431042
24	6	0	2.255927	1.361779	1.361779
25	8	0	3.590364	-1.875449	-1.875449
26	8	0	0.018925	-0.644748	-0.644748
27	8	0	2.851868	2.314295	2.314295

Table S35.The theoretical Cartesian coordinates (in Å) for the structure **Fe12-1** of $C_{12}H_8Fe(CO)_2$ using M06-L method.

Center Number	Atomic Number	Atomic Type	Coordinates(Angstroms)		
			x	y	z
1	6	0	0.200112	1.477187	-0.781153
2	6	0	0.962731	0.284785	-0.602556
3	6	0	0.373587	-0.805089	-1.309724
4	6	0	1.030900	-2.046445	-1.255812
5	1	0	0.644047	-2.908796	-1.782451
6	6	0	2.195732	-2.141044	-0.508035
7	6	0	2.743057	-1.073251	0.211540
8	6	0	2.126924	0.181866	0.199715
9	6	0	2.488340	1.355511	0.904627
10	6	0	1.677517	2.468941	0.848711
11	1	0	1.939316	3.330133	1.451590
12	1	0	3.370815	1.357144	1.531844
13	1	0	2.705448	-3.096201	-0.470131
14	1	0	3.648007	-1.225452	0.786776
15	6	0	-0.855039	-0.303872	-1.854935
16	6	0	-0.941945	1.102428	-1.577551
17	1	0	-1.548816	-0.861507	-2.464167
18	1	0	-1.730733	1.757634	-1.909929
19	6	0	0.510655	2.550037	0.058105
20	1	0	-0.083995	3.453947	0.057516
21	26	0	-1.029008	0.062808	0.160989
22	6	0	-0.765898	-1.100067	1.488806
23	6	0	-2.770535	0.023543	0.337664
24	8	0	-0.582667	-1.904929	2.294011
25	8	0	-3.923169	-0.005957	0.413091

Table S36.The theoretical Cartesian coordinates (in Å) for the structure **Fe12-2** of $C_{12}H_8Fe(CO)_2$ using M06-L method.

Center Number	Atomic Number	Atomic Type	Coordinates(Angstroms)		
			x	y	z
1	6	0	-2.256834	0.325378	-0.250688
2	6	0	-1.142959	-0.112783	0.514502
3	6	0	-0.575802	0.989011	1.215485
4	6	0	0.635818	0.795837	1.917836
5	1	0	1.131045	1.598494	2.446145
6	6	0	1.147526	-0.526330	1.977947
7	6	0	0.583513	-1.590073	1.237921
8	6	0	-0.612461	-1.413061	0.469133
9	6	0	-1.273337	-2.327941	-0.387767
10	6	0	-2.383586	-1.920863	-1.100970
11	1	0	-2.873662	-2.635915	-1.749599
12	1	0	-0.908261	-3.343644	-0.474628
13	1	0	2.076323	-0.703137	2.503692
14	1	0	1.108463	-2.536002	1.204766
15	6	0	-1.402294	2.132306	0.877625
16	6	0	-2.398014	1.734886	0.032274
17	1	0	-1.246776	3.133872	1.249456
18	1	0	-3.162053	2.377224	-0.380116
19	6	0	-2.887648	-0.605374	-1.049892
20	1	0	-3.740559	-0.337874	-1.662007
21	26	0	0.964821	0.051072	-0.017700
22	6	0	2.494140	-0.518770	-0.668638
23	6	0	1.026661	1.385590	-1.187052
24	8	0	3.508117	-0.876924	-1.092786
25	8	0	1.092110	2.255952	-1.940188

Table S37. The theoretical Cartesian coordinates (in Å) for the structure **Fe28-1** of $C_{12}H_8Fe_2(CO)_8$ using M06-L method.

Center Number	Atomic Number	Atomic Type	Coordinates(Angstroms)		
			x	y	z
1	6	0	0.733861	1.487526	1.121221
2	6	0	-0.197311	1.439720	0.072518
3	6	0	-0.404718	0.094858	-0.371961
4	6	0	-1.163410	-0.090673	-1.544323
5	1	0	-1.105934	-1.011890	-2.110070
6	6	0	-1.687532	1.075398	-2.200287
7	6	0	-1.490124	2.343560	-1.738657
8	6	0	-0.704927	2.572698	-0.567347
9	6	0	-0.346257	3.815741	-0.013626
10	6	0	0.510539	3.871587	1.071559
11	1	0	0.775564	4.839024	1.480093
12	1	0	-0.730506	4.730464	-0.448658
13	1	0	-2.260317	0.922993	-3.106969
14	1	0	-1.910549	3.186448	-2.273606
15	6	0	0.546494	-0.736461	0.401073
16	6	0	1.203743	0.113329	1.345804
17	1	0	0.358375	-1.782574	0.588685
18	1	0	1.530224	-0.222731	2.320760
19	6	0	1.081575	2.721524	1.638206
20	1	0	1.799819	2.814991	2.443877
21	26	0	2.643353	-0.563392	-0.117954
22	6	0	2.346618	0.871792	-1.215011
23	6	0	2.824522	-1.611360	-1.578565
24	6	0	2.946234	-1.999776	0.958116
25	6	0	4.192799	0.192002	0.425106
26	8	0	2.229266	1.748210	-1.938175
27	8	0	2.957248	-2.273630	-2.507233
28	8	0	3.137244	-2.899940	1.637296
29	8	0	5.185193	0.666387	0.753848
30	26	0	-2.550569	-0.740453	0.163733
31	6	0	-3.155039	0.948482	0.504160
32	6	0	-2.306819	-0.992160	1.927599
33	6	0	-2.033905	-2.450977	-0.168068
34	6	0	-4.135296	-1.112281	-0.590097
35	8	0	-3.577308	1.983281	0.744694
36	8	0	-2.198570	-1.179451	3.057416
37	8	0	-1.729373	-3.536142	-0.376451
38	8	0	-5.183118	-1.371703	-0.990003

Table S38. The theoretical Cartesian coordinates (in Å) for the structure **Fe28-2** of $C_{12}H_8Fe_2(CO)_8$ using M06-L method.

Center Number	Atomic Number	Atomic Type	Coordinates(Angstroms)		
			x	y	z
1	6	0	0.411578	0.216600	-1.581769
2	6	0	0.201373	1.439753	-0.882928
3	6	0	1.419988	2.076892	-0.597573
4	6	0	1.386215	3.295891	0.050324
5	1	0	2.293768	3.832364	0.299826
6	6	0	0.136325	3.843324	0.383329
7	6	0	-1.057959	3.215894	0.072801
8	6	0	-1.047857	1.976944	-0.591313
9	6	0	-2.184708	1.255749	-1.103177
10	6	0	-1.984543	0.081228	-1.861087
11	1	0	-2.779255	-0.271070	-2.504882
12	1	0	-3.105033	1.812080	-1.225317
13	1	0	0.106982	4.799445	0.891261
14	1	0	-1.999930	3.686355	0.329924
15	6	0	2.491914	1.204191	-1.110752
16	6	0	1.865006	0.046936	-1.685786
17	1	0	3.419001	1.621603	-1.479754
18	1	0	2.291016	-0.507618	-2.510723
19	6	0	-0.670412	-0.456239	-2.074274
20	1	0	-0.564458	-1.368330	-2.649662
21	26	0	-3.029881	-0.510133	0.119067
22	6	0	-4.660063	0.085019	-0.426979
23	6	0	-3.174623	0.357660	1.688497
24	6	0	-1.465769	-1.293783	0.610015
25	6	0	-3.674101	-2.175292	-0.022312
26	8	0	-5.696520	0.443144	-0.760227
27	8	0	-3.274778	0.863590	2.715749
28	8	0	-0.535810	-1.888315	0.918700
29	8	0	-4.122857	-3.235953	-0.036129
30	26	0	2.960733	-0.490625	0.112471
31	6	0	4.320090	-0.894553	-1.026036
32	6	0	2.556409	-2.246389	0.324193
33	6	0	1.658420	0.038055	1.291263
34	6	0	4.171055	0.056514	1.333029
35	8	0	5.176623	-1.139499	-1.743744
36	8	0	2.320987	-3.358899	0.466054
37	8	0	0.924135	0.393230	2.090873
38	8	0	4.951436	0.381266	2.110292

Table S39. The theoretical Cartesian coordinates (in Å) for the structure **Fe28-3** of $C_{12}H_8Fe_2(CO)_8$ using M06-L method.

Center Number	Atomic Number	Atomic Type	Coordinates(Angstroms)		
			x	y	z
1	6	0	1.696530	1.208066	-1.022712
2	6	0	0.271022	1.156354	-0.983295
3	6	0	-0.231886	2.333663	-0.361872
4	6	0	-1.584934	2.553508	-0.366918
5	1	0	-2.015963	3.461450	0.037650
6	6	0	-2.443659	1.602923	-0.995197
7	6	0	-1.926583	0.445598	-1.636840
8	6	0	-0.503216	0.247913	-1.678902
9	6	0	0.190834	-0.714539	-2.464253
10	6	0	1.556399	-0.675277	-2.557716
11	1	0	2.063501	-1.384754	-3.200066
12	1	0	-0.367542	-1.456752	-3.022387
13	1	0	-3.445990	1.929830	-1.236652
14	1	0	-2.521802	-0.049327	-2.393570
15	6	0	0.926384	3.124079	0.006590
16	6	0	2.053037	2.487051	-0.406022
17	1	0	0.892594	4.079551	0.508347
18	1	0	3.060921	2.861306	-0.301249
19	6	0	2.360090	0.278286	-1.855665
20	1	0	3.369666	0.451466	-2.204655
21	26	0	-3.030948	-0.240153	0.241195
22	6	0	-4.515880	-0.452782	-0.788243
23	6	0	-4.064842	0.390639	1.568232
24	6	0	-1.579530	0.011927	1.311833
25	6	0	-2.741515	-2.015073	0.193294
26	8	0	-5.453100	-0.589083	-1.432807
27	8	0	-4.738618	0.715929	2.442507
28	8	0	-0.697607	0.176380	2.022292
29	8	0	-2.614262	-3.156954	0.220598
30	26	0	2.858022	-0.413527	0.273197
31	6	0	4.387763	0.570271	0.197845
32	6	0	3.846704	-1.895418	0.080476
33	6	0	1.376115	-1.469724	0.354713
34	6	0	2.540851	0.206354	1.936695
35	8	0	5.367088	1.163854	0.159154
36	8	0	4.488382	-2.850711	0.052149
37	8	0	0.474012	-2.170556	0.420361
38	8	0	2.396428	0.553639	3.021512

Table S40. The theoretical Cartesian coordinates (in Å) for the structure **Fe28-4** of $C_{12}H_8Fe_2(CO)_8$ using M06-L method.

Center Number	Atomic Number	Atomic Type	Coordinates(Angstroms)		
			x	y	z
1	6	0	0.675537	2.058849	-0.601626
2	6	0	0.013128	0.964638	0.039350
3	6	0	-1.062178	1.442389	0.785508
4	6	0	-1.878209	0.511502	1.446106
5	1	0	-2.605234	0.827154	2.182711
6	6	0	-1.548979	-0.863305	1.317799
7	6	0	-0.445136	-1.301686	0.570327
8	6	0	0.366970	-0.377496	-0.086540
9	6	0	1.531217	-0.654994	-0.908340
10	6	0	2.183556	0.427267	-1.564202
11	1	0	2.777242	0.219891	-2.445097
12	1	0	1.613890	-1.648295	-1.331915
13	1	0	-2.070309	-1.584840	1.932656
14	1	0	-0.222212	-2.361266	0.525764
15	6	0	-1.073289	2.887030	0.619069
16	6	0	-0.047198	3.252155	-0.199220
17	1	0	-1.796575	3.555602	1.063030
18	1	0	0.191916	4.258792	-0.507344
19	6	0	1.750809	1.790856	-1.392664
20	1	0	2.282546	2.572133	-1.924221
21	26	0	3.497288	-0.335705	0.053804
22	6	0	4.229904	-1.484049	-1.154656
23	6	0	3.447823	-1.646226	1.289914
24	6	0	2.796578	0.833892	1.277088
25	6	0	5.012381	0.645913	0.029946
26	8	0	4.692561	-2.206030	-1.911890
27	8	0	3.434698	-2.471570	2.087980
28	8	0	2.414616	1.554587	2.075949
29	8	0	5.997758	1.235436	0.057480
30	26	0	-3.554498	-0.363655	-0.085455
31	6	0	-2.520870	0.019162	-1.537336
32	6	0	-4.529186	1.099864	-0.405190
33	6	0	-4.609582	-0.760386	1.339430
34	6	0	-3.923847	-1.966497	-0.786858
35	8	0	-1.888056	0.252911	-2.462861
36	8	0	-5.226565	1.976071	-0.680273
37	8	0	-5.280141	-1.010755	2.235580
38	8	0	-4.257422	-2.946786	-1.294481

Table S41. The theoretical Cartesian coordinates (in Å) for the structure **Fe27-1** of $C_{12}H_8Fe_2(CO)_7$ using M06-L method.

Center Number	Atomic Number	Atomic Type	Coordinates(Angstroms)		
			x	y	z
1	6	0	-1.226656	0.797697	-1.300460
2	6	0	-0.587717	0.821691	-0.023521
3	6	0	0.106927	-0.412267	0.230658
4	6	0	0.902098	-0.501269	1.392311
5	1	0	1.153829	-1.465599	1.813749
6	6	0	0.869722	0.630202	2.282535
7	6	0	0.219526	1.801913	2.019682
8	6	0	-0.495313	1.976091	0.794134
9	6	0	-1.068350	3.132543	0.278600
10	6	0	-1.643912	3.133188	-1.003721
11	1	0	-2.036296	4.069062	-1.383272
12	1	0	-1.031111	4.054278	0.845412
13	1	0	1.418148	0.537185	3.212592
14	1	0	0.284679	2.626264	2.718336
15	6	0	-0.499830	-1.336485	-0.706827
16	6	0	-1.219599	-0.577979	-1.711375
17	1	0	-0.238876	-2.378838	-0.810437
18	1	0	-1.568027	-0.962487	-2.656559
19	6	0	-1.734200	2.012462	-1.805326
20	1	0	-2.186790	2.064618	-2.786224
21	26	0	-2.300968	-0.638266	0.014812
22	6	0	-3.754359	0.452930	0.039857
23	6	0	-2.220648	-1.042895	1.794470
24	6	0	-3.236969	-2.052341	-0.500338
25	8	0	-4.650434	1.166500	0.061548
26	8	0	-2.187574	-1.341177	2.900067
27	8	0	-3.806879	-2.985270	-0.850805
28	26	0	2.607497	-0.264071	-0.111002
29	6	0	2.457973	-0.196070	-1.891485
30	6	0	2.664365	-2.075045	-0.174031
31	6	0	4.208022	-0.235349	0.692098
32	6	0	2.556837	1.552759	-0.051542
33	8	0	2.409837	-0.153299	-3.043124
34	8	0	2.696600	-3.222137	-0.213253
35	8	0	5.281191	-0.210512	1.112283
36	8	0	2.563156	2.699100	-0.040087

Table S42. The theoretical Cartesian coordinates (in Å) for the structure **Fe27-2** of $C_{12}H_8Fe_2(CO)_7$ using M06-L method.

Center Number	Atomic Number	Atomic Type	Coordinates(Angstroms)		
			x	y	z
1	6	0	-0.551586	0.242185	-1.205497
2	6	0	-0.469147	1.593459	-0.689450
3	6	0	0.809608	2.114431	-0.778548
4	6	0	0.996869	3.419003	-0.316304
5	1	0	1.970845	3.893146	-0.327625
6	6	0	-0.106214	4.106060	0.183478
7	6	0	-1.393520	3.550926	0.232249
8	6	0	-1.584875	2.251495	-0.221307
9	6	0	-2.799145	1.429804	-0.361735
10	6	0	-2.906069	0.582468	-1.516285
11	1	0	-3.858965	0.370417	-1.982807
12	1	0	-3.726721	1.795209	0.064406
13	1	0	0.033004	5.115473	0.550538
14	1	0	-2.219020	4.139936	0.613484
15	6	0	1.665028	1.045851	-1.336844
16	6	0	0.843034	-0.117228	-1.532473
17	1	0	2.522712	1.271787	-1.956398
18	1	0	1.032437	-0.834463	-2.321187
19	6	0	-1.730797	-0.070071	-1.953084
20	1	0	-1.743340	-0.774864	-2.774415
21	26	0	-2.218273	-0.639004	-0.034994
22	6	0	-1.702085	-0.364000	1.680336
23	6	0	-1.611349	-2.306349	-0.318348
24	6	0	-3.870016	-1.237232	0.326832
25	8	0	-1.474251	-0.244509	2.797559
26	8	0	-1.187366	-3.348080	-0.547810
27	8	0	-4.935167	-1.594285	0.565180
28	26	0	2.293893	-0.465092	0.055508
29	6	0	3.224194	-1.344279	-1.235692
30	6	0	1.784251	-2.019785	0.828065
31	6	0	1.452033	0.503363	1.362680
32	6	0	3.847340	0.147757	0.734609
33	8	0	3.811210	-1.898616	-2.046961
34	8	0	1.477284	-2.980935	1.374874
35	8	0	1.040478	1.128819	2.225024
36	8	0	4.847513	0.507943	1.170204

Table S43. The theoretical Cartesian coordinates (in Å) for the structure **Fe27-3** of $C_{12}H_8Fe_2(CO)_7$ using M06-L method.

Center Number	Atomic Number	Atomic Type	Coordinates(Angstroms)		
			x	y	z
1	6	0	1.532190	1.091417	-0.632313
2	6	0	0.472866	0.310985	-0.026842
3	6	0	-0.426608	1.129062	0.615241
4	6	0	-1.496937	0.502642	1.312080
5	1	0	-2.068063	1.051972	2.048550
6	6	0	-1.534169	-0.914811	1.309863
7	6	0	-0.537242	-1.704885	0.668679
8	6	0	0.491809	-1.080020	0.000892
9	6	0	1.708503	-1.613421	-0.616088
10	6	0	2.328877	-0.909534	-1.695191
11	1	0	2.919302	-1.433656	-2.434982
12	1	0	1.908260	-2.676276	-0.543263
13	1	0	-2.186720	-1.416649	2.011355
14	1	0	-0.584336	-2.783253	0.755663
15	6	0	0.051030	2.485618	0.421096
16	6	0	1.205498	2.469892	-0.308472
17	1	0	-0.434051	3.374941	0.798557
18	1	0	1.767988	3.335876	-0.624833
19	6	0	2.271262	0.502693	-1.703048
20	1	0	2.770265	1.084718	-2.465813
21	26	0	3.235563	-0.162941	-0.005035
22	6	0	2.777365	-0.277060	1.751433
23	6	0	4.368631	1.237288	0.027433
24	6	0	4.584173	-1.339664	-0.058889
25	8	0	2.451583	-0.346366	2.846092
26	8	0	5.060243	2.151779	0.051719
27	8	0	5.428230	-2.116567	-0.091624
28	26	0	-3.296860	-0.086933	-0.083170
29	6	0	-2.196538	-0.123911	-1.531259
30	6	0	-3.914104	1.514956	-0.587148
31	6	0	-4.383546	-0.065879	1.372828
32	6	0	-4.106724	-1.574467	-0.662501
33	8	0	-1.512398	-0.149424	-2.449993
34	8	0	-4.378922	2.500167	-0.963991
35	8	0	-5.067827	-0.051293	2.293051
36	8	0	-4.690527	-2.474089	-1.085087

Table S44. The theoretical Cartesian coordinates (in Å) for the structure **Fe27-4** of $C_{12}H_8Fe_2(CO)_7$ using M06-L method.

Center Number	Atomic Number	Atomic Type	Coordinates(Angstroms)		
			x	y	z
1	6	0	2.031831	1.605361	-0.451208
2	6	0	0.628977	1.480172	-0.788561
3	6	0	-0.098396	2.579226	-0.321101
4	6	0	-1.457572	2.605068	-0.597125
5	1	0	-2.094297	3.422732	-0.283135
6	6	0	-2.020186	1.522592	-1.307624
7	6	0	-1.247393	0.406363	-1.724809
8	6	0	0.131551	0.392634	-1.442424
9	6	0	1.169823	-0.609033	-1.719609
10	6	0	2.492695	-0.149866	-2.025249
11	1	0	3.148655	-0.708275	-2.679855
12	1	0	0.874179	-1.572587	-2.119170
13	1	0	-3.030976	1.621433	-1.680090
14	1	0	-1.667490	-0.311258	-2.416651
15	6	0	0.867734	3.409306	0.381881
16	6	0	2.106160	2.844058	0.312388
17	1	0	0.639079	4.340718	0.880124
18	1	0	3.012804	3.267798	0.720249
19	6	0	2.965553	0.994675	-1.346312
20	1	0	3.972119	1.363165	-1.491135
21	26	0	-2.710578	-0.339429	0.138552
22	6	0	-3.766803	-1.042892	-1.159644
23	6	0	-4.185160	0.165896	1.003577
24	6	0	-1.754062	0.467001	1.466864
25	6	0	-1.960129	-1.939192	0.425054
26	8	0	-4.443778	-1.484943	-1.973902
27	8	0	-5.139236	0.382714	1.615182
28	8	0	-1.207661	1.005232	2.317238
29	8	0	-1.570468	-2.996768	0.668488
30	26	0	2.540643	-0.518505	-0.007831
31	6	0	3.917303	-0.059751	1.054670
32	6	0	3.197233	-2.167986	-0.244455
33	6	0	1.335768	-0.935519	1.290362
34	8	0	4.776161	0.283597	1.733457
35	8	0	3.591609	-3.231541	-0.417002
36	8	0	0.672708	-1.274057	2.160397

Table S45. The theoretical Cartesian coordinates (in Å) for the structure **Fe26-1** of $C_{12}H_8Fe_2(CO)_6$ using M06-L method.

Center Number	Atomic Number	Atomic Type	Coordinates(Angstroms)		
			x	y	z
1	6	0	-1.230917	1.139588	-1.064939
2	6	0	-0.397169	0.568255	-0.059324
3	6	0	-0.044940	-0.786797	-0.383254
4	6	0	0.878759	-1.490642	0.415704
5	1	0	0.980981	-2.562027	0.304883
6	6	0	1.450895	-0.831403	1.551660
7	6	0	1.374240	0.603654	1.579083
8	6	0	0.330663	1.327702	0.893987
9	6	0	0.040403	2.679984	0.925864
10	6	0	-0.841187	3.246608	-0.022387
11	1	0	-1.005112	4.316982	0.022432
12	1	0	0.553027	3.331021	1.622758
13	1	0	1.882367	-1.397076	2.364596
14	1	0	1.896887	1.120642	2.374998
15	6	0	-0.951650	-1.140105	-1.438972
16	6	0	-1.643871	0.043880	-1.893724
17	1	0	-1.006028	-2.103319	-1.922720
18	1	0	-2.259608	0.108023	-2.776396
19	6	0	-1.469769	2.534014	-1.017003
20	1	0	-2.103484	3.021061	-1.744803
21	26	0	-2.353314	-0.443341	-0.036889
22	6	0	-3.527968	0.799154	0.552498
23	6	0	-2.065001	-1.263800	1.566702
24	6	0	-3.632812	-1.531451	-0.641942
25	8	0	-4.247532	1.605988	0.928271
26	8	0	-1.897018	-1.786966	2.570472
27	8	0	-4.423406	-2.249423	-1.059291
28	26	0	2.591433	-0.257906	0.018318
29	6	0	4.080163	0.323165	0.794554
30	6	0	2.367280	0.891863	-1.364603
31	6	0	3.464549	-1.620093	-0.737833
32	8	0	5.033704	0.715892	1.310094
33	8	0	2.243825	1.647573	-2.225880
34	8	0	4.012911	-2.503609	-1.236082

Table S46. The theoretical Cartesian coordinates (in Å) for the structure **Fe26-2** of $C_{12}H_8Fe_2(CO)_6$ using M06-L method.

Center Number	Atomic Number	Atomic Type	Coordinates(Angstroms)		
			x	y	z
1	6	0	0.294667	0.048027	-1.600701
2	6	0	0.719259	1.121917	-0.768395
3	6	0	2.133143	1.327834	-0.855657
4	6	0	2.684325	2.452481	-0.195515
5	1	0	3.746567	2.652091	-0.214037
6	6	0	1.807070	3.289479	0.454192
7	6	0	0.402499	3.123042	0.455245
8	6	0	-0.189334	2.059128	-0.202385
9	6	0	-1.582461	1.863497	-0.523865
10	6	0	-1.972132	0.994186	-1.613551
11	1	0	-2.756556	1.252166	-2.313010
12	1	0	-2.241492	2.690805	-0.285594
13	1	0	2.208570	4.160812	0.958242
14	1	0	-0.213839	3.890761	0.906317
15	6	0	2.629987	0.248246	-1.658352
16	6	0	1.512838	-0.568199	-2.063175
17	1	0	3.652078	0.101578	-1.970737
18	1	0	1.577642	-1.412830	-2.731214
19	6	0	-1.091650	-0.141110	-1.838300
20	1	0	-1.382277	-0.886211	-2.568572
21	26	0	-2.313759	-0.072749	-0.028141
22	6	0	-1.458761	-0.353557	1.527934
23	6	0	-2.993746	-1.685368	-0.370013
24	6	0	-3.903236	0.541059	0.481522
25	8	0	-0.951910	-0.486233	2.559304
26	8	0	-3.400592	-2.739538	-0.604258
27	8	0	-4.929094	0.950440	0.814902
28	26	0	1.842381	-0.659838	-0.009634
29	6	0	0.715024	-2.050969	0.329353
30	6	0	1.980542	-0.048039	1.685554
31	6	0	3.344504	-1.624475	0.100042
32	8	0	0.082665	-2.988749	0.484052
33	8	0	2.079617	0.391908	2.734254
34	8	0	4.303051	-2.250951	0.153891

Table S47. The theoretical Cartesian coordinates (in Å) for the structure **Fe26-3** of $C_{12}H_8Fe_2(CO)_6$ using M06-L method.

Center Number	Atomic Number	Atomic Type	Coordinates(Angstroms)		
			x	y	z
1	6	0	-0.630153	1.880676	0.538154
2	6	0	0.052359	0.835023	0.023344
3	6	0	1.189015	1.268864	-0.741248
4	6	0	1.687518	0.391942	-1.749988
5	1	0	2.273410	0.742881	-2.588409
6	6	0	1.370627	-0.979540	-1.596943
7	6	0	0.627908	-1.410646	-0.458167
8	6	0	-0.331012	-0.527830	0.192405
9	6	0	-1.123119	-0.830719	1.339213
10	6	0	-1.894391	0.224046	1.877518
11	1	0	-2.536907	0.045812	2.728804
12	1	0	-1.142946	-1.821294	1.774421
13	1	0	1.770946	-1.703564	-2.294106
14	1	0	0.560740	-2.479661	-0.288275
15	6	0	1.192927	2.717271	-0.600749
16	6	0	0.094260	3.069093	0.144120
17	1	0	1.900594	3.392629	-1.055662
18	1	0	-0.182874	4.084835	0.390506
19	6	0	-1.868398	1.489807	1.208112
20	1	0	-2.573884	2.241239	1.541827
21	26	0	-2.625624	-0.235438	0.009425
22	6	0	-2.521365	0.692485	-1.547544
23	6	0	-4.341122	-0.026916	0.460441
24	6	0	-2.932314	-1.910076	-0.555644
25	8	0	-2.437482	1.285200	-2.527701
26	8	0	-5.441638	0.148689	0.748075
27	8	0	-3.067199	-2.987321	-0.939718
28	26	0	2.541780	-0.329603	-0.017780
29	6	0	2.189206	-0.159811	1.757025
30	6	0	3.985240	0.733173	-0.171185
31	6	0	3.534722	-1.816098	0.005033
32	8	0	1.950204	-0.050813	2.871453
33	8	0	4.892116	1.428231	-0.266869
34	8	0	4.156426	-2.781022	0.022850

Table S48. The theoretical Cartesian coordinates (in Å) for the structure **Fe26-4** of $C_{12}H_8Fe_2(CO)_6$ using M06-L method.

Center Number	Atomic Number	Atomic Type	Coordinates(Angstroms)		
			x	y	z
1	6	0	1.405325	1.195447	-0.999896
2	6	0	-0.000428	1.297869	-0.713731
3	6	0	-0.199698	2.517149	0.081617
4	6	0	-1.461427	2.759014	0.486071
5	1	0	-1.756507	3.610745	1.085555
6	6	0	-2.461825	1.791888	0.045726
7	6	0	-2.323666	1.136970	-1.230818
8	6	0	-1.002239	0.817522	-1.620124
9	6	0	-0.565369	0.034779	-2.748753
10	6	0	0.742299	-0.304250	-2.842594
11	1	0	1.059891	-0.956362	-3.648164
12	1	0	-1.299011	-0.343351	-3.448895
13	1	0	-3.474945	1.935730	0.402152
14	1	0	-3.174068	0.868215	-1.843606
15	6	0	1.086795	3.157085	0.181349
16	6	0	2.019034	2.405063	-0.457635
17	1	0	1.279969	4.065665	0.731713
18	1	0	3.075632	2.623852	-0.526013
19	6	0	1.759657	0.159570	-1.926756
20	1	0	2.783919	0.081479	-2.271639
21	26	0	-1.676161	-0.223050	0.159351
22	6	0	-3.318439	-0.849706	0.369617
23	6	0	-1.277352	-0.246165	1.927540
24	6	0	-1.281725	-1.867508	-0.553680
25	8	0	-4.398292	-1.213528	0.513497
26	8	0	-1.179832	-0.303219	3.068760
27	8	0	-1.184351	-2.895574	-1.052289
28	26	0	1.580355	-0.467094	0.141668
29	6	0	3.333251	-0.525946	0.176669
30	6	0	1.408165	-2.278732	0.264292
31	6	0	1.616995	0.173313	1.828628
32	8	0	4.483969	-0.571971	0.176822
33	8	0	1.442584	-3.416384	0.425686
34	8	0	1.725918	0.627875	2.878436

Table S49.The theoretical Cartesian coordinates (in Å) for the structure **Fe25-1** of $C_{12}H_8Fe_2(CO)_5$ using M06-L method.

Center Number	Atomic Number	Atomic Type	Coordinates(Angstroms)		
			x	y	z
1	6	0	-1.722144	1.011594	-1.173901
2	6	0	-1.731124	0.203208	0.000000
3	6	0	-1.722144	1.011594	1.173901
4	6	0	-1.655857	0.351426	2.443696
5	1	0	-1.737569	0.915131	3.363630
6	6	0	-1.452756	-0.991448	2.460707
7	6	0	-1.275427	-1.783915	1.266994
8	6	0	-1.559141	-1.197746	0.000000
9	6	0	-1.275427	-1.783915	-1.266994
10	6	0	-1.452756	-0.991448	-2.460707
11	1	0	-1.377327	-1.501788	-3.412792
12	1	0	-1.297000	-2.860902	-1.367812
13	1	0	-1.377327	-1.501788	3.412792
14	1	0	-1.297000	-2.860902	1.367812
15	6	0	-1.695390	2.370239	0.711758
16	6	0	-1.695390	2.370239	-0.711758
17	1	0	-1.679292	3.250654	1.334693
18	1	0	-1.679292	3.250654	-1.334693
19	6	0	-1.655857	0.351426	-2.443696
20	1	0	-1.737569	0.915131	-3.363630
21	26	0	0.507443	-1.318172	0.000000
22	6	0	1.554065	-0.800988	1.361189
23	6	0	1.554065	-0.800988	-1.361189
24	6	0	1.005675	-3.026680	0.000000
25	8	0	2.251515	-0.606232	2.254823
26	8	0	2.251515	-0.606232	-2.254823
27	8	0	1.368491	-4.118806	0.000000
28	26	0	0.000000	1.403399	0.000000
29	6	0	1.080818	1.986099	-1.274324
30	6	0	1.080818	1.986099	1.274324
31	8	0	1.732744	2.452492	-2.101508
32	8	0	1.732744	2.452492	2.101508

Table S50. The theoretical Cartesian coordinates (in Å) for the structure **Fe25-2** of $C_{12}H_8Fe_2(CO)_5$ using M06-L method.

Center Number	Atomic Number	Atomic Type	Coordinates(Angstroms)		
			x	y	z
1	6	0	-0.351875	-0.085591	-1.790961
2	6	0	-1.185244	-0.932182	-0.979512
3	6	0	-2.479058	-0.375026	-0.836084
4	6	0	-3.418407	-1.107800	-0.058000
5	1	0	-4.431158	-0.752348	0.074847
6	6	0	-2.990780	-2.265645	0.540245
7	6	0	-1.655220	-2.741072	0.471205
8	6	0	-0.718138	-2.060642	-0.273121
9	6	0	0.718234	-2.265000	-0.383189
10	6	0	1.437760	-1.707296	-1.487248
11	1	0	2.362479	-2.156117	-1.822826
12	1	0	1.145500	-3.133123	0.103705
13	1	0	-3.697883	-2.831707	1.134478
14	1	0	-1.375415	-3.619501	1.039017
15	6	0	-2.424201	0.916048	-1.468789
16	6	0	-1.144243	1.053057	-2.100001
17	1	0	-3.238109	1.617349	-1.556984
18	1	0	-0.826162	1.905765	-2.679168
19	6	0	1.000358	-0.494362	-2.054797
20	1	0	1.581298	-0.011378	-2.828621
21	26	0	1.614071	-0.316191	0.007562
22	6	0	0.970785	-0.154701	1.687907
23	6	0	2.266969	1.333570	-0.270338
24	6	0	3.215100	-0.948583	0.434870
25	8	0	0.791356	-0.182100	2.827616
26	8	0	2.697796	2.378738	-0.477679
27	8	0	4.246474	-1.350797	0.749036
28	26	0	-0.923329	0.920333	-0.031239
29	6	0	-0.433409	2.601728	0.169089
30	6	0	-1.618560	0.880314	1.601650
31	8	0	-0.164515	3.717569	0.270134
32	8	0	-2.148645	0.860647	2.622592

Table S51. The theoretical Cartesian coordinates (in Å) for the structure **Fe25-3** of $C_{12}H_8Fe_2(CO)_5$ using M06-L method.

Center Number	Atomic Number	Atomic Type	Coordinates(Angstroms)		
			x	y	z
1	6	0	0.878808	-1.599971	-0.918456
2	6	0	-0.515306	-1.460520	-0.701562
3	6	0	-1.117302	-0.866996	-1.864869
4	6	0	-2.423393	-0.369384	-1.667063
5	1	0	-2.897177	0.261956	-2.408016
6	6	0	-3.145532	-0.698151	-0.489200
7	6	0	-2.562146	-1.436822	0.561670
8	6	0	-1.203188	-1.853299	0.470625
9	6	0	-0.405283	-2.443523	1.504576
10	6	0	0.948305	-2.469522	1.367508
11	1	0	1.545387	-2.868778	2.179022
12	1	0	-0.879501	-2.794719	2.411511
13	1	0	-4.154046	-0.326287	-0.372298
14	1	0	-3.129607	-1.634483	1.461454
15	6	0	-0.097215	-0.701453	-2.823223
16	6	0	1.110835	-1.091894	-2.244563
17	1	0	-0.202848	-0.211019	-3.777493
18	1	0	2.075296	-1.069983	-2.730910
19	6	0	1.658562	-1.957051	0.222781
20	1	0	2.703992	-2.217889	0.123741
21	26	0	-1.417766	0.308930	0.168664
22	6	0	-1.128643	0.675899	1.873487
23	6	0	-1.838179	1.996748	-0.140365
24	8	0	-1.076534	0.908528	3.000608
25	8	0	-2.175539	3.082861	-0.319010
26	26	0	1.412115	0.197433	0.021525
27	6	0	3.094178	0.357251	-0.490466
28	6	0	1.739225	0.774940	1.688701
29	6	0	0.890435	1.692311	-0.848646
30	8	0	4.189609	0.494451	-0.819392
31	8	0	2.022223	1.150482	2.737668
32	8	0	0.762798	2.664226	-1.454569

Table S52. The theoretical Cartesian coordinates (in Å) for the structure **Fe25-4** of $C_{12}H_8Fe_2(CO)_5$ using M06-L method.

Center Number	Atomic Number	Atomic Type	Coordinates(Angstroms)		
			x	y	z
1	6	0	-1.252258	0.186945	1.667807
2	6	0	-0.439836	0.046393	0.523432
3	6	0	0.528276	1.123155	0.454823
4	6	0	1.063610	1.479156	-0.816017
5	1	0	1.450424	2.465267	-1.033792
6	6	0	1.077985	0.450821	-1.782604
7	6	0	0.627069	-0.850983	-1.393940
8	6	0	-0.464375	-0.982742	-0.419737
9	6	0	-1.441380	-1.969213	-0.222249
10	6	0	-2.301547	-1.857782	0.911247
11	1	0	-3.107421	-2.572928	1.004000
12	1	0	-1.562247	-2.795384	-0.909324
13	1	0	1.499352	0.626907	-2.762915
14	1	0	0.777075	-1.655372	-2.104216
15	6	0	0.273758	1.915263	1.647605
16	6	0	-0.774802	1.388813	2.336645
17	1	0	0.802008	2.820919	1.909127
18	1	0	-1.197030	1.796700	3.243148
19	6	0	-2.242704	-0.793693	1.854343
20	1	0	-2.946331	-0.759195	2.674114
21	26	0	-2.437751	-0.071730	-0.146999
22	6	0	-2.403538	1.442161	-1.048387
23	6	0	-4.115830	-0.246363	-0.643954
24	8	0	-2.368408	2.438235	-1.637242
25	8	0	-5.218531	-0.341933	-0.981181
26	26	0	2.296585	-0.082038	-0.217247
27	6	0	2.146081	-1.348264	1.074204
28	6	0	3.494732	1.026270	0.540579
29	6	0	3.547042	-0.822513	-1.266685
30	8	0	2.027496	-2.151063	1.882860
31	8	0	4.232788	1.744792	1.046607
32	8	0	4.329251	-1.321722	-1.942597

Table S53. The theoretical Cartesian coordinates (in Å) for the structure **Fe25-5** of $C_{12}H_8Fe_2(CO)_5$ using M06-L method.

Center Number	Atomic Number	Atomic Type	Coordinates(Angstroms)		
			x	y	z
1	6	0	-1.441216	1.309140	-1.020909
2	6	0	-0.579006	0.732138	-0.055841
3	6	0	-0.317514	-0.654743	-0.349544
4	6	0	0.473421	-1.425802	0.544138
5	1	0	0.465613	-2.506119	0.497591
6	6	0	1.116519	-0.753198	1.609903
7	6	0	1.194540	0.683683	1.552126
8	6	0	0.141382	1.456053	0.913765
9	6	0	-0.160156	2.799273	1.014024
10	6	0	-1.104553	3.377606	0.136443
11	1	0	-1.313718	4.435205	0.244013
12	1	0	0.352775	3.427690	1.731128
13	1	0	1.558318	-1.311055	2.423217
14	1	0	1.782050	1.178645	2.316349
15	6	0	-1.208151	-0.970748	-1.427429
16	6	0	-1.866713	0.229700	-1.874528
17	1	0	-1.305880	-1.938593	-1.894986
18	1	0	-2.508423	0.305201	-2.737422
19	6	0	-1.745597	2.682916	-0.868746
20	1	0	-2.421828	3.186244	-1.546294
21	26	0	-2.507552	-0.239303	-0.009692
22	6	0	-2.477224	-0.648919	1.738513
23	6	0	-3.816749	-1.342407	-0.405704
24	8	0	-2.382961	-0.974467	2.838596
25	8	0	-4.654702	-2.078419	-0.697529
26	26	0	2.262643	-0.349648	-0.010807
27	6	0	2.278084	1.009894	-1.215051
28	6	0	2.851489	-1.717482	-1.006439
29	6	0	3.837825	-0.214896	0.803912
30	8	0	2.320745	1.897944	-1.944738
31	8	0	3.202761	-2.595914	-1.662810
32	8	0	4.851711	-0.096364	1.337425

Table S54. The theoretical Cartesian coordinates (in Å) for the structure **Fe24-1** of $C_{12}H_8Fe_2(CO)_4$ using M06-L method.

Center Number	Atomic Number	Atomic Type	Coordinates(Angstroms)		
			x	y	z
1	6	0	-2.612556	-0.041003	0.353132
2	6	0	-1.433776	-0.697328	0.795666
3	6	0	-0.631083	0.183739	1.600835
4	6	0	0.676238	-0.251554	2.015848
5	1	0	1.229274	0.306784	2.759345
6	6	0	1.090308	-1.547746	1.646825
7	6	0	0.411931	-2.219846	0.582347
8	6	0	-0.975457	-1.933849	0.282178
9	6	0	-1.839671	-2.605322	-0.553558
10	6	0	-3.075247	-2.015144	-0.918081
11	1	0	-3.723253	-2.571464	-1.584916
12	1	0	-1.555128	-3.554403	-0.990155
13	1	0	1.957605	-1.992616	2.114146
14	1	0	0.819181	-3.165631	0.246296
15	6	0	-1.336339	1.430416	1.622080
16	6	0	-2.531887	1.305174	0.830344
17	1	0	-1.019387	2.324917	2.135380
18	1	0	-3.273588	2.076317	0.697713
19	6	0	-3.464962	-0.757913	-0.525157
20	1	0	-4.385494	-0.321704	-0.888268
21	26	0	1.488599	-0.393047	-0.009940
22	6	0	2.935919	-1.310094	-0.472518
23	6	0	2.417349	1.138038	0.121086
24	8	0	3.859313	-1.906876	-0.815099
25	8	0	2.993822	2.127866	0.214224
26	26	0	-0.777947	0.975737	-0.256632
27	6	0	-0.247180	2.621329	-0.621268
28	6	0	0.455543	-0.064696	-1.444864
29	8	0	0.049437	3.725441	-0.776345
30	8	0	-0.347689	0.096401	-2.303783

Table S55. The theoretical Cartesian coordinates (in Å) for the structure **Fe24-2** of $C_{12}H_8Fe_2(CO)_4$ using M06-L method.

Center Number	Atomic Number	Atomic Type	Coordinates(Angstroms)		
			x	y	z
1	6	0	1.378114	1.895419	0.163303
2	6	0	0.755260	1.014081	1.093569
3	6	0	1.630610	-0.059117	1.438309
4	6	0	1.127860	-1.084920	2.309560
5	1	0	1.787299	-1.847775	2.701622
6	6	0	-0.198806	-1.090790	2.597293
7	6	0	-1.141947	-0.147374	2.034565
8	6	0	-0.635760	1.009660	1.371874
9	6	0	-1.412360	1.930618	0.612279
10	6	0	-0.749262	2.946304	-0.162900
11	1	0	-1.365893	3.719170	-0.604194
12	1	0	-2.447922	2.091493	0.879740
13	1	0	-0.595378	-1.868887	3.237765
14	1	0	-2.148368	-0.132409	2.431876
15	6	0	2.840078	0.175048	0.693389
16	6	0	2.682741	1.348624	-0.093364
17	1	0	3.717511	-0.453016	0.707659
18	1	0	3.428723	1.762972	-0.753172
19	6	0	0.589447	2.944750	-0.403894
20	1	0	1.042250	3.693120	-1.040419
21	26	0	-1.329196	-0.188062	-0.178586
22	6	0	-1.176566	-1.968800	-0.233217
23	6	0	-0.453780	0.188891	-1.692617
24	6	0	-3.095666	-0.100281	-0.398311
25	8	0	-1.118036	-3.116031	-0.241431
26	8	0	0.290938	0.485940	-2.567648
27	8	0	-4.228814	-0.059452	-0.601228
28	26	0	1.248432	-0.065419	-0.598874
29	6	0	1.672817	-1.733005	-1.025969
30	8	0	2.031530	-2.809057	-1.235960

Table S56. The theoretical Cartesian coordinates (in Å) for the structure **Fe24-3** of $C_{12}H_8Fe_2(CO)_4$ using M06-L method.

Center Number	Atomic Number	Atomic Type	Coordinates(Angstroms)		
			x	y	z
1	6	0	1.293317	1.869148	0.363661
2	6	0	0.478623	1.035258	1.187776
3	6	0	1.253021	-0.022752	1.752040
4	6	0	0.564230	-1.020135	2.527872
5	1	0	1.118285	-1.777260	3.067091
6	6	0	-0.791511	-1.004719	2.538237
7	6	0	-1.582888	-0.061303	1.771965
8	6	0	-0.934313	1.095985	1.222864
9	6	0	-1.537864	2.013616	0.332058
10	6	0	-0.717268	2.951066	-0.380794
11	1	0	-1.217521	3.710495	-0.968646
12	1	0	-2.601637	2.199173	0.394803
13	1	0	-1.324985	-1.762544	3.097957
14	1	0	-2.640949	-0.008776	1.995408
15	6	0	2.585589	0.170823	1.264236
16	6	0	2.611683	1.305863	0.403382
17	1	0	3.432052	-0.461910	1.481659
18	1	0	3.483260	1.684944	-0.104994
19	6	0	0.645665	2.905352	-0.381158
20	1	0	1.224848	3.609669	-0.963766
21	26	0	-1.326373	-0.147290	-0.354177
22	6	0	-0.911786	-1.879111	-0.465781
23	6	0	-3.079034	-0.296864	-0.592279
24	8	0	-0.827159	-3.029984	-0.459549
25	8	0	-4.214729	-0.441073	-0.731525
26	26	0	1.282239	-0.126993	-0.347567
27	6	0	0.936715	0.269550	-2.031325
28	6	0	1.867184	-1.745441	-0.740021
29	8	0	0.675646	0.553371	-3.122601
30	8	0	2.314485	-2.779868	-0.985144

Table S57. The theoretical Cartesian coordinates (in Å) for the structure **Fe24-4** of $C_{12}H_8Fe_2(CO)_4$ using M06-L method.

Center Number	Atomic Number	Atomic Type	Coordinates(Angstroms)		
			x	y	z
1	6	0	0.715752	-1.442622	0.702253
2	6	0	0.038676	-0.211237	0.432117
3	6	0	0.134488	0.120832	-0.989915
4	6	0	-0.632482	1.228706	-1.467370
5	1	0	-0.646775	1.500985	-2.512242
6	6	0	-1.224909	2.061879	-0.488794
7	6	0	-1.305116	1.715697	0.881773
8	6	0	-0.674411	0.544521	1.405920
9	6	0	-0.630544	0.046099	2.728329
10	6	0	0.120130	-1.077535	3.013137
11	1	0	0.172614	-1.413648	4.041046
12	1	0	-1.152019	0.571572	3.517566
13	1	0	-1.790290	2.922181	-0.821877
14	1	0	-1.921488	2.323359	1.531103
15	6	0	0.969740	-0.891190	-1.564416
16	6	0	1.315025	-1.837788	-0.543411
17	1	0	1.220074	-0.974880	-2.609490
18	1	0	1.924485	-2.713443	-0.698040
19	6	0	0.823246	-1.815249	2.042208
20	1	0	1.392388	-2.688409	2.332794
21	26	0	2.084990	0.013957	-0.109101
22	6	0	2.403972	1.755034	0.062215
23	6	0	3.732467	-0.303727	-0.615976
24	8	0	2.586057	2.894055	0.107495
25	8	0	4.802659	-0.525305	-0.989756
26	26	0	-1.968550	0.109273	-0.306457
27	6	0	-2.362361	-1.460662	-1.033053
28	6	0	-3.691411	0.419589	-0.189861
29	8	0	-2.639587	-2.472641	-1.510745
30	8	0	-4.826631	0.623166	-0.135408

Table S58. The theoretical Cartesian coordinates (in Å) for the structure **Fe24-5** of $C_{12}H_8Fe_2(CO)_4$ using M06-L method.

Center Number	Atomic Number	Atomic Type	Coordinates(Angstroms)		
			x	y	z
1	6	0	0.702301	1.538130	-0.424048
2	6	0	0.035578	0.419543	0.174496
3	6	0	-0.719641	0.863122	1.305634
4	6	0	-1.511380	-0.070261	2.013597
5	1	0	-2.118700	0.223621	2.857898
6	6	0	-1.458090	-1.422066	1.605158
7	6	0	-0.750337	-1.832093	0.450083
8	6	0	0.056052	-0.922497	-0.308443
9	6	0	0.886857	-1.166325	-1.445364
10	6	0	1.433978	-0.042061	-2.133293
11	1	0	2.041158	-0.229830	-3.008370
12	1	0	0.970761	-2.158867	-1.863998
13	1	0	-2.063069	-2.153158	2.123597
14	1	0	-0.862620	-2.849836	0.102269
15	6	0	-0.505261	2.289027	1.378625
16	6	0	0.343925	2.679267	0.382683
17	1	0	-0.920690	2.932096	2.139705
18	1	0	0.694286	3.686032	0.212611
19	6	0	1.377703	1.282397	-1.634133
20	1	0	1.915039	2.063793	-2.155084
21	26	0	2.133299	-0.084907	-0.180661
22	6	0	2.509590	-0.656064	1.454793
23	6	0	3.838674	-0.176183	-0.550200
24	8	0	2.764788	-1.052108	2.508178
25	8	0	4.968896	-0.235105	-0.783429
26	26	0	-2.063299	-0.252952	-0.017741
27	6	0	-3.063600	1.161887	-0.397657
28	6	0	-3.280440	-1.248699	-0.804885
29	8	0	-3.738641	2.066599	-0.631743
30	8	0	-4.101494	-1.893420	-1.299566

Table S59. The theoretical Cartesian coordinates (in Å) for the structure **Fe24-6** of $C_{12}H_8Fe_2(CO)_4$ using M06-L method.

Center Number	Atomic Number	Atomic Type	Coordinates(Angstroms)		
			x	y	z
1	6	0	0.885563	0.762248	-1.316616
2	6	0	0.000000	0.000000	-0.481613
3	6	0	-0.885563	-0.762248	-1.316616
4	6	0	-1.892433	-1.486518	-0.652567
5	1	0	-2.589021	-2.109979	-1.197457
6	6	0	-1.924846	-1.504682	0.765134
7	6	0	-0.949954	-0.873858	1.585548
8	6	0	0.000000	0.000000	0.967425
9	6	0	0.949954	0.873858	1.585548
10	6	0	1.924846	1.504682	0.765134
11	1	0	2.638601	2.161956	1.243338
12	1	0	1.006152	0.947802	2.661867
13	1	0	-2.638601	-2.161956	1.243338
14	1	0	-1.006152	-0.947802	2.661867
15	6	0	-0.514698	-0.448230	-2.675485
16	6	0	0.514698	0.448230	-2.675485
17	1	0	-1.001355	-0.848690	-3.551734
18	1	0	1.001355	0.848690	-3.551734
19	6	0	1.892433	1.486518	-0.652567
20	1	0	2.589021	2.109979	-1.197457
21	26	0	0.000000	2.058295	0.174387
22	6	0	-1.751124	2.321725	0.168861
23	6	0	0.194861	3.788523	0.366502
24	8	0	-2.889008	2.513210	0.183391
25	8	0	0.303554	4.931349	0.492138
26	26	0	0.000000	-2.058295	0.174387
27	6	0	1.751124	-2.321725	0.168861
28	6	0	-0.194861	-3.788523	0.366502
29	8	0	2.889008	-2.513210	0.183391
30	8	0	-0.303554	-4.931349	0.492138

Table S60. The theoretical Cartesian coordinates (in Å) for the structure **Fe24-7** of $C_{12}H_8Fe_2(CO)_4$ using M06-L method.

Center Number	Atomic Number	Atomic Type	Coordinates(Angstroms)		
			x	y	z
1	6	0	0.096036	-0.079624	-1.680669
2	6	0	0.208641	1.026581	-0.781658
3	6	0	1.560402	1.470706	-0.688575
4	6	0	1.817320	2.641424	0.069982
5	1	0	2.822213	3.025692	0.182001
6	6	0	0.746246	3.276585	0.651066
7	6	0	-0.594352	2.848018	0.510227
8	6	0	-0.898686	1.727984	-0.239301
9	6	0	-2.205214	1.245830	-0.643278
10	6	0	-2.313483	0.361873	-1.756772
11	1	0	-3.233417	0.279006	-2.326666
12	1	0	-3.059403	1.864412	-0.393120
13	1	0	0.931446	4.174519	1.228658
14	1	0	-1.387020	3.441955	0.947981
15	6	0	2.341703	0.503495	-1.402411
16	6	0	1.428468	-0.451745	-2.000103
17	1	0	3.404187	0.543095	-1.582435
18	1	0	1.721636	-1.253750	-2.659519
19	6	0	-1.213462	-0.522371	-2.045234
20	1	0	-1.321865	-1.263652	-2.826887
21	26	0	-2.346599	-0.809017	-0.201339
22	6	0	-3.328964	-0.649414	1.257759
23	6	0	-1.067528	-1.664151	0.528156
24	8	0	-3.947817	-0.502802	2.223051
25	8	0	0.053236	-1.978601	0.779382
26	26	0	1.496372	-0.543439	0.105925
27	6	0	2.796767	-1.742367	0.168663
28	6	0	1.832540	0.042598	1.761043
29	8	0	3.685828	-2.470652	0.157722
30	8	0	2.082442	0.469561	2.797016

Table S61. The theoretical Cartesian coordinates (in Å) for the structure **Fe39-1** of $C_{12}H_8Fe_3(CO)_9$ using M06-L method.

Center Number	Atomic Number	Atomic Type	Coordinates(Angstroms)		
			x	y	z
1	6	0	0.633213	0.423365	-1.434157
2	6	0	-0.268024	0.346461	-0.355930
3	6	0	-1.150250	1.457934	-0.320323
4	6	0	-2.260720	1.378313	0.590454
5	1	0	-2.902405	2.240694	0.715736
6	6	0	-2.205615	0.404426	1.654370
7	6	0	-1.452196	-0.781451	1.438274
8	6	0	-0.567713	-0.885818	0.331430
9	6	0	0.059256	-2.058802	-0.187975
10	6	0	0.818639	-2.025187	-1.412439
11	1	0	0.838540	-2.865483	-2.092928
12	1	0	-0.331987	-3.012838	0.146813
13	1	0	-2.743555	0.557292	2.578650
14	1	0	-1.525372	-1.597409	2.145968
15	6	0	-0.700541	2.340093	-1.341524
16	6	0	0.428886	1.728026	-2.006452
17	1	0	-1.152300	3.280279	-1.617961
18	1	0	0.928012	2.125224	-2.875819
19	6	0	1.422243	-0.741890	-1.738201
20	1	0	2.065035	-0.692574	-2.608586
21	26	0	0.917673	2.200192	-0.064538
22	6	0	0.677159	2.187520	1.734846
23	6	0	1.139910	3.976236	-0.190580
24	6	0	2.706839	1.870947	-0.104074
25	8	0	0.494471	2.192571	2.863134
26	8	0	1.257630	5.112125	-0.281320
27	8	0	3.833355	1.703531	-0.182641
28	26	0	-3.099264	-0.499608	0.088412
29	6	0	-3.597638	-2.206151	0.326214
30	6	0	-2.866122	-0.501204	-1.708821
31	6	0	-4.773492	0.086758	0.292820
32	8	0	-3.888345	-3.307567	0.479205
33	8	0	-2.723696	-0.468513	-2.849443
34	8	0	-5.845247	0.487051	0.409646
35	26	0	2.171738	-1.773364	-0.025124
36	6	0	2.440645	-0.727877	1.415180
37	6	0	3.803759	-1.775222	-0.733157
38	6	0	2.388120	-3.400404	0.686515
39	8	0	2.624439	-0.115915	2.378911
40	8	0	4.853720	-1.743309	-1.207848
41	8	0	2.521432	-4.449894	1.143083

Table S62. The theoretical Cartesian coordinates (in Å) for the structure **Fe39-2** of $C_{12}H_8Fe_3(CO)_9$ using M06-L method.

Center Number	Atomic Number	Atomic Type	Coordinates(Angstroms)		
			x	y	z
1	6	0	1.073138	0.849209	-1.617683
2	6	0	-0.128434	0.188826	-1.224535
3	6	0	-1.253121	0.983629	-1.413755
4	6	0	-2.513500	0.227964	-1.300244
5	1	0	-3.451024	0.765436	-1.220815
6	6	0	-2.525222	-1.046569	-1.962551
7	6	0	-1.342766	-1.805282	-1.872489
8	6	0	-0.239801	-1.242583	-1.131035
9	6	0	1.086760	-1.914105	-1.095690
10	6	0	2.143458	-1.328855	-1.893779
11	1	0	2.842502	-1.928011	-2.460183
12	1	0	1.071335	-2.998178	-1.043801
13	1	0	-3.410302	-1.450384	-2.436787
14	1	0	-1.270098	-2.796258	-2.301944
15	6	0	-0.798837	2.259052	-1.911909
16	6	0	0.657520	2.227149	-1.805553
17	1	0	-1.386278	3.007460	-2.418698
18	1	0	1.299009	3.004670	-2.193591
19	6	0	2.201471	0.097952	-1.968134
20	1	0	3.043886	0.574189	-2.452022
21	26	0	-0.368305	2.392259	0.011780
22	6	0	0.760480	2.003476	1.389479
23	6	0	-1.926315	2.513186	0.903397
24	6	0	-0.125117	4.149737	0.049795
25	8	0	1.454925	1.840800	2.287177
26	8	0	-2.943691	2.599185	1.429909
27	8	0	0.053476	5.284472	0.034006
28	26	0	-2.125585	-1.475545	-0.006387
29	6	0	-3.860296	-1.791381	0.343247
30	6	0	-1.624189	-3.102019	0.581611
31	6	0	-1.741846	-0.557218	1.509546
32	8	0	-4.970916	-1.971142	0.566179
33	8	0	-1.247177	-4.122282	0.942782
34	8	0	-1.571976	-0.014910	2.502942
35	26	0	2.542238	-0.892558	-0.010200
36	6	0	1.614880	-1.122055	1.509832
37	6	0	3.737354	-2.190852	0.136837
38	6	0	3.727174	0.359825	0.492490
39	8	0	1.074972	-1.433947	2.478514
40	8	0	4.499788	-3.046712	0.255172
41	8	0	4.458998	1.194349	0.795763

Table S63. The theoretical Cartesian coordinates (in Å) for the structure **Fe39-3** of $C_{12}H_8Fe_3(CO)_9$ using M06-L method.

Center Number	Atomic Number	Atomic Type	Coordinates(Angstroms)		
			x	y	z
1	6	0	1.297645	1.398964	0.578191
2	6	0	0.751158	0.062837	0.535825
3	6	0	0.835935	-0.428031	-0.811123
4	6	0	0.444403	-1.772609	-0.986496
5	1	0	0.539404	-2.242953	-1.958025
6	6	0	-0.573692	-2.299205	-0.071727
7	6	0	-0.860836	-1.634906	1.174754
8	6	0	-0.187600	-0.406004	1.491251
9	6	0	-0.391151	0.412958	2.609987
10	6	0	0.216484	1.659808	2.704683
11	1	0	0.021865	2.255639	3.589085
12	1	0	-1.067095	0.090322	3.392551
13	1	0	-0.716305	-3.372938	-0.106125
14	1	0	-1.254042	-2.210386	2.004606
15	6	0	1.770736	0.415725	-1.454608
16	6	0	1.871841	1.672698	-0.695600
17	1	0	2.084572	0.306337	-2.482976
18	1	0	2.683495	2.366102	-0.858804
19	6	0	1.042911	2.211459	1.704028
20	1	0	1.580198	3.132507	1.886051
21	26	0	0.005197	2.800489	-0.276589
22	6	0	-1.346751	3.677385	0.492087
23	6	0	-1.053875	1.556590	-0.871977
24	6	0	0.680614	4.185650	-1.223195
25	8	0	-2.217785	4.213390	1.020374
26	8	0	-1.674358	0.623912	-1.250944
27	8	0	1.036661	5.004731	-1.953734
28	26	0	2.417515	-1.342311	-0.093332
29	6	0	3.795676	-0.367287	0.580992
30	6	0	3.350421	-2.294396	-1.294349
31	6	0	2.304422	-2.665178	1.121980
32	8	0	4.672538	0.244937	0.991307
33	8	0	3.943548	-2.886768	-2.077862
34	8	0	2.185887	-3.495488	1.903623
35	26	0	-2.416703	-1.288343	-0.209937
36	6	0	-3.229585	-2.686999	0.461172
37	6	0	-3.611001	-0.128268	0.556645
38	6	0	-3.017077	-1.671948	-1.890229
39	8	0	-3.753128	-3.610124	0.902573
40	8	0	-4.348300	0.590533	1.058584
41	8	0	-3.416611	-1.952097	-2.926896

Table S64. The theoretical Cartesian coordinates (in Å) for the structure **Fe38-1** of $C_{12}H_8Fe_3(CO)_8$ using M06-L method.

Center Number	Atomic Number	Atomic Type	Coordinates(Angstroms)		
			x	y	z
1	6	0	0.622509	0.186015	-1.648594
2	6	0	-0.275746	0.203800	-0.544257
3	6	0	-0.814910	1.489829	-0.340616
4	6	0	-1.930027	1.561617	0.589028
5	1	0	-2.391178	2.522861	0.775767
6	6	0	-2.013744	0.567374	1.627216
7	6	0	-1.486327	-0.722332	1.354233
8	6	0	-0.722557	-0.947427	0.186839
9	6	0	-0.052976	-2.154874	-0.194467
10	6	0	0.734565	-2.230911	-1.362627
11	1	0	1.045498	-3.201380	-1.724237
12	1	0	-0.282199	-3.073322	0.331316
13	1	0	-2.462040	0.782413	2.586293
14	1	0	-1.615914	-1.522219	2.072238
15	6	0	-0.109983	2.346431	-1.219006
16	6	0	0.792060	1.548131	-2.025583
17	1	0	-0.255832	3.409550	-1.329876
18	1	0	1.411854	1.919339	-2.824958
19	6	0	1.225042	-1.065201	-2.015729
20	1	0	1.834190	-1.150407	-2.903660
21	26	0	1.364449	1.429678	-0.039329
22	6	0	1.218341	1.398460	1.740144
23	6	0	2.460083	2.830019	-0.057655
24	8	0	1.076814	1.407396	2.881555
25	8	0	3.138342	3.755500	-0.085214
26	26	0	-3.131664	-0.140147	0.111825
27	6	0	-3.879527	-1.766074	0.281080
28	6	0	-3.071458	0.016903	-1.688649
29	6	0	-4.652213	0.691422	0.525615
30	8	0	-4.332934	-2.817960	0.382897
31	8	0	-3.025308	0.160294	-2.828668
32	8	0	-5.628205	1.244154	0.779809
33	26	0	2.037104	-1.233637	-0.072258
34	6	0	2.136423	-1.530978	1.693312
35	6	0	3.366331	-2.328337	-0.450352
36	6	0	3.160925	0.269112	-0.104162
37	8	0	2.175884	-1.768506	2.816844
38	8	0	4.253491	-3.023856	-0.680623
39	8	0	4.274120	0.628234	-0.149564

Table S65. The theoretical Cartesian coordinates (in Å) for the structure **Fe38-2** of $C_{12}H_8Fe_3(CO)_8$ using M06-L method.

Center Number	Atomic Number	Atomic Type	Coordinates(Angstroms)		
			x	y	z
1	6	0	-0.646965	-0.267033	-1.648614
2	6	0	0.319241	-0.298985	-0.603795
3	6	0	0.856673	-1.581357	-0.442021
4	6	0	2.009470	-1.640816	0.453717
5	1	0	2.533074	-2.580676	0.573119
6	6	0	2.057995	-0.711475	1.549330
7	6	0	1.465210	0.561372	1.367225
8	6	0	0.741792	0.825889	0.181296
9	6	0	-0.017171	2.020620	-0.110689
10	6	0	-0.772313	2.139817	-1.312192
11	1	0	-1.056703	3.119751	-1.669742
12	1	0	0.212597	2.929248	0.432859
13	1	0	2.546274	-0.957185	2.481461
14	1	0	1.544251	1.317765	2.137593
15	6	0	0.097759	-2.439183	-1.284190
16	6	0	-0.822515	-1.622012	-2.042452
17	1	0	0.230629	-3.501670	-1.409748
18	1	0	-1.506685	-1.985961	-2.791831
19	6	0	-1.267689	0.991674	-1.968966
20	1	0	-1.893678	1.093219	-2.844526
21	26	0	-1.273136	-1.477173	-0.032901
22	6	0	-2.023912	0.885669	1.754900
23	6	0	-1.033096	-1.788522	1.696237
24	6	0	-2.726035	-2.492547	-0.105796
25	8	0	-1.981469	0.796839	2.900406
26	8	0	-0.814232	-2.070629	2.792843
27	8	0	-3.633185	-3.198919	-0.182180
28	26	0	3.097014	0.181746	0.059105
29	6	0	3.723501	1.854026	0.267333
30	6	0	3.067501	0.050950	-1.746815
31	6	0	4.679155	-0.535638	0.466835
32	8	0	4.085763	2.937925	0.390610
33	8	0	3.046688	-0.065070	-2.889333
34	8	0	5.693151	-1.017671	0.712859
35	26	0	-2.107521	1.236173	-0.011420
36	6	0	-2.978939	2.783354	0.126226
37	6	0	-3.587074	0.315604	-0.443078
38	8	0	-3.574673	3.758291	0.253944
39	8	0	-4.583367	-0.166056	-0.756714

Table S66. The theoretical Cartesian coordinates (in Å) for the structure **Fe38-3** of $C_{12}H_8Fe_3(CO)_8$ using M06-L method.

Center Number	Atomic Number	Atomic Type	Coordinates(Angstroms)		
			x	y	z
1	6	0	1.742564	0.908044	-1.767847
2	6	0	0.476144	0.233660	-1.705349
3	6	0	-0.583508	1.171814	-1.627762
4	6	0	-1.916963	0.648731	-1.660102
5	1	0	-2.763917	1.285395	-1.869747
6	6	0	-2.042324	-0.732114	-1.595028
7	6	0	-0.955213	-1.650248	-1.545334
8	6	0	0.329466	-1.171474	-1.595047
9	6	0	1.587320	-1.879062	-1.434328
10	6	0	2.809887	-1.277669	-1.867025
11	1	0	3.657762	-1.894000	-2.131842
12	1	0	1.556679	-2.959568	-1.367269
13	1	0	-3.062674	-1.162272	-1.748461
14	1	0	-1.159937	-2.705829	-1.422447
15	6	0	0.029651	2.463509	-1.533333
16	6	0	1.447359	2.294586	-1.669641
17	1	0	-0.481457	3.410489	-1.473011
18	1	0	2.170408	3.094966	-1.658601
19	6	0	2.946347	0.123615	-1.827225
20	1	0	3.892946	0.587854	-2.067804
21	26	0	0.776749	1.334637	0.051294
22	6	0	-0.407886	0.976544	1.319580
23	6	0	1.549814	2.502519	1.124143
24	8	0	-1.186288	0.829775	2.155861
25	8	0	2.021431	3.316131	1.788507
26	26	0	-3.482383	-0.376725	-0.035898
27	6	0	-3.147208	-1.902410	0.859143
28	6	0	-4.029321	0.387665	1.446451
29	6	0	-5.014606	0.124004	-0.774892
30	8	0	-3.103548	-2.912815	1.413441
31	8	0	-4.373867	0.907746	2.413136
32	8	0	-6.076098	0.291069	-1.204817
33	26	0	2.657387	-0.779877	0.117180
34	6	0	1.421834	-1.150269	1.381851
35	6	0	3.794819	-2.083006	0.527096
36	6	0	3.679054	0.447588	0.942245
37	8	0	0.728035	-1.580017	2.193620
38	8	0	4.513410	-2.927803	0.829575
39	8	0	4.369580	1.213152	1.449005

Table S67. Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses, in km/mol) for the structure **Fe14-1**，**Fe14-2** of $C_{12}H_8FeCO_4$ using M06-L.

Fe14-1		**Fe14-2**	
A" 25(0)	A' 841(14)	A 34(0)	A 817(14)
A" 38(0)	A" 843(1)	A 43(0)	A 872(18)
A' 52(0)	A" 905(0)	A 52(0)	A 886(4)
A' 70(0)	A' 919(0)	A 69(0)	A 910(0)
A" 78(0)	A" 943(0)	A 87(1)	A 918(5)
A' 86(0)	A" 975(0)	A 92(0)	A 973(0)
A" 89(0)	A' 984(1)	A 93(0)	A 980(1)
A' 107(1)	A' 1025(9)	A 108(1)	A 1032(4)
A" 129(0)	A" 1054(2)	A 121(0)	A 1044(1)
A' 130(0)	A' 1072(1)	A 130(0)	A 1069(1)
A' 171(2)	A' 1087(12)	A 154(16)	A 1110(14)
A' 222(6)	A" 1128(3)	A 210(1)	A 1121(3)
A" 249(0)	A" 1187(0)	A 233(1)	A 1190(2)
A' 369(58)	A' 1208(4)	A 259(26)	A 1208(4)
A" 383(0)	A" 1232(1)	A 374(0)	A 1213(2)
A" 401(3)	A" 1263(1)	A 384(0)	A 1259(2)
A' 412(3)	A' 1268(0)	A 390(3)	A 1277(3)
A" 418(0)	A" 1325(0)	A 419(4)	A 1348(5)
A' 420(2)	A' 1344(6)	A 422(3)	A 1380(3)
A' 441(5)	A' 1418(3)	A 428(3)	A 1434(9)
A' 451(14)	A" 1424(1)	A 445(31)	A 1445(3)
A' 462(0)	A' 1468(2)	A 461(5)	A 1470(28)
A" 466(4)	A' 1477(5)	A 470(19)	A 1477(6)
A' 478(23)	A" 1501(1)	A 472(4)	A 1517(8)
A' 489(12)	A" 1536(6)	A 474(2)	A 1551(11)
A" 502(1)	A' 1640(9)	A 481(0)	A 1597(34)
A" 520(1)	A' 1653(8)	A 521(1)	A 1647(1)
A' 563(7)	A" 1666(1)	A 557(5)	A 1659(2)
A" 563(0)	A" 2060(956)	A 563(1)	A 2051(1004)
A' 594(68)	A' 2078(572)	A 574(5)	A 2069(574)
A" 597(2)	A' 2089(1158)	A 595(58)	A 2080(1050)
A" 631(72)	A' 2146(523)	A 608(19)	A 2137(571)
A' 639(43)	A' 3170(2)	A 629(78)	A 3172(0)
A' 650(156)	A" 3170(0)	A 649(105	A 3173(1)
A" 667(2)	A" 3179(6)	A 652(36)	A 3182(12)
A' 684(4)	A' 3179(22)	A 673(3)	A 3183(9)
A" 704(10)	A" 3189(2)	A 701(0)	A 3195(26)
A" 768(0)	A" 3193(37)	A 727(22)	A 3195(18)
A' 782(39)	A' 3194(21)	A 761(1)	A 3214(1)
A' 814(27)	A' 3204(9)	A 776(1)	A 3235(8)
A' 822(0)		A 814(63)	

Table S68. Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses, in km/mol) for the structure **Fe13-1**，**Fe13-2** of $C_{12}H_8FeCO_3$ using M06-L.

Fe13-1		**Fe13-2**	
A" 28(0)	A" 857(2)	A 40(0)	A 891(0)
A' 66(1)	A' 875(4)	A 60(0)	A 912(1)
A' 75(0)	A" 895(3)	A 72(0)	A 931(4)
A" 78(0)	A" 972(1)	A 80(0)	A 959(1)
A" 82(0)	A' 978(1)	A 81(0)	A 964(0)
A' 95(0)	A' 1018(5)	A 93(0)	A 1015(3)
A" 124(1)	A" 1061(4)	A 131(1)	A 1047(1)
A' 138(2)	A' 1074(1)	A 161(1)	A 1064(4)
A' 188(5)	A' 1080(1)	A 213(2)	A 1103(11)
A" 225(3)	A" 1127(0)	A 252(3)	A 1111(1)
A' 289(8)	A" 1182(29)	A 290(3)	A 1152(4)
A' 386(3)	A" 1206(0)	A 333(6)	A 1192(3)
A" 387(1)	A' 1209(17)	A 394(1)	A 1203(0)
A" 426(0)	A' 1264(1)	A 402(4)	A 1247(3)
A' 430(5)	A" 1271(2)	A 417(4)	A 1276(4)
A" 448(2)	A' 1328(2)	A 453(15)	A 1336(3)
A" 456(0)	A" 1330(52)	A 456(1)	A 1369(7)
A' 463(3)	A' 1404(12)	A 470(8)	A 1390(18)
A' 475(2)	A" 1417(19)	A 473(5)	A 1427(0)
A" 484(2)	A" 1455(14)	A 478(4)	A 1441(27)
A' 490(2)	A' 1464(60)	A 491(25)	A 1481(2)
A' 506(14)	A' 1477(1)	A 514(1)	A 1501(40)
A" 511(0)	A" 1541(0)	A 537(25)	A 1516(6)
A' 551(22)	A' 1603(105)	A 553(49)	A 1545(3)
A' 566(42)	A' 1617(29)	A 557(14)	A 1629(1)
A" 582(4)	A" 1644(61)	A 593(6)	A 1677(3)
A" 591(48)	A' 2062(804)	A 598(4)	A 2057(718)
A' 609(56)	A" 2067(667)	A 613(62)	A 2072(873)
A' 621(55)	A' 2121(882)	A 624(62)	A 2119(887)
A" 655(2)	A' 3171(4)	A 668(6)	A 3171(6)
A' 688(6)	A" 3171(12)	A 687(5)	A 3173(1)
A" 714(3)	A" 3191(1)	A 701(3)	A 3183(17)
A" 755(1)	A' 3192(32)	A 736(29)	A 3189(4)
A' 771(40)	A" 3204(19)	A 764(8)	A 3196(31)
A' 802(45)	A' 3204(1)	A 798(40)	A 3203(11)
A' 809(12)	A" 3229(2)	A 816(2)	A 3207(3)
A" 846(3)	A' 3241(5)	A 860(16)	A 3228(13)
A' 846(5)		A 885(5)	

Table S69. Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses, in km/mol) for the structure **Fe12-1**，**Fe12-2** of $C_{12}H_8FeCO_2$ using M06-L.

Fe12-1		**Fe12-2**	
A 45(0)	A 893(1)	A 40(0)	A 914(3)
A 59(1)	A 970(0)	A 64(0)	A 948(2)
A 72(1)	A 978(0)	A 81(0)	A 960(1)
A 90(1)	A 1033(3)	A 93(1)	A 1033(1)
A 133(3)	A 1055(3)	A 154(5)	A 1044(3)
A 146(0)	A 1072(0)	A 163(1)	A 1063(3)
A 186(0)	A 1084(5)	A 213(1)	A 1101(21)
A 253(0)	A 1127(0)	A 287(3)	A 1121(1)
A 320(5)	A 1185(4)	A 313(1)	A 1176(4)
A 368(5)	A 1208(4)	A 333(10)	A 1203(6)
A 429(3)	A 1215(4)	A 382(7)	A 1216(1)
A 443(4)	A 1269(0)	A 417(2)	A 1255(1)
A 449(2)	A 1281(2)	A 421(2)	A 1277(6)
A 476(3)	A 1338(2)	A 461(2)	A 1359(15)
A 480(2)	A 1354(10)	A 473(1)	A 1369(5)
A 483(2)	A 1413(4)	A 479(1)	A 1434(3)
A 487(7)	A 1429(2)	A 499(14)	A 1437(3)
A 515(2)	A 1462(4)	A 526(1)	A 1460(48)
A 535(6)	A 1470(9)	A 540(18)	A 1486(24)
A 550(6)	A 1475(0)	A 555(29)	A 1505(13)
A 570(29)	A 1537(5)	A 566(1)	A 1526(10)
A 581(31)	A 1597(18)	A 585(39)	A 1557(26)
A 620(4)	A 1617(12)	A 596(7)	A 1616(7)
A 641(9)	A 1637(15)	A 643(18)	A 1642(0)
A 657(36)	A 2022(864)	A 654(19)	A 2021(774)
A 694(4)	A 2062(1410)	A 683(2)	A 2065(1340)
A 709(3)	A 3176(2)	A 692(16)	A 3177(2)
A 739(3)	A 3176(7)	A 706(2)	A 3187(3)
A 761(2)	A 3191(10)	A 763(1)	A 3187(9)
A 793(63)	A 3194(16)	A 782(45)	A 3197(6)
A 812(2)	A 3203(17)	A 811(1)	A 3200(19)
A 831(19)	A 3203(5)	A 842(14)	A 3209(9)
A 860(1)	A 3234(2)	A 880(5)	A 3219(2)
A 872(1)	A 3248(3)	A 894(9)	A 3239(9)
A 889(2)		A 904(1)	

Table S70. Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses, in km/mol) for the structure **Fe28-1**，**Fe28-2**，**Fe28-3**，**Fe28-4** of $C_{12}H_8Fe_2CO_8$ using M06-L.

Fe28-1		Fe28-2		Fe28-3		Fe28-4	
A 22(0)	A 634(147)	A 11(0)	A 639(34)	A 27(0)	A 633(27)	A 21(0)	A 634(67)
A 28(0)	A 646(273)	A 25(0)	A 648(162)	A 35(0)	A 642(114)	A 25(0)	A 646(280)
A 34(0)	A 655(60)	A 34(0)	A 651(122)	A 41(0)	A 651(78)	A 28(0)	A 647(16)
A 39(0)	A 659(5)	A 44(1)	A 665(5)	A 46(0)	A 652(78)	A 34(0)	A 657(2)
A 47(0)	A 675(2)	A 54(0)	A 685(15)	A 53(0)	A 677(10)	A 42(0)	A 676(0)
A 51(0)	A 703(6)	A 57(0)	A 702(9)	A 56(0)	A 702(1)	A 48(1)	A 692(18)
A 56(0)	A 764(5)	A 64(0)	A 771(24)	A 62(0)	A 736(19)	A 52(0)	A 701(5)
A 70(1)	A 776(6)	A 75(0)	A 783(0)	A 72(6)	A 775(2)	A 55(0)	A 771(3)
A 76(0)	A 814(41)	A 79(2)	A 803(22)	A 74(0)	A 782(12)	A 63(0)	A 785(20)
A 80(0)	A 814(6)	A 83(0)	A 811(2)	A 86(0)	A 807(10)	A 82(1)	A 808(1)
A 86(1)	A 823(2)	A 84(1)	A 830(2)	A 91(2)	A 817(28)	A 86(1)	A 829(10)
A 90(0)	A 837(12)	A 92(0)	A 837(4)	A 95(0)	A 852(11)	A 88(1)	A 857(11)
A 92(0)	A 872(5)	A 94(0)	A 890(4)	A 98(0)	A 872(6)	A 91(1)	A 886(5)
A 94(0)	A 909(1)	A 104(0)	A 909(2)	A 104(1)	A 898(11)	A 91(0)	A 912(8)
A 105(2)	A 942(0)	A 109(1)	A 921(2)	A 107(1)	A 920(4)	A 92(0)	A 924(12)
A 106(1)	A 976(1)	A 111(1)	A 947(2)	A 108(0)	A 934(1)	A 102(1)	A 930(1)
A 117(4)	A 984(0)	A 114(0)	A 974(0)	A 114(2)	A 975(0)	A 106(0)	A 934(12)
A 121(1)	A 1021(5)	A 131(4)	A 1009(8)	A 122(16)	A 1011(3)	A 109(1)	A 1002(4)
A 125(0)	A 1047(1)	A 140(8)	A 1031(5)	A 126(1)	A 1039(1)	A 118(1)	A 1039(4)
A 131(2)	A 1073(1)	A 152(0)	A 1071(1)	A 132(0)	A 1057(0)	A 126(0)	A 1043(8)
A 148(10)	A 1095(6)	A 167(5)	A 1086(13)	A 143(5)	A 1112(12)	A 151(8)	A 1104(29)
A 214(20)	A 1124(7)	A 211(2)	A 1131(2)	A 169(47)	A 1121(1)	A 192(25)	A 1124(2)
A 226(19)	A 1191(0)	A 234(5)	A 1177(2)	A 203(1)	A 1181(2)	A 222(2)	A 1175(5)
A 281(17)	A 1207(4)	A 286(39)	A 1202(1)	A 267(7)	A 1203(2)	A 272(1)	A 1197(3)
A 364(78)	A 1217(3)	A 376(4)	A 1227(1)	A 302(25)	A 1211(2)	A 301(31)	A 1221(1)
A 374(0)	A 1261(1)	A 378(35)	A 1254(2)	A 373(1)	A 1243(6)	A 370(0)	A 1250(1)
A 382(0)	A 1262(1)	A 388(4)	A 1263(1)	A 377(0)	A 1273(1)	A 379(1)	A 1277(6)
A 388(2)	A 1323(6)	A 388(5)	A 1328(2)	A 381(17)	A 1353(9)	A 381(1)	A 1358(6)
A 400(3)	A 1343(5)	A 401(4)	A 1339(12)	A 385(1)	A 1376(7)	A 394(18)	A 1376(25)
A 414(7)	A 1399(2)	A 410(3)	A 1403(3)	A 388(1)	A 1421(4)	A 397(16)	A 1418(2)
A 417(28)	A 1431(3)	A 413(1)	A 1423(4)	A 416(10)	A 1433(4)	A 413(15)	A 1425(3)
A 417(10)	A 1454(1)	A 421(4)	A 1438(6)	A 423(10)	A 1451(27)	A 415(1)	A 1437(49)
A 425(1)	A 1460(7)	A 429(6)	A 1452(4)	A 426(2)	A 1469(10)	A 422(3)	A 1488(17)
A 427(0)	A 1477(2)	A 431(1)	A 1498(3)	A 426(6)	A 1494(4)	A 427(2)	A 1499(4)
A 440(3)	A 1529(3)	A 441(1)	A 1516(3)	A 428(0)	A 1548(8)	A 430(0)	A 1533(13)
A 449(15)	A 1598(11)	A 450(16)	A 1622(1)	A 445(24)	A 1591(17)	A 450(14)	A 1609(16)
A 453(8)	A 1646(3)	A 452(9)	A 1647(11)	A 452(8)	A 1619(4)	A 456(3)	A 1630(16)
A 466(9)	A 1650(8)	A 465(4)	A 1653(14)	A 463(7)	A 1651(5)	A 464(8)	A 1648(42)
A 467(1)	A 2044(926)	A 472(5)	A 2044(1002)	A 466(6)	A 2047(2067)	A 467(23)	A 2031(1089)
A 473(15)	A 2059(614)	A 476(8)	A 2057(1480)	A 471(35)	A 2048(80)	A 468(11)	A 2051(572)
A 474(0)	A 2062(699)	A 478(24)	A 2064(500)	A 472(6)	A 2063(694)	A 473(7)	A 2060(856)
A 476(15)	A 2074(829)	A 481(8)	A 2069(748)	A 475(4)	A 2066(687)	A 474(6)	A 2063(1518)
A 485(4)	A 2080(544)	A 485(25)	A 2085(508)	A 477(7)	A 2074(1338)	A 480(14)	A 2078(578)
A 487(13)	A 2088(1484)	A 490(12)	A 2089(779)	A 483(1)	A 2076(184)	A 482(1)	A 2088(1230)
A 490(4)	A 2130(994)	A 507(1)	A 2126(1069)	A 493(1)	A 2122(1249)	A 492(4)	A 2130(882)
A 518(2)	A 2149(300)	A 528(11)	A 2149(481)	A 522(7)	A 2143(394)	A 522(17)	A 2146(389)
A 556(18)	A 3173(1)	A 560(8)	A 3172(0)	A 552(6)	A 3175(0)	A 556(5)	A 3171(2)
A 563(0)	A 3174(1)	A 564(3)	A 3178(5)	A 565(2)	A 3179(2)	A 565(1)	A 3177(6)
A 564(0)	A 3183(10)	A 569(1)	A 3181(9)	A 567(0)	A 3184(8)	A 566(4)	A 3178(5)
A 592(17)	A 3185(6)	A 590(29)	A 3184(7)	A 570(1)	A 3187(6)	A 570(0)	A 3191(1)
A 595(58)	A 3194(3)	A 593(70)	A 3189(2)	A 596(87)	A 3197(11)	A 595(65)	A 3192(6)
A 600(52)	A 3196(24)	A 601(49)	A 3195(23)	A 599(10)	A 3201(6)	A 608(72)	A 3205(7)
A 623(19)	A 3196(14)	A 629(18)	A 3203(7)	A 613(47)	A 3216(0)	A 615(4)	A 3216(1)
A 632(31)	A 3220(3)	A 633(105)	A 3203(8)	A 629(105)	A 3237(8)	A 633(41)	A 3238(9)

Table S71. Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses, in km/mol) for the structure **Fe27-1**，**Fe27-2**，**Fe27-3**，**Fe27-4** of $C_{12}H_8Fe_2CO_7$ using M06-L.

Fe27-1		Fe27-2		Fe27-3		Fe27-4	
A 22(0)	A 649(12)	A 21(0)	A 650(136)	A 27(0)	A 651(112)	A 21(0)	A 649(83)
A 29(0)	A 658(96)	A 34(0)	A 673(23)	A 31(0)	A 663(8)	A 27(0)	A 660(13)
A 35(0)	A 682(3)	A 45(0)	A 693(7)	A 31(0)	A 684(8)	A 39(0)	A 687(3)
A 45(1)	A 706(1)	A 54(0)	A 694(6)	A 41(0)	A 698(5)	A 48(0)	A 700(0)
A 55(0)	A 750(8)	A 64(0)	A 761(22)	A 49(0)	A 720(22)	A 51(0)	A 728(17)
A 57(7)	A 767(1)	A 70(0)	A 787(12)	A 57(0)	A 772(2)	A 57(0)	A 768(4)
A 65(2)	A 791(42)	A 78(0)	A 818(11)	A 65(1)	A 789(25)	A 71(0)	A 795(41)
A 76(0)	A 808(51)	A 80(0)	A 824(4)	A 76(0)	A 806(2)	A 74(1)	A 813(7)
A 80(1)	A 835(39)	A 84(0)	A 836(15)	A 77(0)	A 849(17)	A 81(0)	A 854(17)
A 84(0)	A 848(3)	A 87(0)	A 882(7)	A 85(1)	A 875(10)	A 85(0)	A 878(4)
A 88(1)	A 865(5)	A 92(0)	A 899(2)	A 90(0)	A 886(2)	A 88(0)	A 889(8)
A 91(0)	A 886(2)	A 109(0)	A 912(0)	A 91(0)	A 911(1)	A 93(0)	A 912(2)
A 96(2)	A 905(2)	A 110(0)	A 938(1)	A 96(0)	A 919(1)	A 97(0)	A 916(1)
A 100(6)	A 971(9)	A 124(0)	A 961(0)	A 105(1)	A 925(4)	A 106(0)	A 942(4)
A 110(2)	A 983(1)	A 128(0)	A 966(1)	A 107(1)	A 964(0)	A 108(1)	A 966(0)
A 111(1)	A 1023(1)	A 142(1)	A 1004(6)	A 112(1)	A 1012(15)	A 127(3)	A 1012(3)
A 141(4)	A 1041(4)	A 143(0)	A 1044(2)	A 126(1)	A 1023(8)	A 135(1)	A 1027(0)
A 143(2)	A 1068(2)	A 183(12)	A 1063(3)	A 166(1)	A 1052(1)	A 155(1)	A 1052(1)
A 151(1)	A 1076(1)	A 220(2)	A 1075(10)	A 174(30)	A 1101(17)	A 169(3)	A 1104(10)
A 218(0)	A 1122(3)	A 235(1)	A 1110(6)	A 234(0)	A 1111(1)	A 237(2)	A 1110(0)
A 281(38)	A 1188(17)	A 276(0)	A 1143(2)	A 276(4)	A 1153(9)	A 271(7)	A 1146(4)
A 289(3)	A 1202(7)	A 351(32)	A 1187(1)	A 294(2)	A 1184(3)	A 279(4)	A 1182(2)
A 372(0)	A 1209(9)	A 371(27)	A 1192(0)	A 364(19)	A 1200(0)	A 332(9)	A 1203(1)
A 377(4)	A 1261(10)	A 393(17)	A 1241(4)	A 373(0)	A 1246(8)	A 373(0)	A 1241(1)
A 383(1)	A 1270(1)	A 400(2)	A 1253(0)	A 383(1)	A 1271(5)	A 379(0)	A 1271(2)
A 392(2)	A 1321(8)	A 404(5)	A 1308(11)	A 393(1)	A 1337(0)	A 394(2)	A 1336(5)
A 415(47)	A 1353(30)	A 406(3)	A 1337(2)	A 403(8)	A 1370(12)	A 401(2)	A 1365(3)
A 423(4)	A 1396(6)	A 416(1)	A 1357(3)	A 417(6)	A 1394(2)	A 419(4)	A 1390(15)
A 433(1)	A 1423(19)	A 428(6)	A 1395(12)	A 427(3)	A 1428(18)	A 421(5)	A 1418(3)
A 435(3)	A 1445(22)	A 440(6)	A 1415(3)	A 428(4)	A 1438(12)	A 425(1)	A 1436(30)
A 452(1)	A 1462(6)	A 447(9)	A 1442(0)	A 453(11)	A 1480(0)	A 441(15)	A 1470(3)
A 455(0)	A 1479(24)	A 450(7)	A 1463(9)	A 453(11)	A 1495(53)	A 453(2)	A 1485(21)
A 460(2)	A 1534(15)	A 460(0)	A 1500(12)	A 457(1)	A 1502(6)	A 458(4)	A 1503(9)
A 468(6)	A 1581(102)	A 464(4)	A 1523(5)	A 470(4)	A 1531(10)	A 468(14)	A 1538(3)
A 472(1)	A 1607(16)	A 476(26)	A 1625(2)	A 472(4)	A 1614(3)	A 472(9)	A 1606(3)
A 475(3)	A 1641(54)	A 480(12)	A 1672(7)	A 474(16)	A 1643(20)	A 474(15)	A 1682(7)
A 479(3)	A 2031(938)	A 487(2)	A 2052(819)	A 475(3)	A 2035(1102)	A 476(1)	A 2028(1199)
A 481(9)	A 2048(595)	A 493(10)	A 2061(502)	A 480(10)	A 2053(624)	A 483(6)	A 2047(367)
A 483(11)	A 2057(901)	A 500(1)	A 2064(379)	A 487(0)	A 2063(1310)	A 486(0)	A 2059(909)
A 498(9)	A 2068(873)	A 514(19)	A 2077(431)	A 491(30)	A 2066(725)	A 508(43)	A 2066(1100)
A 504(22)	A 2070(739)	A 521(5)	A 2092(1359)	A 513(2)	A 2079(929)	A 518(1)	A 2077(419)
A 511(13)	A 2113(1685)	A 546(72)	A 2111(1140)	A 539(16)	A 2121(1684)	A 537(19)	A 2114(1182)
A 548(40)	A 2129(202)	A 559(4)	A 2149(529)	A 551(36)	A 2132(43)	A 551(38)	A 2134(522)
A 563(43)	A 3176(1)	A 566(49)	A 3170(8)	A 557(22)	A 3175(6)	A 554(10)	A 3172(4)
A 567(0)	A 3178(7)	A 566(2)	A 3173(0)	A 568(0)	A 3184(4)	A 571(1)	A 3185(3)
A 577(126)	A 3190(3)	A 593(56)	A 3177(3)	A 588(22)	A 3192(4)	A 592(11)	A 3190(3)
A 580(28)	A 3194(9)	A 602(18)	A 3183(13)	A 594(3)	A 3192(4)	A 599(7)	A 3194(3)
A 592(65)	A 3199(10)	A 613(59)	A 3185(3)	A 605(68)	A 3206(13)	A 608(67)	A 3204(12)
A 604(80)	A 3206(7)	A 621(50)	A 3196(27)	A 612(62)	A 3206(3)	A 611(35)	A 3208(5)
A 616(106)	A 3226(1)	A 626(43)	A 3197(13)	A 620(134)	A 3209(3)	A 623(79)	A 3209(0)
A 633(37)	A 3244(1)	A 632(48)	A 3199(15)	A 634(54)	A 3232(7)	A 633(38)	A 3229(13)

Table S72. Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses, in km/mol) for the structure **Fe26-1**，**Fe26-2**，**Fe26-3**，**Fe26-4** of $C_{12}H_8Fe_2CO_6$ using M06-L.

Fe26-1		Fe26-2		Fe26-3		Fe26-4	
A 18(0)	A 694(5)	A 29(0)	A 694(6)	A 29(0)	A 679(8)	A 17(0)	A 685(1)
A 25(1)	A 712(2)	A 51(0)	A 720(28)	A 36(0)	A 685(21)	A 31(0)	A 709(4)
A 40(4)	A 743(25)	A 54(2)	A 761(28)	A 37(2)	A 701(9)	A 52(0)	A 739(33)
A 50(1)	A 771(39)	A 57(0)	A 775(4)	A 45(0)	A 740(21)	A 63(0)	A 769(12)
A 67(0)	A 794(4)	A 66(1)	A 790(16)	A 60(0)	A 806(8)	A 67(0)	A 780(12)
A 70(0)	A 810(2)	A 79(0)	A 815(11)	A 70(0)	A 849(20)	A 74(0)	A 794(19)
A 76(2)	A 845(3)	A 82(1)	A 850(14)	A 74(0)	A 855(2)	A 85(0)	A 837(12)
A 78(0)	A 859(7)	A 87(1)	A 867(15)	A 78(1)	A 880(7)	A 88(0)	A 861(19)
A 79(0)	A 866(7)	A 90(0)	A 873(6)	A 81(1)	A 893(0)	A 96(0)	A 881(2)
A 84(1)	A 884(1)	A 98(2)	A 890(8)	A 85(0)	A 904(1)	A 98(0)	A 896(6)
A 94(0)	A 892(4)	A 104(3)	A 894(1)	A 93(0)	A 909(3)	A 104(0)	A 924(4)
A 99(0)	A 923(28)	A 106(3)	A 924(42)	A 96(0)	A 943(1)	A 121(0)	A 947(1)
A 115(12)	A 982(1)	A 114(2)	A 982(1)	A 119(8)	A 956(2)	A 140(1)	A 968(8)
A 123(8)	A 1021(3)	A 128(4)	A 1017(0)	A 128(1)	A 1001(17)	A 144(0)	A 972(4)
A 144(1)	A 1031(0)	A 141(12)	A 1020(2)	A 135(4)	A 1042(1)	A 149(1)	A 1021(0)
A 158(1)	A 1062(0)	A 154(2)	A 1056(2)	A 157(5)	A 1047(0)	A 173(1)	A 1044(1)
A 227(1)	A 1070(2)	A 209(4)	A 1064(1)	A 219(15)	A 1089(16)	A 191(0)	A 1098(2)
A 309(10)	A 1118(3)	A 248(12)	A 1114(4)	A 247(67)	A 1097(5)	A 224(2)	A 1108(4)
A 346(26)	A 1153(3)	A 293(3)	A 1135(4)	A 295(4)	A 1142(4)	A 275(3)	A 1149(1)
A 358(6)	A 1192(9)	A 360(11)	A 1190(3)	A 337(3)	A 1163(14)	A 314(7)	A 1195(7)
A 380(4)	A 1207(16)	A 366(3)	A 1207(32)	A 378(4)	A 1188(2)	A 331(6)	A 1203(2)
A 384(5)	A 1259(14)	A 383(3)	A 1259(22)	A 386(2)	A 1229(3)	A 388(3)	A 1236(1)
A 391(16)	A 1267(7)	A 395(3)	A 1264(3)	A 395(1)	A 1247(9)	A 395(0)	A 1256(0)
A 414(24)	A 1331(1)	A 413(9)	A 1327(10)	A 405(11)	A 1306(0)	A 401(3)	A 1324(4)
A 432(40)	A 1375(32)	A 433(7)	A 1338(15)	A 408(1)	A 1360(15)	A 407(15)	A 1354(5)
A 438(12)	A 1384(7)	A 439(19)	A 1368(5)	A 439(70)	A 1396(0)	A 416(9)	A 1379(1)
A 451(3)	A 1405(8)	A 447(2)	A 1390(18)	A 446(2)	A 1431(9)	A 432(3)	A 1408(3)
A 455(4)	A 1430(75)	A 452(0)	A 1426(77)	A 450(11)	A 1437(11)	A 438(5)	A 1417(1)
A 460(1)	A 1447(1)	A 458(5)	A 1443(10)	A 457(4)	A 1442(5)	A 446(2)	A 1443(6)
A 466(12)	A 1466(9)	A 467(1)	A 1453(6)	A 459(1)	A 1481(21)	A 450(2)	A 1480(6)
A 472(4)	A 1518(4)	A 471(17)	A 1514(97)	A 464(1)	A 1487(3)	A 452(2)	A 1526(22)
A 476(4)	A 1550(169)	A 481(1)	A 1524(163)	A 471(0)	A 1498(13)	A 459(5)	A 1552(18)
A 478(11)	A 1591(149)	A 482(0)	A 1582(171)	A 474(4)	A 1535(23)	A 470(3)	A 1615(13)
A 484(2)	A 1633(50)	A 490(26)	A 1627(60)	A 480(43)	A 1663(27)	A 481(1)	A 1678(2)
A 494(10)	A 2024(748)	A 502(16)	A 1997(590)	A 486(4)	A 2037(641)	A 488(1)	A 2033(230)
A 498(17)	A 2029(741)	A 504(7)	A 2021(716)	A 491(15)	A 2047(857)	A 493(9)	A 2037(377)
A 505(16)	A 2076(1190)	A 518(11)	A 2073(1093)	A 504(7)	A 2065(770)	A 505(4)	A 2059(72)
A 531(11)	A 2081(883)	A 538(11)	A 2082(881)	A 512(56)	A 2075(851)	A 510(23)	A 2071(1109)
A 540(40)	A 2082(1370)	A 560(18)	A 2104(659)	A 543(58)	A 2092(2056)	A 538(67)	A 2081(1798)
A 561(43)	A 2132(810)	A 570(28)	A 2144(771)	A 548(20)	A 2122(648)	A 540(21)	A 2121(1004)
A 567(62)	A 3175(9)	A 573(100)	A 3165(5)	A 554(36)	A 3169(4)	A 546(9)	A 3166(3)
A 572(31)	A 3177(6)	A 577(35)	A 3174(10)	A 581(17)	A 3179(9)	A 576(33)	A 3173(9)
A 580(32)	A 3191(5)	A 586(33)	A 3176(12)	A 594(10)	A 3190(3)	A 586(49)	A 3178(10)
A 594(64)	A 3193(11)	A 604(28)	A 3184(17)	A 606(113)	A 3193(2)	A 596(27)	A 3191(6)
A 605(68)	A 3210(6)	A 620(74)	A 3192(11)	A 615(73)	A 3204(9)	A 606(73)	A 3196(9)
A 620(22)	A 3211(5)	A 622(19)	A 3211(6)	A 618(120)	A 3208(7)	A 619(63)	A 3198(10)
A 623(122)	A 3231(1)	A 632(86)	A 3231(1)	A 627(3)	A 3209(10)	A 628(5)	A 3209(1)
A 657(53)	A 3247(1)	A 674(10)	A 3244(1)	A 647(8)	A 3242(5)	A 655(29)	A 3233(8)

Table S73. Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses, in km/mol) for the structure **Fe25-1**，**Fe25-2**，**Fe25-3** of $C_{12}H_8Fe_2CO_5$ using M06-L.

Fe25-1		Fe25-2		Fe25-3	
A" 37(0)	A' 743(1)	A 32(0)	A 724(5)	A 33(0)	A 734(40)
A" 42(0)	A" 764(1)	A 39(1)	A 766(39)	A 36(0)	A 756(13)
A' 69(0)	A' 772(53)	A 61(0)	A 797(8)	A 65(0)	A 774(24)
A" 73(0)	A' 814(13)	A 72(0)	A 824(9)	A 71(0)	A 809(4)
A' 84(0)	A' 840(16)	A 83(0)	A 849(2)	A 81(1)	A 851(24)
A" 89(0)	A" 853(3)	A 84(0)	A 869(4)	A 87(0)	A 867(6)
A' 90(1)	A" 883(0)	A 92(0)	A 873(8)	A 91(0)	A 872(10)
A' 100(0)	A" 899(3)	A 94(1)	A 883(0)	A 94(1)	A 899(0)
A" 123(0)	A' 902(0)	A 102(0)	A 898(3)	A 112(2)	A 908(1)
A' 125(0)	A" 965(0)	A 125(0)	A 963(3)	A 124(0)	A 949(1)
A" 153(0)	A' 968(4)	A 139(0)	A 974(0)	A 126(0)	A 968(3)
A' 165(1)	A" 1020(1)	A 157(2)	A 1025(1)	A 151(1)	A 1037(3)
A' 176(5)	A' 1034(1)	A 174(2)	A 1042(1)	A 176(5)	A 1038(1)
A' 183(2)	A' 1053(1)	A 186(9)	A 1059(3)	A 177(6)	A 1052(1)
A" 209(4)	A' 1090(5)	A 230(0)	A 1078(3)	A 190(2)	A 1089(17)
A" 294(1)	A" 1107(0)	A 310(2)	A 1113(1)	A 281(1)	A 1122(1)
A' 314(0)	A" 1189(1)	A 351(4)	A 1167(2)	A 303(1)	A 1181(1)
A' 360(1)	A" 1204(0)	A 359(6)	A 1197(2)	A 330(2)	A 1203(2)
A" 392(2)	A' 1206(2)	A 365(11)	A 1203(3)	A 343(12)	A 1214(6)
A' 393(4)	A" 1242(0)	A 384(12)	A 1252(4)	A 382(4)	A 1250(2)
A" 403(7)	A' 1296(0)	A 422(7)	A 1280(0)	A 401(1)	A 1286(2)
A' 437(0)	A' 1330(1)	A 433(0)	A 1334(2)	A 416(1)	A 1332(39)
A' 441(19)	A" 1389(6)	A 445(3)	A 1379(5)	A 431(2)	A 1383(8)
A" 447(0)	A' 1402(0)	A 445(8)	A 1395(7)	A 434(7)	A 1412(1)
A" 459(2)	A" 1423(3)	A 460(3)	A 1418(4)	A 439(13)	A 1431(8)
A" 476(0)	A' 1429(2)	A 473(0)	A 1435(9)	A 463(1)	A 1449(19)
A' 483(1)	A" 1473(3)	A 476(4)	A 1470(2)	A 473(5)	A 1479(16)
A" 484(2)	A' 1519(5)	A 491(1)	A 1482(6)	A 478(1)	A 1492(5)
A' 500(22)	A' 1537(3)	A 494(1)	A 1519(1)	A 484(6)	A 1506(80)
A' 503(2)	A" 1561(4)	A 499(14)	A 1542(12)	A 495(1)	A 1562(18)
A" 512(0)	A" 1606(3)	A 514(6)	A 1601(37)	A 499(8)	A 1572(17)
A" 528(4)	A' 1645(0)	A 524(2)	A 1648(17)	A 501(6)	A 1619(7)
A' 535(24)	A" 2023(13)	A 536(19)	A 2014(91)	A 509(16)	A 2017(43)
A' 545(12)	A' 2036(6)	A 546(14)	A 2034(66)	A 535(33)	A 2030(70)
A" 549(33)	A' 2059(1648)	A 548(60)	A 2055(1189)	A 537(18)	A 2052(1327)
A" 557(29)	A" 2059(1221)	A 557(41)	A 2067(1432)	A 543(22)	A 2060(1334)
A' 567(74)	A' 2111(1122)	A 583(23)	A 2108(1188)	A 561(40)	A 2107(1249)
A" 585(38)	A" 3182(3)	A 590(48)	A 3178(7)	A 574(24)	A 3175(2)
A' 587(64)	A' 3182(0)	A 604(27)	A 3181(4)	A 588(62)	A 3188(1)
A' 613(22)	A' 3195(7)	A 614(38)	A 3193(9)	A 615(84)	A 3192(6)
A' 633(46)	A" 3196(1)	A 624(66)	A 3194(4)	A 628(56)	A 3196(2)
A" 649(0)	A" 3205(19)	A 645(33)	A 3206(10)	A 638(9)	A 3202(10)
A' 659(54)	A' 3205(4)	A 654(12)	A 3207(9)	A 651(16)	A 3210(8)
A' 687(7)	A" 3233(1)	A 692(1)	A 3234(1)	A 676(4)	A 3221(2)
A" 695(1)	A' 3246(3)	A 702(1)	A 3249(2)	A 708(1)	A 3247(3)

Table S74. Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses, in km/mol) for the structure **Fe25-4**，**Fe25-5** of $C_{12}H_8Fe_2CO_5$ using M06-L.

Fe25-4		**Fe25-5**	
A 21(0)	A 704(7)	A 29(1)	A 753(9)
A 37(0)	A 785(34)	A 38(5)	A 786(18)
A 45(1)	A 804(7)	A 43(0)	A 800(5)
A 51(1)	A 835(15)	A 54(2)	A 825(5)
A 70(0)	A 850(3)	A 68(0)	A 835(11)
A 75(0)	A 858(11)	A 70(0)	A 864(1)
A 80(1)	A 882(5)	A 76(0)	A 882(2)
A 86(1)	A 910(0)	A 77(3)	A 886(0)
A 95(0)	A 931(7)	A 91(1)	A 899(0)
A 96(0)	A 934(2)	A 92(1)	A 934(2)
A 139(0)	A 959(0)	A 116(20)	A 983(1)
A 153(8)	A 1008(1)	A 123(1)	A 1021(2)
A 168(1)	A 1019(2)	A 137(3)	A 1035(2)
A 180(3)	A 1051(1)	A 154(2)	A 1059(1)
A 259(3)	A 1104(5)	A 233(0)	A 1072(5)
A 295(16)	A 1106(3)	A 302(5)	A 1113(1)
A 322(7)	A 1152(2)	A 325(6)	A 1159(7)
A 333(1)	A 1179(4)	A 353(19)	A 1198(8)
A 372(8)	A 1200(1)	A 380(6)	A 1200(3)
A 386(1)	A 1242(1)	A 383(16)	A 1253(1)
A 396(3)	A 1261(2)	A 408(4)	A 1271(2)
A 407(1)	A 1324(3)	A 416(78)	A 1329(3)
A 420(3)	A 1369(7)	A 432(28)	A 1372(8)
A 451(18)	A 1399(1)	A 441(2)	A 1381(4)
A 454(1)	A 1417(2)	A 452(8)	A 1403(5)
A 469(1)	A 1441(6)	A 462(11)	A 1417(5)
A 472(10)	A 1472(2)	A 464(4)	A 1459(6)
A 476(4)	A 1486(5)	A 469(5)	A 1469(4)
A 483(3)	A 1510(5)	A 475(5)	A 1514(4)
A 490(24)	A 1542(2)	A 483(9)	A 1536(10)
A 499(0)	A 1578(5)	A 486(13)	A 1592(10)
A 510(8)	A 1595(5)	A 508(4)	A 1639(34)
A 528(8)	A 2002(596)	A 518(10)	A 2032(495)
A 543(45)	A 2047(2170)	A 532(46)	A 2036(1163)
A 546(59)	A 2062(704)	A 541(9)	A 2038(785)
A 562(15)	A 2071(784)	A 550(39)	A 2063(3406)
A 569(21)	A 2118(978)	A 558(73)	A 2094(502)
A 589(32)	A 3178(6)	A 575(11)	A 3176(6)
A 600(29)	A 3194(2)	A 586(49)	A 3177(5)
A 614(55)	A 3196(1)	A 611(25)	A 3194(11)
A 618(86)	A 3204(6)	A 616(78)	A 3198(2)
A 649(22)	A 3208(6)	A 639(69)	A 3207(11)
A 657(23)	A 3211(7)	A 655(15)	A 3210(4)
A 676(4)	A 3214(1)	A 699(5)	A 3228(1)
A 694(2)	A 3234(7)	A 706(3)	A 3247(1)

Table S75. Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses, in km/mol) for the structure **Fe24-1**，**Fe24-2**，**Fe24-3**，**Fe24-4** of $C_{12}H_8Fe_2CO_4$ using M06-L.

Fe24-1		Fe24-2		Fe24-3		Fe24-4	
A 49(0)	A 797(5)	A 50(0)	A 771(40)	A 29(0)	A 772(44)	A 38(0)	A 794(0)
A 60(0)	A 815(13)	A 65(0)	A 811(5)	A 50(0)	A 812(12)	A 46(0)	A 819(2)
A 68(0)	A 840(4)	A 79(0)	A 814(20)	A 62(0)	A 815(10)	A 50(1)	A 827(4)
A 84(0)	A 866(3)	A 87(0)	A 846(2)	A 77(0)	A 857(4)	A 57(1)	A 855(5)
A 88(0)	A 875(4)	A 91(0)	A 879(6)	A 82(1)	A 881(6)	A 68(0)	A 874(6)
A 93(0)	A 890(4)	A 105(0)	A 895(0)	A 90(1)	A 893(1)	A 77(0)	A 882(2)
A 110(1)	A 897(1)	A 130(0)	A 903(1)	A 96(0)	A 914(1)	A 92(3)	A 890(8)
A 129(0)	A 946(4)	A 151(0)	A 960(0)	A 123(0)	A 958(1)	A 95(0)	A 953(2)
A 151(1)	A 977(0)	A 174(2)	A 964(4)	A 134(1)	A 965(3)	A 132(8)	A 963(0)
A 174(5)	A 1024(1)	A 178(1)	A 1014(1)	A 165(2)	A 1019(0)	A 150(0)	A 1028(0)
A 197(2)	A 1042(1)	A 197(4)	A 1032(1)	A 171(2)	A 1034(1)	A 164(2)	A 1040(2)
A 219(7)	A 1060(2)	A 215(1)	A 1051(1)	A 189(5)	A 1053(1)	A 185(1)	A 1061(3)
A 248(1)	A 1077(4)	A 240(5)	A 1087(7)	A 208(3)	A 1087(7)	A 226(1)	A 1074(5)
A 311(3)	A 1114(0)	A 298(0)	A 1103(0)	A 283(1)	A 1105(1)	A 317(6)	A 1113(3)
A 342(3)	A 1166(2)	A 315(1)	A 1187(2)	A 319(2)	A 1187(2)	A 338(9)	A 1174(1)
A 372(1)	A 1195(4)	A 350(3)	A 1201(1)	A 348(2)	A 1202(0)	A 359(4)	A 1198(2)
A 374(7)	A 1204(6)	A 394(12)	A 1204(2)	A 399(7)	A 1205(1)	A 372(7)	A 1205(4)
A 402(4)	A 1255(4)	A 405(2)	A 1239(0)	A 401(5)	A 1240(1)	A 403(2)	A 1256(1)
A 432(4)	A 1275(0)	A 414(6)	A 1295(0)	A 407(17)	A 1293(0)	A 429(4)	A 1273(2)
A 437(2)	A 1334(3)	A 427(0)	A 1325(1)	A 431(8)	A 1325(1)	A 437(4)	A 1295(0)
A 454(4)	A 1382(4)	A 440(0)	A 1383(5)	A 442(0)	A 1389(6)	A 454(2)	A 1356(12)
A 457(1)	A 1393(5)	A 452(6)	A 1398(1)	A 459(4)	A 1399(0)	A 469(2)	A 1384(2)
A 467(5)	A 1419(4)	A 464(5)	A 1421(3)	A 478(3)	A 1419(1)	A 474(8)	A 1407(1)
A 477(1)	A 1428(8)	A 477(0)	A 1428(2)	A 485(2)	A 1423(4)	A 476(5)	A 1447(4)
A 485(10)	A 1467(0)	A 487(4)	A 1469(4)	A 498(5)	A 1473(4)	A 486(16)	A 1458(1)
A 502(9)	A 1482(10)	A 508(25)	A 1511(7)	A 509(6)	A 1512(4)	A 493(2)	A 1471(12)
A 511(10)	A 1514(2)	A 512(1)	A 1527(2)	A 512(6)	A 1526(2)	A 500(17)	A 1490(1)
A 520(18)	A 1537(10)	A 519(17)	A 1558(5)	A 517(25)	A 1553(2)	A 513(4)	A 1545(3)
A 529(19)	A 1593(24)	A 537(51)	A 1601(2)	A 526(10)	A 1603(5)	A 527(4)	A 1579(4)
A 540(6)	A 1645(40)	A 542(15)	A 1634(1)	A 538(25)	A 1633(1)	A 536(14)	A 1616(21)
A 545(36)	A 1833(358)	A 544(7)	A 1829(368)	A 545(29)	A 2008(135)	A 552(31)	A 2019(594)
A 559(15)	A 2032(190)	A 556(14)	A 2031(250)	A 554(13)	A 2014(678)	A 561(32)	A 2026(951)
A 568(9)	A 2048(1362)	A 564(20)	A 2047(1403)	A 565(38)	A 2040(1579)	A 579(39)	A 2050(3618)
A 595(34)	A 2092(1403)	A 570(10)	A 2092(1141)	A 572(64)	A 2080(1281)	A 590(18)	A 2075(252)
A 619(53)	A 3175(8)	A 593(48)	A 3181(2)	A 605(3)	A 3179(2)	A 591(31)	A 3183(4)
A 626(40)	A 3181(4)	A 632(34)	A 3183(2)	A 640(39)	A 3182(2)	A 625(4)	A 3190(1)
A 648(55)	A 3193(12)	A 646(5)	A 3196(4)	A 646(5)	A 3189(4)	A 645(11)	A 3199(6)
A 657(27)	A 3195(2)	A 665(83)	A 3198(4)	A 657(11)	A 3198(4)	A 651(71)	A 3200(5)
A 697(4)	A 3207(12)	A 685(7)	A 3205(13)	A 688(8)	A 3205(17)	A 686(1)	A 3206(10)
A 704(3)	A 3208(8)	A 694(1)	A 3207(11)	A 695(2)	A 3205(8)	A 704(0)	A 3220(3)
A 737(6)	A 3230(2)	A 729(2)	A 3229(2)	A 733(3)	A 3234(1)	A 720(4)	A 3239(1)
A 772(40)	A 3246(3)	A 756(13)	A 3244(3)	A 763(8)	A 3251(3)	A 764(24)	A 3251(1)

Table S76. Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses, in km/mol) for the structure **Fe24-5**，**Fe24-6**，**Fe24-7** of $C_{12}H_8Fe_2CO_4$ using M06-L.

Fe24-5		Fe24-6		Fe24-7	
A 33(0)	A 798(0)	A 34(0)	A 796(0)	A 30(0)	A 779(1)
A 42(0)	A 823(4)	B 40(0)	A 815(0)	A 49(0)	A 797(8)
A 45(1)	A 837(8)	B 45(1)	B 821(8)	A 65(0)	A 838(7)
A 52(1)	A 875(7)	A 53(1)	B 880(6)	A 79(1)	A 845(20)
A 69(0)	A 883(16)	A 73(0)	A 887(0)	A 84(1)	A 863(1)
A 88(0)	A 884(2)	B 79(1)	B 887(33)	A 99(0)	A 869(2)
A 94(2)	A 906(2)	B 93(2)	A 902(2)	A 120(0)	A 886(3)
A 95(0)	A 936(1)	A 97(0)	A 948(4)	A 126(1)	A 927(10)
A 143(3)	A 945(5)	B 147(1)	B 950(5)	A 133(1)	A 979(0)
A 161(2)	A 1023(4)	A 150(0)	A 1024(1)	A 159(2)	A 1017(5)
A 166(2)	A 1028(2)	B 182(6)	B 1025(1)	A 171(1)	A 1022(6)
A 181(4)	A 1050(1)	A 191(1)	A 1038(2)	A 219(1)	A 1057(4)
A 284(2)	A 1103(14)	A 287(1)	A 1105(12)	A 261(7)	A 1064(2)
A 313(5)	A 1110(1)	B 319(7)	B 1108(2)	A 292(11)	A 1114(5)
A 331(0)	A 1169(1)	A 334(2)	B 1175(4)	A 312(2)	A 1155(4)
A 338(4)	A 1185(7)	B 338(6)	A 1184(4)	A 367(6)	A 1191(0)
A 354(8)	A 1208(1)	B 367(4)	B 1213(1)	A 391(5)	A 1202(11)
A 376(13)	A 1243(1)	A 377(1)	B 1241(1)	A 404(16)	A 1251(6)
A 399(1)	A 1270(3)	B 393(0)	A 1271(1)	A 421(1)	A 1261(0)
A 412(1)	A 1330(3)	A 404(3)	A 1318(0)	A 434(2)	A 1331(4)
A 423(2)	A 1372(12)	A 428(2)	B 1368(13)	A 449(4)	A 1368(4)
A 461(2)	A 1404(1)	B 470(2)	A 1399(0)	A 452(1)	A 1381(1)
A 470(3)	A 1421(4)	B 471(1)	B 1413(5)	A 472(1)	A 1413(3)
A 473(1)	A 1443(9)	A 473(0)	A 1420(6)	A 476(1)	A 1425(15)
A 480(10)	A 1478(2)	B 483(18)	B 1471(8)	A 479(6)	A 1435(3)
A 496(18)	A 1484(2)	B 494(2)	B 1486(4)	A 485(6)	A 1470(1)
A 500(19)	A 1508(1)	A 503(1)	A 1492(3)	A 508(1)	A 1518(7)
A 512(3)	A 1542(9)	B 511(14)	A 1538(5)	A 517(1)	A 1529(57)
A 535(14)	A 1554(5)	A 528(16)	A 1552(4)	A 530(32)	A 1587(54)
A 541(19)	A 1569(8)	B 539(24)	B 1575(7)	A 544(14)	A 1637(27)
A 547(24)	A 2020(721)	A 547(4)	A 2021(5)	A 552(51)	A 1798(278)
A 561(45)	A 2024(760)	B 567(43)	B 2022(1313)	A 563(4)	A 2032(1437)
A 567(22)	A 2054(3648)	A 570(17)	B 2057(3435)	A 585(20)	A 2056(788)
A 579(17)	A 2076(35)	B 597(18)	A 2075(29)	A 600(1)	A 2096(1149)
A 596(31)	A 3192(1)	A 599(35)	A 3190(2)	A 626(2)	A 3157(3)
A 632(1)	A 3195(1)	A 626(0)	B 3191(0)	A 632(50)	A 3174(9)
A 647(24)	A 3202(5)	A 647(7)	B 3201(10)	A 667(2)	A 3175(7)
A 651(54)	A 3205(2)	B 650(62)	A 3201(1)	A 680(15)	A 3189(7)
A 656(13)	A 3213(8)	B 660(4)	B 3214(3)	A 688(7)	A 3191(11)
A 681(2)	A 3214(3)	A 678(1)	A 3215(5)	A 709(8)	A 3205(10)
A 705(4)	A 3223(1)	B 709(3)	B 3223(1)	A 758(19)	A 3232(1)
A 771(25)	A 3242(5)	B 768(34)	A 3242(6)	A 772(15)	A 3244(3)

Table S77. Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses, in km/mol) for the structure **Fe39-1**，**Fe39-2**，**Fe39-3** of $C_{12}H_8Fe_3CO_9$ using M06-L.

Fe39-1		Fe39-2		Fe39-3	
A 23(0)	A 585(29)	A 13(18)	A 608(97)	A 26(0)	A 596(194)
A 28(1)	A 602(79)	A 31(5)	A 613(44)	A 34(0)	A 602(36)
A 39(5)	A 607(63)	A 33(0)	A 617(111)	A 36(0)	A 609(23)
A 44(1)	A 615(50)	A 48(4)	A 623(84)	A 42(1)	A 622(114)
A 48(2)	A 617(72)	A 52(14)	A 629(16)	A 50(1)	A 629(47)
A 55(0)	A 624(96)	A 57(2)	A 644(7)	A 53(0)	A 639(40)
A 60(0)	A 654(14)	A 62(3)	A 659(4)	A 59(0)	A 681(1)
A 68(1)	A 692(6)	A 71(0)	A 690(4)	A 62(0)	A 700(0)
A 73(0)	A 712(8)	A 75(0)	A 714(5)	A 70(0)	A 710(2)
A 77(0)	A 724(31)	A 77(1)	A 740(12)	A 72(0)	A 747(55)
A 80(1)	A 783(4)	A 80(2)	A 784(7)	A 75(0)	A 790(2)
A 83(0)	A 795(8)	A 86(2)	A 800(5)	A 79(0)	A 809(17)
A 86(1)	A 833(1)	A 88(0)	A 825(15)	A 80(1)	A 837(11)
A 91(1)	A 843(0)	A 91(2)	A 844(9)	A 85(0)	A 845(6)
A 95(1)	A 856(6)	A 96(1)	A 864(18)	A 89(0)	A 854(4)
A 99(0)	A 884(2)	A 101(2)	A 882(9)	A 95(0)	A 857(25)
A 104(6)	A 894(12)	A 107(14)	A 889(8)	A 109(0)	A 860(7)
A 107(5)	A 901(3)	A 111(1)	A 910(1)	A 116(1)	A 896(2)
A 110(3)	A 919(17)	A 114(0)	A 942(2)	A 127(0)	A 930(17)
A 120(1)	A 925(32)	A 122(0)	A 954(1)	A 131(1)	A 959(1)
A 133(10)	A 1012(3)	A 127(0)	A 990(2)	A 143(1)	A 986(1)
A 139(2)	A 1019(0)	A 135(2)	A 1018(5)	A 157(4)	A 1017(1)
A 156(1)	A 1035(2)	A 164(10)	A 1034(3)	A 160(2)	A 1054(4)
A 184(23)	A 1052(2)	A 218(3)	A 1051(4)	A 172(0)	A 1078(1)
A 264(16)	A 1101(0)	A 246(2)	A 1089(1)	A 201(0)	A 1122(3)
A 305(48)	A 1124(7)	A 256(5)	A 1117(7)	A 261(5)	A 1171(7)
A 361(12)	A 1163(6)	A 295(11)	A 1145(3)	A 265(1)	A 1192(20)
A 369(18)	A 1192(7)	A 358(19)	A 1182(8)	A 313(3)	A 1208(2)
A 376(8)	A 1245(38)	A 372(8)	A 1200(4)	A 334(9)	A 1231(11)
A 384(0)	A 1252(6)	A 380(5)	A 1233(10)	A 371(6)	A 1252(12)
A 391(7)	A 1313(4)	A 388(4)	A 1273(8)	A 394(1)	A 1327(7)
A 395(6)	A 1352(26)	A 401(1)	A 1329(9)	A 398(4)	A 1373(46)
A 406(4)	A 1367(11)	A 409(4)	A 1339(15)	A 403(27)	A 1378(28)
A 432(5)	A 1378(10)	A 431(10)	A 1381(15)	A 409(2)	A 1405(9)
A 435(22)	A 1411(7)	A 434(15)	A 1405(14)	A 417(3)	A 1410(8)
A 440(40)	A 1436(25)	A 445(13)	A 1410(9)	A 432(2)	A 1437(75)
A 444(15)	A 1453(21)	A 448(11)	A 1430(8)	A 435(5)	A 1453(35)
A 448(10)	A 1485(17)	A 451(0)	A 1465(16)	A 443(5)	A 1502(48)
A 452(12)	A 1506(144)	A 452(13)	A 1489(12)	A 446(9)	A 1560(2)
A 463(4)	A 1550(53)	A 459(1)	A 1530(72)	A 449(3)	A 1575(44)
A 465(6)	A 1567(147)	A 463(8)	A 1561(44)	A 452(7)	A 1594(60)
A 472(4)	A 2001(545)	A 470(14)	A 2023(434)	A 453(8)	A 1829(273)
A 474(4)	A 2031(556)	A 480(9)	A 2037(586)	A 462(7)	A 2024(1369)
A 476(12)	A 2043(635)	A 483(1)	A 2052(641)	A 467(26)	A 2057(211)
A 478(18)	A 2049(627)	A 485(31)	A 2057(143)	A 472(14)	A 2061(1155)
A 483(15)	A 2075(1867)	A 492(10)	A 2070(108)	A 474(5)	A 2065(642)
A 484(1)	A 2085(1132)	A 494(13)	A 2079(1038)	A 476(16)	A 2070(550)
A 489(52)	A 2098(675)	A 497(5)	A 2081(1814)	A 482(10)	A 2073(2199)
A 491(54)	A 2100(1445)	A 513(15)	A 2106(1435)	A 490(12)	A 2107(2914)
A 494(1)	A 2142(727)	A 514(9)	A 2133(898)	A 494(18)	A 2127(275)
A 506(24)	A 3169(3)	A 521(30)	A 3155(9)	A 505(3)	A 3162(3)
A 517(14)	A 3176(8)	A 529(21)	A 3176(2)	A 508(7)	A 3172(4)
A 534(37)	A 3188(0)	A 545(31)	A 3185(6)	A 516(7)	A 3173(7)
A 542(58)	A 3190(5)	A 552(55)	A 3191(3)	A 542(15)	A 3181(5)
A 562(32)	A 3193(10)	A 563(22)	A 3197(14)	A 549(5)	A 3189(7)
A 570(21)	A 3214(2)	A 567(56)	A 3203(9)	A 558(61)	A 3204(5)
A 574(86)	A 3231(1)	A 573(43)	A 3218(5)	A 564(21)	A 3213(1)
A 578(60)	A 3247(1)	A 577(8)	A 3243(3)	A 572(78)	A 3224(2)
A 581(92)		A 591(27)		A 584(34)	

Table S78. Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses, in km/mol) for the structure **Fe38-1**，**Fe38-2**，**Fe38-3** of $C_{12}H_8Fe_3CO_8$ using M06-L.

Fe38-1		Fe38-2		Fe38-3	
A 26(1)	A 614(93)	A 20(0)	A 612(146)	A 19(1)	A 620(63)
A 37(4)	A 619(83)	A 29(1)	A 618(63)	A 27(1)	A 622(25)
A 39(1)	A 628(65)	A 39(2)	A 624(17)	A 38(0)	A 633(34)
A 45(0)	A 630(102)	A 42(3)	A 633(56)	A 46(1)	A 641(30)
A 49(1)	A 655(7)	A 48(0)	A 655(4)	A 48(1)	A 656(21)
A 64(0)	A 686(1)	A 64(0)	A 688(1)	A 59(0)	A 690(1)
A 69(0)	A 705(17)	A 69(0)	A 701(9)	A 67(1)	A 698(3)
A 73(1)	A 715(26)	A 74(1)	A 714(21)	A 70(1)	A 725(21)
A 74(0)	A 793(3)	A 74(0)	A 793(4)	A 74(0)	A 738(9)
A 78(1)	A 819(3)	A 80(1)	A 832(8)	A 82(0)	A 796(12)
A 82(0)	A 830(14)	A 85(0)	A 837(3)	A 87(1)	A 826(7)
A 89(1)	A 839(1)	A 93(1)	A 851(3)	A 92(0)	A 847(2)
A 97(0)	A 861(1)	A 97(0)	A 857(3)	A 98(1)	A 853(21)
A 100(2)	A 868(0)	A 102(0)	A 876(2)	A 101(0)	A 877(6)
A 110(1)	A 876(9)	A 112(3)	A 883(8)	A 104(0)	A 883(5)
A 113(10)	A 904(4)	A 114(11)	A 908(2)	A 111(1)	A 899(5)
A 125(17)	A 933(6)	A 123(0)	A 941(3)	A 119(1)	A 963(7)
A 139(0)	A 961(9)	A 132(4)	A 968(3)	A 134(0)	A 980(3)
A 154(2)	A 1017(1)	A 143(2)	A 1017(1)	A 149(4)	A 1020(6)
A 161(1)	A 1034(2)	A 166(1)	A 1038(3)	A 152(1)	A 1038(2)
A 199(1)	A 1049(0)	A 174(2)	A 1051(0)	A 178(1)	A 1054(1)
A 233(19)	A 1059(5)	A 195(15)	A 1061(4)	A 189(16)	A 1077(6)
A 242(20)	A 1111(1)	A 267(37)	A 1107(1)	A 197(0)	A 1115(0)
A 323(2)	A 1150(5)	A 316(4)	A 1149(3)	A 275(2)	A 1169(1)
A 359(30)	A 1182(9)	A 353(2)	A 1177(7)	A 315(15)	A 1194(3)
A 362(17)	A 1193(1)	A 363(13)	A 1193(1)	A 349(4)	A 1202(9)
A 373(25)	A 1245(26)	A 366(5)	A 1239(10)	A 356(9)	A 1250(6)
A 377(15)	A 1258(3)	A 379(37)	A 1260(1)	A 358(1)	A 1276(1)
A 389(5)	A 1317(3)	A 396(2)	A 1315(2)	A 373(21)	A 1326(3)
A 403(12)	A 1374(10)	A 401(11)	A 1374(5)	A 393(5)	A 1379(1)
A 427(2)	A 1385(4)	A 422(7)	A 1380(2)	A 407(14)	A 1391(4)
A 436(4)	A 1418(3)	A 438(36)	A 1420(2)	A 414(3)	A 1417(6)
A 438(2)	A 1444(3)	A 446(1)	A 1446(10)	A 425(12)	A 1436(8)
A 445(15)	A 1459(30)	A 449(15)	A 1452(16)	A 439(1)	A 1468(7)
A 448(38)	A 1483(14)	A 451(10)	A 1477(1)	A 444(4)	A 1483(8)
A 455(3)	A 1494(5)	A 458(1)	A 1494(3)	A 447(9)	A 1504(2)
A 460(8)	A 1520(19)	A 459(5)	A 1524(21)	A 458(23)	A 1533(7)
A 467(11)	A 1571(57)	A 468(4)	A 1566(16)	A 460(2)	A 1587(24)
A 469(5)	A 1579(43)	A 474(0)	A 1587(7)	A 471(2)	A 1621(55)
A 477(7)	A 1912(477)	A 476(6)	A 2019(69)	A 472(1)	A 2007(1174)
A 477(3)	A 2038(40)	A 481(1)	A 2037(45)	A 479(8)	A 2017(123)
A 482(1)	A 2044(649)	A 485(4)	A 2051(527)	A 485(3)	A 2033(426)
A 488(1)	A 2047(633)	A 492(3)	A 2053(595)	A 488(2)	A 2041(101)
A 493(50)	A 2057(1287)	A 496(32)	A 2059(1304)	A 494(11)	A 2058(672)
A 497(12)	A 2079(1407)	A 498(3)	A 2063(1651)	A 504(23)	A 2066(1243)
A 504(17)	A 2092(3002)	A 504(24)	A 2095(3247)	A 511(1)	A 2087(1927)
A 515(16)	A 2113(191)	A 512(43)	A 2115(123)	A 521(7)	A 2114(1135)
A 534(19)	A 3186(1)	A 529(13)	A 3180(2)	A 534(38)	A 2830(20)
A 541(76)	A 3187(2)	A 541(63)	A 3187(4)	A 546(28)	A 3183(3)
A 555(21)	A 3189(6)	A 551(32)	A 3191(3)	A 548(17)	A 3196(2)
A 561(41)	A 3202(2)	A 555(92)	A 3197(1)	A 550(23)	A 3198(3)
A 564(98)	A 3214(2)	A 562(48)	A 3210(5)	A 557(61)	A 3208(9)
A 574(28)	A 3218(3)	A 575(30)	A 3212(2)	A 582(17)	A 3225(2)
A 588(29)	A 3236(1)	A 583(4)	A 3239(1)	A 589(44)	A 3236(1)
A 593(46)	A 3255(0)	A 597(88)	A 3251(1)	A 602(45)	A 3252(1)
A 600(13)		A 604(61)		A 612(44)	