Binuclear Cyclooctatetraene-Iron Carbonyl Complexes: Examples of Fluxionality and Valence Tautomerism

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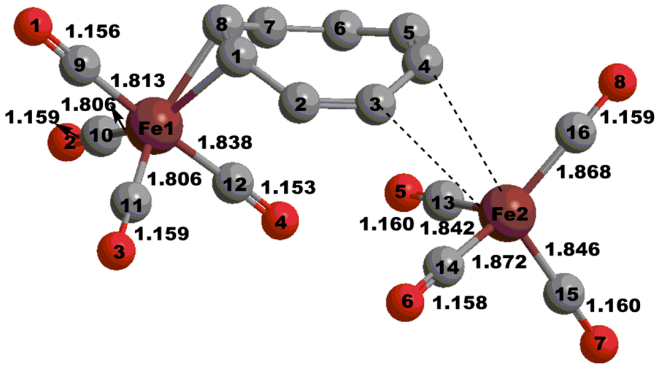
Supplementary Material

1. Complete Gaussian reference
2. Higher energy optimized $C_8H_8Fe_2(CO)_n$ structures(Figures S1);
3. Energies, relative energies, and iron-iron distances for the $(C_8H_8)Fe_2(CO)_n$ (n = 8, 7, 6, 5, 4, 3) structures by the M06L, B3LYP and BP86 methods(Table S1);
4. Complete tables of iron-carbon and carbon-carbon distances (in Å) for the $(C_8H_8)Fe_2(CO)_n$ (n = 8, 7, 6, 5, 4, 3) structures by the M06L, B3LYP and BP86 methods(Table S2);
5. Coordinates of the optimized $(C_8H_8)Fe_2(CO)_n$ (n = 8, 7, 6, 5, 4, 3) structures (Table S3) by the M06L method;
6. Harmonic vibrational frequencies of the $(C_8H_8)Fe_2(CO)_n$ (n = 8, 7, 6, 5, 4, 3) structures (Table S4) by the M06Lmethod.

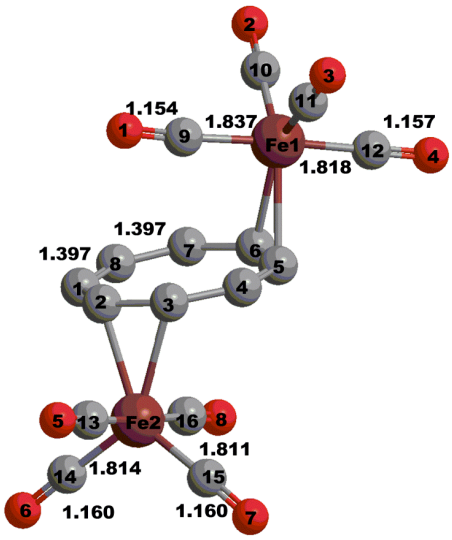
1. Complete Gaussian reference (reference 28).

Gaussian 09, Revision A.1, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2009.

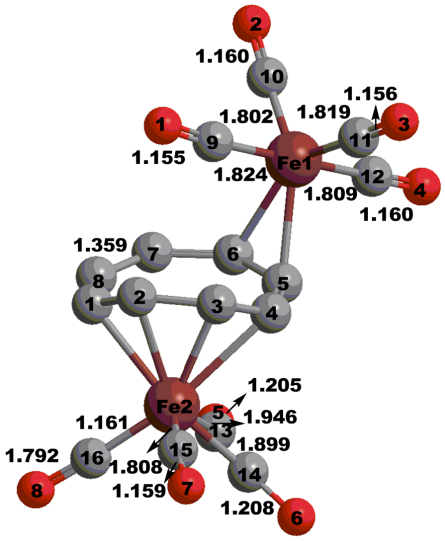
Figures S1: Higher energy optimized $C_8H_8Fe_2(CO)_n$ (n=8, 7, 6, 5, 3) structures



8-cis-T(C_1,13.7)



8-trans-T(C_2,14.8)



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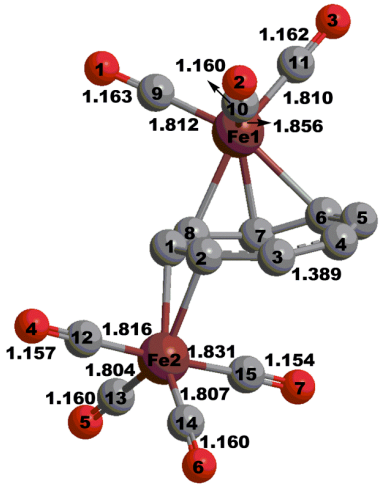

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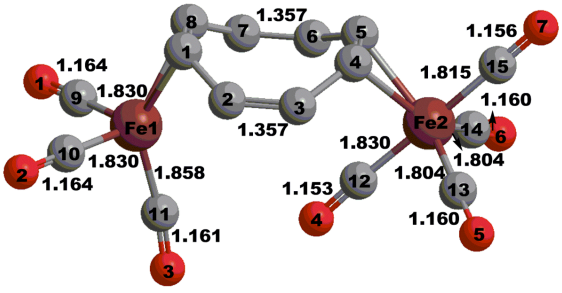

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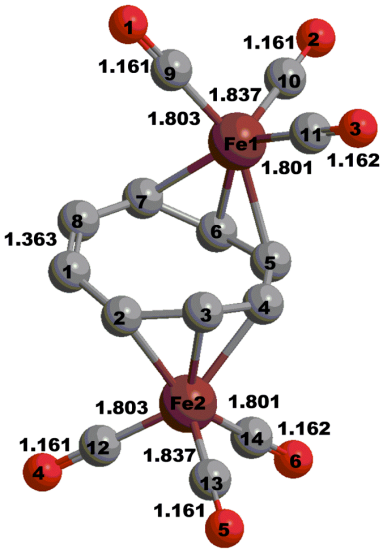
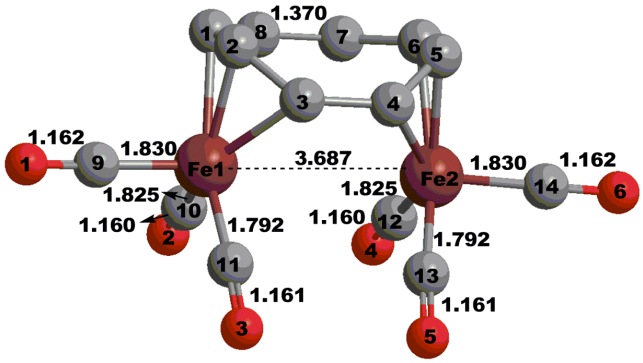


6-trans-T(C_2,14.8)



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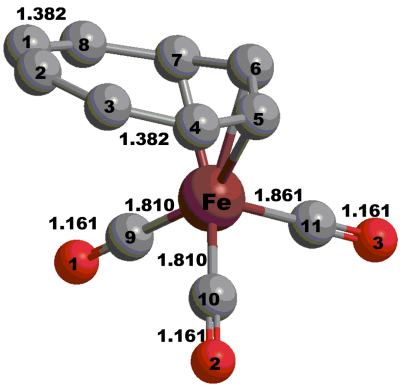
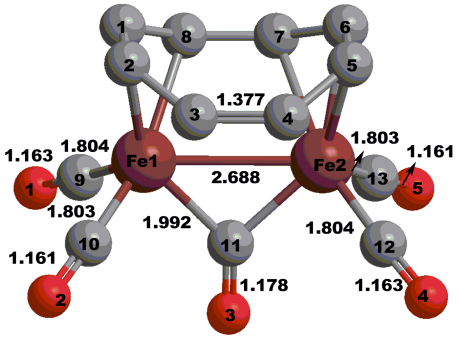
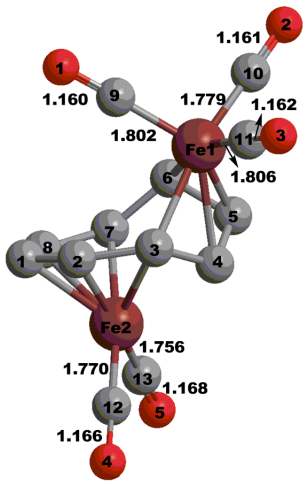


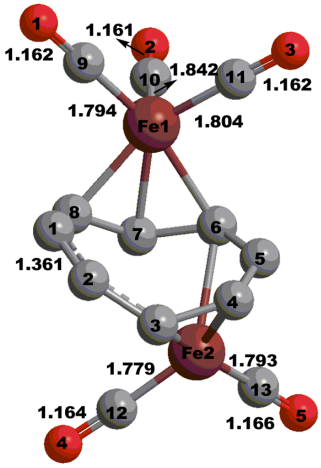
$C_8H_8Fe(CO)_3$-T(C_s,20.9)



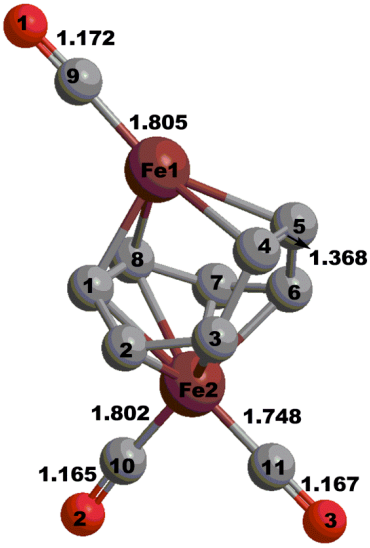
5-cis-T (C2v, 20.9)



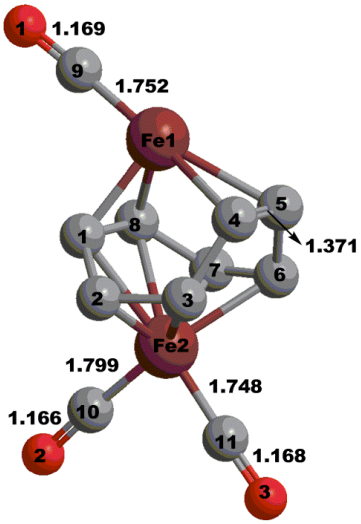
5-trans-S (C1, 21.2)



5-trans-T (C1, 20.9)



3-trans-T(C_1,28.4)



3-trans-S(C_1,42.0)

Table S1. Energies, relative energies, and metal-metal distances for the $(C_8H_8)Fe_2(CO)_n$ (n = 8,7,6,5,4,3) the M06L, B3LYP and BP86 method.

	$C_8H_8Fe(CO)_3$-S(C_{2v})			$C_8H_8Fe(CO)_3$-T(C_s)		
	M06L	B3LYP	BP86	M06L	B3LYP	BP86
–E	1913.38970	1913.49619	1913.74339	1913.35305	1913.46922	1913.70095
ZPE	0.16073	0.16097	0.15638	0.15736	0.15755	0.15379
ΔE	0.00	0.00	0.00	23.00	16.92	26.63
ΔE(ZPE)	0.00	0.00	0.00	20.88	14.78	25.01
$\langle S^2 \rangle$	---	---	---	2.1	2.1	2.0

	8-cis-S(C_{2v})			8-trans-S(C_1)		
	M06L	B3LYP	BP86	M06L	B3LYP	BP86
Fe_1-Fe_2	6.427	6.496	6.478	---	---	---
–E	3743.85752	3744.05559	3744.55795	3743.78753	3743.96477	3744.48986
ZPE	0.20208	0.20330	0.19764	0.20349	0.20399	0.19819
ΔE	0.00	0.00	0.00	43.92	56.99	42.73
ΔE(ZPE)	0.00	0.00	0.00	44.80	57.42	43.07
	8-cis-T(C_1)			8-trans-T(C_2)		
	M06L	B3LYP	BP86	M06L	B3LYP	BP86
Fe_1-Fe_2	6.478	6.807	7.463	---	---	---
–E	3743.83365	3744.03832	3744.51716	3743.83184	3744.02682	3744.52616
ZPE	0.20003	0.19949	0.19496	0.19998	0.20030	0.19573
ΔE	14.98	10.84	25.60	16.11	18.05	19.95
ΔE(ZPE)	13.69	8.45	23.91	14.80	16.17	18.75
$\langle S^2 \rangle$	2.1	2.0	2.0	2.1	2.1	2.1

	7-cis-S(C_1)			7-trans-S(C_1)		
	M06L	B3LYP	BP86	M06L	B3LYP	BP86
Fe_1-Fe_2	4.755	4.859	4.832	---	---	---
–E	3630.51570	3630.69799	3631.19999	3630.53084	3630.71278	3631.21538
ZPE	0.19531	0.19601	0.19072	0.19569	0.19642	0.19108
ΔE	9.50	9.28	9.66	0.00	0.00	0.00
ΔE(ZPE)	9.26	9.02	9.43	0.00	0.00	0.00
	7-cis-T(C_s)			7-trans-T(C_1)		
	M06L	B3LYP	BP86	M06L	B3LYP	BP86
Fe_1-Fe_2	5.623	5.871	5.871	---	---	---
–E	3630.49296	3630.68833	3631.16960	3630.50270	3630.69171	3631.17970
ZPE	0.19167	0.19238	0.18744	0.19248	0.19264	0.18839
ΔE	23.77	15.34	28.73	17.66	13.22	22.39
ΔE(ZPE)	21.25	12.81	26.44	15.64	10.85	20.70
$\langle S^2 \rangle$	2.1	2.1	2.0	2.1	2.1	2.0

	6-cis-S(C_s)			6-trans-S(C_i)		
	M06L	B3LYP	BP86	M06L	B3LYP	BP86
Fe_1-Fe_2	2.990	3.084	3.041	---	---	---
–E	3517.17731	3517.34287	3517.84548	3517.19393	3517.36109	3517.86077
ZPE	0.18831	0.18876	0.18355	0.18838	0.18888	0.18377
ΔE	10.43	11.43	9.59	0.00	0.00	0.00
ΔE(ZPE)	10.39	11.36	9.46	0.00	0.00	0.00
	6-cis-T(C_s)			6-trans-T(C_2)		
	M06L	B3LYP	BP86	M06L	B3LYP	BP86
Fe_1-Fe_2	3.687	3.846	3.837	---	---	---
–E	3517.16277	3517.34255	3517.82393	3517.16731	3517.35151	3517.83089
ZPE	0.18506	0.18537	0.18080	0.18535	0.18574	0.18118
ΔE	19.55	11.63	23.12	16.70	6.01	18.75
ΔE(ZPE)	17.47	9.43	21.25	14.80	4.04	17.12
$\langle S^2 \rangle$	2.1	2.1	2.0	2.1	2.1	2.0

	5-cis-S(C_{2v})			5-cis-S′(C_{2v})			5-trans-S(C_1)		
	M06L	B3LYP	BP86	M06L	B3LYP	BP86	M06L	B3LYP	BP86
Fe_1-Fe_2	2.776	2.814	2.809	2.739	2.791	2.781	---	---	---
–E	3403.84635	3404.00699	3404.50246	3403.84331	3404.00107	3404.49862	3403.80500	3403.96595	3404.462423
ZPE	0.18037	0.18087	0.17605	0.17976	0.18014	0.17538	0.17848	0.17897	0.17415
ΔE	0.00	0.00	0.00	1.91	3.71	2.41	25.95	25.75	25.12
ΔE(ZPE)	0.00	0.00	0.00	24.76	24.56	23.93	21.23	16.53	24.57

	5-cis-T(C_{2v})			5-trans-T(C_1)		
	M06L	B3LYP	BP86	M06L	B3LYP	BP86
Fe_1-Fe_2	2.640	2.709	2.688	---	---	---
–E	3403.80908	3403.97687	3404.46019	3403.80969	3403.98919	3404.45430
ZPE	0.17694	0.17710	0.17293	0.17699	0.17754	0.17265
ΔE	23.39	18.90	26.52	23.00	11.17	30.22
ΔE(ZPE)	20.88	9.08	28.09	20.88	9.08	28.09
$\langle S^2 \rangle$	2.1	2.1	2.0	2.1	2.1	2.0

	4-cis-S(C_2)			4-trans-S(C_2)		
	M06L	B3LYP	BP86	M06L	B3LYP	BP86
Fe_1-Fe_2	2.635	2.632	2.635	---	---	---
–E	3290.44796	3290.59680	3291.084264	3290.42728	3290.57912	3291.06999
ZPE	0.17056	0.17040	0.16582	0.16975	0.16982	0.16531
ΔE	11.03	20.91	4.44	24.01	32.01	13.40
ΔE(ZPE)	11.73	21.40	4.80	24.20	32.13	13.43
	4-cis-T(C_2)			4-trans-T(C_2)		
	M06L	B3LYP	BP86	M06L	B3LYP	BP86
Fe_1-Fe_2	2.497	2.594	2.514	---	---	---
–E	3290.46554	3290.63013	3291.09134	3290.44561	3290.62633	3291.06672
ZPE	0.16944	0.16962	0.16525	0.16930	0.16995	0.16513
ΔE	0.00	0.00	0.00	12.51	2.38	15.45
ΔE(ZPE)	0.00	0.00	0.00	12.42	2.59	15.37
$\langle S^2 \rangle$	2.1	2.1	2.0	2.1	2.1	2.0

	3-cis-S(C_{2v})			3-trans-S(C_s)		
	M06L	B3LYP	BP86	M06L	B3LYP	BP86
Fe_1-Fe_2	2.243	2.231	2.249	---	---	---
–E	3177.07557	3177.21545	3177.70341	3177.01878	3177.17526	3177.65092
ZPE	0.16129	0.16132	0.15698	0.15831	0.15900	0.15392
ΔE	7.66	15.14	0.63	43.30	40.36	33.57
ΔE(ZPE)	8.26	16.20	1.11	42.03	39.96	32.13
	3-cis-T(C_s)			3-trans-T(C_s)		
	M06L	B3LYP	BP86	M06L	B3LYP	BP86
Fe_1-Fe_2	2.446	2.478	2.452	---	---	---
–E	3177.08778	3177.23958	3177.70442	3177.05593	3177.21175	3177.67042
ZPE	0.16033	0.159641	0.15622	0.15774	0.15799	0.15375
ΔE	0.00	0.00	0.00	19.99	17.46	21.34
ΔE(ZPE)	0.00	0.00	0.00	18.36	16.43	19.79
$\langle S^2 \rangle$	2.3	2.5	2.1	2.3	2.3	2.1

Table S2. Complete tables of metal-carbon, carbon-carbon distances (in Å) for the $(C_8H_8)Fe_2(CO)_n$ (n = 8,7,6,5,4,3) structures by the M06L, B3LYP and BP86 method;

Table S2-1. Iron-carbon and Carbon-carbon distances (in Å) for the $C_8H_8Fe(CO)_3$ structures

	$C_8H_8Fe(CO)_3$-S			$C_8H_8Fe(CO)_3$-T		
	M06L	B3LYP	BP86	M06L	B3LYP	BP86
Fe-C1	3.822	3.848	3.885	3.679	3.756	3.806
Fe-C2	3.822	3.848	3.885	3.931	4.020	4.080
Fe-C3	3.197	3.225	3.247	3.679	3.756	3.806
Fe-C4	2.202	2.218	2.249	3.021	3.071	3.093
Fe-C5	2.051	2.073	2.066	2.198	2.226	2.211
Fe-C6	2.051	2.073	2.066	2.105	2.122	2.097
Fe-C7	2.202	2.218	2.249	2.198	2.226	2.211
Fe-C8	3.197	3.225	3.247	3.021	3.071	3.093
C1-C2	1.426	1.438	1.435	1.413	1.420	1.426
C2-C3	1.366	1.367	1.383	1.413	1.420	1.426
C3-C4	1.447	1.461	1.456	1.382	1.387	1.395
C4-C5	1.438	1.441	1.450	1.447	1.457	1.461
C5-C6	1.413	1.415	1.426	1.421	1.423	1.435
C6-C7	1.438	1.441	1.450	1.421	1.423	1.435
C7-C8	1.447	1.461	1.456	1.447	1.457	1.461
C8-C1	1.366	1.367	1.383	1.382	1.387	1.395
Fe-C9	1.794	1.795	1.784	1.810	1.813	1.793
C9-O1	1.159	1.156	1.171	1.161	1.158	1.174
Fe-C10	1.792	1.798	1.781	1.810	1.813	1.793
C10-O2	1.161	1.158	1.175	1.161	1.158	1.174
Fe-C11	1.792	1.798	1.781	1.861	1.878	1.817
C11-O3	1.161	1.158	1.175	1.161	1.157	1.175

Table S2-2. Iron-carbon and Carbon-carbon distances (in Å) for the $C_8H_8Fe_2(CO)_8$ structures

	8-cis-S			8-trans-S			8-cis-T			8-trans-T		
	M06L	B3LYP	BP86	M06L	B3LYP	BP86	M06L	B3LYP	BP86	M06L	B3LYP	BP86
Fe1-C1	2.168	2.197	2.186	4.559	4.649	4.644	2.146	2.173	2.161	4.537	4.088	4.094
Fe1-C2	3.083	3.131	3.125	4.396	4.490	4.486	3.017	3.088	3.069	4.547	4.654	4.645
Fe1-C3	4.263	4.310	4.312	3.821	3.912	3.895	4.097	4.251	4.217	4.004	4.641	4.624
Fe1-C4	5.037	5.091	5.091	3.110	3.142	3.147	4.834	5.019	4.978	3.125	4.085	4.077
Fe1-C5	5.037	5.091	5.092	2.204	2.209	2.220	4.831	5.020	4.977	2.302	3.148	3.153
Fe1-C6	4.263	4.310	4.312	2.189	2.198	2.207	4.091	4.252	4.217	2.262	2.272	2.268
Fe1-C7	3.083	3.131	3.125	3.157	3.192	3.198	3.014	3.088	3.071	3.109	2.326	2.306
Fe1-C8	2.168	2.197	2.186	4.071	4.132	4.141	2.146	2.172	2.162	4.008	3.178	3.176
Fe2-C1	5.037	5.091	5.091	2.336	2.376	2.409	5.911	6.250	6.526	3.109	2.326	2.306
Fe2-C2	4.263	4.310	4.312	2.132	2.154	2.149	4.963	5.321	5.654	2.262	2.272	2.268
Fe2-C3	3.083	3.131	3.125	2.110	2.149	2.108	3.895	4.463	4.482	2.302	3.148	3.153
Fe2-C4	2.168	2.197	2.186	2.411	2.530	2.431	3.380	4.270	3.658	3.125	4.085	4.077
Fe2-C5	2.168	2.197	2.186	3.318	3.428	3.369	3.590	4.312	3.621	4.004	4.641	4.624
Fe2-C6	3.083	3.131	3.125	3.879	3.960	3.961	4.334	4.561	4.404	4.547	4.654	4.645
Fe2-C7	4.263	4.310	4.312	3.827	3.888	3.929	5.323	5.403	5.593	4.537	4.088	4.094
Fe2-C8	5.037	5.091	5.091	3.223	3.278	3.322	6.042	6.279	6.504	4.008	3.178	3.176
C1-C2	1.472	1.483	1.484	1.408	1.402	1.421	1.468	1.485	1.484	1.430	1.438	1.448
C2-C3	1.349	1.351	1.363	1.427	1.437	1.440	1.354	1.354	1.368	1.435	1.440	1.445
C3-C4	1.472	1.483	1.484	1.413	1.408	1.429	1.450	1.466	1.462	1.418	1.403	1.409
C4-C5	1.413	1.410	1.426	1.453	1.465	1.466	1.362	1.358	1.377	1.418	1.402	1.409
C5-C6	1.472	1.483	1.484	1.421	1.420	1.433	1.448	1.465	1.462	1.435	1.440	1.445
C6-C7	1.349	1.351	1.363	1.445	1.461	1.457	1.335	1.353	1.367	1.430	1.438	1.448
C7-C8	1.472	1.483	1.484	1.359	1.359	1.374	1.467	1.485	1.484	1.397	1.425	1.432
C8-C1	1.413	1.410	1.426	1.450	1.467	1.462	1.419	1.413	1.429	1.397	1.425	1.432

Table S2-3. Iron-carbon and Carbon-carbon distances (in Å) for the $C_8H_8Fe_2(CO)_7$ structures

	7-cis-S			7-trans-S			7-cis-T			7-trans-T		
	M06L	B3LYP	BP86	M06L	B3LYP	BP86	M06L	B3LYP	BP86	M06L	B3LYP	BP86
Fe1-C1	2.071	2.093	2.085	3.813	3.831	3.859	2.212	2.248	2.160	3.078	3.120	4.165
Fe1-C2	2.036	2.058	2.058	3.156	3.176	3.189	2.815	2.938	2.729	3.785	3.864	3.834
Fe1-C3	2.163	2.187	2.202	2.158	2.181	2.197	3.839	3.997	3.745	4.111	4.226	3.103
Fe1-C4	3.404	3.432	3.444	2.063	2.085	2.082	4.628	4.795	4.532	3.878	4.010	2.217
Fe1-C5	4.025	4.042	4.073	2.059	2.079	2.075	4.628	4.795	4.532	3.169	3.292	2.068
Fe1-C6	3.837	3.849	3.895	2.186	2.203	2.223	3.839	3.997	3.745	2.307	2.408	2.301
Fe1-C7	3.093	3.118	3.151	3.233	3.263	3.278	2.815	2.938	2.729	2.070	2.088	3.198
Fe1-C8	2.153	2.174	2.185	3.842	3.868	3.895	2.212	2.248	2.160	2.208	2.239	3.924
Fe2-C1	5.128	5.208	5.197	2.208	2.229	2.213	4.983	5.032	5.092	2.192	2.213	3.158
Fe2-C2	4.530	4.592	4.586	2.225	2.259	2.240	4.210	4.260	4.307	2.225	2.231	2.246
Fe2-C3	3.202	3.268	3.254	3.147	3.213	3.182	3.055	3.101	3.117	3.104	3.132	2.203
Fe2-C4	2.158	2.197	2.176	3.786	3.893	3.871	2.160	2.177	2.185	4.074	4.128	3.128
Fe2-C5	2.193	2.225	2.212	4.451	4.575	4.558	2.160	2.177	2.185	4.665	4.744	3.982
Fe2-C6	3.101	3.177	3.154	4.620	4.728	4.715	3.055	3.101	3.117	4.629	4.718	4.712
Fe2-C7	4.129	4.235	4.199	4.101	4.175	4.177	4.210	4.260	4.307	3.919	4.013	4.752
Fe2-C8	4.860	4.968	4.929	3.168	3.208	3.204	4.983	5.032	5.092	3.095	3.142	4.154
C1-C2	1.412	1.415	1.425	1.414	1.411	1.428	1.457	1.470	1.467	1.423	1.421	1.450
C2-C3	1.448	1.449	1.456	1.467	1.480	1.478	1.357	1.357	1.378	1.439	1.453	1.436
C3-C4	1.494	1.508	1.506	1.438	1.440	1.448	1.466	1.480	1.477	1.389	1.388	1.479
C4-C5	1.409	1.404	1.421	1.408	1.411	1.421	1.416	1.415	1.427	1.405	1.418	1.424
C5-C6	1.453	1.466	1.465	1.439	1.441	1.450	1.466	1.480	1.477	1.419	1.417	1.438
C6-C7	1.354	1.355	1.368	1.459	1.473	1.470	1.357	1.357	1.378	1.426	1.433	1.438
C7-C8	1.463	1.477	1.474	1.356	1.357	1.371	1.457	1.470	1.467	1.410	1.409	1.414
C8-C1	1.439	1.441	1.452	1.444	1.458	1.457	1.389	1.388	1.411	1.467	1.480	1.404

Table S2-4. Iron-carbon and Carbon-carbon distances (in Å) for the $C_8H_8Fe_2(CO)_6$ structures

	6-cis-S			6-trans-S			6-cis-T			6-trans-T		
	M06L	B3LYP	BP86	M06L	B3LYP	BP86	M06L	B3LYP	BP86	M06L	B3LYP	BP86
Fe1-C1	2.205	2.222	2.232	3.667	3.690	3.714	2.190	2.217	2.193	3.750	3.795	3.828
Fe1-C2	2.062	2.074	2.066	3.667	3.690	3.714	2.077	2.094	2.071	3.965	4.025	4.086
Fe1-C3	2.189	2.224	2.205	3.201	3.232	3.240	2.204	2.239	2.218	3.520	3.582	3.649
Fe1-C4	3.020	3.071	3.051	2.108	2.139	2.140	3.205	3.274	3.257	2.972	3.028	3.032
Fe1-C5	3.775	3.830	3.820	2.056	2.077	2.075	4.066	4.136	4.140	2.183	2.217	2.199
Fe1-C6	3.848	3.908	3.900	2.056	2.077	2.075	4.165	4.250	4.241	2.074	2.095	2.067
Fe1-C7	3.704	3.749	3.759	2.108	2.139	2.141	3.649	3.740	3.688	2.197	2.220	2.210
Fe1-C8	3.108	3.142	3.156	3.201	3.233	3.241	2.875	2.954	2.877	3.073	3.110	3.098
Fe2-C1	3.848	3.908	3.900	2.056	2.077	2.075	4.165	4.250	4.241	3.073	3.110	3.142
Fe2-C2	3.775	3.830	3.820	2.056	2.077	2.075	4.066	4.136	4.139	2.197	2.220	2.215
Fe2-C3	3.020	3.071	3.051	2.108	2.139	2.141	3.205	3.274	3.257	2.074	2.095	2.066
Fe2-C4	2.189	2.224	2.205	3.201	3.233	3.241	2.204	2.239	2.218	2.183	2.217	2.200
Fe2-C5	2.062	2.074	2.066	3.667	3.690	3.714	2.077	2.094	2.071	2.972	3.028	2.995
Fe2-C6	2.205	2.222	2.232	3.667	3.690	3.714	2.190	2.217	2.193	3.520	3.582	3.580
Fe2-C7	3.108	3.142	3.156	3.201	3.232	3.240	2.875	2.954	2.877	3.965	4.025	4.047
Fe2-C8	3.704	3.749	3.759	2.108	2.138	2.140	3.649	3.740	3.688	3.750	3.795	3.844
C1-C2	1.430	1.431	1.443	1.408	1.411	1.421	1.419	1.420	1.433	1.447	1.460	1.457
C2-C3	1.412	1.415	1.425	1.439	1.441	1.450	1.418	1.419	1.433	1.420	1.421	1.434
C3-C4	1.448	1.454	1.461	1.501	1.514	1.514	1.469	1.482	1.483	1.415	1.416	1.427
C4-C5	1.412	1.415	1.425	1.439	1.441	1.450	1.418	1.419	1.433	1.467	1.479	1.478
C5-C6	1.430	1.431	1.443	1.408	1.411	1.421	1.419	1.420	1.433	1.415	1.416	1.431
C6-C7	1.445	1.458	1.456	1.439	1.441	1.450	1.440	1.455	1.450	1.420	1.421	1.431
C7-C8	1.356	1.357	1.371	1.501	1.514	1.514	1.370	1.369	1.389	1.447	1.460	1.457
C8-C1	1.445	1.458	1.456	1.439	1.441	1.450	1.440	1.455	1.450	1.363	1.365	1.381

Table S2-5. Iron-carbon and Carbon-carbon distances (in Å) for the $C_8H_8Fe_2(CO)_5$ structures

	5-cis-S			5-cis-S′			5-trans-S			5-cis-T			5-trans-T		
	M06	B3LY	BP86	M06	B3LY	BP86	M06	B3LY	BP86	M06	B3LY	BP86	M06	B3LY	BP86
Fe1-C	2.105	2.125	2.11	2.131	2.137	2.14	3.840	3.852	3.87	2.100	2.106	2.10	2.892	2.956	2.91
Fe1-C	2.105	2.125	2.11	2.131	2.165	2.14	3.122	3.148	3.14	2.209	2.237	2.21	3.697	3.744	3.75
Fe1-C	2.214	2.254	2.23	2.436	2.549	2.48	2.144	2.173	2.15	2.749	2.879	2.78	4.106	4.140	4.17
Fe1-C	2.981	3.023	3.01	3.432	3.480	3.46	2.218	2.244	2.26	3.345	3.466	3.39	3.874	3.849	3.94
Fe1-C	3.746	3.780	3.77	3.859	3.894	3.89	1.999	2.020	2.02	3.741	3.789	3.77	3.115	3.120	3.15
Fe1-C	3.746	3.780	3.77	3.432	3.480	3.46	2.074	2.094	2.09	3.672	3.707	3.71	2.165	2.191	2.18
Fe1-C	2.981	3.023	3.01	2.436	2.549	2.48	3.216	3.249	3.24	2.919	2.957	2.96	2.129	2.126	2.15
Fe1-C	2.214	2.254	2.23	2.131	2.165	2.14	3.906	3.915	3.93	2.172	2.192	2.20	2.120	2.169	2.11
Fe2-C	3.746	3.780	3.77	3.859	3.894	3.89	2.128	2.152	2.14	3.672	3.707	3.71	3.544	3.636	3.53
Fe2-C	3.746	3.780	3.77	3.432	3.480	3.46	2.095	2.129	2.12	3.741	3.789	3.77	3.131	3.160	3.14
Fe2-C	2.981	3.023	3.01	2.436	2.549	2.48	2.233	2.282	2.25	3.345	3.466	3.39	2.177	2.204	2.21
Fe2-C	2.214	2.254	2.23	2.131	2.165	2.14	2.207	2.227	2.18	2.749	2.879	2.78	2.074	2.080	2.09
Fe2-C	2.105	2.125	2.11	2.131	2.137	2.14	2.954	2.947	2.95	2.209	2.237	2.21	2.095	2.123	2.10
Fe2-C	2.105	2.125	2.11	2.131	2.165	2.14	3.002	3.031	3.02	2.100	2.106	2.10	2.305	2.495	2.25
Fe2-C	2.214	2.254	2.23	2.436	2.549	2.48	2.218	2.288	2.25	2.172	2.192	2.20	2.448	2.763	2.33
Fe2-C	2.981	3.023	3.01	3.432	3.480	3.46	2.113	2.147	2.12	2.919	2.957	2.96	3.281	3.480	3.22
C1-C2	1.408	1.413	1.42	1.411	1.416	1.42	1.408	1.409	1.42	1.409	1.413	1.42	1.356	1.361	1.37
C2-C3	1.423	1.424	1.43	1.433	1.431	1.44	1.448	1.455	1.46	1.438	1.452	1.44	1.457	1.464	1.46
C3-C4	1.435	1.443	1.44	1.433	1.431	1.44	1.507	1.500	1.52	1.377	1.374	1.39	1.429	1.430	1.43
C4-C5	1.423	1.424	1.43	1.411	1.416	1.42	1.432	1.434	1.44	1.438	1.452	1.44	1.405	1.408	1.42
C5-C6	1.408	1.413	1.42	1.411	1.416	1.42	1.442	1.444	1.45	1.409	1.413	1.42	1.457	1.471	1.46
C6-C7	1.423	1.424	1.43	1.433	1.431	1.44	1.489	1.500	1.50	1.420	1.422	1.43	1.455	1.442	1.47
C7-C8	1.435	1.443	1.44	1.433	1.431	1.44	1.406	1.401	1.41	1.441	1.453	1.44	1.429	1.422	1.44
C8-C1	1.423	1.424	1.43	1.411	1.416	1.42	1.414	1.422	1.42	1.420	1.422	1.43	1.446	1.457	1.45

Table S2-6. Iron-carbon and Carbon-carbon distances (in Å) for the $C_8H_8Fe_2(CO)_4$ structures

	4-cis-S			4-trans-S			4-cis-T			4-trans-T		
	M06L	B3LYP	BP86	M06L	B3LYP	BP86	M06L	B3LYP	BP86	M06L	B3LYP	BP86
Fe1-C1	2.139	2.149	2.139	3.106	3.126	3.133	2.167	2.190	2.172	2.779	2.894	2.831
Fe1-C2	2.037	2.036	2.037	3.504	3.482	3.515	2.133	2.178	2.131	3.319	3.436	3.406
Fe1-C3	2.303	2.265	2.303	2.985	2.958	2.985	2.402	2.547	2.414	3.783	3.869	3.875
Fe1-C4	3.334	3.304	3.334	2.177	2.246	2.178	3.383	3.470	3.399	3.613	3.661	3.691
Fe1-C5	3.779	3.769	3.779	2.127	2.152	2.153	3.758	3.813	3.778	2.990	3.023	3.039
Fe1-C6	3.386	3.406	3.386	2.102	2.158	2.129	3.289	3.328	3.310	2.152	2.180	2.169
Fe1-C7	2.329	2.348	2.329	2.044	2.068	2.062	2.271	2.368	2.295	2.049	2.062	2.050
Fe1-C8	2.126	2.133	2.126	2.100	2.125	2.134	2.106	2.142	2.119	2.124	2.165	2.141
Fe2-C1	3.779	3.769	3.779	2.100	2.125	2.134	3.758	3.813	3.778	2.124	2.165	2.141
Fe2-C2	3.386	3.406	3.386	2.044	2.068	2.062	3.289	3.328	3.310	2.049	2.062	2.050
Fe2-C3	2.329	2.348	2.329	2.102	2.158	2.129	2.271	2.368	2.295	2.152	2.180	2.169
Fe2-C4	2.126	2.133	2.126	2.127	2.152	2.153	2.106	2.142	2.119	2.990	3.023	3.039
Fe2-C5	2.139	2.149	2.139	2.177	2.246	2.178	2.167	2.190	2.172	3.613	3.661	3.691
Fe2-C6	2.037	2.036	2.037	2.985	2.958	2.985	2.133	2.178	2.131	3.783	3.869	3.875
Fe2-C7	2.303	2.265	2.303	3.504	3.483	3.515	2.402	2.547	2.414	3.319	3.436	3.406
Fe2-C8	3.779	3.304	3.334	3.106	3.126	3.133	3.383	3.470	3.399	2.779	2.894	2.831
C1-C2	1.428	1.418	1.428	1.422	1.421	1.431	1.399	1.403	1.414	1.418	1.419	1.430
C2-C3	1.460	1.456	1.460	1.410	1.417	1.425	1.460	1.459	1.471	1.423	1.423	1.434
C3-C4	1.463	1.461	1.463	1.442	1.435	1.454	1.433	1.426	1.446	1.447	1.458	1.462
C4-C5	1.423	1.411	1.423	1.485	1.475	1.496	1.422	1.428	1.434	1.363	1.368	1.377
C5-C6	1.428	1.418	1.428	1.442	1.435	1.454	1.399	1.403	1.414	1.447	1.458	1.462
C6-C7	1.460	1.456	1.460	1.410	1.417	1.425	1.460	1.459	1.471	1.423	1.423	1.434
C7-C8	1.463	1.461	1.463	1.422	1.421	1.431	1.433	1.426	1.446	1.418	1.419	1.430
C8-C1	1.423	1.411	1.423	1.499	1.511	1.510	1.422	1.428	1.434	1.464	1.476	1.479

Table S2-7. Iron-carbon and Carbon-carbon distances (in Å) for the $C_8H_8Fe_2(CO)_3$ structures

	3-cis-S			3-trans-S			3-cis-T			3-trans-T		
	M06L	B3LYP	BP86	M06L	B3LYP	BP86	M06L	B3LYP	BP86	M06L	B3LYP	BP86
Fe1-C1	2.038	2.063	2.055	1.931	1.953	1.939	2.117	2.140	2.123	2.076	2.101	2.065
Fe1-C2	2.046	2.077	2.068	2.870	2.868	2.868	2.097	2.148	2.079	2.872	2.890	2.876
Fe1-C3	2.314	2.373	2.371	2.962	2.981	2.957	2.430	2.542	2.426	2.966	3.009	2.971
Fe1-C4	3.192	3.211	3.214	2.215	2.258	2.201	3.297	3.345	3.299	2.251	2.328	2.244
Fe1-C5	3.562	3.575	3.581	2.215	2.258	2.201	3.701	3.735	3.714	2.251	2.328	2.244
Fe1-C6	3.192	3.211	3.214	2.962	2.981	2.957	3.294	3.337	3.315	2.966	3.009	2.971
Fe1-C7	2.314	2.373	2.371	2.870	2.868	2.868	2.273	2.358	2.338	2.872	2.890	2.876
Fe1-C8	2.046	2.077	2.068	1.931	1.953	1.939	2.087	2.128	2.104	2.076	2.101	2.065
Fe2-C1	3.562	3.575	3.581	2.228	2.301	2.271	3.701	3.735	3.714	2.216	2.274	2.269
Fe2-C2	3.192	3.211	3.214	1.984	2.005	2.005	3.297	3.345	3.299	1.996	2.274	2.269
Fe2-C3	2.314	2.373	2.371	2.089	2.120	2.112	2.430	2.542	2.426	2.101	2.020	2.013
Fe2-C4	2.046	2.077	2.068	2.886	2.936	2.920	2.097	2.148	2.079	2.945	2.133	2.117
Fe2-C5	2.038	2.063	2.055	2.886	2.936	2.920	2.117	2.140	2.123	2.945	2.982	2.972
Fe2-C6	2.046	2.077	2.068	2.087	2.120	2.112	2.087	2.128	2.104	2.101	2.982	2.972
Fe2-C7	2.314	2.373	2.371	1.984	2.005	2.005	2.273	2.358	2.338	1.996	2.133	2.117
Fe2-C8	3.192	3.211	3.214	2.228	2.301	2.272	3.294	3.337	3.315	2.216	2.020	2.013
C1-C2	1.422	1.424	1.437	1.462	1.474	1.472	1.426	1.433	1.440	1.457	1.464	1.470
C2-C3	1.435	1.437	1.444	1.421	1.418	1.434	1.426	1.427	1.442	1.422	1.420	1.436
C3-C4	1.435	1.437	1.444	1.490	1.499	1.504	1.426	1.427	1.442	1.489	1.499	1.504
C4-C5	1.422	1.424	1.437	1.371	1.368	1.388	1.426	1.433	1.440	1.368	1.363	1.382
C5-C6	1.422	1.424	1.437	1.490	1.499	1.504	1.402	1.403	1.418	1.489	1.499	1.504
C6-C7	1.435	1.437	1.444	1.421	1.418	1.434	1.451	1.451	1.456	1.422	1.420	1.436
C7-C8	1.435	1.437	1.444	1.462	1.474	1.472	1.451	1.451	1.456	1.457	1.464	1.470
C8-C1	1.422	1.424	1.437	1.646	1.596	1.656	1.402	1.403	1.418	1.514	1.506	1.524

Table S3. Coordinates of the optimized $(C_8H_8)Fe_2(CO)_n$ (n = 8, 7, 6, 5, 4, 3) structures (Table S3) by the M06L method

$C_8H_8Fe(CO)_3$-S(C_{2v})				$C_8H_8Fe(CO)_3$-T(C_s)			
	x	y	z		x	y	z
6	-0.348606	-2.030537	1.611785	6	2.695361	0.265932	1.307882
6	-0.839565	-2.934035	0.712823	6	3.204276	0.100921	0.000000
6	-0.839565	-2.934035	-0.712823	6	2.695361	0.265932	-1.307882
6	0.519884	-0.876111	1.522617	6	1.509925	0.733649	1.843398
6	1.659384	-0.555496	0.706314	6	0.311490	1.319580	1.284106
1	-0.687390	-2.194967	2.635094	1	3.394466	-0.074275	2.071151
1	-1.424212	-3.737327	1.158880	1	4.216863	-0.302977	0.000000
1	-1.424212	-3.737327	-1.158880	1	3.394466	-0.074275	-2.071151
1	0.636281	-0.427421	2.510067	1	1.449126	0.642158	2.927656
1	2.524165	-0.115519	1.199752	1	-0.334572	1.728618	2.060351
6	-0.348606	-2.030537	-1.611785	6	1.509925	0.733649	-1.843398
1	-0.687390	-2.194967	-2.635094	1	1.449126	0.642158	-2.927656
6	0.519884	-0.876111	-1.522617	6	0.311490	1.319580	-1.284106
1	0.636281	-0.427421	-2.510067	1	-0.334572	1.728618	-2.060351
6	1.659384	-0.555496	-0.706314	6	0.000000	1.842386	0.000000
1	2.524165	-0.115519	-1.199752	1	-0.835798	2.539418	0.000000
6	0.386814	1.891988	1.303421	6	-0.791722	-1.335934	1.353623
6	0.386814	1.891988	-1.303421	6	-2.520712	0.331911	0.000000
8	0.519884	2.696487	2.130547	8	-0.834158	-2.111974	2.216190
8	0.519884	2.696487	-2.130547	8	-3.642617	0.630674	0.000000
26	0.181737	0.678816	0.000000	26	-0.719783	-0.135889	0.000000
6	-1.607143	0.537192	0.000000	6	-0.791722	-1.335934	-1.353623
8	-2.754197	0.373074	0.000000	8	-0.834158	-2.111974	-2.216190

8-cis-S(C_{2v})				8-trans-S(C_1)			
	x	y	z		x	y	z
6	0.706600	1.607769	1.240678	6	0.692106	-0.768437	-0.561022
6	-0.706600	1.607769	1.240678	6	1.104363	0.352734	-1.331267
6	-1.636372	0.674291	0.584785	6	0.596170	1.704210	-1.385302
6	1.636372	0.674291	0.584785	6	-0.265058	-0.967532	0.513771
6	1.636372	-0.674291	0.584785	6	-0.835044	-0.174992	1.535588
1	1.182754	2.153054	2.057598	1	0.859976	-1.711749	-1.079102
1	-1.182754	2.153054	2.057598	1	1.566469	0.073089	-2.275892
1	-2.517887	1.147105	0.148949	1	1.077394	2.301088	-2.158497
1	2.517887	1.147105	0.148949	1	-0.340622	-2.027642	0.758803
1	2.517887	-1.147105	0.148949	1	-1.062985	-0.699623	2.460515
6	-1.636372	-0.674291	0.584785	6	-0.427800	2.334895	-0.752793
1	-2.517887	-1.147105	0.148949	1	-0.643219	3.322704	-1.156959
6	-0.706600	-1.607769	1.240678	6	-1.304607	2.029758	0.361297
1	-1.182754	-2.153054	2.057598	1	-1.981559	2.865110	0.543372
6	0.706600	-1.607769	1.240678	6	-1.251031	1.189655	1.489665
1	1.182754	-2.153054	2.057598	1	-1.770980	1.543142	2.375948
26	0.000000	3.213680	-0.032844	26	2.700081	-0.131926	0.086333
6	1.519097	3.972102	-0.630829	6	3.067403	-1.229353	1.469206
6	0.000000	2.100905	-1.480609	6	3.352710	-1.351746	-1.095311
8	2.491513	4.471225	-1.023736	8	3.322496	-1.917185	2.367979
8	0.000000	1.458207	-2.439506	8	3.771388	-2.124846	-1.845648
6	1.519097	-3.972102	-0.630829	6	-3.600985	-0.615070	1.435446
6	-1.519097	3.972102	-0.630829	6	4.069751	0.970990	-0.308901
6	-1.519097	-3.972102	-0.630829	6	-3.661198	1.048969	-0.614634
8	-2.491513	4.471225	-1.023736	8	4.974692	1.658346	-0.542279
8	2.491513	-4.471225	-1.023736	8	-4.394497	-1.119947	2.112761
8	-2.491513	-4.471225	-1.023736	8	-4.434391	1.777978	-1.081677
26	0.000000	-3.213680	-0.032844	26	-2.448268	0.000572	0.186694
6	0.000000	-2.100905	-1.480609	6	-1.995203	-0.634819	-1.596062
8	0.000000	-1.458207	-2.439506	8	-1.479930	-0.404809	-2.660730
6	0.000000	-4.327013	1.398298	6	2.064486	1.142782	1.226033
6	0.000000	4.327013	1.398298	8	1.739498	1.974413	1.959154
8	0.000000	5.037437	2.311864	6	-2.734467	-1.587535	-0.813866
8	0.000000	-5.037437	2.311864	8	-3.184407	-2.708699	-0.809307

8-cis-T(C_1)				8-trans-T(C_2)			
	x	y	z		x	y	z
6	2.235591	1.730615	-0.068606	6	-0.927203	-0.656830	0.922827
6	2.172870	1.072065	-1.323903	6	-1.341940	0.671297	1.274374
6	1.063863	0.448582	-2.055643	6	-0.941858	1.987514	0.882742
6	1.213353	2.014656	0.944952	6	0.000000	-1.202901	0.000000
6	-0.113574	2.272889	0.857075	6	0.927207	-0.656864	-0.922810
1	3.102536	2.383750	0.051232	1	-1.262707	-1.402214	1.642737
1	2.999883	1.311674	-1.995708	1	-1.878146	0.692399	2.222421
1	1.404921	-0.328469	-2.741556	1	-1.506347	2.750889	1.418392
1	1.638513	2.116932	1.944568	1	0.000000	-2.292813	0.000000
1	-0.576641	2.551312	1.804491	1	1.262712	-1.402273	-1.642694
6	-0.259306	0.729806	-2.120431	6	0.000000	2.520920	0.000000
1	-0.802869	0.141067	-2.861465	1	0.000000	3.610080	0.000000
6	-1.091434	1.722587	-1.469478	6	0.941853	1.987483	-0.882830
1	-1.978009	1.971803	-2.057161	1	1.506335	2.750840	-1.418512
6	-1.031635	2.347560	-0.260674	6	1.341945	0.671252	-1.274405
1	-1.882796	2.999364	-0.055732	1	1.878150	0.692319	-2.222453
26	3.017381	-0.258398	0.132224	26	-2.954795	-0.186016	-0.060070
6	3.502816	-0.417366	1.864127	6	-3.462399	-1.655165	-0.989631
6	1.325441	-0.847026	0.542237	6	-3.726044	-0.840287	1.450799
8	3.815692	-0.513835	2.976314	8	-3.820734	-2.579087	-1.593371
8	0.282954	-1.251466	0.822936	8	-4.223000	-1.253363	2.410921
6	-2.353295	-1.592663	-0.929629	6	3.726049	-0.840344	-1.450778
6	3.352875	-1.788267	-0.766427	6	-4.222325	1.105452	-0.188011
6	-4.317435	1.351985	-0.288756	6	4.222341	1.105442	0.187981
8	3.568224	-2.767097	-1.349144	8	-5.051691	1.910044	-0.289366
8	-1.700831	-2.432019	-1.388045	8	4.223012	-1.253447	-2.410885
8	-4.853721	2.377616	-0.345059	8	5.051678	1.910059	0.289375
26	-3.455004	-0.298524	-0.144827	26	2.954797	-0.186017	0.060068
6	-4.873209	-1.366774	0.360087	6	2.103022	0.476155	1.546674
8	-5.759032	-2.036287	0.696428	8	1.628264	0.879287	2.518006
6	-2.680307	-0.123601	1.517368	6	-2.103025	0.476085	-1.546710
6	4.651858	0.397665	-0.298555	8	-1.628270	0.879173	-2.518061
8	5.686073	0.831129	-0.579858	6	3.462393	-1.655129	0.989703
8	-2.204130	-0.006007	2.568497	8	3.820723	-2.579021	1.593490

7-cis-S(C_1)				7-trans-S(C_1)			
	x	y	z		x	y	z
6	0.798725	0.124474	-1.370988	6	0.496629	0.604964	0.771816
6	1.252660	-1.202454	-1.238342	6	0.950540	-0.613809	1.327864
6	0.560546	-2.285733	-0.560982	6	0.450406	-1.957029	1.150463
6	-0.521177	0.757559	-1.071210	6	-0.520936	0.958627	-0.224089
6	-1.631590	0.481422	-1.957806	6	-1.006008	0.351400	-1.433501
1	1.261690	0.676792	-2.194005	1	0.682695	1.460980	1.420073
1	2.042261	-1.523444	-1.917377	1	1.474629	-0.498377	2.275363
1	1.201682	-3.064592	-0.148475	1	1.005891	-2.707588	1.710971
1	-0.363627	1.833417	-0.951639	1	-0.524348	2.045024	-0.332038
1	-2.086152	1.246132	-2.586106	1	-1.145364	0.990077	-2.304017
6	-0.770769	-2.471668	-0.401372	6	-0.655385	-2.415551	0.512613
1	-1.040787	-3.349237	0.186766	1	-0.865239	-3.468818	0.699807
6	-1.960408	-1.782691	-0.900694	6	-1.664781	-1.821679	-0.357867
1	-2.823164	-2.442648	-0.791147	1	-2.454261	-2.553660	-0.534907
6	-2.236226	-0.793711	-1.908608	6	-1.560930	-0.941787	-1.491426
1	-3.149233	-0.930800	-2.487092	1	-2.096044	-1.210328	-2.400250
26	2.402644	0.126864	0.072957	26	2.510231	0.131038	-0.047066
6	2.374224	1.867042	0.523208	6	2.700773	1.459884	-1.241585
6	1.344929	-0.260684	1.504799	6	3.187215	1.172073	1.276474
8	2.356196	2.988796	0.824396	8	2.837642	2.301783	-2.030852
8	0.803679	-0.502825	2.496287	8	3.618768	1.835375	2.121438
6	-4.126695	-0.085036	-0.003312	6	-3.143107	1.836628	-0.232876
6	3.667613	-0.893916	0.849618	6	3.923123	-0.969709	0.112820
6	-2.032746	-0.485932	1.572910	6	-4.139975	-0.535046	-0.383194
8	4.495956	-1.526322	1.363665	8	4.864438	-1.646690	0.189617
8	-5.274930	-0.249941	0.035913	8	-3.545666	2.919657	-0.345566
8	-1.954437	-0.962960	2.625615	8	-5.190505	-0.982409	-0.592131
26	-2.349703	0.168343	-0.078198	26	-2.520238	0.165935	-0.045094
6	-2.521598	1.907488	0.327843	6	-2.462496	0.032959	1.743216
8	-2.616228	3.032435	0.593675	8	-2.361903	-0.077070	2.893009
6	3.564230	0.471672	-1.276340	6	1.851991	-0.980619	-1.329522
8	4.316084	0.694818	-2.127926	8	1.494708	-1.708949	-2.153775

7-cis-T(C_s)				7-trans-T(C_1)			
	x	y	z		x	y	z
6	1.438149	-1.464150	0.707940	6	-0.530645	-1.715454	1.449262
6	1.438149	-1.464150	-0.707940	6	0.346260	-2.617553	0.861658
6	0.985333	-0.442489	-1.657172	6	1.311484	-2.555978	-0.157345
6	0.985333	-0.442489	1.657172	6	-0.784597	-0.306023	1.311196
6	1.144276	0.905489	1.651276	6	-0.380937	0.697595	0.386129
1	2.126154	-2.170946	1.176062	1	-1.121335	-2.149350	2.255974
1	2.126154	-2.170946	-1.176062	1	0.299078	-3.601830	1.326099
1	0.570274	-0.855935	-2.577438	1	1.897796	-3.469541	-0.246404
1	0.570274	-0.855935	2.577438	1	-1.168213	0.110048	2.242345
1	0.852205	1.407993	2.574303	1	-0.444347	1.704227	0.799635
6	1.144276	0.905489	-1.651276	6	1.683073	-1.582833	-1.121095
1	0.852205	1.407993	-2.574303	1	2.375172	-1.979620	-1.862763
6	1.796670	1.789768	-0.694635	6	1.137470	-0.328346	-1.525201
1	2.423990	2.549125	-1.160641	1	1.484692	-0.000369	-2.506149
6	1.796670	1.789768	0.694635	6	0.503862	0.690358	-0.783414
1	2.423990	2.549125	1.160641	1	0.395690	1.613590	-1.353431
26	-0.151434	-2.743851	0.000000	26	-2.463226	0.183017	-0.064884
6	-0.935294	-3.372882	1.498506	6	-2.955534	1.488432	1.098227
6	-1.291688	-1.312423	0.000000	6	-2.851018	1.239860	-1.474778
8	-1.444595	-3.778992	2.458261	8	-3.261058	2.323286	1.837968
8	-2.054342	-0.447499	0.000000	8	-3.109384	1.911837	-2.384630
6	0.031215	4.103366	1.357791	6	4.314582	-0.267154	-0.365604
6	-0.935294	-3.372882	-1.498506	6	-1.906663	-1.156167	-1.182824
6	0.031215	4.103366	-1.357791	6	2.394780	-0.044510	1.572484
8	-1.444595	-3.778992	-2.458261	8	-1.599926	-2.001418	-1.905919
8	0.036144	4.889400	2.216297	8	5.406442	-0.656600	-0.449184
8	0.036144	4.889400	-2.216297	8	2.316916	-0.229232	2.714606
26	-0.000325	2.876777	0.000000	26	2.612122	0.332947	-0.231757
6	-1.829743	2.550208	0.000000	6	2.946177	2.106478	-0.065521
8	-2.988527	2.484339	0.000000	6	-3.896496	-0.809206	0.409456
6	1.009488	-4.139382	0.000000	8	-4.834746	-1.429198	0.693546
8	1.753264	-5.024681	0.000000	8	3.134178	3.246425	0.066308

6-cis-S(C_s)				6-trans-S(C_i)			
	x	y	z		x	y	z
6	1.091013	-1.663723	1.671760	6	1.005145	-0.647445	1.608058
6	1.970746	-0.536603	1.662865	6	1.005630	0.759975	1.557674
6	2.824282	0.088023	0.678095	6	0.650815	1.412360	0.324717
6	0.126388	-2.069936	0.724212	6	0.649770	-1.386069	0.424805
6	0.126388	-2.069936	-0.724212	6	-0.650815	-1.412360	-0.324717
1	0.982680	-2.145496	2.641642	1	1.451151	-1.147526	2.465682
1	2.339570	-0.340375	2.670111	1	1.452116	1.319700	2.377355
1	3.584129	0.722578	1.131663	1	1.024952	2.439933	0.312629
1	-0.597672	-2.774221	1.131985	1	1.023236	-2.412114	0.486119
1	-0.597672	-2.774221	-1.131985	1	-1.024952	-2.439933	-0.312629
6	2.824282	0.088023	-0.678095	6	-0.649770	1.386069	-0.424805
1	3.584129	0.722578	-1.131663	1	-1.023236	2.412114	-0.486119
6	1.970746	-0.536603	-1.662865	6	-1.005145	0.647445	-1.608058
1	2.339570	-0.340375	-2.670111	1	-1.451151	1.147526	-2.465682
6	1.091013	-1.663723	-1.671760	6	-1.005630	-0.759975	-1.557674
1	0.982680	-2.145496	-2.641642	1	-1.452116	-1.319700	-2.377355
26	-0.172063	-0.042860	-1.495039	26	-2.194950	-0.001259	-0.061347
6	-0.340672	-0.067844	-3.256071	6	-3.433547	-1.296819	-0.213513
6	-1.957782	-0.094908	-1.401885	8	-4.218019	-2.147921	-0.300221
8	-0.428660	-0.046951	-4.415018	6	3.432527	-1.281235	0.304992
8	-3.116620	-0.136161	-1.463491	6	-3.432527	1.281235	-0.304992
6	-0.340672	-0.067844	3.256071	6	2.046345	-0.062228	-1.719652
6	0.169116	1.722981	-1.367979	8	-4.216391	2.124652	-0.451576
8	0.403578	2.856106	-1.462435	8	4.216391	-2.124652	0.451576
8	-0.428660	-0.046951	4.415018	8	1.937007	-0.103518	-2.874656
26	-0.172063	-0.042860	1.495039	26	2.194950	0.001259	0.061347
6	0.169116	1.722981	1.367979	6	3.433547	1.296819	0.213513
8	0.403578	2.856106	1.462435	8	4.218019	2.147921	0.300221
6	-1.957782	-0.094908	1.401885	6	-2.046345	0.062228	1.719652
8	-3.116620	-0.136161	1.463491	8	-1.937007	0.103518	2.874656

6-cis-T(C_s)				6-trans-T(C_2)			
	x	y	z		x	y	z
6	1.216387	-1.652328	1.656908	6	0.861630	-0.073649	-1.496458
6	2.030789	-0.491341	1.702527	6	1.166430	1.290305	-1.245655
6	2.471342	0.427799	0.684942	6	0.494608	2.309798	-0.469149
6	0.181300	-1.950080	0.734542	6	0.434669	-1.073572	-0.590628
6	0.181300	-1.950080	-0.734542	6	-0.434687	-1.073554	0.590782
1	1.205013	-2.238192	2.573329	1	1.241496	-0.460393	-2.439064
1	2.558725	-0.365133	2.646411	1	1.772346	1.725921	-2.038715
1	2.934310	1.314681	1.117167	1	0.836138	3.308636	-0.737326
1	-0.515024	-2.696525	1.114186	1	0.507105	-2.074998	-1.013179
1	-0.515024	-2.696525	-1.114186	1	-0.507119	-2.074961	1.013376
6	2.471342	0.427799	-0.684942	6	-0.494561	2.309820	0.469194
1	2.934310	1.314681	-1.117167	1	-0.836008	3.308677	0.737405
6	2.030789	-0.491341	-1.702527	6	-1.166487	1.290354	1.245647
1	2.558725	-0.365133	-2.646411	1	-1.772450	1.726002	2.038653
6	1.216387	-1.652328	-1.656908	6	-0.861706	-0.073594	1.496534
1	1.205013	-2.238192	-2.573329	1	-1.241626	-0.460294	2.439137
26	-0.113211	-0.068157	-1.843400	26	2.315372	-0.124439	-0.018790
6	-0.248482	-0.173568	-3.665588	6	2.555162	-1.321416	1.305455
6	-1.885985	-0.170977	-1.599732	6	3.655405	-0.738821	-1.115605
8	-0.322659	-0.228947	-4.823442	8	2.705602	-2.104646	2.150475
8	-3.041380	-0.256836	-1.517722	8	4.512863	-1.132028	-1.792363
6	-0.248482	-0.173568	3.665588	6	-2.555211	-1.321653	-1.305234
6	0.023421	1.747275	-1.716031	6	3.241845	1.229856	0.727867
8	0.117517	2.902853	-1.672378	6	-3.655549	-0.738491	1.115621
8	-0.322659	-0.228947	4.823442	8	3.832208	2.111695	1.198662
26	-0.113211	-0.068157	1.843400	8	-2.705689	-2.105024	-2.150118
6	0.023421	1.747275	1.716031	8	-4.513100	-1.131475	1.792390
8	0.117517	2.902853	1.672378	26	-2.315369	-0.124451	0.018792
6	-1.885985	-0.170977	1.599732	6	-3.241615	1.229819	-0.728203
8	-3.041380	-0.256836	1.517722	8	-3.831828	2.111644	-1.199212

5-cis-S(C_{2v})				5-cis-S′(C_{2v})				5-trans-S(C_1)			
	x	y	z		x	y	z		x	y	z
6	0.703823	1.730064	-1.950432	6	-0.501549	-1.062001	-1.235675	6	1.246530	1.321555	-1.717880
6	-0.703823	1.730064	-1.950432	6	0.137575	0.219247	-1.240735	6	0.000000	1.889615	-2.056577
6	-1.553494	0.717340	-1.424257	6	0.009410	1.178248	-0.085389	6	-1.246530	1.321555	-1.717880
6	1.553494	0.717340	-1.424257	6	-0.576310	-1.624601	0.089849	6	1.561657	0.000000	-1.263567
6	1.553494	-0.717340	-1.424257	6	0.744802	-1.693853	0.773441	6	1.246530	-1.321555	-1.717880
1	1.182736	2.679788	-2.175628	6	-0.760113	-1.559793	-2.166413	6	-1.561657	0.000000	-1.263567
1	-1.182736	2.679788	-2.175628	6	0.152755	0.735818	-2.199979	6	-1.246530	-1.321555	-1.717880
1	-2.539954	1.105199	-1.175233	6	-0.049020	2.177335	-0.519590	6	0.000000	-1.889615	-2.056577
1	2.539954	1.105199	-1.175233	26	-1.118509	-2.569480	0.173339	26	0.000000	-1.369355	0.009465
1	2.539954	-1.105199	-1.175233	6	1.173920	-2.690549	0.629181	6	1.256471	-2.275312	0.847013
6	-1.553494	-0.717340	-1.424257	6	0.706068	1.310090	1.176627	6	0.000000	0.000000	1.406455
1	-2.539954	-1.105199	-1.175233	8	0.881545	2.350211	1.443914	8	2.063416	-2.920056	1.383598
6	-0.703823	-1.730064	-1.950432	8	1.309516	0.384741	2.050009	8	0.000000	0.000000	2.591574
1	-1.182736	-2.679788	-2.175628	26	1.871286	0.800719	2.881396	26	0.000000	1.369355	0.009465
6	0.703823	-1.730064	-1.950432	6	1.404340	-1.005032	1.805924	6	-1.256471	2.275312	0.847013
1	1.182736	-2.679788	-2.175628	8	2.165022	-1.543885	2.368105	8	-2.063416	2.920056	1.383598
26	0.000000	-1.387894	0.003591	6	1.924051	0.036965	0.042517	6	-1.256471	-2.275312	0.847013
6	1.258875	-2.287869	0.852500	6	2.971571	-1.128819	-0.749001	6	1.256471	2.275312	0.847013
6	0.000000	0.000000	1.405720	8	3.687909	-1.899418	-1.256183	8	2.063416	2.920056	1.383598
8	2.067907	-2.925103	1.394139	8	-3.166340	-1.034603	-0.582324	8	-2.063416	-2.920056	1.383598
8	0.000000	0.000000	2.587807	1	3.076426	1.301240	-0.410051	1	2.088663	-2.009885	-1.719999
6	1.258875	2.287869	0.852500	1	-2.146110	0.261262	1.577429	1	2.532438	0.000000	-0.766152
6	-1.258875	-2.287869	0.852500	1	3.884225	2.086305	-0.712736	1	0.000000	-2.922662	-2.391896
8	-2.067907	-2.925103	1.394139	1	-4.061634	-1.726178	-0.844246	1	-2.088663	-2.009885	-1.719999
8	2.067907	2.925103	1.394139	1	-2.327617	0.362821	2.718470	1	-2.532438	0.000000	-0.766152
26	0.000000	1.387894	0.003591	1	-1.798886	0.029026	-0.175935	1	2.088663	2.009885	-1.719999
6	-1.258875	2.287869	0.852500	1	-2.619605	1.431215	-0.963999	1	0.000000	2.922662	-2.391896
8	-2.067907	2.925103	1.394139	1	-3.141624	2.346601	-1.452519	1	-2.088663	2.009885	-1.719999

5-cis-T(C_{2v})				5-trans-T(C_1)			
	x	y	z		xy		z
6	-2.036858	0.352451	1.725814	6	0.502164	1.197922	-1.044695
6	-1.753888	-1.027749	1.718626	6	-0.080490	-0.105052	-0.983241
6	-1.111896	-1.807922	0.720372	6	-0.094763	-1.018966	0.148411
6	-2.168409	1.339336	0.688589	6	0.316880	2.308973	-0.137615
6	-2.168409	1.339336	-0.688589	6	-0.592526	2.451732	0.857736
1	-2.292526	0.737925	2.710695	1	0.796777	1.497730	-2.050201
1	-1.804766	-1.502567	2.695748	1	-0.093074	-0.626327	-1.938696
1	-0.725356	-2.745871	1.115576	1	-0.086282	-2.063159	-0.160366
1	-2.265587	2.340004	1.108121	1	0.932870	3.178150	-0.362177
1	-2.265587	2.340004	-1.108121	1	-0.646778	3.449558	1.294191
6	-1.111896	-1.807922	-0.720372	6	-0.720038	-0.876899	1.457086
1	-0.725356	-2.745871	-1.115576	1	-0.746836	-1.794604	2.039336
6	-1.753888	-1.027749	-1.718626	6	-1.336326	0.246515	2.033429
1	-1.804766	-1.502567	-2.695748	1	-1.920359	0.022390	2.925655
6	-2.036858	0.352451	-1.725814	6	-1.557141	1.524777	1.434170
1	-2.292526	0.737925	-2.710695	1	-2.352420	2.062226	1.952670
26	0.087087	-0.099515	-1.320047	26	-2.224121	-0.138592	0.198740
6	0.654456	1.496982	-1.935670	6	-3.037482	0.872908	-1.018051
6	1.567055	0.084578	0.000000	8	-3.527744	1.548195	-1.830014
8	1.039941	2.497807	-2.381537	6	3.153579	1.112553	-0.150015
8	2.735135	0.235495	0.000000	6	-3.057898	-1.668446	-0.226433
6	0.654456	1.496982	1.935670	6	2.469775	-1.028775	1.329221
6	1.039778	-1.051807	-2.520357	8	-3.650860	-2.640311	-0.478640
8	1.640454	-1.653502	-3.313621	8	3.986169	1.921341	-0.193314
8	1.039941	2.497807	2.381537	8	2.843102	-1.615406	2.259812
26	0.087087	-0.099515	1.320047	26	1.863963	-0.134684	-0.115550
6	1.039778	-1.051807	2.520357	6	2.603985	-1.216237	-1.409922
8	1.640454	-1.653502	3.313621	8	3.107069	-1.892172	-2.208320

4-cis-S(C_2)				4-trans-S(C_2)			
	x	y	z		x	y	z
6	-0.261327	-1.809227	-2.006427	6	-1.741424	-0.597073	0.092331
6	1.035867	-1.361519	-1.689781	6	-0.742262	-0.019733	0.956719
6	1.502574	-0.147777	-1.034436	6	0.742262	0.019733	0.956719
6	-1.447854	-1.225944	-1.502614	6	-1.470762	-1.099258	-1.197626
6	-1.502574	0.147777	-1.034436	6	-0.206382	-0.720592	-1.726839
1	-0.331593	-2.827843	-2.381189	1	-2.708158	-0.759243	0.562252
1	1.795749	-2.137991	-1.775800	1	-1.089115	0.000489	1.988720
1	2.453418	-0.345504	-0.537829	1	1.089115	-0.000489	1.988720
1	-2.373422	-1.792354	-1.568399	1	-2.185079	-1.762034	-1.680235
1	-2.453418	0.345504	-0.537829	1	0.105922	-1.243750	-2.635587
6	1.447854	1.225944	-1.502614	6	1.741424	0.597073	0.092331
1	2.373422	1.792354	-1.568399	1	2.708158	0.759243	0.562252
6	0.261327	1.809227	-2.006427	6	1.470762	1.099258	-1.197626
1	0.331593	2.827843	-2.381189	1	2.185079	1.762034	-1.680235
6	-1.035867	1.361519	-1.689781	6	0.206382	0.720592	-1.726839
1	-1.795749	2.137991	-1.775800	1	-0.105922	1.243750	-2.635587
26	0.154321	1.287337	0.048720	26	0.024662	1.809554	0.059588
6	-0.354510	2.870960	0.644727	6	-0.456300	3.234118	-0.851676
6	1.035867	1.069669	1.565843	8	-0.754856	4.178954	-1.466457
8	-0.647654	3.915804	1.072867	6	0.456300	-3.234118	-0.851676
8	1.620883	0.963633	2.568713	6	0.262903	2.832740	1.502765
6	-1.035867	-1.069669	1.565843	8	0.456300	3.536643	2.411645
8	-1.620883	-0.963633	2.568713	8	0.754856	-4.178954	-1.466457
26	-0.154321	-1.287337	0.048720	26	-0.024662	-1.809554	0.059588
6	0.354510	-2.870960	0.644727	6	-0.262903	-2.832740	1.502765
8	0.647654	-3.915804	1.072867	8	-0.456300	-3.536643	2.411645

4-cis-T(C_2)				4-trans-T(C_2)			
	x	y	z		x	y	z
6	-0.591356	-1.796671	-2.013341	6	0.386544	1.652166	-1.204013
6	0.786133	-1.642714	-1.697320	6	0.189738	0.654606	-2.233798
6	1.462135	-0.489717	-1.181762	6	-0.189738	-0.654606	-2.233798
6	-1.587621	-0.897730	-1.619262	6	-0.029232	1.722902	0.154641
6	-1.462135	0.489717	-1.181762	6	0.029232	0.731408	1.167284
1	-0.912134	-2.783823	-2.334695	1	0.554063	2.640656	-1.628975
1	1.373832	-2.558141	-1.710971	1	0.355681	1.061570	-3.230079
1	2.391521	-0.794011	-0.698973	1	-0.355681	-1.061570	-3.230079
1	-2.608510	-1.273235	-1.630736	1	-0.114626	2.735129	0.549502
1	-2.391521	0.794011	-0.698973	1	-0.135152	1.129457	2.166525
6	1.587621	0.897730	-1.619262	6	-0.386544	-1.652166	-1.204013
1	2.608510	1.273235	-1.630736	1	-0.554063	-2.640656	-1.628975
6	0.591356	1.796671	-2.013341	6	0.029232	-1.722902	0.154641
1	0.912134	2.783823	-2.334695	1	0.114626	-2.735129	0.549502
6	-0.786133	1.642714	-1.697320	6	-0.029232	-0.731408	1.167284
1	-1.373832	2.558141	-1.710971	1	0.135152	-1.129457	2.166525
26	0.301493	1.211719	0.053378	26	-1.895314	-1.021850	0.194320
6	-0.370742	2.602700	0.950205	6	-2.890539	-0.538321	1.592558
6	1.459524	0.896405	1.360055	8	-3.539371	-0.252904	2.518062
8	-0.786133	3.508526	1.553941	6	2.890539	0.538321	1.592558
8	2.221385	0.699121	2.220573	6	-3.230989	-1.145820	-0.979507
6	-1.459524	-0.896405	1.360055	8	-4.096535	-1.226789	-1.754597
8	-2.221385	-0.699121	2.220573	8	3.539371	0.252904	2.518062
26	-0.301493	-1.211719	0.053378	26	1.895314	1.021850	0.194320
6	0.370742	-2.602700	0.950205	6	3.230989	1.145820	-0.979507
8	0.786133	-3.508526	1.553941	8	4.096535	1.226789	-1.754597

3-cis-S(C_{2v})				3-trans-S(C_s)			
	x	y	z		x	y	z
6	1.338389	-1.271651	-1.466702	6	-1.064279	-0.149474	0.822944
6	1.902960	0.000000	-1.761858	6	-1.064279	-0.149474	-0.822944
6	1.338389	1.271651	-1.466702	6	0.018482	0.271360	-1.710331
6	0.000000	-1.623101	-1.088133	6	0.018482	0.271360	1.710331
6	-1.338389	-1.271651	-1.466702	6	1.277189	-0.302090	1.385435
1	2.057792	-2.087429	-1.426608	1	-2.040903	0.240486	1.112661
1	2.963740	0.000000	-2.000708	1	-2.040903	0.240486	-1.112661
1	2.057792	2.087429	-1.426608	1	-0.181914	0.856045	-2.605471
1	0.000000	-2.614409	-0.632333	1	-0.181914	0.856045	2.605471
1	-2.057792	-2.087429	-1.426608	1	2.137279	-0.079973	2.016782
6	0.000000	1.623101	-1.088133	6	1.277189	-0.302090	-1.385435
1	0.000000	2.614409	-0.632333	1	2.137279	-0.079973	-2.016782
6	-1.338389	1.271651	-1.466702	6	1.277189	-1.617327	-0.685426
1	-2.057792	2.087429	-1.426608	1	1.412777	-2.547047	-1.254570
6	-1.902960	0.000000	-1.761858	6	1.277189	-1.617327	0.685426
1	-2.963740	0.000000	-2.000708	1	1.412777	-2.547047	1.254570
26	-1.121321	0.000000	0.120770	26	-0.812380	-1.878439	0.000000
6	-2.620309	0.000000	1.067671	6	2.110693	1.957045	0.000000
6	0.000000	0.000000	1.736119	6	-2.528633	-2.231022	0.000000
8	-3.587459	0.000000	1.723239	8	-3.681369	-2.424203	0.000000
8	0.000000	0.000000	2.911581	8	3.139674	2.509433	0.000000
26	1.121321	0.000000	0.120770	26	0.586804	1.100127	0.000000
6	2.620309	0.000000	1.067671	6	-0.286500	2.672986	0.000000
8	3.587459	0.000000	1.723239	8	-0.791534	3.723945	0.000000

3-cis-T(C_s)				3-trans-T(C_s)			
	x	y	z		x	y	z
6	1.805831	-1.025894	1.328101	6	-1.147585	0.081027	0.757212
6	1.832682	0.260963	1.883408	6	-1.147585	0.081027	-0.757212
6	1.193621	1.405823	1.322879	6	-0.039368	0.317644	-1.673770
6	1.378427	-1.422738	0.000000	6	-0.039368	0.317644	1.673770
6	1.805831	-1.025894	-1.328101	6	1.203988	-0.302708	1.370399
1	2.014431	-1.842341	2.018305	1	-2.099939	0.476994	1.107001
1	2.132004	0.338161	2.925471	1	-2.099939	0.476994	-1.107001
1	0.959256	2.183462	2.047017	1	-0.242329	0.841289	-2.605753
1	1.149043	-2.490454	0.000000	1	-0.242329	0.841289	2.605753
1	2.014431	-1.842341	-2.018305	1	2.030474	-0.115278	2.056390
6	0.742655	1.688095	0.000000	6	1.203988	-0.302708	-1.370399
1	0.069549	2.545032	0.000000	1	2.030474	-0.115278	-2.056390
6	1.193621	1.405823	-1.322879	6	1.203988	-1.624487	-0.683779
1	0.959256	2.183462	-2.047017	1	1.343033	-2.544344	-1.261815
6	1.832682	0.260963	-1.883408	6	1.203988	-1.624487	0.683779
1	2.132004	0.338161	-2.925471	1	1.343033	-2.544344	1.261815
26	-0.118587	-0.226452	-1.223142	26	-0.930222	-1.839392	0.000000
6	-1.172582	0.182745	-2.599602	6	2.221895	1.884194	0.000000
6	-1.623177	-0.446946	0.000000	6	-2.556089	-2.623167	0.000000
8	-1.864438	0.423048	-3.508874	8	-3.627297	-3.097510	0.000000
8	-2.791811	-0.650064	0.000000	8	3.294642	2.343635	0.000000
26	-0.118587	-0.226452	1.223142	26	0.621688	1.180179	0.000000
6	-1.172582	0.182745	2.599602	6	-0.076567	2.841868	0.000000
8	-1.864438	0.423048	3.508874	8	-0.445881	3.947269	0.000000

Table S4. Harmonic vibrational frequencies of the $(C_8H_8)Fe_2(CO)_n$ (n = 8, 7, 6, 5, 4, 3) structures (Table S4) by the M06Lmethod.

$C_8H_8Fe(CO)_3$-S(C_{2v})			$C_8H_8Fe(CO)_3$-T(C_s)		
43	72	74	13	53	66
82	92	95	67	80	84
128	166	264	107	120	186
268	327	328	257	306	313
389	391	397	316	338	377
457	459	485	391	426	449
498	499	544	459	470	506
567	597	615	524	545	566
634	713	717	590	676	732
746	802	822	736	746	772
872	872	905	827	870	878
936	939	963	916	918	947
980	1001	1010	949	962	984
1151	1202	1273	1187	1198	1280
1316	1334	1393	1307	1327	1368
1435	1462	1504	1402	1453	1463
1509	1537	1625	1503	1529	1557
1672	2044	2057	1592	2033	2044
2107	3121	3122	2096	3133	3138
3139	3143	3154	3140	3150	3151
3159	3169	3174	3164	3166	3172

8-cis-S(C_{2v})			8-trans-S(C_1)			8-cis-T(C_1)			8-trans-T(C_2)		
26	31	34	23	28	30	18	25	28	23	27	30
39	55	56	43	51	60	31	38	42	43	51	52
60	65	70	67	71	78	55	59	61	61	63	72
86	87	89	84	87	95	68	71	76	84	86	86
90	97	100	99	106	115	79	84	88	89	93	93
110	118	145	120	127	141	89	91	106	99	105	110
154	166	166	166	205	221	121	131	154	114	118	160
257	262	269	249	302	309	165	280	284	202	293	317
344	374	384	317	327	343	306	320	324	322	322	358
386	402	404	381	392	402	327	343	348	359	369	369
422	427	435	421	426	432	387	397	407	393	394	414
438	448	452	440	447	456	411	418	422	417	434	436
468	469	471	461	477	481	436	455	461	443	444	460
479	482	489	483	507	517	464	478	485	460	471	472
513	516	562	534	548	555	496	499	501	490	492	545
563	597	598	560	587	591	510	522	527	547	564	570
620	639	644	613	627	632	560	590	631	570	608	613
649	650	658	643	713	732	643	645	687	618	625	697
702	703	790	761	767	831	690	725	773	732	737	745
802	804	868	845	858	867	806	835	873	746	810	847
871	884	921	872	920	934	880	909	940	851	877	879
947	984	989	956	969	998	974	983	993	906	933	947
1016	1095	1200	1003	1154	1211	996	1111	1225	984	1184	1190
1220	1251	1274	1295	1323	1341	1276	1306	1308	1315	1324	1327
1351	1393	1417	1397	1433	1459	1380	1426	1439	1403	1450	1455
1449	1527	1531	1496	1536	1538	1483	1534	1655	1467	1509	1512
1688	1691	2047	1548	1666	1778	1682	1686	2039	1537	1546	2048
2049	2065	2066	1898	2053	2055	2040	2048	2060	2050	2065	2065
2069	2087	2131	2072	2076	2092	2077	2088	2121	2075	2077	2117
2149	3118	3118	2135	3133	3134	2144	3112	3116	2132	3131	3136
3125	3127	3133	3147	3152	3164	3123	3129	3131	3136	3148	3148
3136	3148	3151	3170	3175	3187	3141	3149	3156	3160	3163	3169

7-cis-S(C_1)			7-trans-S(C_1)			7-cis-T(C_s)			7-trans-T(C_1)		
18	29	41	29	31	43	13	32	37	29	29	37
48	60	62	52	56	67	42	53	60	47	57	64
75	83	84	73	77	81	61	63	69	66	69	76
87	91	96	86	90	99	78	86	87	83	86	87
105	116	134	107	114	118	93	96	110	95	96	109
142	161	208	140	143	181	122	125	156	114	124	131
254	292	325	274	287	308	167	252	268	192	259	290
340	349	386	338	360	380	281	317	322	318	325	346
401	402	420	392	398	405	346	366	375	349	378	383
429	433	447	425	433	442	384	397	399	386	402	413
449	462	464	453	458	461	419	430	435	420	429	446
470	478	488	467	480	482	436	450	462	452	456	468
499	504	519	487	500	502	468	477	493	473	478	492
552	562	573	546	561	570	499	520	528	518	523	553
600	608	615	595	607	616	539	560	592	556	562	583
639	646	656	622	641	649	631	635	643	601	624	637
683	740	761	700	730	768	659	699	714	693	726	739
783	839	856	782	838	852	780	796	811	748	805	825
877	895	928	879	882	934	861	869	913	855	864	888
941	971	979	943	966	971	916	949	968	918	934	954
1006	1057	1121	1004	1019	1145	976	981	1097	961	989	1171
1154	1237	1248	1184	1262	1308	1203	1243	1262	1199	1300	1317
1306	1368	1388	1324	1389	1420	1287	1363	1406	1324	1396	1438
1422	1450	1489	1455	1481	1495	1429	1466	1530	1442	1460	1509
1516	1542	1681	1538	1549	1674	1584	1646	1653	1532	1556	1565
2045	2051	2056	2044	2049	2056	2014	2023	2056	2030	2034	2054
2063	2080	2108	2062	2067	2103	2072	2078	2086	2071	2078	2089
2141	3085	3097	2131	3114	3120	2143	3116	3128	2133	3128	3133
3116	3137	3145	3139	3142	3154	3131	3134	3145	3137	3146	3147
3147	3160	3162	3157	3168	3171	3151	3153	3164	3156	3161	3172

6-cis-S(C_s)			6-trans-S(C_i)			6-cis-T(C_s)			6-trans-T(C_2)		
14i	44	59	32	52	53	16i	46	46	2i	14	43
59	69	82	61	73	77	56	56	69	45	65	67
89	90	99	77	81	86	75	85	87	69	71	73
101	115	135	100	101	110	90	97	99	87	89	94
159	167	169	156	173	173	102	126	162	112	126	130
183	254	270	313	365	370	169	241	257	152	269	270
303	323	359	380	384	410	301	330	332	304	312	321
371	393	403	419	420	430	335	341	365	335	354	362
434	443	450	441	463	464	406	410	418	400	404	414
458	482	486	467	473	483	422	430	438	415	439	440
495	498	501	484	510	511	443	444	478	466	468	475
527	527	554	517	524	563	492	499	527	485	496	534
558	581	589	576	606	607	528	556	557	540	552	562
597	613	620	622	624	626	564	566	586	563	578	600
644	704	739	642	663	789	645	712	727	624	723	724
744	780	860	810	813	835	753	794	839	759	773	825
874	897	901	874	886	930	851	865	898	864	869	909
936	942	952	937	957	989	919	923	943	918	928	947
968	993	1021	1016	1029	1048	944	980	997	963	985	1000
1178	1199	1308	1124	1127	1189	1160	1183	1280	1172	1193	1300
1318	1327	1398	1267	1274	1362	1295	1322	1383	1305	1334	1393
1443	1450	1505	1383	1418	1436	1421	1451	1490	1430	1454	1496
1520	1554	1560	1460	1476	1517	1516	1539	1549	1513	1540	1548
1676	2026	2029	1525	2049	2050	1626	2026	2029	1649	2034	2037
2047	2066	2070	2051	2052	2102	2039	2059	2074	2043	2045	2088
2118	3130	3132	2114	3085	3085	2110	3139	3141	2106	3141	3146
3142	3151	3151	3103	3105	3157	3151	3156	3158	3149	3157	3157
3160	3166	3173	3157	3173	3173	3166	3172	3176	3170	3174	3177

5-cis-S(C_{2v})			5-cis-S′(C_{2v})			5-trans-S(C_1)			5-cis-T(C_{2v})			5-trans-T(C_1)		
30	52	65	-44	4	66	40	51	58	25	41	56	21	42	49
72	86	87	67	73	88	66	76	80	59	62	75	55	66	71
90	98	105	92	92	107	83	92	101	75	84	100	73	82	90
118	159	202	118	119	211	111	168	180	101	134	136	93	118	136
250	263	278	247	253	255	187	225	286	194	196	244	142	177	245
312	329	338	274	310	341	295	334	374	267	292	305	304	316	326
350	383	415	356	394	416	390	409	418	335	355	356	337	351	366
417	428	446	429	452	468	436	452	460	377	402	402	397	411	417
452	473	500	478	485	501	470	475	478	424	426	438	451	452	466
502	508	516	502	514	526	491	507	510	450	462	465	473	483	485
534	549	582	538	541	571	540	551	557	482	486	530	497	525	539
592	609	629	579	596	639	580	595	613	536	550	570	542	566	585
635	647	708	654	659	691	623	642	675	580	611	721	608	622	674
750	806	827	780	813	831	758	794	824	738	745	785	730	778	815
845	874	894	842	872	884	837	851	875	839	853	878	827	860	894
895	927	932	887	916	935	897	933	947	906	906	932	898	913	935
952	952	1004	937	979	997	973	985	1021	943	957	965	956	975	990
1006	1164	1167	1009	1144	1164	1027	1108	1121	991	1171	1202	1002	1135	1171
1258	1306	1333	1237	1276	1310	1182	1256	1300	1299	1314	1342	1262	1266	1285
1383	1426	1466	1376	1411	1454	1326	1378	1393	1394	1439	1461	1372	1414	1430
1529	1533	1548	1517	1523	1536	1417	1451	1471	1522	1526	1563	1449	1482	1500
1556	1577	1906	1549	1563	1894	1536	1566	2014	1567	1606	1918	1539	1668	2022
2033	2039	2067	2032	2038	2063	2046	2052	2059	2028	2036	2054	2036	2043	2069
2095	3142	3143	2094	3134	3134	2108	3085	3111	2091	3142	3145	2102	3125	3140
3157	3159	3171	3165	3167	3169	3115	3150	3159	3155	3159	3164	3143	3148	3150
3173	3184	3186	3171	3197	3198	3161	3185	3194	3169	3177	3180	3163	3172	3182

4-cis-S(C_2)			4-trans-S(C_2)			4-cis-T(C_2)			4-trans-T(C_2)		
30	52	72	47	48	56	27	45	55	-26	-5	42
73	81	87	64	80	87	68	77	83	49	63	80
91	105	164	99	106	150	86	108	129	85	87	89
185	203	243	177	195	289	147	209	255	112	127	148
271	319	343	296	330	364	261	293	311	282	292	323
346	367	405	379	394	420	312	326	381	344	352	353
447	454	462	434	445	458	404	435	448	392	403	459
466	483	509	472	476	486	455	467	470	460	485	491
516	523	537	499	521	542	491	494	512	498	498	507
538	570	578	543	548	588	526	529	535	531	538	546
626	628	637	597	621	636	609	611	615	604	618	625
662	776	807	647	798	804	676	765	794	728	730	759
828	838	861	829	831	856	816	818	855	774	822	852
868	898	899	901	904	906	868	872	901	873	901	912
959	959	984	953	953	981	931	932	980	922	937	951
1009	1029	1123	989	1031	1103	999	1014	1129	978	989	1167
1139	1217	1249	1121	1169	1186	1163	1233	1268	1189	1291	1303
1274	1363	1395	1285	1325	1355	1296	1372	1400	1327	1386	1425
1429	1443	1484	1395	1420	1466	1446	1479	1495	1449	1490	1507
1494	1538	1542	1470	1513	1524	1517	1549	1560	1537	1540	1655
2009	2019	2038	2018	2019	2046	2016	2021	2040	2022	2024	2067
2080	3127	3127	2076	3089	3096	2084	3131	3131	2084	3138	3138
3143	3144	3169	3137	3147	3172	3162	3165	3168	3145	3153	3158
3170	3181	3182	3172	3190	3190	3170	3193	3194	3163	3171	3174

3-cis-S(C_{2v})			3-trans-S(C_s)			3-cis-T(C_s)			3-trans-T(C_s)		
53	60	70	-30	56	57	43	55	64	42	49	62
89	109	114	82	92	94	77	91	95	83	87	100
127	174	242	192	192	223	159	215	222	175	182	220
254	267	269	266	307	312	245	264	269	263	270	302
281	317	359	360	414	435	322	327	338	343	354	379
381	427	428	439	452	462	390	394	424	402	428	432
432	463	509	469	501	511	435	441	468	444	457	471
517	529	534	513	536	551	501	510	513	481	493	507
546	552	585	563	574	605	516	537	555	533	552	604
618	681	766	620	646	717	602	674	748	608	657	718
807	816	850	732	788	803	790	804	819	766	793	796
855	855	872	816	818	890	851	852	873	818	840	883
908	937	939	893	927	952	902	926	928	891	920	921
975	980	1009	963	971	1002	974	985	1017	948	954	981
1148	1153	1248	1035	1089	1118	1143	1159	1244	1035	1115	1122
1278	1305	1378	1118	1135	1256	1265	1303	1375	1144	1199	1300
1415	1451	1503	1285	1340	1344	1411	1446	1479	1307	1355	1357
1513	1526	1535	1383	1445	1454	1512	1533	1548	1403	1448	1459
1548	1942	2017	1592	2011	2018	1548	1880	2019	1601	2006	2015
2043	3126	3127	2063	3049	3073	2044	3113	3144	2067	3088	3109
3154	3157	3158	3119	3128	3148	3149	3153	3159	3138	3141	3142
3161	3179	3180	3148	3170	3170	3166	3185	3185	3149	3165	3166