Binuclear Iron Carbonyl Complexes of Thialene

Rong Jin,[a] Xiaohong Chen,[a] Quan Du,[a] Hao Feng,[a]*
Yaoming Xie,[b] R. Bruce King,*[b] and Henry F. Schaefer[b]
[a]*School of Physics and Chemistry, Research Center for Advanced Computation, Xihua University, Chengdu, China 610039*
[b]*Department of Chemistry and Center for Computational Chemistry University of Georgia, Athens, Georgia 30602, USA*
E-mail: Fenghao@mail.xhu.edu.cn; rbking@chem.uga.edu

Supporting Information

Table S1-S4: Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses, in km/mol) for the (thialene)$Fe_2(CO)_n$ (n = 6, 5) structures **6S-1, 6S-2**, **6S-3**, and **5S-1**

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Tables S19-S23: Cartesian coordinates and total energies for the (thialene)$Fe_2(CO)_4$ structures **4T-*n*** (n = 1-5)

Tables S24-S28: Cartesian coordinates and total energies for the (thialene)$Fe_2(CO)_4$ structures **4S-*n*** (n = 1-5)

Table S29: Total energies (E, in hartree), relative energies (E, in kcal mol-1), and Fe–Fe and S-Fe distances (in Å) for the (thialene)$Fe_2(CO)_6$ and (thialene)$Fe_2(CO)_5$ structures **6S-*n*** (n = 1-3) and **5S-1**

Table S30: Total energies (E, in hartree), relative energies (E, in kcal mol^{-1}), and Fe–Fe and S-Fe distances (in Å) for the (thialene)$Fe_2(CO)_4$ structures **4T-*n*** (n = 1-5)

Table S31: Total energies (E, in hartree), relative energies (E, in kcal mol-1), and Fe–Fe and S-Fe distances (in Å) for the (thialene)$Fe_2(CO)_4$ structures **4S-*n*** (n = 1-5)

Table S32: Harmonic ν(CO) vibrational frequencies (in cm^{-1}) predicted by the BP86 method for (thialene)$Fe_2(CO)_n$ (n = 6, 5) structures

Table S33: Harmonic ν(CO) vibrational frequencies (in cm^{-1}) predicted by the BP86 method for $(C_8H_6S)Fe_2(CO)_4$ structures

Figure S1: The (thialene)$Fe_2(CO)_6$ structures **6S-*n*** (n = 1 to 3)

Figure S2: The (thialene)$Fe_2(CO)_5$ structure **5S-1**

Figure S3: The triplet (thialene)$Fe_2(CO)_4$ structures **4T-*n*** (n = 1 to 5)

Figure S4: The singlet (thialene)$Fe_2(CO)_4$ structures **4S-*n*** (n = 1 to 5).

Complete Gaussian reference

Table S1. Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses, in km/mol) for the $(C_8H_6S)Fe_2(CO)_6$ structure **6S-1.**

	M06L		BP86		B3LYP	
1	26	(0)	24	(0)	26	(1)
2	38	(1)	35	(0)	38	(1)
3	48	(2)	45	(4)	47	(4)
4	52	(1)	49	(1)	52	(1)
5	71	(1)	68	(1)	71	(1)
6	72	(0)	74	(0)	76	(0)
7	76	(0)	78	(0)	81	(0)
8	77	(0)	79	(0)	82	(0)
9	77	(1)	81	(1)	83	(2)
10	90	(0)	92	(0)	96	(0)
11	96	(0)	99	(0)	103	(0)
12	101	(0)	102	(0)	105	(0)
13	124	(16)	119	(13)	125	(18)
14	148	(2)	142	(1)	146	(2)
15	168	(6)	156	(14)	164	(11)
16	210	(4)	201	(7)	207	(7)
17	324	(19)	308	(43)	308	(56)
18	335	(85)	319	(56)	324	(66)
19	354	(4)	341	(5)	348	(1)
20	368	(53)	357	(45)	362	(57)
21	383	(1)	383	(0)	382	(2)
22	392	(4)	385	(5)	391	(13)
23	408	(13)	392	(2)	401	(1)
24	414	(13)	409	(11)	410	(29)
25	447	(18)	433	(23)	441	(34)
26	454	(4)	450	(19)	452	(9)
27	461	(3)	452	(9)	456	(4)
28	466	(2)	457	(2)	462	(1)
29	469	(3)	472	(5)	470	(8)
30	471	(4)	479	(22)	473	(1)
31	483	(54)	488	(3)	483	(48)
32	485	(9)	497	(15)	489	(22)
33	499	(8)	503	(3)	505	(7)
34	503	(54)	507	(11)	509	(3)
35	508	(3)	512	(40)	512	(66)
36	520	(26)	517	(3)	521	(11)
37	535	(4)	530	(6)	539	(9)
38	561	(53)	554	(7)	560	(36)
39	568	(70)	569	(81)	567	(105)
40	588	(3)	582	(7)	586	(3)
41	605	(151)	595	(25)	607	(129)
42	608	(141)	598	(95)	611	(112)
43	613	(65)	609	(59)	613	(129)
44	617	(11)	614	(206)	620	(28)
45	630	(49)	617	(28)	627	(55)
46	667	(3)	650	(8)	664	(6)

47	687	(36)	661	(37)	681	(28)
48	795	(9)	772	(11)	800	(6)
49	822	(2)	803	(2)	827	(2)
50	849	(4)	827	(5)	860	(3)
51	853	(5)	832	(8)	862	(8)
52	870	(1)	851	(1)	887	(2)
53	903	(3)	881	(3)	921	(5)
54	911	(1)	887	(2)	929	(2)
55	931	(5)	901	(3)	941	(5)
56	1003	(9)	974	(9)	1003	(11)
57	1056	(6)	1024	(4)	1055	(7)
58	1073	(1)	1041	(0)	1069	(1)
59	1100	(10)	1069	(11)	1097	(16)
60	1121	(5)	1094	(4)	1127	(6)
61	1171	(3)	1138	(3)	1176	(3)
62	1237	(0)	1200	(1)	1236	(1)
63	1306	(20)	1268	(24)	1310	(21)
64	1325	(6)	1282	(5)	1319	(1)
65	1378	(9)	1335	(10)	1380	(13)
66	1413	(4)	1362	(4)	1408	(7)
67	1442	(6)	1387	(8)	1430	(7)
68	1461	(14)	1410	(15)	1454	(19)
69	1542	(36)	1488	(34)	1532	(60)
70	2037	(723)	1957	(585)	2045	(767)
71	2042	(708)	1963	(647)	2047	(693)
72	2056	(847)	1974	(702)	2064	(870)
73	2059	(876)	1978	(755)	2067	(833)
74	2091	(2117)	2008	(1915)	2088	(2656)
75	2114	(390)	2029	(366)	2114	(380)
76	3169	(5)	3110	(1)	3181	(2)
77	3180	(8)	3123	(1)	3195	(2)
78	3198	(16)	3136	(3)	3212	(3)
79	3211	(4)	3157	(0)	3227	(0)
80	3238	(1)	3174	(0)	3247	(0)
81	3253	(3)	3187	(0)	3260	(0)

Table S2. Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses, in km/mol) for the $(C_8H_6S)Fe_2(CO)_6$ structure **6S-2.**

	M06L		BP86		B3LYP	
1	25	(0)	24	(0)	26	(0)
2	44	(0)	41	(0)	42	(0)
3	59	(0)	55	(0)	56	(0)
4	67	(0)	60	(0)	64	(0)
5	75	(0)	74	(0)	78	(0)
6	78	(0)	79	(0)	82	(0)
7	80	(0)	81	(0)	84	(0)
8	89	(0)	86	(1)	89	(1)
9	94	(0)	95	(0)	98	(0)
10	101	(0)	98	(0)	103	(0)
11	104	(0)	103	(0)	107	(0)
12	126	(0)	113	(0)	122	(0)
13	134	(0)	128	(1)	135	(0)
14	150	(0)	138	(0)	146	(1)
15	201	(10)	180	(24)	193	(15)
16	215	(5)	201	(1)	208	(1)
17	288	(2)	270	(5)	276	(3)
18	343	(2)	326	(2)	327	(6)
19	357	(5)	339	(7)	338	(8)
20	375	(9)	364	(12)	369	(9)
21	395	(0)	388	(1)	395	(6)
22	400	(4)	397	(2)	397	(3)
23	409	(3)	404	(10)	406	(3)
24	415	(18)	411	(8)	412	(19)
25	449	(2)	441	(0)	446	(5)
26	453	(1)	447	(20)	451	(12)
27	460	(18)	448	(5)	451	(26)
28	462	(3)	455	(16)	457	(5)
29	471	(10)	468	(6)	467	(18)
30	475	(8)	480	(2)	475	(6)
31	484	(9)	491	(7)	484	(11)
32	487	(1)	496	(1)	489	(7)
33	494	(5)	501	(6)	500	(4)
34	508	(17)	506	(12)	510	(22)
35	510	(17)	517	(2)	517	(4)
36	522	(17)	529	(24)	531	(26)
37	553	(77)	540	(22)	551	(74)
38	564	(85)	563	(88)	566	(82)
39	574	(12)	570	(23)	573	(21)
40	597	(46)	587	(29)	593	(44)
41	611	(108)	607	(54)	615	(130)
42	613	(42)	614	(140)	616	(17)
43	617	(71)	615	(10)	620	(71)
44	638	(52)	622	(23)	633	(54)
45	648	(21)	637	(74)	644	(45)
46	677	(39)	652	(33)	670	(44)

47	722	(6)	697	(7)	725	(1)
48	795	(11)	772	(11)	798	(9)
49	811	(14)	787	(15)	814	(15)
50	837	(9)	823	(16)	862	(18)
51	864	(7)	838	(4)	869	(2)
52	867	(12)	847	(15)	883	(17)
53	897	(4)	875	(5)	914	(6)
54	918	(1)	885	(1)	930	(1)
55	934	(4)	906	(2)	952	(5)
56	993	(8)	962	(9)	993	(7)
57	1058	(6)	1016	(5)	1049	(7)
58	1064	(1)	1031	(1)	1063	(1)
59	1080	(6)	1049	(9)	1079	(10)
60	1121	(1)	1092	(1)	1127	(2)
61	1161	(3)	1122	(4)	1156	(4)
62	1213	(1)	1177	(1)	1212	(0)
63	1273	(15)	1224	(14)	1253	(7)
64	1313	(10)	1273	(10)	1319	(9)
65	1363	(7)	1316	(8)	1361	(7)
66	1404	(5)	1347	(7)	1398	(8)
67	1427	(3)	1373	(5)	1417	(4)
68	1440	(4)	1386	(4)	1434	(2)
69	1484	(2)	1428	(4)	1473	(1)
70	2039	(990)	1962	(929)	2046	(825)
71	2048	(48)	1966	(114)	2055	(341)
72	2056	(903)	1975	(814)	2062	(884)
73	2062	(774)	1983	(502)	2071	(648)
74	2093	(1159)	2012	(1041)	2092	(1418)
75	2119	(823)	2036	(738)	2122	(930)
76	3169	(0)	3111	(0)	3183	(0)
77	3177	(11)	3117	(1)	3190	(2)
78	3190	(30)	3130	(7)	3204	(9)
79	3199	(5)	3148	(1)	3217	(1)
80	3226	(5)	3164	(0)	3236	(1)
81	3242	(9)	3176	(1)	3249	(1)

Table S3. Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses, in km/mol) for the $(C_8H_6S)Fe_2(CO)_6$ structure **6S-3.**

	M06L		BP86		B3LYP	
1	36	(0)	35	(0)	36	(0)
2	45	(0)	44	(1)	45	(0)
3	62	(0)	62	(1)	63	(1)
4	66	(0)	66	(1)	70	(1)
5	67	(0)	68	(2)	73	(1)
6	73	(1)	76	(0)	77	(1)
7	88	(0)	91	(0)	96	(0)
8	91	(1)	96	(3)	99	(2)
9	95	(2)	97	(1)	100	(2)
10	104	(1)	102	(0)	105	(0)
11	109	(0)	106	(2)	112	(2)
12	141	(0)	137	(1)	145	(0)
13	156	(6)	153	(7)	157	(7)
14	189	(8)	182	(6)	192	(6)
15	208	(2)	202	(2)	204	(2)
16	230	(19)	227	(23)	232	(25)
17	277	(11)	263	(11)	247	(11)
18	297	(4)	299	(4)	300	(5)
19	325	(8)	318	(8)	309	(6)
20	343	(4)	334	(9)	339	(1)
21	355	(6)	348	(6)	347	(9)
22	374	(0)	352	(1)	356	(0)
23	390	(6)	389	(8)	394	(5)
24	413	(52)	403	(34)	411	(42)
25	423	(1)	417	(2)	424	(7)
26	434	(0)	425	(2)	433	(0)
27	441	(3)	437	(17)	440	(4)
28	457	(4)	450	(3)	455	(2)
29	460	(3)	462	(16)	457	(45)
30	464	(43)	471	(2)	467	(11)
31	469	(1)	483	(4)	471	(7)
32	493	(30)	487	(5)	493	(16)
33	497	(11)	496	(79)	499	(10)
34	506	(43)	511	(18)	510	(90)
35	510	(40)	520	(9)	519	(41)
36	534	(5)	532	(6)	534	(3)
37	556	(35)	553	(21)	558	(31)
38	575	(73)	562	(20)	570	(39)
39	577	(14)	569	(17)	581	(43)
40	589	(71)	580	(58)	592	(41)
41	595	(114)	589	(92)	598	(95)
42	604	(27)	598	(81)	606	(83)
43	621	(18)	604	(17)	626	(30)
44	638	(49)	636	(55)	644	(55)
45	663	(6)	645	(2)	657	(10)

46	679	(2)	654	(15)	677	(1)
47	707	(14)	686	(11)	704	(12)
48	790	(11)	769	(19)	797	(27)
49	793	(46)	773	(46)	803	(41)
50	856	(8)	832	(8)	862	(7)
51	873	(4)	854	(5)	885	(5)
52	887	(1)	862	(6)	894	(4)
53	888	(4)	866	(1)	897	(3)
54	900	(5)	878	(7)	914	(9)
55	976	(3)	943	(1)	1003	(3)
56	1008	(3)	979	(3)	1012	(3)
57	1056	(5)	1024	(5)	1053	(6)
58	1077	(1)	1044	(1)	1077	(2)
59	1121	(8)	1089	(8)	1122	(5)
60	1152	(1)	1124	(1)	1166	(2)
61	1188	(1)	1153	(1)	1198	(1)
62	1255	(0)	1213	(0)	1252	(1)
63	1324	(10)	1282	(10)	1330	(11)
64	1384	(5)	1333	(3)	1374	(3)
65	1399	(4)	1349	(6)	1400	(7)
66	1420	(0)	1365	(1)	1408	(2)
67	1454	(12)	1399	(11)	1453	(14)
68	1485	(3)	1431	(3)	1488	(3)
69	1522	(1)	1464	(1)	1518	(0)
70	1848	(199)	1775	(177)	1798	(239)
71	2032	(178)	1955	(287)	2038	(49)
72	2046	(424)	1964	(230)	2056	(576)
73	2061	(1407)	1979	(1209)	2068	(1609)
74	2080	(1484)	2000	(1285)	2086	(1483)
75	2115	(964)	2028	(809)	2118	(1004)
76	3173	(4)	3110	(1)	3186	(2)
77	3181	(7)	3118	(1)	3193	(1)
78	3192	(13)	3126	(3)	3206	(2)
79	3229	(4)	3166	(1)	3239	(0)
80	3240	(3)	3174	(0)	3246	(0)
81	3264	(4)	3194	(0)	3268	(0)

Table S4. Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses, in km/mol) for the $(C_8H_6S)Fe_2(CO)_5$ structure **5S-1.**

	M06L		BP86		B3LYP	
1	34	(1)	34	(0)	24	(2)
2	43	(1)	54	(0)	44	(1)
3	59	(0)	57	(1)	61	(0)
4	74	(0)	79	(0)	76	(0)
5	82	(0)	79	(0)	80	(0)
6	87	(0)	83	(0)	91	(0)
7	90	(0)	94	(0)	96	(0)
8	97	(0)	100	(0)	101	(0)
9	103	(0)	103	(1)	103	(0)
10	131	(0)	135	(0)	131	(0)
11	157	(2)	167	(0)	158	(3)
12	180	(2)	185	(1)	166	(1)
13	189	(11)	210	(21)	187	(13)
14	226	(0)	219	(2)	219	(1)
15	326	(7)	310	(10)	305	(8)
16	339	(4)	327	(3)	332	(2)
17	366	(14)	339	(8)	349	(7)
18	370	(18)	361	(10)	360	(16)
19	389	(4)	369	(32)	375	(13)
20	399	(1)	389	(3)	385	(7)
21	430	(10)	409	(7)	419	(12)
22	443	(10)	431	(2)	436	(8)
23	452	(4)	445	(12)	443	(6)
24	455	(2)	449	(1)	451	(1)
25	468	(2)	466	(1)	467	(3)
26	477	(3)	474	(7)	474	(2)
27	485	(5)	483	(1)	484	(10)
28	500	(11)	506	(8)	501	(18)
29	504	(1)	510	(1)	504	(0)
30	517	(4)	516	(10)	516	(4)
31	533	(10)	525	(59)	542	(2)
32	550	(97)	543	(22)	548	(109)
33	556	(49)	552	(8)	558	(57)
34	575	(31)	560	(18)	569	(18)
35	583	(24)	570	(42)	578	(36)
36	591	(33)	581	(54)	591	(40)
37	609	(80)	603	(15)	604	(38)
38	626	(42)	619	(9)	626	(86)
39	639	(47)	628	(52)	639	(47)
40	643	(9)	636	(46)	644	(12)
41	674	(7)	650	(36)	673	(8)
42	700	(21)	673	(26)	696	(11)
43	802	(12)	780	(9)	807	(12)
44	826	(16)	804	(21)	834	(23)
45	847	(3)	822	(3)	857	(3)
46	858	(7)	831	(16)	868	(11)

47	864	(9)	847	(4)	879	(9)
48	896	(1)	870	(1)	911	(2)
49	898	(4)	880	(6)	913	(5)
50	949	(2)	906	(5)	965	(2)
51	1014	(2)	982	(2)	1016	(2)
52	1058	(4)	1027	(4)	1055	(4)
53	1077	(0)	1043	(0)	1075	(1)
54	1111	(8)	1073	(8)	1107	(10)
55	1142	(1)	1106	(1)	1151	(2)
56	1189	(1)	1152	(1)	1198	(1)
57	1258	(0)	1217	(1)	1258	(0)
58	1317	(11)	1273	(12)	1321	(9)
59	1381	(0)	1318	(2)	1368	(1)
60	1397	(8)	1347	(7)	1399	(7)
61	1425	(1)	1373	(1)	1413	(1)
62	1452	(7)	1400	(13)	1449	(10)
63	1489	(5)	1432	(6)	1485	(7)
64	1559	(9)	1487	(9)	1544	(7)
65	2005	(148)	1849	(299)	2000	(192)
66	2031	(74)	1955	(151)	2038	(75)
67	2050	(1192)	1971	(884)	2056	(1219)
68	2065	(1450)	1992	(1184)	2064	(1683)
69	2104	(1060)	2019	(879)	2106	(1170)
70	3172	(2)	3111	(0)	3183	(1)
71	3185	(10)	3122	(3)	3195	(1)
72	3200	(16)	3139	(3)	3209	(4)
73	3227	(2)	3166	(0)	3241	(0)
74	3238	(3)	3173	(0)	3248	(0)
75	3258	(6)	3190	(0)	3265	(0)

Table S5. Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses, in km/mol) for the $(C_8H_6S)Fe_2(CO)_4$ structure **4T-1.**

	M06L		BP86		B3LYP	
1	34	(0)	34	(0)	32	(0)
2	52	(1)	54	(1)	44	(2)
3	60	(0)	63	(0)	60	(0)
4	71	(0)	77	(0)	74	(0)
5	76	(0)	80	(0)	80	(0)
6	88	(0)	92	(0)	90	(0)
7	90	(0)	98	(0)	97	(0)
8	124	(1)	135	(2)	114	(1)
9	145	(0)	156	(3)	132	(1)
10	179	(5)	185	(2)	151	(3)
11	191	(2)	210	(1)	172	(2)
12	218	(0)	214	(0)	211	(1)
13	290	(3)	274	(6)	258	(3)
14	304	(4)	297	(3)	266	(4)
15	344	(19)	330	(1)	311	(2)
16	351	(5)	344	(3)	336	(17)
17	375	(35)	365	(10)	360	(33)
18	379	(3)	388	(22)	361	(3)
19	405	(5)	396	(10)	389	(5)
20	434	(5)	415	(2)	394	(5)
21	449	(12)	443	(5)	429	(10)
22	451	(3)	450	(5)	447	(22)
23	470	(2)	462	(1)	458	(2)
24	476	(27)	467	(13)	464	(23)
25	480	(6)	475	(11)	475	(10)
26	488	(13)	496	(14)	477	(9)
27	496	(7)	502	(17)	492	(5)
28	510	(12)	509	(7)	500	(5)
29	522	(14)	531	(32)	522	(9)
30	552	(48)	538	(3)	543	(72)
31	566	(7)	553	(8)	564	(8)
32	573	(11)	560	(34)	571	(26)
33	589	(46)	589	(36)	586	(33)
34	620	(108)	615	(27)	612	(109)
35	639	(13)	618	(75)	638	(12)
36	670	(3)	645	(9)	670	(2)
37	692	(23)	663	(26)	691	(10)
38	776	(6)	763	(12)	787	(27)
39	795	(23)	777	(9)	802	(22)
40	799	(19)	778	(26)	804	(24)
41	836	(1)	811	(2)	849	(5)
42	849	(9)	824	(12)	862	(15)
43	885	(1)	865	(2)	896	(1)
44	895	(1)	872	(1)	916	(0)
45	941	(4)	906	(6)	960	(2)

46	1008	(3)	976	(3)	1010	(3)
47	1058	(5)	1023	(7)	1057	(2)
48	1078	(2)	1045	(2)	1077	(4)
49	1101	(9)	1065	(9)	1097	(7)
50	1136	(1)	1103	(1)	1151	(2)
51	1188	(0)	1152	(0)	1198	(0)
52	1256	(0)	1215	(1)	1257	(0)
53	1316	(10)	1272	(8)	1320	(6)
54	1349	(2)	1293	(2)	1345	(17)
55	1395	(5)	1349	(6)	1396	(8)
56	1420	(16)	1367	(12)	1408	(12)
57	1455	(4)	1402	(4)	1458	(7)
58	1491	(8)	1432	(6)	1483	(8)
59	1547	(10)	1486	(7)	1539	(1)
60	1942	(426)	1819	(361)	1965	(533)
61	2035	(528)	1956	(491)	2041	(469)
62	2046	(1564)	1965	(1369)	2054	(1626)
63	2084	(1151)	2002	(996)	2087	(1376)
64	3172	(3)	3111	(0)	3182	(1)
65	3186	(9)	3123	(2)	3195	(1)
66	3200	(19)	3135	(4)	3209	(4)
67	3223	(2)	3162	(1)	3234	(0)
68	3241	(3)	3173	(0)	3245	(0)
69	3254	(5)	3184	(1)	3257	(0)

Table S6. Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses, in km/mol) for the $(C_6H_4S_2)Fe_2(CO)_4$ structure **4T-2.**

	M06L		BP86		B3LYP	
1	37	(0)	42	(0)	41	(0)
2	47	(0)	47	(0)	45	(0)
3	54	(1)	58	(1)	55	(1)
4	72	(0)	73	(0)	73	(0)
5	77	(0)	80	(0)	79	(0)
6	84	(0)	84	(0)	86	(0)
7	88	(1)	92	(0)	91	(0)
8	103	(0)	99	(0)	95	(0)
9	136	(2)	138	(2)	128	(1)
10	163	(4)	160	(5)	150	(1)
11	172	(1)	168	(2)	162	(2)
12	202	(1)	198	(0)	193	(0)
13	305	(10)	292	(10)	282	(8)
14	335	(3)	322	(3)	306	(4)
15	345	(1)	337	(1)	328	(2)
16	361	(1)	340	(2)	341	(1)
17	372	(1)	370	(6)	366	(4)
18	385	(19)	378	(16)	368	(5)
19	393	(0)	386	(2)	382	(7)
20	412	(8)	396	(7)	403	(7)
21	433	(0)	424	(4)	426	(0)
22	439	(4)	432	(1)	437	(2)
23	463	(16)	463	(5)	457	(0)
24	468	(1)	471	(3)	463	(22)
25	484	(1)	486	(23)	485	(1)
26	491	(8)	492	(12)	488	(23)
27	500	(35)	505	(8)	497	(20)
28	509	(24)	524	(50)	520	(27)
29	536	(53)	535	(9)	529	(11)
30	542	(25)	538	(4)	540	(35)
31	557	(3)	553	(35)	551	(9)
32	575	(39)	561	(4)	582	(48)
33	592	(2)	575	(41)	592	(1)
34	611	(52)	603	(6)	618	(44)
35	625	(5)	609	(43)	620	(13)
36	656	(0)	634	(1)	653	(0)
37	687	(4)	666	(4)	687	(2)
38	782	(5)	765	(9)	788	(9)
39	804	(15)	785	(20)	806	(28)
40	819	(7)	805	(14)	844	(11)
41	846	(2)	823	(3)	856	(4)
42	849	(11)	828	(5)	862	(10)
43	851	(2)	829	(6)	871	(3)
44	884	(2)	858	(3)	904	(4)
45	918	(2)	888	(1)	939	(1)

46	1004	(2)	973	(1)	1007	(1)
47	1057	(4)	1023	(4)	1055	(4)
48	1073	(2)	1041	(2)	1075	(4)
49	1101	(12)	1067	(10)	1098	(10)
50	1143	(1)	1113	(1)	1151	(2)
51	1181	(2)	1145	(1)	1188	(2)
52	1244	(0)	1205	(0)	1242	(1)
53	1317	(8)	1276	(8)	1319	(10)
54	1358	(5)	1308	(4)	1354	(4)
55	1398	(2)	1351	(3)	1399	(2)
56	1424	(6)	1369	(5)	1412	(8)
57	1460	(6)	1407	(4)	1459	(9)
58	1491	(4)	1436	(4)	1489	(3)
59	1511	(0)	1456	(0)	1496	(2)
60	2010	(235)	1932	(75)	2015	(494)
61	2023	(746)	1945	(946)	2035	(579)
62	2043	(1268)	1962	(953)	2051	(1345)
63	2086	(1297)	1999	(1131)	2092	(1350)
64	3183	(2)	3118	(0)	3192	(1)
65	3198	(10)	3131	(1)	3208	(1)
66	3210	(10)	3141	(1)	3217	(1)
67	3234	(2)	3169	(0)	3240	(0)
68	3243	(3)	3176	(0)	3248	(0)
69	3260	(5)	3191	(0)	3265	(0)

Table S7. Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses, in km/mol) for the $(C_8H_6S)Fe_2(CO)_4$ structure **4T-3**.

	M06L		BP86		B3LYP	
1	37	(0)	40	(0)	34	(0)
2	46	(0)	42	(0)	39	(0)
3	57	(0)	51	(0)	47	(0)
4	78	(0)	72	(0)	64	(0)
5	82	(0)	81	(0)	72	(1)
6	87	(0)	84	(0)	85	(0)
7	93	(0)	88	(0)	87	(0)
8	104	(0)	94	(0)	95	(1)
9	140	(0)	141	(1)	110	(1)
10	146	(0)	156	(2)	137	(0)
11	168	(3)	161	(2)	161	(1)
12	197	(2)	191	(1)	193	(0)
13	312	(6)	290	(11)	291	(6)
14	337	(5)	320	(5)	315	(7)
15	339	(4)	329	(6)	328	(1)
16	363	(4)	348	(0)	345	(1)
17	371	(9)	358	(18)	361	(7)
18	401	(0)	375	(6)	383	(10)
19	406	(11)	390	(1)	392	(1)
20	416	(2)	404	(4)	407	(3)
21	436	(2)	416	(3)	437	(1)
22	452	(3)	441	(12)	456	(0)
23	464	(1)	449	(3)	458	(0)
24	468	(7)	463	(2)	476	(9)
25	491	(5)	484	(5)	485	(14)
26	492	(23)	485	(16)	488	(3)
27	498	(5)	512	(5)	497	(1)
28	526	(30)	520	(12)	513	(8)
29	538	(40)	535	(17)	532	(19)
30	548	(33)	546	(34)	539	(71)
31	555	(3)	555	(16)	553	(4)
32	587	(39)	562	(28)	588	(28)
33	589	(8)	578	(38)	594	(32)
34	622	(12)	602	(10)	623	(37)
35	627	(33)	627	(34)	632	(18)
36	674	(0)	646	(2)	664	(0)
37	683	(7)	665	(7)	683	(5)
38	788	(3)	765	(5)	796	(9)
39	805	(5)	793	(33)	807	(26)
40	812	(24)	797	(7)	827	(15)
41	831	(6)	809	(6)	854	(6)
42	848	(1)	824	(0)	858	(4)
43	862	(1)	838	(1)	880	(2)
44	889	(1)	862	(0)	901	(3)
45	927	(3)	893	(2)	954	(2)

46	1010	(2)	980	(2)	1013	(3)
47	1047	(5)	1014	(5)	1044	(6)
48	1073	(3)	1040	(2)	1073	(2)
49	1112	(7)	1078	(8)	1108	(6)
50	1145	(1)	1120	(0)	1152	(2)
51	1187	(1)	1152	(1)	1194	(4)
52	1252	(0)	1213	(1)	1246	(1)
53	1312	(13)	1274	(10)	1314	(14)
54	1386	(3)	1331	(1)	1367	(11)
55	1398	(4)	1350	(4)	1396	(10)
56	1424	(0)	1371	(1)	1411	(5)
57	1445	(14)	1393	(9)	1439	(30)
58	1492	(1)	1440	(1)	1484	(2)
59	1543	(4)	1485	(4)	1529	(6)
60	2007	(123)	1931	(84)	2020	(127)
61	2028	(602)	1945	(623)	2041	(1447)
62	2040	(1420)	1956	(1292)	2059	(651)
63	2090	(1294)	2005	(1133)	2095	(1393)
64	3161	(4)	3094	(0)	3164	(1)
65	3195	(8)	3130	(0)	3198	(2)
66	3206	(11)	3137	(1)	3211	(3)
67	3233	(2)	3170	(0)	3240	(0)
68	3244	(3)	3178	(0)	3250	(0)
69	3257	(5)	3190	(0)	3263	(0)

Table S8. Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses, in km/mol) for the $(C_8H_6S)Fe_2(CO)_4$ structure **4T-4.**

	M06L		BP86		B3LYP	
1	39	(0)	30	(1)	41	(0)
2	41	(0)	40	(0)	45	(0)
3	48	(0)	48	(0)	55	(1)
4	65	(2)	66	(0)	73	(0)
5	75	(0)	76	(1)	79	(0)
6	82	(0)	85	(1)	86	(0)
7	87	(1)	91	(1)	91	(0)
8	97	(1)	95	(0)	95	(0)
9	120	(7)	117	(3)	128	(1)
10	149	(3)	148	(2)	150	(1)
11	171	(5)	171	(5)	162	(2)
12	210	(1)	204	(3)	193	(0)
13	273	(19)	264	(14)	282	(8)
14	304	(15)	303	(6)	306	(4)
15	325	(11)	321	(12)	328	(2)
16	341	(8)	337	(14)	341	(1)
17	376	(5)	357	(0)	366	(4)
18	388	(0)	361	(1)	368	(5)
19	401	(4)	403	(2)	382	(7)
20	409	(19)	408	(2)	403	(7)
21	427	(12)	416	(1)	426	(0)
22	435	(4)	428	(13)	437	(2)
23	437	(12)	446	(24)	457	(0)
24	445	(10)	459	(5)	463	(22)
25	457	(28)	469	(9)	485	(1)
26	475	(2)	488	(5)	488	(23)
27	500	(2)	502	(19)	497	(20)
28	512	(4)	514	(16)	520	(27)
29	527	(37)	520	(14)	529	(11)
30	554	(13)	537	(43)	540	(35)
31	565	(34)	555	(20)	551	(9)
32	570	(26)	566	(7)	582	(48)
33	591	(22)	574	(29)	592	(1)
34	624	(8)	601	(8)	618	(44)
35	643	(33)	631	(33)	620	(13)
36	675	(4)	649	(2)	653	(0)
37	703	(11)	677	(8)	687	(2)
38	783	(4)	767	(7)	788	(9)
39	810	(19)	782	(29)	806	(28)
40	827	(1)	802	(2)	844	(11)
41	838	(4)	815	(5)	856	(4)
42	848	(3)	825	(3)	862	(10)
43	859	(1)	851	(2)	871	(3)
44	881	(2)	852	(1)	904	(4)
45	917	(1)	893	(2)	939	(1)
46	1011	(1)	979	(1)	1007	(1)

47	1052	(5)	1019	(6)	1055	(4)
48	1073	(2)	1041	(1)	1075	(4)
49	1120	(10)	1083	(10)	1098	(10)
50	1157	(2)	1126	(1)	1151	(2)
51	1185	(0)	1150	(1)	1188	(2)
52	1257	(0)	1214	(1)	1242	(1)
53	1327	(6)	1281	(7)	1319	(10)
54	1386	(2)	1329	(2)	1354	(4)
55	1400	(2)	1350	(3)	1399	(2)
56	1425	(1)	1369	(1)	1412	(8)
57	1451	(5)	1396	(6)	1459	(9)
58	1489	(7)	1436	(4)	1489	(3)
59	1554	(4)	1489	(2)	1496	(2)
60	2003	(51)	1926	(34)	2015	(494)
61	2023	(1123)	1942	(941)	2035	(579)
62	2035	(1354)	1955	(1189)	2051	(1345)
63	2082	(1292)	1996	(1120)	2092	(1350)
64	3189	(1)	3123	(0)	3192	(1)
65	3195	(6)	3130	(0)	3208	(1)
66	3209	(9)	3140	(1)	3217	(1)
67	3237	(2)	3171	(0)	3240	(0)
68	3245	(3)	3179	(0)	3248	(0)
69	3260	(7)	3192	(0)	3265	(0)

Table S9. Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses, in km/mol) for the $(C_8H_6S)Fe_2(CO)_4$ structure **4T-5.**

	M06L		BP86		B3LYP	
1	32	(0)	32	(0)	28	(0)
2	38	(1)	39	(1)	37	(1)
3	48	(0)	46	(1)	43	(0)
4	59	(1)	57	(1)	56	(1)
5	60	(0)	62	(0)	62	(0)
6	81	(0)	85	(0)	85	(0)
7	86	(0)	90	(0)	87	(0)
8	95	(0)	96	(0)	94	(0)
9	127	(2)	130	(3)	122	(2)
10	151	(0)	147	(0)	139	(1)
11	158	(1)	153	(2)	144	(2)
12	195	(3)	190	(2)	173	(2)
13	285	(3)	267	(5)	271	(4)
14	318	(1)	317	(1)	307	(5)
15	350	(8)	344	(6)	337	(0)
16	367	(1)	346	(3)	345	(5)
17	372	(6)	369	(6)	359	(7)
18	406	(1)	392	(2)	392	(2)
19	409	(2)	395	(1)	395	(4)
20	425	(3)	410	(1)	412	(2)
21	431	(2)	412	(3)	416	(3)
22	462	(1)	458	(5)	459	(2)
23	475	(1)	467	(2)	464	(0)
24	478	(4)	482	(1)	477	(9)
25	499	(2)	488	(4)	492	(7)
26	501	(2)	500	(1)	496	(2)
27	509	(3)	513	(1)	501	(2)
28	529	(42)	528	(7)	521	(20)
29	544	(28)	540	(21)	532	(25)
30	549	(25)	550	(39)	540	(44)
31	564	(35)	556	(19)	557	(40)
32	580	(5)	576	(38)	578	(1)
33	600	(46)	589	(16)	599	(58)
34	633	(10)	621	(34)	633	(3)
35	642	(58)	637	(54)	638	(68)
36	685	(0)	654	(0)	681	(0)
37	714	(5)	694	(5)	705	(6)
38	783	(9)	768	(6)	793	(22)
39	790	(14)	779	(20)	796	(16)
40	832	(1)	810	(1)	843	(5)
41	835	(5)	818	(4)	849	(3)
42	850	(6)	827	(4)	861	(7)
43	851	(2)	829	(3)	871	(4)
44	874	(2)	852	(2)	888	(2)
45	929	(2)	896	(5)	950	(2)

46	1000	(1)	972	(0)	1007	(1)
47	1034	(4)	1002	(4)	1029	(5)
48	1060	(3)	1029	(2)	1065	(1)
49	1104	(7)	1069	(7)	1107	(7)
50	1138	(3)	1108	(2)	1149	(2)
51	1180	(1)	1145	(1)	1188	(1)
52	1245	(1)	1205	(1)	1240	(4)
53	1291	(14)	1252	(12)	1304	(24)
54	1372	(3)	1325	(2)	1369	(2)
55	1386	(1)	1333	(3)	1379	(3)
56	1426	(2)	1368	(3)	1416	(1)
57	1446	(16)	1392	(11)	1448	(23)
58	1487	(5)	1433	(9)	1488	(10)
59	1524	(13)	1466	(20)	1515	(10)
60	2021	(643)	1941	(563)	2026	(693)
61	2024	(1235)	1943	(1074)	2030	(1302)
62	2066	(2498)	1980	(2418)	2072	(2570)
63	2080	(44)	1995	(12)	2085	(48)
64	3166	(3)	3098	(0)	3169	(1)
65	3186	(11)	3121	(1)	3192	(2)
66	3213	(3)	3146	(1)	3221	(1)
67	3234	(2)	3169	(0)	3241	(0)
68	3246	(3)	3179	(0)	3252	(0)
69	3260	(6)	3192	(0)	3266	(0)

Table S10. Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses, in km/mol) for the $(C_8H_6S)Fe_2(CO)_5$ structure **4S-1.**

	M06L		BP86		B3LYP	
1	51	(0)	52	(1)	55	(1)
2	63	(0)	58	(0)	58	(0)
3	72	(0)	64	(0)	65	(0)
4	87	(0)	86	(0)	89	(0)
5	92	(0)	95	(0)	97	(0)
6	98	(0)	96	(0)	99	(0)
7	131	(0)	119	(0)	126	(0)
8	140	(1)	129	(0)	134	(0)
9	186	(5)	180	(5)	184	(7)
10	204	(3)	195	(5)	194	(4)
11	239	(0)	227	(4)	222	(6)
12	244	(6)	228	(4)	233	(3)
13	316	(7)	300	(10)	299	(7)
14	342	(4)	324	(2)	332	(1)
15	360	(6)	346	(7)	340	(7)
16	386	(3)	376	(6)	372	(5)
17	402	(5)	387	(2)	386	(1)
18	410	(2)	403	(2)	407	(5)
19	431	(5)	414	(9)	420	(5)
20	449	(3)	434	(5)	445	(3)
21	460	(5)	446	(3)	458	(5)
22	468	(3)	469	(7)	468	(9)
23	474	(7)	475	(3)	477	(8)
24	485	(2)	480	(1)	489	(11)
25	495	(10)	495	(3)	493	(3)
26	514	(31)	508	(10)	510	(29)
27	523	(10)	531	(59)	520	(18)
28	543	(36)	540	(6)	541	(28)
29	554	(78)	548	(16)	553	(18)
30	567	(8)	550	(8)	559	(53)
31	580	(9)	559	(30)	573	(37)
32	592	(27)	573	(44)	582	(5)
33	615	(91)	614	(83)	619	(108)
34	637	(31)	617	(32)	631	(36)
35	656	(59)	644	(28)	660	(56)
36	684	(13)	663	(45)	684	(13)
37	698	(20)	671	(16)	695	(8)
38	801	(13)	778	(14)	807	(12)
39	820	(17)	794	(25)	831	(31)
40	839	(1)	817	(2)	852	(1)
41	848	(2)	821	(5)	854	(6)
42	855	(9)	839	(6)	868	(10)
43	884	(1)	859	(2)	902	(2)
44	896	(0)	875	(1)	917	(0)
45	941	(3)	905	(3)	953	(4)
46	1014	(2)	983	(2)	1017	(2)

47	1050	(4)	1016	(4)	1049	(4)
48	1077	(1)	1044	(0)	1076	(1)
49	1113	(6)	1079	(6)	1109	(8)
50	1144	(2)	1115	(1)	1153	(2)
51	1184	(0)	1150	(1)	1195	(0)
52	1254	(0)	1212	(1)	1254	(0)
53	1316	(9)	1273	(9)	1318	(9)
54	1378	(1)	1321	(1)	1364	(0)
55	1392	(4)	1344	(5)	1394	(3)
56	1420	(2)	1366	(3)	1415	(3)
57	1455	(3)	1399	(5)	1447	(6)
58	1478	(3)	1423	(4)	1476	(4)
59	1546	(1)	1485	(1)	1532	(2)
60	1837	(402)	1757	(362)	1839	(450)
61	2029	(258)	1950	(249)	2041	(212)
62	2046	(1284)	1963	(1103)	2052	(1444)
63	2087	(1211)	2004	(1059)	2091	(1353)
64	3170	(4)	3109	(1)	3181	(1)
65	3185	(7)	3121	(1)	3196	(1)
66	3198	(19)	3133	(4)	3209	(4)
67	3224	(3)	3163	(0)	3239	(0)
68	3233	(3)	3168	(0)	3244	(0)
69	3252	(7)	3186	(0)	3262	(0)

Table S11. Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses, in km/mol) for the $(C_8H_6S)Fe_2(CO)_4$ structure **4S-2.**

	M06L		BP86		B3LYP	
1	31	(0)	29	(0)	35	(0)
2	48	(3)	58	(0)	51	(3)
3	60	(1)	68	(1)	59	(0)
4	70	(0)	76	(0)	73	(0)
5	80	(0)	80	(0)	85	(0)
6	89	(1)	90	(1)	94	(1)
7	93	(0)	98	(1)	99	(0)
8	129	(1)	131	(0)	127	(1)
9	147	(2)	149	(2)	145	(1)
10	172	(5)	183	(5)	166	(2)
11	185	(10)	192	(9)	172	(12)
12	215	(3)	212	(14)	209	(3)
13	320	(4)	309	(5)	293	(4)
14	351	(4)	334	(5)	340	(4)
15	357	(4)	343	(5)	344	(3)
16	373	(16)	351	(7)	357	(2)
17	394	(32)	380	(26)	382	(38)
18	414	(3)	393	(12)	405	(10)
19	431	(9)	406	(14)	418	(11)
20	440	(1)	438	(2)	437	(2)
21	466	(2)	451	(2)	452	(0)
22	472	(5)	468	(6)	468	(3)
23	493	(12)	484	(5)	476	(18)
24	503	(9)	505	(5)	502	(2)
25	509	(4)	514	(13)	507	(21)
26	533	(32)	519	(2)	528	(14)
27	537	(11)	530	(26)	531	(3)
28	553	(18)	535	(60)	549	(14)
29	561	(45)	549	(7)	557	(113)
30	565	(73)	565	(8)	563	(44)
31	584	(7)	579	(32)	578	(0)
32	596	(65)	587	(41)	593	(74)
33	622	(8)	604	(15)	613	(7)
34	635	(10)	617	(18)	628	(9)
35	637	(43)	628	(47)	642	(47)
36	675	(4)	645	(27)	671	(2)
37	692	(15)	669	(14)	693	(10)
38	795	(6)	770	(14)	804	(5)
39	811	(11)	791	(13)	820	(19)
40	829	(11)	799	(18)	845	(15)
41	849	(8)	825	(5)	860	(9)
42	859	(4)	841	(5)	872	(5)
43	892	(4)	856	(3)	904	(9)
44	895	(6)	869	(7)	912	(3)
45	934	(2)	895	(3)	954	(1)

46	1009	(4)	977	(3)	1011	(3)
47	1056	(5)	1022	(3)	1052	(3)
48	1065	(1)	1032	(2)	1062	(2)
49	1101	(9)	1062	(8)	1096	(9)
50	1139	(3)	1103	(2)	1152	(3)
51	1188	(1)	1149	(0)	1197	(0)
52	1256	(1)	1211	(1)	1258	(1)
53	1307	(9)	1261	(8)	1310	(7)
54	1384	(1)	1319	(2)	1372	(3)
55	1391	(3)	1342	(5)	1395	(3)
56	1422	(1)	1368	(4)	1407	(3)
57	1450	(7)	1392	(7)	1446	(9)
58	1491	(10)	1431	(11)	1487	(9)
59	1567	(4)	1492	(9)	1554	(2)
60	1980	(190)	1834	(292)	1999	(134)
61	2028	(754)	1951	(921)	2028	(893)
62	2040	(1440)	1962	(824)	2046	(1531)
63	2081	(1203)	2005	(981)	2083	(1330)
64	3169	(3)	3106	(0)	3181	(0)
65	3179	(8)	3115	(2)	3188	(1)
66	3192	(17)	3127	(3)	3203	(3)
67	3232	(3)	3166	(0)	3241	(0)
68	3240	(4)	3175	(0)	3249	(0)
69	3261	(5)	3191	(0)	3266	(0)

Table S12. Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses, in km/mol) for the $(C_8H_6S)Fe_2(CO)_4$ structure **4S-3.**

	M06L		BP86		B3LYP	
1	37	(0)	38	(0)	39	(0)
2	45	(0)	44	(0)	49	(0)
3	70	(1)	72	(1)	75	(1)
4	85	(0)	79	(0)	87	(0)
5	89	(0)	85	(0)	89	(0)
6	90	(1)	87	(0)	94	(1)
7	99	(0)	93	(0)	97	(0)
8	107	(0)	97	(0)	101	(0)
9	139	(2)	134	(1)	139	(2)
10	170	(3)	163	(3)	169	(3)
11	187	(1)	174	(2)	178	(3)
12	213	(1)	196	(1)	200	(2)
13	277	(18)	253	(18)	239	(19)
14	333	(1)	321	(2)	323	(2)
15	355	(4)	346	(5)	336	(4)
16	381	(3)	357	(0)	362	(2)
17	388	(5)	376	(6)	371	(5)
18	406	(5)	393	(5)	404	(10)
19	433	(1)	414	(1)	420	(2)
20	446	(2)	430	(1)	437	(1)
21	451	(2)	433	(2)	444	(3)
22	472	(2)	458	(1)	464	(2)
23	477	(2)	465	(3)	473	(1)
24	485	(20)	488	(1)	488	(52)
25	497	(7)	500	(21)	496	(2)
26	499	(1)	509	(0)	502	(3)
27	519	(3)	514	(1)	515	(1)
28	540	(23)	529	(2)	541	(10)
29	562	(40)	550	(17)	555	(20)
30	565	(11)	570	(14)	561	(53)
31	578	(39)	572	(49)	568	(55)
32	598	(39)	580	(39)	593	(28)
33	609	(46)	603	(31)	611	(50)
34	627	(7)	615	(19)	621	(6)
35	641	(39)	635	(26)	640	(43)
36	682	(4)	652	(13)	680	(4)
37	693	(8)	676	(7)	694	(6)
38	781	(2)	753	(4)	782	(3)
39	821	(18)	800	(22)	829	(26)
40	828	(6)	808	(7)	838	(6)
41	842	(4)	824	(6)	858	(4)
42	849	(5)	825	(3)	860	(7)
43	858	(4)	827	(7)	866	(10)
44	888	(2)	862	(2)	905	(4)
45	931	(2)	894	(2)	953	(1)

46	1011	(2)	981	(2)	1014	(2)
47	1050	(3)	1017	(3)	1048	(4)
48	1072	(1)	1039	(0)	1072	(0)
49	1113	(10)	1078	(10)	1111	(11)
50	1148	(0)	1123	(0)	1164	(1)
51	1188	(1)	1154	(1)	1198	(1)
52	1253	(1)	1214	(1)	1253	(0)
53	1320	(9)	1282	(10)	1329	(8)
54	1383	(1)	1329	(0)	1370	(1)
55	1398	(4)	1351	(5)	1403	(4)
56	1423	(2)	1369	(1)	1414	(1)
57	1451	(9)	1397	(12)	1451	(10)
58	1504	(3)	1454	(3)	1505	(7)
59	1544	(13)	1488	(14)	1534	(13)
60	2005	(164)	1927	(156)	2011	(304)
61	2029	(585)	1955	(584)	2027	(672)
62	2043	(1305)	1962	(1046)	2049	(1414)
63	2091	(1234)	2006	(1083)	2097	(1362)
64	3131	(9)	3066	(1)	3136	(1)
65	3198	(5)	3136	(0)	3211	(0)
66	3204	(10)	3138	(1)	3214	(1)
67	3232	(2)	3171	(0)	3243	(0)
68	3240	(3)	3176	(0)	3249	(0)
69	3258	(7)	3190	(0)	3265	(0)

Table S13. Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses, in km/mol) for the $(C_8H_6S)Fe_2(CO)_4$ structure **4S-4.**

	M06L		BP86		B3LYP	
1	41	(0)	38	(0)	42	(0)
2	65	(0)	56	(0)	56	(0)
3	75	(0)	69	(1)	71	(0)
4	85	(0)	81	(0)	85	(0)
5	93	(0)	91	(0)	93	(0)
6	98	(0)	96	(0)	99	(0)
7	131	(0)	124	(1)	133	(0)
8	169	(1)	144	(3)	157	(2)
9	183	(2)	165	(0)	174	(0)
10	200	(2)	188	(3)	189	(3)
11	221	(7)	205	(15)	210	(15)
12	250	(3)	234	(3)	238	(6)
13	301	(6)	288	(7)	281	(9)
14	341	(7)	326	(6)	327	(4)
15	348	(4)	336	(2)	337	(1)
16	360	(9)	356	(15)	358	(8)
17	385	(2)	367	(1)	368	(1)
18	398	(2)	382	(8)	391	(5)
19	428	(2)	414	(5)	420	(1)
20	449	(7)	444	(5)	446	(3)
21	463	(2)	445	(0)	452	(4)
22	463	(1)	453	(3)	459	(3)
23	480	(4)	475	(1)	482	(9)
24	488	(3)	476	(7)	484	(3)
25	494	(4)	506	(19)	502	(7)
26	512	(25)	515	(18)	509	(39)
27	518	(29)	518	(22)	517	(11)
28	545	(22)	542	(6)	542	(7)
29	555	(69)	555	(16)	554	(34)
30	579	(13)	560	(15)	577	(29)
31	585	(29)	568	(16)	581	(19)
32	588	(8)	577	(27)	585	(20)
33	592	(48)	593	(54)	595	(58)
34	632	(18)	614	(40)	631	(70)
35	637	(118)	631	(97)	646	(90)
36	683	(2)	658	(26)	682	(7)
37	690	(17)	662	(9)	686	(7)
38	796	(15)	774	(21)	802	(20)
39	799	(11)	777	(16)	809	(22)
40	844	(5)	818	(5)	853	(8)
41	849	(8)	824	(10)	858	(7)
42	862	(5)	833	(6)	874	(4)
43	887	(2)	856	(2)	890	(5)
44	891	(7)	862	(7)	903	(10)
45	956	(1)	916	(1)	972	(1)

46	1010	(2)	980	(2)	1013	(1)
47	1056	(7)	1021	(7)	1054	(9)
48	1076	(1)	1042	(1)	1073	(2)
49	1111	(10)	1078	(9)	1110	(8)
50	1150	(0)	1120	(1)	1161	(1)
51	1187	(1)	1150	(1)	1196	(1)
52	1256	(1)	1212	(0)	1253	(0)
53	1318	(9)	1274	(9)	1324	(9)
54	1383	(0)	1328	(1)	1371	(2)
55	1398	(10)	1346	(11)	1401	(7)
56	1414	(0)	1360	(0)	1403	(2)
57	1444	(4)	1389	(5)	1446	(5)
58	1491	(2)	1433	(3)	1487	(2)
59	1556	(3)	1493	(3)	1535	(2)
60	1829	(402)	1754	(382)	1821	(436)
61	2024	(314)	1948	(286)	2040	(260)
62	2046	(1302)	1963	(1144)	2053	(1482)
63	2093	(1040)	2008	(925)	2095	(1192)
64	3176	(2)	3115	(0)	3190	(1)
65	3187	(7)	3124	(1)	3199	(0)
66	3199	(18)	3135	(4)	3211	(4)
67	3218	(3)	3157	(0)	3233	(0)
68	3233	(4)	3170	(0)	3246	(0)
69	3253	(6)	3186	(0)	3264	(0)

Table S14. Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses, in km/mol) for the $(C_8H_6S)Fe_2(CO)_4$ structure **4S-5.**

	M06L		BP86		B3LYP	
1	29	(0)	39	(0)	36	(1)
2	45	(0)	43	(0)	45	(0)
3	56	(1)	50	(0)	47	(2)
4	71	(0)	59	(1)	54	(1)
5	82	(0)	72	(0)	78	(0)
6	90	(0)	92	(1)	89	(2)
7	92	(0)	95	(0)	97	(1)
8	107	(0)	100	(1)	98	(1)
9	115	(2)	113	(2)	109	(1)
10	151	(2)	140	(1)	146	(0)
11	201	(10)	161	(11)	171	(9)
12	219	(1)	201	(2)	205	(2)
13	287	(6)	285	(5)	272	(7)
14	313	(3)	322	(4)	320	(2)
15	337	(4)	330	(6)	333	(3)
16	351	(3)	347	(0)	343	(7)
17	389	(4)	352	(4)	354	(0)
18	391	(1)	397	(9)	390	(8)
19	425	(5)	408	(12)	408	(13)
20	434	(0)	419	(2)	432	(3)
21	449	(0)	432	(1)	438	(5)
22	467	(2)	453	(3)	457	(1)
23	479	(3)	467	(3)	468	(4)
24	497	(14)	492	(7)	490	(34)
25	498	(2)	496	(2)	496	(10)
26	507	(1)	516	(12)	504	(11)
27	521	(9)	520	(6)	523	(25)
28	541	(22)	531	(53)	531	(42)
29	548	(98)	544	(3)	539	(23)
30	572	(12)	564	(12)	563	(22)
31	578	(35)	580	(35)	569	(46)
32	599	(51)	584	(40)	598	(35)
33	630	(10)	602	(11)	615	(11)
34	639	(20)	618	(19)	632	(21)
35	648	(13)	639	(8)	647	(38)
36	656	(30)	646	(38)	658	(4)
37	713	(11)	680	(9)	698	(11)
38	757	(2)	746	(9)	773	(6)
39	795	(14)	779	(24)	807	(26)
40	839	(0)	817	(6)	850	(2)
41	842	(7)	819	(1)	853	(6)
42	846	(8)	824	(7)	859	(8)
43	854	(18)	830	(17)	866	(18)
44	871	(3)	847	(4)	889	(8)
45	917	(4)	887	(3)	944	(3)

46	1000	(1)	972	(1)	1006	(1)
47	1047	(5)	1015	(5)	1047	(6)
48	1066	(1)	1035	(0)	1066	(1)
49	1109	(8)	1075	(10)	1107	(10)
50	1152	(2)	1124	(1)	1164	(1)
51	1188	(0)	1153	(0)	1198	(0)
52	1262	(1)	1217	(1)	1259	(0)
53	1307	(15)	1272	(14)	1317	(13)
54	1387	(3)	1336	(2)	1379	(2)
55	1409	(1)	1348	(2)	1399	(1)
56	1416	(1)	1360	(2)	1404	(2)
57	1447	(7)	1394	(7)	1448	(7)
58	1510	(1)	1452	(1)	1502	(3)
59	1566	(5)	1497	(11)	1544	(5)
60	2009	(48)	1933	(5)	2016	(99)
61	2031	(738)	1953	(1122)	2026	(954)
62	2036	(1209)	1961	(685)	2043	(1365)
63	2087	(1357)	2003	(1159)	2090	(1433)
64	3182	(6)	3118	(1)	3193	(1)
65	3199	(9)	3136	(1)	3209	(1)
66	3223	(1)	3154	(1)	3230	(1)
67	3238	(2)	3172	(0)	3245	(0)
68	3246	(3)	3179	(0)	3251	(0)
69	3261	(6)	3193	(0)	3268	(0)

Table S15. Cartesian coordinates and total energy for the $(C_8H_6S)Fe_2(CO)_6$ structure **6S-1.**

	M06L			BP86			B3LYP		
	E=-3914.197202a.u.			E=-3914. 908724a.u.			E=-3914.371787 a.u.		
	x	y	z	x	y	z	x	y	z
C	0.112640	0.424103	0.208787	0.091506	0.427260	0.180710	0.096102	0.435605	0.226377
C	-0.473855	-0.742879	-0.475530	-0.472728	-0.775108	-0.485984	-0.478234	-0.744054	-0.467455
C	1.689520	-1.697139	0.643649	1.718042	-1.702048	0.672031	1.721575	-1.699457	0.645718
C	1.609138	-0.745733	1.725192	1.620688	-0.712661	1.731400	1.638582	-0.733131	1.716820
C	0.814735	0.392919	1.443562	0.831014	0.433637	1.406847	0.834673	0.405873	1.436591
C	-0.739941	1.506267	-0.288750	-0.772687	1.501693	-0.343439	-0.775836	1.517355	-0.266154
C	-1.316850	1.110295	-1.540527	-1.387633	1.060157	-1.575436	-1.352802	1.113855	-1.517530
C	-1.159546	-0.297325	-1.651487	-1.223624	-0.364611	-1.647329	-1.175906	-0.297799	-1.633912
H	2.384149	-2.526643	0.760677	2.412749	-2.539098	0.819688	2.408710	-2.534187	0.778215
H	2.164808	-0.835292	2.653672	2.164752	-0.782536	2.679887	2.192170	-0.816575	2.648783
H	0.780890	1.243155	2.119819	0.791171	1.302169	2.074530	0.815159	1.256283	2.114934
H	-0.693885	2.531301	0.064367	-0.730923	2.544301	-0.013887	-0.733024	2.544954	0.082650
H	-1.794907	1.756844	-2.264955	-1.871764	1.689672	-2.325845	-1.824926	1.758009	-2.251025
H	-1.488069	-0.926753	-2.468516	-1.559204	-1.021890	-2.453085	-1.492639	-0.922967	-2.461453
S	0.183970	-2.321585	-0.153748	0.219351	-2.346421	-0.153604	0.207445	-2.328616	-0.157055
Fe	-2.385317	0.188054	-0.051506	-2.455720	0.186572	-0.038528	-2.448614	0.179892	-0.030065
Fe	2.386396	0.165024	0.086363	2.445756	0.160416	0.077410	2.433440	0.166881	0.065743
C	2.748942	1.925640	0.131449	2.841527	1.904837	0.086884	2.827695	1.926719	0.117787
C	-2.280331	-0.012615	1.740972	-2.383335	0.057943	1.752178	-2.371833	-0.011602	1.763348
C	4.087383	-0.303853	0.374462	4.132384	-0.289083	0.407435	4.127713	-0.320601	0.360475
C	2.239104	-0.082192	-1.681977	2.375356	-0.119561	-1.683022	2.323529	-0.074711	-1.706168
C	-3.475817	-1.196741	-0.387480	-3.564589	-1.179705	-0.321039	-3.542012	-1.204658	-0.389106
C	-3.715112	1.388251	-0.132380	-3.773280	1.376109	-0.154736	-3.774485	1.387697	-0.126909
O	-2.193356	-0.142532	2.889225	-2.366769	-0.013522	2.921235	-2.334965	-0.122563	2.913374
O	-4.553397	2.189783	-0.165218	-4.631047	2.174634	-0.205679	-4.601972	2.195402	-0.166068
O	-4.148574	-2.116243	-0.603468	-4.282116	-2.089890	-0.498321	-4.217035	-2.115724	-0.615190
O	5.193222	-0.618123	0.545273	5.254240	-0.579842	0.601382	5.223349	-0.655797	0.535709
O	2.106717	-0.295266	-2.816711	2.339694	-0.340096	-2.835880	2.261578	-0.270134	-2.847029
O	2.949813	3.070973	0.154520	3.104349	3.050626	0.080570	3.058719	3.062530	0.143438

Table S16. Cartesian coordinates and total energy for the $(C_8H_6S)Fe_2(CO)_6$ structure **6S-2.**

	M06L			BP86			B3LYP		
	E=-3914.181754a.u.			E=- 3914.891437a.u.			E=-3914.354821 a.u.		
	x	y	z	x	y	z	x	y	z
C	-0.273899	-0.172021	-1.192353	-0.268379	-0.238385	-1.176865	-0.274557	-0.163204	-1.143770
C	0.539849	-1.283318	-0.617950	0.535541	-1.346031	-0.547847	0.538041	-1.289890	-0.558850
C	-1.946370	-1.851438	-0.045232	-1.976973	-1.883748	0.047845	-1.980330	-1.871205	-0.029572
C	-2.380704	-1.320795	-1.311155	-2.396165	-1.407993	-1.257513	-2.364365	-1.358370	-1.320191
C	-1.494988	-0.404329	-1.921243	-1.496825	-0.505125	-1.899326	-1.468475	-0.432509	-1.907304
C	0.848127	0.695651	-1.654249	0.864832	0.607103	-1.687579	0.862784	0.688510	-1.637936
C	1.937241	-0.154946	-2.040329	1.961054	-0.278337	-2.029834	1.922243	-0.197761	-2.037389
C	1.759823	-1.398862	-1.368660	1.772738	-1.493119	-1.279921	1.730568	-1.432582	-1.340288
H	-2.676913	-2.411305	0.535031	-2.715240	-2.427666	0.650972	-2.723704	-2.446370	0.520612
H	-3.376364	-1.502669	-1.707033	-3.385295	-1.630352	-1.675491	-3.338288	-1.563459	-1.760568
H	-1.769140	0.157674	-2.810727	-1.759181	0.008685	-2.832349	-1.715535	0.100455	-2.823726
H	0.726671	1.709324	-2.024937	0.744866	1.606741	-2.117415	0.748440	1.692615	-2.037230
H	2.765558	0.106219	-2.687774	2.778110	-0.073222	-2.726878	2.728863	0.021300	-2.729505
H	2.407217	-2.265060	-1.424292	2.417834	-2.375353	-1.295299	2.359732	-2.313722	-1.407711
S	-0.317785	-2.566712	0.193232	-0.332463	-2.581323	0.339933	-0.337649	-2.558059	0.284497
Fe	2.080572	0.135350	-0.032655	2.156550	0.143897	-0.042598	2.163341	0.137988	-0.027795
Fe	-2.021390	0.234044	-0.032110	-2.084689	0.222951	-0.041094	-2.086042	0.237562	-0.035396
C	-1.860204	1.982151	-0.417842	-1.967890	1.947178	-0.495808	-1.949631	1.988814	-0.436908
C	3.627196	1.019060	-0.253905	3.652975	1.053633	-0.358662	3.645899	1.099396	-0.343839
C	-3.764518	0.384235	0.399775	-3.827586	0.386872	0.323970	-3.854283	0.357707	0.306292
C	-1.363513	0.167742	1.636342	-1.502679	0.269950	1.645250	-1.528961	0.227191	1.670513
C	2.727613	-0.914432	1.263523	2.921961	-0.815009	1.244409	2.977787	-0.911973	1.179978
C	1.266958	1.384617	0.969830	1.365133	1.386596	0.972390	1.368132	1.303240	1.082708
O	4.623996	1.600840	-0.388350	4.634635	1.670613	-0.547502	4.586862	1.744018	-0.547928
O	0.816030	2.274646	1.564117	0.946546	2.281847	1.603193	0.945799	2.135579	1.768010
O	3.085523	-1.636098	2.098743	3.397491	-1.465785	2.097258	3.456804	-1.618082	1.962113
O	-4.883414	0.493765	0.688830	-4.964785	0.525387	0.579028	-4.985587	0.439527	0.535556
O	-0.967804	0.021599	2.715007	-1.186017	0.226315	2.770978	-1.230770	0.143482	2.783089
O	-1.707690	3.103883	-0.674272	-1.884934	3.080720	-0.786646	-1.825108	3.109180	-0.697281

Table S17. Cartesian coordinates and total energy for the $(C_8H_6S)Fe_2(CO)_6$ structure **6S-3.**

	M06L			BP86			B3LYP		
	E=-3914.170379a.u.			E=-3914.878276a.u.			E=-3914.340683 a.u.		
	x	y	z	x	y	z	x	y	z
C	0.646270	-0.904619	-1.403576	0.642912	-0.924741	-1.403367	0.650465	-0.954127	-1.395706
C	1.086330	-1.762203	-0.338626	1.086344	-1.789943	-0.329087	1.115061	-1.774482	-0.306676
C	-1.522334	-1.989520	0.174817	-1.540995	-2.014581	0.186686	-1.501340	-2.029303	0.239604
C	-1.728977	-1.545178	-1.158198	-1.760093	-1.559493	-1.154989	-1.720446	-1.614349	-1.099228
C	-0.766905	-0.653680	-1.714573	-0.779292	-0.678618	-1.725997	-0.777046	-0.743547	-1.711641
C	1.815574	-0.436337	-2.077069	1.822913	-0.443612	-2.078783	1.802581	-0.482578	-2.093744
C	2.966996	-0.976116	-1.434601	2.985923	-0.994401	-1.433654	2.975420	-0.995418	-1.451707
C	2.512116	-1.762301	-0.332320	2.528506	-1.784532	-0.320045	2.545262	-1.772446	-0.330950
H	-2.325948	-2.543126	0.654180	-2.353355	-2.561312	0.681549	-2.299033	-2.576122	0.738807
H	-2.656637	-1.775246	-1.673132	-2.687692	-1.808465	-1.682679	-2.656850	-1.861820	-1.592828
H	-0.973820	-0.222912	-2.691407	-0.985639	-0.242342	-2.711000	-0.998754	-0.365358	-2.707838
H	1.814591	0.237811	-2.925457	1.822592	0.227706	-2.942259	1.783589	0.164138	-2.965285
H	3.998270	-0.792522	-1.702506	4.027093	-0.804112	-1.701608	4.001950	-0.811600	-1.745535
H	3.136247	-2.288967	0.378396	3.160066	-2.323220	0.390965	3.187897	-2.289661	0.373349
S	0.032245	-2.610391	0.747529	0.022578	-2.657009	0.751319	0.074218	-2.622255	0.816243
Fe	1.847794	0.225687	-0.085234	1.848866	0.230462	-0.064056	1.846540	0.246830	-0.077648
Fe	-1.812919	0.164179	-0.038219	-1.829145	0.163869	-0.044898	-1.822892	0.164693	-0.037841
C	-1.361291	1.862906	-0.439099	-1.383974	1.842968	-0.485680	-1.404200	1.841192	-0.514950
C	-2.450473	0.230545	1.643576	-2.456683	0.219841	1.627843	-2.448679	0.292747	1.649312
C	-3.482943	0.352597	-0.700183	-3.497555	0.371634	-0.664923	-3.507726	0.296496	-0.694826
C	0.207120	0.522576	1.038698	0.228773	0.619885	1.012325	0.195030	0.632991	0.973461
C	2.933248	0.495567	1.281790	2.925031	0.468289	1.305110	2.883753	0.489788	1.347884
C	1.904913	1.940278	-0.521255	1.995346	1.928056	-0.516379	1.987144	1.951867	-0.559265
O	-2.834287	0.243184	2.735106	-2.863300	0.236882	2.725061	-2.834006	0.345426	2.735554
O	2.034052	3.053708	-0.831809	2.185431	3.043580	-0.832415	2.152108	3.047009	-0.899322
O	3.673478	0.650646	2.163193	3.683763	0.607174	2.190201	3.586572	0.619966	2.256847
O	-4.553587	0.549159	-1.105882	-4.587240	0.600477	-1.039336	-4.576919	0.473348	-1.102260
O	0.171115	0.893685	2.166707	0.168788	1.092231	2.112282	0.150412	1.112236	2.064966
O	-1.112429	2.955573	-0.740698	-1.167440	2.945502	-0.822993	-1.177266	2.922506	-0.864194

Table S18. Cartesian coordinates and total energy for the $(C_8H_6S)Fe_2(CO)_5$ structure **5S-1.**

	M06L			BP86			B3LYP		
	E=-3800. 846562a.u.			E=-3801.552602a.u.			E=-3801.022021 a.u.		
	x	y	z	x	y	z	x	y	z
C	0.400803	-0.902310	-1.517897	-0.230409	0.976737	-1.466075	0.499583	-0.952785	-1.491822
C	1.029523	-1.707573	-0.489913	-0.881684	1.782142	-0.425475	1.072098	-1.735616	-0.408281
C	-1.447826	-1.905809	0.325303	1.586922	1.862006	0.451259	-1.4665	-1.921335	0.304652
C	-1.908522	-1.579196	-0.998136	2.096241	1.587073	-0.88069	-1.847218	-1.603721	-1.04913
C	-1.001094	-0.920905	-1.847233	1.179508	1.018314	-1.80467	-0.899663	-0.949205	-1.857247
C	1.425923	-0.075239	-2.075316	-1.284655	0.211559	-2.102646	1.567588	-0.187274	-2.062525
C	2.671988	-0.403643	-1.458271	-2.548889	0.590365	-1.538221	2.781294	-0.510502	-1.375725
C	2.426029	-1.420689	-0.488977	-2.297072	1.561093	-0.500384	2.472743	-1.480653	-0.368003
H	-2.182572	-2.311560	1.017506	2.308629	2.183655	1.21275	-2.23521	-2.346859	0.948028
H	-2.945406	-1.707912	-1.295499	3.155889	1.696916	-1.140798	-2.865342	-1.742867	-1.406226
H	-1.322782	-0.524221	-2.805458	1.506926	0.670897	-2.790573	-1.1816	-0.569952	-2.83688
H	1.267946	0.681977	-2.834343	-1.131635	-0.51878	-2.902125	1.463585	0.525255	-2.874063
H	3.634647	0.030457	-1.692369	-3.529677	0.219499	-1.84405	3.766145	-0.115544	-1.596729
H	3.157503	-1.870842	0.170353	-3.048445	2.043461	0.130144	3.173693	-1.920693	0.333149
S	0.116825	-2.756549	0.556567	0.04105	2.791936	0.663948	0.099939	-2.76533	0.625245
Fe	1.363056	0.297623	-0.018242	-1.372931	-0.279877	-0.018301	1.412668	0.319094	-0.003026
Fe	-1.395200	0.157934	-0.038443	1.407794	-0.176013	-0.060267	-1.437275	0.164106	-0.050647
C	-1.313994	1.726647	-0.917943	1.573481	-1.697525	-0.986762	-1.43959	1.741465	-0.93136
C	1.581506	2.051874	-0.109666	-1.651164	-2.003233	-0.272557	1.615258	2.071267	-0.217521
C	-3.077376	0.423455	0.428122	2.876566	-0.556371	0.80873	-3.141492	0.350745	0.392706
C	-0.711415	0.609853	1.569437	0.319461	-0.706849	1.340836	-0.785676	0.656292	1.547638
C	1.946374	0.247142	1.648425	-2.261601	-0.315418	1.496461	1.962069	0.387973	1.681249
O	1.776701	3.195929	-0.195486	-1.901964	-3.13339	-0.471091	1.803916	3.203238	-0.38504
O	2.420545	0.185123	2.708751	-2.916052	-0.334128	2.470691	2.415898	0.409247	2.747611
O	-4.174471	0.614335	0.762380	3.863717	-0.815232	1.392246	-4.246187	0.48164	0.717918
O	-0.605748	0.920697	2.689482	0.262959	-1.142872	2.447787	-0.693222	0.993671	2.659137
O	-1.263814	2.721510	-1.515010	1.730695	-2.695983	-1.585203	-1.458342	2.743809	-1.510059

Table S19. Cartesian coordinates and total energy for the $(C_8H_6S)Fe_2(CO)_4$ structure **4T-1.**

	M06L			BP86			B3LYP		
	E=-3687.478895a.u.			E=-3688.144659a.u.			E=-3687.6481954a.u.		
	x	y	z	x	y	z	x	y	z
C	0.579433	1.138473	1.204269	0.563475	1.104027	1.220818	-0.818647	-1.105917	1.199138
C	1.127321	1.685376	-0.035469	1.127536	1.685941	-0.018500	-1.262416	-1.671469	-0.074254
C	-1.418258	1.679092	-0.672712	-1.438018	1.720153	-0.649969	1.353413	-1.814832	-0.504977
C	-1.780841	1.680481	0.722315	-1.809148	1.695735	0.753776	1.571726	-1.728017	0.919155
C	-0.795378	1.251909	1.628718	-0.814066	1.248573	1.662602	0.540432	-1.188796	1.705080
C	1.671578	0.511343	1.892919	1.658306	0.438476	1.898660	-1.965782	-0.494348	1.812017
C	2.829568	0.641167	1.103115	2.833995	0.591999	1.110904	-3.059753	-0.638451	0.931376
C	2.511799	1.392760	-0.080941	2.523408	1.388877	-0.062277	-2.638898	-1.379957	-0.229725
H	-2.204395	1.904629	-1.390080	-2.224305	1.950692	-1.379920	2.186980	-2.163236	-1.113010
H	-2.795910	1.871881	1.058504	-2.831599	1.893427	1.096857	2.542528	-1.939015	1.362109
H	-1.033851	1.093348	2.676277	-1.051137	1.086947	2.720254	0.711743	-0.976579	2.758429
H	1.588223	-0.037653	2.823945	1.573477	-0.131044	2.828528	-1.969135	0.038959	2.757272
H	3.808586	0.247965	1.346241	3.820541	0.187308	1.351666	-4.062362	-0.258037	1.098221
H	3.198379	1.665781	-0.871611	3.221926	1.679431	-0.850856	-3.263943	-1.661434	-1.070247
S	0.112499	2.462816	-1.218802	0.110045	2.526267	-1.176067	-0.176490	-2.541333	-1.145879
Fe	1.332482	-0.411134	-0.085824	1.343544	-0.427611	-0.106881	-1.360256	0.488621	-0.162462
Fe	-1.281631	-0.222714	0.145706	-1.28301	-0.210992	0.157368	1.321602	0.190618	0.143620
C	-0.427579	-0.932577	-1.302387	-0.300398	-0.923851	-1.235894	0.649888	0.850525	-1.384998
C	-1.196022	-1.551082	1.359673	-1.381269	-1.540486	1.357101	1.294521	1.622997	1.244257
C	-2.912707	-0.669435	-0.358257	-2.826893	-0.683168	-0.522724	3.050465	0.420476	-0.225180
C	2.242158	-1.855003	-0.690055	2.323177	-1.831031	-0.643352	-2.041600	2.126047	-0.632899
O	-1.116859	-2.395102	2.155508	-1.481079	-2.412244	2.138441	1.289223	2.542199	1.950624
O	2.864269	-2.760674	-1.073332	2.996817	-2.73359	-0.978804	-2.509332	3.148925	-0.908333
O	-3.978230	-0.974644	-0.711188	-3.857419	-1.007742	-0.986492	4.166263	0.580221	-0.497116
O	-0.302878	-1.307826	-2.411800	-0.233837	-1.328278	-2.359268	0.509213	1.225020	-2.485521

Table S20. Cartesian coordinates and total energy for the $(C_8H_6S)Fe_2(CO)_4$ structure **4T-2.**

	M06L			BP86			B3LYP		
	E=-3687.476531a.u.			E=-3688.143432a.u.			E=-3687.645350a.u.		
	x	y	z	x	y	z	x	y	z
C	-0.163637	1.176237	-1.258681	-0.220333	1.187653	-1.267381	-0.167681	1.158737	-1.252042
C	-0.739962	1.761005	-0.066126	-0.777703	1.777326	-0.051208	-0.791900	1.752993	-0.088658
C	1.756788	1.733679	0.752173	1.759756	1.738196	0.723506	1.708992	1.821458	0.788971
C	2.187357	1.551915	-0.587086	2.167951	1.553612	-0.635367	2.160708	1.655958	-0.547894
C	1.244871	1.140034	-1.568200	1.190514	1.157951	-1.607646	1.254668	1.181587	-1.534438
C	-1.274190	0.625135	-2.020689	-1.353300	0.619044	-2.008962	-1.249277	0.606158	-2.062760
C	-2.476664	0.913287	-1.344721	-2.552012	0.894275	-1.290804	-2.480102	0.910248	-1.446045
C	-2.145890	1.579644	-0.110327	-2.194571	1.583815	-0.060259	-2.197638	1.570458	-0.191628
H	2.501405	1.918352	1.521032	2.524399	1.915704	1.488866	2.436163	2.051726	1.564204
H	3.246587	1.526074	-0.826768	3.230392	1.545442	-0.906012	3.224044	1.684703	-0.777922
H	1.562642	0.878298	-2.571810	1.493085	0.888871	-2.625199	1.601016	0.946559	-2.537110
H	-1.172063	0.103764	-2.964491	-1.272443	0.096858	-2.966074	-1.110254	0.089322	-3.006864
H	-3.473856	0.651094	-1.671534	-3.564629	0.621372	-1.595595	-3.465898	0.653772	-1.816866
H	-2.844927	1.915727	0.644728	-2.885640	1.915336	0.718668	-2.931580	1.919506	0.526586
S	0.213979	2.566505	1.150759	0.216765	2.588737	1.153815	0.117159	2.602353	1.152957
Fe	-1.269579	-0.336978	-0.146273	-1.286175	-0.350679	-0.122349	-1.311210	-0.396503	-0.149951
Fe	1.269591	-0.190541	0.036551	1.264691	-0.197300	0.009261	1.345788	-0.169900	0.077198
C	2.512183	-1.420968	-0.423881	2.523555	-1.374527	-0.465112	2.561298	-1.376575	-0.527583
C	-0.611969	-1.891603	-0.711599	-0.633267	-1.893695	-0.687152	-0.738781	-1.996123	-0.681235
C	0.975833	-0.862962	1.665404	1.105500	-0.860939	1.647469	1.171511	-0.931007	1.679804
C	-2.496559	-1.168343	0.856953	-2.479478	-1.200519	0.880598	-2.546259	-1.131269	0.930299
O	-0.320196	-2.939302	-1.133243	-0.366694	-2.961362	-1.111627	-0.461695	-3.055506	-1.067586
O	-3.312939	-1.713907	1.478382	-3.290205	-1.773091	1.509971	-3.365799	-1.603397	1.598512
O	0.826111	-1.279549	2.744052	1.069731	-1.284205	2.745415	1.116677	-1.419085	2.734106
O	3.325431	-2.212774	-0.687922	3.380357	-2.137479	-0.731446	3.380781	-2.121076	-0.878597

Table S21. Cartesian coordinates and total energy for the $(C_8H_6S)Fe_2(CO)_4$ **4T-3.**

	M06L			BP86			B3LYP		
	E=-3687.475175a.u.			E=-3688.137369a.u.			E=-3687.646646.a.u.		
	x	y	z	x	y	z	x	y	z
C	0.134480	-1.425416	-1.112194	0.249486	-1.434751	-1.147375	0.230804	-1.297164	-1.127472
C	-0.004398	-1.868815	0.253232	0.111952	-1.912477	0.222162	0.284077	-1.830938	0.214484
C	-2.449096	-0.878262	0.026418	-2.403091	-1.046888	-0.016984	-2.335807	-1.262386	0.199866
C	-2.260583	-0.837372	-1.385392	-2.185212	-0.919263	-1.429343	-2.255353	-1.191338	-1.223674
C	-0.955309	-0.909500	-1.916146	-0.858530	-0.922189	-1.946244	-1.004021	-0.967217	-1.836748
C	1.528614	-1.425788	-1.409380	1.659532	-1.364755	-1.427553	1.579308	-1.180836	-1.585808
C	2.230804	-1.921898	-0.258860	2.377662	-1.822167	-0.254268	2.446198	-1.701242	-0.560841
C	1.287178	-2.208816	0.761621	1.425802	-2.168772	0.758736	1.647155	-2.114931	0.543572
H	-3.449665	-0.720247	0.418841	-3.424470	-0.946898	0.368965	-3.320525	-1.333298	0.657484
H	-3.075461	-0.501402	-2.025008	-3.013179	-0.591493	-2.073898	-3.165320	-1.060754	-1.811697
H	-0.783327	-0.735418	-2.973355	-0.679345	-0.681138	-2.999786	-0.946455	-0.791441	-2.907918
H	1.973139	-1.121408	-2.348803	2.107550	-1.016401	-2.361785	1.889224	-0.819067	-2.560550
H	3.301876	-2.057587	-0.183916	3.463627	-1.898628	-0.161370	3.525493	-1.783099	-0.628152
H	1.495567	-2.582989	1.755237	1.644292	-2.537301	1.763582	1.998433	-2.541015	1.476469
S	-1.546802	-2.033547	1.066700	-1.447523	-2.186858	1.008616	-1.143276	-2.230282	1.162698
Fe	1.252802	-0.132603	0.219331	1.251659	-0.087965	0.211759	1.461258	0.059493	0.153425
Fe	-1.219668	0.708936	-0.550212	-1.225696	0.649164	-0.501933	-1.559271	0.583419	-0.466392
C	-0.065391	1.848098	-1.382651	-0.218536	1.944344	-1.252488	-0.872238	1.945137	-1.446869
C	2.674900	0.928615	0.187223	2.555368	1.096209	0.108712	2.846780	1.170478	0.015055
C	-1.819051	1.838639	0.696304	-1.980973	1.711677	0.706057	-2.080645	1.502575	0.981460
C	0.653343	0.622719	1.717562	0.707508	0.616034	1.737915	0.938676	0.796239	1.698914
O	3.621265	1.605727	0.183699	3.454452	1.854054	0.069877	3.769446	1.870139	-0.058285
O	0.350984	1.043063	2.761051	0.446418	1.038483	2.805627	0.694187	1.233402	2.745350
O	-2.269541	2.586814	1.465980	-2.536635	2.440960	1.443376	-2.468680	2.084788	1.906365
O	0.633824	2.601635	-1.932443	0.353396	2.842553	-1.754507	-0.456164	2.822571	-2.083842

Table S22. Cartesian coordinates and total energy for the $(C_8H_6S)Fe_2(CO)_4$ structure **4T-4.**

	M06L			BP86			B3LYP (Collapsesto **4T-2**)		
	E=-3687.466016a.u.			E=-3688.133521a.u.			E=-3687.645350a.u.		
	x	y	z	x	y	z	x	y	z
C	1.088801	-0.739219	-1.397639	1.061222	-0.864019	-1.338082	-0.167681	1.158758	-1.252031
C	1.294315	-1.498636	-0.185706	1.240272	-1.575820	-0.079052	-0.791879	1.753003	-0.088631
C	-1.308082	-2.018157	-0.359429	-1.390312	-2.031155	-0.257087	1.709020	1.821432	0.788975
C	-1.307055	-1.397178	-1.628395	-1.366674	-1.483787	-1.577150	2.160721	1.655942	-0.547898
C	-0.193310	-0.606117	-2.021905	-0.214467	-0.758596	-2.015212	1.254667	1.181588	-1.534436
C	2.219830	0.128995	-1.537126	2.227344	-0.026680	-1.512642	-1.249291	0.606213	-2.062753
C	3.117388	-0.115178	-0.448978	3.116675	-0.242359	-0.392489	-2.480105	0.910304	-1.446017
C	2.546743	-1.114181	0.384058	2.507355	-1.190878	0.492233	-2.197620	1.570484	-0.191589
H	-2.191479	-2.569349	-0.049211	-2.302580	-2.531908	0.088902	2.436202	2.051686	1.564203
H	-2.215310	-1.381644	-2.221935	-2.277982	-1.477301	-2.185636	3.224056	1.684668	-0.777933
H	-0.265461	0.001831	-2.919368	-0.254730	-0.207375	-2.961955	1.601005	0.946567	-2.537113
H	2.347974	0.866815	-2.319008	2.390455	0.667632	-2.340920	-1.110282	0.089401	-3.006873
H	4.069234	0.373310	-0.289412	4.088558	0.234576	-0.247275	-3.465910	0.653856	-1.816836
H	2.966522	-1.506742	1.301163	2.914713	-1.553665	1.438863	-2.931556	1.919523	0.526635
S	0.149309	-2.679149	0.423472	0.056888	-2.729075	0.555496	0.117199	2.602341	1.152983
Fe	1.236619	0.543079	0.234199	1.220908	0.527968	0.241406	-1.311220	-0.396497	-0.149976
Fe	-1.220393	0.128339	-0.173680	-1.194451	0.112991	-0.198176	1.345788	-0.169911	0.077195
C	-2.239140	1.332495	-1.106465	-1.998917	1.423047	-1.128663	2.561301	-1.376587	-0.527576
C	1.248398	2.305328	0.157126	1.333324	2.274700	0.084801	-0.738793	-1.996118	-0.681258
C	-2.356303	-0.003482	1.251017	-2.447724	0.131553	1.081524	1.171468	-0.931027	1.679795
C	0.596689	0.572315	1.879644	0.536455	0.699007	1.858248	-2.546255	-1.131276	0.930276
O	1.266533	3.470280	0.103803	1.430999	3.444620	-0.013891	-0.461707	-3.055504	-1.067600
O	0.261636	0.585267	2.999468	0.197105	0.836694	2.980500	-3.365784	-1.603408	1.598501
O	-3.119624	-0.093900	2.120233	-3.318437	0.149737	1.869978	1.116598	-1.419112	2.734091
O	-2.880040	2.106276	-1.694566	-2.532647	2.286228	-1.724395	3.380797	-2.121082	-0.878576

Table S23. Cartesian coordinates and total energy for the $(C_8H_6S)Fe_2(CO)_4$ structure **4T-5.**

	M06L			BP86			B3LYP		
	E=-3687.463399a.u.			E=-3688.130477a.u.			E=-3687.644450a.u.		
	x	y	z	x	y	z	x	y	z
C	0.363129	0.995170	-0.224591	0.357024	0.960079	-0.25846	0.349929	0.949976	-0.206673
C	0.437985	0.151965	0.915640	0.431124	0.079852	0.872794	0.449773	0.068002	0.905206
C	-1.151913	-1.567851	-0.509960	-1.229994	-1.581683	-0.593733	-1.226310	-1.576391	-0.538464
C	-0.886817	-0.684565	-1.573646	-0.972787	-0.661866	-1.646651	-0.960987	-0.670844	-1.584234
C	-0.565422	0.685410	-1.313755	-0.59576	0.697086	-1.35108	-0.603474	0.684208	-1.299832
C	1.414964	1.940797	-0.105400	1.400589	1.929908	-0.099209	1.366356	1.932130	-0.050283
C	2.073095	1.729131	1.165461	2.056329	1.693673	1.182945	2.020452	1.709791	1.227042
C	1.473902	0.616423	1.801246	1.461997	0.540683	1.787194	1.456168	0.552669	1.820628
H	-1.394447	-2.615552	-0.651192	-1.504817	-2.628401	-0.760304	-1.487798	-2.615655	-0.717321
H	-1.117446	-1.023481	-2.581850	-1.235732	-0.965012	-2.669654	-1.224590	-0.976543	-2.597743
H	-0.565906	1.361902	-2.164625	-0.616091	1.415889	-2.179332	-0.599927	1.384437	-2.133105
H	1.664900	2.708954	-0.826737	1.647459	2.728319	-0.804082	1.580845	2.743579	-0.737883
H	2.896708	2.314673	1.552275	2.871191	2.28915	1.60106	2.811301	2.322004	1.645760
H	1.732932	0.192037	2.761892	1.718209	0.096351	2.751335	1.717897	0.113332	2.776289
S	-0.831975	-1.050872	1.168738	-0.874839	-1.111988	1.104669	-0.805841	-1.163491	1.159066
Fe	2.297604	0.019784	-0.052448	2.331975	0.004654	-0.068396	2.382708	0.019285	-0.064494
Fe	-2.411360	0.031255	-0.403467	-2.453618	0.037473	-0.393078	-2.498633	0.048408	-0.403069
C	-2.983494	1.619739	0.183981	-2.981132	1.596207	0.279207	-3.056724	1.657594	0.159302
C	-3.962050	-0.841097	-0.182624	-4.006823	-0.801824	-0.177502	-4.037365	-0.843488	-0.124221
C	2.724754	-1.664720	0.277415	2.885295	-1.621194	0.311429	2.882104	-1.667386	0.201760
C	3.837083	0.351317	-0.857124	3.852526	0.414179	-0.852829	3.919088	0.462296	-0.841699
O	4.864357	0.582976	-1.358320	4.884674	0.703905	-1.343026	4.933408	0.766127	-1.320478
O	2.999427	-2.769865	0.529646	3.271801	-2.696276	0.602885	3.217047	-2.760367	0.410268
O	-4.985361	-1.390147	-0.079888	-5.053334	-1.333694	-0.073059	-5.042029	-1.408316	0.020346
O	-3.328272	2.646797	0.609104	-3.311945	2.612267	0.770696	-3.388959	2.694222	0.560414

Table S24. Cartesian coordinates and total energy for the $(C_8H_6S)Fe_2(CO)_4$ structure **4S-1.**

	M06L			BP86			B3LYP		
	E=-3687.477876a.u.			E=-3688.152738a.u.			E=-3687.635906a.u.		
	x	y	z	x	y	z	x	y	z
C	-0.771511	-0.771293	1.326071	-0.863950	-0.763445	1.299335	-0.874715	-0.790292	1.302030
C	-1.127538	-1.689380	0.262844	-1.226306	-1.665399	0.204345	-1.205939	-1.681926	0.203225
C	1.463391	-1.824451	-0.033584	1.391349	-1.904678	-0.004217	1.418265	-1.864412	-0.001477
C	1.648809	-1.296601	1.293500	1.553607	-1.396292	1.345443	1.547258	-1.360479	1.346105
C	0.560919	-0.605038	1.863443	0.461538	-0.667524	1.895740	0.450662	-0.658321	1.883439
C	-1.921909	0.056781	1.552277	-2.009611	0.101664	1.512719	-2.033669	0.025645	1.536369
C	-2.979217	-0.378832	0.680424	-3.067231	-0.294551	0.600381	-3.069857	-0.381586	0.623732
C	-2.479773	-1.435441	-0.121886	-2.569707	-1.359065	-0.217325	-2.550096	-1.421754	-0.198358
H	2.336044	-2.260714	-0.515491	2.265423	-2.376785	-0.471116	2.297125	-2.339280	-0.435324
H	2.611892	-1.319883	1.795166	2.500771	-1.478255	1.891312	2.485361	-1.413781	1.894009
H	0.681608	-0.066947	2.799502	0.570704	-0.149921	2.856020	0.547643	-0.141672	2.836103
H	-1.974140	0.874232	2.261869	-2.065535	0.906696	2.250798	-2.110107	0.812420	2.279498
H	-3.973771	0.044513	0.630509	-4.060279	0.156362	0.537441	-4.069088	0.035290	0.569015
H	-3.009048	-1.942693	-0.919369	-3.098712	-1.841731	-1.044012	-3.066648	-1.906795	-1.020263
S	0.012011	-2.790657	-0.452898	-0.097950	-2.808243	-0.493968	-0.048672	-2.799447	-0.491653
Fe	-1.308838	0.276581	-0.361865	-1.327928	0.360297	-0.392136	-1.346103	0.342923	-0.387361
Fe	1.295121	0.265666	0.021482	1.312346	0.211322	0.082807	1.336528	0.244130	0.052414
C	0.339517	0.269858	-1.491408	0.351805	0.337686	-1.420685	0.375850	0.373766	-1.430137
C	1.135503	1.949444	0.645415	1.381812	1.874719	0.753890	1.366392	1.928419	0.715754
C	3.007241	0.479849	-0.377641	2.989015	0.325546	-0.428557	3.043012	0.328853	-0.416040
C	-1.757527	1.984282	-0.514296	-1.709699	2.078319	-0.484779	-1.772774	2.073980	-0.475216
O	1.011768	3.030962	1.050128	1.448433	2.969097	1.172266	1.379838	3.007316	1.135249
O	-2.118897	3.092452	-0.531198	-2.039621	3.209752	-0.481401	-2.125527	3.179378	-0.466057
O	4.121652	0.633011	-0.674050	4.101374	0.424967	-0.798166	4.146478	0.386479	-0.769087
O	-0.416463	0.092142	-2.403230	-0.289657	0.252630	-2.444217	-0.303653	0.308108	-2.410674

Table S25. Cartesian coordinates and total energy for the $(C_8H_6S)Fe_2(CO)_4$ structure **4S-2.**

	M06L			BP86			B3LYP		
	E=-3687.473158a.u.			E=-3688.152065a.u.			E=-3687.631676a.u.		
	x	y	z	x	y	z	x	y	z
C	0.234607	-1.453718	-1.049395	-0.033762	-1.417659	-1.089295	0.372190	-1.475708	-1.023039
C	0.578867	-1.726590	0.331439	0.283292	-1.782256	0.293647	0.673439	-1.715580	0.377542
C	-1.967355	-1.203063	0.721750	-2.202579	-0.989438	0.686579	-1.941734	-1.302170	0.684507
C	-2.210771	-1.419326	-0.690001	-2.483781	-1.157878	-0.738369	-2.097867	-1.516335	-0.742282
C	-1.106235	-1.376670	-1.556052	-1.368964	-1.254279	-1.614241	-0.965043	-1.413573	-1.563253
C	1.466835	-1.200220	-1.735719	1.243694	-1.265990	-1.768455	1.618893	-1.225622	-1.685149
C	2.547640	-1.345625	-0.818641	2.302611	-1.592408	-0.859612	2.671630	-1.309751	-0.723394
C	1.993325	-1.680639	0.457458	1.705092	-1.898878	0.422289	2.081795	-1.625743	0.548584
H	-2.830176	-1.146486	1.381995	-3.045042	-0.811343	1.367309	-2.837896	-1.334562	1.302412
H	-3.219707	-1.468209	-1.089476	-3.502422	-1.089258	-1.138492	-3.086038	-1.603500	-1.188995
H	-1.253989	-1.323023	-2.631583	-1.504964	-1.171857	-2.699610	-1.082494	-1.365302	-2.644697
H	1.547448	-0.921214	-2.779049	1.361550	-0.975423	-2.815939	1.730447	-0.984931	-2.737048
H	3.600494	-1.250475	-1.046337	3.369117	-1.625612	-1.091873	3.731291	-1.195238	-0.919004
H	2.543732	-1.835884	1.376815	2.235965	-2.178377	1.335822	2.611178	-1.748143	1.487271
S	-0.622889	-2.053997	1.562723	-0.965950	-2.045960	1.510233	-0.572665	-2.084020	1.574194
Fe	1.316027	0.187196	-0.176114	1.314527	0.114259	-0.132361	1.351768	0.239556	-0.173604
Fe	-1.309386	0.354415	-0.306223	-1.304023	0.449863	-0.324737	-1.338708	0.344826	-0.279031
C	-0.614300	1.408803	0.962864	-0.263872	1.279170	0.917422	-0.821575	1.438765	1.031539
C	1.578345	1.608797	-1.195225	1.777030	1.476558	-1.149125	1.564075	1.633463	-1.246097
C	-2.834857	1.206753	-0.328017	-2.565308	1.625633	-0.163522	-2.936375	1.080102	-0.434421
C	1.984298	1.001949	1.239124	2.276278	0.736210	1.199717	1.905207	1.154781	1.234104
O	1.780860	2.524233	-1.887855	2.128820	2.352624	-1.851140	1.733174	2.527135	-1.970970
O	2.513159	1.501146	2.148382	2.979015	1.126381	2.055965	2.368961	1.716196	2.139468
O	-3.835774	1.805161	-0.343675	-3.412511	2.443305	-0.077539	-3.966482	1.602599	-0.545797
O	-0.520327	2.145043	1.869065	-0.164135	1.998607	1.865388	-0.759556	2.159859	1.943500

Table S26. Cartesian coordinates and total energy for the $(C_8H_6S)Fe_2(CO)_4$ structure **4S-3.**

	M06L			BP86			B3LYP		
	E=-3687.468912a.u.			E=-3688.143070a.u.			E=-3687.627437a.u.		
	x	y	z	x	Y	z	x	y	z
C	-0.488509	-0.878731	-1.464833	-0.320306	-1.074360	-1.399518	-0.422047	-1.072504	-1.394864
C	-0.786569	-1.698004	-0.311436	-0.516084	-1.833976	-0.167607	-0.735923	-1.780510	-0.170529
C	-2.613342	0.146903	0.168874	-2.669850	-0.282798	0.124500	-2.670680	0.039216	0.076540
C	-2.447583	0.591055	-1.164721	-2.504594	0.117022	-1.231262	-2.419780	0.393558	-1.266843
C	-1.303282	0.238889	-1.914580	-1.282866	-0.107050	-1.934109	-1.231044	0.017743	-1.936650
C	0.803584	-1.261510	-1.924926	1.021501	-1.330317	-1.844575	0.873053	-1.500110	-1.809854
C	1.289458	-2.326914	-1.095371	1.652059	-2.240310	-0.910692	1.357971	-2.469706	-0.863923
C	0.301372	-2.603858	-0.110785	0.698239	-2.559272	0.115514	0.355957	-2.652398	0.134282
H	-3.445032	0.542237	0.744756	-3.573401	0.024076	0.663536	-3.542631	0.454571	0.575878
H	-3.063453	1.423985	-1.509493	-3.236259	0.826518	-1.650339	-3.031758	1.189348	-1.701508
H	-1.143227	0.647444	-2.906961	-1.154739	0.263587	-2.956657	-1.044203	0.358127	-2.951596
H	1.334659	-0.796548	-2.746614	1.492014	-0.878480	-2.721675	1.409650	-1.128090	-2.676113
H	2.235576	-2.838986	-1.208229	2.668505	-2.632943	-0.985526	2.308413	-2.988396	-0.913231
H	0.369342	-3.337426	0.682394	0.864087	-3.212933	0.975296	0.420489	-3.308028	0.995788
S	-2.231011	-1.521860	0.662612	-2.009599	-1.814718	0.774379	-2.233873	-1.563827	0.739613
Fe	0.957355	-0.637665	0.066153	1.083931	-0.485799	0.101397	1.001896	-0.621905	0.123878
Fe	-0.827881	1.334747	-0.192763	-1.033975	1.165499	-0.274966	-0.856423	1.299779	-0.278494
C	0.555780	2.150678	-0.916874	0.175915	2.209423	-0.979465	0.466237	2.207060	-1.017696
C	2.528819	0.167002	-0.043147	2.524413	0.498972	-0.131786	2.544582	0.221828	-0.114808
C	-0.530329	1.759535	1.505812	-0.935980	1.793427	1.375039	-0.663213	1.914434	1.380366
C	1.024038	-0.679227	1.829975	1.220753	-0.341102	1.846848	1.098898	-0.464276	1.888431
O	3.591818	0.635612	-0.125331	3.535391	1.081951	-0.284628	3.585552	0.708221	-0.279350
O	1.075495	-0.789821	2.987480	1.355173	-0.312161	3.015424	1.183376	-0.432708	3.044787
O	-0.336379	2.047426	2.617039	-0.872930	2.235575	2.463792	-0.539973	2.340142	2.452680
O	1.424237	2.725533	-1.443402	0.909282	2.979070	-1.491992	1.285501	2.845967	-1.539330

Table S27. Cartesian coordinates and total energy for the $(C_8H_6S)Fe_2(CO)_4$ structure **4S-4.**

	M06L			BP86			B3LYP		
	E=-3687.468615a.u.			E=-3688.142987a.u.			E=-3687. 627768a.u.		
	x	y	z	x	Y	z	x	y	z
C	0.796728	-1.540545	-0.689764	0.847495	-1.426679	-0.858336	0.853389	-1.483577	-0.762358
C	1.353652	-1.211976	0.608027	1.470263	-1.211103	0.447860	1.445049	-1.215383	0.535324
C	-1.147261	-1.315836	1.404649	-1.004382	-1.513176	1.359442	-1.057788	-1.439547	1.408860
C	-1.491448	-1.962046	0.179592	-1.395864	-2.044846	0.084371	-1.405731	-2.018996	0.155725
C	-0.602810	-1.863763	-0.909646	-0.554271	-1.803922	-1.041885	-0.553108	-1.830887	-0.956742
C	1.770581	-1.185854	-1.662324	1.764594	-0.936498	-1.847303	1.804248	-1.088457	-1.748524
C	2.925975	-0.655358	-1.008645	2.953654	-0.440456	-1.193617	2.977634	-0.592000	-1.095706
C	2.669597	-0.686791	0.398814	2.778121	-0.625419	0.225305	2.756435	-0.683554	0.318659
H	-1.892627	-1.315135	2.196605	-1.708064	-1.615638	2.194924	-1.777858	-1.521364	2.220982
H	-2.481657	-2.383485	0.034304	-2.374991	-2.517858	-0.053213	-2.384333	-2.471713	0.013086
H	-0.902638	-2.232951	-1.886257	-0.887583	-2.104384	-2.041921	-0.867663	-2.179438	-1.937781
H	1.605184	-1.203956	-2.734068	1.548343	-0.861263	-2.917549	1.624870	-1.082828	-2.819448
H	3.842865	-0.333079	-1.483463	3.841090	-0.034035	-1.684004	3.882715	-0.240937	-1.577506
H	3.331906	-0.342382	1.183540	3.487448	-0.352119	1.010870	3.447811	-0.381377	1.097967
S	0.497445	-1.436390	2.113753	0.697400	-1.634091	1.971186	0.623248	-1.529711	2.062320
Fe	1.263669	0.475492	-0.503941	1.273490	0.606598	-0.471694	1.291346	0.566891	-0.505938
Fe	-1.327549	0.068312	-0.185289	-1.339531	0.020877	-0.112827	-1.362409	0.049569	-0.133929
C	-1.369827	1.333820	1.080371	-1.669475	1.113223	1.252590	-1.630601	1.241374	1.177045
C	-0.459303	0.983441	-1.448906	-0.486209	1.158316	-1.188933	-0.487199	1.088607	-1.276540
C	-3.037339	0.154703	-0.673184	-2.964126	0.088288	-0.806048	-3.021742	0.053297	-0.781301
C	1.542116	1.870148	0.545556	1.519801	1.838780	0.761327	1.562441	1.917091	0.627352
O	0.303610	1.504652	-2.214105	0.074520	1.879988	-1.986244	0.154071	1.718015	-2.070039
O	1.810037	2.739233	1.276349	1.773428	2.624448	1.603260	1.818270	2.752634	1.391461
O	-4.143053	0.276546	-1.013086	-4.038512	0.192797	-1.273137	-4.090494	0.113896	-1.226842
O	-1.408751	2.121404	1.931095	-1.922585	1.819940	2.153725	-1.820352	1.995112	2.034339

Table S28. Cartesian coordinates and total energy for the $(C_8H_6S)Fe_2(CO)_4$ structure **4S-5.**

	M06L			BP86			B3LYP		
	E=-3687.467889a.u.			E=-3688.142451a.u.			E=-3687. 625363a.u.		
	x	y	z	x	Y	z	x	y	z
C	0.733409	-1.332796	-1.114318	0.275121	-1.434890	-1.128140	0.430135	-1.378957	-1.172758
C	0.655910	-1.737739	0.264950	0.105191	-1.778012	0.276979	0.341603	-1.794142	0.208296
C	-2.121116	-1.755200	-0.215914	-2.556764	-1.098287	-0.156679	-2.387129	-1.364510	-0.122855
C	-1.751797	-1.474943	-1.540805	-2.185207	-0.920642	-1.515109	-2.065591	-1.123247	-1.475070
C	-0.449518	-1.039767	-1.884047	-0.813230	-0.878149	-1.917603	-0.732557	-0.915863	-1.906451
C	2.094892	-1.006092	-1.362999	1.682332	-1.494128	-1.405114	1.815473	-1.270038	-1.488273
C	2.842775	-1.185571	-0.152320	2.378360	-1.869889	-0.193484	2.579506	-1.607027	-0.319936
C	1.947718	-1.657578	0.854763	1.398670	-2.060518	0.845181	1.661506	-1.947868	0.725536
H	-3.097002	-2.120811	0.082140	-3.599277	-1.088443	0.176811	-3.408838	-1.504729	0.217257
H	-2.553192	-1.388998	-2.269966	-2.957233	-0.579800	-2.215999	-2.881049	-0.850842	-2.142896
H	-0.307813	-0.586129	-2.860192	-0.576476	-0.507046	-2.920742	-0.570988	-0.509545	-2.901831
H	2.480561	-0.625169	-2.300085	2.144963	-1.243675	-2.363169	2.215337	-0.940530	-2.441191
H	3.908810	-1.048646	-0.033663	3.454662	-2.021707	-0.090027	3.660060	-1.644107	-0.249479
H	2.191298	-1.869553	1.887522	1.595987	-2.345531	1.881176	1.919728	-2.243591	1.736279
S	-0.900029	-1.947384	1.086485	-1.496796	-1.910296	1.062505	-1.211021	-2.093750	1.039094
Fe	1.328057	0.219620	0.148847	1.336897	-0.066171	0.140071	1.346313	0.073052	0.102349
Fe	-1.271929	0.085608	-0.207555	-1.194868	0.428931	-0.238480	-1.227999	0.330046	-0.170001
C	-1.464263	1.513593	-1.194211	-0.956767	1.884033	-1.138175	-1.362725	1.806761	-1.100685
C	1.713217	1.764500	-0.603160	2.282187	1.227363	-0.579027	1.995390	1.529091	-0.664262
C	-1.986633	0.979421	1.144425	-1.678645	1.418696	1.139912	-1.675205	1.209226	1.314785
C	1.082332	0.987606	1.709764	1.396403	0.728821	1.696462	1.393120	0.828082	1.696666
O	1.981354	2.774659	-1.122115	2.959909	2.064184	-1.058287	2.448278	2.464915	-1.185160
O	0.920794	1.472917	2.758906	1.467762	1.241825	2.755424	1.458061	1.298611	2.758304
O	-2.482166	1.604348	1.992885	-2.046214	2.131866	2.000956	-2.011383	1.815523	2.244187
O	-1.602870	2.464191	-1.854662	-0.853026	2.883722	-1.755681	-1.469359	2.781420	-1.724163

Table S29. Total energies (E, in hartree), relative energies (E, in kcal mol-1), and Fe–Fe and S-Fe distances (in Å) for the structures of $(C_8H_6S)Fe_2(CO)_6$ and $(C_8H_6S)Fe_2(CO)_5$ **6S-1(n=1-3) and 5S-1**.

	6S-1c	**6S-2**	**6S-3**	**5S-1**
M06L				
-E	3914.197202	3914.181754	3914.170379	3800.862415
ΔE	0.0	9.7	16.8	0.0
Fe-Fe	—	4.103	3.662	2.762
Fe-S	3.330, 3.593	3.286, 3.620	3.423, 3.469	3.337, 3.348
Image	0	0	0	0
BP86				
-E	3914.908724	3914.891437	3914.878276	3801.552602
ΔE	0.0	10.8	19.1	0.0
Fe-Fe	—	4.242	3.679	2,783
Fe-S	3.361, 3.686	3.329, 3.711	3.467, 3.513	3.347, 3.450
Image	0	0	0	0
B3LYP				
-E	3914.371787	3914.354821	3914.340683	3801.022021
ΔE	0.0	10. 6	19. 5	0.0
Fe-Fe	—	4.251	3.671	2.855
Fe-S	3.351, 3.656	3.313, 3.691	3.478, 3.489	3.377, 3.411
Image	0	0	0	0

Table S30. Total energies (E, in hartree), relative energies (E, in kcal mol^{-1}), and Fe–Fe and S-Fe distances (in Å) for the $(C_8H_6S)Fe_2(CO)_4$ structures **4T-n(n=1-5) .**

	4T-1	**4T-2**	**4T-3**	**4T-4**	**4T-5**
M06L					
-E	3687.478895	3687.476531	3687.475175	3687.466016	3687.463399
ΔE	0.0	1.5	2.3	8.1	9.7
Fe-Fe	2.631	2.550	2.723	2.525	—
Fe-S	3.319, 3.321	3.155, 3.509	3.200, 3.488	3.180, 3.406	2.477, 3.526
Image	0	0	0	0	0
$<S^2>$	2.214	2.119	2.107	2.142	2.092
BP86					
-E	3688.144659	3688.143432	3688.137109	3688.133521	3688.130477
ΔE	0.0	0.8	4.7	7.0	8.9
Fe-Fe	2.649	2.559	2.681	2.490	—
Fe-S	3.348, 3.375	3.189, 3.539	3.221, 3.511	3.196, 3.473	2.461, 2.593
Image	0	0	0	0	0
$<S^2>$	2.042	2.036	2.037	2.044	2.028
B3LYP				Collapses to **4T-2**	
-E	3687.648195	3687.646350	3687.646646	3687.646350	3687.644450
ΔE	0.0	1.2	1.0	1.2	2.3
Fe-Fe	2.703	2.676	3.128	2.676	—
Fe-S	3.372, 3.398	3.217, 3.568	3.278, 3,612	3.217, 3.568	2.603, 3.614
Image	0	0	0	0	0
$<S^2>$	2.449	2.2.112	2.081	2. 112	2.075

Table S31. Total energies (E, in hartree), relative energies (E, in kcal mol-1), and Fe–Fe and S-Fe distances (in Å) for the $(C_6H_8S)Fe_2(CO)_4$ structures **4S-n (n=1-5)**

	4S-1	**4S-2**	**4S-3**	**4S-4**	**4S-5**
M06L					
-E	3687.477876	3687.473158	3687.468912	3687.468615	3687.467889
ΔE	0.6	3.6	6.3	6.5	6.9
Fe-Fe	2.632	2.634	2.673	2.642	2.628
Fe-S	3.349, 3.341	3.125, 3.436	3.296, 3.362	3.299, 3.331	2.438, 3.246
Image	0	0	0	0	0
BP86					
-E	3688.152738	3688.152065	3688.143070	3688.142987	3688.142451
ΔE	-5.1	-4.6	1.0	1.0	1.4
Fe-Fe	2. 687	2. 647	2.712	2.702	2. 607
Fe-S	3.382, 3.400	3.116, 3.545	3.307, 3.433	3.351，3.365	2.694, 3.505
Image	0	0	0	0	0
B3LYP					
-E	3687.635906	3687.631676	3687.627437	3687.627768	3687.625363
ΔE	7.7	10.4	13.0	12.8	14.3
Fe-Fe	2.720	2.695	2.703	2.729	2.601
Fe-S	3.388, 3.401	3.150, 3.487	3.337, 3.426	3.356, 3.382	2.709, 3.480
Image	0	0	0	0	0

Table S32. Harmonic ν(CO) vibrational frequencies (in cm^{-1}) predicted by the BP86 method for $(C_8H_6S)Fe_2(CO)_n$ (n=6,5) structures. The infrared intensities (in km/mol) are in parentheses.

	BP86
6S-1	1957(585),1963(647),1974(702),1978(755),2008(1915),2029(366)
6S-2	1962(929),1966(114),1974(814),1983(502),2011(1041),2036(738)
6S-3	**1775(177)**,1955(287),1964(230),1979(1209),2000(1285), 2028(809)
5S-1	**1849(299)**,1955(151),1971(884),1992(1184),2019(879)

Table S33. Harmonic ν(CO) vibrational frequencies (in cm^{-1}) predicted by the BP86 method for $(C_8H_6S)Fe_2(CO)_4$ structures. The infrared intensities (in km/mol) are in parentheses.

	BP86
4T-1	**1819(361)**,1956(191),1965(1369),2002(996)
4T-2	1932(75),1945(946),1962(953),1999(1131)
4T-3	1931(84),1945(623),1956(1292),2005(1133)
4T-4	1926(34),1942(941),1955(1189),1996(1119)
4T-5	1941(563),1943(1074),1980(2418),1995(12)
4S-1	**1757(362)**,1950(249),1963(1103),2004(1059)
4S-2	**1834(292)**,1951(921),1962(824),2005(981)
4S-3	1927(156),1955(584),1961(1046),2006(1083)
4S-4	1753(382),1948(286),1963(1144),2008(925)
4S-5	1933(5),1953(1122),1961(685),2003(1159)

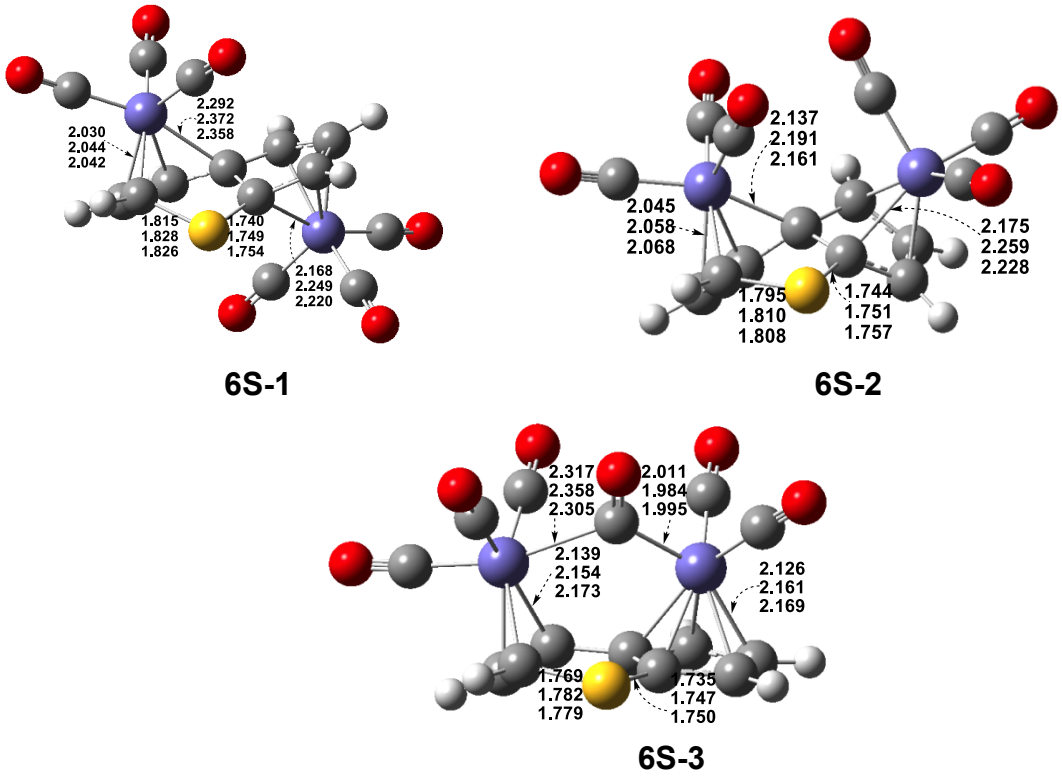

Figure S1. The $(C_8H_6S)Fe_2(CO)_6$ structures**.**

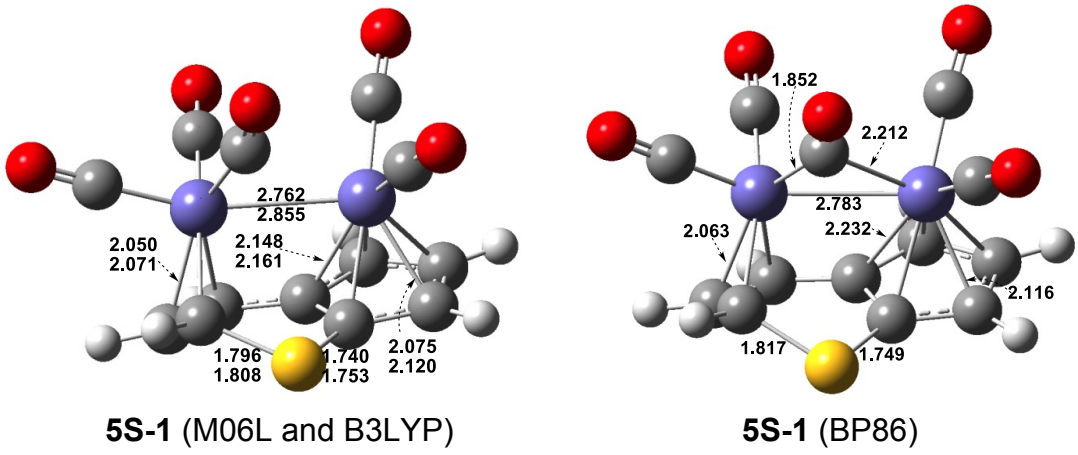

Figure S2. The only $(C_8H_6S)Fe_2(CO)_5$ structure **5S-1 .**

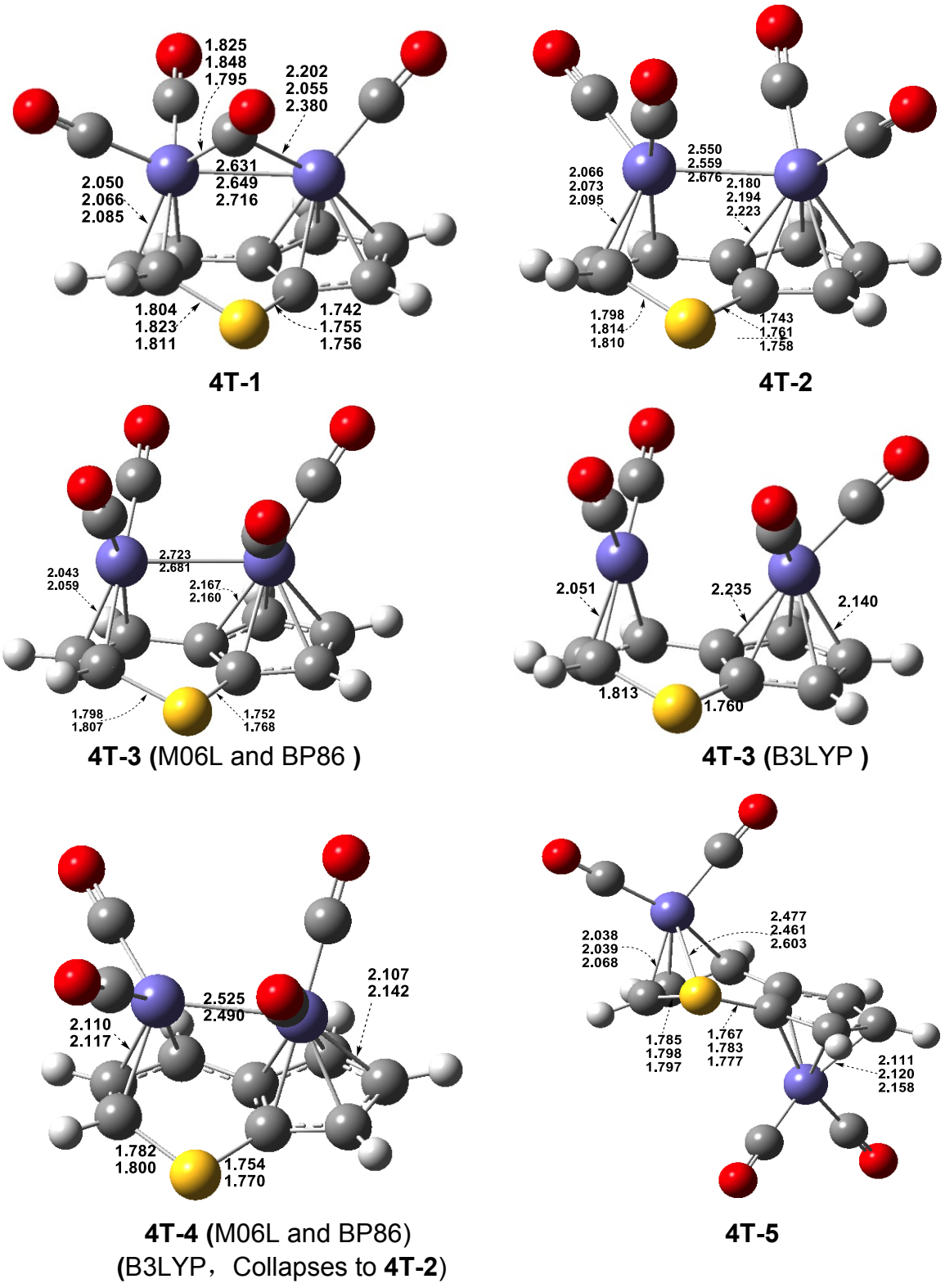

Figure S3. The triplet $(C_8H_6S)Fe_2(CO)_4$ structures.

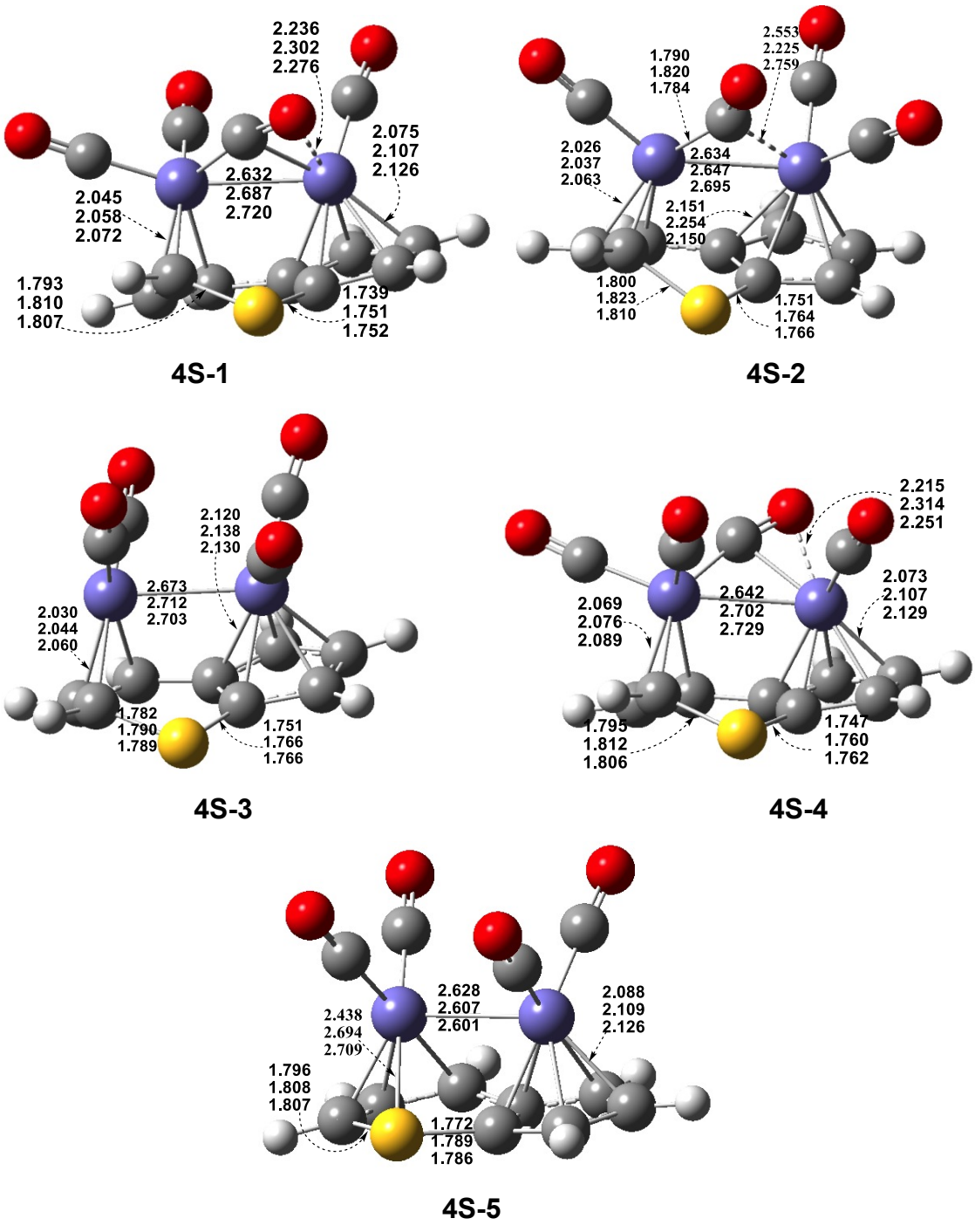

Figure S4. The singlet $(C_8H_6S)Fe_2(CO)_4$ structures.

Complete Gaussian Reference

Gaussian 09, Revision A.02,

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