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Theoretical Studies on the Desulfurization of Benzothiophene (Thianaphthene) and Thienothiophene (Thiophthene) by Carbon-Sulfur Bond Cleavage: Binuclear Iron Carbonyl Intermediates

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*

Supporting Information

Table S1-S4. Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses, in km/mol) for the $(C_8H_6S)Fe_2(CO)_n$ (n = 6,5) structures **BTh6-1, BTh5-1**, **BTh5-2** and **BTh5-3.**

Table S5-S8. Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses, in km/mol) for the $(C_6H_4S_2)Fe_2(CO)_n$ (n = 6,5) structures ***anti*-ThTh6-1, *anti*-ThTh5-1**, ***anti*-ThTh5-2** and ***anti*-ThTh5-3.**

Table S9-S12. Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses, in km/mol) for the $(C_6H_4S_2)Fe_2(CO)_n$ (n = 6,5) structures ***syn*-ThTh6-1, *syn*-ThTh5-1**, ***syn*-ThTh5-2** and ***syn*-ThTh5-3.**

Table S13-S16. Cartesian coordinates and total energy for the $(C_8H_6S)Fe_2(CO)_n$ (n = 6,5) structures **BTh6-1, BTh5-1**, **BTh5-2** and **BTh5-3.**

Table S17-S20. Cartesian coordinates and total energy for the $(C_6H_4S_2)Fe_2(CO)_5$ (n = 6,5) structures ***anti*-ThTh6-1, *anti*-ThTh5-1**, ***anti*-ThTh5-2** and ***anti*-ThTh5-3.**

Table S21-S24. Cartesian coordinates and total energy for the "cis" $(C_6H_4S_2)Fe_2(CO)$ (n = 6,5) structures ***syn*-ThTh6-1, *syn*-ThTh5-1**, ***syn*-ThTh5-2** and ***syn*-ThTh5-3.**

Table S25. Total energies (E, in hartree), relative energies (E, in kcal/mol), and Fe–Fe and S-Fe distances (in Å) for the structures of $(C_8H_6S)Fe_2(CO)_6$ and $(C_8H_6S)Fe_2(CO)_5$ **BTh6-1, BTh5-1**, **BTh5-2** and **BTh5-3.**

Table S26. Total energies (E, in hartree), relative energies (E, in kcal/mol), and Fe–Fe and S-Fe distances (in Å) for the $(C_6H_4S_2)Fe_2(CO)_6$ structures ***anti*-ThTh6-1** and ***syn*-ThTh6-1.**

Table S27. Total energies (E, in hartree), relative energies (E, in kcal/mol), and Fe–Fe and S-Fe distances (in Å) for the $(C_6H_4S_2)Fe_2(CO)_5$ structures ***anti*-ThTh5-n** (n=1-3) and ***syn*-ThTh5-n** (n=1-3).

Table S28. Harmonic ν(CO) vibrational frequencies (in cm^{-1}) predicted for the $(C_8H_6S)Fe_2(CO)_n$ and $(C_6H_4S_2)Fe_2(CO)_n$ (n = 6, 5) structures.

Complete Gaussian reference.

Figure S1. The $(C_8H_6S)Fe_2(CO)_6$ and $(C_8H_6S)Fe_2(CO)_5$ structures **BTh6-1, BTh5-1**, **BTh5-2** and **BTh5-3.**

Figure S2. The lowest-lying $(C_6H_4S_2)Fe_2(CO)_6$ and $(C_6H_4S_2)Fe_2(CO)_5$ structures ***anti*-ThTh6-1** and ***anti*-ThTh5-1.**

Figure S3. The $(C_6H_4S_2)Fe_2(CO)_5$ structures ***anti*-ThTh5-2** and ***anti*-ThTh5-3.**

Figure S4. The lowest-lying $(C_6H_4S_2)Fe_2(CO)_6$ and $(C_6H_4S_2)Fe_2(CO)_5$ structures ***syn*-ThTh6-1** and ***syn*-ThTh5-1.**

Figure S5. The "cis" $(C_6H_4S_2)Fe_2(CO)_5$ structures ***syn*-ThTh5-2** and ***syn*-ThTh5-3.**

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 **BTh6-1.**

	M06L		BP86		B3LYP	
1	34	(0)	36	(0)	38	(0)
2	39	(0)	40	(0)	41	(0)
3	47	(0)	48	(0)	50	(0)
4	55	(0)	58	(0)	60	(0)
5	71	(0)	73	(0)	76	(0)
6	75	(0)	77	(0)	81	(0)
7	77	(0)	80	(0)	82	(0)
8	83	(0)	82	(0)	85	(0)
9	90	(0)	92	(0)	95	(0)
10	91	(0)	93	(0)	96	(0)
11	96	(0)	97	(0)	100	(0)
12	102	(0)	100	(0)	104	(0)
13	116	(0)	117	(0)	122	(0)
14	133	(0)	133	(0)	138	(0)
15	199	(2)	194	(3)	192	(3)
16	222	(2)	219	(2)	222	(3)
17	244	(1)	239	(1)	243	(1)
18	254	(1)	252	(1)	255	(2)
19	278	(1)	278	(1)	282	(1)
20	337	(4)	337	(5)	338	(4)
21	369	(2)	367	(0)	371	(2)
22	388	(3)	383	(3)	391	(5)
23	404	(7)	397	(3)	406	(5)
24	419	(3)	410	(5)	415	(2)
25	425	(3)	420	(4)	424	(2)
26	442	(3)	439	(4)	440	(3)
27	448	(4)	444	(7)	444	(7)
28	457	(5)	454	(2)	456	(5)
29	461	(4)	468	(5)	461	(6)
30	465	(1)	471	(1)	466	(3)
31	469	(1)	486	(3)	469	(3)
32	474	(8)	495	(1)	481	(15)
33	486	(5)	498	(5)	498	(4)
34	498	(6)	506	(5)	506	(7)
35	504	(20)	513	(0)	511	(14)
36	513	(10)	518	(27)	519	(19)
37	539	(17)	527	(3)	534	(13)
38	546	(8)	534	(3)	547	(6)
39	560	(9)	551	(5)	561	(13)
40	564	(9)	571	(7)	565	(11)
41	590	(49)	591	(52)	591	(52)
42	608	(124)	612	(133)	608	(119)
43	615	(68)	616	(52)	615	(83)
44	624	(97)	624	(82)	624	(123)
45	639	(32)	639	(16)	638	(33)

46	668	(36)	655	(51)	672	(26)
47	703	(3)	681	(7)	702	(4)
48	749	(16)	724	(25)	755	(23)
49	767	(25)	741	(27)	771	(31)
50	841	(3)	813	(1)	838	(3)
51	873	(3)	845	(1)	880	(2)
52	883	(8)	864	(10)	893	(8)
53	945	(1)	911	(1)	954	(1)
54	980	(0)	945	(0)	989	(0)
55	999	(3)	968	(3)	1021	(3)
56	1055	(4)	1018	(3)	1047	(4)
57	1073	(2)	1034	(0)	1072	(2)
58	1143	(6)	1106	(5)	1140	(5)
59	1162	(1)	1127	(2)	1169	(2)
60	1174	(0)	1143	(0)	1176	(0)
61	1241	(1)	1203	(2)	1244	(1)
62	1275	(6)	1235	(6)	1278	(6)
63	1301	(31)	1255	(24)	1321	(24)
64	1394	(1)	1347	(2)	1353	(1)
65	1421	(0)	1372	(0)	1418	(1)
66	1482	(5)	1427	(7)	1479	(6)
67	1506	(13)	1451	(16)	1501	(24)
68	1631	(2)	1566	(1)	1619	(2)
69	1645	(2)	1581	(2)	1631	(1)
70	2051	(58)	1973	(10)	2058	(106)
71	2058	(102)	1978	(155)	2069	(48)
72	2070	(1173)	1987	(1062)	2078	(1138)
73	2074	(991)	1991	(818)	2081	(1057)
74	2101	(1849)	2021	(1595)	2101	(2101)
75	2135	(634)	2049	(525)	2137	(651)
76	3080	(10)	3032	(4)	3099	(8)
77	3105	(41)	3055	(15)	3129	(16)
78	3168	(10)	3104	(2)	3178	(2)
79	3181	(0)	3113	(1)	3188	(2)
80	3192	(27)	3123	(8)	3198	(8)
81	3206	(49)	3136	(19)	3211	(18)

Table S2. Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses, in km/mol) for the $(C_8H_6S)Fe_2(CO)_5$ structure **BTh5-1.**

	M06L		BP86		B3LYP	
1	38	(0)	36	(0)	39	(0)
2	44	(0)	44	(0)	46	(0)
3	50	(0)	52	(0)	54	(0)
4	54	(0)	56	(0)	57	(0)
5	67	(0)	69	(0)	73	(0)
6	77	(0)	82	(0)	83	(0)
7	83	(0)	86	(0)	89	(0)
8	87	(0)	89	(0)	91	(0)
9	90	(0)	93	(0)	96	(0)
10	93	(0)	95	(0)	98	(0)
11	109	(0)	111	(0)	115	(0)
12	137	(0)	136	(0)	141	(0)
13	195	(1)	188	(1)	188	(2)
14	227	(4)	216	(4)	225	(6)
15	232	(1)	226	(2)	230	(1)
16	252	(1)	248	(0)	248	(1)
17	286	(2)	283	(1)	287	(2)
18	344	(8)	341	(8)	344	(8)
19	368	(6)	361	(2)	365	(6)
20	390	(2)	381	(3)	387	(5)
21	403	(12)	399	(3)	408	(5)
22	434	(8)	422	(7)	429	(5)
23	439	(10)	429	(13)	436	(9)
24	444	(1)	438	(1)	439	(1)
25	452	(3)	446	(5)	449	(5)
26	462	(7)	463	(1)	462	(4)
27	464	(5)	469	(5)	466	(2)
28	470	(1)	488	(2)	477	(15)
29	486	(10)	497	(3)	493	(6)
30	497	(5)	503	(7)	499	(8)
31	500	(10)	511	(7)	507	(15)
32	530	(23)	519	(4)	522	(9)
33	536	(13)	530	(3)	534	(22)
34	547	(2)	544	(7)	545	(4)
35	560	(19)	569	(23)	558	(17)
36	568	(17)	571	(15)	569	(26)
37	606	(30)	597	(29)	605	(40)
38	615	(102)	616	(119)	615	(126)
39	626	(54)	625	(53)	621	(16)
40	636	(60)	633	(34)	633	(83)
41	683	(15)	666	(7)	681	(11)
42	703	(4)	689	(9)	703	(3)
43	745	(17)	720	(23)	752	(20)
44	765	(26)	739	(31)	769	(35)
45	838	(6)	810	(4)	835	(6)
46	864	(10)	840	(3)	873	(6)

47	873	(2)	848	(8)	884	(3)
48	942	(1)	908	(1)	952	(1)
49	966	(3)	932	(2)	986	(1)
50	978	(0)	944	(0)	991	(2)
51	1055	(9)	1018	(8)	1048	(7)
52	1067	(4)	1027	(2)	1065	(5)
53	1137	(2)	1102	(2)	1139	(5)
54	1146	(4)	1109	(5)	1148	(2)
55	1173	(0)	1143	(0)	1176	(0)
56	1234	(0)	1194	(2)	1235	(0)
57	1271	(14)	1222	(26)	1276	(6)
58	1274	(27)	1234	(6)	1292	(22)
59	1389	(2)	1340	(1)	1347	(1)
60	1412	(0)	1364	(0)	1408	(1)
61	1476	(7)	1423	(9)	1474	(8)
62	1505	(20)	1449	(23)	1498	(31)
63	1627	(4)	1562	(3)	1614	(3)
64	1645	(1)	1579	(1)	1630	(0)
65	2030	(387)	1947	(465)	2045	(349)
66	2040	(810)	1968	(581)	2053	(852)
67	2066	(661)	1985	(490)	2071	(770)
68	2079	(1924)	1994	(1573)	2087	(2094)
69	2116	(617)	2033	(651)	2119	(594)
70	3085	(5)	3038	(1)	3106	(4)
71	3105	(35)	3055	(12)	3130	(14)
72	3168	(10)	3105	(2)	3179	(2)
73	3181	(1)	3114	(1)	3188	(2)
74	3192	(27)	3124	(8)	3198	(9)
75	3206	(47)	3136	(18)	3211	(17)

Table S3. Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses, in km/mol) for the $(C_8H_6S)Fe_2(CO)_5$ structure **BTh5-2.**

	M06L		BP86		B3LYP	
1	32	(0)	30	(0)	34	(0)
2	39	(0)	44	(0)	46	(0)
3	50	(0)	49	(0)	48	(0)
4	57	(0)	57	(0)	60	(0)
5	70	(0)	72	(0)	74	(0)
6	76	(0)	79	(0)	81	(0)
7	82	(0)	85	(0)	87	(0)
8	87	(0)	88	(1)	92	(0)
9	91	(1)	94	(0)	96	(0)
10	95	(0)	97	(0)	101	(0)
11	112	(0)	112	(0)	118	(0)
12	137	(0)	137	(0)	142	(0)
13	187	(0)	177	(0)	178	(1)
14	228	(2)	220	(1)	229	(3)
15	236	(1)	230	(1)	236	(2)
16	263	(3)	262	(1)	265	(4)
17	283	(1)	280	(2)	284	(3)
18	357	(1)	350	(3)	357	(2)
19	365	(5)	363	(3)	367	(4)
20	385	(8)	380	(12)	382	(11)
21	406	(4)	401	(6)	402	(3)
22	417	(3)	410	(4)	418	(4)
23	425	(2)	418	(1)	422	(2)
24	444	(2)	443	(6)	444	(4)
25	452	(0)	444	(2)	451	(5)
26	460	(10)	463	(1)	460	(10)
27	467	(2)	468	(5)	465	(2)
28	470	(4)	487	(3)	472	(3)
29	477	(11)	498	(4)	478	(20)
30	499	(18)	507	(3)	506	(19)
31	515	(5)	515	(24)	515	(15)
32	517	(24)	517	(4)	520	(11)
33	527	(6)	527	(4)	526	(15)
34	545	(19)	538	(22)	534	(13)
35	563	(25)	558	(16)	563	(15)
36	568	(7)	570	(16)	569	(14)
37	584	(52)	589	(35)	585	(58)
38	594	(74)	602	(76)	595	(68)
39	626	(47)	625	(88)	625	(38)
40	627	(77)	627	(29)	629	(112)
41	671	(19)	657	(21)	674	(14)
42	702	(6)	680	(9)	701	(5)
43	748	(16)	723	(22)	754	(21)
44	768	(23)	743	(27)	772	(32)
45	841	(2)	815	(2)	838	(3)
46	874	(0)	846	(0)	883	(1)

47	901	(8)	874	(11)	905	(7)
48	946	(0)	914	(1)	956	(1)
49	980	(2)	944	(3)	990	(0)
50	985	(4)	950	(1)	1004	(6)
51	1054	(3)	1017	(2)	1047	(3)
52	1071	(3)	1032	(2)	1070	(3)
53	1142	(5)	1105	(8)	1141	(4)
54	1154	(5)	1110	(7)	1155	(9)
55	1174	(1)	1143	(1)	1176	(1)
56	1237	(3)	1198	(6)	1239	(2)
57	1268	(15)	1220	(20)	1270	(12)
58	1285	(19)	1238	(5)	1303	(16)
59	1390	(1)	1341	(3)	1353	(1)
60	1408	(2)	1362	(1)	1402	(2)
61	1477	(9)	1424	(12)	1474	(10)
62	1498	(3)	1441	(3)	1494	(12)
63	1623	(1)	1557	(0)	1612	(0)
64	1640	(6)	1575	(14)	1629	(3)
65	2037	(176)	1956	(318)	2052	(172)
66	2057	(1048)	1975	(747)	2065	(872)
67	2060	(787)	1978	(662)	2067	(1037)
68	2079	(1955)	1995	(1648)	2086	(2181)
69	2118	(706)	2032	(674)	2121	(653)
70	3077	(13)	3031	(5)	3097	(9)
71	3100	(40)	3051	(15)	3125	(17)
72	3167	(9)	3104	(2)	3178	(2)
73	3181	(1)	3114	(1)	3188	(2)
74	3192	(25)	3124	(7)	3199	(8)
75	3205	(49)	3136	(19)	3210	(19)

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 **BTh5-3.**

	M06L		BP86		B3LYP	
1	31	(0)	30	(0)	34	(0)
2	41	(0)	44	(0)	47	(0)
3	61	(0)	63	(0)	64	(0)
4	68	(0)	66	(0)	68	(0)
5	76	(0)	77	(0)	79	(0)
6	86	(0)	87	(0)	89	(0)
7	93	(0)	94	(0)	93	(0)
8	95	(0)	99	(0)	101	(1)
9	103	(0)	102	(0)	103	(0)
10	126	(0)	106	(0)	108	(0)
11	146	(1)	141	(0)	138	(1)
12	155	(0)	147	(1)	149	(1)
13	177	(7)	172	(9)	178	(6)
14	220	(0)	211	(0)	215	(0)
15	295	(5)	283	(5)	284	(4)
16	321	(8)	317	(8)	306	(11)
17	349	(6)	336	(3)	343	(1)
18	361	(5)	344	(10)	349	(7)
19	411	(8)	402	(13)	403	(14)
20	415	(3)	405	(2)	408	(2)
21	433	(5)	415	(3)	419	(5)
22	444	(6)	424	(4)	435	(6)
23	446	(1)	432	(2)	440	(4)
24	463	(21)	456	(19)	455	(22)
25	473	(0)	464	(1)	468	(1)
26	483	(3)	471	(2)	482	(9)
27	493	(9)	485	(5)	485	(10)
28	496	(5)	493	(2)	489	(6)
29	497	(14)	502	(13)	496	(4)
30	501	(4)	508	(4)	503	(16)
31	514	(3)	520	(3)	509	(4)
32	534	(2)	526	(11)	531	(4)
33	546	(33)	548	(10)	550	(31)
34	558	(51)	561	(34)	557	(52)
35	577	(44)	564	(29)	566	(29)
36	589	(70)	583	(104)	587	(100)
37	603	(76)	588	(22)	597	(43)
38	630	(61)	619	(23)	625	(77)
39	642	(7)	628	(57)	645	(31)
40	646	(42)	638	(49)	646	(19)
41	681	(12)	654	(11)	684	(6)
42	705	(7)	683	(6)	706	(6)
43	745	(22)	720	(18)	747	(17)
44	794	(6)	778	(5)	809	(5)
45	826	(10)	800	(8)	827	(8)

46	835	(12)	809	(21)	837	(22)
47	893	(8)	864	(9)	905	(9)
48	930	(5)	901	(6)	942	(6)
49	933	(4)	904	(3)	944	(3)
50	959	(3)	928	(3)	976	(3)
51	1034	(2)	998	(2)	1028	(2)
52	1056	(7)	1028	(7)	1062	(9)
53	1069	(16)	1037	(13)	1072	(16)
54	1123	(11)	1086	(11)	1119	(8)
55	1158	(0)	1128	(0)	1165	(0)
56	1206	(1)	1173	(1)	1211	(0)
57	1244	(8)	1206	(9)	1248	(8)
58	1293	(2)	1255	(1)	1299	(2)
59	1353	(9)	1309	(10)	1349	(8)
60	1410	(10)	1362	(10)	1403	(3)
61	1448	(9)	1397	(10)	1446	(11)
62	1490	(10)	1434	(12)	1465	(19)
63	1534	(0)	1478	(1)	1531	(2)
64	1572	(10)	1512	(8)	1560	(14)
65	2011	(231)	1935	(186)	2021	(75)
66	2026	(176)	1947	(181)	2033	(127)
67	2052	(1200)	1971	(1062)	2055	(1539)
68	2063	(1133)	1985	(936)	2057	(1247)
69	2105	(1098)	2021	(953)	2106	(1205)
70	3184	(6)	3127	(1)	3196	(1)
71	3194	(2)	3133	(0)	3208	(0)
72	3197	(14)	3134	(0)	3209	(2)
73	3197	(3)	3139	(2)	3210	(0)
74	3209	(6)	3143	(0)	3219	(0)
75	3226	(10)	3156	(1)	3233	(1)

Table S5. Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses, in km/mol) for the $(C_6H_4S_2)Fe_2(CO)_6$ structure ***anti*-ThTh6-1.**

	M06L		BP86		B3LYP	
1	28	(1)	27	(1)	26	(1)
2	49	(1)	46	(1)	49	(1)
3	56	(0)	54	(0)	56	(0)
4	66	(0)	66	(0)	69	(0)
5	70	(0)	72	(0)	74	(0)
6	76	(2)	76	(1)	79	(2)
7	87	(0)	89	(0)	92	(1)
8	89	(0)	91	(0)	95	(0)
9	92	(0)	92	(0)	96	(0)
10	104	(2)	102	(1)	106	(1)
11	112	(1)	108	(3)	110	(2)
12	121	(1)	112	(0)	114	(1)
13	128	(0)	114	(0)	117	(0)
14	135	(1)	136	(0)	138	(0)
15	169	(0)	164	(0)	167	(0)
16	189	(1)	182	(2)	179	(3)
17	207	(1)	205	(0)	210	(1)
18	238	(1)	238	(2)	238	(1)
19	285	(7)	273	(6)	279	(10)
20	328	(2)	329	(1)	332	(2)
21	365	(5)	360	(5)	368	(4)
22	377	(12)	375	(9)	380	(12)
23	411	(6)	404	(9)	410	(7)
24	422	(4)	414	(4)	418	(5)
25	431	(15)	422	(10)	428	(15)
26	437	(3)	433	(2)	436	(5)
27	443	(1)	445	(2)	442	(2)
28	453	(8)	449	(6)	447	(13)
29	457	(5)	457	(1)	452	(7)
30	468	(3)	474	(15)	467	(1)
31	477	(7)	480	(1)	474	(19)
32	482	(6)	480	(0)	484	(4)
33	487	(11)	498	(7)	492	(13)
34	493	(9)	512	(5)	496	(18)
35	507	(15)	519	(9)	513	(6)
36	512	(11)	523	(7)	524	(17)
37	533	(3)	532	(6)	532	(5)
38	554	(12)	549	(2)	553	(5)
39	559	(69)	568	(49)	559	(70)
40	580	(49)	582	(38)	580	(52)
41	606	(13)	608	(24)	604	(13)
42	615	(62)	610	(8)	617	(66)
43	625	(97)	616	(62)	623	(124)
44	628	(45)	625	(117)	631	(63)
45	637	(33)	631	(30)	636	(15)
46	664	(12)	645	(27)	662	(11)

47	767	(34)	742	(50)	768	(16)
48	775	(13)	750	(10)	780	(41)
49	829	(10)	799	(8)	827	(11)
50	844	(13)	823	(13)	857	(19)
51	898	(0)	866	(1)	901	(42)
52	907	(40)	874	(36)	915	(0)
53	965	(4)	943	(2)	991	(6)
54	1084	(6)	1053	(8)	1091	(7)
55	1134	(13)	1107	(10)	1147	(23)
56	1180	(5)	1143	(5)	1183	(18)
57	1200	(29)	1163	(22)	1194	(24)
58	1302	(12)	1261	(11)	1321	(16)
59	1379	(37)	1327	(34)	1371	(60)
60	1406	(64)	1349	(47)	1389	(89)
61	1453	(25)	1398	(16)	1452	(24)
62	1522	(92)	1461	(86)	1510	(97)
63	2023	(246)	1945	(219)	2028	(299)
64	2040	(249)	1959	(256)	2049	(175)
65	2063	(360)	1983	(259)	2071	(573)
66	2077	(1108)	1993	(941)	2084	(1434)
67	2086	(1750)	2005	(1513)	2088	(1511)
68	2134	(870)	2048	(776)	2135	(929)
69	3116	(14)	3067	(5)	3125	(11)
70	3142	(23)	3087	(8)	3163	(7)
71	3224	(1)	3153	(1)	3228	(1)
72	3244	(2)	3171	(1)	3247	(0)

Table S6. Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses, in km/mol) for the $(C_6H_4S_2)Fe_2(CO)_5$ structure ***anti*-ThTh5-1**.

	M06L	BP86	B3LYP
1	33 (0)	34 (0)	36 (0)
2	41 (0)	43 (0)	42 (0)
3	48 (0)	46 (0)	46 (0)
4	64 (1)	62 (1)	62 (1)
5	72 (0)	74 (0)	76 (0)
6	78 (0)	81 (0)	84 (0)
7	88 (0)	90 (0)	90 (0)
8	90 (0)	92 (0)	95 (0)
9	94 (0)	95 (0)	99 (0)
10	97 (0)	100 (0)	101 (0)
11	128 (1)	128 (1)	129 (2)
12	147 (1)	142 (1)	146 (1)
13	190 (4)	184 (6)	178 (5)
14	210 (2)	206 (2)	211 (5)
15	236 (1)	235 (2)	237 (1)
16	263 (4)	267 (6)	265 (3)
17	318 (5)	312 (13)	312 (0)
18	327 (10)	321 (3)	316 (15)
19	367 (7)	360 (9)	369 (8)
20	391 (5)	382 (1)	385 (4)
21	394 (0)	388 (2)	390 (1)
22	406 (3)	399 (2)	408 (3)
23	424 (4)	416 (4)	424 (3)
24	431 (3)	430 (3)	431 (4)
25	447 (2)	445 (1)	443 (6)
26	457 (4)	461 (2)	452 (6)
27	465 (2)	481 (5)	465 (3)
28	495 (14)	486 (0)	491 (10)
29	495 (7)	499 (7)	498 (8)
30	499 (18)	504 (5)	501 (25)
31	506 (1)	514 (17)	510 (14)
32	520 (10)	518 (6)	526 (13)
33	527 (3)	529 (3)	528 (2)
34	533 (25)	552 (10)	541 (23)
35	560 (18)	556 (21)	560 (23)
36	583 (50)	576 (28)	584 (50)
37	607 (61)	601 (29)	609 (41)
38	617 (109)	609 (45)	618 (119)
39	618 (23)	616 (122)	630 (32)
40	629 (34)	629 (14)	631 (43)
41	648 (13)	638 (32)	649 (13)
42	736 (39)	711 (49)	745 (43)
43	772 (2)	744 (4)	767 (3)
44	819 (4)	799 (2)	821 (5)
45	837 (9)	806 (11)	836 (14)
46	882 (1)	852 (1)	902 (1)

47	908	(37)	879	(31)	910	(29)
48	954	(6)	924	(6)	969	(10)
49	1091	(7)	1059	(8)	1098	(7)
50	1158	(0)	1119	(2)	1159	(1)
51	1180	(7)	1143	(6)	1175	(9)
52	1213	(13)	1176	(12)	1218	(12)
53	1319	(17)	1271	(16)	1331	(17)
54	1364	(5)	1317	(7)	1360	(5)
55	1427	(18)	1369	(20)	1421	(27)
56	1496	(1)	1440	(1)	1475	(3)
57	1557	(17)	1491	(16)	1540	(15)
58	2023	(291)	1946	(302)	2029	(297)
59	2053	(642)	1974	(596)	2055	(1507)
60	2059	(743)	1975	(480)	2068	(1465)
61	2065	(2073)	1987	(1845)	2070	(918)
62	2118	(992)	2032	(818)	2119	(1059)
63	3115	(9)	3063	(3)	3125	(8)
64	3138	(26)	3083	(8)	3163	(6)
65	3228	(2)	3158	(2)	3232	(3)
66	3257	(1)	3184	(2)	3259	(2)

Table S7. Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses, in km/mol) for the $(C_6H_4S_2)Fe_2(CO)_5$ structure ***anti*-ThTh5-2.**

	M06L	BP86	B3LYP
1	31 (0)	26 (0)	27 (1)
2	48 (1)	43 (1)	47 (0)
3	59 (7)	60 (3)	62 (0)
4	66 (0)	67 (0)	72 (0)
5	72 (0)	72 (0)	76 (0)
6	78 (0)	78 (1)	81 (1)
7	84 (1)	87 (0)	84 (1)
8	86 (0)	88 (0)	93 (0)
9	94 (1)	98 (0)	99 (1)
10	102 (4)	107 (3)	107 (1)
11	129 (0)	132 (0)	112 (3)
12	157 (1)	154 (1)	132 (0)
13	182 (0)	181 (1)	162 (1)
14	202 (2)	211 (1)	184 (3)
15	228 (7)	231 (4)	196 (2)
16	260 (2)	264 (3)	264 (2)
17	299 (1)	278 (2)	291 (12)
18	328 (1)	332 (0)	337 (0)
19	362 (18)	361 (4)	370 (5)
20	373 (5)	381 (6)	380 (6)
21	397 (1)	386 (3)	410 (3)
22	402 (3)	393 (3)	418 (10)
23	428 (3)	419 (4)	436 (9)
24	446 (1)	438 (0)	438 (9)
25	460 (6)	450 (1)	445 (13)
26	465 (4)	454 (3)	452 (8)
27	474 (3)	459 (0)	462 (5)
28	476 (16)	487 (2)	482 (7)
29	488 (18)	493 (15)	487 (30)
30	501 (4)	506 (11)	494 (12)
31	503 (6)	509 (1)	502 (15)
32	511 (3)	517 (4)	521 (5)
33	533 (20)	536 (9)	532 (7)
34	547 (55)	548 (23)	551 (12)
35	572 (24)	568 (30)	573 (100)
36	587 (37)	583 (30)	577 (14)
37	595 (11)	593 (33)	582 (30)
38	603 (54)	595 (19)	605 (42)
39	620 (16)	609 (49)	622 (76)
40	641 (64)	634 (33)	636 (20)
41	651 (1)	640 (11)	656 (5)
42	745 (39)	732 (44)	753 (13)
43	765 (1)	738 (4)	778 (46)
44	825 (9)	793 (10)	822 (6)
45	851 (9)	832 (10)	852 (17)
46	890 (2)	863 (0)	897 (47)

47	903	(34)	874	(34)	914	(0)
48	974	(7)	943	(4)	976	(10)
49	1089	(8)	1055	(9)	1089	(2)
50	1119	(5)	1090	(3)	1109	(25)
51	1161	(4)	1136	(2)	1174	(6)
52	1194	(20)	1157	(18)	1187	(36)
53	1296	(10)	1253	(12)	1307	(12)
54	1361	(14)	1327	(12)	1363	(83)
55	1410	(33)	1348	(40)	1387	(57)
56	1487	(9)	1425	(10)	1451	(27)
57	1541	(33)	1470	(47)	1508	(96)
58	1927	(401)	1835	(361)	2024	(279)
59	2045	(611)	1962	(554)	2046	(546)
60	2067	(856)	1979	(788)	2063	(916)
61	2076	(1951)	1993	(1732)	2076	(2003)
62	2111	(767)	2022	(612)	2114	(841)
63	3097	(13)	3053	(3)	3095	(9)
64	3141	(18)	3077	(5)	3166	(4)
65	3227	(2)	3155	(2)	3228	(1)
66	3252	(1)	3176	(2)	3247	(1)

Table S8. Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses, in km/mol) for the $(C_6H_4S_2)Fe_2(CO)_5$ structure ***anti*-ThTh5-3.**

	M06L	BP86	B3LYP
1	35 (0)	34 (0)	33 (0)
2	55 (2)	54 (1)	46 (0)
3	67 (0)	67 (0)	66 (0)
4	71 (0)	73 (0)	67 (0)
5	82 (1)	84 (1)	71 (1)
6	87 (0)	90 (0)	88 (0)
7	97 (1)	103 (1)	95 (0)
8	105 (0)	107 (0)	99 (0)
9	122 (1)	117 (1)	103 (1)
10	128 (1)	131 (1)	106 (0)
11	155 (1)	151 (1)	140 (1)
12	186 (5)	186 (8)	151 (0)
13	206 (3)	199 (3)	165 (9)
14	226 (1)	211 (1)	219 (0)
15	234 (1)	221 (3)	235 (0)
16	331 (6)	321 (5)	323 (6)
17	359 (26)	341 (31)	336 (0)
18	387 (6)	371 (7)	345 (11)
19	396 (5)	374 (1)	397 (5)
20	409 (34)	385 (6)	411 (1)
21	412 (15)	401 (52)	413 (10)
22	421 (11)	411 (3)	421 (3)
23	439 (3)	421 (2)	437 (5)
24	461 (4)	444 (5)	444 (2)
25	471 (4)	459 (11)	461 (17)
26	480 (6)	472 (2)	468 (3)
27	485 (6)	489 (8)	484 (6)
28	493 (21)	492 (0)	495 (9)
29	498 (17)	500 (9)	500 (7)
30	503 (18)	513 (7)	504 (15)
31	513 (5)	517 (10)	526 (11)
32	530 (54)	532 (28)	542 (11)
33	544 (43)	541 (31)	549 (52)
34	558 (10)	545 (10)	552 (60)
35	587 (15)	573 (21)	565 (65)
36	592 (54)	583 (25)	581 (9)
37	608 (25)	600 (23)	590 (40)
38	615 (55)	607 (71)	624 (98)
39	629 (125)	616 (53)	644 (41)
40	638 (13)	625 (100)	647 (9)
41	710 (26)	687 (21)	696 (21)
42	751 (16)	721 (15)	742 (16)
43	789 (3)	768 (3)	756 (2)
44	796 (4)	779 (7)	788 (4)
45	804 (11)	784 (11)	809 (7)

46	840	(5)	822	(4)	886	(14)
47	898	(7)	869	(6)	895	(10)
48	936	(8)	904	(6)	942	(8)
49	1056	(8)	1026	(6)	1041	(10)
50	1065	(9)	1038	(8)	1070	(6)
51	1148	(0)	1111	(0)	1143	(2)
52	1196	(2)	1162	(1)	1205	(2)
53	1273	(0)	1235	(0)	1266	(1)
54	1332	(6)	1286	(3)	1319	(4)
55	1374	(10)	1327	(7)	1361	(9)
56	1410	(26)	1353	(30)	1400	(9)
57	1459	(15)	1403	(9)	1462	(23)
58	1960	(312)	1870	(295)	2023	(116)
59	2008	(303)	1928	(245)	2032	(124)
60	2047	(894)	1967	(796)	2055	(1278)
61	2061	(1394)	1979	(1168)	2058	(1606)
62	2101	(1170)	2017	(1007)	2106	(1183)
63	3193	(3)	3139	(1)	3198	(1)
64	3210	(5)	3151	(0)	3213	(1)
65	3229	(0)	3162	(2)	3238	(2)
66	3242	(1)	3173	(2)	3258	(6)

Table S9. Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses, in km/mol) for the $(C_6H_4S_2)Fe_2(CO)_6$ structure **syn-ThTh6-1.**

	M06L		BP86		B3LYP	
1	28	(1)	29	(1)	28	(1)
2	46	(2)	46	(1)	49	(1)
3	50	(0)	51	(0)	55	(1)
4	58	(0)	57	(1)	59	(0)
5	69	(1)	68	(1)	73	(1)
6	73	(1)	73	(0)	75	(0)
7	86	(0)	89	(1)	92	(1)
8	88	(0)	90	(0)	94	(0)
9	91	(0)	93	(0)	96	(0)
10	102	(2)	100	(2)	105	(2)
11	108	(0)	104	(1)	109	(1)
12	112	(0)	110	(1)	114	(0)
13	125	(0)	117	(0)	116	(0)
14	131	(2)	132	(2)	134	(1)
15	174	(1)	166	(1)	173	(0)
16	190	(2)	182	(3)	179	(4)
17	216	(0)	214	(0)	220	(0)
18	231	(0)	226	(0)	227	(1)
19	311	(4)	284	(5)	293	(10)
20	322	(2)	323	(0)	327	(1)
21	347	(3)	345	(5)	353	(3)
22	368	(16)	369	(12)	375	(15)
23	405	(6)	398	(8)	405	(10)
24	419	(4)	412	(4)	415	(5)
25	432	(11)	425	(8)	430	(10)
26	442	(1)	442	(2)	441	(2)
27	449	(2)	456	(1)	443	(3)
28	461	(0)	462	(13)	457	(4)
29	469	(0)	470	(20)	466	(0)
30	471	(28)	474	(2)	471	(40)
31	480	(3)	480	(3)	483	(17)
32	481	(5)	492	(5)	484	(4)
33	488	(10)	506	(1)	496	(12)
34	500	(7)	511	(8)	506	(8)
35	503	(20)	518	(8)	515	(15)
36	530	(8)	531	(13)	530	(4)
37	534	(1)	533	(0)	541	(3)
38	554	(78)	547	(14)	557	(73)
39	563	(4)	567	(47)	560	(5)
40	572	(64)	572	(32)	573	(70)
41	593	(15)	586	(4)	596	(17)
42	607	(32)	610	(34)	607	(30)
43	617	(50)	615	(65)	620	(84)
44	625	(116)	625	(121)	626	(84)
45	634	(37)	630	(27)	632	(68)
46	661	(18)	645	(27)	661	(17)

47	715	(12)	691	(19)	716	(11)
48	735	(15)	710	(21)	736	(22)
49	820	(9)	789	(8)	817	(10)
50	849	(9)	829	(10)	866	(14)
51	890	(1)	858	(1)	907	(2)
52	940	(50)	909	(50)	938	(51)
53	979	(16)	951	(10)	1000	(13)
54	1055	(41)	1026	(42)	1051	(52)
55	1119	(6)	1090	(4)	1123	(6)
56	1162	(12)	1128	(11)	1174	(16)
57	1212	(13)	1173	(18)	1212	(24)
58	1310	(26)	1268	(22)	1328	(24)
59	1353	(2)	1300	(6)	1345	(11)
60	1417	(61)	1348	(51)	1394	(92)
61	1492	(19)	1430	(14)	1479	(28)
62	1594	(14)	1534	(10)	1582	(18)
63	2021	(249)	1943	(229)	2028	(298)
64	2042	(244)	1960	(268)	2051	(192)
65	2064	(407)	1984	(267)	2072	(627)
66	2080	(1053)	1994	(900)	2086	(1436)
67	2087	(1771)	2005	(1552)	2090	(1463)
68	2135	(849)	2048	(756)	2136	(918)
69	3113	(15)	3066	(4)	3125	(10)
70	3141	(29)	3086	(11)	3160	(10)
71	3204	(4)	3141	(2)	3211	(2)
72	3256	(1)	3183	(2)	3258	(3)

Table S10. Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses, in km/mol) for the $(C_6H_4S_2)Fe_2(CO)_5$ structure **syn-ThTh5-1.**

	M06L	BP86	B3LYP
1	33 (0)	33 (0)	35 (0)
2	43 (0)	43 (0)	43 (0)
3	48 (0)	46 (0)	46 (0)
4	64 (1)	63 (1)	62 (0)
5	72 (0)	74 (0)	76 (0)
6	78 (0)	81 (0)	83 (0)
7	88 (0)	90 (0)	91 (0)
8	90 (1)	93 (0)	95 (0)
9	94 (0)	95 (0)	100 (0)
10	97 (0)	100 (0)	101 (0)
11	129 (2)	129 (1)	129 (2)
12	147 (0)	142 (0)	149 (0)
13	188 (4)	182 (6)	175 (4)
14	215 (1)	211 (1)	214 (3)
15	226 (2)	223 (2)	228 (3)
16	271 (4)	274 (4)	274 (2)
17	312 (2)	311 (6)	307 (1)
18	328 (16)	316 (14)	317 (16)
19	368 (0)	367 (1)	365 (1)
20	390 (4)	382 (2)	389 (3)
21	396 (4)	385 (7)	392 (6)
22	415 (5)	403 (3)	414 (4)
23	426 (3)	416 (4)	423 (3)
24	432 (2)	430 (2)	434 (3)
25	453 (2)	451 (2)	449 (3)
26	460 (6)	458 (1)	454 (16)
27	466 (4)	474 (9)	465 (4)
28	475 (16)	485 (2)	476 (17)
29	497 (8)	493 (2)	497 (2)
30	503 (2)	507 (3)	507 (16)
31	506 (7)	515 (12)	511 (8)
32	515 (10)	524 (4)	519 (15)
33	533 (25)	540 (5)	535 (13)
34	540 (5)	555 (11)	541 (13)
35	577 (38)	562 (27)	575 (40)
36	583 (44)	575 (42)	583 (39)
37	604 (79)	604 (56)	607 (63)
38	618 (91)	611 (25)	618 (118)
39	628 (27)	617 (93)	630 (37)
40	632 (3)	629 (10)	641 (4)
41	652 (17)	641 (29)	652 (12)
42	724 (2)	700 (3)	722 (3)
43	743 (47)	721 (56)	755 (54)
44	831 (3)	808 (6)	834 (5)
45	838 (17)	810 (14)	836 (19)

46	881	(1)	852	(1)	902	(1)
47	952	(6)	922	(8)	959	(10)
48	970	(28)	939	(25)	980	(23)
49	1043	(5)	1008	(4)	1039	(4)
50	1115	(7)	1083	(8)	1120	(8)
51	1197	(5)	1162	(5)	1209	(8)
52	1224	(1)	1185	(1)	1223	(1)
53	1323	(17)	1277	(13)	1335	(11)
54	1364	(8)	1314	(11)	1360	(11)
55	1415	(17)	1357	(17)	1410	(24)
56	1521	(1)	1463	(2)	1499	(3)
57	1576	(8)	1510	(6)	1560	(6)
58	2024	(306)	1946	(309)	2029	(299)
59	2053	(621)	1974	(622)	2055	(1534)
60	2059	(749)	1975	(453)	2068	(1346)
61	2065	(2080)	1988	(1848)	2070	(1022)
62	2119	(980)	2033	(804)	2120	(1040)
63	3115	(7)	3064	(2)	3127	(7)
64	3137	(37)	3084	(12)	3162	(11)
65	3217	(5)	3149	(1)	3222	(2)
66	3253	(1)	3180	(2)	3255	(2)

Table S11. Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses, in km/mol) for the $(C_6H_4S_2)Fe_2(CO)_5$ structure **syn-ThTh5-2.**

	M06L	BP86	B3LYP
1	35 (0)	30 (0)	8 (0)
2	50 (1)	44 (1)	43 (1)
3	66 (0)	54 (2)	54 (1)
4	73 (1)	68 (0)	70 (0)
5	73 (2)	73 (0)	77 (0)
6	81 (0)	80 (1)	82 (1)
7	85 (0)	85 (0)	86 (0)
8	90 (2)	91 (1)	94 (4)
9	96 (0)	98 (0)	101 (0)
10	112 (4)	105 (2)	110 (3)
11	128 (0)	131 (0)	127 (0)
12	162 (2)	157 (3)	157 (2)
13	189 (3)	191 (2)	169 (4)
14	200 (1)	212 (1)	196 (3)
15	230 (7)	231 (5)	212 (5)
16	252 (1)	246 (0)	253 (1)
17	310 (2)	296 (1)	304 (4)
18	323 (1)	323 (1)	329 (4)
19	358 (19)	356 (2)	352 (17)
20	372 (4)	375 (9)	371 (3)
21	399 (4)	390 (3)	401 (1)
22	407 (2)	392 (6)	407 (2)
23	432 (6)	424 (6)	439 (1)
24	446 (2)	440 (2)	449 (2)
25	457 (4)	451 (2)	456 (14)
26	468 (4)	459 (3)	469 (13)
27	477 (28)	483 (2)	475 (12)
28	478 (9)	490 (16)	483 (3)
29	486 (9)	501 (9)	488 (28)
30	494 (7)	504 (3)	498 (2)
31	512 (5)	509 (1)	511 (17)
32	520 (10)	519 (4)	528 (11)
33	544 (45)	545 (32)	544 (27)
34	564 (12)	549 (10)	560 (6)
35	568 (38)	566 (12)	563 (52)
36	573 (26)	574 (48)	578 (46)
37	595 (19)	585 (6)	589 (39)
38	605 (59)	594 (46)	606 (41)
39	620 (14)	611 (47)	618 (14)
40	641 (57)	636 (46)	639 (61)
41	657 (7)	639 (4)	656 (13)
42	716 (11)	692 (12)	712 (7)
43	742 (29)	720 (36)	746 (27)
44	829 (14)	794 (11)	820 (13)
45	860 (8)	840 (7)	860 (9)
46	881 (2)	858 (3)	905 (1)

47	914	(35)	893	(39)	931	(32)
48	981	(16)	952	(12)	995	(24)
49	1029	(8)	1009	(10)	1030	(25)
50	1108	(5)	1081	(4)	1116	(5)
51	1133	(5)	1107	(5)	1143	(13)
52	1222	(2)	1182	(4)	1216	(8)
53	1300	(8)	1259	(7)	1313	(12)
54	1363	(12)	1309	(15)	1352	(16)
55	1398	(20)	1346	(22)	1402	(52)
56	1512	(0)	1453	(1)	1489	(11)
57	1569	(5)	1513	(2)	1568	(9)
58	1936	(383)	1841	(362)	1939	(436)
59	2049	(580)	1965	(515)	2050	(656)
60	2067	(870)	1980	(772)	2079	(681)
61	2079	(1915)	1996	(1738)	2080	(1972)
62	2112	(733)	2023	(572)	2121	(862)
63	3094	(13)	3047	(3)	3102	(7)
64	3138	(27)	3079	(8)	3163	(7)
65	3211	(6)	3144	(2)	3216	(2)
66	3248	(2)	3178	(2)	3256	(2)

Table S12. Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses, in km/mol) for the $(C_6H_4S_2)Fe_2(CO)_5$ structure ***syn*-ThTh5-3.**

	M06L		BP86		B3LYP	
1	31	(0)	32	(0)	33	(0)
2	54	(1)	46	(1)	53	(1)
3	65	(0)	66	(0)	62	(1)
4	69	(0)	67	(0)	67	(0)
5	81	(0)	79	(0)	81	(0)
6	89	(0)	88	(0)	88	(0)
7	92	(0)	93	(1)	97	(1)
8	97	(0)	98	(1)	98	(0)
9	109	(0)	104	(0)	102	(1)
10	121	(0)	110	(0)	115	(0)
11	146	(1)	139	(1)	139	(1)
12	155	(0)	148	(0)	142	(1)
13	185	(6)	179	(7)	181	(4)
14	223	(0)	211	(1)	216	(1)
15	282	(2)	258	(2)	254	(3)
16	321	(6)	305	(8)	300	(15)
17	339	(7)	322	(5)	324	(0)
18	368	(2)	337	(1)	342	(1)
19	399	(9)	385	(17)	398	(8)
20	416	(6)	404	(10)	409	(7)
21	424	(17)	414	(18)	418	(12)
22	440	(9)	417	(5)	430	(3)
23	446	(7)	430	(11)	435	(2)
24	460	(20)	450	(10)	453	(24)
25	470	(1)	458	(8)	469	(1)
26	481	(15)	480	(1)	476	(4)
27	484	(3)	492	(4)	481	(11)
28	494	(2)	497	(7)	495	(5)
29	505	(6)	502	(10)	499	(20)
30	512	(5)	518	(0)	511	(4)
31	531	(13)	526	(10)	523	(11)
32	543	(30)	543	(28)	542	(40)
33	548	(65)	547	(27)	549	(47)
34	573	(5)	554	(26)	565	(15)
35	576	(101)	569	(63)	574	(74)
36	600	(26)	588	(8)	594	(28)
37	611	(8)	598	(37)	613	(13)
38	627	(95)	622	(81)	622	(110)
39	638	(35)	627	(40)	643	(35)
40	659	(13)	632	(16)	658	(15)
41	664	(14)	643	(14)	666	(7)
42	735	(23)	711	(17)	739	(18)
43	788	(12)	766	(14)	794	(13)
44	801	(7)	777	(5)	812	(8)
45	807	(5)	783	(10)	817	(5)

46	844	(1)	817	(1)	874	(2)
47	910	(6)	878	(5)	922	(5)
48	1007	(1)	974	(0)	1007	(1)
49	1051	(9)	1027	(6)	1054	(14)
50	1065	(22)	1034	(24)	1068	(30)
51	1089	(20)	1054	(18)	1090	(8)
52	1199	(5)	1166	(6)	1210	(8)
53	1264	(0)	1230	(0)	1275	(0)
54	1298	(3)	1259	(1)	1308	(3)
55	1352	(23)	1298	(18)	1343	(16)
56	1397	(9)	1348	(8)	1405	(8)
57	1528	(4)	1471	(6)	1505	(1)
58	2011	(94)	1936	(53)	2021	(13)
59	2024	(173)	1943	(154)	2032	(108)
60	2046	(1220)	1965	(1115)	2052	(1435)
61	2059	(1372)	1980	(1169)	2055	(1558)
62	2103	(1105)	2018	(937)	2105	(1214)
63	3179	(4)	3123	(1)	3189	(1)
64	3191	(13)	3134	(1)	3202	(2)
65	3228	(0)	3165	(2)	3239	(2)
66	3244	(1)	3178	(5)	3258	(7)

Table S13. Cartesian coordinates and total energy for the $(C_8H_6S)Fe_2(CO)_6$ structure **BTh6-1.**

	M06L			BP86			B3LYP		
	E=-3914.241814a.u.			E=-3914.951050 a.u.			E=-3914.428194		
	x	y	z	x	y	z	x	y	z
C	-2.143632	-0.406860	0.582766	-2.141173	-0.405918	0.589344	-2.134902	-0.420152	0.585579
C	-2.265503	0.199318	-0.674154	-2.271264	0.188715	-0.685166	-2.259991	0.168400	-0.684256
C	-3.527261	0.244006	-1.274281	-3.545170	0.217419	-1.290122	-3.526606	0.207394	-1.286117
C	-4.632058	-0.330899	-0.641498	-4.655229	-0.359432	-0.636752	-4.638623	-0.351376	-0.637595
C	-4.485369	-0.962077	0.594591	-4.500303	-0.975070	0.621447	-4.491962	-0.958840	0.616808
C	-3.232708	-1.001865	1.214342	-3.232013	-1.001284	1.243267	-3.230899	-0.993940	1.234592
C	0.150469	-0.021119	-1.486909	0.179210	-0.018296	-1.483680	0.174447	-0.029415	-1.490137
C	-1.067018	0.696476	-1.369987	-1.062046	0.691761	-1.384093	-1.055541	0.668463	-1.391447
H	-3.638807	0.722645	-2.245686	-3.666678	0.684635	-2.276834	-3.641782	0.667567	-2.267369
H	-5.609230	-0.284876	-1.114734	-5.644240	-0.325374	-1.111038	-5.618280	-0.311593	-1.111649
H	-5.345763	-1.404507	1.089122	-5.365811	-1.416075	1.131713	-5.355031	-1.388343	1.123183
H	-3.109071	-1.463429	2.190925	-3.102461	-1.452793	2.235199	-3.109225	-1.440336	2.220338
H	0.676299	0.175770	-2.426780	0.706153	0.154155	-2.436520	0.699134	0.175114	-2.428362
H	-1.296686	1.387399	-2.187129	-1.288062	1.382490	-2.213288	-1.290461	1.352953	-2.211478
Fe	1.017205	-1.138365	-0.141926	1.014591	-1.154949	-0.141371	1.025819	-1.154407	-0.162164
C	-0.595933	2.672946	0.627153	-0.587808	2.683014	0.626451	-0.625055	2.670223	0.642220
Fe	0.457613	1.327498	0.054903	0.458554	1.347271	0.056376	0.457701	1.347998	0.070145
C	1.836529	1.313572	1.215276	1.830399	1.402089	1.206403	1.814350	1.414538	1.254761
C	0.224168	-2.653038	-0.628302	0.217745	-2.639323	-0.667582	0.226612	-2.666125	-0.654140
O	-0.335471	-3.606346	-0.976129	-0.325734	-3.603305	-1.052665	-0.323631	-3.618825	-1.007390
O	-1.289189	3.525323	0.990902	-1.264427	3.560880	1.000419	-1.316337	3.515657	1.016331
O	2.713757	1.363596	1.973020	2.719352	1.518642	1.960775	2.668391	1.518640	2.028513
S	-0.556104	-0.322944	1.358853	-0.528141	-0.309462	1.350432	-0.530221	-0.337941	1.351983
C	2.433242	-1.208064	-1.226666	2.443191	-1.268797	-1.191596	2.448072	-1.251587	-1.256950
C	1.986259	-1.725712	1.293852	1.950656	-1.809862	1.271554	1.994752	-1.772678	1.273603
C	1.400860	2.274770	-1.123208	1.379690	2.327741	-1.099223	1.388958	2.335036	-1.105564
O	3.340798	-1.225519	-1.947015	3.383869	-1.350119	-1.884997	3.353402	-1.300560	-1.972439
O	2.607370	-2.105054	2.193485	2.563237	-2.265612	2.158059	2.605683	-2.178294	2.164055
O	2.010655	2.868992	-1.909590	1.982985	2.980442	-1.862567	1.978241	2.963217	-1.875576

Table S14. Cartesian coordinates and total energy for the $(C_8H_6S)Fe_2(CO)_5$ structure **BTh5-1.**

	M06L			BP86			B3LYP		
	E=-3800.858136a.u.			E=- 3081.554174a.u.			E=-3801.041608 a.u.		
	x	y	z	x	y	z	x	y	z
C	-2.088900	0.058970	-0.541593	-2.086298	0.002852	-0.559005	-2.078752	0.024437	-0.566853
C	-1.970067	-0.334060	0.800809	-1.971210	-0.364406	0.804220	-1.965373	-0.331763	0.791590
C	-3.141279	-0.475767	1.552948	-3.156936	-0.527868	1.553121	-3.143688	-0.494523	1.537394
C	-4.388182	-0.202480	0.987247	-4.416266	-0.302763	0.958982	-4.398591	-0.282497	0.947474
C	-4.480842	0.222865	-0.338613	-4.505477	0.094207	-0.389988	-4.489663	0.099928	-0.397534
C	-3.323679	0.354547	-1.112050	-3.330863	0.248942	-1.159382	-3.321438	0.253593	-1.161824
C	0.441858	0.394857	1.287018	0.450714	0.433568	1.288472	0.440714	0.454057	1.289932
C	-0.641542	-0.522582	1.408023	-0.630532	-0.508013	1.426394	-0.629546	-0.476609	1.424310
H	-3.069075	-0.791612	2.592152	-3.091230	-0.822300	2.609237	-3.077363	-0.778599	2.587429
H	-5.288896	-0.322326	1.583282	-5.329859	-0.439716	1.551197	-5.303787	-0.416144	1.538026
H	-5.451011	0.431107	-0.781350	-5.485325	0.262084	-0.854411	-5.462937	0.260544	-0.858776
H	-3.383261	0.655243	-2.154967	-3.387961	0.529975	-2.218544	-3.380800	0.525020	-2.214568
H	1.076883	0.493003	2.172838	1.073436	0.584865	2.184928	1.070027	0.561923	2.178095
H	-0.667637	-1.091436	2.342555	-0.639929	-1.071216	2.374334	-0.655102	-1.035200	2.364077
Fe	0.851957	1.379457	-0.266885	0.792380	1.430538	-0.265137	0.811795	1.440023	-0.259064
C	0.049280	-2.690073	-0.449781	0.118304	-2.687982	-0.375411	0.064730	-2.689081	-0.368179
Fe	0.832941	-1.111531	-0.052078	0.870639	-1.094137	-0.033835	0.862197	-1.101498	-0.044121
C	2.145921	-0.812559	-1.245601	2.175749	-0.918418	-1.246035	2.155504	-0.966911	-1.287477
C	-0.105969	2.849261	-0.083479	-0.189594	2.871300	-0.093764	-0.182825	2.894744	-0.061908
O	-0.789177	3.760280	0.150074	-0.879780	3.795465	0.137421	-0.870983	3.794789	0.177049
O	-0.470291	-3.692502	-0.705026	-0.363947	-3.730004	-0.598670	-0.443509	-3.703167	-0.584028
O	2.994087	-0.636694	-2.023336	3.036984	-0.842428	-2.040416	2.981386	-0.909021	-2.099047
S	-0.586613	0.093416	-1.485705	-0.550106	0.077173	-1.479595	-0.553861	0.101090	-1.492245
C	2.313984	2.033592	0.500326	2.222236	2.163556	0.462903	2.294241	2.123356	0.487055
C	1.970492	-1.773714	1.141648	2.030593	-1.706144	1.153901	2.025556	-1.714838	1.170143
O	3.274735	2.456909	0.998050	3.182279	2.668478	0.917026	3.257978	2.559973	0.955293
O	2.700020	-2.194474	1.938785	2.794654	-2.118745	1.941340	2.765470	-2.105073	1.968197

Table S15. Cartesian coordinates and total energy for the $(C_8H_6S)Fe_2(CO)_5$ structure **BTh5-2.**

	M06L			BP86			B3LYP		
	E=-3800.846878a.u.			E=-3801.544228a.u.			E=-3801.029509 a.u.		
	x	y	z	x	y	z	x	y	z
C	-1.964487	-0.698173	0.438840	-1.936525	-0.729148	0.447192	-1.948557	-0.712262	0.445645
C	-2.073264	0.086395	-0.722668	-2.062849	0.008977	-0.760087	-2.054577	0.019322	-0.755249
C	-3.285288	0.081638	-1.424851	-3.282035	-0.061091	-1.475216	-3.261422	-0.036140	-1.474038
C	-4.344539	-0.718799	-0.999987	-4.32882	-0.880717	-1.015464	-4.323816	-0.826979	-1.019334
C	-4.207480	-1.521838	0.136273	-4.174831	-1.633462	0.170232	-4.193648	-1.570831	0.164202
C	-3.015599	-1.509716	0.863463	-2.977018	-1.554457	0.910329	-3.003179	-1.510626	0.902844
C	0.411973	0.309942	-1.320302	0.45209	0.293803	-1.328854	0.443638	0.277819	-1.331693
C	-0.913587	0.848465	-1.204642	-0.915494	0.795495	-1.258187	-0.895257	0.792510	-1.258656
H	-3.386879	0.704117	-2.312222	-3.400336	0.525363	-2.396523	-3.362393	0.538065	-2.394947
H	-5.279730	-0.717161	-1.553331	-5.269735	-0.933095	-1.57758	-5.253661	-0.863971	-1.585027
H	-5.034198	-2.144671	0.467149	-4.993709	-2.270572	0.527823	-5.019788	-2.185768	0.518231
H	-2.907746	-2.107167	1.765184	-2.858621	-2.113743	1.847041	-2.900254	-2.065688	1.833887
H	0.958701	0.711330	-2.180259	0.992984	0.642592	-2.22424	0.988700	0.661507	-2.199949
H	-1.177604	1.634594	-1.918931	-1.191075	1.551655	-2.011881	-1.169005	1.535725	-2.012892
Fe	1.314905	-0.844155	-0.057027	1.339892	-0.825298	-0.031704	1.340440	-0.832029	-0.048396
C	-0.976769	2.562566	0.916994	-1.017207	2.576357	0.885336	-1.042253	2.559993	0.914809
Fe	0.287122	1.388576	0.398107	0.236966	1.427460	0.339571	0.255797	1.431470	0.369272
C	2.283838	-1.283653	1.426523	2.314663	-1.239896	1.443300	2.323021	-1.218915	1.451202
O	2.918507	-1.548685	2.359629	2.976221	-1.500027	2.374485	2.960903	-1.447110	2.387538
O	-1.824509	3.315706	1.159752	-1.859349	3.344497	1.162081	-1.898359	3.284473	1.193681
S	-0.475598	-0.544031	1.381833	-0.439906	-0.491692	1.391804	-0.452883	-0.511437	1.389450
C	0.930506	-2.473938	-0.696348	0.963492	-2.45738	-0.632318	0.944070	-2.478064	-0.627129
C	2.792039	-0.498403	-0.982238	2.826116	-0.542626	-0.949269	2.825498	-0.567482	-1.010343
C	1.374908	2.535637	-0.406758	1.226421	2.651618	-0.449537	1.295171	2.646886	-0.439959
O	0.646005	-3.508175	-1.136130	0.70032	-3.517375	-1.057655	0.655389	-3.522273	-1.030969
O	3.739386	-0.238717	-1.599850	3.809548	-0.362237	-1.562073	3.774729	-0.387550	-1.645996
O	2.109460	3.248341	-0.957251	1.902343	3.465618	-0.962187	1.983367	3.413244	-0.967640

Table S16. Cartesian coordinates and total energy for the $(C_8H_6S)Fe_2(CO)_5$ structure **BTh5-3.**

	M06L			BP86			B3LYP		
	E=-3800. 846562a.u.			E=-3801.537724a.u.			E=-3801.014010 a.u.		
	x	y	z	x	y	z	x	y	z
C	-1.038092	-1.749067	-0.367282	-1.025461	-1.795069	-0.272874	-1.055495	-1.766919	-0.297621
C	-0.432358	-0.945006	-1.408828	-0.456768	-1.010100	-1.368647	-0.491965	-0.964522	-1.364412
C	-1.257206	0.027183	-2.039202	-1.328305	-0.097506	-2.047438	-1.362202	-0.055605	-2.032141
C	-2.606692	0.196376	-1.661800	-2.687911	0.056713	-1.644875	-2.718278	0.071955	-1.648890
C	-3.176658	-0.572003	-0.615133	-3.217041	-0.674943	-0.534610	-3.241828	-0.673920	-0.559524
C	-2.381708	-1.562959	0.017199	-2.375648	-1.615741	0.141109	-2.401196	-1.614879	0.100349
C	1.446614	-1.893394	-0.391781	1.480868	-1.915701	-0.372375	1.447428	-1.898976	-0.409506
C	0.982941	-1.173244	-1.563552	0.969968	-1.220216	-1.550245	0.934289	-1.164786	-1.551064
H	-0.811853	0.716820	-2.750623	-0.916924	0.563222	-2.818738	-0.957362	0.607524	-2.792932
H	-3.180612	1.002994	-2.106067	-3.305719	0.817767	-2.134394	-3.338876	0.820606	-2.135151
H	-4.198092	-0.402395	-0.294751	-4.245729	-0.513028	-0.197039	-4.270091	-0.538291	-0.237125
H	-2.775852	-2.113085	0.866384	-2.746561	-2.143074	1.027464	-2.774713	-2.163033	0.962049
H	2.381231	-2.447272	-0.397709	2.430646	-2.461770	-0.387490	2.376502	-2.461091	-0.464438
H	1.489056	-1.113685	-2.522114	1.459862	-1.167495	-2.528147	1.401850	-1.113193	-2.530975
Fe	-1.415020	0.333994	0.090387	-1.454304	0.336676	0.086198	-1.490952	0.354972	0.111481
C	1.582327	0.318193	1.689421	1.659791	0.323701	1.656208	1.698370	0.300959	1.680581
Fe	1.438090	0.133500	-0.102794	1.469590	0.134376	-0.121509	1.503432	0.141139	-0.112813
C	3.164177	0.158335	-0.388893	3.179883	0.181573	-0.442141	3.228962	0.114138	-0.450881
O	1.779247	0.425982	2.829973	1.905719	0.441052	2.798573	1.912283	0.389971	2.815633
O	4.314417	0.161205	-0.572028	4.339545	0.217604	-0.645649	4.369246	0.077232	-0.665565
S	0.106588	-2.799806	0.407793	0.164655	-2.817950	0.502400	0.136212	-2.803452	0.456047
C	-1.448156	2.096028	0.209941	-1.554114	2.090522	0.093545	-1.520435	2.125676	0.110819
C	-1.288537	0.282822	1.851656	-1.311856	0.441933	1.834826	-1.339551	0.417018	1.875751
C	1.261641	1.776559	-0.827049	1.309084	1.778995	-0.824159	1.371485	1.804650	-0.818645
O	-1.513921	3.250869	0.325505	-1.678340	3.257940	0.141105	-1.593116	3.283200	0.134112
O	-1.288828	0.250660	3.013437	-1.316278	0.542511	3.005395	-1.317089	0.469607	3.034212
O	1.201727	2.816250	-1.350065	1.304052	2.850801	-1.310910	1.348841	2.859374	-1.302445

Table S17. Cartesian coordinates and total energy for the $(C_6H_4S_2)Fe_2(CO)_6$ structure ***anti*-ThTh6.**

	M06L			BP86			B3LYP		
	E=-4234.963658a.u.			E=-4235.710454a.u.			E=- 4235.150055a.u.		
	x	y	z	x	y	z	x	y	z
Fe	-0.589407	1.119224	-0.006366	-0.602975	1.138159	-0.010027	-0.608989	1.150970	-0.000507
C	-0.129740	0.686005	1.683496	-0.096262	0.790270	1.676797	-0.145780	0.854230	1.712360
Fe	1.584451	-0.408613	-0.147370	1.588997	-0.415917	-0.130566	1.605891	-0.420386	-0.146231
C	2.625945	1.020729	-0.377292	2.637413	1.002581	-0.330805	2.685635	0.985497	-0.442596
C	0.269906	2.663463	-0.201367	0.175855	2.702318	-0.295753	0.239890	2.695612	-0.282729
O	0.795948	3.689864	-0.333179	0.644882	3.761802	-0.481707	0.765796	3.708824	-0.474140
O	-0.009483	0.505950	2.828013	0.053857	0.715720	2.841450	-0.000343	0.778462	2.862445
O	3.337562	1.919059	-0.546156	3.379846	1.897230	-0.468355	3.412775	1.858302	-0.646957
C	-2.070873	2.077619	0.266923	-2.081436	2.059358	0.324040	-2.117289	2.097948	0.222120
C	2.577343	-1.410296	-1.245360	2.575125	-1.382395	-1.244312	2.554427	-1.482087	-1.225871
C	2.352490	-0.779637	1.471467	2.378220	-0.803608	1.457193	2.379591	-0.742098	1.489697
O	-3.002043	2.739563	0.478304	-3.022380	2.714449	0.578980	-3.058276	2.746485	0.407043
O	3.204876	-2.043758	-1.984065	3.219700	-1.997932	-2.003577	3.141478	-2.156352	-1.957058
O	2.844643	-1.029157	2.487322	2.914925	-1.066095	2.461662	2.869982	-0.956575	2.510611
C	-0.969782	0.033314	-1.726406	-0.974414	0.014352	-1.719022	-0.962165	-0.002401	-1.694112
C	0.405523	0.242101	-1.602967	0.412012	0.239581	-1.581443	0.417649	0.207155	-1.577246
C	-1.313585	-1.810711	0.062001	-1.300005	-1.852249	0.061444	-1.301955	-1.826986	0.115836
C	-1.705699	-0.629730	-0.665820	-1.712705	-0.643101	-0.644631	-1.710730	-0.663748	-0.635503
C	-3.634488	-1.962696	0.202643	-3.639041	-2.066340	0.158625	-3.631730	-2.041084	0.222446
H	-1.537998	0.412606	-2.576341	-1.535814	0.381117	-2.590389	-1.519050	0.356619	-2.560464
H	0.845618	0.807340	-2.427859	0.865116	0.789175	-2.420236	0.838987	0.755348	-2.423927
H	-4.619028	-2.311690	0.491870	-4.629195	-2.451995	0.422908	-4.613778	-2.416640	0.496530
S	0.274515	-2.321738	0.316071	0.309670	-2.330816	0.317588	0.297507	-2.321700	0.387080
S	-3.486254	-0.538286	-0.724781	-3.512915	-0.588249	-0.718639	-3.500583	-0.621066	-0.732740
C	-2.439461	-2.536406	0.544140	-2.423118	-2.632260	0.499176	-2.425348	-2.576920	0.597540
H	-2.349421	-3.438441	1.138170	-2.321250	-3.563970	1.064455	-2.320856	-3.470134	1.206420

Table S18. Cartesian coordinates and total energy for the $(C_6H_4S_2)Fe_2(CO)_5$ structure ***anti*-ThTh5-1.**

	M06L			BP86			B3LYP		
	E=-4121.600310a.u.			E=-4122.337011a.u.			E=-4121.780518a.u.		
	x	y	z	x	y	z	x	y	z
Fe	-0.612824	0.947684	-0.046377	-0.628014	1.003222	-0.056758	-0.606932	1.037356	-0.047671
Fe	1.659409	-0.426307	-0.012116	1.672197	-0.412256	0.001854	1.668228	-0.430532	-0.016728
C	2.911775	0.368130	-1.021962	2.969286	0.279304	-1.011085	2.975319	0.212246	-1.081796
C	0.484121	2.320559	-0.097648	0.398261	2.41704	-0.107653	0.4373	2.457704	-0.133702
O	1.188147	3.248303	-0.135918	1.045296	3.400223	-0.135927	1.097343	3.412148	-0.187895
O	3.717858	0.878570	-1.679548	3.838807	0.705456	-1.670628	3.811808	0.610426	-1.771582
C	-1.968461	2.056560	0.256194	-1.98384	2.105271	0.223155	-1.984752	2.109018	0.317708
C	1.976553	-2.117068	-0.465540	1.870124	-2.11067	-0.444941	1.869787	-2.155863	-0.384413
C	2.759785	-0.222725	1.427582	2.800135	-0.27573	1.413142	2.783804	-0.215946	1.424656
O	-2.824554	2.827856	0.424181	-2.83378	2.904705	0.376412	-2.848664	2.855572	0.52726
O	2.179001	-3.211738	-0.793130	2.008615	-3.230401	-0.766241	1.984643	-3.276253	-0.65044
O	3.506867	-0.111777	2.306930	3.585647	-0.209348	2.280211	3.527028	-0.09817	2.301102
C	-0.934919	-0.328464	-1.720599	-0.917799	-0.307818	-1.719847	-0.914174	-0.263206	-1.71507
C	0.430376	-0.086795	-1.518046	0.453478	-0.019715	-1.500531	0.46082	-0.049242	-1.507115
C	-1.521767	-0.931084	0.705644	-1.501987	-0.915568	0.723733	-1.503495	-0.932378	0.695662
C	-1.792532	-0.814894	-0.689996	-1.772946	-0.828152	-0.690318	-1.77272	-0.798345	-0.697161
C	-3.820998	-1.316554	0.677975	-3.78993	-1.455705	0.683008	-3.782591	-1.469914	0.644626
H	-1.403815	-0.127116	-2.684823	-1.380753	-0.117237	-2.699382	-1.37162	-0.057418	-2.683703
H	0.899058	0.333706	-2.410702	0.930124	0.405106	-2.396867	0.930659	0.361044	-2.404531
H	-4.828339	-1.551611	0.996845	-4.791506	-1.760301	0.999212	-4.775233	-1.78247	0.952069
H	-2.712535	-1.320192	2.536242	-2.687359	-1.369407	2.568709	-2.683056	-1.444342	2.515185
S	-0.010310	-0.587687	1.497594	0.011577	-0.493239	1.507899	-0.010544	-0.504908	1.500159
S	-3.499416	-1.056697	-0.996011	-3.473563	-1.187028	-1.008454	-3.462161	-1.148937	-1.029378
C	-2.715353	-1.199354	1.459361	-2.688813	-1.255609	1.480354	-2.687372	-1.297827	1.439151

Table S19. Cartesian coordinates and total energy for the $(C_6H_4S_2)Fe_2(CO)_5$ ***anti*-ThTh5-2.**

	M06L			BP86			B3LYP		
	E=-4121.579526a.u.			E=-4122.316628a.u.			E=-4121.765955a.u.		
	x	y	z	x	y	z	x	y	z
Fe	0.591474	0.943671	0.204163	0.548487	1.046955	0.160475	-0.606187	1.139263	-0.101987
C	-0.650474	1.304611	-1.117892	-0.757200	1.280692	-1.136134	-0.151392	0.967865	1.622792
Fe	-1.731999	-0.007368	0.189659	-1.686290	-0.061370	0.169560	1.695852	-0.076292	-0.237589
C	0.719557	2.491007	1.043737	0.760035	2.598719	0.964749	0.204210	2.691367	-0.401135
O	0.790748	3.512894	1.593647	0.874324	3.644899	1.488541	0.748037	3.694944	-0.606353
O	-0.91899	1.913206	-2.092117	-1.077129	1.879026	-2.118395	-0.013199	0.922585	2.776244
C	1.975691	1.384924	-0.82414	1.824582	1.491806	-0.985916	-2.211151	1.954062	-0.006691
C	-2.800528	-0.950285	1.285854	-2.764851	-0.874602	1.344407	2.963825	-0.809367	-1.262879
C	-2.961919	0.144931	-1.126423	-2.958636	-0.022642	-1.092399	2.653316	0.097080	1.324183
O	2.8879	1.65843	-1.488725	2.676479	1.792202	-1.735653	-3.213901	2.525325	0.091171
O	-3.472138	-1.586333	1.982904	-3.470063	-1.414669	2.108164	3.760961	-1.272283	-1.961204
O	-3.769909	0.254453	-1.94784	-3.829340	0.027006	-1.873643	3.286345	0.199334	2.284370
C	0.792759	-0.441167	1.843953	0.845114	-0.311443	1.800244	-0.871902	-0.144983	-1.711651
C	-0.490898	0.107209	1.715592	-0.471604	0.190715	1.700772	0.467860	0.249500	-1.675779
C	0.818604	-1.505978	-0.494166	0.867367	-1.722115	-0.396061	-0.752867	-1.905353	0.193855
C	1.430901	-1.038659	0.719172	1.480014	-0.927230	0.662522	-1.418643	-0.873178	-0.571247
C	3.077997	-1.975083	-0.893435	3.145094	-2.234199	-0.701874	-2.995552	-2.489814	0.530795
H	1.380746	-0.324821	2.755376	1.458082	-0.147576	2.699453	-1.533944	0.067320	-2.551554
H	-0.863249	0.604141	2.617037	-0.860732	0.674269	2.611228	0.814423	0.790059	-2.564562
H	3.987276	-2.30245	-1.382218	4.063731	-2.649243	-1.128107	-3.872739	-3.003013	0.915011
H	1.570507	-2.363012	-2.395133	1.610430	-3.048853	-2.032478	-1.383847	-3.612830	1.463607
S	-0.849531	-1.861702	-0.745965	-0.816025	-1.951770	-0.648324	0.931262	-2.126800	0.355415
C	1.818184	-1.986791	-1.409502	1.860565	-2.425099	-1.168647	-1.687785	-2.792731	0.819627
S	3.16567	-1.337502	0.703848	3.249419	-1.182551	0.671256	-3.187553	-1.129745	-0.497826

Table S20. Cartesian coordinates and total energy for the $(C_6H_4S_2)Fe_2(CO)_5$ structure ***anti*-ThTh5-3.**

	M06L			BP86			B3LYP		
	E=-4121.577305a.u.			E=-4122.308990a.u.			E=-4121.747212a.u.		
	x	y	z	x	y	z	x	y	z
C	-2.993515	-0.249809	-0.408701	-3.001018	-0.201198	-0.427179	-2.859825	-0.641338	-0.889287
C	-1.300536	-1.713095	0.247867	-1.332960	-1.708535	0.262792	-0.975054	-1.802199	-0.088216
C	-0.836919	-1.258537	-1.022765	-0.852200	-1.272659	-1.026023	-0.374984	-1.122490	-1.204333
C	1.170557	-1.96377	-0.052828	1.149894	-2.018100	-0.027964	1.523614	-1.882942	-0.139014
C	0.558711	-1.468053	-1.266966	0.554196	-1.512143	-1.252256	1.029723	-1.328188	-1.400461
H	-3.944366	0.267542	-0.443456	-3.953767	0.334169	-0.470740	-3.894310	-0.393024	-1.098557
H	2.071722	-2.569793	-0.083082	2.064268	-2.621147	-0.035292	2.467223	-2.422716	-0.100891
H	0.968801	-1.60099	-2.261773	0.985015	-1.640672	-2.249446	1.512518	-1.386571	-2.371607
S	-0.065783	-2.602538	1.093593	-0.110753	-2.626636	1.127637	0.205473	-2.741084	0.796613
Fe	-1.223886	0.418153	0.175856	-1.207419	0.457266	0.153368	-1.407931	0.344774	0.159168
Fe	1.361107	0.131297	-0.190502	1.365071	0.117772	-0.171962	1.464929	0.167646	-0.112612
C	-0.095199	0.3973	1.598179	-0.052994	0.424615	1.563178	-1.473328	0.459361	1.920226
O	0.109652	0.420498	2.754921	0.111228	0.476626	2.739081	-1.572559	0.541149	3.071916
C	2.732576	0.05377	-1.306781	2.706634	0.077171	-1.318144	3.204963	0.208881	-0.393828
O	3.637373	0.021474	-2.036283	3.612644	0.091755	-2.066862	4.353772	0.220731	-0.560671
C	-1.715031	2.067925	0.60048	-1.719719	2.082419	0.604952	-1.625528	2.100346	0.079961
O	-2.067699	3.136594	0.891164	-2.116630	3.141408	0.924947	-1.814881	3.244357	0.054171
O	3.223488	0.680742	2.033931	3.310107	0.577872	2.000102	1.685774	0.766101	2.777393
C	2.457907	0.479799	1.185171	2.504199	0.405242	1.165756	1.533371	0.539455	1.650474
C	0.825782	1.726346	-0.845451	0.845485	1.722096	-0.795693	1.262804	1.762165	-0.944327
O	0.654453	2.781671	-1.313894	0.742591	2.801678	-1.260180	1.187042	2.780639	-1.495720
C	-2.532654	-1.113326	0.628175	-2.559912	-1.069839	0.635301	-2.367006	-1.582107	0.049474
S	-2.039505	-0.345584	-1.916144	-2.065555	-0.379214	-1.961313	-1.616117	-0.246345	-2.114971
H	-3.067497	-1.291637	1.552915	-3.102678	-1.218847	1.572719	-2.982757	-2.011234	0.833620

Table S21. Cartesian coordinates and total energy for the "cis" $(C_6H_4S_2)Fe_2(CO)_6$ structure ***syn*-ThTh 6-1.**

	M06L			BP86			B3LYP		
	E=-4234.962832a.u.			E=-4235.708897a.u.			E=- 4235.149780a.u.		
	x	y	z	x	y	z	x	y	z
Fe	-0.525364	1.187715	-0.027752	-0.475812	1.259234	-0.047216	-0.491963	1.264963	-0.027023
C	-0.143343	0.635467	1.650112	-0.041652	0.818620	1.640954	-0.125892	0.859253	1.689282
Fe	1.549232	-0.460545	-0.135085	1.521618	-0.527494	-0.124194	1.543923	-0.522711	-0.132133
C	2.694645	0.906678	-0.141275	2.735587	0.765036	-0.178888	2.785619	0.770422	-0.251495
C	0.394533	2.702211	-0.090950	0.442486	2.753020	-0.254252	0.495545	2.737509	-0.193865
O	0.970775	3.708667	-0.137805	1.012236	3.770574	-0.386362	1.117460	3.706490	-0.311162
O	-0.086618	0.408704	2.791393	0.069977	0.724309	2.808811	-0.034479	0.740749	2.841222
O	3.464271	1.772200	-0.160359	3.576848	1.578056	-0.218895	3.609748	1.573578	-0.340067
C	-2.001893	2.147073	0.265509	-1.894743	2.269908	0.282921	-1.941395	2.303572	0.175325
C	2.533519	-1.438001	-1.263911	2.441018	-1.549518	-1.247359	2.438169	-1.616328	-1.228371
C	2.171482	-1.053093	1.482430	2.164941	-1.101061	1.474408	2.159988	-1.045127	1.521359
O	-2.949957	2.783694	0.478440	-2.811544	2.963170	0.524162	-2.861272	2.987411	0.337252
O	3.156266	-2.051716	-2.022424	3.045006	-2.198222	-2.011864	2.992411	-2.304823	-1.971259
O	2.569118	-1.445083	2.494145	2.606138	-1.486678	2.485266	2.549919	-1.386928	2.550469
C	-0.818026	0.301836	-1.899941	-0.861510	0.275690	-1.848826	-0.837790	0.272222	-1.830077
C	0.548240	0.393822	-1.617881	0.527933	0.329357	-1.605020	0.542435	0.317335	-1.595246
C	-1.433671	-1.484794	-0.174195	-1.507000	-1.516699	-0.112662	-1.496383	-1.517646	-0.108030
C	-1.749333	-0.381006	-1.030091	-1.796190	-0.339620	-0.913709	-1.777677	-0.367150	-0.921203
C	-3.900272	-1.038998	-0.363457	-3.986113	-1.042535	-0.335808	-3.965428	-1.051176	-0.353790
C	-3.181771	-0.183121	-1.123372	-3.241661	-0.126288	-1.018648	-3.218071	-0.158709	-1.045851
H	-1.251834	0.815271	-2.759090	-1.298026	0.760291	-2.734504	-1.270281	0.756974	-2.706700
H	1.102933	1.008543	-2.330862	1.098486	0.868635	-2.375854	1.086177	0.874705	-2.362305
H	-4.973966	-1.076141	-0.233269	-5.073591	-1.089950	-0.233683	-5.045744	-1.095516	-0.266492
H	-3.623212	0.599292	-1.733452	-3.675432	0.699906	-1.593033	-3.642529	0.645133	-1.643072
S	0.040391	-2.276496	0.081002	-0.018479	-2.287425	0.161428	-0.013868	-2.289308	0.190695
S	-2.887266	-2.143103	0.518089	-2.989662	-2.230654	0.493957	-2.975107	-2.212987	0.504101

Table S22. Cartesian coordinates and total energy for the "cis" $(C_6H_4S_2)Fe_2(CO)_5$ structure ***syn*-ThTh5-1.**

	M06L			BP86			B3LYP		
	E=-4121.599582a.u.			E=-4122.336223a.u.			E=-4121.780034a.u.		
	x	y	z	x	y	z	x	y	z
Fe	-0.617152	0.974423	-0.085084	-0.635371	1.024770	-0.085048	-0.610713	1.060491	-0.091011
Fe	1.639466	-0.428447	-0.015665	1.652481	-0.411008	-0.007810	1.649832	-0.431017	-0.009981
C	2.974876	0.475669	-0.799350	3.026707	0.401947	-0.803491	3.046147	0.316307	-0.872150
C	0.481796	2.333415	0.113372	0.389286	2.425799	0.127253	0.437882	2.473044	0.060793
O	1.187972	3.250971	0.243664	1.033890	3.399087	0.279134	1.100531	3.421434	0.164900
O	3.834958	1.058801	-1.312047	3.946889	0.907451	-1.323417	3.940860	0.782646	-1.434333
C	-1.991108	2.053721	0.236867	-2.011854	2.096082	0.208172	-2.014546	2.103538	0.255170
C	1.997989	-2.05162	-0.651243	1.900022	-2.037719	-0.655100	1.889725	-2.107015	-0.548052
C	2.609007	-0.420729	1.528570	2.655572	-0.466276	1.499968	2.630640	-0.385051	1.540727
O	-2.857291	2.807947	0.429063	-2.874386	2.877213	0.384129	-2.893786	2.833690	0.458631
O	2.232546	-3.096519	-1.097884	2.075312	-3.105248	-1.108485	2.033853	-3.190903	-0.926638
O	3.277015	-0.430436	2.475839	3.364849	-0.517789	2.431381	3.293033	-0.369842	2.486984
C	-0.789159	-0.085838	-1.925463	-0.777633	-0.063165	-1.920230	-0.764474	-0.050758	-1.909132
C	0.551558	0.105226	-1.575593	0.567693	0.176371	-1.552084	0.584522	0.119378	-1.557755
C	-1.567346	-0.960949	0.325913	-1.545630	-0.958044	0.347542	-1.551467	-0.958932	0.333314
C	-1.766719	-0.67346	-1.059788	-1.747421	-0.693841	-1.058849	-1.740867	-0.672170	-1.051554
C	-3.940607	-1.221582	-0.389099	-3.906646	-1.383475	-0.398648	-3.900138	-1.362113	-0.431471
C	-3.151344	-0.82757	-1.420406	-3.126540	-0.941122	-1.436876	-3.113162	-0.910885	-1.447051
H	-1.164588	0.244884	-2.895114	-1.152286	0.262272	-2.902131	-1.129036	0.269317	-2.886322
H	1.105203	0.621652	-2.362886	1.124233	0.703567	-2.341320	1.139592	0.615081	-2.357879
H	-5.002166	-1.432913	-0.415002	-4.961454	-1.670972	-0.432852	-4.947852	-1.640921	-0.482215
H	-3.511660	-0.661793	-2.429847	-3.491214	-0.809106	-2.460932	-3.462184	-0.762858	-2.465536
S	-0.161304	-0.737912	1.310979	-0.132953	-0.658316	1.329980	-0.162767	-0.641988	1.333750
S	-3.080085	-1.390277	1.095930	-3.046915	-1.483473	1.114001	-3.052179	-1.486461	1.077773

Table S23. Cartesian coordinates and total energy for the "cis" $(C_6H_4S_2)Fe_2(CO)_5$ structure **cis-ThTh5-2.**

	M06L			BP86			B3LYP		
	E=-4121.582253a.u.			E=-4122.317325a.u.			E=-4121.764731a.u.		
	x	y	z	x	y	z	x	y	z
Fe	-0.625261	0.971431	-0.162248	-0.574350	1.047801	-0.156412	-0.638269	1.115203	-0.126904
C	0.466757	1.072942	1.327320	0.624805	1.145733	1.264914	0.339640	1.081812	1.402919
Fe	1.709688	0.055805	-0.112977	1.681780	-0.018908	-0.106744	1.694047	0.028179	-0.118630
C	-0.660359	2.660931	-0.681614	-0.695664	2.700373	-0.740767	-0.455896	2.813117	-0.589271
O	-0.674988	3.772314	-1.020745	-0.757117	3.813045	-1.114132	-0.325760	3.922929	-0.898457
O	0.622569	1.464389	2.427828	0.845036	1.640314	2.327588	0.528598	1.372108	2.525860
C	-2.124338	1.227701	0.766556	-1.967377	1.354924	0.897723	-2.214266	1.485462	0.632828
C	2.894782	-0.654561	-1.259409	2.850678	-0.721995	-1.263359	2.883100	-0.644928	-1.284154
C	2.798253	-0.053608	1.326132	2.822826	-0.161998	1.266703	2.747779	-0.118390	1.368603
O	-3.106539	1.384500	1.364555	-2.895036	1.570800	1.582924	-3.233228	1.723010	1.129037
O	3.644053	-1.137252	-1.999134	3.619344	-1.187605	-2.014959	3.625484	-1.086183	-2.050083
O	3.517545	-0.111263	2.231006	3.610400	-0.229034	2.130639	3.444958	-0.214614	2.281362
C	-0.640419	-0.038170	-2.075689	-0.676124	-0.021781	-2.038838	-0.696891	0.034458	-1.973184
C	0.615460	0.459951	-1.703029	0.618170	0.435719	-1.701183	0.588425	0.498033	-1.664436
C	-0.848830	-1.411050	0.020476	-0.935469	-1.512529	0.027205	-0.835669	-1.612666	-0.027945
C	-1.412516	-0.833008	-1.173133	-1.478072	-0.777946	-1.108430	-1.428462	-0.808753	-1.056038
C	-3.324768	-1.780583	-0.229050	-3.438756	-1.774629	-0.251873	-3.330399	-1.918664	-0.227883
C	-2.823569	-1.089783	-1.285861	-2.911453	-0.986972	-1.241263	-2.860774	-1.040218	-1.151351
H	-1.123958	0.267236	-3.004862	-1.163895	0.287707	-2.975637	-1.215716	0.339943	-2.883111
H	1.068910	1.136198	-2.435165	1.104459	1.060714	-2.468314	1.037486	1.141525	-2.428917
H	-4.357900	-2.060265	-0.063029	-4.486358	-2.057848	-0.114599	-4.357103	-2.234855	-0.074947
H	-3.424374	-0.729231	-2.114219	-3.506312	-0.532795	-2.041037	-3.488675	-0.533866	-1.880355
S	0.761197	-1.946888	0.316892	0.685207	-1.977555	0.363107	0.814048	-2.038232	0.245291
S	-2.137547	-2.157370	0.967411	-2.247925	-2.300104	0.916904	-2.074433	-2.511410	0.827766

Table S24. Cartesian coordinates and total energy for ***syn*-ThTh5-3.**

	M06L			BP86			B3LYP		
	E=-4121.574013a.u.			E=-4122.304418a.u.			E=-4121.743215a.u.		
	x	y	z	x	y	z	x	y	z
C	-2.738640	0.155802	-1.239892	-2.786101	0.059130	-1.235520	-2.795236	-0.012277	-1.297702
C	-1.296702	-1.557513	-0.211168	-1.263955	-1.608185	-0.188462	-1.242886	-1.583900	-0.182477
C	-0.667968	-0.938135	-1.344269	-0.661698	-0.970904	-1.345333	-0.637569	-0.951586	-1.317528
C	1.133992	-1.988979	-0.265631	1.193555	-2.000071	-0.293946	1.213735	-1.975411	-0.277868
C	0.720887	-1.298580	-1.480879	0.743519	-1.304157	-1.502204	0.769514	-1.272377	-1.475326
H	-3.576339	0.792650	-1.495244	-3.660627	0.660295	-1.498411	-3.667990	0.560143	-1.592299
H	-1.253900	0.657871	-2.781750	-1.336626	0.565484	-2.838787	-1.305653	0.571390	-2.805012
H	1.974845	-2.678019	-0.265389	2.060471	-2.670866	-0.299953	2.062447	-2.655523	-0.299780
H	1.190163	-1.416580	-2.452846	1.214047	-1.391198	-2.487202	1.217662	-1.382223	-2.459903
S	-0.281349	-2.669675	0.646037	-0.203493	-2.707060	0.657180	-0.181571	-2.678986	0.671763
Fe	-1.273666	0.520955	0.112180	-1.301012	0.524967	0.095822	-1.365287	0.528309	0.120701
Fe	1.467204	0.036355	-0.159828	1.490963	0.047728	-0.167155	1.542432	0.056853	-0.160444
C	-0.574909	0.460155	1.752661	-0.598084	0.583454	1.724564	-0.786846	0.629845	1.797613
O	-0.376399	0.437413	2.899269	-0.407935	0.672358	2.882120	-0.589374	0.720421	2.937652
C	3.068568	-0.126775	-0.854834	3.076335	-0.031138	-0.892162	3.182855	-0.128621	-0.771878
O	4.128959	-0.235044	-1.322895	4.148611	-0.064158	-1.377422	4.262765	-0.260219	-1.175763
C	-1.479358	2.267639	0.272125	-1.615803	2.249158	0.208690	-1.590792	2.281668	0.117716
O	-1.619076	3.418478	0.371780	-1.853095	3.398630	0.285962	-1.754038	3.431412	0.102454
O	2.677574	0.355555	2.527084	2.710171	0.187981	2.529476	2.528648	0.332426	2.622865
C	2.128154	0.255645	1.508435	2.145888	0.161177	1.500272	2.073121	0.252029	1.561399
C	1.257678	1.686160	-0.860037	1.302212	1.732196	-0.754286	1.413846	1.718914	-0.871347
O	1.182930	2.736375	-1.359933	1.284675	2.835932	-1.163510	1.379224	2.774826	-1.351269
S	-2.938591	-1.031178	0.059721	-2.927687	-1.119369	0.104218	-2.934343	-1.177907	0.023466
C	-1.518307	0.028825	-1.939922	-1.565292	-0.050139	-1.964337	-1.545646	-0.056393	-1.952749

Table S25. 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 $(C_8H_6S)Fe_2(CO)_5$ **BTh6-1**, **BTh5-1**, **BTh5-2**, and **BTh5-3**.

	BTh6-1	**BTh5-1**	**BTh5-2**	**BTh5-3**
BP86				
-E	3914.951050	3801.554174	3801.544228	3801.537724
ΔE	0.0	0.0	6.2	10.3
Fe-Fe	2.571	2.536	2.536	2.938
Fe-S	2.307, 2.322	2.260, 2.341,	2.303, 2.291	3.288, 3.570
M06L				
-E	3914.241814	3800.858136	3800.846878	3800.846562
ΔE	0.0	0.0	7.1	7.3
	2.536	2.500	2.500	2.867
	2.322, 2.335	2.282, 2.350,	2.317, 2.299	3.262, 3.498
B3LYP				
-E	3914.428194	3801.041608	3801.029509	3801.014010
ΔE	0.0	0.0	7.6	17.3
Fe-Fe	2.577	2.551	2.544	3.010
Fe-S	2.320, 2.337	2.276, 2.356	2.321, 2.306	3.296, 3.570

Table S26. Total energies (E, in hartree), relative energies (E, in kcal mol-1), and Fe–Fe and S-Fe distances (in Å) for the $(C_6H_4S_2)Fe_2(CO)_6$ structures ***anti*-ThTh6-1** and **cis-ThTh6-1.**

	***anti*-ThTh6-1** (C_1 ^1A)	**cis-ThTh 6-1** (C_1 ^1A)
BP86		
-E	4235.710454	4235.708897
ΔE	0.0	1.0
Fe-Fe	2.690	2.681
Fe-S	2.346, 3.602	2.356, 3.582
M06L		
-E	4234.963658	4234.962832
ΔE	0.0	0.5
Fe-Fe	2.661	2.652
Fe-S	2.364, 3.562	2.371
B3LYP		
-E	4235.150055	4235.149780
ΔE	0.0	0. 2
Fe-Fe	2.720	2.711
Fe-S	2.369, 3.610	2.377, 3.593

Table S27. Total energies (E, in hartree), relative energies (E, in kcal mol-1), and Fe–Fe and S-Fe distances (in Å) for the $(C_6H_4S_2)Fe_2(CO)_5$ structures **ThTh5-n (n=1-3)** and the "cis" $(C_6H_4S_2)Fe_2(CO)_5$ structures "cis" **ThTh5-n** (n=1-3).

	ThTh5-1	**ThTh5-2**	**ThTh5-3**	**"cis"ThTh5-1**	**"cis"ThTh5-2**	**"cis"ThTh5-3**
BP86						
-E	4122.337011	4122.316628	4122.308990	4122.336223	4122.317325	4122.304418
ΔE	0.0	12.8	17.6	0.5	12.4	20.5
Fe-Fe	2.701	2.495	2.615	2.702	2.496	2.845
Fe-S	2.243, 2.258	2.236, 3.392	3.376, 2.431	2.245, 2.256	2.247, 3.318	3.338, 2.313
M06L						
-E	4121.600310	4121.579526	4121.577305	4121.599582	4121.582253	4121.574013
ΔE	0.0	13.0	14.4	0.5	11.3	16.5
Fe-Fe	2.656	2.511	2.627	2.658	2.509	2.797
Fe-S	2.257, 2.259	2.257, 3.293	3.340, 2.372,	2.258,2.256	2.257	3.321, 2.277
B3LYP						
-E	4121.780518	4121.765955	4121.747212	4121.780034	4121.764731	4121.743215
ΔE	0.0	9.1	20.9	0.3	9.9	23.4
Fe-Fe	2.708	2.607	2.891	2.709	2.573	2.959
Fe-S	2.264, 2.265	2.267, 3.639	3.298, 2.359	2.266, 2.265	2.275, 3.492	3.339, 2.320

Table S28. Harmonic ν(CO) vibrational frequencies (in cm^{-1}) predicted for the $(C_8H_6S)Fe_2(CO)_n$ and $(C_6H_4S_2)Fe_2(CO)_n$ (n = 6, 5) structures. Infrared intensities (in km/mol) are in parentheses. None of the structures has any imaginary vibrational frequencies.

	BP86
BTh6-1	1973(10), 1978(155), 1987(1062), 1991(818), 2021(1595), 2049(525)
Expt (KBr)	1992(m), 2004(s), 2044(vs), 2076(m)
Expt (hexane)	1961, 1994, 2006, 2044, 2077
BTh5-1	1947(465), 1968(581), 1985(490), 1994(1573), 2033(651)
BTh5-2	1956(318), 1975(747), 1978(662), 1995(1648), 2032(674)
BTh5-3	1935(186), 1947(181), 1971(1062), 1985(936), 2121(953)
ThTh6-1	1945(219), 1959(256), 1983(259), 1993(941), 2005(1513), 2048(776)
ThTh5-1	1946(302), 1974(596), 1975(480), 1987(1845), 2032(818)

Complete Gaussian Reference

Gaussian 09, Revision A.02,

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.

Figure S1. The $(C_8H_6S)Fe_2(CO)_6$ and $(C_8H_6S)Fe_2(CO)_5$ structures **BTh6-1, BTh5-1**, **BTh5-2**, and **BTh5-3.**

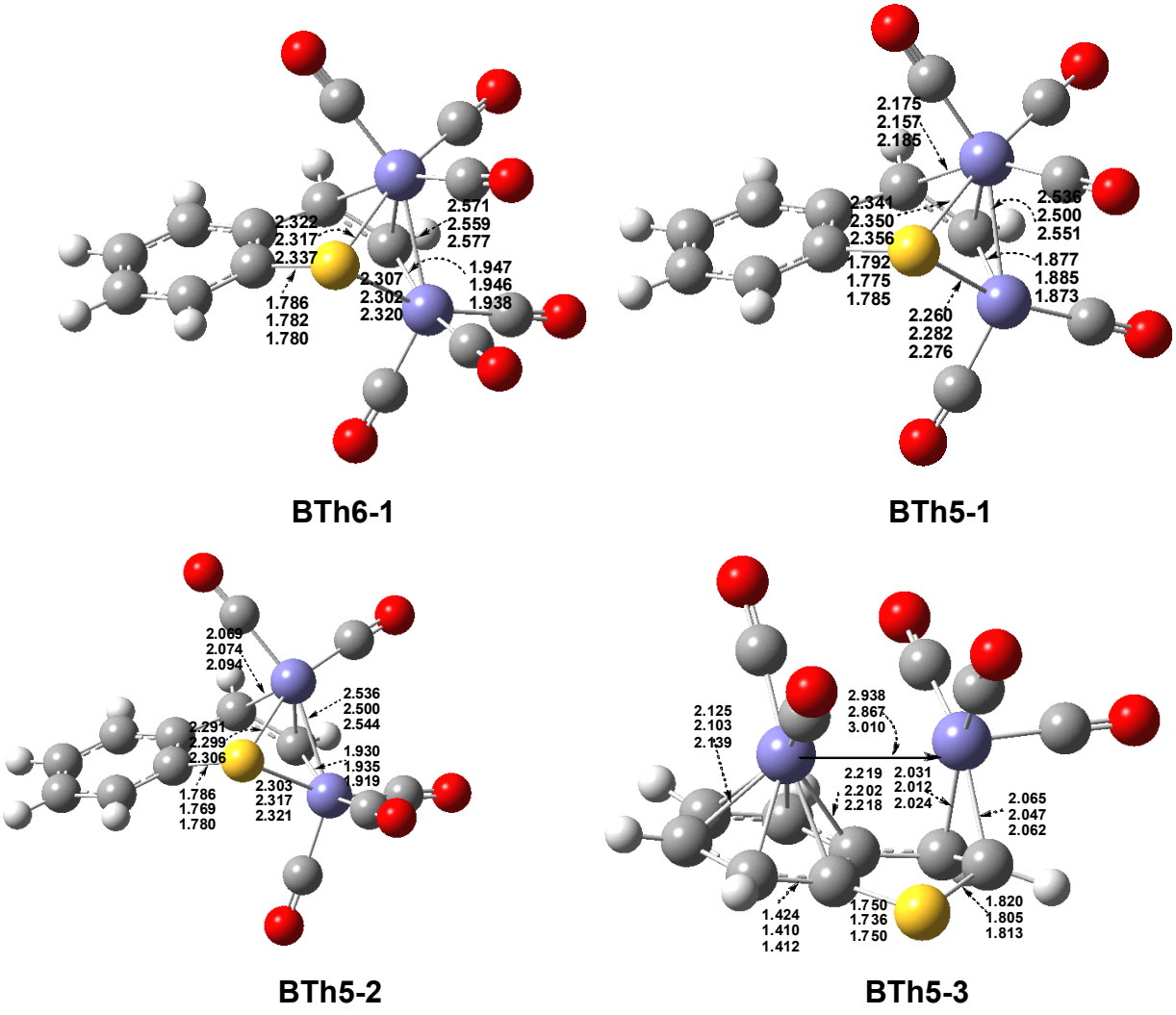
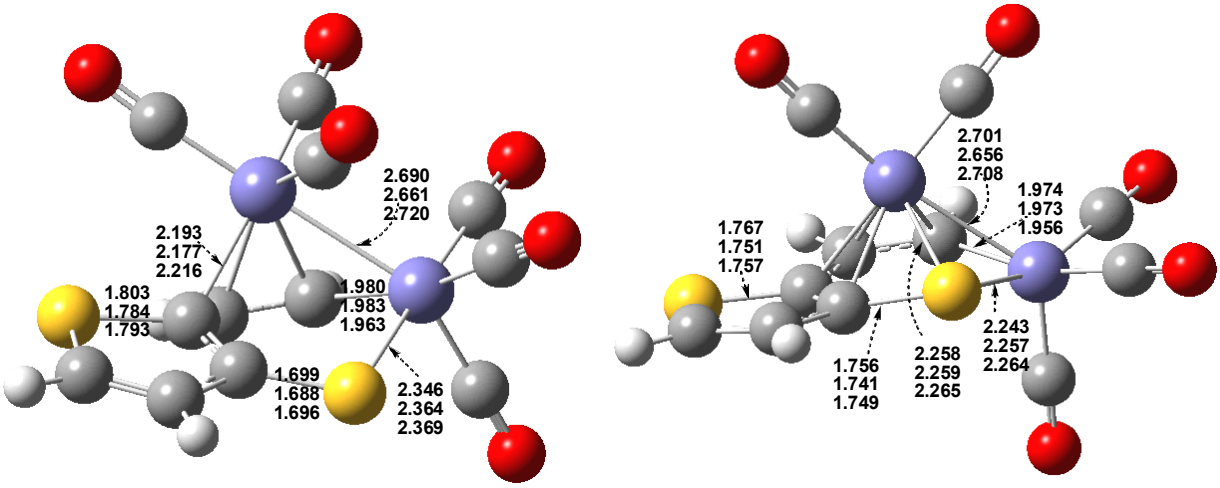
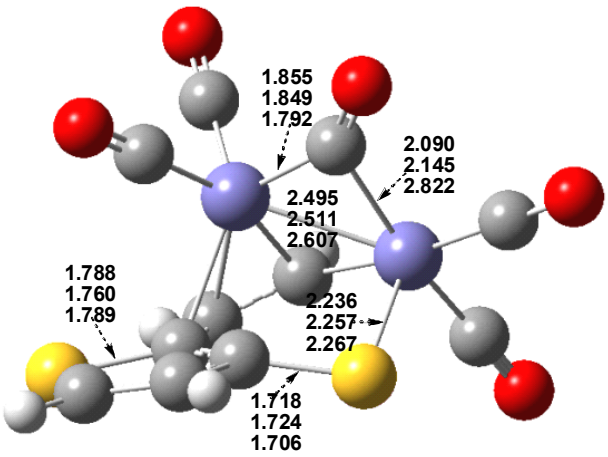


Figure S2. The lowest-lying $(C_6H_4S_2)Fe_2(CO)_6$ and $(C_6H_4S_2)Fe_2(CO)_5$ structures ***anti*-ThTh6-1** and ***anti*-ThTh5-1.**

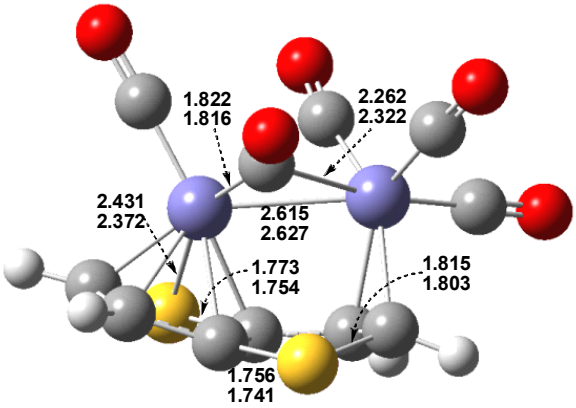


***anti*-ThTh6-1** ***anti*-ThTh5-1**

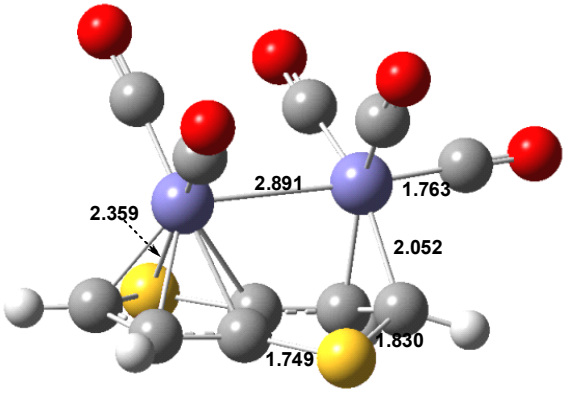
Figure S3. The $(C_6H_4S_2)Fe_2(CO)_5$ structures ***anti*-ThTh5-2 and *anti*-ThTh5-3.**



***anti*-ThTh5-2**

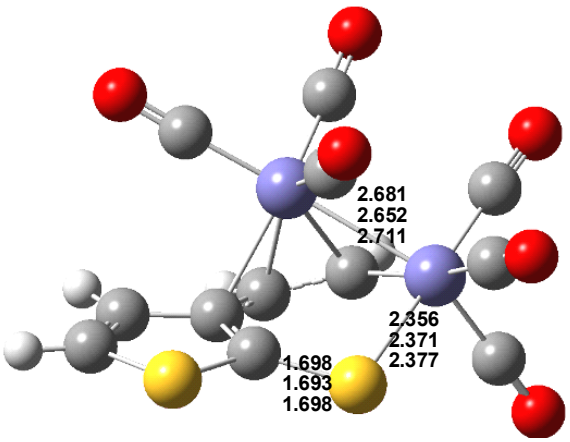


***anti*-ThTh5-3 (** bythe BP86 and M06L method**)**

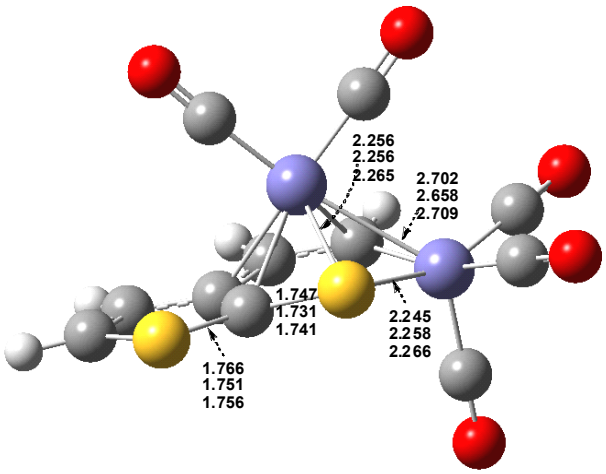


ThTh5-3 (by the B3LYP method**)**

Figure S4. The lowest-lying *syn*-$(C_6H_4S_2)Fe_2(CO)_6$ and *syn*-$(C_6H_4S_2)Fe_2(CO)_5$ structures ***syn*-ThTh6-1** and ***syn*-ThTh5-1.**

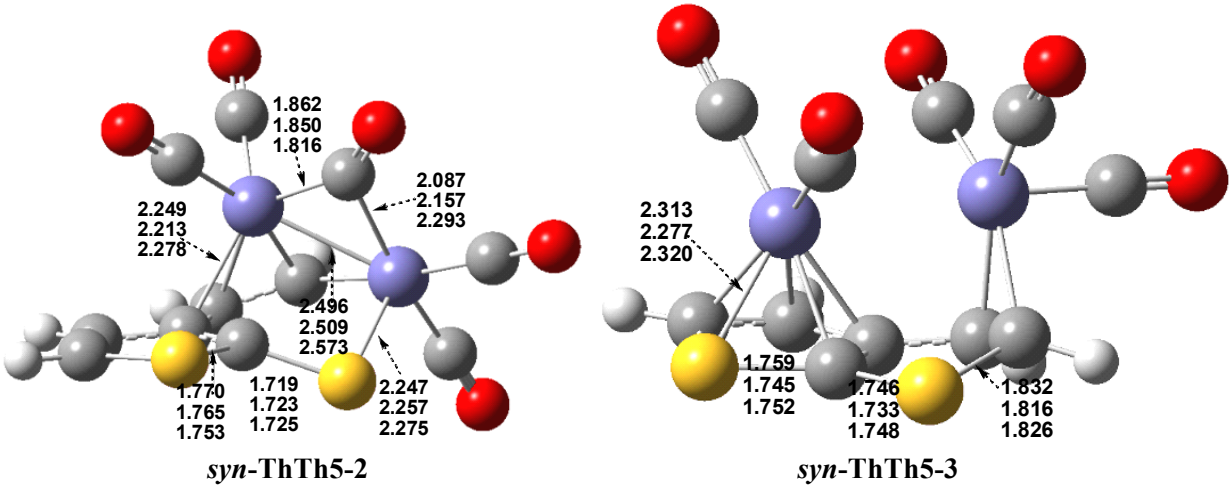


***syn*-ThTh6-1**



***syn*-ThTh5-1**

Figure S5. The *syn*-$(C_6H_4S_2)Fe_2(CO)_5$ structures ***syn*-ThTh5-2** and ***syn*-ThTh5-3.**



***syn*-ThTh5-2** ***syn*-ThTh5-3**