Supporting Information

Bonding in Homoleptic Iron Carbonyl Cluster Cations: A Combined Infrared Photodissociation

Spectroscopic and Theoretical Study

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Table S1. Harmonic vibrational frequencies (cm^{-1}) and IR intensities (km/mol) of $Fe(CO)_5^+$ and $Fe(CO)_6^+$.

Freq.	IR Int.	Freq.	IR Int.
$Fe(CO)_6^+$		$Fe(CO)_5^+$	
26.2	0.2	47.7	0
26.2	0.2	80.0	0
49.0	0.0	80.0	0
50.6	3.0	98.6	0
78.2	0.1	103.2	1.6
78.2	0.1	103.2	1.6
86.0	0.4	107.1	1.1
86.0	0.4	316.9	0.1
98.5	0.0	321.1	1.5
102.7	1.3	338.5	0
102.7	1.3	343.3	0
103.9	1.5	361.1	6.4
307.8	2.9	385.6	26
315.2	0.0	385.6	26
315.2	0.0	415.3	0
337.6	0.0	470.0	2.8
340.4	0.0	470.0	2.8
357.7	3.9	532.6	56.0
386.2	25.7	571.9	79.2
386.2	25.7	571.9	79.2
422.8	0.0	573.8	56.0
463.9	2.9	2197.0	954.6
463.9	2.9	2197.0	954.6
530.6	0.0	2202.9	416.5
571.9	55.9	2211.4	0.0

572.6	81.3	2256.2	0.6
572.6	81.3		
2192.5	954.3		
2192.5	954.3		
2198.3	434.0		
2207.3	0.0		
2244.5	64.4		
2253.1	1.9		

Table S2: Harmonic vibrational frequencies (cm^{-1}) and IR intensities (km/mol) of $Fe_2(CO)_8^+$.

C_s, $^4A''$		C_{2v}, $^2B_1$		D_{2d}, ^2A		C_{2v}, $^4B_1$	
Freq.	IR Int.	Freq.	IR Int.	Freq.	IR Int.	Freq.	IR Int.
5.5	0.0	24.3	0.7	-15.0	0.3	-154.5	0.0
36.9	0.3	31.5	0.0	-11.2	0.0	35.8	0.0
38.8	0.4	36.5	0.1	42.6	1.0	36.8	0.0
42.3	0.1	41.2	0.3	63.5	0.9	43.1	0.4
51.3	0.0	65.9	1.8	68.2	1.9	72.8	0.0
57.9	0.0	70.9	0.6	70.8	1.3	75.9	0.0
62.7	0.0	80.5	0.7	72.4	0.0	80.7	0.3
69.8	1.9	81.2	0.0	79.8	0.0	83.3	0.0
69.9	1.2	81.9	0.2	80.5	0.1	85.1	2.6
91.3	0.0	86.9	0.0	85.1	0.6	91.0	0.3
91.6	0.0	91.4	0.5	90.4	0.8	97.9	0.6
102.1	0.0	93.4	0.8	91.2	0.5	98.9	1.6
108.5	1.5	99.1	0.8	92.6	0.0	114.4	0.9
112.4	0.4	104.8	0.3	113.1	0.4	120.2	0.0
112.6	0.6	117.6	1.1	115.3	1.2	200.8	0.1
147.4	3.3	178.4	0.9	183.6	2.0	204.1	5.5
237.6	35.9	324.5	0.9	303.4	0.1	249.4	0.0
251.8	0.6	336.6	1.4	320.7	0.0	323.4	0.2
279.0	18.3	340.4	0.0	349.8	8.8	335.7	1.5
280.2	1.0	346.0	3.5	351.9	0.0	335.8	6.6
298.1	23.4	352.6	38.5	354.3	4.2	339.1	0.9
307.2	1.7	353.0	0.2	355.0	0.0	347.5	0.0
350.7	0.6	355.3	0.0	358.3	66.7	348.7	171.8
362.2	0.0	366.5	14.7	380.9	0.2	362.6	0.2
371.2	0.0	384.0	35.7	392.9	9.5	366.4	0.0
375.0	0.0	407.1	1.4	398.4	6.5	368.1	12.8
376.0	0.0	416.1	2.0	413.5	0.3	370.0	25.1
386.5	2.9	426.3	8.3	414.1	37.0	372.7	70.8
398.4	5.7	461.9	0.0	461.6	4.0	386.0	24.0
399.0	0.5	462.7	14.3	473.4	47.9	422.7	3.5
420.4	0.0	468.8	5.6	480.2	5.8	436.9	187.7
432.3	7.3	477.6	1.3	485.5	0.0	443.1	0.0
453.1	14.6	504.7	183.2	491.0	0.0	483.1	4.2
453.3	14.3	508.3	0.0	500.9	108.1	504.0	0.0

524.0	10.0	510.6	39.7	515.7	3.7	509.2	56.5
524.9	10.4	545.3	84.9	535.3	61.0	512.2	78.3
557.9	0.1	550.2	50.6	544.1	102.2	516.4	0.0
617.5	94.3	572.0	109.6	555.7	85.1	524.8	41.9
618.4	97.4	577.0	60.2	561.6	50.1	535.2	23.3
642.0	250.4	607.2	41.8	587.6	51.4	546.2	16.2
2130.2	480.8	2124.3	614.2	2129.3	646.6	2024.0	743.8
2131.1	573.0	2127.2	894.2	2129.6	910.4	2040.7	126.2
2140.4	57.1	2140.3	15.2	2136.5	98.8	2161.5	0.2
2156.7	1131.3	2153.5	3.6	2153.9	0.8	2164.0	0.0
2163.5	1319.7	2161.6	1043.5	2169.3	933.3	2165.8	1196.2
2165.7	170.5	2170.4	783.9	2170.6	708.9	2170.2	1147.9
2199.0	838.0	2179.1	1416.1	2179.0	1530.6	2184.0	1534.1
2226.3	15.6	2217.2	0.0	2217.5	10.5	2215.7	16.3

Table S3: Harmonic vibrational frequencies (cm^{-1}) and IR intensities (km/mol) of $Fe_2(CO)_9^+$.

C_{2v}, $^1B_1$		C_{4v}, $^2A_1$		C_{4v}, $^2A_1$	
Freq.	IR Int.	Freq.	IR Int.	Freq.	IR Int.
12.9	0.1	33.8	0.0	-9.6	0.0
16.6	0.0	52.0	0.0	40.0	0.0
35.4	0.1	52.4	0.0	40.7	0.0
64.9	0.3	52.4	0.0	40.7	0.0
72.0	0.1	59.5	0.0	70.1	0.1
72.3	0.0	60.5	0.0	70.1	0.1
72.5	0.1	60.5	0.0	82.6	7.1
92.4	0.5	80.0	2.1	86.3	0.0
93.3	0.8	93.0	0.1	96.0	1.3
93.8	0.0	93.0	0.1	96.0	1.3
96.8	1.0	98.6	1.4	98.2	0.0
97.5	0.7	98.6	1.4	99.7	0.3
106.5	0.2	99.9	0.0	99.7	0.3
109.1	0.3	104.5	0.0	102.4	0.0
112.1	0.7	111.0	0.6	110.6	1.7
113.1	0.5	111.0	0.6	112.2	0.4
116.7	0.0	114.5	1.0	112.2	0.4
140.0	2.5	125.4	6.4	125.5	1.9
319.0	1.4	348.6	0.0	343.2	0.0
345.8	0.0	363.3	0.0	360.8	0.0
361.1	0.0	367.4	0.0	365.2	0.0
369.1	0.1	369.7	0.1	368.4	0.3
372.2	12.4	369.7	0.1	368.4	0.3
380.5	1.3	370.0	27.9	369.3	0.0
381.4	36.9	377.2	0.0	370.8	30.7
382.2	0.6	385.4	0.2	377.8	0.3
382.9	0.0	385.4	0.2	377.8	0.3
388.3	0.5	395.6	9.8	396.3	11.4
396.8	0.1	412.3	30.8	412.1	26.4
422.1	0.0	412.3	30.8	412.1	26.4
429.1	5.0	418.9	0.0	420.4	0.0
443.9	14.6	438.1	0.0	438.0	7.8
451.0	16.1	438.2	6.3	442.3	0.0
460.6	8.7	452.3	11.6	451.9	10.8
466.9	32.8	452.3	11.6	451.9	10.8
526.4	7.8	529.6	10.5	531.9	7.3
530.8	0.0	529.6	10.5	531.9	7.3
532.1	0.2	549.1	0.0	548.3	0.0
555.3	1.0	555.8	0.0	555.2	0.0
555.6	50.0	573.9	39.8	569.5	25.0
575.1	28.8	591.5	42.9	582.7	52.9
587.1	187.9	591.5	42.9	582.7	52.9
614.3	95.6	620.1	101.7	617.0	99.3

617.4	83.2	620.1	101.7	617.0	99.3
638.7	202.4	642.6	254.5	643.5	263.8
2124.9	142.5	2124.5	192.9	2123.5	225.2
2140.0	9.5	2124.5	192.9	2123.5	225.2
2145.6	4.0	2138.7	0.0	2135.7	0.0
2152.7	1708.5	2150.2	18.6	2149.2	27.0
2155.3	1727.7	2155.4	1794.3	2159.1	1745.9
2156.1	0.0	2155.4	1794.3	2159.1	1745.9
2168.4	57.6	2167.3	0.0	2172.2	0.0
2185.0	1333.5	2181.3	1259.4	2179.7	1415.3
2226.0	27.1	2228.2	0.5	2229.0	4.6

Table S4: Harmonic vibrational frequencies (cm^{-1}) and IR intensities (km/mol) of Fe$_3$(CO)$_{12}$$^+$.

C_1, ^4A		C_1, ^4A		C_2, ^2A		C_{2v}, $^4B_1$		C_s, $^2A''$		C_s, $^2A'$		D_{3h}, ^2A	
Freq.	IR Int.	Freq.	IR Int.	Freq.	IR Int.	Freq.	IR Int.	Freq.	IR Int.	Freq.	IR Int.	Freq.	IR Int.
2.1	0.0	17.0	0.1	20.3	0.1	21.0	0.0	9.3	0.0	39.8	0.0	-377.6	51.2
25.2	0.0	20.4	0.0	40.8	0.0	23.9	0.0	25.0	0.0	44.5	0.2	-51.4	27.4
27.9	0.0	28.7	0.0	46.9	0.0	29.4	0.0	33.2	0.1	55.6	0.1	55.6	0.1
35.0	0.0	41.4	0.3	50.4	0.1	35.5	0.0	33.5	0.1	58.9	0.5	55.7	0.1
38.1	0.1	41.5	0.1	53.9	0.0	42.7	0.1	40.8	0.0	60.1	0.0	56.9	0.0
44.7	0.1	45.4	0.1	64.9	0.2	44.3	0.1	44.7	0.2	63.1	0.0	60.2	0.6
47.3	0.1	48.0	0.3	65.9	0.4	65.9	0.3	58.5	0.1	70.4	0.0	67.6	0.2
50.0	0.1	53.2	0.2	69.2	0.0	69.4	1.3	65.2	0.2	71.0	2.9	68.3	0.0
52.1	0.1	53.8	0.1	78.3	0.0	75.0	1.1	72.2	0.0	80.3	0.1	87.1	16.6
61.0	0.2	60.1	0.3	79.8	0.5	75.6	0.8	72.9	0.6	86.8	1.2	88.3	0.1
62.2	1.5	67.3	0.1	82.1	0.0	79.2	0.1	81.2	0.1	86.9	0.0	88.7	10.5
63.7	0.0	71.9	0.0	82.9	0.0	79.8	0.5	84.8	1.3	95.3	0.9	89.0	0.0
67.9	0.0	79.3	1.8	86.4	2.0	82.3	0.0	84.8	1.3	96.0	1.5	94.3	1.4
87.4	1.3	83.7	0.6	88.4	0.7	87.4	0.1	86.5	0.5	98.7	1.6	95.4	2.1
89.7	0.8	85.2	0.1	93.7	0.0	88.0	0.0	87.5	0.1	99.6	1.3	98.4	1.0
91.4	0.0	90.2	15.0	98.7	0.7	89.6	0.0	89.4	0.5	103.9	0.5	100.9	0.0
91.7	0.2	92.8	0.9	101.4	0.2	92.5	1.1	91.3	0.2	105.4	0.1	101.4	0.1
95.8	0.2	97.6	0.2	103.5	0.3	92.9	0.4	91.9	1.2	106.8	0.2	106.1	1.6
104.7	5.4	99.6	0.0	105.7	0.0	98.9	1.0	95.4	1.0	109.1	1.6	110.1	19.3
105.2	2.2	103.4	0.3	106.8	0.3	99.6	0.4	100.7	4.3	111.3	0.1	118.1	0.0
108.4	0.2	105.0	0.0	110.7	0.1	102.8	1.5	102.5	0.2	118.8	0.0	120.8	0.0
110.6	1.5	109.1	0.5	111.5	0.0	105.7	0.0	105.9	0.7	120.1	0.0	125.4	0.9
113.0	0.7	111.1	0.7	118.6	0.0	108.5	0.7	110.3	0.1	124.9	0.1	128.9	0.0
114.9	0.1	111.3	1.3	120.2	0.1	109.7	0.1	132.0	0.2	131.3	0.4	152.8	0.2
116.4	0.1	113.6	0.2	131.7	0.0	127.6	1.3	135.7	9.6	138.0	3.8	159.3	17.1
126.6	6.6	115.5	1.3	142.1	0.5	132.3	0.2	140.3	0.1	155.0	0.2	187.9	2.2
129.8	0.4	118.9	0.1	147.4	0.0	191.5	3.0	146.3	7.6	225.5	16.0	203.3	18.3
288.3	14.9	312.5	0.0	349.4	6.3	306.6	6.9	312.9	3.3	337.5	8.1	212.6	36.6
297.7	46.6	339.8	5.9	349.5	0.9	327.9	1.2	327.7	1.7	341.7	31.9	244.9	62.0
315.0	13.9	361.8	0.0	355.6	0.9	336.2	3.3	330.2	0.3	354.2	11.4	293.2	106.8
321.7	0.0	363.0	0.1	361.5	2.1	337.4	0.0	337.4	0.4	362.7	0.3	298.1	13.1
338.6	6.5	363.6	0.0	361.5	0.3	345.3	0.0	338.9	0.0	378.2	0.0	332.7	1.1
363.5	0.1	368.8	1.4	371.6	2.4	354.9	0.9	350.8	0.5	379.8	42.6	368.5	0.3
365.5	0.0	375.1	0.1	372.4	0.4	355.6	4.1	352.8	4.8	384.1	37.7	369.2	0.0
367.6	0.4	375.1	0.5	377.1	2.0	363.0	0.0	366.6	0.2	385.9	1.1	379.3	8.2
369.6	0.6	375.8	0.0	388.0	3.5	366.8	9.7	370.4	14.1	388.4	22.3	379.4	2.8
375.8	0.1	384.3	18.0	390.4	30.1	370.0	1.8	370.4	13.2	389.7	0.6	390.1	0.1
376.2	0.2	386.0	1.1	394.0	11.7	370.1	1.6	371.3	37.7	394.8	0.3	398.4	0.0
377.5	0.3	395.0	62.5	399.5	1.1	372.8	64.1	374.1	48.3	402.0	1.2	398.7	3.3
377.7	0.2	397.5	14.5	401.5	26.2	378.0	0.1	376.5	15.1	402.7	1.1	399.3	0.0
401.3	12.4	399.4	0.8	404.6	9.6	379.8	14.7	381.2	3.8	404.7	79.9	408.3	6.7
402.2	0.8	422.5	0.1	405.2	5.7	389.8	0.0	388.6	36.5	428.2	39.4	429.8	38.3
413.6	1.5	423.1	1.2	407.6	0.0	407.5	16.1	398.1	1.2	437.7	31.9	433.0	104.7

423.1	1.5	444.0	8.6	413.2	5.6	418.8	6.8	410.4	7.9	444.7	8.0	441.7	0.0
425.5	0.1	444.8	3.2	416.6	0.5	440.7	13.0	415.2	97.7	445.3	46.3	444.9	21.0
441.8	10.0	451.4	2.2	469.0	0.1	457.1	6.1	451.0	17.3	452.7	16.2	451.2	5.9
442.6	7.7	451.6	19.1	477.1	1.0	467.3	0.1	453.4	22.8	456.3	21.6	457.4	2.4
457.6	11.4	455.7	4.5	477.3	4.7	470.3	9.2	468.7	1.3	460.6	21.1	459.9	0.0
459.2	11.6	462.7	16.4	492.3	31.0	473.5	9.3	470.9	20.6	468.7	0.1	460.6	0.4
459.8	12.0	463.0	11.6	495.7	0.7	473.8	6.1	479.7	0.5	483.6	0.5	463.2	0.0
463.0	9.1	467.0	1.0	500.3	10.6	481.9	24.1	492.7	6.8	494.6	2.4	484.8	33.6
524.5	9.3	502.3	5.4	530.3	8.8	504.1	0.0	494.2	205.7	546.2	1.0	520.2	60.0
525.9	11.3	503.7	7.5	531.1	3.2	520.3	0.0	513.1	167.6	546.6	28.8	524.0	0.0
533.0	7.0	549.0	16.2	542.9	2.3	523.4	0.0	522.2	1.3	548.8	2.9	568.4	46.9
534.4	15.5	549.6	2.8	552.1	111.6	535.5	484.9	522.6	1.1	552.7	33.0	573.8	0.0
560.7	0.2	557.4	0.4	562.2	1.5	536.0	23.4	539.0	75.3	581.4	7.8	586.0	0.0
560.9	0.6	558.0	0.5	566.1	0.4	548.3	88.5	550.8	13.2	586.9	1.1	588.4	3.1
621.5	38.7	613.2	117.0	571.5	180.0	553.5	59.3	552.9	72.0	598.8	101.1	592.3	44.0
624.3	13.2	613.4	23.4	575.1	101.4	556.4	45.7	560.4	166.3	599.2	128.1	599.0	56.0
627.1	147.6	629.0	80.0	576.0	171.4	560.1	8.1	563.5	15.4	611.1	96.4	602.0	14.2
628.8	149.7	632.4	129.9	587.7	35.3	560.2	52.2	567.1	6.0	619.8	274.1	604.0	73.2
641.8	428.3	640.4	435.9	591.4	11.0	579.6	105.7	580.0	112.0	625.7	36.7	609.5	11.3
654.4	88.6	650.4	65.1	597.2	125.9	586.1	28.6	582.7	33.5	631.3	4.7	1192.2	17881.6
2095.6	32.4	2082.8	423.2	2078.8	319.0	2049.5	442.7	2014.0	591.6	1954.8	781.6	2004.9	330.5
2101.5	151.2	2097.8	758.7	2080.0	187.4	2072.2	503.0	2047.6	302.4	2047.8	435.4	2038.0	78.0
2110.1	530.6	2100.4	480.2	2108.1	267.5	2072.5	58.8	2072.7	376.2	2089.8	330.0	2086.0	1448.3
2125.1	584.4	2115.1	334.4	2122.4	5.4	2104.7	10.6	2127.0	88.4	2112.9	172.5	2116.8	12.1
2126.0	1032.7	2120.5	88.4	2125.4	160.8	2122.4	1169.7	2129.0	159.5	2129.9	2.8	2120.9	0.0
2129.1	361.0	2136.1	420.8	2137.3	78.8	2141.7	502.7	2149.4	117.1	2134.1	230.9	2135.4	238.7
2139.1	1894.3	2144.1	82.3	2142.4	1619.9	2143.4	78.1	2150.9	1915.1	2146.5	92.4	2137.2	0.6
2150.5	35.4	2147.6	2596.0	2143.2	37.0	2156.4	1512.4	2152.7	1398.9	2155.5	36.6	2146.8	7.5
2152.2	421.5	2153.4	433.5	2146.0	546.2	2158.2	884.7	2157.3	100.4	2158.2	2264.4	2151.8	2392.9
2168.1	910.1	2161.4	431.8	2164.5	2028.7	2168.2	37.3	2163.1	387.1	2162.8	1596.0	2159.8	1408.5
2194.3	755.4	2191.9	832.4	2167.2	1692.0	2184.8	1484.1	2191.3	1277.3	2170.4	1205.4	2207.5	2.9
2211.4	0.7	2210.9	6.7	2206.3	0.0	2214.7	119.3	2212.4	25.3	2214.1	12.9	2368.5	8512.1

Table S5. Cartesian Coordinates of the Optimized Structures:

$Fe(CO)_5^+$

C_{4v}, $^2A_1$

Fe	0.000000	0.000000	0.213134
C	0.000000	1.885952	0.425413
O	0.000000	3.013774	0.548123
C	1.885952	0.000000	0.425413
O	3.013774	0.000000	0.548123
C	0.000000	-1.885952	0.425413
O	0.000000	-3.013774	0.548123
C	0.000000	0.000000	-1.729427
O	0.000000	0.000000	-2.864346
C	-1.885952	0.000000	0.425413
O	-3.013774	0.000000	0.548123

$Fe(CO)_6^+$:

C_{4v}, $^2A_1$

Fe	0.000000000000	0.000000000000	0.306416850000
C	0.000000000000	1.885967900000	0.103524030000
O	0.000000000000	3.014923940000	-0.013785870000
C	1.885967900000	0.000000000000	0.103524030000
O	3.014923940000	0.000000000000	-0.013785870000
C	-1.885967900000	0.000000000000	0.103524030000
O	-3.014923940000	0.000000000000	-0.013785870000
C	0.000000000000	0.000000000000	2.261357850000
O	0.000000000000	0.000000000000	3.396650850000
C	0.000000000000	0.000000000000	-2.977987150000
O	0.000000000000	0.000000000000	-4.110181150000
C	0.000000000000	-1.885967900000	0.103524030000
O	0.000000000000	-3.014923940000	-0.013785870000

$Fe_2CO_8^+$:

C_s, $^4A''$

C	-1.575630864676	-2.384517503254	0.000000000000
O	-2.537231415053	-2.990281280627	0.000000000000
C	-0.177194285636	3.173308112910	0.000000000000
O	-0.264919409751	4.308614430294	0.000000000000
C	-1.302326114704	0.972102033531	1.298167584662
O	-2.089898022421	0.786700580895	2.105818900013
C	-1.302326114704	0.972102033531	-1.298167584662
O	-2.089898022421	0.786700580895	-2.105818900013
C	1.276677124180	1.170695315572	-1.291089876591
O	2.091221313437	1.115643595706	-2.091508217149
C	1.276677124180	1.170695315572	1.291089876591
O	2.091221313437	1.115643595706	2.091508217149
C	0.852140165890	-2.267196026440	1.635392926762
O	1.235311050432	-2.760807152707	2.584544093858
C	0.852140165890	-2.267196026440	-1.635392926762

O	1.235311050432	-2.760807152707	-2.584544093858
Fe	0.159310107037	-1.321202663626	0.000000000000
Fe	-0.035074955777	1.319232774798	0.000000000000

C_{2v}, $^2B_1$

Fe	0.000000000000	0.000000000000	1.189443877774
Fe	0.000000000000	0.000000000000	-1.259161303097
C	1.283086151430	0.000000000000	-2.570441681515
O	2.140689262815	0.000000000000	-3.319861532793
C	0.000000000000	1.461056709468	2.409715094483
O	0.000000000000	2.341834947353	3.131853260818
C	0.000000000000	1.818977765836	-0.860876065500
O	0.000000000000	2.955819389902	-0.740987877498
C	1.848355472865	0.000000000000	1.059261809377
O	2.990290984774	0.000000000000	1.012839255288
C	0.000000000000	-1.461056709468	2.409715094483
O	0.000000000000	-2.341834947353	3.131853260818
C	-1.848355472865	0.000000000000	1.059261809377
O	-2.990290984774	0.000000000000	1.012839255288
C	-1.283086151430	0.000000000000	-2.570441681515
O	-2.140689262815	0.000000000000	-3.319861532793
C	0.000000000000	-1.818977765836	-0.860876065500
O	0.000000000000	-2.955819389902	-0.740987877498

D_{2d}, ^2A

Fe	0.000000	0.000000	1.20909063
Fe	0.000000	0.000000	-1.20909063
C	-1.83769471	0.000000	-0.93906958
O	-2.97650945	0.000000	-0.83919241
C	0.000000	1.83769471	0.93906958
O	0.000000	2.97650945	0.83919241
C	-1.37403938	0.000000	2.48939961
O	-2.24039518	0.000000	3.22786618
C	0.000000	-1.83769471	0.93906958
O	0.000000	-2.97650945	0.83919241
C	1.37403938	0.000000	2.48939961
O	2.24039518	0.000000	3.22786618
C	1.83769471	0.000000	-0.93906958
O	2.97650945	0.000000	-0.83919241
C	0.000000	1.37403938	-2.48939961
O	0.000000	2.24039518	-3.22786618
C	0.000000	-1.37403938	-2.48939961
O	0.000000	-2.24039518	-3.22786618

C_{2v}, $^4B_1$

Fe	0.000000	1.26385011	-0.33636867
Fe	0.000000	-1.26385011	-0.33636867
C	-1.34533735	-2.29558026	-1.16920498
C	1.34533735	-2.29558026	-1.16920498

C	-1.34533735	2.29558026	-1.16920498
C	1.34533735	2.29558026	-1.16920498
O	-2.1527085	-2.92345835	-1.66830301
O	-2.1527085	2.92345835	-1.66830301
O	2.1527085	2.92345835	-1.66830301
O	2.1527085	-2.92345835	-1.66830301
C	1.45738322	0.000000	0.30494817
C	-1.45738322	0.000000	0.30494817
O	2.51764043	0.000000	0.76193107
O	-2.51764043	0.000000	0.76193107
C	0.000000	2.17913718	1.33218621
C	0.000000	-2.17913718	1.33218621
O	0.000000	2.75294777	2.31602338
O	0.000000	-2.75294777	2.31602338

$Fe_2(CO)_9^+$:

C_{2v}, $^1B_1$

Fe	0.000000000000	0.000000000000	-1.447005975187
Fe	0.000000000000	0.000000000000	1.413390785203
C	0.000000000000	1.855487032054	1.398099787115
O	0.000000000000	2.996037209674	1.458314850231
C	1.316736811159	-1.289122788005	-1.242546991478
O	2.139451393393	-2.076175841661	-1.163161761622
C	0.000000000000	0.000000000000	-3.300450300038
O	0.000000000000	0.000000000000	-4.438803770176
C	-1.316736811159	1.289122788005	-1.242546991478
O	-2.139451393393	2.076175841661	-1.163161761622
C	-1.316736811159	-1.289122788005	-1.242546991478
O	-2.139451393393	-2.076175841661	-1.163161761622
C	0.000000000000	-1.855487032054	1.398099787115
O	0.000000000000	-2.996037209674	1.458314850231
C	1.481699190151	0.000000000000	2.568637088730
O	2.381208860870	0.000000000000	3.269633090223
C	-1.481699190151	0.000000000000	2.568637088730
O	-2.381208860870	0.000000000000	3.269633090223
C	1.316736811159	1.289122788005	-1.242546991478
O	2.139451393393	2.076175841661	-1.163161761622

C_{4v}, $^2A_1$

Fe	0. 000000	0.000000	-1.79721995
Fe	0.000000	0.000000	1.27647947
C	1.32285831	-1.32285831	-1.91593646
C	1.32285831	1.32285831	-1.91593646
C	-1.32285831	1.32285831	-1.91593646
C	1.32285831	-1.32285831	-1.91593646
O	-2.12629122	-2.12629122	-2.00462382
O	2.12629122	-2.12629122	-2.00462382
O	2.12629122	2.12629122	-2.00462382

O	-2.12629122	2.12629122	-2.00462382
C	0.000000	1.8304273	1.03404621
C	1.8304273	0.000000	1.03404621
C	0.000000	-1.8304273	1.03404621
C	-1.8304273	0.000000	1.03404621
O	0.000000	2.96809238	0.91901647
O	2.96809238	0.000000	0.91901647
O	0.000000	-2.96809238	0.91901647
O	-2.96809238	0.000000	0.91901647
C	0.000000	0.000000	3.1235757
O	0.000000	0.000000	4.26303122

C_{4v}, $^2A_1$

Fe	0.000000000000	0.000000000000	1.794706019747
Fe	0.000000000000	0.000000000000	-1.436651650286
C	0.000000000000	-1.870393878785	1.921736760600
O	0.000000000000	-3.003681575437	2.038855749652
C	-1.870393878785	0.000000000000	1.921736760600
O	-3.003681575437	0.000000000000	2.038855749652
C	0.000000000000	1.870393878785	1.921736760600
O	0.000000000000	3.003681575437	2.038855749652
C	1.870393878785	0.000000000000	1.921736760600
O	3.003681575437	0.000000000000	2.038855749652
C	0.000000000000	1.832780763250	-1.214948254588
O	0.000000000000	2.973867040321	-1.140017117324
C	-1.832780763250	0.000000000000	-1.214948254588
O	-2.973867040321	0.000000000000	-1.140017117324
C	0.000000000000	-1.832780763250	-1.214948254588
O	0.000000000000	-2.973867040321	-1.140017117324
C	1.832780763250	0.000000000000	-1.214948254588
O	2.973867040321	0.000000000000	-1.140017117324
C	0.000000000000	0.000000000000	-3.279753850899
O	0.000000000000	0.000000000000	-4.419581359919

$Fe_3(CO)_{12}^+$:
C_1, ^4A

Fe	-2.544690197202	-0.389972134095	-0.076579227980
Fe	-0.006335953376	0.928929044758	0.102923978538
C	-2.958984572997	0.526042245315	1.467885695983
O	-3.243196771919	1.086310343603	2.423918291283
C	-4.107885392821	-1.353043261612	-0.297247678035
O	-5.067937563530	-1.952524549930	-0.436368724003
C	-1.623227712042	-0.950113005672	-1.558507608301
O	-1.080735640273	-1.304637271706	-2.505287653480
C	-3.053186222123	1.110733014916	-1.020095982575
O	-3.390607867041	2.036511231035	-1.600310285604
C	0.032627688956	2.213739414002	-1.374304323684
O	0.056059936972	2.942725404213	-2.251448582197
C	-0.012063044367	1.868045395424	1.822303884146

O	-0.012877245836	2.393394417094	2.834925240826
C	-1.655501493759	-1.612064924240	0.965396969138
O	-1.130488002007	-2.377676559165	1.636650024067
Fe	2.534705186572	-0.428409803662	-0.008479088343
C	3.015198935385	1.310336162961	0.359922560160
O	3.335897411330	2.385902744633	0.585182551538
C	4.235434830623	-1.153815990925	0.001857417874
O	5.284906584936	-1.600019720847	0.009888931848
C	1.618357370864	-1.972127440227	-0.394851128251
O	1.075883941489	-2.949231441829	-0.643218732276
C	2.099191824553	-0.660450361206	1.762488216999
O	1.855587106663	-0.825046332305	2.869629834251
C	2.411261820232	0.018624122752	-1.789956870323
O	2.362286933955	0.277805415077	-2.903794439973

C_1, ^4A

Fe	2.767090619275	0.088097621316	-0.225048895165
Fe	-0.001084251695	-0.013703409528	1.154581775838
Fe	-2.761903904914	-0.086941119809	-0.242161259380
C	-0.060319695846	1.881181762375	1.411314823276
O	-0.094192178241	3.015003500119	1.549953149516
C	3.152703452298	-1.534113150895	0.566569317525
O	3.413349694549	-2.535496492669	1.051095951391
C	4.403948650140	0.178907433950	-1.073018071058
O	5.414839091762	0.235019596016	-1.599334233851
C	2.213648118402	1.708306294927	-0.913043141746
O	1.899585540485	2.718293061109	-1.345699379673
C	1.683159265745	-0.778921700965	-1.417398018918
O	1.042275731228	-1.331731892090	-2.194276500519
C	0.056910932874	-1.913615143238	1.371241782904
O	0.090270785670	-3.050141846555	1.485719491362
C	3.043987076981	0.893357304876	1.403240069132
O	3.247224479334	1.390920125208	2.416442993036
C	-3.151934152905	1.518488148891	0.580757505137
O	-3.415285738883	2.509689287473	1.084392546340
C	-4.394528896698	-0.160294330463	-1.099916372187
O	-5.402862892988	-0.205571259884	-1.632165728244
C	-2.204791819973	-1.692440176905	-0.961024162832
O	-1.888432033606	-2.693163931593	-1.413073976582
C	-1.672004230788	0.804898192526	-1.410510267237
O	-1.027289881358	1.374103918397	-2.172231992347
C	-3.046552233103	-0.925876669846	1.367630522319
O	-3.25458554876	-1.444722322819	2.369150524745

C_2, ^2A

Fe	0.213332002851	1.603698252544	0.005433205321
Fe	1.250899994655	-1.026594710874	0.040398399755
Fe	-1.475702360191	-0.663647440196	-0.046285091280
C	-2.366980465240	-2.232125187778	-0.538221703855

O	-2.931203471969	-3.180698540126	-0.825239736376
C	-1.982181893095	0.220514507323	-1.598101105157
O	-2.392115635664	0.712643473880	-2.545557249926
C	-2.868958335674	0.132115754065	0.883309676185
O	-3.738431169711	0.619153239687	1.440652210778
C	-0.867239577597	-1.425989630915	1.517470718713
O	-0.710583682487	-1.918011292686	2.544230039506
C	0.655837996063	1.452694708460	-1.778191869196
O	0.946731826420	1.434448404093	-2.885344565973
C	-0.976374485132	2.981904432942	-0.334713882802
O	-1.699224982720	3.840941010535	-0.544301803641
C	1.721565988758	2.620779984486	0.353757588515
O	2.643601919245	3.259634174089	0.568464598712
C	-0.254831930970	1.561622390382	1.788405328688
O	-0.541357631814	1.612598298959	2.895675816380
C	2.804533171198	-0.616515809595	-0.885096396308
O	3.771569275452	-0.369984989415	-1.439927330382
C	1.700736491703	-2.776768499861	0.521009234446
O	1.997112039458	-3.841736814153	0.801147911372
C	1.969551134693	-0.316009590573	1.597630754295
O	2.493069696085	0.045460508450	2.547980061787
C	0.465678782201	-1.592873002047	-1.527876072198
O	0.186773857113	-2.019941791126	-2.557773320014

C_{2v}, $^4B_1$

Fe	0.144952985388	-0.013202808155	0.002719665781
Fe	2.687179533489	-0.282974533250	-0.002005324162
Fe	-2.665156872151	0.284889524854	0.007801237688
C	2.420852027006	-1.544701562793	-1.325824220162
O	2.285257391933	-2.329974454633	-2.146450716181
C	0.733511566429	1.212604452719	-1.238767396671
O	1.027630715249	1.997684236646	-2.025274302061
C	0.467695240799	-1.335693297134	1.242544616794
O	0.593403375500	-2.165293335775	2.028298549409
C	-0.575689435421	1.226858160175	1.199118609702
O	-0.740313455774	2.030376883179	2.006755594379
C	2.696385893302	1.005935125123	1.322371557261
O	2.731595423904	1.801758514197	2.143269116354
C	3.775066448025	-1.445453138762	1.004512673791
O	4.430402692922	-2.151365677374	1.616339512494
C	3.990819166055	0.625970500256	-1.013111608269
O	4.777240527802	1.179096581745	-1.627703780917
C	-0.824155892526	-1.073973701285	-1.190611365247
O	-1.156590771286	-1.824738020654	-1.997373923880
C	-2.730036627556	-1.055657813250	1.304904391955
O	-2.795475639363	-1.871902355368	2.097313158606
C	-2.451989678719	1.609634221291	-1.289656859524
O	-2.347563540281	2.421638598360	-2.082269197185
C	-3.980127079815	-0.583624795089	-1.025369719954

O	-4.789789650321	-1.097493622882	-1.640147780032
C	-3.764789441100	1.409655620438	1.045421479391
O	-4.446306903487	2.081798697463	1.662930030609

C_s, $^2A''$

Fe	-2.4466133259	0.193080573	-0.5807842796
Fe	-0.0239444943	1.446995486	-0.2091404395
Fe	2.4781343875	0.3054128876	-0.0913508316
C	4.1558812907	0.8993073485	-0.7178390853
O	5.1756890024	1.2465266727	-1.0896534166
C	2.9781776058	-1.3519741459	0.6482717616
O	3.2935552615	-2.3545950577	1.0901379798
C	2.0768922571	-0.4748197243	-1.726247618
O	1.8574620014	-0.9625466018	-2.7350494369
C	2.7106585592	1.1705463008	1.5401966662
O	2.8732712187	1.6905445455	2.5421348055
C	1.3435273589	2.3991268816	-0.9897868611
O	2.0098485697	3.1686386874	-1.5311264465
C	-0.0835846875	-0.1235384883	0.7433669377
O	-0.1338040873	-1.0347088003	1.4561470271
C	-1.250274337	2.3394157047	-1.2512864387
O	-1.8295388674	3.0795159478	-1.9189296426
C	-0.1979261518	2.5860712533	1.2728851387
O	-0.3032911822	3.2808549958	2.1753362802
C	-3.9908207515	0.7145619713	-1.5316103882
O	-4.9304694085	1.0178011747	-2.1007297241
C	-1.6930863045	-0.5689961404	-2.095367276
O	-1.2475355092	-1.0564168746	-3.0268422713
C	-3.0355440109	1.0418583328	0.9675495362
O	-3.4162739366	1.5503636002	1.9147434135
C	-3.0105805896	-1.4862412057	0.0558558947
O	-3.3631458686	-2.5027763247	0.4331097147

C_s, $^2A'$

Fe	0.922910001745	-1.364577984879	0.000000000000
Fe	-1.591460142955	0.012461273035	0.000000000000
Fe	0.955318520146	1.490895701978	0.000000000000
C	-3.366831485226	-0.383516887725	0.000000000000
O	-4.483827565966	-0.617566021371	0.000000000000
C	-1.672271589975	-0.006390856534	1.853824892945
O	-1.804549580440	-0.008855285876	2.987362067296
C	-1.050175537438	-1.933754896256	0.000000000000
O	-1.593143684287	-2.965405471172	0.000000000000
C	-1.672271589975	-0.006390856534	-1.853824892945
O	-1.804549580440	-0.008855285876	-2.987362067296
C	0.989837103923	1.554403033571	1.856494256294
O	1.038312516211	1.670427975188	2.992520750251
C	2.443721278631	-0.328872588589	0.000000000000
O	3.513582618257	0.107098220251	0.000000000000

C	0.934767503472	-1.485469423284	-1.851099307921
O	0.991375467499	-1.635323045115	-2.981231301746
C	0.934767503472	-1.485469423284	1.851099307921
O	0.991375467499	-1.635323045115	2.981231301746
C	1.573065758275	-3.062747633806	0.000000000000
O	2.004872397278	-4.119441386354	0.000000000000
C	1.239146984907	3.304134703173	0.000000000000
O	1.421603363905	4.431866711129	0.000000000000
C	0.989837103923	1.554403033571	-1.856494256294
O	1.038312516211	1.670427975188	-2.992520750251
C	-1.662390536401	1.868927352058	0.000000000000
O	-2.007799052250	2.964714862627	0.000000000000

D_{3h}, ^2A

Fe	0.000000	0.000000	1.562141
Fe	1.352854	0.000000	-0.781070
Fe	-1.352854	0.000000	-0.781070
C	0.000000	0.000000	3.381691
O	0.000000	0.000000	4.524327
C	2.928630	0.000000	-1.690845
O	3.918182	0.000000	-2.262163
C	-2.928630	0.000000	-1.690845
O	-3.918182	0.000000	-2.262163
C	2.016893	0.000000	1.164454
O	3.017076	0.000000	1.741910
C	0.000000	0.000000	-2.328907
O	0.000000	0.000000	-3.483820
C	-2.016893	0.000000	1.164454
O	-3.017076	0.000000	1.741910
C	0.000000	-1.853358	1.702241
O	0.000000	-2.978410	1.899175
C	1.474184	-1.853358	-0.851121
O	1.644733	-2.978410	-0.949587
C	-1.474184	-1.853358	-0.851121
O	-1.644733	-2.978410	-0.949587
C	0.000000	1.853358	1.702241
O	0.000000	2.978410	1.899175
C	1.474184	1.853358	-0.851121
O	1.644733	2.978410	-0.949587
C	-1.474184	1.853358	-0.851121
O	-1.644733	2.978410	-0.949587