Supporting Information For:

Infrared Photodissociation Spectra of Mas Selected Homoleptic Dinuclear Iron Carbonyl Cluster Anions in the Gas Phase

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Table S1 Harmonic vibration frequencies (cm^{-1}) of the $Fe_2(CO)_4^-$ anion calculated at the B3LYP/6-31+G(d) level.

$Fe_2(CO)_4^-(C_s, {}^4A')$	$Fe_2(CO)_4^-(C_1, {}^4A)$	$Fe_2(CO)_4^-(C_{2v}, {}^4B_1)$	$Fe_2(CO)_4^-(C_{3v}, {}^4A)$[a]
25	27	16	46
51	40	67	49
53	55	80	88
78	71	83	91
79	75	88	92
100	87	89	94
189	102	94	107
248	218	236	216
262	338	386	392
351	367	393	392
380	382	442	401
388	388	460	457
427	414	501	502
436	444	509	507
461	475	535	526
487	509	552	537
514	529	587	547
534	544	612	609
558	577	624	645
591	600	646	648
1626	1832	1873	1920
1833	1879	1879	1921
1912	1908	1935	1939
1968	1979	1994	2006

[a] The wavefunction has an undefined symmetry due to symmetry breaking.

Table S2 Harmonic vibration frequencies (cm^{-1}) of the $Fe_2(CO)_5^-$ anion calculated at the B3LYP/6-31+G(d) level.

$Fe_2(CO)_5^-$(C_s, $^4A'$)	$Fe_2(CO)_5^-$(C_{3v}, ^4A) [a]	$Fe_2(CO)_5^-$(C_{2v}, $^4A_2$)	$Fe_2(CO)_5^-$(C_s, $^4A''$)	$Fe_2(CO)_5^-$(C_s_1, $^4A''$)
19	-85	-58	9	11
36	-84	-50	18	19
46	16	22	44	36
51	16	70	74	61
61	75	77	78	82
63	75	92	93	89
71	89	93	95	91
91	89	94	110	99
114	89	97	128	107
168	212	217	223	224
288	298	322	334	326
327	298	323	373	372
345	389	387	387	390
346	393	399	400	392
372	393	428	401	393
382	468	465	460	466
441	477	497	490	479
468	523	522	511	513
483	523	526	523	514
503	523	531	524	519
513	562	570	554	555
557	562	570	569	562
557	625	640	634	622
563	653	647	634	647
599	653	647	647	647
1871	1893	1859	1851	1861
1918	1893	1879	1908	1915
1925	1923	1946	1947	1932
1967	1972	1978	1970	1973
2021	2015	2021	2023	2020

[a] The wavefunction has an undefined symmetry due to symmetry breaking.

Table S3 Harmonic vibration frequencies (cm^{-1}) of the $Fe_2(CO)_6^-$ anion calculated at the B3LYP/6-31+G(d) level.

$Fe_2(CO)_6^-(D_{3d}, {}^2A_{2u})$	$Fe_2(CO)_6^-(D_{3h}, {}^2A)$[a]	$Fe_2(CO)_6^-(C_{2h}, {}^2B_g)$	$Fe_2(CO)_6^-(C_s, {}^2A'')$	$Fe_2(CO)_6^-(C_{2v}, {}^2A_1)$
-34	-29	-1551	8	12
-33	-29	-317	22	26
-3	8	33	47	38
37	40	40	56	73
37	40	64	56	75
55	57	66	74	75
71	72	67	75	75
71	72	84	76	76
77	77	84	81	85
78	78	90	87	91
78	78	147	105	109
151	148	149	154	194
331	334	193	312	341
331	335	245	331	354
331	335	275	343	376
341	344	350	357	390
365	369	376	377	405
365	369	410	383	420
415	417	424	420	442
433	437	436	437	473
472	473	453	456	504
472	473	460	466	506
476	477	464	504	516
476	477	498	529	519
500	502	518	533	522
529	535	552	540	522
529	535	567	543	580
544	544	573	547	585
545	544	593	578	630
545	545	619	593	644
1949	1946	1582	1916	1903
1949	1946	1809	1937	1917
1967	1970	1953	1957	1956
1967	1970	1957	1970	1970
2002	2002	1967	1999	1999
2061	2062	2043	2059	2052

[a] The wavefunction has an undefined symmetry due to symmetry breaking.

Table S4 Harmonic vibration frequencies (cm^{-1}) of the $Fe_2(CO)_7^-$ anion calculated at the B3LYP/6-31+G(d) level.

$Fe_2(CO)_7^-(C_{2v}, {}^2A)^a$	$Fe_2(CO)_7^-(C_{2v}, {}^2A_1)$	$Fe_2(CO)_7^-(C_s, {}^2A')$
-346	24	9
-124	31	18
24	36	54
47	54	60
62	59	68
68	66	72
76	79	73
79	80	76
80	87	81
87	88	83
90	92	87
91	99	104
91	107	123
158	174	163
173	344	322
249	368	356
331	377	360
358	385	371
359	388	382
375	414	387
377	419	425
390	457	431
412	473	452
412	492	471
413	505	485
430	516	487
433	521	514
457	537	524
461	547	529
463	567	538
484	584	549
506	589	553
527	637	555
536	637	612
544	639	614
1904	1939	1932
2060	1947	1966
2066	1951	1972
2075	1980	1983
2081	2001	1987
2102	2002	2023

2147	2084	2077

[a] The wavefunction has an undefined symmetry due to symmetry breaking.

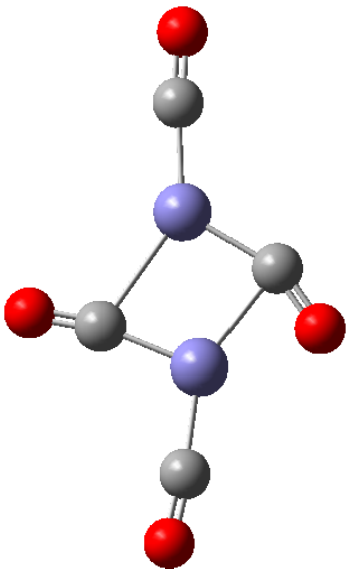
Table S5 Harmonic vibration frequencies (cm^{-1}) of the $Fe_2(CO)_8^-$ anion calculated at the B3LYP/6-31+G(d) level.

$Fe_2(CO)_8^-(D_{2h}, {}^2B_{2g})$	$Fe_2(CO)_8^-(D_{2d}, {}^2A)$	$^aFe_2(CO)_8^-(C_{2v}, {}^2B_2)$	$Fe_2(CO)_8^-(C_s, {}^2A')$	$Fe_2(CO)_8^-(C_s, {}^2A'')$
-145	-50	-163	23	17
-52	-31	27	34	31
50	29	29	36	32
68	32	35	64	42
88	67	72	75	72
91	74	76	79	73
91	77	82	80	77
93	80	83	87	82
96	84	94	89	85
102	86	96	92	89
104	90	101	99	92
114	93	102	101	98
123	95	113	117	102
123	107	162	182	105
187	119	205	213	143
220	176	231	235	183
273	343	285	311	342
321	351	320	372	347
341	360	375	383	365
348	362	386	393	382
360	376	392	394	384
375	401	395	400	414
393	419	421	424	415
422	437	425	425	446
435	468	440	448	465
439	471	471	468	467
442	478	476	474	467
464	485	477	482	491
466	502	479	485	507
508	505	485	491	514
514	522	511	512	521
517	533	519	521	526
548	539	520	530	542
561	568	565	564	557
603	571	586	582	577
616	587	594	593	582
624	596	613	607	585
627	603	625	624	616
646	615	627	626	639
669	616	630	650	646
1877	1967	1812	1822	1906

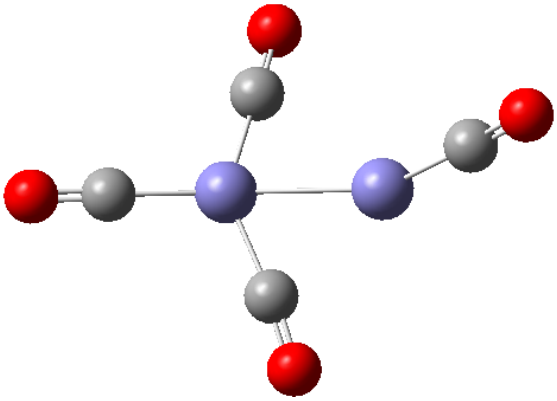
1891	1967	1863	1865	1978
1960	1983	1997	1996	1979
1970	1991	2000	1997	1991
1982	1997	2006	2005	2003
2020	2001	2009	2009	2007
2020	2023	2011	2026	2029
2095	2095	2095	2095	2096

[a] The wavefunction has an undefined symmetry due to symmetry breaking.

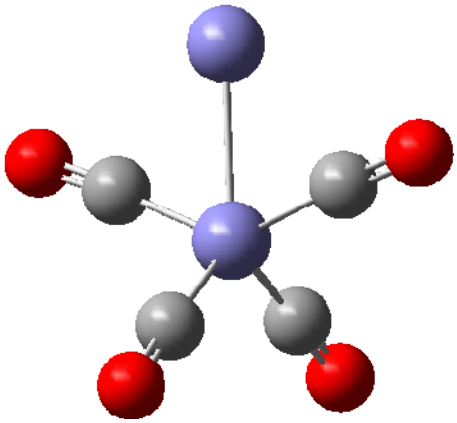
Figure S1 Geometries of the $Fe_2(CO)_4^-$ anion isomers.



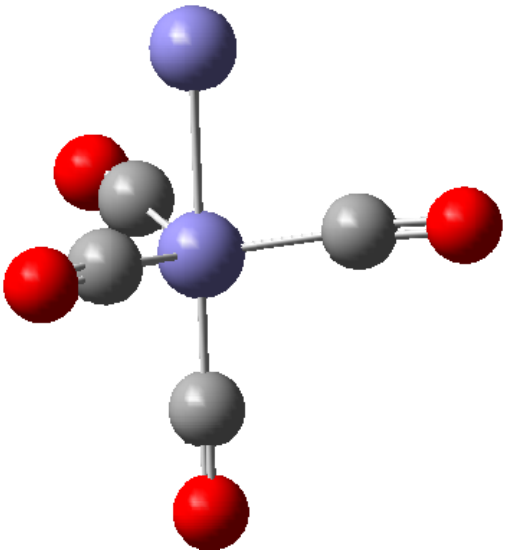
$Fe_2(CO)_4^-(C_s, {}^4A')$



$Fe_2(CO)_4^-(C_1, {}^4A)$

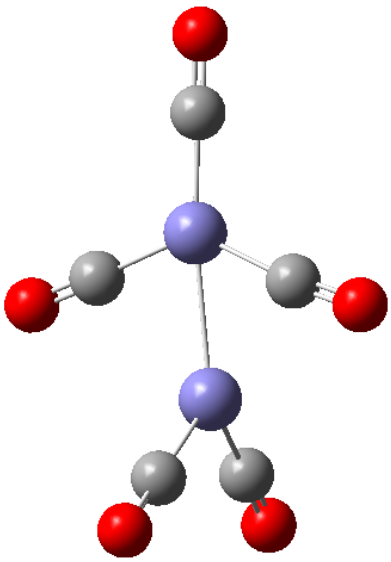


$Fe_2(CO)_4^-(C_{2v}, {}^4B_1)$

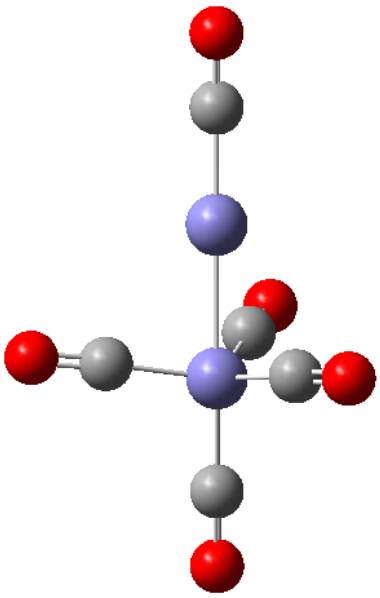


$Fe_2(CO)_4^-(C_{3v}, {}^4A)$

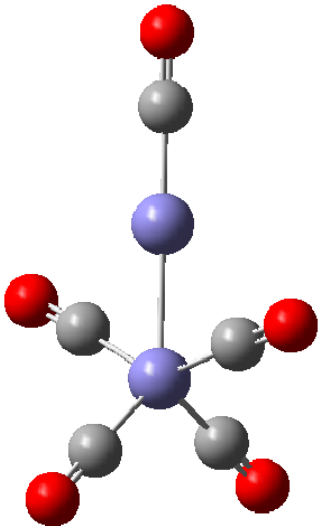
Figure S2 Geometries of the $Fe_2(CO)_5^-$ anion isomers.



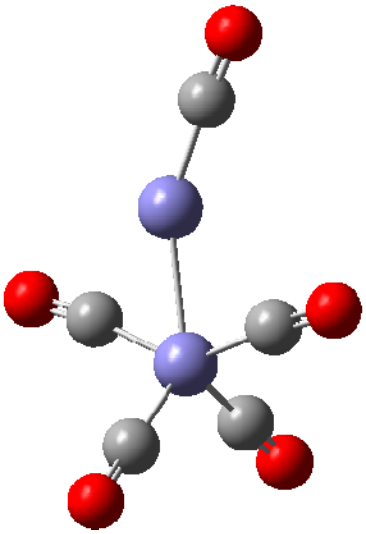
$Fe_2(CO)_5^-(C_s, {}^4A')$



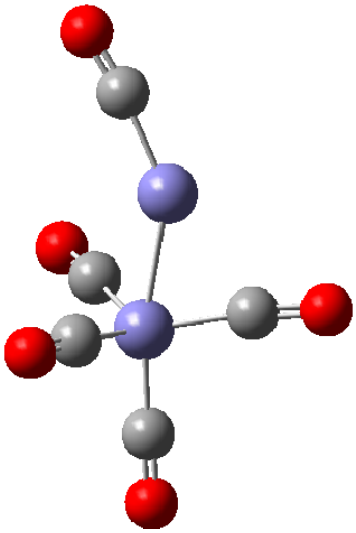
$Fe_2(CO)_5^-(C_{3v}, {}^4A)$



$Fe_2(CO)_5^-(C_{2v}, {}^4A_2)$

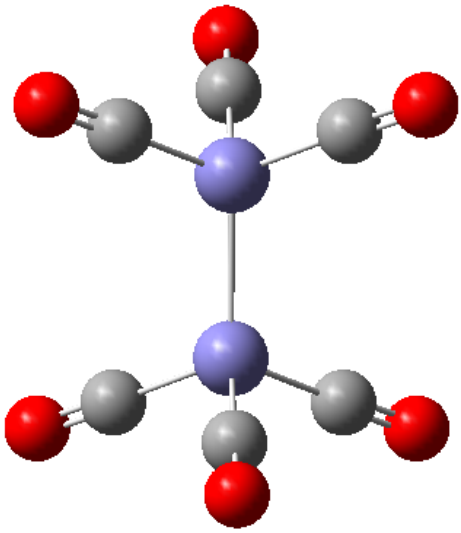


$Fe_2(CO)_5^-(C_s, {}^4A'')$

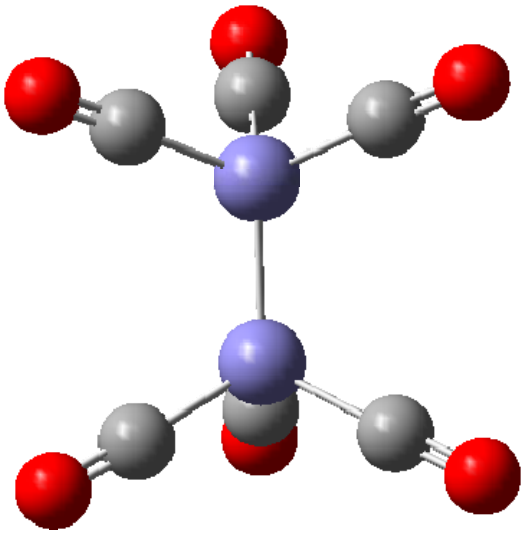


$Fe_2(CO)_5^-(C_s\_1, {}^4A'')$

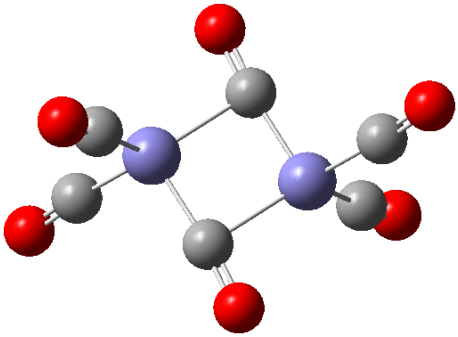
Figure S3 Geometries of the $Fe_2(CO)_6^-$ anion isomers.



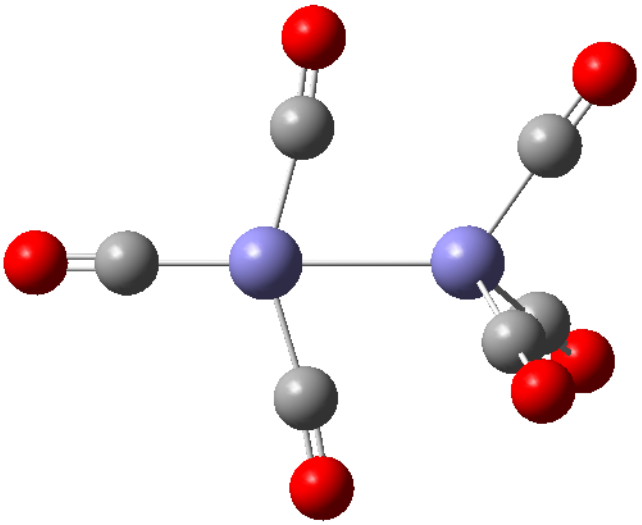
$Fe_2(CO)_6^-(D_{3d}, {}^2A_{2u})$



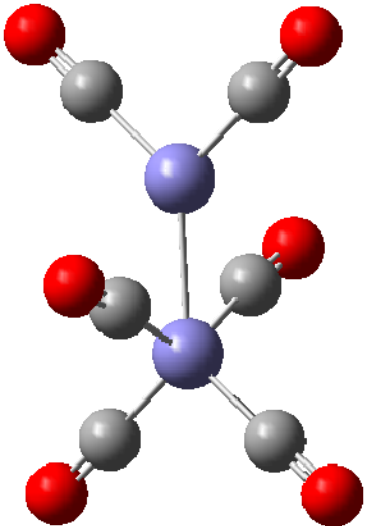
$Fe_2(CO)_6^-(D_{3h}, {}^2A)$



$Fe_2(CO)_6^-(C_{2h}, {}^2B_g)$

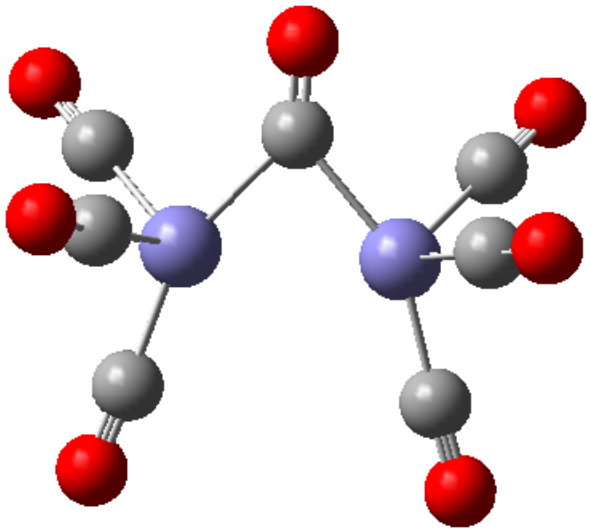


$Fe_2(CO)_6^-(C_s, {}^2A'')$

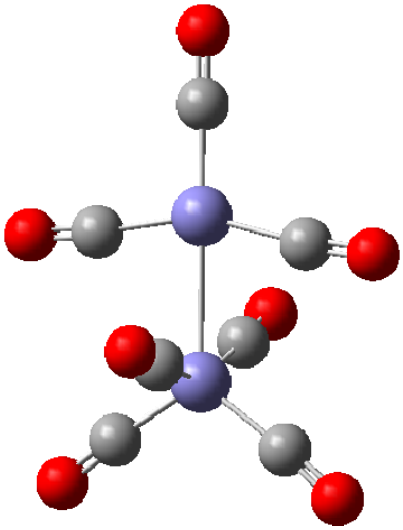


$Fe_2(CO)_6^-(C_{2v}, {}^2A_1)$

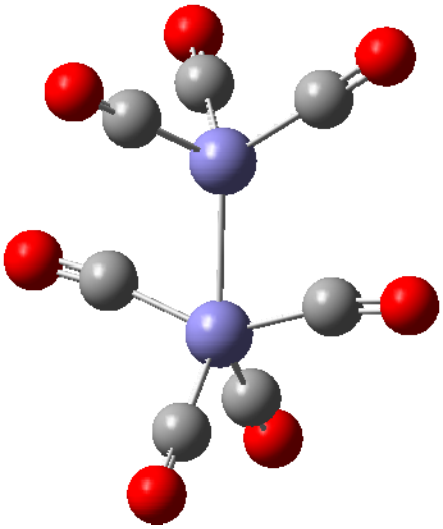
Figure S4 Geometries of the $Fe_2(CO)_7^-$ anion isomers.



$Fe_2(CO)_7^-(C_{2v}, {}^2A)$

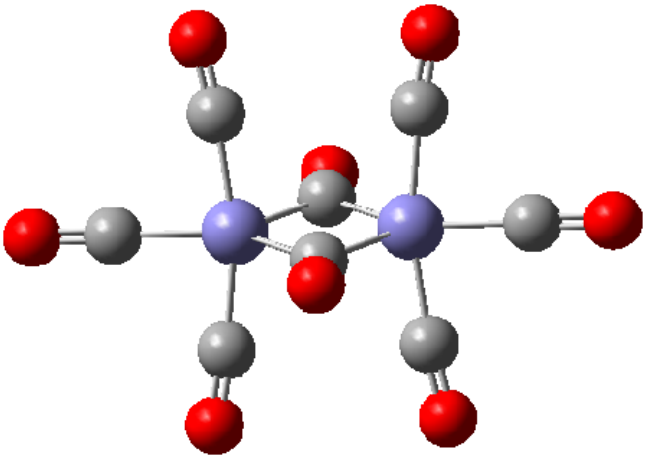


$Fe_2(CO)_7^-(C_{2v}, {}^2A_1)$

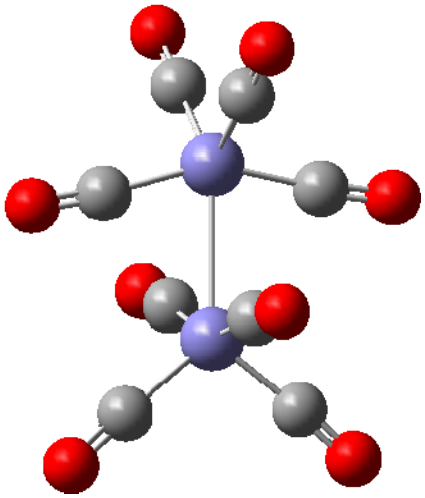


$Fe_2(CO)_7^-(C_s, {}^2A')$

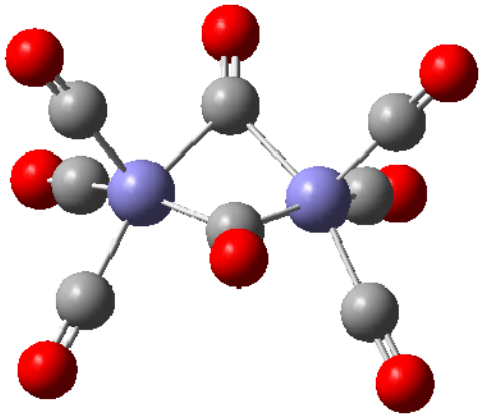
Figure S5 Geometries of the $Fe_2(CO)_8^-$ anion isomers.



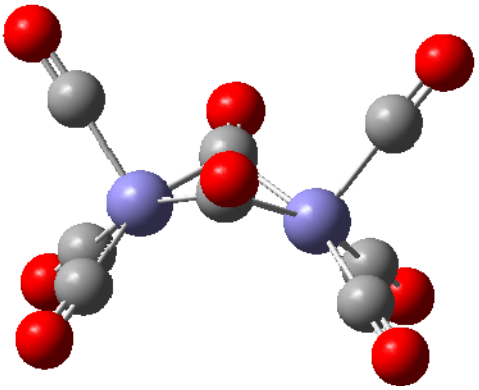
$Fe_2(CO)_8^-(D_{2h}, {}^2B_{2g})$



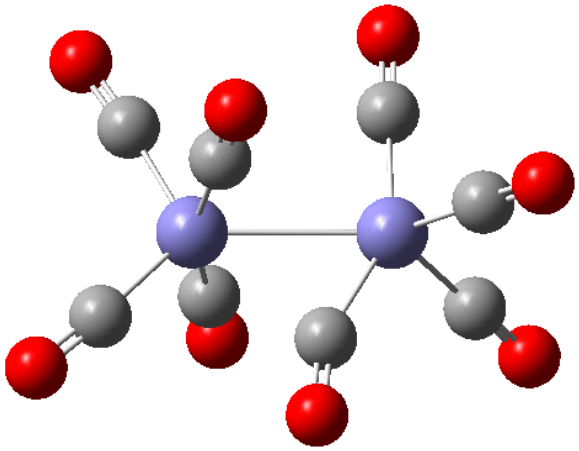
$Fe_2(CO)_8^-(D_{2d}, {}^2A)$



$Fe_2(CO)_8^-(C_{2v}, {}^2B_2)$



$Fe_2(CO)_8^-(C_s, {}^2A')$



$Fe_2(CO)_8^-(C_s, {}^2A'')$

Cartesian Coordinates of the Structures of the $Fe_2(CO)_n^-$ (n = 4–8) anions.

$Fe_2(CO)_4^-$ (C_s, $^4A'$)

Fe	-0.2257300	-1.3490870	0.0000000
Fe	0.0000000	1.2205770	0.0000000
C	-0.5051700	-3.1251330	0.0000000
C	1.4691530	0.2401410	0.0000000
C	-1.5715640	-0.1270080	0.0000000
C	0.5772460	2.9027260	0.0000000
O	-0.8009950	-4.2646130	0.0000000
O	2.5731870	-0.2045070	0.0000000
O	-2.0726030	0.9923720	0.0000000
O	1.0567850	3.9763580	0.0000000

$Fe_2(CO)_4^-$ (C_1, ^4A)

Fe	-1.0713982	0.0417465	-0.3945070
Fe	1.2679192	-0.2094232	-0.3903167
C	-2.5141452	0.0282340	0.6561624
C	-0.5107537	1.7298206	-0.6458643
C	-0.5275936	-1.6460368	-0.6491524
C	2.7530745	0.1180200	0.5575374
O	-3.4145707	0.0098687	1.4098036
O	-0.2025120	2.8534709	-0.8304031
O	-0.2975122	-2.7977798	-0.8361954
O	3.6908785	0.3585230	1.2256484

$Fe_2(CO)_4^-$ (C_{2v}, $^4B_1$)

Fe	0.000000	0.000000	-0.434043
Fe	0.000000	0.000000	1.984638
C	0.000000	1.440033	-1.454826
O	0.000000	2.366143	-2.173363
C	0.000000	-1.440033	-1.454826
O	0.000000	-2.366143	-2.173363
C	-1.659828	0.000000	0.217568
O	-2.785229	0.000000	0.581590
C	1.659828	0.000000	0.217568
O	2.785229	0.000000	0.581590

$Fe_2(CO)_4^-$ (C_{3v}, ^4A)

Fe	0.000000	0.000000	-0.355364
Fe	0.000000	0.000000	1.985042
C	0.000000	0.000000	-2.124220
O	0.000000	0.000000	-3.294046
C	0.000000	1.765105	-0.110071
O	0.000000	2.937918	-0.053860
C	1.528626	-0.882552	-0.110071
O	2.544312	-1.468959	-0.053860

C	-1.528626	-0.882552	-0.110071
O	-2.544312	-1.468959	-0.053860

$Fe_2(CO)_5^-(C_s, {}^4A')$

Fe	0.653659	1.229072	0.000000
Fe	-0.414631	-1.022400	0.000000
C	-1.125876	-1.942376	-1.383701
O	-1.607256	-2.546792	-2.264038
C	1.624899	2.741032	0.000000
O	2.261535	3.723765	0.000000
C	1.702958	-0.233129	0.000000
O	2.492187	-1.113732	0.000000
C	-1.125876	1.502212	0.000000
O	-2.278722	1.717835	0.000000
C	-1.125876	-1.942376	1.383701
O	-1.607256	-2.546792	2.264038

$Fe_2(CO)_5^-(C_{3v}, {}^4A)$

Fe	0.000000	0.000000	-0.935063
Fe	0.000000	0.000000	1.462934
C	0.000000	0.000000	-2.704498
O	0.000000	0.000000	-3.875061
C	0.000000	1.740729	-0.613973
O	0.000000	2.909307	-0.455990
C	1.507516	-0.870365	-0.613973
O	2.519534	-1.454654	-0.455990
C	-1.507516	-0.870365	-0.613973
O	-2.519534	-1.454654	-0.455990
C	0.000000	0.000000	3.297170
O	0.000000	0.000000	4.464387

$Fe_2(CO)_5^-(C_{2v}, {}^4A_2)$

Fe	0.000000	0.000000	-0.936770
Fe	0.000000	0.000000	1.472453
C	0.000000	0.000000	3.299506
O	0.000000	0.000000	4.468049
C	0.000000	1.416695	-1.998774
O	0.000000	2.342515	-2.714993
C	0.000000	-1.416695	-1.998774
O	0.000000	-2.342515	-2.714993
C	-1.647127	0.000000	-0.281421
O	-2.774552	0.000000	0.083315
C	1.647127	0.000000	-0.281421
O	2.774552	0.000000	0.083315

$Fe_2(CO)_5^-(C_s, {}^4A'')$

Fe	0.060178	-0.868047	0.000000
Fe	0.245509	1.478204	0.000000
C	-0.505404	3.141666	0.000000
O	-1.061908	4.168898	0.000000
C	0.056309	-1.929507	1.418364
O	0.056309	-2.640830	2.347648
C	-1.608526	-0.230569	0.000000
O	-2.744452	0.080892	0.000000
C	0.056309	-1.929507	-1.418364
O	0.056309	-2.640830	-2.347648
C	1.736480	-0.276974	0.000000
O	2.898883	-0.032471	0.000000

$Fe_2(CO)_5^-(C_s\_1, {}^4A")$

Fe	0.851031	0.179099	0.000000
Fe	-1.488952	0.081224	0.000000
C	-2.997637	-0.953739	0.000000
O	-3.874166	-1.724431	0.000000
C	2.571360	0.607113	0.000000
O	3.706276	0.891989	0.000000
C	0.741839	-0.797921	1.478195
O	0.741839	-1.434886	2.466287
C	0.741839	-0.797921	-1.478195
O	0.741839	-1.434886	-2.466287
C	0.170336	1.814193	0.000000
O	-0.163351	2.952371	0.000000

$Fe_2(CO)_6^-(D_{3d}, {}^2A_{2u})$

Fe	0.000000	0.000000	1.169664
Fe	0.000000	0.000000	-1.169664
C	1.440642	0.831755	-1.903948
C	0.000000	1.663510	1.903948
C	1.440642	-0.831755	1.903948
C	-1.440642	-0.831755	1.903948
C	-1.440642	0.831755	-1.903948
C	0.000000	-1.663510	-1.903948
O	0.000000	2.742136	2.345007
O	2.374759	-1.371068	2.345007
O	-2.374759	-1.371068	2.345007
O	2.374759	1.371068	-2.345007
O	-2.374759	1.371068	-2.345007
O	0.000000	-2.742136	-2.345007

$Fe_2(CO)_6^-(D_{3h}, {}^2A)$

Fe	0.000000	0.000000	1.169782
Fe	0.000000	0.000000	-1.169782

C	0.000000	1.660052	-1.909731
C	0.000000	1.660052	1.909731
C	1.437647	-0.830026	1.909731
C	-1.437647	-0.830026	1.909731
C	-1.437647	-0.830026	-1.909731
C	1.437647	-0.830026	-1.909731
O	0.000000	2.735454	2.358479
O	2.368973	-1.367727	2.358479
O	-2.368973	-1.367727	2.358479
O	0.000000	2.735454	-2.358479
O	-2.368973	-1.367727	-2.358479
O	2.368973	-1.367727	-2.358479

$Fe_2(CO)_6^-(C_{2h}, {}^2B_g)$

Fe	-0.559497	-1.148007	0.000000
Fe	0.559497	1.148007	0.000000
C	0.701662	2.209420	1.456732
C	-1.154475	0.758270	0.000000
C	-0.701662	-2.209420	1.456732
C	-0.701662	-2.209420	-1.456732
C	0.701662	2.209420	-1.456732
C	1.154475	-0.758270	0.000000
O	-2.344574	0.628006	0.000000
O	-0.693851	-2.916425	2.383298
O	-0.693851	-2.916425	-2.383298
O	0.693851	2.916425	2.383298
O	0.693851	2.916425	-2.383298
O	2.344574	-0.628006	0.000000

$Fe_2(CO)_6^-(C_s, {}^2A")$

Fe	-1.530437	0.044372	0.000000
Fe	1.070815	0.040097	0.000000
C	2.145864	1.535766	0.000000
O	2.859512	2.455123	0.000000
C	-1.035413	-1.693550	0.000000
O	-0.843030	-2.847168	0.000000
C	-3.315216	0.050875	0.000000
O	-4.486258	0.059166	0.000000
C	-1.039418	1.779489	0.000000
O	-0.874585	2.939058	0.000000
C	1.812437	-0.861998	-1.410354
O	2.276307	-1.421071	-2.321184
C	1.812437	-0.861998	1.410354
O	2.276307	-1.421071	2.321184

$Fe_2(CO)_6^-(C_{2v}, {}^2A_1)$

Fe	0.000000	0.000000	-1.154445
Fe	0.000000	0.000000	1.222391
C	0.000000	1.354512	2.399047
O	0.000000	2.234728	3.163942
C	0.000000	-1.336372	-2.325290
O	0.000000	-2.234798	-3.069408
C	-1.619008	0.000000	-0.376523
O	-2.725558	0.000000	0.022128
C	0.000000	1.336372	-2.325290
O	0.000000	2.234798	-3.069408
C	0.000000	-1.354512	2.399047
O	0.000000	-2.234728	3.163942
C	1.619008	0.000000	-0.376523
O	2.725558	0.000000	0.022128

$Fe_2(CO)_7^-(C_{2v}, {}^2A)$

Fe	0.000000	1.300506	-0.093123
Fe	0.000000	-1.300506	-0.093123
C	1.349532	-2.321160	0.579997
O	2.194154	-2.975748	1.005919
C	1.349532	2.321160	0.579997
O	2.194154	2.975748	1.005919
C	-1.349532	2.321160	0.579997
O	-2.194154	2.975748	1.005919
C	0.000000	0.000000	1.412068
O	0.000000	0.000000	2.584369
C	0.000000	1.815300	-1.889656
O	0.000000	2.167463	-2.983649
C	-1.349532	-2.321160	0.579997
O	-2.194154	-2.975748	1.005919
C	0.000000	-1.815300	-1.889656
O	0.000000	-2.167463	-2.983649

$Fe_2(CO)_7^-(C_{2v}, {}^2A_1)$

Fe	0.000000	0.000000	-1.201391
Fe	0.000000	0.000000	1.435853
C	0.000000	1.798402	1.090194
O	0.000000	2.953071	0.978926
C	1.725455	0.000000	-0.747967
O	2.850574	0.000000	-0.422276
C	0.000000	1.461804	-2.203191
O	0.000000	2.371660	-2.936686
C	-1.725455	0.000000	-0.747967
O	-2.850574	0.000000	-0.422276
C	0.000000	-1.461804	-2.203191
O	0.000000	-2.371660	-2.936686

C	0.000000	-1.798402	1.090194
O	0.000000	-2.953071	0.978926
C	0.000000	0.000000	3.213005
O	0.000000	0.000000	4.379764

$Fe_2(CO)_7^-(C_s, {}^2A')$

Fe	0.036289	-1.288889	0.000000
Fe	0.018746	1.198404	0.000000
C	-0.844774	1.984182	1.397434
O	-1.383143	2.479235	2.301527
C	1.749212	-0.718377	0.000000
O	2.910347	-0.581208	0.000000
C	0.034454	-2.468659	-1.346362
O	0.034454	-3.215663	-2.239298
C	-1.672556	-0.702811	0.000000
O	-2.826621	-0.522097	0.000000
C	0.034454	-2.468659	1.346362
O	0.034454	-3.215663	2.239298
C	-0.844774	1.984182	-1.397434
O	-1.383143	2.479235	-2.301527
C	1.529721	2.256143	0.000000
O	2.445485	2.970734	0.000000

$Fe_2(CO)_8^-(D_{2h}, {}^2B_{2g})$

Fe	-1.277784	0.000000	0.000000
Fe	1.277784	0.000000	0.000000
C	0.000000	0.000000	1.522088
O	0.000000	0.000000	2.701279
C	-1.470636	1.801733	0.000000
O	-1.689228	2.941371	0.000000
C	0.000000	0.000000	-1.522088
O	0.000000	0.000000	-2.701279
C	-1.470636	-1.801733	0.000000
O	-1.689228	-2.941371	0.000000
C	-3.043599	0.000000	0.000000
O	-4.212692	0.000000	0.000000
C	1.470636	-1.801733	0.000000
O	1.689228	-2.941371	0.000000
C	1.470636	1.801733	0.000000
O	1.689228	2.941371	0.000000
C	3.043599	0.000000	0.000000
O	4.212692	0.000000	0.000000

$Fe_2(CO)_8^-(D_{2d}, {}^2A)$

Fe	0.000000	0.000000	1.321559
Fe	0.000000	0.000000	-1.321559

C	-1.764659	0.000000	-0.916918
O	-2.917166	0.000000	-0.753278
C	0.000000	1.764659	0.916918
O	0.000000	2.917166	0.753278
C	-1.413056	0.000000	2.427846
O	-2.290350	0.000000	3.191067
C	0.000000	-1.764659	0.916918
O	0.000000	-2.917166	0.753278
C	1.413056	0.000000	2.427846
O	2.290350	0.000000	3.191067
C	1.764659	0.000000	-0.916918
O	2.917166	0.000000	-0.753278
C	0.000000	1.413056	-2.427846
O	0.000000	2.290350	-3.191067
C	0.000000	-1.413056	-2.427846
O	0.000000	-2.290350	-3.191067

$Fe_2(CO)_8^-(C_{2v}, {}^2B_2)$

Fe	0.000000	1.270481	-0.024748
Fe	0.000000	-1.270481	-0.024748
C	-1.314339	-2.040083	-0.989516
O	-2.150870	-2.562225	-1.602065
C	0.000000	2.282604	1.458990
O	0.000000	2.965430	2.397896
C	-1.418985	0.000000	0.495609
O	-2.530383	0.000000	0.904990
C	-1.314339	2.040083	-0.989516
O	-2.150870	2.562225	-1.602065
C	1.314339	2.040083	-0.989516
O	2.150870	2.562225	-1.602065
C	1.418985	0.000000	0.495609
O	2.530383	0.000000	0.904990
C	0.000000	-2.282604	1.458990
O	0.000000	-2.965430	2.397896
C	1.314339	-2.040083	-0.989516
O	2.150870	-2.562225	-1.602065

$Fe_2(CO)_8^-(C_s, {}^2A')$

Fe	-0.067651	1.268920	0.000000
Fe	0.000451	-1.286716	0.000000
C	-1.033265	-2.006224	1.284552
O	-1.690735	-2.508427	2.100284
C	1.447773	2.266316	0.000000
O	2.402171	2.925236	0.000000
C	0.521930	-0.070808	1.408461
O	0.951775	-0.019402	2.510227

C	-0.961483	2.076983	1.348727
O	-1.526419	2.621479	2.203408
C	-0.961483	2.076983	-1.348727
O	-1.526419	2.621479	-2.203408
C	0.521930	-0.070808	-1.408461
O	0.951775	-0.019402	-2.510227
C	1.455464	-2.313292	0.000000
O	2.378791	-3.019395	0.000000
C	-1.033265	-2.006224	-1.284552
O	-1.690735	-2.508427	-2.100284

$Fe_2(CO)_8^-(C_s, {}^2A")$

Fe	0.432094	1.240279	0.000000
Fe	-0.445438	-1.243599	0.000000
C	-0.413531	-0.934640	1.774935
O	-0.413531	-0.770337	2.926504
C	1.642999	-0.148178	0.000000
O	2.697809	-0.666353	0.000000
C	1.124634	2.200779	1.367608
O	1.580166	2.829147	2.231624
C	-1.294734	1.828680	0.000000
O	-2.380376	2.236528	0.000000
C	1.124634	2.200779	-1.367608
O	1.580166	2.829147	-2.231624
C	-0.413531	-0.934640	-1.774935
O	-0.413531	-0.770337	-2.926504
C	0.357071	-2.829128	0.000000
O	0.808837	-3.901829	0.000000
C	-2.212386	-1.469904	0.000000
O	-3.352537	-1.710489	0.000000

$Fe_2(CO)_8^-(C_{2v}\_1, {}^2B_2)$

Fe	0.000000	0.000000	-1.324119
Fe	0.000000	0.000000	1.339197
C	0.000000	1.773757	1.035750
O	0.000000	2.925790	0.866247
C	-1.757421	0.000000	-0.840765
O	-2.912060	0.000000	-0.707177
C	0.000000	1.371210	-2.509058
O	0.000000	2.242808	-3.275301
C	1.757421	0.000000	-0.840765
O	2.912060	0.000000	-0.707177
C	0.000000	-1.371210	-2.509058
O	0.000000	-2.242808	-3.275301
C	0.000000	-1.773757	1.035750
O	0.000000	-2.925790	0.866247

C	-1.467848	0.000000	2.333911
O	-2.367355	0.000000	3.076853
C	1.467848	0.000000	2.333911
O	2.367355	0.000000	3.076853