

Alternative Modes of Bonding of C₄F₈ Units in Mononuclear and Binuclear Iron Carbonyl Complexes

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Supporting Information

Table S1. Comparison of total energies and relative energies for various optimized low-lying structures of the C₄F₈Fe(CO)₄ complexes using four different methods: M06-L, B3LYP, BP86 and BPW91.

Table S2: Total energies, relative energies, ZPE (zero point energy) corrected total energies, and ZPE corrected relative energies for optimized low-lying structures of the (C₄F₈)₂Fe₂(CO)_n (n=7, 6) and C₄F₈Fe(CO)₄ complexes at the M06-L/cc-pVTZ level.

Table S3: Vibrational frequencies and infrared intensities for optimized low-lying structures of the (C₄F₈)₂Fe₂(CO)_n (n=7, 6) and C₄F₈Fe(CO)₄ complexes at the M06-L/cc-pVTZ level.

Table S4: Cartesian coordinates for optimized low-lying structures of the (C₄F₈)₂Fe₂(CO)_n (n=7, 6) and C₄F₈Fe(CO)₄ complexes at the M06-L/cc-pVTZ level.

Complete Gaussian 09 reference.

Table S1. Comparison of total energies (E_{tot} , in hartree) and relative energies (ΔE , in kcal/mol) for various optimized low-lying structures of the $\text{C}_4\text{F}_8\text{Fe}(\text{CO})_4$ complexes using four different methods: M06-L, B3LYP, BP86 and BPW91.

Structure	M06-L/cc-pVTZ		B3LYP/cc-pVTZ		BP86/cc-pVTZ		BPW91/cc-pVTZ	
	E_{tot}	ΔE	E_{tot}	ΔE	E_{tot}	ΔE	E_{tot}	ΔE
14-1S	-2668.58169180	0.0	-2668.84332674	0.0	-2669.09026006	0.0	-2668.89381868	0.0
14-2S	-2668.57425707	4.7	-2668.83914191	2.6	-2669.08492792	3.3	-2668.88907588	3.0
14-3S	-2668.55817624	14.8	-2668.82219648	13.3	-2669.06915151	13.2	-2668.87335328	12.8
14-4S	-2668.55490472	16.8	-2668.82036169	14.4	-2669.06418926	16.4	-2668.86715271	16.7
14-5S	-2668.55436045	17.2	-2668.81792658	15.9	-2669.06388574	16.6	-2668.86741204	16.6
14-6S	-2668.54814075	21.1	-2668.81409848	18.3	-2669.06085218	18.5	-2668.86464492	18.3
14-7S	-2668.54645253	22.1	-2668.81191783	19.7	-2669.06030179	18.8	-2668.86358924	19.0
14-8S	-2668.54084053	25.6	-2668.80615985	23.3	-2669.05284907	23.5	-2668.85570051	23.9
14-9S	-2668.53658183	28.3	-2668.80381794	24.8	-2669.05181971	24.1	-2668.85537242	24.1

Table S2. Total energies (E_{tot} , in hartree), relative energies (ΔE , in kcal/mol), ZPE (zero point energy)-corrected total energies (E_0 , in hartree) and ZPE-corrected relative energies (ΔE_0 , in kcal/mol) for various optimized low-lying structures of the $(\text{C}_4\text{F}_8)_2\text{Fe}_2(\text{CO})_n$ ($n=7, 6$) and $\text{C}_4\text{F}_8\text{Fe}(\text{CO})_4$ complexes at the M06-L/cc-pVTZ level.

Complex	Structure	Multiplicity	M06-L/cc-pVTZ			
			E_{tot}	ΔE	E_0	ΔE_0
$(\text{C}_4\text{F}_8)_2\text{Fe}_2(\text{CO})_7$	27-1S	1	-5223.79152253	0.0	-5223.635347	0.0
	27-2S	1	-5223.78906426	1.5	-5223.633056	1.4
	27-3S	1	-5223.78886839	1.7	-5223.633265	1.3
	27-4S	1	-5223.78769683	2.4	-5223.631455	2.4
	27-5S	1	-5223.78676204	3.0	-5223.630402	3.1
	27-6S	1	-5223.78303182	5.3	-5223.626907	5.3
	27-7S	1	-5223.78294558	5.4	-5223.626883	5.3
	27-8S	1	-5223.78270145	5.5	-5223.626980	5.3
	27-9S	1	-5223.78208549	5.9	-5223.625348	6.3
	27-10S	1	-5223.78206107	5.9	-5223.626378	5.6
	27-11S	1	-5223.78178415	6.1	-5223.626490	5.6
	27-12S	1	-5223.77895509	7.9	-5223.623174	7.6
	27-13S	1	-5223.77852105	8.2	-5223.623281	7.6
	27-14S	1	-5223.77678661	9.2	-5223.621179	8.9
	27-15S	1	-5223.77187559	12.3	-5223.615972	12.2
	27-16S	1	-5223.77037817	13.3	-5223.615397	12.5
	27-17S	1	-5223.76873735	14.3	-5223.613231	13.9
	27-18S	1	-5223.76731052	15.2	-5223.612225	14.5
	27-19S	1	-5223.76220868	18.4	-5223.606956	17.8
	27-20S	1	-5223.76140204	18.9	-5223.605942	18.5
	27-21S	1	-5223.76061874	19.4	-5223.605303	18.9
	27-22S	1	-5223.75979384	19.9	-5223.604333	19.5
	27-23S	1	-5223.75866437	20.6	-5223.603761	19.8
$(\text{C}_4\text{F}_8)_2\text{Fe}_2(\text{CO})_6$	26-1S	1	-5110.43461222	0.0	-5110.286876	0.0
	26-2S	1	-5110.42457643	6.3	-5110.276785	6.3
	26-3S	1	-5110.41662375	11.3	-5110.269617	10.8
	26-4S	1	-5110.41482556	12.4	-5110.267832	12.0
	26-5S	1	-5110.41355884	13.2	-5110.266480	12.8
	26-6S	1	-5110.41151560	14.5	-5110.264619	14.0
	26-7S	1	-5110.41143198	14.5	-5110.264195	14.2
	26-8S	1	-5110.41056340	15.1	-5110.263482	14.7
	26-9S	1	-5110.40503730	18.6	-5110.257702	18.3
	26-10S	1	-5110.40503290	18.6	-5110.258813	17.6
	26-11S	1	-5110.40208500	20.4	-5110.255302	19.8
$\text{C}_4\text{F}_8\text{Fe}(\text{CO})_4$	14-1S	1	-2668.58169180	0.0	-2668.500119	0.0
	14-2S	1	-2668.57425707	4.7	-2668.492966	4.5
	14-3S	1	-2668.55817624	14.8	-2668.477051	14.5
	14-4S	1	-2668.55490472	16.8	-2668.473991	16.4
	14-5S	1	-2668.55436045	17.2	-2668.473363	16.8
	14-6S	1	-2668.54814075	21.1	-2668.467339	20.6
	14-7S	1	-2668.54645253	22.1	-2668.465445	21.8
	14-8S	1	-2668.54084053	25.6	-2668.459896	25.2
	14-9S	1	-2668.53658183	28.3	-2668.455663	27.9

Table S3. Vibrational frequencies (in cm^{-1}) and infrared intensities (in km/mol , given in parentheses) for optimized low-lying structures of the $(\text{C}_4\text{F}_8)_2\text{Fe}_2(\text{CO})_n$ ($n=7, 6$) and $\text{C}_4\text{F}_8\text{Fe}(\text{CO})_4$ complexes at the M06-L/cc-pVTZ level.

Structure	ν
27-1S	26(0), 41(0), 48(0), 58(0), 62(0), 64(0), 74(1), 81(0), 88(0), 89(0), 93(0), 98(0), 103(0), 105(0), 114(0), 116(0), 122(0), 126(0), 130(0), 131(1), 135(1), 137(2), 143(0), 159(1), 163(0), 170(2), 175(2), 181(1), 194(2), 202(0), 215(1), 219(2), 228(1), 233(1), 237(1), 242(2), 259(3), 273(10), 309(0), 314(1), 318(2), 324(1), 344(0), 355(0), 360(1), 371(1), 375(1), 377(21), 390(3), 396(6), 406(13), 414(0), 424(8), 442(7), 443(37), 451(5), 457(38), 462(7), 465(18), 488(16), 495(35), 500(12), 514(16), 519(7), 535(12), 538(2), 543(1), 551(11), 553(34), 561(23), 566(13), 571(54), 580(221), 592(4), 597(34), 614(27), 619(186), 623(48), 636(101), 658(87), 701(88), 715(26), 718(31), 746(7), 747(52), 787(3), 839(44), 917(42), 976(80), 995(149), 1041(23), 1058(27), 1097(191), 1113(1), 1120(2), 1147(58), 1153(302), 1171(260), 1190(125), 1197(222), 1217(121), 1221(51), 1232(375), 1251(608), 1285(336), 1292(125), 1466(215), 2052(243), 2075(371), 2100(715), 2114(383), 2124(648), 2139(1341), 2172(138)
27-2S	35(0), 41(0), 45(0), 51(0), 60(0), 67(0), 69(0), 77(0), 87(0), 91(0), 93(0), 97(0), 102(0), 105(0), 110(0), 114(0), 117(0), 120(3), 122(1), 126(1), 129(0), 137(0), 143(0), 149(1), 154(1), 173(2), 181(5), 182(1), 197(8), 209(2), 214(0), 222(3), 229(0), 242(2), 255(0), 262(4), 265(1), 273(2), 292(6), 305(3), 308(2), 327(2), 343(32), 345(1), 360(2), 366(0), 369(0), 372(4), 380(1), 415(5), 420(5), 429(1), 441(14), 443(2), 445(2), 450(14), 452(7), 453(2), 472(2), 481(10), 494(3), 509(12), 518(13), 522(7), 527(18), 535(25), 537(7), 539(8), 548(1), 555(0), 582(45), 590(3), 590(39), 597(28), 600(43), 608(18), 620(57), 626(109), 638(30), 654(167), 696(37), 706(68), 719(88), 738(43), 751(97), 794(79), 846(78), 916(30), 992(81), 1045(22), 1054(32), 1072(90), 1101(87), 1110(165), 1126(100), 1154(208), 1171(29), 1174(291), 1179(89), 1192(142), 1218(89), 1223(270), 1227(220), 1228(501), 1257(24), 1299(143), 1339(153), 1990(396), 2104(35), 2108(869), 2114(205), 2121(1100), 2145(1582), 2171(18)
27-3S	23(0), 32(0), 39(1), 45(0), 56(0), 59(0), 64(1), 65(1), 74(1), 83(0), 86(0), 88(1), 94(0), 95(0), 99(5), 105(0), 113(3), 120(1), 125(1), 126(1), 135(1), 139(4), 144(1), 152(15), 155(1), 164(8), 170(2), 177(3), 185(1), 190(0), 209(2), 211(4), 212(14), 222(18), 231(1), 241(8), 283(12), 291(1), 311(0), 312(1), 322(1), 325(1), 341(57), 347(4), 347(0), 358(18), 361(31), 372(152), 382(8), 383(3), 387(17), 394(7), 397(2), 413(11), 418(4), 441(27), 447(7), 458(13), 462(9), 471(13), 487(11), 497(35), 515(2), 515(4), 529(11), 541(6), 543(4), 545(5), 545(12), 564(0), 564(1), 584(19), 598(276), 603(32), 611(13), 619(128), 621(24), 625(19), 638(18), 675(166), 691(198), 714(25), 717(40), 760(39), 764(29), 795(2), 797(3), 973(46), 975(152), 998(283), 1000(142), 1094(3), 1106(2), 1108(4), 1119(6), 1151(495), 1171(291), 1181(174), 1190(81), 1202(28), 1204(39), 1250(480), 1260(642), 1287(48), 1289(630), 1410(256), 1443(227), 2009(443), 2071(182), 2079(125), 2106(715), 2113(950), 2133(574), 2172(191)
27-4S	38(0), 44(0), 47(0), 57(0), 60(0), 64(0), 72(0), 77(0), 82(0), 86(0), 90(0), 94(0), 96(0), 105(0), 107(0), 110(0), 117(0), 124(1), 126(0), 132(1), 134(0), 140(0), 146(1), 152(0), 155(1), 161(0), 169(1), 173(2), 179(0), 191(1), 203(1), 207(0), 232(0), 235(2), 242(1), 255(6), 275(6), 277(4), 283(2), 296(1), 314(1), 315(2), 323(1), 347(1), 362(1), 371(0), 378(7), 394(1), 398(6), 412(5), 413(5), 419(1), 422(0), 442(3), 446(17), 457(14), 459(6), 464(38), 466(11), 485(22), 492(10), 497(9), 500(4), 517(5), 520(5), 535(10), 538(11), 551(0), 565(6), 567(15), 576(14), 586(119), 592(8), 599(21), 611(17), 615(25), 623(88), 629(148), 645(111), 667(159), 696(66), 700(79), 716(34), 746(49), 760(0), 778(20), 838(45), 901(62), 916(58), 1039(25), 1060(27), 1084(62), 1096(192), 1100(56), 1142(32), 1148(85), 1155(234), 1168(94), 1191(253), 1195(166), 1205(421), 1216(101), 1234(362), 1260(322), 1291(243), 1306(261), 1455(48), 2085(21), 2098(499), 2105(809), 2113(391), 2123(695), 2141(1254), 2176(93)
27-5S	35(0), 45(0), 48(0), 59(0), 62(0), 67(0), 81(0), 88(0), 90(0), 92(0), 95(0), 101(0), 105(0), 110(0), 114(0), 116(0), 118(1), 125(1), 126(0), 130(0), 140(0), 144(1), 148(1), 153(1), 160(1), 178(1), 180(3), 188(0), 192(2), 204(1), 213(6), 218(2), 231(0), 242(2), 263(2), 264(2), 265(1), 287(2), 303(3), 308(1), 315(1), 327(1), 329(1), 346(9), 355(19), 358(1), 368(0), 382(3), 397(2), 416(2), 423(5), 431(2), 438(14), 443(5), 450(6), 452(3), 454(9), 470(1), 481(8), 495(4), 509(27), 523(10), 524(10), 528(14), 533(9), 540(13), 541(15), 543(4), 548(2), 556(1), 560(3), 587(70), 591(8), 599(76), 600(11), 620(34), 627(82), 632(57), 641(24), 645(136), 706(76), 719(113), 726(104), 738(16), 751(42), 798(32), 845(68), 914(29), 956(22), 1037(69), 1048(57), 1065(53), 1099(45), 1110(161), 1144(29), 1154(267), 1159(35), 1175(257), 1190(80), 1192(49), 1215(92), 1218(275), 1228(422), 1231(173), 1244(353), 1271(431), 1297(139), 1986(372), 2101(124), 2107(792), 2111(385), 2123(905), 2144(1511), 2170(52)
27-6S	23(0), 37(0), 41(0), 44(0), 62(0), 64(0), 72(0), 82(0), 86(0), 91(0), 94(0), 95(0), 98(0), 104(0), 106(0), 115(0), 118(0), 121(0), 127(0), 133(0), 135(0), 141(1), 148(0), 149(1), 159(0), 163(1), 174(0), 182(0), 191(1), 193(0), 206(2), 218(1), 222(0), 237(1), 239(1), 262(7), 272(1), 288(4), 300(4), 309(0), 316(2), 321(2), 329(0), 346(0), 352(0), 365(0), 385(2), 387(1), 392(4), 403(5), 409(3), 417(3), 421(15), 426(2), 429(19), 442(10), 462(78), 468(4), 480(6), 486(15), 495(35), 504(13), 513(21), 518(2), 537(2), 537(47), 541(8), 544(5), 551(13), 563(4), 564(1), 574(32), 582(13), 588(73), 599(37), 613(45), 627(252), 633(18), 638(117), 654(224), 663(58), 716(31), 725(110), 734(2), 750(6), 792(4), 799(31), 968(44), 975(62), 978(123), 987(139), 1093(59), 1096(3), 1119(3), 1149(51), 1152(52), 1161(188), 1177(195), 1178(13), 1210(59), 1226(269), 1235(246), 1246(494), 1254(396), 1281(350), 1288(327), 1449(256), 2084(2), 2093(584), 2104(379), 2111(712), 2115(869), 2135(1243), 2174(91)

27-7S	38(0), 41(0), 47(0), 49(0), 57(0), 65(0), 73(0), 79(0), 84(0), 89(0), 90(0), 93(0), 94(0), 96(0), 98(0), 108(0), 112(0), 114(1), 116(0), 120(0), 134(0), 137(0), 147(0), 156(2), 159(1), 181(5), 184(0), 189(1), 199(0), 203(2), 206(0), 227(1), 233(6), 262(0), 263(2), 267(0), 269(1), 288(1), 289(3), 311(1), 312(0), 328(2), 329(0), 346(3), 347(1), 355(7), 364(22), 389(0), 392(1), 401(1), 421(11), 422(0), 429(2), 441(27), 451(1), 458(5), 460(1), 468(3), 479(6), 489(0), 515(30), 520(7), 526(0), 531(7), 531(7), 536(16), 540(1), 541(14), 546(0), 549(3), 557(9), 561(1), 597(116), 599(32), 601(72), 623(2), 631(90), 633(1), 635(28), 640(2), 666(352), 725(268), 733(13), 736(8), 745(8), 800(77), 808(3), 958(0), 961(54), 1004(84), 1060(121), 1107(74), 1113(65), 1141(3), 1145(67), 1160(52), 1162(91), 1189(4), 1189(0), 1222(14), 1226(320), 1228(168), 1228(231), 1242(525), 1245(287), 1271(581), 1276(316), 1967(360), 2097(1), 2101(966), 2111(92), 2118(1293), 2142(1447), 2168(18)
27-8S	36(0), 37(0), 42(0), 44(0), 51(0), 61(0), 70(0), 73(0), 76(0), 84(0), 86(0), 87(0), 95(0), 95(0), 99(0), 102(0), 107(0), 109(1), 111(0), 115(0), 123(0), 131(0), 140(0), 150(1), 165(1), 178(1), 180(4), 199(1), 207(5), 211(0), 215(3), 224(2), 235(3), 249(0), 262(1), 265(0), 269(1), 277(0), 288(5), 291(3), 308(1), 329(1), 330(5), 345(9), 349(6), 355(13), 370(3), 377(1), 389(1), 396(1), 415(8), 421(2), 432(1), 439(24), 447(2), 450(6), 452(1), 461(4), 465(2), 479(11), 490(0), 513(10), 517(16), 525(7), 530(11), 534(11), 536(10), 541(6), 545(5), 547(0), 559(4), 587(12), 596(47), 598(71), 602(78), 605(18), 625(118), 631(35), 634(24), 640(20), 665(264), 697(80), 731(150), 735(57), 748(45), 798(115), 808(15), 961(25), 998(115), 1012(31), 1071(118), 1100(88), 1112(49), 1125(123), 1144(37), 1163(74), 1174(73), 1179(97), 1188(3), 1223(177), 1226(242), 1228(315), 1229(231), 1245(369), 1257(14), 1274(459), 1339(163), 1976(375), 2098(52), 2103(980), 2110(304), 2120(1064), 2142(1433), 2169(30)
27-9S	33(0), 49(0), 54(0), 60(0), 63(0), 65(1), 76(0), 93(0), 94(0), 99(1), 106(0), 107(0), 111(0), 112(1), 122(0), 125(0), 126(1), 128(1), 130(0), 132(0), 152(7), 154(0), 157(0), 161(0), 170(0), 179(4), 181(3), 186(11), 191(0), 193(1), 221(0), 234(0), 237(1), 251(2), 253(3), 256(3), 257(0), 263(4), 304(4), 305(1), 325(1), 327(1), 346(41), 348(0), 355(4), 369(0), 370(0), 373(0), 416(1), 422(1), 427(12), 432(1), 441(6), 444(0), 447(0), 450(18), 460(4), 472(6), 491(5), 499(0), 506(24), 517(0), 520(26), 523(1), 529(29), 534(10), 543(22), 550(2), 559(1), 559(0), 583(50), 584(66), 593(23), 594(1), 599(3), 621(51), 624(105), 631(92), 643(9), 701(4), 709(117), 719(67), 727(21), 742(63), 751(57), 834(55), 841(66), 901(17), 908(32), 1042(25), 1044(41), 1062(14), 1067(27), 1112(89), 1114(255), 1155(334), 1160(308), 1173(23), 1187(113), 1187(370), 1193(153), 1204(197), 1218(7), 1230(459), 1235(183), 1290(185), 1293(118), 2005(433), 2106(218), 2113(367), 2115(553), 2124(898), 2146(1648), 2172(41)
27-10S	19(0), 28(0), 34(0), 42(0), 45(0), 57(0), 63(0), 69(0), 73(0), 77(0), 84(0), 89(0), 93(0), 99(0), 103(0), 106(1), 108(0), 111(1), 121(0), 128(0), 131(0), 134(1), 142(1), 146(0), 158(1), 165(0), 174(0), 196(1), 200(0), 207(2), 215(3), 217(1), 225(1), 231(1), 242(0), 246(0), 268(8), 282(3), 293(4), 300(7), 311(0), 321(2), 343(2), 346(0), 359(0), 368(1), 374(2), 383(3), 389(3), 398(11), 403(2), 409(5), 418(4), 425(3), 432(10), 446(5), 451(10), 453(108), 468(2), 476(4), 488(6), 491(30), 501(4), 514(14), 522(13), 537(1), 538(37), 544(3), 561(9), 564(1), 571(16), 578(57), 588(6), 589(91), 597(56), 605(37), 616(12), 627(171), 637(167), 647(304), 664(18), 697(27), 716(32), 743(93), 750(9), 790(4), 806(83), 977(85), 990(123), 992(95), 1002(120), 1100(0), 1110(78), 1119(1), 1125(76), 1163(244), 1171(61), 1178(79), 1180(173), 1211(61), 1223(330), 1227(190), 1253(527), 1258(136), 1289(330), 1334(159), 1452(247), 2080(32), 2094(556), 2102(716), 2109(493), 2116(800), 2135(1193), 2173(98)
27-11S	32(0), 35(0), 46(0), 46(0), 50(0), 57(0), 63(0), 72(0), 72(0), 75(0), 80(0), 83(0), 89(0), 91(0), 94(0), 100(0), 101(1), 105(2), 106(0), 111(0), 115(0), 125(0), 137(0), 140(0), 163(5), 165(0), 197(7), 203(8), 205(0), 213(0), 220(2), 222(1), 234(4), 247(0), 251(1), 261(0), 269(2), 271(1), 279(1), 290(10), 291(1), 311(7), 343(23), 344(7), 348(2), 369(0), 371(5), 376(0), 377(2), 378(0), 414(8), 425(0), 431(2), 439(24), 446(0), 446(3), 449(11), 453(4), 455(4), 468(0), 480(11), 491(0), 509(1), 519(21), 525(16), 529(14), 535(11), 537(1), 542(4), 545(0), 582(7), 590(30), 596(10), 598(48), 599(90), 603(10), 610(60), 622(129), 632(0), 645(2), 662(340), 695(4), 699(153), 736(3), 751(145), 799(13), 803(191), 996(157), 1005(0), 1025(26), 1074(130), 1100(126), 1101(30), 1123(110), 1125(121), 1173(3), 1173(97), 1178(42), 1181(232), 1222(432), 1223(257), 1229(190), 1230(213), 1258(1), 1258(34), 1337(333), 1339(12), 1981(392), 2100(1), 2104(1063), 2113(133), 2120(1232), 2144(1462), 2171(2)
27-12S	36(0), 38(0), 42(0), 53(0), 58(0), 68(0), 68(0), 70(0), 79(0), 86(0), 88(0), 91(1), 94(0), 99(0), 101(0), 105(1), 109(0), 114(0), 119(0), 126(0), 130(0), 137(0), 140(0), 142(0), 143(0), 156(1), 163(2), 181(3), 188(0), 190(1), 195(0), 206(1), 234(2), 241(1), 265(1), 269(5), 274(3), 279(4), 284(4), 293(2), 302(5), 309(1), 315(2), 327(1), 344(0), 347(0), 385(7), 391(2), 398(7), 403(2), 415(6), 416(5), 423(1), 424(1), 432(5), 452(25), 462(47), 470(0), 476(1), 484(26), 485(18), 499(13), 503(5), 518(3), 520(1), 536(1), 537(14), 538(18), 553(3), 562(4), 571(2), 579(8), 585(31), 599(37), 611(56), 614(121), 625(101), 633(86), 640(49), 658(234), 672(88), 695(63), 726(95), 738(27), 764(0), 777(19), 805(46), 901(74), 957(51), 976(85), 1081(54), 1095(61), 1110(77), 1139(28), 1145(36), 1159(52), 1165(102), 1184(171), 1185(110), 1200(333), 1228(213), 1230(197), 1241(299), 1260(338), 1274(509), 1305(276), 1450(51), 2079(49), 2095(633), 2104(399), 2112(206), 2114(1385), 2139(1064), 2176(81)

27-13S	21(0), 30(0), 33(0), 40(0), 52(0), 55(0), 58(0), 69(0), 69(0), 76(0), 80(0), 81(1), 86(0), 88(0), 93(0), 96(4), 101(1), 114(1), 117(1), 123(1), 125(0), 132(0), 138(1), 155(0), 162(0), 166(0), 175(5), 183(3), 185(0), 199(5), 204(1), 213(3), 221(21), 233(0), 234(30), 241(7), 279(7), 287(9), 296(1), 306(6), 311(1), 320(2), 335(3), 337(1), 346(0), 357(76), 359(22), 374(23), 378(11), 390(14), 396(73), 398(59), 409(51), 415(29), 422(9), 425(0), 436(25), 442(27), 456(1), 466(12), 477(12), 488(16), 496(48), 517(6), 536(6), 538(16), 542(1), 544(11), 547(7), 563(15), 568(26), 573(16), 586(36), 602(410), 606(43), 610(103), 613(28), 624(29), 633(15), 670(95), 680(120), 716(46), 717(40), 757(10), 769(2), 778(22), 798(1), 935(102), 977(99), 1002(171), 1058(101), 1104(2), 1109(44), 1121(5), 1154(35), 1161(257), 1167(305), 1178(249), 1194(96), 1206(286), 1212(49), 1254(1009), 1263(112), 1290(172), 1293(376), 1420(68), 1449(201), 1969(408), 2077(39), 2088(215), 2103(905), 2118(770), 2137(645), 2172(107)
27-14S	28(0), 36(0), 42(0), 45(0), 54(0), 59(0), 62(0), 66(0), 70(0), 77(0), 81(1), 88(0), 88(0), 97(0), 103(0), 103(0), 110(0), 113(0), 120(0), 122(0), 129(0), 134(1), 137(1), 140(0), 146(1), 151(1), 162(0), 179(0), 185(1), 208(1), 209(2), 217(0), 227(1), 242(1), 246(0), 270(2), 272(8), 274(3), 287(3), 293(3), 295(4), 299(4), 315(2), 341(2), 346(0), 369(1), 376(2), 387(7), 397(3), 402(3), 411(3), 417(4), 421(3), 422(1), 433(5), 452(18), 454(44), 462(28), 470(3), 475(6), 485(16), 487(16), 500(10), 503(5), 518(4), 524(4), 536(24), 538(1), 558(4), 570(3), 576(18), 581(39), 587(16), 596(55), 607(69), 611(13), 616(85), 625(104), 641(72), 649(298), 670(74), 695(69), 698(27), 744(91), 763(0), 777(19), 809(89), 902(77), 991(68), 1008(113), 1082(53), 1096(63), 1113(88), 1123(61), 1139(41), 1164(89), 1171(63), 1179(89), 1185(267), 1200(340), 1223(305), 1228(241), 1255(23), 1260(313), 1305(413), 1333(139), 1451(52), 2080(37), 2095(554), 2104(771), 2111(313), 2117(965), 2138(1139), 2175(77)
27-15S	24(0), 36(0), 46(0), 53(0), 61(0), 64(0), 73(0), 76(0), 86(0), 88(0), 91(0), 95(0), 105(0), 106(0), 107(0), 117(0), 120(0), 128(1), 130(1), 134(1), 138(0), 142(0), 144(0), 152(0), 158(0), 166(1), 168(1), 177(1), 182(1), 185(1), 199(0), 217(1), 225(2), 234(0), 238(2), 249(3), 258(5), 267(2), 286(5), 295(2), 315(2), 322(1), 324(1), 348(1), 360(1), 370(0), 372(1), 386(14), 394(3), 397(6), 411(13), 415(2), 420(3), 433(17), 443(7), 446(14), 449(3), 460(45), 466(5), 470(6), 490(18), 497(16), 499(9), 519(11), 520(1), 533(13), 538(3), 551(8), 555(50), 564(28), 566(36), 585(70), 592(5), 596(33), 602(28), 615(13), 624(59), 625(283), 635(13), 640(131), 664(143), 701(73), 716(28), 746(50), 747(32), 769(18), 838(46), 909(117), 918(77), 1040(21), 1056(29), 1086(23), 1094(211), 1107(82), 1148(43), 1151(85), 1153(262), 1181(29), 1196(147), 1199(585), 1219(283), 1221(153), 1234(395), 1257(67), 1294(140), 1340(114), 1471(71), 2074(99), 2093(447), 2099(789), 2112(459), 2124(588), 2139(1348), 2174(103)
27-16S	26(0), 29(1), 36(0), 43(1), 50(0), 54(0), 60(0), 66(0), 67(0), 72(0), 75(1), 81(0), 82(0), 88(0), 90(0), 95(0), 98(3), 107(1), 113(0), 117(0), 124(0), 124(0), 132(1), 133(2), 143(0), 152(0), 165(1), 166(1), 187(6), 199(3), 204(2), 225(44), 229(4), 232(5), 242(17), 270(3), 273(2), 282(9), 286(2), 293(7), 298(1), 311(8), 312(2), 331(4), 344(0), 346(0), 354(81), 371(124), 387(3), 391(55), 396(74), 406(5), 418(0), 423(23), 425(1), 434(9), 438(7), 440(43), 454(4), 462(2), 474(5), 486(13), 495(29), 505(1), 517(1), 536(4), 536(8), 537(20), 551(19), 566(14), 571(13), 576(5), 584(46), 603(298), 606(56), 613(57), 619(61), 625(24), 630(10), 676(187), 683(85), 697(74), 717(53), 768(4), 772(1), 778(26), 783(29), 908(66), 934(99), 1061(110), 1084(51), 1099(76), 1110(55), 1143(55), 1148(56), 1163(214), 1171(255), 1183(329), 1185(151), 1202(205), 1207(243), 1261(370), 1266(438), 1292(332), 1305(292), 1425(59), 1449(35), 1973(424), 2082(38), 2086(90), 2109(954), 2114(862), 2140(629), 2174(105)
27-17S	22(0), 26(0), 38(0), 43(0), 51(0), 57(0), 64(0), 70(0), 71(0), 79(1), 85(0), 88(0), 91(0), 95(0), 102(0), 107(0), 110(0), 119(0), 120(0), 126(0), 127(0), 133(0), 140(0), 148(0), 152(1), 161(3), 164(1), 167(1), 174(1), 181(0), 191(1), 201(1), 228(2), 240(1), 248(2), 256(3), 260(1), 289(0), 306(0), 315(2), 322(2), 325(1), 335(3), 345(1), 358(1), 366(8), 373(0), 382(9), 396(7), 406(8), 413(8), 415(1), 428(2), 440(2), 449(5), 453(1), 464(1), 466(10), 470(4), 490(9), 496(17), 499(26), 519(8), 524(7), 526(11), 537(1), 538(8), 539(9), 551(1), 556(6), 561(17), 571(98), 590(2), 597(14), 609(39), 618(20), 626(189), 635(83), 637(94), 661(30), 701(110), 715(54), 737(18), 742(66), 746(57), 825(85), 840(60), 920(55), 981(62), 1042(13), 1047(28), 1093(205), 1112(116), 1134(9), 1142(20), 1154(365), 1162(90), 1170(44), 1196(126), 1196(101), 1223(23), 1226(69), 1230(603), 1240(240), 1256(416), 1284(713), 1299(68), 2049(287), 2059(293), 2091(742), 2107(110), 2110(1151), 2132(1387), 2164(121)
27-18S	27(0), 31(0), 35(0), 43(0), 50(0), 54(0), 58(0), 63(0), 71(0), 82(0), 85(0), 88(0), 91(2), 93(0), 97(0), 100(0), 109(1), 115(1), 118(1), 123(1), 127(1), 133(0), 138(0), 153(0), 160(2), 163(1), 169(2), 181(1), 183(2), 203(4), 207(2), 210(1), 219(25), 228(2), 239(17), 245(1), 255(2), 278(4), 289(8), 301(1), 312(0), 323(0), 327(1), 345(2), 347(4), 356(0), 361(94), 371(2), 376(111), 383(8), 388(94), 394(4), 397(9), 416(3), 419(36), 422(14), 438(1), 446(39), 457(19), 462(3), 469(9), 488(20), 496(29), 515(1), 524(5), 534(7), 541(21), 542(2), 545(4), 564(11), 564(13), 570(21), 596(20), 602(258), 605(36), 614(61), 617(158), 626(25), 634(14), 636(1), 677(176), 689(152), 715(33), 754(35), 763(43), 774(29), 793(3), 914(165), 974(101), 998(215), 1088(14), 1095(2), 1108(3), 1110(94), 1149(161), 1150(253), 1181(205), 1185(88), 1202(454), 1204(43), 1222(408), 1255(571), 1265(80), 1290(334), 1335(117), 1415(249), 1464(91), 1983(454), 2075(191), 2079(128), 2109(659), 2112(945), 2137(702), 2174(92)

27-19S	19(0), 35(0), 39(0), 52(0), 55(0), 62(0), 66(0), 73(0), 83(0), 84(0), 91(0), 94(0), 100(0), 103(0), 108(0), 110(0), 115(0), 120(1), 124(2), 130(0), 135(1), 146(1), 152(1), 154(2), 161(4), 171(1), 182(1), 196(10), 210(3), 214(2), 218(1), 224(6), 230(1), 245(1), 247(0), 259(1), 265(1), 274(5), 282(1), 294(7), 301(2), 307(3), 322(0), 337(1), 344(4), 356(29), 364(1), 371(8), 376(0), 403(2), 411(4), 420(0), 429(18), 434(9), 439(14), 444(5), 448(1), 453(16), 463(0), 487(4), 495(5), 500(2), 515(13), 521(17), 527(27), 531(17), 535(3), 543(6), 549(4), 566(31), 569(34), 582(9), 590(12), 595(113), 602(30), 604(35), 609(22), 619(111), 625(41), 646(121), 688(117), 692(74), 699(41), 739(116), 793(48), 802(33), 808(124), 898(5), 985(63), 1015(27), 1046(27), 1073(72), 1099(64), 1118(36), 1129(97), 1143(212), 1162(31), 1176(152), 1183(87), 1197(122), 1204(208), 1224(341), 1225(242), 1233(195), 1266(16), 1294(442), 1333(164), 1981(377), 2100(7), 2107(829), 2126(79), 2129(1102), 2153(1521), 2176(67)
27-20S	37(0), 42(0), 56(0), 59(0), 68(0), 75(0), 81(0), 84(1), 89(0), 92(0), 100(0), 101(0), 104(0), 107(0), 109(0), 113(2), 119(0), 120(1), 129(0), 132(1), 135(0), 143(2), 146(1), 151(2), 161(1), 176(1), 180(0), 182(1), 195(2), 201(0), 208(2), 216(2), 225(3), 229(1), 251(0), 258(1), 267(2), 288(2), 298(5), 308(1), 315(0), 323(2), 329(2), 335(1), 341(0), 351(1), 366(10), 382(2), 390(3), 398(3), 403(1), 416(6), 423(5), 438(2), 444(12), 452(2), 459(3), 464(11), 476(12), 502(2), 511(32), 519(16), 525(15), 529(13), 532(12), 538(8), 541(1), 543(4), 546(11), 556(6), 566(25), 570(14), 584(11), 589(19), 598(39), 606(105), 618(144), 625(122), 640(22), 653(18), 692(130), 721(113), 726(55), 740(17), 784(38), 799(44), 833(25), 937(91), 947(96), 959(32), 1008(24), 1046(102), 1091(58), 1096(2), 1134(7), 1144(34), 1150(54), 1160(66), 1181(435), 1190(25), 1209(388), 1221(120), 1225(125), 1231(431), 1245(262), 1257(465), 1275(455), 2039(212), 2090(250), 2104(658), 2112(558), 2136(778), 2145(1165), 2178(255)
27-21S	24(0), 32(0), 37(0), 44(0), 48(0), 54(0), 61(0), 68(0), 76(0), 77(0), 83(0), 86(0), 91(0), 95(0), 98(0), 101(0), 108(0), 113(0), 119(0), 123(1), 127(0), 131(1), 134(0), 142(0), 150(0), 163(0), 177(1), 180(0), 195(0), 200(1), 215(2), 217(2), 228(1), 234(1), 248(0), 252(1), 261(4), 276(2), 285(4), 288(6), 300(1), 304(5), 326(1), 342(1), 348(1), 361(1), 372(1), 379(2), 388(6), 402(6), 406(6), 412(13), 417(9), 424(4), 432(13), 436(7), 448(9), 453(25), 456(67), 470(0), 480(3), 486(19), 493(13), 499(12), 522(4), 529(4), 532(16), 533(21), 555(39), 563(4), 575(31), 581(21), 587(1), 600(30), 601(35), 612(46), 618(0), 628(63), 634(91), 640(132), 643(393), 671(95), 697(24), 745(86), 749(24), 764(22), 811(82), 905(152), 989(39), 1003(145), 1081(18), 1103(74), 1106(155), 1131(36), 1144(38), 1163(68), 1165(54), 1183(101), 1196(467), 1217(351), 1221(212), 1231(331), 1252(6), 1259(115), 1334(165), 1335(126), 1460(73), 2085(9), 2093(633), 2106(548), 2112(322), 2118(1261), 2139(1022), 2177(77)
27-22S	14(0), 34(0), 36(0), 44(0), 51(0), 60(0), 67(0), 77(0), 80(0), 82(0), 86(0), 94(0), 96(0), 99(0), 102(0), 103(0), 111(0), 117(0), 122(0), 126(0), 129(0), 130(0), 135(1), 154(1), 165(1), 172(0), 178(1), 179(1), 182(1), 192(1), 199(0), 216(2), 224(2), 237(1), 251(1), 262(5), 266(1), 281(5), 285(2), 295(2), 303(4), 312(1), 323(1), 326(1), 346(0), 348(0), 374(1), 388(6), 393(4), 400(18), 407(0), 416(16), 418(1), 423(2), 432(10), 438(9), 447(11), 459(69), 470(2), 479(1), 486(8), 490(33), 506(15), 519(1), 521(6), 533(16), 536(3), 538(18), 554(4), 556(42), 564(2), 579(12), 584(18), 598(32), 601(29), 612(48), 626(70), 632(232), 635(54), 639(65), 656(292), 671(62), 726(86), 737(21), 750(27), 770(19), 804(39), 905(136), 956(68), 972(70), 1083(22), 1102(98), 1108(81), 1143(56), 1144(29), 1157(72), 1166(73), 1183(6), 1199(457), 1216(367), 1226(244), 1232(168), 1239(330), 1257(130), 1275(355), 1336(121), 1463(73), 2080(46), 2094(653), 2105(472), 2110(283), 2116(1288), 2138(1050), 2176(84)
27-23S	33(0), 38(0), 44(0), 48(0), 58(0), 64(0), 72(0), 76(0), 78(0), 85(1), 89(0), 90(0), 97(0), 100(0), 104(0), 109(2), 118(0), 118(2), 125(1), 129(2), 135(2), 140(1), 145(1), 154(1), 158(1), 165(2), 174(0), 185(0), 202(1), 203(1), 208(1), 215(5), 225(2), 232(1), 245(0), 251(1), 256(1), 270(2), 293(5), 299(5), 308(1), 323(2), 332(1), 341(0), 344(0), 357(11), 367(5), 376(0), 381(3), 396(4), 400(1), 416(8), 420(4), 436(5), 441(13), 444(4), 451(6), 462(7), 465(9), 470(16), 505(3), 510(22), 522(12), 524(25), 530(6), 535(19), 536(2), 542(2), 544(3), 562(33), 568(4), 583(14), 587(35), 590(7), 597(33), 601(59), 610(74), 625(119), 632(52), 661(96), 691(127), 698(103), 721(106), 729(83), 782(43), 785(42), 835(26), 936(102), 948(88), 988(78), 1009(26), 1062(70), 1093(35), 1098(71), 1124(124), 1137(12), 1156(59), 1163(47), 1178(91), 1184(365), 1210(404), 1223(291), 1224(46), 1230(518), 1261(413), 1266(14), 1337(151), 2030(254), 2093(277), 2106(644), 2115(544), 2136(700), 2146(1285), 2178(227)
26-1S	37(0), 41(0), 46(0), 52(0), 55(0), 62(0), 66(0), 68(0), 74(0), 81(0), 83(0), 96(0), 99(0), 101(0), 104(0), 109(0), 118(0), 121(0), 126(0), 132(0), 139(0), 143(2), 153(1), 158(1), 160(1), 174(0), 191(1), 192(0), 205(4), 211(2), 225(1), 236(1), 242(0), 261(1), 284(3), 306(2), 307(0), 314(1), 319(1), 331(1), 342(0), 359(0), 370(0), 372(2), 388(0), 399(7), 408(3), 417(2), 426(3), 436(0), 440(31), 449(20), 450(8), 460(7), 463(41), 484(24), 488(19), 511(7), 517(1), 524(6), 532(14), 541(1), 544(3), 547(14), 562(7), 564(16), 574(61), 587(82), 588(7), 594(95), 602(49), 617(7), 630(141), 643(131), 661(77), 690(29), 715(31), 719(97), 747(30), 755(12), 804(1), 851(99), 884(40), 960(19), 983(107), 995(138), 1074(128), 1104(62), 1104(25), 1120(2), 1158(77), 1168(302), 1181(123), 1184(130), 1206(55), 1215(459), 1221(152), 1259(480), 1273(345), 1299(398), 1323(115), 1463(233), 2071(105), 2093(756), 2109(737), 2111(562), 2128(1019), 2168(306)

26-2S	33(0), 46(0), 54(0), 56(0), 61(0), 69(0), 72(0), 75(0), 76(0), 81(0), 84(1), 91(0), 99(0), 105(0), 106(0), 114(0), 118(0), 122(0), 128(0), 130(0), 134(0), 137(1), 141(1), 149(1), 154(1), 163(1), 178(0), 198(6), 205(0), 213(1), 227(1), 247(1), 255(3), 266(6), 273(1), 288(3), 294(2), 305(0), 315(0), 317(3), 328(2), 343(1), 369(1), 372(0), 396(6), 406(1), 420(1), 422(2), 426(3), 432(4), 447(2), 453(10), 461(0), 462(42), 473(12), 488(21), 492(24), 504(5), 512(0), 521(2), 524(4), 535(18), 543(7), 547(4), 561(65), 568(43), 575(35), 581(24), 588(0), 602(26), 616(4), 618(8), 634(107), 646(145), 666(120), 691(21), 695(64), 716(90), 748(37), 764(2), 774(13), 850(94), 882(32), 905(75), 958(20), 1073(131), 1094(69), 1102(70), 1125(62), 1144(33), 1160(62), 1170(153), 1182(152), 1183(183), 1197(320), 1216(360), 1223(218), 1268(179), 1271(500), 1319(417), 1325(118), 1476(40), 2059(150), 2095(747), 2105(796), 2110(314), 2119(1095), 2166(413)
26-3S	29(0), 31(0), 38(0), 42(0), 51(0), 57(0), 64(0), 65(0), 71(0), 79(0), 84(0), 89(0), 93(1), 97(0), 100(1), 103(0), 111(0), 118(1), 119(1), 123(0), 129(0), 136(1), 142(1), 146(3), 155(0), 171(0), 181(1), 196(0), 203(0), 208(1), 227(2), 238(2), 249(0), 252(0), 278(1), 288(6), 303(2), 306(1), 309(4), 326(1), 342(0), 347(1), 361(1), 369(1), 380(1), 389(0), 401(5), 409(4), 414(5), 424(2), 435(12), 438(1), 445(20), 454(12), 465(66), 468(2), 486(9), 496(14), 505(1), 524(15), 530(1), 532(1), 535(7), 553(3), 558(8), 562(8), 571(42), 587(9), 596(43), 601(31), 606(27), 607(60), 619(2), 637(228), 646(294), 662(35), 704(79), 705(24), 748(41), 750(46), 798(5), 817(90), 931(128), 995(135), 997(45), 1014(156), 1045(68), 1109(128), 1120(36), 1133(44), 1153(251), 1164(61), 1178(71), 1184(112), 1222(249), 1226(221), 1230(286), 1257(4), 1290(590), 1337(135), 1349(327), 1436(266), 2066(145), 2091(755), 2109(517), 2113(946), 2126(917), 2170(230)
26-4S	28(0), 34(0), 40(0), 46(0), 55(0), 61(0), 64(0), 72(0), 75(0), 83(0), 91(1), 93(0), 97(0), 99(0), 102(2), 103(0), 112(1), 116(1), 128(1), 130(2), 144(0), 148(6), 151(1), 153(2), 164(2), 167(3), 179(1), 191(0), 203(2), 211(1), 223(5), 226(3), 238(1), 246(21), 290(4), 302(1), 307(2), 312(1), 324(0), 331(1), 343(12), 346(0), 357(12), 360(7), 377(8), 384(6), 388(187), 393(14), 399(38), 414(15), 426(10), 436(11), 452(5), 455(6), 466(49), 474(42), 494(29), 498(0), 504(30), 515(1), 529(7), 537(3), 543(3), 544(6), 552(5), 564(0), 566(22), 573(133), 593(24), 601(19), 610(41), 621(48), 625(75), 628(50), 679(135), 687(201), 704(34), 715(35), 756(30), 763(30), 794(3), 801(7), 886(142), 975(104), 997(229), 1006(160), 1045(115), 1100(1), 1109(8), 1130(129), 1151(256), 1157(317), 1184(141), 1197(161), 1203(33), 1236(359), 1255(505), 1290(342), 1303(418), 1357(342), 1420(239), 1426(268), 1976(469), 2072(42), 2081(299), 2098(1026), 2111(719), 2157(422)
26-5S	21(0), 28(0), 37(0), 43(0), 54(0), 64(0), 66(0), 75(1), 82(0), 87(0), 88(1), 94(1), 97(1), 99(0), 107(0), 110(0), 117(0), 120(0), 123(0), 127(0), 135(2), 139(1), 149(1), 154(0), 167(0), 169(1), 179(0), 187(1), 194(1), 207(0), 218(1), 239(1), 248(0), 261(1), 283(4), 293(3), 302(0), 304(0), 309(0), 326(1), 331(0), 343(0), 346(1), 367(1), 387(0), 393(0), 404(9), 409(1), 419(5), 425(11), 430(7), 432(5), 448(9), 464(9), 472(61), 483(16), 506(9), 512(5), 515(6), 531(7), 534(7), 538(8), 540(2), 551(4), 556(10), 560(37), 563(8), 569(20), 587(27), 599(29), 601(52), 616(96), 631(16), 637(180), 654(195), 665(109), 706(28), 730(74), 737(31), 751(9), 802(4), 810(51), 939(82), 962(166), 973(47), 991(107), 1049(70), 1109(71), 1119(26), 1148(52), 1151(48), 1153(273), 1179(65), 1181(8), 1218(254), 1227(192), 1234(303), 1247(307), 1281(481), 1291(389), 1344(317), 1437(264), 2066(130), 2090(656), 2108(614), 2112(951), 2126(941), 2168(249)
26-6S	28(0), 40(0), 46(0), 52(0), 61(0), 64(1), 72(0), 76(1), 79(0), 84(0), 88(0), 90(0), 92(1), 96(1), 104(1), 108(1), 114(0), 116(3), 119(0), 129(0), 136(0), 144(1), 161(0), 162(5), 168(2), 188(4), 194(0), 212(1), 221(3), 230(2), 234(4), 240(1), 257(1), 262(4), 280(2), 288(1), 292(6), 306(2), 312(11), 324(1), 342(26), 343(10), 358(1), 374(1), 376(5), 377(1), 386(1), 418(8), 431(0), 431(20), 444(3), 448(4), 451(5), 458(14), 463(12), 466(16), 480(16), 506(3), 515(17), 517(30), 526(5), 531(4), 540(1), 543(2), 544(3), 558(52), 586(7), 590(19), 594(27), 598(35), 602(39), 608(23), 618(18), 628(179), 649(58), 693(10), 697(33), 710(94), 741(17), 750(76), 820(86), 850(86), 876(46), 949(10), 999(71), 1057(86), 1072(117), 1106(164), 1110(50), 1127(85), 1160(48), 1172(85), 1175(83), 1179(97), 1216(341), 1222(289), 1226(233), 1233(262), 1254(29), 1257(454), 1318(122), 1339(149), 2012(396), 2082(646), 2109(572), 2115(1446), 2125(505), 2167(345)
26-7S	37(1), 48(0), 57(0), 61(0), 67(0), 74(1), 76(1), 84(0), 87(0), 93(0), 96(0), 102(0), 107(0), 109(0), 114(0), 120(2), 123(1), 131(0), 133(0), 139(5), 144(1), 149(2), 151(1), 160(0), 167(3), 175(1), 185(3), 189(1), 210(1), 224(1), 233(5), 243(0), 249(3), 259(1), 282(0), 293(15), 305(4), 310(2), 322(4), 324(1), 345(13), 352(4), 355(22), 369(0), 377(1), 378(0), 411(21), 426(6), 428(2), 441(1), 446(2), 450(6), 453(17), 461(3), 466(3), 482(10), 501(7), 517(5), 520(20), 525(4), 526(1), 537(29), 543(6), 545(7), 553(3), 557(5), 586(12), 589(47), 590(19), 596(33), 602(35), 617(19), 619(79), 635(95), 692(14), 698(38), 707(80), 717(36), 739(47), 754(30), 837(35), 859(62), 869(59), 917(38), 945(15), 1045(28), 1065(21), 1071(156), 1100(125), 1115(135), 1155(31), 1158(291), 1170(47), 1180(132), 1199(202), 1211(263), 1220(256), 1225(27), 1228(500), 1254(440), 1290(159), 1309(123), 2047(270), 2080(822), 2114(1326), 2120(491), 2135(482), 2174(410)

26-8S	36(0), 39(0), 45(0), 59(0), 62(0), 68(0), 72(0), 79(1), 85(0), 86(0), 89(0), 90(0), 97(1), 102(0), 104(1), 110(0), 114(3), 124(0), 127(1), 130(0), 144(1), 147(0), 160(1), 165(2), 180(1), 187(0), 195(1), 202(4), 211(4), 233(2), 234(8), 258(2), 261(0), 265(6), 284(1), 291(1), 302(4), 309(0), 312(6), 328(0), 332(2), 344(24), 350(11), 358(2), 375(0), 387(0), 402(3), 426(3), 428(10), 435(15), 444(2), 449(5), 455(20), 465(5), 469(18), 481(9), 505(11), 516(20), 523(14), 525(6), 530(1), 538(3), 540(3), 544(4), 550(1), 556(36), 565(29), 585(17), 589(10), 596(50), 605(23), 617(36), 628(182), 635(17), 647(31), 695(24), 708(91), 733(87), 741(22), 746(44), 813(50), 849(71), 874(46), 949(10), 959(26), 1043(80), 1071(119), 1105(174), 1108(20), 1143(31), 1156(52), 1161(60), 1173(100), 1190(1), 1215(310), 1224(312), 1226(133), 1230(157), 1244(550), 1252(456), 1275(330), 1315(120), 1997(407), 2085(586), 2107(596), 2118(1477), 2122(547), 2163(291)
26-9S	23(0), 33(0), 48(0), 48(0), 55(0), 58(0), 71(0), 72(0), 79(0), 80(0), 89(0), 95(0), 97(0), 100(0), 106(0), 114(1), 121(0), 125(0), 126(0), 134(0), 140(1), 141(1), 144(0), 155(1), 164(1), 178(0), 186(1), 191(0), 202(3), 225(0), 230(2), 236(2), 243(7), 255(0), 268(1), 276(5), 291(3), 305(0), 313(1), 321(2), 337(1), 350(1), 369(0), 370(0), 375(1), 400(6), 407(3), 417(2), 426(3), 433(14), 440(4), 445(11), 451(18), 454(26), 460(1), 474(27), 484(23), 490(20), 512(2), 517(2), 523(4), 533(16), 542(8), 552(12), 556(36), 565(6), 582(72), 588(1), 594(58), 599(40), 603(39), 618(15), 630(134), 637(10), 646(163), 662(79), 687(34), 716(97), 747(30), 751(38), 771(15), 843(107), 880(33), 907(132), 955(26), 1073(123), 1086(29), 1102(88), 1112(86), 1144(58), 1157(109), 1176(26), 1183(178), 1197(479), 1215(279), 1219(413), 1221(236), 1265(138), 1273(289), 1324(116), 1337(112), 1485(71), 2069(109), 2092(769), 2107(763), 2109(479), 2122(1075), 2167(348)
26-10S	24(0), 30(0), 34(0), 42(0), 45(0), 53(0), 58(1), 59(0), 64(0), 70(1), 77(0), 78(0), 88(0), 90(1), 96(0), 98(2), 101(1), 106(1), 108(0), 121(1), 125(1), 131(1), 133(3), 139(1), 162(1), 164(0), 170(0), 183(1), 199(2), 215(6), 229(18), 232(10), 249(17), 267(2), 271(2), 286(4), 295(5), 305(1), 309(1), 312(6), 323(2), 342(0), 343(0), 359(29), 367(146), 375(1), 389(2), 393(12), 399(1), 417(2), 422(8), 434(173), 443(12), 449(44), 457(12), 474(46), 482(20), 500(2), 505(1), 517(1), 525(1), 529(8), 536(6), 542(4), 553(3), 560(2), 569(28), 572(45), 583(33), 595(57), 608(91), 618(72), 621(118), 625(19), 680(115), 685(127), 698(70), 703(32), 752(21), 773(3), 782(34), 801(1), 910(73), 913(148), 1006(155), 1044(79), 1083(51), 1097(75), 1128(87), 1142(37), 1164(197), 1169(233), 1182(202), 1183(91), 1199(272), 1234(268), 1268(354), 1292(818), 1307(141), 1353(333), 1426(233), 1447(35), 1963(423), 2077(63), 2093(540), 2100(617), 2123(1140), 2162(76)
26-11S	33(0), 42(0), 44(0), 53(0), 58(0), 67(0), 73(0), 79(0), 83(0), 86(0), 89(0), 90(0), 94(0), 103(0), 106(1), 110(1), 110(1), 115(0), 121(1), 128(2), 137(1), 151(5), 154(0), 163(2), 184(1), 189(0), 201(2), 205(2), 211(4), 230(8), 239(6), 263(0), 267(1), 269(0), 280(6), 286(2), 288(1), 304(2), 309(3), 318(7), 329(3), 331(9), 339(17), 349(0), 352(6), 380(0), 397(3), 406(6), 424(11), 426(2), 432(2), 446(19), 447(4), 461(3), 474(5), 479(16), 505(12), 512(16), 517(10), 525(9), 530(8), 535(4), 536(2), 540(2), 545(2), 553(3), 559(4), 567(35), 578(21), 592(64), 605(42), 617(6), 625(102), 635(6), 642(14), 679(247), 723(97), 730(17), 735(91), 749(24), 804(43), 817(40), 952(91), 964(26), 1002(100), 1062(63), 1082(193), 1106(26), 1114(55), 1133(42), 1142(32), 1162(78), 1186(2), 1196(72), 1204(95), 1226(176), 1232(243), 1243(303), 1259(357), 1273(536), 1282(197), 1309(392), 1970(409), 2085(585), 2097(576), 2111(1278), 2119(915), 2159(261)
14-1S	37(0), 41(0), 54(0), 63(0), 78(0), 87(0), 93(0), 100(0), 129(1), 135(0), 141(0), 163(2), 178(1), 198(1), 209(0), 234(0), 273(0), 311(1), 320(0), 347(0), 356(1), 377(1), 404(1), 408(2), 423(6), 427(7), 437(2), 457(35), 468(7), 494(28), 516(3), 541(3), 545(5), 557(12), 564(2), 612(45), 615(5), 626(128), 649(104), 687(197), 715(40), 760(17), 797(4), 975(128), 1002(223), 1093(1), 1112(6), 1157(281), 1179(127), 1203(71), 1258(535), 1294(374), 1416(284), 2087(837), 2112(997), 2115(403), 2176(236)
14-2S	40(0), 44(0), 48(0), 56(0), 61(0), 83(0), 89(0), 97(0), 105(0), 119(0), 123(0), 138(0), 165(1), 208(1), 230(0), 250(3), 273(1), 274(2), 288(2), 312(1), 338(2), 399(0), 405(1), 414(2), 427(6), 438(3), 438(1), 456(8), 467(24), 489(26), 505(0), 518(2), 536(11), 564(0), 570(3), 607(64), 610(4), 636(58), 645(121), 684(151), 699(106), 771(0), 775(26), 912(96), 1083(32), 1090(82), 1147(32), 1165(143), 1177(197), 1190(456), 1269(373), 1305(295), 1448(49), 2091(949), 2113(242), 2120(1081), 2180(197)
14-3S	40(0), 47(0), 55(0), 71(0), 77(0), 85(0), 93(0), 100(0), 107(0), 116(1), 130(0), 158(0), 179(0), 202(1), 228(1), 235(2), 245(1), 277(3), 295(1), 322(1), 344(1), 370(0), 399(0), 404(2), 424(5), 427(1), 437(6), 445(3), 459(8), 476(27), 493(22), 523(1), 532(9), 560(3), 568(7), 602(20), 608(48), 625(64), 639(36), 645(125), 692(226), 758(35), 769(22), 916(203), 1082(14), 1101(115), 1141(46), 1171(41), 1192(469), 1217(393), 1265(122), 1332(140), 1437(95), 2089(924), 2111(408), 2117(1000), 2178(172)
14-4S	63(0), 69(0), 70(0), 77(0), 91(0), 99(0), 100(1), 105(0), 117(0), 122(1), 168(0), 187(1), 221(0), 223(1), 232(3), 239(4), 252(1), 269(0), 279(1), 291(3), 325(0), 351(0), 372(1), 390(1), 411(7), 424(1), 429(1), 429(3), 439(11), 468(3), 493(10), 521(7), 528(1), 548(0), 584(0), 589(11), 604(49), 612(55), 634(128), 641(52), 659(30), 837(1), 907(317), 983(303), 1032(22), 1074(10), 1079(154), 1121(157), 1167(306), 1170(38), 1235(106), 1264(154), 1346(108), 2115(680), 2134(371), 2135(1022), 2193(153)

14-5S	53(0), 57(0), 71(0), 74(0), 81(0), 88(0), 93(0), 102(0), 120(0), 133(1), 141(0), 162(0), 207(3), 212(0), 224(3), 242(2), 259(2), 280(1), 296(0), 308(0), 330(0), 334(0), 394(2), 408(0), 412(6), 420(2), 438(1), 446(0), 462(5), 482(26), 514(0), 522(3), 530(3), 552(2), 575(3), 600(13), 603(15), 612(38), 631(100), 641(146), 720(45), 824(8), 870(191), 925(207), 1040(110), 1089(27), 1110(160), 1132(76), 1173(110), 1187(305), 1229(109), 1295(285), 1299(235), 2108(741), 2127(979), 2129(381), 2187(202)
14-6S	33(0), 47(0), 63(0), 68(0), 75(0), 85(0), 93(0), 104(0), 116(0), 122(0), 130(0), 191(0), 208(1), 215(0), 218(4), 242(2), 248(4), 265(1), 269(0), 314(0), 340(1), 363(0), 387(0), 395(2), 417(6), 428(1), 431(1), 432(2), 463(5), 490(24), 513(3), 520(0), 536(0), 549(0), 578(0), 599(49), 610(22), 628(99), 630(83), 639(2), 685(229), 810(117), 811(0), 996(235), 1072(31), 1080(6), 1101(199), 1151(46), 1164(19), 1209(388), 1237(429), 1258(81), 1299(275), 2105(776), 2123(600), 2127(833), 2185(185)
14-7S	15(0), 31(0), 48(0), 59(0), 67(0), 73(0), 87(0), 93(0), 98(0), 108(0), 125(1), 148(1), 153(0), 175(0), 206(2), 252(1), 291(1), 307(0), 322(2), 333(3), 346(0), 387(3), 396(0), 396(3), 414(1), 437(3), 451(0), 458(8), 485(23), 496(15), 524(5), 528(8), 537(4), 545(17), 558(1), 568(4), 597(65), 636(25), 651(79), 680(112), 735(25), 744(64), 833(102), 981(88), 1086(210), 1132(15), 1161(57), 1167(65), 1187(2), 1229(195), 1243(414), 1253(268), 1286(548), 2076(995), 2096(395), 2103(1109), 2165(255)
14-8S	16(0), 24(0), 44(0), 50(0), 68(0), 78(0), 91(0), 97(0), 102(0), 121(1), 139(0), 147(0), 172(1), 214(3), 217(2), 230(5), 277(2), 299(0), 312(0), 329(0), 376(0), 393(4), 398(0), 401(1), 416(7), 443(1), 455(0), 457(8), 489(17), 496(16), 509(11), 531(17), 549(1), 557(0), 587(2), 591(14), 592(27), 630(63), 648(97), 697(66), 721(25), 748(41), 873(95), 939(65), 1049(38), 1083(97), 1103(193), 1148(118), 1184(65), 1201(450), 1228(11), 1241(508), 1293(321), 2086(932), 2107(272), 2112(1060), 2172(316)
14-9S	16(0), 30(0), 33(0), 53(0), 69(0), 72(0), 88(0), 93(0), 104(0), 107(0), 128(0), 141(0), 152(1), 201(1), 223(2), 235(0), 284(4), 292(1), 331(1), 347(3), 364(2), 371(1), 389(3), 397(0), 415(1), 431(1), 451(0), 453(12), 458(8), 488(23), 501(0), 513(14), 540(9), 548(21), 559(0), 591(5), 598(80), 618(10), 652(68), 654(120), 709(56), 748(62), 829(101), 998(34), 1124(55), 1128(301), 1159(21), 1172(17), 1182(186), 1213(261), 1232(424), 1256(95), 1338(194), 2077(1001), 2097(401), 2104(1111), 2166(239)

Table S4. Cartesian coordinates (in Å) for optimized low-lying structures of the $(C_4F_8)_2Fe_2(CO)_n$ ($n=7, 6$) and $C_4F_8Fe(CO)_4$ complexes at the M06-L/cc-pVTZ level.

<p>$(C_4F_8)_2Fe_2(CO)_7$ (27-1S) M06-L/cc-pVTZ</p> <p>Fe,0,-0.6807147449,-0.25875079,0.0356696106 C,0,0.6093703163,0.9473224667,-1.9916268341 C,0,-0.9380048442,-1.52571316,1.3252883036 O,0,-0.3779166429,-2.2178859208,-2.2107783175 O,0,0.3352595837,0.7863071065,-3.0904553261 O,0,-1.1515755565,-2.3176955939,2.1130272816 Fe,0,1.2324066173,1.536547711,-0.3675303601 C,0,1.7856363879,2.2788494166,1.2337561761 C,0,0.4365047792,3.1430233396,-0.737012228 C,0,-0.7619966797,1.1750716736,1.1909817599 O,0,-0.0495550633,4.154130693,-0.9379006944 O,0,2.1757707313,2.8542586393,2.1333788873 O,0,-0.9714266206,1.9760263786,1.9836229202 C,0,-0.4730210594,-1.4872397876,-1.3470511263 C,0,2.852470493,1.8099371554,-1.1031038552 O,0,3.8427162561,2.030821277,-1.6231064893 C,0,1.4204263696,-0.3594098711,0.3798227906 C,0,2.1933310548,-1.3966038103,-0.4295220464 C,0,1.8096688658,-0.5015049262,1.8417860239 C,0,3.7326500117,-1.5973919616,-0.2152843555 F,0,2.1067410439,-1.1140744745,-1.7622227047 F,0,1.6698797789,-2.6477919861,-0.27114497 F,0,3.0559422973,-0.0384344976,2.0836373529 F,0,1.0103417635,0.1753056802,2.689634413 F,0,1.7818286865,-1.7756564299,2.2634132783 F,0,4.0141052171,-2.2021092836,0.9276156321 F,0,4.1941771986,-2.359346425,-1.2033175798 F,0,4.376732495,-0.4295293821,-0.2610919326 C,0,-3.5761307571,-1.4366523648,-0.5046745594 C,0,-3.5862188737,0.5802069433,0.9624175055 C,0,-2.8291637469,-0.1553704972,-0.1439050241 C,0,-2.1787027563,0.560629057,-1.1864757887 F,0,-3.2413484363,0.1368156061,2.1794079293 F,0,-3.9631104811,-2.0727655692,0.6059696448 F,0,-4.9037930739,0.3846136376,0.8370992678 F,0,-3.3960971265,1.8976377775,0.9428712406 F,0,-2.2724850536,0.0847819818,-2.4297954986 F,0,-2.2014777046,1.890879689,-1.2560652413 F,0,-2.8604458777,-2.3051434706,-1.2198637377 F,0,-4.6689878482,-1.1611090275,-1.2253663485</p>	<p>$(C_4F_8)_2Fe_2(CO)_7$ (27-2S) M06-L/cc-pVTZ</p> <p>Fe,0,1.76191355,1.6846356362,-0.3708733082 C,0,0.359018975,2.5867836495,-1.1413479073 C,0,2.8101934952,3.0474044276,-0.9902285773 O,0,1.5724366867,2.8834253411,2.3190937062 O,0,-0.4389485148,3.2487750668,-1.6114310771 O,0,3.3585925986,3.947333773,-1.4231144948 Fe,0,2.3430416484,-0.7022192996,-0.75762801 C,0,3.8259059942,-1.2244962651,-1.6801171179 C,0,1.3799304767,-1.8736279399,-1.792835635 C,0,2.1569517424,0.7518784887,-2.1390477168 O,0,0.8653501225,-2.6616536675,-2.4328765694 O,0,4.6821904804,-1.6166061935,-2.3215824975 O,0,2.2737772501,0.9727036424,3.266798928 C,0,1.6025063825,2.3988247799,1.2901127433 C,0,2.634029949,-1.8742359958,0.6079819298 O,0,2.9054649106,-2.6088415401,1.4320655384 C,0,7.2686893544,0.4409970908,-0.2640246425 C,0,5.9400449105,0.273114937,0.5216360366 C,0,4.7590673667,1.1473720418,-0.013234098 C,0,3.365016029,0.654985691,0.3690403897 F,0,3.4955652203,0.4648739663,1.7129696865 F,0,4.9596302283,2.3869859278,0.5054910552 F,0,4.8774646944,1.2623291245,-1.3610933195 F,0,6.183631708,0.5935903099,1.7949427956 F,0,5.6042726361,-1.0345597143,0.4690103402 F,0,7.566622116,1.7293243814,-0.3951069358 F,0,8.2449688254,-0.1592839709,0.4067426073 F,0,7.1837923642,-0.1114744904,-1.4681695697 C,0,0.5742949142,0.0483091776,0.0360582681 C,0,0.2024598296,-0.4017873726,1.4397155823 C,0,-0.6419652666,-0.0823222288,-0.8685900308 C,0,-1.0645780138,0.1929226264,2.1369083283 F,0,1.209177744,-0.1477423005,2.3051340822 F,0,0.0114677763,-1.7560536184,1.4757265758 F,0,-1.6049491481,0.8117467238,-0.570040022 F,0,-0.3633032869,0.126668532,-2.1758997785 F,0,-1.2153857885,-1.2943607938,-0.8064914063 F,0,-2.1853128761,-0.3239363567,1.6543671714 F,0,-1.0139124041,-0.082448386,3.4359235373 F,0,-1.099876371,1.5227301382,1.997828448</p>
<p>$(C_4F_8)_2Fe_2(CO)_7$ (27-3S) M06-L/cc-pVTZ</p> <p>Fe,0,-1.4963976771,0.9505531727,0.2114136873 C,0,0.0731572185,-0.5405904303,0.5234305384 C,0,-1.4664389135,1.3515167808,-1.5873146315 C,0,-1.4310709162,2.7419837919,0.417411526 O,0,0.0220803895,-1.5362422313,1.1006328424 O,0,-1.4437022936,1.7777274411,-2.6449181392 O,0,-1.4422242448,3.8784434109,0.5538049472 Fe,0,1.3177534363,0.7552736614,-0.3004017669 C,0,1.0249498948,-0.0238546399,-1.9586430242 C,0,1.3667121973,1.6968049169,1.2858772644 C,0,1.2342854186,2.3860393009,-1.1187783857 O,0,0.7527627773,-0.4200913342,-2.9873613488 O,0,1.3441232869,2.3744320713,2.1997656653 O,0,1.2454579414,3.403640661,-1.6347063697 C,0,-1.5051169771,0.9283921327,2.0547325243 O,0,-1.4689918355,1.0633513172,3.1837170576 C,0,3.2784780915,-0.9040167373,1.5282970805 C,0,3.0436182154,-1.776293458,-0.8035548438 C,0,2.9194636425,-0.5506331634,0.0917321313</p>	<p>$(C_4F_8)_2Fe_2(CO)_7$ (27-4S) M06-L/cc-pVTZ</p> <p>Fe,0,-0.5979229429,-0.4104750844,0.5108354461 C,0,0.2978326952,1.3854661794,-1.5964982554 C,0,-0.4066885131,-2.0282573875,1.3092230556 O,0,-0.9705584704,-1.790937918,-2.1199752009 O,0,-0.1454307973,1.429279444,-2.6458035706 O,0,-0.3318642691,-3.0393809965,1.8264522534 Fe,0,1.0935528057,1.5946154936,0.0450539364 C,0,1.8681824367,2.0117767152,1.6669223088 C,0,0.045249067,3.0783519956,0.2879171453 C,0,-0.463883322,0.5308347354,2.0866425203 O,0,-0.581050914,4.0106177565,0.4801323499 O,0,2.3787110877,2.4202100073,2.597618572 O,0,-0.4788747199,1.0882686613,3.0817471009 C,0,-0.7888535931,-1.2081614423,-1.1632679744 C,0,2.5466672434,2.2673586955,-0.771062661 O,0,3.4395152873,2.7360682188,-1.3040063289 C,0,-2.3753656218,0.6628382669,0.2703619525 C,0,-2.6427443395,-0.6689314758,0.7029277114 C,0,-2.9630218331,1.1993668893,-1.0214476741</p>

<p>C,0,3.3198239647,0.7366893535,-0.395120781 F,0,1.9538235261,-2.5522697275,-0.742277071 F,0,2.7740546532,-2.0901224725,1.8660997351 F,0,4.0875483338,-2.5293107986,-0.4416246218 F,0,3.2229619597,-1.4635909828,-2.0920731604 F,0,3.9385104735,1.5653021313,0.4571259797 F,0,3.8700152846,0.9043705198,-1.5943097605 F,0,2.8320566813,-0.0156716861,2.4282193572 F,0,4.6072213156,-0.9646893313,1.6864156248 C,0,-2.7405679135,-1.3740388866,-1.394394201 C,0,-3.0377578305,-1.7139739205,1.0502580132 C,0,-2.785327611,-0.6873617947,-0.0449323886 C,0,-3.4365019374,0.5916624992,0.1205145513 F,0,-2.3781205951,-2.8495426781,0.8180832438 F,0,-1.5367418424,-1.9398842724,-1.6114750538 F,0,-4.3430047113,-2.0190164602,1.1200301393 F,0,-2.6838927721,-1.2942192818,2.2730049225 F,0,-4.1211941891,1.1561092298,-0.8803485907 F,0,-4.1409618551,0.785887781,1.2459144975 F,0,-2.9624616888,-0.5462031352,-2.4227054697 F,0,-3.6503538985,-2.3499437509,-1.4894337208</p>	<p>C,0,-3.3445406475,-0.9875827929,2.0104301855 F,0,-2.8156200747,-0.3628690375,3.0587632726 F,0,-3.3048447483,-2.299463733,2.2463463317 F,0,-4.6298131196,-0.6277673388,1.9220091642 F,0,-2.4675252992,2.4139564265,-1.2867481003 F,0,-2.7365173489,0.4190597484,-2.0730780344 F,0,-4.2871972502,1.3315522304,-0.8872549333 F,0,-2.5768212389,1.6389180769,1.2082581318 F,0,-3.1743671953,-1.5034211877,-0.2335979454 C,0,1.53227801,-0.3845531945,0.2517803281 C,0,2.0575130594,-1.1852227162,-0.9393549493 C,0,2.3340236741,-0.7952942189,1.4777874622 C,0,3.5966403181,-1.2822961709,-2.17286633 F,0,1.5800835733,-0.675106277,-2.1105458597 F,0,1.6287239968,-2.4809491831,-0.8978954682 F,0,3.5653181619,-0.2372079487,1.4770643876 F,0,1.77729452,-0.425887002,2.6486579253 F,0,2.5069736327,-2.1219132064,1.5757559353 F,0,4.2363087272,-2.0399714262,-0.3420565268 F,0,3.7698003069,-1.8186708583,-2.4222513871 F,0,4.1456299656,-0.0655439145,-1.2237679167</p>
<p>(C₄F₈)₂Fe₂(CO)₇ (27-5S) M06-L/cc-pVTZ Fe,0,-0.4826826911,1.2147758032,-0.5378075342 C,0,-1.7435015797,2.0228879372,-1.5926179259 C,0,0.6745252445,2.3222091695,-1.4242416948 O,0,-0.8683217939,2.9115806753,1.840584875 O,0,-2.4554517467,2.6365965774,-2.2353374395 O,0,1.2412711988,3.016596581,-2.1281865611 Fe,0,-0.0142991497,-1.217948143,-0.4798632868 C,0,1.5578043792,-1.8946722239,-1.1071112676 C,0,-0.8959416323,-2.5133643363,-1.4287791021 C,0,0.0449539352,-0.060927979,-2.0778998555 O,0,-1.3654701555,-3.3769942905,-2.0022833518 O,0,2.4834705629,-2.3651370468,-1.5768418492 O,0,0.2936049466,-0.0155179351,-3.2060182229 C,0,-0.7595114837,2.2425659846,0.9254539335 C,0,-0.0158255308,-2.1790859731,1.0777759143 O,0,0.0490834183,-2.8015338858,2.0259603959 C,0,0.9369021833,0.2761741937,0.6179651622 F,0,0.8104476683,0.2072834489,1.977484282 C,0,-1.8251538765,-0.2715584286,-0.0485014337 C,0,-2.4214024242,-0.4550502102,1.3396054921 C,0,-2.9159515231,-0.5153202128,-1.0838150724 C,0,-3.72501149,0.3168265208,1.7318509441 F,0,-1.5336385546,-0.1013175491,2.2929061111 F,0,-2.7146650891,-1.7711573072,1.5710750042 F,0,-3.8643728855,0.4411218944,-1.0731215216 F,0,-2.4591898638,-0.5373272425,-2.3569526617 F,0,-3.5530191001,-1.6837725426,-0.9052750296 F,0,-4.8082937111,-0.2242334405,1.1941026498 F,0,-3.8667097971,0.2812782175,3.0529366932 F,0,-3.6421354991,1.5995360726,1.3607857747 C,0,3.3408790776,-0.5103815987,1.1927687822 C,0,2.8795580145,1.9586911279,1.0636604893 C,0,2.4345106023,0.5713768397,0.4818941887 F,0,2.4694530243,2.1456853741,2.3078577289 F,0,3.6262583126,-0.1556357987,2.4401053885 F,0,2.4021227031,2.9634993646,0.3279548018 F,0,4.2096095593,2.0461734619,1.028391729 F,0,2.7836600366,0.5962586838,-0.8427274388 F,0,4.4727265689,-0.6533115041,0.5172538074 F,0,2.7539127112,-1.7104906792,1.2582807512</p>	<p>(C₄F₈)₂Fe₂(CO)₇ (27-6S) M06-L/cc-pVTZ Fe,0,0.7539141277,-0.3788342097,0.3481176426 C,0,0.1829663591,2.3663749449,1.5697885193 C,0,0.8879792934,-2.1564718633,0.7223335837 O,0,1.4046332731,-0.0510419926,3.2408641947 O,0,0.7276125426,2.8020622468,2.4706487723 O,0,1.0809366711,-3.2625470798,0.9135618761 Fe,0,-0.7317619308,1.838925713,0.076182968 C,0,-1.5864943937,1.4677958694,-1.5137915332 C,0,0.2391414532,3.0656891822,-0.8955430108 C,0,0.0528120623,-0.7603394239,-1.2967457435 O,0,0.7857580326,3.8657914658,-1.4954437762 O,0,-2.1061936587,1.4215060403,-2.5258588863 O,0,-0.4064306589,-1.0565558371,-2.2967454081 C,0,1.2041536277,-0.0886550804,2.122653271 C,0,-2.1026213104,2.8876864984,0.5636380309 O,0,-2.9277187535,3.618868782,0.8601374455 C,0,-1.1896040541,0.0844648181,0.9881093176 F,0,-1.2761847625,0.1799612956,2.3765276044 C,0,3.8056737169,-0.5217310289,0.946069232 C,0,3.2502144807,-1.3567316943,-1.3415635034 C,0,2.8154300737,-0.4425549699,-0.2060019748 C,0,2.2023664041,0.8005398114,-0.5404893299 F,0,3.6766706809,-2.5303201615,-0.8623590698 F,0,3.6021090943,-1.6137902108,1.7017285378 F,0,4.2574824648,-0.8127475004,-2.0365888669 F,0,2.2812537137,-1.6224335279,-2.2221037224 F,0,2.5892661727,1.9340385435,0.0573251934 F,0,2.0322140795,1.06974263,-1.8470122427 F,0,3.7474298343,0.5310973609,1.7663086367 F,0,5.0615617219,-0.5914897892,0.4923166185 C,0,-3.7103398833,-0.2800381489,1.4420628336 C,0,-2.2778036384,-2.2782989604,0.8823479981 C,0,-2.4428492012,-0.7471008692,0.6516866416 F,0,-1.6237419322,-2.5312947977,2.0135031486 F,0,-3.7418050815,-0.8151484183,2.6586011163 F,0,-1.5967555191,-2.8145255529,-0.1345006254 F,0,-3.4519322794,-2.9014158469,0.9336884829 F,0,-2.7524453203,-0.6242689542,-0.6777156548 F,0,-4.8086713089,-0.6471321511,0.7889788695 F,0,-3.7546188332,1.0459838971,1.5710712628</p>

<p>(C₄F₈)₂Fe₂(CO)₇ (27-7S) M06-L/cc-pVTZ Fe,0,0.0060038087,-1.2294162794,0.5779352227 C,0,-1.3230567229,-2.1383871997,1.4442792547 C,0,1.2271611416,-2.127415967,1.6156925907 O,0,0.200818831,-2.9787243869,-1.7911935498 O,0,-2.1038224447,-2.7528749781,2.0034409339 O,0,1.8577451528,-2.7220262424,2.3554862852 Fe,0,-0.0060038087,1.2294162794,0.5779352227 C,0,1.3230567229,2.1383871997,1.4442792547 C,0,-1.2271611416,2.127415967,1.6156925907 C,0,0,0,2.1493306968 O,0,-1.8577451528,2.7220262424,2.3554862852 O,0,2.1038224447,2.7528749781,2.0034409339 O,0,0,0,3.3088922004 C,0,0.1142800084,-2.3120297413,-0.8733155093 C,0,-0.1142800084,2.3120297413,-0.8733155093 O,0,-0.200818831,2.9787243869,-1.7911935498 C,0,1.3103445505,0.01259829,-0.421699469 F,0,1.2338624539,0.0780388051,-1.7911271008 C,0,3.5451718403,1.2572010338,-0.7931519335 C,0,3.5561250036,-1.2625524613,-0.728998206 C,0,2.8175034437,0.0019972262,-0.1783403346 F,0,3.2729158334,-1.5070655846,-1.9993176409 F,0,3.9638274568,1.0096881528,-2.029876568 F,0,3.22343729,-2.3468396371,-0.0249853729 F,0,4.8743385057,-1.1037691169,-0.6052619782 F,0,3.0589491005,0.0066252368,1.1710948165 F,0,4.5897974148,1.581670275,-0.0428867794 F,0,2.7475572843,2.3286814318,-0.8590903266 C,0,-1.3103445505,-0.01259829,-0.421699469 F,0,-1.2338624539,-0.0780388051,-1.7911271008 C,0,-3.5451718403,-1.2572010338,-0.7931519335 C,0,-3.5561250036,1.2625524613,-0.728998206 C,0,-2.8175034437,-0.0019972262,-0.1783403346 F,0,-3.2729158334,-1.5070655846,-1.9993176409 F,0,-3.9638274568,-1.0096881528,-2.029876568 F,0,-3.22343729,2.3468396371,-0.0249853729 F,0,-4.8743385057,1.1037691169,-0.6052619782 F,0,-3.0589491005,-0.0066252368,1.1710948165 F,0,-4.5897974148,-1.581670275,-0.0428867794 F,0,-2.7475572843,-2.3286814318,-0.8590903266</p>	<p>(C₄F₈)₂Fe₂(CO)₇ (27-8S) M06-L/cc-pVTZ Fe,0,-0.0497373806,-1.0038975749,0.6651164024 C,0,-1.5387615796,-1.6379058972,1.5142693783 C,0,0.9614556815,-2.0161972913,1.8267927878 O,0,-0.1858442795,-2.8720250664,-1.6065369964 O,0,-2.4260829077,-2.1046261463,2.0567659584 O,0,1.4530125075,-2.646280901,2.6391247793 Fe,0,0.4423250127,1.4129298802,0.5573468999 C,0,1.9075538558,2.0802060072,1.4346236502 C,0,-0.6481280075,2.6779533888,1.3081155764 C,0,0.0676629806,0.3645247025,2.1783386744 O,0,-1.2598853132,3.506141234,1.795917888 O,0,2.7840332609,2.5440202204,1.9967849483 O,0,-0.045945429,0.4145287764,3.3298236516 C,0,-0.1338510492,-2.1620040657,-0.7181214028 C,0,0.631194295,2.3572110821,-0.986435212 O,0,0.7180187576,2.9416505545,-1.957460048 C,0,1.4866263673,-0.1183704094,-0.3460611107 F,0,1.4226402662,-0.0978211215,-1.7191166542 C,0,3.9347877486,0.5970838916,-0.7630645534 C,0,3.3993144687,-1.858218495,-0.5435251665 C,0,2.9579637808,-0.4291051554,-0.082225679 F,0,3.0115102222,-2.130628342,-1.7807259291 F,0,4.2359888112,0.2198753937,-2.0010403341 F,0,2.8806696357,-2.790652689,0.2583101603 F,0,4.7252790394,-1.9751244884,-0.4740945494 F,0,3.1959954325,-0.3835443006,1.2665950798 F,0,5.0537702622,0.6910952854,-0.056885761 F,0,3.4072735441,1.8238066744,-0.8418021031 C,0,-4.9927091116,0.0110137422,-0.0648588359 C,0,-3.6011068327,-0.0560206356,-0.748655888 C,0,-2.4974839516,0.8095558034,-0.0619560336 C,0,-1.0709054253,0.387557985,-0.3700388816 F,0,-3.7530706344,0.3473805516,-2.0134392473 F,0,-5.8906576925,-0.5693324912,-0.05835783117 F,0,-3.2219330642,-1.3529775512,-0.7575280356 F,0,-2.7040207694,2.0845585349,-0.4862035561 F,0,-2.7148844066,0.8044302543,1.2791855256 F,0,-1.0535166702,0.3181790931,-1.7371466666 F,0,-5.3499758096,1.2758463958,0.1325837491 F,0,-4.9826925961,-0.6255581694,1.1000814464</p>
<p>(C₄F₈)₂Fe₂(CO)₇ (27-9S) M06-L/cc-pVTZ Fe,0,0.9089796326,-1.2363955496,0. Fe,0,-1.2908523152,-0.0851625329,0. C,0,-0.8809322711,-2.1418245313,0. O,0,-1.4424091361,-3.1478098925,0. C,0,1.5439590088,-2.3974247893,1.2560483019 C,0,-2.6395459777,-0.3337527329,1.2075315056 C,0,1.5439590088,-2.3974247893,-1.2560483019 C,0,-2.6395459777,-0.3337527329,-1.2075315056 C,0,2.4434180314,-0.2256431064,0. C,0,-1.3782590593,1.7305580113,0. C,0,0.0805898916,-0.1092195354,1.5693895143 C,0,-0.3626112413,-0.935750845,-2.7839908644 C,0,0.0805898916,-0.1092195354,-1.5693895143 C,0,0.8609502625,1.0882893719,-2.1181103061 C,0,0.2427430167,1.9809670081,-3.2501836918 C,0,0.8609502625,1.0882893719,2.1181103061 C,0,-0.3626112413,-0.935750845,2.7839908644 C,0,0.2427430167,1.9809670081,3.2501836918 F,0,-0.8919687322,-2.1356561529,-2.4749544894 F,0,0.6460399652,-1.1927109551,-3.6298967475</p>	<p>(C₄F₈)₂Fe₂(CO)₇ (27-10S) M06-L/cc-pVTZ Fe,0,-0.8736832804,-0.3024444525,-0.1572482346 C,0,-0.2148761472,2.3418919086,-1.2810103566 C,0,-0.7806147445,-2.114539865,-0.3107918279 O,0,-1.1968257247,-0.1584168423,-3.1238739581 O,0,-0.7368429506,2.7752886956,-2.1969884888 O,0,-0.809419661,-3.2526157083,-0.3438599882 Fe,0,0.7168600017,1.8114178991,0.2033367931 C,0,1.7052347299,1.367335495,1.6893049308 C,0,-0.2702883799,2.9832693536,1.2286085979 C,0,-0.4237381463,-0.4000496879,1.6133303244 O,0,-0.8569858191,3.7242849368,1.8655373462 O,0,2.3708416605,1.2190074088,2.6008077137 O,0,-0.1746100706,-0.5093635693,2.7217056662 C,0,-1.1277195007,-0.145260224,-1.9898149937 C,0,2.0973406254,2.7998297711,-0.3742486969 O,0,2.954341248,3.4450832736,-0.7643173503 C,0,4.6623376057,-1.4932901661,0.2609506425 C,0,3.6442070813,-0.6086082806,-0.5115559155 C,0,2.1489768437,-0.9691204142,-0.2576555603 C,0,1.1151575865,0.0682595686,-0.6837971504</p>

<p>F,0,-1.3143978932,-0.3106789545,-3.5026547777 F,0,0.2914835676,1.404508494,-4.4411819665 F,0,0.934747319,3.1130049094,-3.3218276605 F,0,-1.0251325791,2.2903439726,-2.9574814331 F,0,2.0662448561,0.6730858087,-2.613832881 F,0,1.1454203501,1.9715762131,-1.1474560495 F,0,1.1454203501,1.9715762131,1.1474560495 F,0,2.0662448561,0.6730858087,2.613832881 F,0,-1.3143978932,-0.3106789545,3.5026547777 F,0,-0.8919687322,-2.1356561529,2.4749544894 F,0,0.6460399652,-1.1927109551,3.6298967475 F,0,0.2914835676,1.404508494,4.4411819665 F,0,0.934747319,3.1130049094,3.3218276605 F,0,-1.0251325791,2.2903439726,2.9574814331 O,0,2.0012667015,-3.1660942633,-1.9597738028 O,0,2.0012667015,-3.1660942633,1.9597738028 O,0,3.4479240131,0.3052050928,0. O,0,-3.5805210131,-0.4678496073,1.8346130889 O,0,-1.5046062155,2.8613931278,0. O,0,-3.5805210131,-0.4678496073,-1.8346130889</p>	<p>F,0,1.35735534,0.1777057417,-2.0452537322 F,0,1.9335590729,-2.1256414129,-0.9336476833 F,0,2.0226546751,-1.2519668939,1.0633083012 F,0,3.9122006626,-0.7150191108,-1.8157535525 F,0,3.8810861996,0.6664783787,-0.129252099 F,0,4.3841694061,-2.7820387827,0.1071031251 F,0,5.8807548834,-1.2583547611,-0.2153901758 F,0,4.6536556834,-1.1974824246,1.5558660046 C,0,-3.8097955995,-0.6343358944,-1.139163784 C,0,-3.5176738063,-1.3294288601,1.2393235997 C,0,-2.9839589895,-0.442685688,0.1232066155 C,0,-2.482522709,0.8474021867,0.467565561 F,0,-3.8122887426,-2.5459421894,0.7673066712 F,0,-3.4486183327,-1.7420107526,-1.8076519445 F,0,-4.6358288248,-0.8172836008,1.7688842127 F,0,-2.6615930219,-1.5003824385,2.2498364206 F,0,-2.7959309654,1.9366839728,-0.2375328381 F,0,-2.5104070315,1.1900286526,1.7663866148 F,0,-3.7073615151,0.3879271599,-1.9931459705 F,0,-5.1077933424,-0.7642463833,-0.8448748398</p>
<p>(C₄F₈)₂Fe₂(CO)₇ (27-11S) M06-L/cc-pVTZ C,0,5.1987805249,0.019915938,-0.2029994367 C,0,3.8157985251,0.0894225555,-0.9040158978 C,0,2.6859981242,-0.7158488693,-0.1890836704 C,0,1.2706761497,-0.28559489,-0.5343473979 Fe,0,-0.2814866513,-1.2068667392,0.4033647794 C,0,-1.7621625246,-1.8496610492,1.2710183782 C,0,0.7782065298,-2.4249655933,1.2791927109 O,0,-0.6132191984,-2.8377426025,-2.0315469795 O,0,-2.6446119429,-2.3148275571,1.8223125466 O,0,1.3644065076,-3.2252665255,1.8396302901 C,0,-5.1987805249,-0.019915938,-0.2029994367 C,0,-3.8157985251,-0.0894225555,-0.9040158978 C,0,-2.6859981242,-0.7158488693,-0.1890836704 C,0,-1.2706761497,0.28559489,-0.5343473979 Fe,0,0.2814866513,1.2068667392,0.4033647794 C,0,1.7621625246,1.8496610492,1.2710183782 C,0,-0.7782065298,2.4249655933,1.2791927109 C,0,0,0,1.9858710118 O,0,-1.3644065076,3.2252665255,1.8396302901 O,0,2.6446119429,2.3148275571,1.8223125466 O,0,0,0,3.1430262973 F,0,3.9676168753,-0.3736590982,-2.1479494821 F,0,6.1196024705,0.5341064842,-1.0108566808 F,0,3.4704178085,1.3944577606,-0.9737191643 F,0,2.8705930322,-2.0156929603,-0.5407285405 F,0,2.887290029,-0.6402730949,1.1524544693 F,0,1.2619455917,-0.2791791735,-1.905055211 F,0,5.5196854788,-1.2416288541,0.0643129218 F,0,5.193961638,0.7171902843,0.9268961579 F,0,-1.2619455917,0.2791791735,-1.905055211 F,0,-2.8705930322,2.0156929603,-0.5407285405 F,0,-2.887290029,0.6402730949,1.1524544693 F,0,-3.9676168753,0.3736590982,-2.1479494821 F,0,-3.4704178085,-1.3944577606,-0.9737191643 F,0,-5.5196854788,1.2416288541,0.0643129218 F,0,-6.1196024705,-0.5341064842,-1.0108566808 F,0,-5.193961638,-0.7171902843,0.9268961579 C,0,-0.4870901159,-2.2205895677,-1.0846144581 C,0,0.4870901159,2.2205895677,-1.0846144581 O,0,0.6132191984,2.8377426025,-2.0315469795</p>	<p>(C₄F₈)₂Fe₂(CO)₇ (27-12S) M06-L/cc-pVTZ Fe,0,0.7295649857,0.5037881797,-0.0732201125 C,0,-0.0806206761,-2.0068687968,-1.493255145 C,0,0.488754972,2.2707031334,0.2253805962 O,0,0.7975196694,0.9433988862,-3.0284109547 O,0,0.2457306747,-2.262328157,-2.5540111493 O,0,0.422922624,3.3738899228,0.5070218187 Fe,0,-0.7408325256,-1.7190104564,0.1931612526 C,0,-1.3892566029,-1.5176587664,1.9050787178 C,0,0.4151538142,-2.9746791073,0.9020150286 C,0,0.5729435986,0.2941953315,1.7332488599 O,0,1.0831479492,-3.7697145792,1.3699393956 O,0,-1.7828276225,-1.5455651714,2.9725296767 O,0,0.5127752078,0.2783888514,2.873106659 C,0,0.795553399,0.7142257441,-1.9167605988 C,0,-2.1968766239,-2.6732797063,-0.2290353684 O,0,-3.1167827932,-3.2886754793,-0.5098544306 C,0,-1.3250892405,0.0662609244,-0.468196044 F,0,-1.6501835231,0.0630672866,-1.8241243229 C,0,3.1132471974,-1.43296514,-1.0440147498 C,0,2.524787986,-0.5266286844,0.0187814246 C,0,2.7557872815,0.8804392585,-0.0290373995 C,0,3.4813407914,1.6289561764,1.071988998 F,0,4.4448097922,-1.4671137466,-0.9262675643 F,0,2.6726839505,-2.6895719545,-0.8913077411 F,0,2.82378471,-1.0455569671,-2.2841837598 F,0,3.2320613921,1.3681121583,-1.2112297203 F,0,3.4190496248,2.9437351478,0.8575292657 F,0,4.7731464422,1.2792459282,1.0752164025 F,0,2.9892409118,1.3842347524,2.284646008 F,0,2.7705720783,-1.1233714557,1.2273298259 C,0,-3.8041547637,0.2661865116,0.269156177 C,0,-2.6477744327,2.2672969347,-0.7329249852 C,0,-2.4153654311,0.9610645033,0.1181332138 F,0,-3.5926176118,2.0759828899,-1.6492904899 F,0,-4.1454897835,-0.3885055761,-0.8347034102 F,0,-1.5519965845,2.6675585799,-1.3822442656 F,0,-3.023125028,3.2553734795,0.0698548813 F,0,-2.0604544217,1.338953072,1.3876558007 F,0,-4.7520115174,1.1570632662,0.5525353469 F,0,-3.7833689603,-0.6121218643,1.2756944056</p>

<p>(C₄F₈)₂Fe₂(CO)₇ (27-13S) M06-L/cc-pVTZ C,0,2.9129858658,0.8682366945,-0.1857890593 C,0,3.4764211997,-0.3981378177,0.2100431856 C,0,3.0207498688,1.5184313018,-1.5577911811 C,0,4.2771064806,-1.3462814445,-0.6589526516 F,0,3.920637384,-1.2909429364,-1.943491884 F,0,4.1209075065,-2.6110870274,-0.2460448306 F,0,5.5760082701,-1.0574862281,-0.584336658 F,0,2.4983616221,0.7870824136,-2.5468276909 F,0,2.380968426,2.6857833427,-1.5502854782 F,0,4.302177817,1.7562136475,-1.8674221623 F,0,3.1299916239,1.8565607824,0.7240295675 F,0,4.1038466944,-0.3777326133,1.4206293757 Fe,0,1.4756260888,-0.4901536115,0.3296525614 C,0,0.191399796,1.1826645627,0.2918651651 C,0,1.2756897491,-1.194593676,-1.3558191699 C,0,1.2516641094,-2.2015318757,0.9409456261 O,0,0.3638015426,2.3077763751,0.5108720593 O,0,1.1209672566,-1.7466989202,-2.3425049105 O,0,1.1615592316,-3.2719836457,1.3282077959 Fe,0,-1.2623706314,-0.0950433511,-0.0859719161 C,0,-0.9549878489,0.4885861256,-1.8206589611 C,0,-1.2367068988,-0.6218719049,1.6767690262 C,0,-1.4808279075,-1.8701782669,-0.6136684241 O,0,-0.6336459502,0.8700077613,-2.8410996956 O,0,-1.156119143,-0.9871951757,2.75351021 O,0,-1.6661693544,-2.9442042196,-0.9415453102 C,0,1.6262431473,0.0704141739,2.0869068859 O,0,1.71005397,0.3847420548,3.1746640218 C,0,-4.0865085789,0.2884963625,-1.3312230444 C,0,-4.0721554332,-0.3613965503,1.0766207893 C,0,-3.2932038294,0.3335100993,-0.0340261138 C,0,-2.4891664167,1.4882794779,0.2416715728 F,0,-3.8782908185,-1.6932521615,1.0549020493 F,0,-4.5682995512,-0.9437364975,-1.5357701154 F,0,-5.3855432127,-0.1608760561,0.9473996528 F,0,-3.7323845466,0.0581682314,2.2968393262 F,0,-2.4562478594,2.4666698985,-0.6688888103 F,0,-2.4534838685,2.0499692265,1.4449470977 F,0,-3.3757326851,0.6136828572,-2.4169390626 F,0,-5.1215886307,1.1334387411,-1.2936653988</p>	<p>(C₄F₈)₂Fe₂(CO)₇ (27-14S) M06-L/cc-pVTZ Fe,0,-0.7973603699,-0.6550948303,0.0210295225 C,0,-0.4884330508,1.8587389894,-1.5163780985 C,0,-0.3427433203,-2.4031233807,0.1566379201 O,0,-1.4020614367,-1.0824921985,-2.8746535714 O,0,-1.0363219752,2.0677608939,-2.4936459509 O,0,-0.1392866623,-3.5152729898,0.299774883 Fe,0,0.5276951822,1.6716072171,-0.005141859 C,0,1.6292541747,1.5558997266,1.4632272718 C,0,-0.5702608588,2.7998420442,0.9639622282 C,0,-0.3229249624,-0.3704003855,1.7656463284 O,0,-1.204128313,3.5068091365,1.5928933319 O,0,2.3430343156,1.6151768084,2.3480507335 O,0,-0.0614238981,-0.2711894126,2.8724069625 C,0,-1.2030940819,-0.8600271253,-1.7793566976 C,0,1.7223805767,2.7726297143,-0.7597237243 O,0,2.4633825764,3.4807272846,-1.2627791915 C,0,4.8798720392,-1.0380795406,0.230713242 C,0,3.7141478839,-0.3803900345,-0.559632537 C,0,2.2962498407,-0.9186026098,-0.199784294 C,0,1.1078985909,-0.0991454284,-0.6922523871 F,0,1.2365152653,-0.1795384753,-2.068902035 F,0,2.2409047101,-2.1649027239,-0.7315236101 F,0,2.2432115753,-1.0566443218,1.150224469 F,0,3.9368491437,-0.5712055029,-1.8632871329 F,0,3.7867051506,0.9452552896,-0.3053245355 F,0,4.7940727361,-2.361784443,0.1965471936 F,0,6.0308851296,-0.6692890768,-0.3224820705 F,0,4.8729101236,-0.6338076958,1.495979918 C,0,-3.4939722514,1.0336797897,-0.4441450979 C,0,-2.6327798385,0.190299873,0.4743119712 C,0,-2.726909757,-1.2328507062,0.4550643355 C,0,-3.1365407834,-2.0421709552,1.6695702182 F,0,-4.7736108198,0.9560962785,-0.0645582228 F,0,-3.1380094787,2.3237413977,-0.3721141001 F,0,-3.4244274406,0.6611350373,-1.7203052604 F,0,-3.3744734421,-1.7763007247,-0.6161360805 F,0,-2.9777709419,-3.345190855,1.4334555882 F,0,-4.4319660901,-1.8321504922,1.9321565389 F,0,-2.4429424077,-1.7331405949,2.7631849029 F,0,-2.6976472056,0.7702314628,1.7135431076</p>
<p>(C₄F₈)₂Fe₂(CO)₇ (27-15S) M06-L/cc-pVTZ Fe,0,-0.6445594838,-0.0704523516,-0.2932122643 C,0,1.3165911064,1.5070470515,-1.5747145891 C,0,-1.2011852235,-1.7362642459,0.2085352792 O,0,-0.4175368575,-1.0068550385,-3.124554567 O,0,1.2674737218,1.7880072461,-2.6797454349 O,0,-1.5762349755,-2.7782325925,0.4689696113 Fe,0,1.5541846792,1.3264212705,0.2344788153 C,0,1.7558471278,1.3514196642,2.0714723675 C,0,1.024805037,3.0702265346,0.3875793074 C,0,-0.8823370798,0.731796101,1.3379193119 O,0,0.7147103168,4.1597208481,0.516480252 O,0,1.9703646116,1.5089674007,3.1772884249 O,0,-1.1500525917,1.2199071957,2.3360425265 C,0,-0.4308414373,-0.6495217703,-2.0470540524 C,0,3.3304412072,1.5235922507,0.0378576667 O,0,4.4461939834,1.7099244006,-0.1073420883 C,0,1.3291048132,-0.7017955004,0.2050205558 C,0,2.0266593359,-1.5317465219,-0.8687666451 C,0,1.4580968876,-1.4262825756,1.5338216122 C,0,3.4623200472,-2.107952643,-0.6255641273</p>	<p>(C₄F₈)₂Fe₂(CO)₇ (27-16S) M06-L/cc-pVTZ C,0,-2.8580604414,0.8279221562,0.5328833606 C,0,-3.3285016032,-0.1041595077,-0.4453781515 C,0,-3.0550142352,2.321813734,0.3328321843 C,0,-4.3239991695,-1.2041310308,-0.1417400739 F,0,-4.0239228748,-1.8849930367,0.9658534241 F,0,-4.3753325143,-2.07294834,-1.1551411447 F,0,-5.5442829032,-0.685577427,0.0140916253 F,0,-2.5748782462,3.0035851245,1.3642917409 F,0,-2.4723433124,2.7736447978,-0.7812585193 F,0,-4.3649839704,2.5946919152,0.2414686417 F,0,-3.1818320934,0.5489282219,1.8303923131 F,0,-3.6901973011,0.4351264476,-1.6477511311 Fe,0,-1.3433651123,-0.3179976871,-0.2323352908 C,0,-0.0024019732,0.948821562,0.579352784 C,0,-1.4303836653,-1.342297792,1.2932608492 C,0,-1.2490591943,-1.852373626,-1.2491964642 O,0,0.0230997186,2.0229152302,1.0120383631 O,0,-1.4436200893,-1.9869874049,2.231819971 O,0,-1.2503917327,-2.806992458,-1.8727134572 C,0,3.3738258119,-0.3630238641,0.5592644495</p>

<p>F,0,2.1866472989,-0.8007359883,-2.0098839 F,0,1.2766035842,-2.6163526502,-1.2275382896 F,0,2.6973169246,-1.2967999264,2.059509712 F,0,0.6168067104,-0.9732254854,2.4855760044 F,0,1.2113544143,-2.7420917712,1.4429970331 F,0,3.4793564945,-3.0981410351,0.2515856215 F,0,3.9264549619,-2.5781531294,-1.7802680966 F,0,4.2882440213,-1.145584484,-0.2097029811 C,0,-4.2710094812,-0.6053197196,0.8646884291 C,0,-3.7825919505,0.6449765916,0.0945976378 C,0,-2.5943228234,0.4413823515,-0.8317355779 C,0,-1.6820329767,1.4959429755,-1.1498514143 F,0,-3.5357928688,1.5939302762,1.0137761259 F,0,-5.442581418,-0.358679734,1.4317763094 F,0,-4.8195538581,1.0641477005,-0.6654792174 F,0,-1.4850846044,1.7691300774,-2.4412070792 F,0,-3.0231823415,-0.2700092816,-1.9116313311 F,0,-1.7147154931,2.650888781,-0.4752511394 F,0,-3.3959321024,-0.9135603337,1.8269192017 F,0,-4.3948027182,-1.6491759389,0.0523419294</p>	<p>C,0,2.7621254383,0.9392709347,0.5433309544 C,0,4.3278810574,-0.9044181575,-0.4845896969 C,0,2.9861428658,2.0180336039,-0.5151170768 F,0,2.4456065096,3.1611339789,-0.1132216922 F,0,2.4487637279,1.7187140538,-1.7049211891 F,0,4.2950009954,2.230780764,-0.708903393 F,0,4.2312000647,-2.237218829,-0.5747157943 F,0,4.0892258647,-0.3961441643,-1.6968156872 F,0,5.5859533306,-0.6136259656,-0.1597889292 F,0,3.8613508526,-0.7492023801,1.7709471596 F,0,2.7864816238,1.557981339,1.7539096505 Fe,0,1.3863510098,-0.5666011063,0.3769002284 C,0,1.2710758279,-0.5707884556,2.225939807 C,0,1.4291618209,-0.6811636978,-1.4582335008 C,0,1.2915271382,-2.4007487059,0.3990649759 O,0,1.1907673715,-0.5984264469,3.3577788826 O,0,1.4228661256,-0.8672393812,-2.5834271904 O,0,1.2848725808,-3.5414801851,0.4327444863 C,0,-1.0878771887,0.7201511806,-1.7492587784 O,0,-0.8733440954,1.3040956054,-2.6989221849</p>
<p>(C₄F₈)₂Fe₂(CO)₇ (27-17S) M06-L/cc-pVTZ Fe,0,-0.1499542556,-0.6646860963,0.1396944534 C,0,0.4565976183,0.6370115749,-1.9517415914 C,0,-0.1147446477,-1.800407231,1.5338592171 O,0,0.4529096525,-2.8470318623,-1.8209698367 O,0,0.1175502871,0.3100055686,-2.9982730396 O,0,-0.1639215417,-2.507779712,2.4268146787 Fe,0,1.0479341439,1.5572738328,-0.4737656656 C,0,1.427908428,2.5553024305,1.0343269777 C,0,-0.2246563926,2.8009997115,-0.8671734196 C,0,-0.7176293576,0.6921714265,1.2216704349 O,0,-1.0228024932,3.5870205098,-1.0874899506 O,0,1.6598904672,3.2891412188,1.8723878841 O,0,-1.1860073907,1.431792053,1.961357006 C,0,0.3152174402,-1.97325195,-1.1083413661 C,0,2.4403938881,2.2239851868,-1.3973285114 O,0,3.2689621744,2.6752155371,-2.0386362381 C,0,1.8815396045,-0.1240476157,0.3739467084 C,0,2.8730113232,-0.9360855458,-0.4395491313 C,0,2.3579550466,-0.0259249493,1.8062837662 C,0,4.4042609948,-0.6307202152,-0.3575455547 F,0,2.5949469616,-0.8260406962,-1.7742053006 F,0,2.7872032595,-2.2715975513,-0.1544308921 F,0,3.4134603565,0.8063902623,1.953141518 F,0,1.4168117938,0.44551502,2.6535922767 F,0,2.7309067707,-1.2137056972,2.3118233125 F,0,4.931891834,-1.0310949513,0.7896594798 F,0,5.0230702859,-1.2803689746,-1.3405423924 F,0,4.6423285905,0.673029409,-0.5119981774 C,0,-4.0266422705,-2.1007462345,0.0357683811 C,0,-4.0178307803,0.4452932771,-0.377258186 C,0,-1.8579043401,-0.8877512671,-0.5120654748 C,0,-3.2236187768,-0.7730338446,0.1598507087 F,0,-4.1579513416,0.3904014129,-1.6964312638 F,0,-4.5652804062,-2.2480255127,-1.1675697684 F,0,-3.3515206907,1.5609268923,-0.0731602392 F,0,-5.2203860425,0.5119147001,0.1792459505 F,0,-2.1055520529,-1.3616330057,-1.736640712 F,0,-3.0589597899,-0.5698017156,1.4978529619 F,0,-4.9928490044,-2.1364759603,0.941008804 F,0,-3.2038098364,-3.1295672253,0.2653192124</p>	<p>(C₄F₈)₂Fe₂(CO)₇ (27-18S) M06-L/cc-pVTZ Fe,0,-1.4051440953,0.0000470924,0.2125875221 C,0,-0.0788488961,1.28089051,-0.8422624533 C,0,-1.0863106601,0.501327426,1.9562319296 C,0,-1.1813052174,-1.6979563945,0.8004982506 O,0,-0.265485781,2.0554381705,-1.6809466413 O,0,-0.8554317036,0.676677228,3.059514985 O,0,-1.0919743566,-2.774646552,1.1764097444 Fe,0,1.3995821578,0.4247124534,0.1513966586 C,0,1.3710688148,1.929106829,1.2375483542 C,0,1.3423105363,-1.0489685909,-0.9445986026 C,0,1.5579230213,-0.6688424776,1.6462476009 O,0,1.33786812,2.8438157465,1.9078302191 O,0,1.26576532,-1.9809046944,-1.5943446686 O,0,1.6908557795,-1.316185013,2.5745017406 C,0,-1.6109237198,-0.766473417,-1.4523611453 O,0,-1.6826275053,-1.355662327,-2.4225253228 C,0,4.6769223189,-1.383864207,0.4647098833 C,0,4.3797343181,-0.2989648388,-0.601989729 C,0,3.3712183167,0.7596259706,-0.1974748882 C,0,2.5509431911,1.4553962928,-1.1492930015 F,0,3.9842287591,-0.9504815462,-1.7132443295 F,0,5.7720377132,-2.0536148669,0.1434309971 F,0,5.5488549173,0.3179609946,-0.8749718864 F,0,2.5233177521,2.7861148965,-1.0873117646 F,0,3.9501166277,1.563487762,0.7398910169 F,0,2.5173880616,1.0846591751,-2.4289389244 F,0,3.6576777442,-2.2509227426,0.5203810688 F,0,4.8336614308,-0.8461367476,1.6695122098 C,0,-2.8404242917,2.6369395462,0.9494574148 C,0,-3.3578469133,1.9359596349,-1.3833314291 C,0,-2.8953544541,1.4653852087,-0.0127409492 C,0,-3.3649554282,0.1725952441,0.4247123675 F,0,-2.8168898377,3.1127314139,-1.7009579572 F,0,-1.6700987754,3.2991162932,0.8503602684 F,0,-4.6913291113,2.0882063104,-1.4080508084 F,0,-3.0591952974,1.0840757408,-2.3739051368 F,0,-3.8665955097,-0.013982969,1.6485642993 F,0,-4.1262763604,-0.5293276978,-0.4303779785 F,0,-2.9661904226,2.2767791996,2.2314694046 F,0,-3.8099009235,3.5257241829,0.7085352613</p>

<p>(C₄F₈)₂Fe₂(CO)₇ (27-19S) M06-L/cc-pVTZ Fe,0,-0.6973259799,-1.4580921426,0.1873341926 C,0,-1.9758897685,-2.6916391249,0.6361831746 C,0,0.4688062717,-2.5718607693,1.0963731187 O,0,-0.2892759178,-2.6842608274,-2.4675328793 O,0,-2.6703622936,-3.5387137494,0.9436004007 O,0,1.0612159555,-3.3762224004,1.6438558093 Fe,0,-0.1422299562,0.9409165144,1.0336377602 C,0,1.2384840832,0.7244124597,2.2390768373 C,0,-1.0360622841,1.9802496009,2.2606566846 C,0,-1.1997004981,-0.5964923582,1.9202620442 O,0,-1.5467272423,2.6497171077,3.0234740833 O,0,2.0499349253,0.7086411653,3.0388736856 O,0,-1.7383704155,-0.8039683431,2.922375844 C,0,-0.4224674511,-2.213649396,-1.4427199185 C,0,0.6005440284,2.417445909,0.2936452636 O,0,1.0650184123,3.3739261823,-0.1090860035 C,0,4.7759924816,-0.1315008554,-0.4136193472 C,0,3.3371613689,0.319792596,-0.7984117826 C,0,2.2150241618,-0.6651031929,-0.3620526642 C,0,0.7727270839,-0.1387304024,-0.4064203649 F,0,0.6660720192,0.3613410676,-1.6706992709 F,0,2.3197250515,-1.7454161924,-1.1808592943 F,0,2.5427708931,-1.0875847623,0.8847858887 F,0,3.3024689852,0.4929573109,-2.1210084271 F,0,3.1392511274,1.5115176773,-0.1949908753 F,0,4.9926630622,-1.3912654095,-0.7724712131 F,0,5.6474138452,0.6491107641,-1.0423828941 F,0,4.9726824587,-0.0121895825,0.89461095 C,0,-3.4996721341,-0.7626923264,-0.8404824882 C,0,-2.0660784845,-0.2087979248,-0.8321321433 C,0,-1.8924493181,1.1261848073,-0.1387796402 C,0,-2.000222855,2.3747669509,-1.0185496378 F,0,-4.360846257,0.0567033374,-1.4354899243 F,0,-3.5139888484,-1.918676934,-1.5320874556 F,0,-3.9732769916,-1.0291025873,0.3828153621 F,0,-2.9535557924,1.2641188795,0.761305707 F,0,-1.9409251321,3.46816185,-0.2313340675 F,0,-3.1551894993,2.4373790476,-1.6786029258 F,0,-1.0148225637,2.4684385038,-1.9088883298 F,0,-1.7706271015,-0.0771184506,-2.1754772585</p>	<p>(C₄F₈)₂Fe₂(CO)₇ (27-20S) M06-L/cc-pVTZ Fe,0,-0.6064371183,-0.972955764,0.7087870157 C,0,-1.8347465882,-1.2964659277,2.0691474838 C,0,0.5248822309,-1.5718784164,2.0074524605 O,0,-0.8228698426,-3.5893754605,-0.5853372257 O,0,-2.3776006271,-1.5738763577,3.0312571337 O,0,1.0699558297,-1.9974473348,2.9147224544 Fe,0,0.0401456192,1.5930019089,0.4563167613 C,0,1.7206593329,2.0760712143,1.0443940952 C,0,-0.6964813644,3.1744980807,0.9686285025 C,0,-0.346138379,0.9696703247,2.1547738532 O,0,-1.1539073645,4.1656876303,1.2861259721 O,0,2.704445847,2.4758764979,1.4547219838 O,0,-0.4999984608,0.9632695899,3.2929599916 C,0,-0.7510453961,-2.5592841092,-0.1032148591 C,0,0.3141366146,2.2556921304,-1.2510346885 O,0,0.5018710913,2.7684428529,-2.2443341609 C,0,0.8608536095,-0.3098976642,-0.4106117976 F,0,0.7848236914,-0.3328992721,-1.7725096508 C,0,-1.9744558358,-0.3144900577,-2.1587024937 C,0,-3.5942093716,-0.7653761766,-0.3709025092 C,0,-2.1813374329,-0.2101910333,-0.6329734079 C,0,-1.9921283887,1.1785251478,-0.1068246859 F,0,-3.7303665539,-1.9568314835,-0.976507703 F,0,-1.4108494619,-1.4759757867,-2.5180809519 F,0,-4.552250311,0.0488415307,-0.832724385 F,0,-3.9058065941,-0.9679006979,0.9161343091 F,0,-2.4455194779,2.1630026553,-0.9440917512 F,0,-2.7422922441,1.3365637201,1.0342379463 F,0,-1.221113434,0.6760694379,-2.654332318 F,0,-3.1273113777,-0.2422468394,-2.8413273049 C,0,3.329497356,0.1663886752,-1.102524064 C,0,2.6411637384,-2.1775321535,-0.4839470078 C,0,2.3453217945,-0.6632869606,-0.2024491213 F,0,2.0856191974,-2.5898584471,-1.6133109705 F,0,3.4819074755,-0.3949686975,-2.2952029113 F,0,2.1715353555,-2.9374810488,0.5079225355 F,0,3.9545172727,-2.3895293187,-0.5475529254 F,0,2.7191802941,-0.4509684991,1.097841425 F,0,4.5136940551,0.2517271093,-0.5107935471 F,0,2.897740029,1.4177115509,-1.3054091727</p>
<p>(C₄F₈)₂Fe₂(CO)₇ (27-21S) M06-L/cc-pVTZ Fe,0,0.980390127,-0.4301863862,0.3154907783 C,0,-0.040328498,2.1059689909,1.8129475072 C,0,0.7854174283,-2.2308722724,0.5184948859 O,0,1.4460840198,-0.3165090452,3.2630156848 O,0,0.2966527627,2.4447132121,2.8466730159 O,0,0.7218979202,-3.3582300959,0.670876789 Fe,0,-0.6432773179,1.7016229368,0.1344475565 C,0,-1.2010756102,1.4058739,-1.5937564593 C,0,0.3716730079,3.100027786,-0.5025413075 C,0,0.7596063127,-0.5394159874,-1.4953813249 O,0,0.9667951236,3.9959085953,-0.8798433946 O,0,-1.5716789798,1.3591007033,-2.6689767878 O,0,0.6675728387,-0.6561748934,-2.6255718246 C,0,1.2588994321,-0.3088195315,2.1430283525 C,0,-2.2118386272,2.4807838727,0.5186657213 O,0,-3.1967395033,2.9957723059,0.7802963004 C,0,-4.6226930782,-1.6789909496,-0.0987444979 C,0,-3.5572307648,-0.5775649252,0.1521324576 C,0,-2.0789287189,-1.0670978302,0.0896382092 C,0,-1.0437569816,-0.1544094091,0.7371706566</p>	<p>(C₄F₈)₂Fe₂(CO)₇ (27-22S) M06-L/cc-pVTZ Fe,0,0.6598323994,-0.148137619,0.351453751 C,0,-0.8464901096,1.9827840624,1.9120036342 C,0,0.8114529875,-1.9273517939,0.0087124765 O,0,0.4551775576,-0.7673013198,3.2646760859 O,0,-0.7163615245,2.1524485148,3.0302652175 O,0,0.9855214624,-3.0284968152,-0.2287026925 Fe,0,-1.1432943808,1.8212778788,0.1110516405 C,0,-1.357080807,1.7459481259,-1.7155764303 C,0,-0.249528654,3.4123123159,-0.1446707862 C,0,0.7964073433,0.1429138753,-1.4424388338 O,0,0.239228715,4.4306812117,-0.2968429454 O,0,-1.5130354579,1.8370947966,-2.8394263654 O,0,0.9370287512,0.229843327,-2.571830106 C,0,0.5271377581,-0.4847696752,2.1673514111 C,0,-2.8265589137,2.4043029664,0.3101052307 O,0,-3.8880566752,2.7998679214,0.4523139605 C,0,4.0521112543,-1.5863023528,-0.8881415317 C,0,3.8039527212,-0.1342621685,-0.4086198662 C,0,2.7108314787,0.0579123626,0.6261591062 C,0,2.0317460232,1.3102183437,0.7667832312</p>

<p>F,0,-1.3118997859,-0.2868893536,2.0906906381 F,0,-2.0458736661,-2.2881317844,0.6821733394 F,0,-1.7952449564,-1.2511221727,-1.2222488589 F,0,-3.8232557434,-0.0250076272,1.3443804454 F,0,-3.7307797499,0.3670929288,-0.7975665251 F,0,-4.7129768255,-2.4961368008,0.9405617762 F,0,-5.8048254116,-1.0974136551,-0.2816829208 F,0,-4.3213600309,-2.3826899803,-1.1848992594 C,0,3.7479301653,-2.6681494883,-1.0813209417 C,0,3.8407118205,-1.1245619014,-0.9911217359 C,0,3.0515283075,-0.4805821412,0.1317802701 C,0,2.5378278056,0.8540496996,0.0455476424 F,0,3.4666278167,-0.6494588479,-2.1937706912 F,0,4.6899572361,-3.1352244572,-1.8879647082 F,0,5.1464611223,-0.8198624239,-0.8125224816 F,0,2.8331019379,1.7002806243,1.0453337377 F,0,3.6761425925,-0.7743247912,1.3098343039 F,0,2.6316205422,1.5241496044,-1.1123180477 F,0,2.558483101,-3.018388983,-1.5817801946 F,0,3.8851659088,-3.2313549558,0.1143380734</p>	<p>F,0,3.5663621863,0.5923054502,-1.5168397274 F,0,5.214644345,-1.6625032816,-1.5204590799 F,0,4.9632604723,0.304017413,0.1346466985 F,0,2.0060124624,1.8687741762,1.9857992076 F,0,3.1326208129,-0.4955031445,1.8002226103 F,0,2.2551285728,2.2792530282,-0.1324153324 F,0,3.0884957627,-1.9438155884,-1.7415641239 F,0,4.0578840991,-2.4414751858,0.1284703799 C,0,-3.7045492173,-0.6015963414,-0.8015705624 C,0,-2.4300151808,-2.5122694956,0.2286789208 C,0,-1.4661200146,-0.1261743772,0.429022943 C,0,-2.2708664978,-1.0924784399,-0.4392849795 F,0,-3.5561703142,-2.5837422761,0.9340650478 F,0,-4.3549978783,-0.1633601335,0.2706836369 F,0,-1.4318457944,-2.8133517574,1.0601957338 F,0,-2.4604618269,-3.4421881243,-0.7187151662 F,0,-1.992361541,-0.3656230392,1.6999549771 F,0,-1.6372275922,-1.2584022638,-1.6444288913 F,0,-4.4125416168,-1.5779155666,-1.365572076 F,0,-3.6503551686,0.3990979899,-1.6862354041</p>
<p>(C₄F₈)₂Fe₂(CO)₇ (27-23S) M06-L/cc-pVTZ Fe,0,-0.768742516,-1.0060354103,0.755469306 C,0,-2.0026059786,-1.2964812111,2.1225594279 C,0,0.3471836699,-1.8216515677,1.9346228266 O,0,-1.0446261974,-3.551694022,-0.663070207 O,0,-2.552446728,-1.5525808544,3.0862524999 O,0,0.9151519476,-2.4420240978,2.705507484 Fe,0,0.0401077774,1.5106108848,0.4779851821 C,0,1.7312971296,1.9867087103,1.0352216926 C,0,-0.6346402139,3.1109988064,1.0425014252 C,0,-0.3079267149,0.8306998006,2.1805990568 O,0,-1.0463627277,4.1127779076,1.386864278 O,0,2.71562424,2.4094384655,1.4194752079 O,0,-0.3825174823,0.8229973984,3.327666165 C,0,-0.9638401176,-2.5444466241,-0.1370409897 C,0,0.373415634,2.1575647644,-1.2200408073 O,0,0.6448662101,2.6321188993,-2.2134243883 C,0,4.7156551751,-0.4243891774,-0.3862475561 C,0,3.2785086759,-0.3228262604,-0.9682617408 C,0,2.1575302083,-0.8417093255,-0.0160376795 C,0,0.7332811601,-0.3700866533,-0.3365223486 F,0,0.6969232481,-0.4980158637,-1.6932532251 F,0,2.196366614,-2.1977447357,-0.1007189929 F,0,2.5098459792,-0.5248900872,1.2580542879 F,0,3.2589085696,-1.0199321847,-2.1058897653 F,0,3.0582335259,0.9807203887,-1.2573064884 F,0,4.9347725613,-1.6426640645,0.0954109805 F,0,5.5896858315,-0.1821700469,-1.3561113861 F,0,4.9039321473,0.4663855862,0.5807138735 C,0,-2.0985029,-0.2382954127,-2.1107181009 C,0,-3.7390727689,-0.6186906766,-0.3223358065 C,0,-2.2976252705,-0.1442138199,-0.5843236648 C,0,-2.0210859518,1.2223904947,-0.0499175678 F,0,-3.9509290526,-1.7867041051,-0.9511149396 F,0,-1.6516460164,-1.4390927387,-2.4984204633 F,0,-4.649319235,0.260412024,-0.7605749892 F,0,-4.0518826462,-0.8276096784,0.9633570556 F,0,-2.4232301565,2.2404993135,-0.8728527557 F,0,-2.7421925801,1.4133177702,1.1044181314 F,0,-1.2482390717,0.6815423194,-2.5854586744 F,0,-3.2396249786,-0.0353139156,-2.7869833436</p>	

<p>(C₄F₈)₂Fe₂(CO)₆ (26-1S) M06-L/cc-pVTZ Fe,0,-0.615397251,-0.2969285139,-0.2071342214 C,0,-0.3533549565,-0.0848385598,-1.9218716276 O,0,-1.032006923,-3.2142730853,-0.5778915317 O,0,-0.1968419834,0.0263262196,-3.0511456469 Fe,0,1.2158421651,1.5351287258,-0.0235516151 C,0,2.7641694304,2.0569564856,0.7428542725 C,0,0.4218293424,3.0384506397,-0.6837412367 C,0,0.3524190739,1.9046760291,1.5485262103 O,0,-0.0744957282,3.9768936176,-1.1016251144 O,0,3.7254765939,2.3784701575,1.2664894715 O,0,-0.1231343143,2.2632727856,2.5184181823 C,0,-0.8411549451,-2.1113254351,-0.3741871224 C,0,2.0487138436,1.4072167132,-1.6645521302 O,0,2.5893397264,1.4919082694,-2.6616917924 C,0,1.2961717041,-0.4757109052,0.3248126463 C,0,2.2572866736,-1.3810423962,-0.3991838322 C,0,1.0427410563,-0.8619844668,1.7510500171 C,0,3.7527251315,-1.2415049828,-0.0105402897 F,0,2.2020778933,-1.1729250813,-1.7425559217 F,0,1.9549729991,-2.6951722873,-0.2235276385 F,0,1.6854150874,-0.1722056376,2.6934786388 F,0,-0.3349933142,-0.5393326079,1.9523912455 F,0,1.1341881529,-2.1395899024,2.0748772106 F,0,3.882472836,-1.2493345262,1.3175222174 F,0,4.4707511185,-2.2311892824,-0.5159596336 F,0,4.2512382703,-0.089039856,-0.4721164423 C,0,-3.5426382862,-0.7394849204,-1.2022558968 C,0,-3.2340987952,-0.4470929255,1.2803294415 C,0,-2.6962038293,-0.1281864239,-0.1014295259 C,0,-2.0973267598,1.1385237362,-0.3497892638 F,0,-2.979726238,-1.7161062551,1.6324231331 F,0,-3.9377060119,-1.9735312199,-0.8734010544 F,0,-4.5635011172,-0.2894028762,1.3197872433 F,0,-2.7117202801,0.3337238929,2.2277000527 F,0,-2.2661439345,1.6933771259,-1.5576650832 F,0,-2.1609141902,2.122764479,0.5522429721 F,0,-2.8947108078,-0.8294934497,-2.3698843655 F,0,-4.6435044328,-0.0111032803,-1.4238989683</p>	<p>(C₄F₈)₂Fe₂(CO)₆ (26-2S) M06-L/cc-pVTZ Fe,0,-0.6026608204,-0.5395601015,-0.1815315694 C,0,1.5977753367,1.7682902966,-1.7150136181 C,0,-0.460122197,-2.2445759996,-0.8004870553 O,0,-0.7962395737,0.4621755595,-2.8912243157 O,0,1.9973712424,2.0571880453,-2.7402529519 O,0,-0.4398541067,-3.275907539,-1.284384751 Fe,0,0.9386941852,1.5816909437,0.0007129328 C,0,0.126230537,1.606890573,1.6387502216 C,0,-0.011392502,3.0856795867,-0.4019955965 O,0,-0.5613493944,4.0439738012,-0.6859915851 O,0,-0.3201032214,1.773963448,2.6732952687 C,0,-0.7027626799,0.1295447426,-1.797177097 C,0,2.4587333813,2.2176392517,0.7326266721 O,0,3.4064804771,2.6062791674,1.2346917946 C,0,-2.3706921891,0.2401482125,0.4953107045 C,0,-2.6135630664,-1.0108812055,-0.1262222138 C,0,-3.0557457798,1.5107861116,0.0491599322 C,0,-3.1204608052,-2.2014304926,0.6639467027 F,0,-2.3087948029,-2.5084827618,1.6766344516 F,0,-3.2259172817,-3.2698324895,-0.1248492629 F,0,-4.3332700706,-1.9469888059,1.1676481386 F,0,-2.6178553318,2.5509203082,0.7686250216 F,0,-2.8509313078,1.7794281386,-1.2395587905 F,0,-4.3758332123,1.4221665349,0.2444691765 F,0,-2.3878675862,0.1903135838,1.8578500711 F,0,-3.2091122519,-0.9839684995,-1.3430867518 C,0,1.3787292092,-0.4099990885,0.0869924263 C,0,2.3660675918,-1.0413236202,-0.8591314058 C,0,1.3796111286,-0.9988086437,1.4687470334 C,0,3.8560953931,-0.6618449003,-0.6481597497 F,0,2.068722149,-0.7204681805,-2.1482057123 F,0,2.3366174213,-2.399702606,-0.8081658548 F,0,1.9677075169,-0.2841868561,2.4272693676 F,0,-0.0020611472,-1.0167378564,0.8344038417 F,0,1.776591936,-2.2492172837,1.6156788541 F,0,4.176366001,-0.7898750928,0.6413709618 F,0,4.6505846652,-1.4393231292,-1.3652245073 F,0,4.0807501566,0.6060278471,-1.0099677846</p>
<p>(C₄F₈)₂Fe₂(CO)₆ (26-3S) M06-L/cc-pVTZ Fe,0,0.9201820963,-0.2982907481,-0.2935312742 C,0,0.2651988289,2.0389025088,1.4381573599 C,0,0.7571330114,-2.1280510659,-0.1656864261 O,0,0.7795024317,2.2686658701,2.4260199591 O,0,0.7231305987,-3.2656238789,-0.1837337196 Fe,0,-0.6533228101,1.7645952027,-0.1226886193 C,0,-1.5585806305,1.5276999131,-1.7055399306 C,0,0.2969419536,3.1188117632,-0.9260577855 C,0,0.5316844901,-0.3154712384,-1.9880329308 O,0,0.8791552691,3.9658732277,-1.4198978248 O,0,-2.1312463877,1.4953613172,-2.6884882387 O,0,0.3310784822,-0.3546294164,-3.1163766234 C,0,-2.0871177001,2.5817014123,0.5886672195 O,0,-2.9857494935,3.1113679822,1.0535545182 C,0,-4.6145364842,-1.5821874013,0.3854102583 C,0,-3.5014733638,-0.5012760405,0.4278034658 C,0,-2.0817176331,-0.998293794,0.0304494508 C,0,-0.9266834907,-0.1114240638,0.4669570858 F,0,-0.8011708932,-0.3373960575,1.8280167438 F,0,-1.9412133223,-2.2389785794,0.5638078334 F,0,-2.0718279629,-1.1356601835,-1.3177028396 F,0,-3.4777604781,0.0088475873,1.6691581904</p>	<p>(C₄F₈)₂Fe₂(CO)₆ (26-4S) M06-L/cc-pVTZ Fe,0,-1.3941327987,0.8851566431,0.1380930814 C,0,0.0701792101,-0.428773196,0.8206427085 C,0,-0.980602345,0.8783405999,-1.6569004009 C,0,-1.5588274116,2.6816607146,-0.0284572368 O,0,0.0584476957,-1.3723515872,1.4912745855 O,0,-0.6945693482,1.0132262458,-2.7524348893 O,0,-1.7467625246,3.8035578104,-0.1437130606 Fe,0,1.3874164303,0.8782609662,0.07125294 C,0,1.4935346523,1.6450643318,1.646663377 C,0,1.2713658388,2.5143520548,-0.7689377763 O,0,1.5527717925,2.1550232645,2.6681226621 O,0,1.29754934,3.5320472903,-1.283943994 C,0,-1.6174713033,1.1798249501,1.9438598676 O,0,-1.6928270401,1.4829925333,3.037558927 C,0,3.40251447668,-1.2092948894,1.4068162808 C,0,2.4436447341,-1.2995163876,-0.9966152646 C,0,2.8590623923,-0.5051208522,0.1957171845 C,0,3.3347525168,0.8112508506,-0.1521550929 F,0,1.7437114676,-2.380337801,-0.7483340567 F,0,2.7933755504,-2.3696958905,1.637644705 F,0,3.3839127089,-1.6014812361,-1.8717413757 F,0,1.5572394048,-0.4062426837,-1.6798920041</p>

<p>F,0,-3.8669392373,0.4790939093,-0.4249688677 F,0,-4.4890212253,-2.4335410795,1.3930585501 F,0,-5.7985605949,-0.9844329378,0.4839911304 F,0,-4.5687874324,-2.2510598813,-0.7622267766 C,0,3.1725457745,-0.6151587925,1.1138209982 C,0,3.7681335032,-1.1894689012,-1.3114116101 C,0,2.9556657788,-0.3794270014,-0.3456669291 C,0,2.4760729162,0.9397813065,-0.6470832847 F,0,3.6147321901,-2.5066614647,-1.1239312559 F,0,3.3523120217,-1.8838108864,1.438881982 F,0,5.0790387954,-0.9272680014,-1.1679911938 F,0,3.4373311748,-0.9294349843,-2.5765405673 F,0,2.7244587879,1.9243330073,0.2458269881 F,0,2.6714764604,1.4447910974,-1.8657566467 F,0,1.9663548508,-0.2210451964,1.7211171222 F,0,4.1249157241,0.0947764895,1.6943504887</p>	<p>F,0,4.1189025055,1.4467756413,0.7182518417 F,0,3.8010402552,1.0483398027,-1.388645799 F,0,3.2729016766,-0.4523570446,2.5031145445 F,0,4.7126434363,-1.4714374821,1.2581827773 C,0,-2.508959892,-1.6348485053,-1.26115699 C,0,-3.0556205136,-1.6132548509,1.1716128785 C,0,-2.6898860096,-0.760951635,-0.0341821782 C,0,-3.3274822913,0.5243426948,-0.1390754695 F,0,-2.3627781648,-2.7523158122,1.1865276472 F,0,-1.2839029224,-2.1885729792,-1.2960565885 F,0,-4.3581022158,-1.9361189964,1.1471036269 F,0,-2.8418517568,-1.0034881797,2.3454237518 F,0,-3.8669255881,0.9510740031,-1.282619285 F,0,-4.1454819249,0.8968519764,0.8570068997 F,0,-2.6608897832,-0.9684825628,-2.4113354138 F,0,-3.3918125412,-2.6401608527,-1.283716411</p>
<p>(C₄F₈)₂Fe₂(CO)₆ (26-5S) M06-L/cc-pVTZ Fe,0,0.707280312,-0.2527282145,-0.2644716178 C,0,-0.20961164,2.0483814843,1.461842647 C,0,0.8436201905,-2.0794051626,-0.0486392648 O,0,0.1678246635,2.2734871475,2.5106031829 O,0,1.0526589984,-3.1961155526,0.0127256833 Fe,0,-0.8951903463,1.7858847587,-0.2163773368 C,0,-1.524176808,1.5892041552,-1.9344536195 C,0,0.0543517174,3.230316567,-0.8434822601 C,0,0.4149383421,-0.4214518831,-1.9671947447 O,0,0.6024963387,4.1553601799,-1.2229173275 O,0,-1.902451002,1.6118097851,-3.0080308841 O,0,0.2464010525,-0.5661891676,-3.0920906864 C,0,-2.4265349455,2.6093946727,0.2372546962 O,0,-3.3756560382,3.1863914082,0.5024907471 C,0,-1.2034055997,-0.134128353,0.3306687526 F,0,-1.1009535248,-0.3955632063,1.7032459962 C,0,2.9509480243,-0.319918642,1.2721762849 C,0,3.6930265365,-0.8505911844,-1.12686593 C,0,2.7550970051,-0.1339327667,-0.1999994633 C,0,2.1673765361,1.1280335161,-0.5403952694 F,0,3.7314030491,-2.1682195796,-0.8973153105 F,0,3.2491323268,-1.5597170774,1.6262703439 F,0,4.9480826885,-0.3927041599,-0.9763886853 F,0,3.350831295,-0.6822771768,-2.4053458886 F,0,2.3045772238,2.1375242234,0.3503831894 F,0,2.3681534465,1.6345513016,-1.7585279886 F,0,1.7054954225,-0.0366125155,1.8437035822 F,0,3.8216789958,0.4886389842,1.854708575 C,0,-3.6441782502,-0.7087057554,0.919711946 C,0,-2.2659876006,-2.4237434907,-0.3185308885 C,0,-2.4618604494,-0.9018149947,-0.0919140672 F,0,-1.6641012741,-3.0007121075,0.7172417062 F,0,-3.5767326252,-1.5915587486,1.9116061272 F,0,-1.5204911711,-2.6257483158,-1.4096915912 F,0,-3.4315305457,-3.0346718109,-0.516816854 F,0,-2.9038272816,-0.4379589912,-1.3055270589 F,0,-4.8037825714,-0.8683315823,0.2903673337 F,0,-3.6488234913,0.5109202555,1.4584119435</p>	<p>(C₄F₈)₂Fe₂(CO)₆ (26-6S) M06-L/cc-pVTZ Fe,0,0.6264548311,1.3168421373,0.2486666443 C,0,2.0886066296,2.2758290577,0.7866678029 C,0,-0.5013649915,-2.7318059904,0.4549249278 O,0,0.7833030782,2.0946162366,-2.6131873968 O,0,2.9937628598,2.9120610263,1.0540502459 O,0,-1.1411053979,3.6584161057,0.6272267135 Fe,0,0.0345318452,-1.0139750666,0.8195333015 C,0,-1.4078635019,-1.4563958872,1.840408516 C,0,0.0796383677,0.8214872646,2.0038969464 O,0,-2.2601282148,-1.7871196124,2.5259896701 O,0,-0.157696185,1.0147533249,3.1141261767 C,0,0.7839091076,1.7433775294,-1.5330589367 C,0,0.0431888972,-2.5668553582,-0.058843323 O,0,-0.0112860583,-3.5202263729,-0.6860008289 C,0,-4.7975849767,-0.2613497708,-0.2901428271 C,0,-3.3828155216,-0.5230771105,-0.8717470777 C,0,-2.2945836077,0.4948893523,-0.403387199 C,0,-0.8681433927,-0.0321600669,-0.4979237669 F,0,-0.7572110959,-0.4054347606,-1.8061585295 F,0,-2.4418502595,1.5976437957,-1.1819653214 F,0,-2.5736165297,0.8719343636,0.8701595434 F,0,-3.4739481162,-0.4809643817,-2.2042607575 F,0,-3.0261544333,-1.7722954908,-0.5075235696 F,0,-5.1374908595,1.0131091727,-0.4569687922 F,0,-5.6768291155,-1.0258739111,-0.9274282689 F,0,-4.8391257753,-0.5582351803,1.0029541827 C,0,1.8090216113,-0.4217255448,0.1732281233 C,0,2.5445902713,-0.7921797548,-1.0841425325 C,0,2.55686975,-0.7921640587,1.4323403194 C,0,3.8425595422,0.0142637215,-1.3772848979 F,0,1.7695580059,-0.6298560485,-2.1823867619 F,0,2.9117500708,-2.1031548601,-1.0789681497 F,0,3.0694703142,0.2097213474,2.1529777311 F,0,1.5856364159,-1.3620380406,2.3061631847 F,0,3.4861399383,-1.723432754,1.3346443624 F,0,4.6330933278,0.0599677595,-0.3040213023 F,0,4.5170566506,-0.5216297782,-2.3814454923 F,0,3.536462518,1.2770066256,-1.7071876602</p>

<p>(C₄F₈)₂Fe₂(CO)₆ (26-7S) M06-L/cc-pVTZ Fe,0,1.316336734,0.3009122841,0.6105817034 Fe,0,-1.1118093906,-0.2898838773,0.5806185689 C,0,0.3887673861,0.205902312,2.2579092631 O,0,0.1767109504,0.3170175712,3.3785970557 C,0,2.0876772525,1.8791886958,1.1065628151 C,0,2.6755541753,-0.6972535247,1.3043710117 C,0,-1.9551153156,-1.4257524527,1.724176213 C,0,2.1973548027,0.3258418431,-1.0238454802 C,0,-2.285078156,-0.4819789055,-0.7364455866 C,0,-0.352053053,1.4063882525,-0.1487474834 C,0,0.5541135189,-2.683988012,1.0408024013 C,0,0.2817552339,-1.0741624302,0.0741624302 C,0,0.4743333424,-2.031447732,-1.3484115174 C,0,-0.2799589434,-3.3248716494,-1.8041697406 C,0,-0.3066883788,2.0732528421,-1.5068665587 C,0,-1.0692073379,2.29201632,0.8552367576 C,0,0.5192391219,3.3933773252,-1.609608402 F,0,0.6584001379,-2.2945776736,2.3314940258 F,0,1.6927017113,-3.3432552546,0.7720561846 F,0,-0.4352711246,-3.5940924805,1.025649854 F,0,0.2764625313,-4.424208885,-1.3144384993 F,0,-0.2321181521,-3.3999789789,-3.1303710149 F,0,-1.5615084972,-3.2808325369,-1.4360411303 F,0,1.7906465902,-2.2839046323,-1.6261415233 F,0,0.0771002111,-1.0893215272,-2.2272041913 F,0,0.2307715154,1.2910290911,-2.4652082289 F,0,-1.563332744,2.3716849145,-1.9345638247 F,0,-1.9042240659,3.1974724172,0.3866240751 F,0,-1.9015829518,1.426227915,1.6162237702 F,0,-0.3116529423,2.8907540835,1.7829758041 F,0,1.827827384,3.1071276666,-1.5215334864 F,0,0.3042417124,3.9850313462,-2.7727142263 F,0,0.2328667044,4.2525423719,-0.6331976577 O,0,3.5631749806,-1.2530898984,1.7480524138 O,0,2.6200354235,2.833693851,1.4216014198 O,0,2.8719901975,0.3676764335,-1.9344906255 O,0,-3.0133728357,-0.6070330977,-1.6088631652 O,0,-2.5871807286,-2.0256260266,2.4628855752</p>	<p>(C₄F₈)₂Fe₂(CO)₆ (26-8S) M06-L/cc-pVTZ Fe,0,-0.3822445628,-1.0016904083,0.7944392757 C,0,-1.8272651124,-1.773319905,1.5970199679 C,0,0.7340467098,-2.0802223736,1.7483542459 O,0,-0.2593333283,-2.8723888294,-1.5048995882 O,0,-2.7119367873,-2.3280288937,2.0508220794 O,0,1.3073239464,-2.7549324766,2.4657172852 Fe,0,0.0309999745,1.3881870666,0.4764891912 C,0,1.3776292651,2.2719031732,1.3237089286 C,0,0.0070158378,0.2180237697,2.2284192602 O,0,2.1741482174,2.8705615012,1.8829744002 O,0,0.1557581444,0.4490518202,3.3494084639 C,0,-0.3599911519,-2.1220372522,-0.6566716715 C,0,-0.0496065882,2.542174149,-0.8995266264 O,0,-0.0486929507,3.2338165737,-1.8068758047 C,0,1.0737869312,0.0769179067,-0.4091565759 F,0,0.9333477552,0.0112125354,-1.7666855897 C,0,-1.6608840932,0.4552273391,-0.0050212981 C,0,-2.3348927048,0.2408011633,-1.3339952404 C,0,-2.5249571504,1.225286308,0.9701024264 C,0,-3.5666953706,-0.7116269533,-1.3211665233 F,0,-1.4978509994,-0.298783004,-2.2493563201 F,0,-2.7679198409,1.4138451842,-1.8728068746 F,0,-3.0438604829,0.5442954405,1.9955340284 F,0,-1.6621964556,2.1641993693,1.6043374633 F,0,-3.4887819114,1.970957906,0.4629323561 F,0,-4.4245436136,-0.3907904521,-0.3523499079 F,0,-4.201759223,-0.6744645252,-2.4815284956 F,0,-3.1649916044,-1.9721933766,-1.105100601 C,0,3.4550257213,0.9349489571,-0.8885707531 C,0,3.0996111931,-1.5539640474,-0.7055120691 C,0,2.5701453144,-0.1730661707,-0.200184452 F,0,2.7449472021,-1.813110449,-1.9539402313 F,0,3.7819066466,0.5772819343,-2.1266496031 F,0,2.6337907753,-2.5451954106,0.0602961124 F,0,4.4293069128,-1.5863602213,-0.6199720111 F,0,2.8442200893,-0.1403820596,1.1422822259 F,0,4.5650880589,1.1190333503,-0.1866153004 F,0,2.8298682362,2.1114463606,-0.9736651732</p>
<p>(C₄F₈)₂Fe₂(CO)₆ (26-9S) M06-L/cc-pVTZ Fe,0,0.5549390083,-0.145178502,0.4961004031 C,0,-2.2236670105,1.310091404,1.9243280468 C,0,0.9080266759,-1.9153066909,0.7908209741 O,0,0.2333229139,0.2352052577,3.3442712853 O,0,-2.7420456366,1.3506946274,2.9363113337 O,0,1.1699939654,-2.9719910254,1.1254593175 Fe,0,-1.4453984049,1.4981216669,0.2639001191 C,0,-0.6470970233,1.9267673887,-1.326591328 C,0,-0.7851332362,3.0799308567,0.8815866478 O,0,-0.3704413149,4.0709441297,1.2665985864 O,0,-0.2218298283,2.3150392045,-2.3085036885 C,0,0.3380420481,0.1042296066,2.2107979622 C,0,-3.0484432932,1.860207063,-0.480823381 O,0,-4.0442325582,2.0843167119,-0.9911470536 C,0,-1.3283191884,-0.5183156295,-0.0466017771 C,0,-2.2001914435,-1.4986313889,0.6897051608 C,0,-0.9962952796,-0.9057353388,-1.4550506186 C,0,-3.7074658214,-1.4879357943,0.3238571063 F,0,-2.1392117479,-1.2795358342,2.0325608322 F,0,-1.7956868373,-2.7846715374,0.5128347669 F,0,-1.691526186,-0.3262900583,-2.4320272701 F,0,0.3422015229,-0.4149621252,-1.6317322901</p>	<p>(C₄F₈)₂Fe₂(CO)₆ (26-10S) M06-L/cc-pVTZ C,0,-2.8994824224,0.7622747464,0.405974234 C,0,-3.1893197412,-0.3704176923,-0.4207053257 C,0,-3.2645902036,2.165799623,-0.0427241372 C,0,-4.0434168891,-1.534607741,0.0319389361 F,0,-3.7159507036,-1.9772915143,1.2481335271 F,0,-3.9225359316,-2.5561771832,-0.8209247936 F,0,-5.3305215301,-1.1782540508,0.0601438336 F,0,-2.8915383108,3.0631432533,0.8615319552 F,0,-2.7101253742,2.4946419969,-1.2134690924 F,0,-4.5946082885,2.2642544461,-0.1858888666 F,0,-3.2600169716,0.6550113534,1.7202013951 F,0,-3.550283317,-0.0878277483,-1.7085807529 Fe,0,-1.2126960931,-0.268516533,-0.0946235149 C,0,-0.081370562,1.1877888977,0.6003201961 C,0,-1.2278060758,-1.0551688452,1.5696935075 C,0,-0.8273290835,-1.872401986,-0.9014406842 O,0,-0.1444910099,2.2741518869,1.0034574061 O,0,-1.1634012952,-1.5227662129,2.6058171948 O,0,-0.6488102481,-2.8713630633,-1.4246882278 Fe,0,1.4272315078,-0.1785426564,0.3992183105 C,0,1.7189991829,0.1253178183,2.0993846759 C,0,1.5699236307,-2.017370616,0.7123093059</p>

<p>F,0,-0.9112616902,-2.1909499914,-1.7468469214 F,0,-3.8526280962,-1.5150430291,-1.0027600638 F,0,-4.3316346943,-2.533081004,0.8427521597 F,0,-4.2979927843,-0.3809334039,0.7872588188 C,0,3.6868311594,-1.6776911976,-1.0086672108 C,0,3.4329495658,-0.1743933221,-0.734177126 C,0,2.5948797293,0.1605575347,0.48120205 C,0,1.8982721481,1.3985870056,0.5709547454 F,0,2.8713913641,0.3271885863,-1.8510186208 F,0,4.5975267635,-1.8095827949,-1.9633019284 F,0,4.6488016991,0.4013787782,-0.5796207648 F,0,1.9991952084,2.0936579785,1.7085850678 F,0,3.2264040434,-0.2352541443,1.6183877826 F,0,1.9216712457,2.2596627587,-0.4551287867 F,0,2.558237304,-2.2607914836,-1.4255535139 F,0,4.1106917099,-2.3056402632,0.0814091774</p>	<p>O,0,1.8956228388,0.3177623458,3.2124449482 O,0,1.7478958576,-3.1155273337,0.9614059312 C,0,-0.9636288267,0.5603307143,-1.7303050345 O,0,-0.7404673517,1.011241345,-2.748565866 C,0,4.5273226779,0.0765623017,0.4694051384 C,0,3.1251502867,-0.411406954,-1.5992807494 C,0,3.2421463935,0.2796992495,-0.279378084 C,0,2.4038518006,1.4530615745,-0.1683784022 F,0,3.6366618327,-1.6282243408,-1.6227244737 F,0,4.6848452632,-1.2025600062,0.8414269101 F,0,3.5588928872,0.2435356268,-2.6571864064 F,0,1.7291678062,-0.5687870499,-1.7840868155 F,0,2.7106253009,2.4040439418,0.7031392571 F,0,1.9729305168,2.0396043478,-1.3023976438 F,0,4.585863425,0.8200968221,1.5717787421 F,0,5.5817050209,0.3917812357,-0.2999345339</p>
<p>(C₄F₈)₂Fe₂(CO)₆ (26-11S) M06-L/cc-pVTZ Fe,0,-0.2204243189,1.1231135955,0.3578188578 C,0,0.5863053479,2.2835892811,1.533347689 O,0,-0.1197452501,2.9076998907,-1.98707273 O,0,0.9277545798,3.0268474833,2.3301743716 Fe,0,-0.0267167683,-1.3153707874,0.5242197415 C,0,-1.2714795843,-2.4466670494,1.2420959096 C,0,1.2986356734,-2.0773474299,1.5333434845 C,0,-0.2913854585,-0.052611838,2.0107027818 O,0,2.0772527785,-2.6021402388,2.1803586883 O,0,-1.9833941244,-3.2212585492,1.68192726 O,0,-0.4804377184,0.062549119,3.1476011687 C,0,-0.2063909487,2.2394604958,-1.0665650531 C,0,0.1930461041,-2.351295194,-0.9581801045 O,0,0.295836123,-2.9909097935,-1.8926366395 C,0,-1.3609529806,-0.1978334547,-0.5476301112 F,0,-1.3927946367,-0.3264698963,-1.9094304673 C,0,-3.8095854933,-0.9494675167,-0.9344861268 C,0,-3.2368984091,1.3893207727,-0.0392309805 C,0,-2.8291211378,-0.0918672529,-0.0988357046 F,0,-3.0882377961,2.0142642657,-1.1933046164 F,0,-4.0554429032,-0.4010446276,-2.1183004089 F,0,-2.3741282256,1.9755883739,0.8630395695 F,0,-4.4571949125,1.5911563027,0.4126349858 F,0,-2.9705792363,-0.5057412016,1.2063374865 F,0,-4.9653274639,-1.0849195103,-0.2895319299 F,0,-3.2975773038,-2.1677142994,-1.1182708141 C,0,1.2325316291,0.0870946716,-0.3568920287 F,0,1.2656841941,-0.0117639854,-1.7328990702 C,0,3.3208530643,1.621556064,-0.4253788154 C,0,3.6184467681,-0.8797789851,-0.5599961502 C,0,2.7039525351,0.254626364,0.0214690082 F,0,4.0263467342,-0.5763625673,-1.7883237937 F,0,3.0067665565,1.9251560101,-1.6776958194 F,0,2.9839470675,-2.0552615367,-0.6333269155 F,0,4.6796980553,-1.0517621479,0.2177187436 F,0,2.8248430617,0.2228222247,1.3859272713 F,0,4.6497074891,1.5932996577,-0.3147184747 F,0,2.8861569087,2.6089742892,0.357191737</p>	

<p>$C_4F_8Fe(CO)_4$ (14-1S) M06-L/cc-pVTZ</p> <p>C,0,-1.8297603017,-1.0648932777,-1.3440287321 C,0,1.5886261763,0.1329183714,-0.8362124992 C,0,-0.4658303195,-0.1649909957,0.4807078838 C,0,-0.3838202244,0.8641868402,-2.39015336 Fe,0,-0.07040977,-0.5465815774,-1.2395397784 O,0,-0.7033199097,0.0506837105,1.5780441811 O,0,2.5430113134,0.6524302069,-0.4994846498 O,0,-2.9426605756,-1.2917615201,-1.285466778 O,0,-0.5620989042,1.6977275731,-3.1460930901 C,0,-0.2001866982,-2.5378230987,-3.6429096315 C,0,2.0598942068,-1.6298593723,-3.1374003211 C,0,0.6936655973,-1.9597346116,-2.5627858453 C,0,0.5522160097,-2.4569701216,-1.213806184 F,0,2.0643402767,-0.4315984221,-3.7522759137 F,0,-0.1138378227,-1.8071285768,-4.7627651484 F,0,2.4445114002,-2.5284108969,-4.0503590696 F,0,3.0236967918,-1.5856780875,-2.2107324478 F,0,-0.372366985,-3.409405027,-1.0014191252 F,0,1.6206934591,-2.7689242181,-0.4746944004 F,0,-1.4977737648,-2.5867650476,-3.311874284 F,0,0.1505491244,-3.7933295812,-3.9513054363</p>	<p>$C_4F_8Fe(CO)_4$ (14-2S) M06-L/cc-pVTZ</p> <p>Fe,0,0,0,1.0956118945 C,0,-0.765906064,1.3148656845,2.1047781056 C,0,0.765906064,-1.3148656845,2.1047781056 C,0,-1.5947101482,-0.9092554759,1.1808496472 C,0,1.5947101482,0.9092554759,1.1808496472 O,0,2.5929714516,1.4320926548,1.328015481 O,0,1.2461917475,-2.1659116372,2.6945581234 O,0,-1.2461917475,2.1659116372,2.6945581234 O,0,-2.5929714516,-1.4320926548,1.328015481 C,0,-0.0933713355,1.9101070038,-1.3777953753 C,0,-0.4505447793,0.5590488805,-0.8016704187 C,0,0.4505447793,-0.5590488805,-0.8016704187 C,0,0.0933713355,-1.9101070038,-1.3777953753 F,0,-0.1440926861,1.8788160971,-2.7140307885 F,0,-0.966840675,2.8329577253,-0.9628995921 F,0,1.1287413837,2.3213248469,-1.0296824528 F,0,1.7378605487,-0.2969926398,-1.1886543953 F,0,0.966840675,-2.8329577253,-0.9628995921 F,0,0.1440926861,-1.8788160971,-2.7140307885 F,0,-1.1287413837,-2.3213248469,-1.0296824528 F,0,-1.7378605487,0.2969926398,-1.1886543953</p>
<p>$C_4F_8Fe(CO)_4$ (14-3S) M06-L/cc-pVTZ</p> <p>C,0,2.1712769086,0.0135817492,-2.0570096651 C,0,1.6679790713,-0.2746459883,1.5654052116 C,0,3.3282401595,0.9288564097,0.0494590425 C,0,2.44993462056,-1.9055928625,-0.3229555826 Fe,0,1.8970995143,-0.1526774062,-0.2490938895 O,0,4.198756601,1.6452182711,0.2339557219 O,0,1.6122289167,-0.3494205885,2.699129485 O,0,2.3800017457,0.1131805079,-3.1696432423 O,0,2.7612898722,-3.0012461848,-0.3871225977 C,0,-1.0349740439,-2.4159184831,0.3458703574 C,0,-1.1395446568,-0.8712053888,0.2632016016 C,0,-0.1116253165,-0.2058340551,-0.6230165523 C,0,0.370464662,1.1400838591,-0.4067626945 F,0,-1.0651979324,-0.4166711675,1.5319074435 F,0,-2.1316768287,-2.9217822803,0.8930121079 F,0,-2.3747085607,-0.5851481918,-0.2058654629 F,0,0.3325762315,1.9721425995,-1.4572148801 F,0,-0.4382577136,-0.4787592713,-1.9245347124 F,0,-0.003361308,1.825850617,0.6827444926 F,0,0.0075806221,-2.7594437302,1.112866213 F,0,-0.8639091399,-2.956412355,-0.8556777174</p>	<p>$C_4F_8Fe(CO)_4$ (14-4S) M06-L/cc-pVTZ</p> <p>C,0,0.2900768281,1.3737990581,2.2606081885 C,0,-0.2900768281,-1.3737990581,2.2606081885 C,0,-1.8001899617,0.3735757678,0.9380314275 C,0,1.8001899617,-0.3735757678,0.9380314275 C,0,0.2170942832,-0.7334582063,-1.7879052528 C,0,-0.2170942832,0.7334582063,-1.7879052528 Fe,0,0,0,1.0693755243 O,0,-2.909826793,0.6020888345,0.8840955112 O,0,-0.4791908179,-2.2434246254,2.9695247534 O,0,0.4791908179,2.2434246254,2.9695247534 O,0,2.909826793,-0.6020888345,0.8840955112 C,0,-0.2427074289,-1.3788668864,-0.4686908529 C,0,0.2427074289,1.3788668864,-0.4686908529 F,0,0.4753928445,-2.5207456161,-0.2824162129 F,0,-1.5341928106,-1.7795512884,-0.6210466133 F,0,-0.2494158291,-1.3790763798,-2.8661428956 F,0,1.5702037428,-0.7664807056,-1.8284443075 F,0,-1.5702037428,0.7664807056,-1.8284443075 F,0,0.2494158291,1.3790763798,-2.8661428956 F,0,1.5341928106,1.7795512884,-0.6210466133 F,0,-0.4753928445,2.5207456161,-0.2824162129</p>
<p>$C_4F_8Fe(CO)_4$ (14-5S) M06-L/cc-pVTZ</p> <p>C,0,-2.0448579971,-0.1245975978,-1.5962237599 C,0,-0.5390671914,0.849905197,1.6186709001 C,0,-2.9454248926,0.6643490729,0.7141866865 C,0,-0.8671970596,2.075898475,-0.7005050127 Fe,0,-1.2822824806,0.4148006403,-0.0043678471 O,0,-3.9835474988,0.7619599296,1.1734489286 O,0,-0.1582250456,1.1636763151,2.6413910904 O,0,-2.5632150268,-0.3932521953,-2.5695095519 O,0,-0.5561701128,3.0748058652,-1.147490006 C,0,1.7787021404,-0.0981898179,-0.0008452155 C,0,0.4826642302,-0.4391523356,-0.7133680546 C,0,-0.0361016229,-1.8616347903,-0.4612816889 C,0,-1.1788672825,-1.574520149,0.5217730445 F,0,0.8783777472,-2.7545872237,-0.0246236975 F,0,2.8293516326,-0.6664175352,-0.5896185254 F,0,0.7237765093,-0.2158754774,-2.0476374602</p>	<p>$C_4F_8Fe(CO)_4$ (14-6S) M06-L/cc-pVTZ</p> <p>C,0,1.792451612,-1.2810266835,0. C,0,-1.8789390381,-1.1664694616,0. C,0,-0.077006939,-2.4825174633,-1.4310581387 C,0,-0.077006939,-2.4825174633,-1.4310581387 Fe,0,-0.0525857483,-1.3266043778,0. O,0,-0.092034767,-3.1479842134,2.3554636529 O,0,-3.0108987604,-1.078674475,0. O,0,2.9269006065,-1.3389847374,0. O,0,-0.092034767,-3.1479842134,-2.3554636529 C,0,-0.0056444114,0.37468712,-1.1644230096 C,0,-0.1177470749,2.7471244966,0. C,0,0.4004701557,1.3013381206,0. C,0,-0.0056444114,0.37468712,1.1644230096 F,0,0.3306061955,3.3870749572,-1.0822120422 F,0,1.7658336954,1.3913522358,0. F,0,0.3306061955,3.3870749572,1.0822120422</p>

<p>F,0,-2.266866208,-2.3403207879,0.2932361278 F,0,-0.5542848629,-2.348058501,-1.6101839477 F,0,-0.7953755137,-1.8183753026,1.7965752346 F,0,1.7532832031,-0.5038323024,1.2756723199 F,0,1.9936438424,1.229215681,0.0009801552</p>	<p>F,0,-1.4454782289,2.8096172978,0. F,0,0.890339669,0.4227117621,2.1717372512 F,0,-1.1968441527,0.7505053176,1.7017082797 F,0,-1.1968441527,0.7505053176,-1.7017082797 F,0,0.890339669,0.4227117621,-2.1717372512</p>
<p>C₄F₈Fe(CO)₄ (14-7S) M06-L/cc-pVTZ C,0,-2.3517074021,-0.7419856846,-0.6775361139 C,0,-0.4407446364,1.2314946633,0.2706089256 C,0,-0.2859191573,-1.3224396648,0.6851601046 C,0,-0.9522368781,0.7502645196,-2.2471158293 Fe,0,-0.5997941062,-0.2547198839,-0.7716167736 O,0,-0.2267736819,-1.9432926239,1.6390365087 O,0,-0.2861101868,2.1645864694,0.9127262377 O,0,-3.443288619,-1.0825088259,-0.6629810378 O,0,-1.1875387002,1.3890010919,-3.1604181775 C,0,3.195794027,-1.7088209173,-2.0260257745 C,0,1.3594988063,-3.4821508295,-1.7668242412 C,0,0.7399258746,-1.0276803628,-1.7533183348 C,0,1.8176198374,-2.0499118327,-1.3926299738 F,0,0.9306489586,-3.5366558243,-3.0234634144 F,0,3.2538158955,-2.0669165384,-3.3050163111 F,0,0.3579739162,-3.8424120263,-0.9625975888 F,0,2.3439212946,-4.3645282537,-1.6163803302 F,0,0.9482583557,-0.77454011,-3.0648234187 F,0,2.0269512717,-2.0630003592,-0.0420506886 F,0,4.1671682089,-2.3373851081,-1.3725969634 F,0,3.4260105915,-0.3982655088,-1.9367879649</p>	<p>C₄F₈Fe(CO)₄ (14-8S) M06-L/cc-pVTZ C,0,2.7120563374,0.289939019,-2.4680931814 C,0,1.2564485966,-0.7844436605,-0.2794900898 C,0,1.2239004345,1.6971583513,-0.9689697767 C,0,0.9555436812,-1.5305618824,-2.7073831049 Fe,0,1.0089657068,0.0995948337,-1.853453207 O,0,1.5023057531,2.6479720411,-0.4103615407 O,0,1.3482212563,-1.3204053222,0.7242122498 O,0,3.7554866392,0.4225287688,-2.9125361348 O,0,1.0580021071,-2.5842000524,-3.123701986 C,0,-1.3013601503,1.9303306452,-2.1245416736 C,0,-0.5921223729,0.674275648,-2.6059219801 C,0,-1.307177806,0.0336964581,-3.7719032754 C,0,-2.4163793016,-0.9877721954,-3.3855996639 F,0,-0.6560729084,3.0294375992,-2.5692620755 F,0,-1.3057875624,2.0070482024,-0.7759939002 F,0,-2.5787873855,2.0611495807,-2.4881368177 F,0,-1.8580739445,-2.0488616656,-2.7911829037 F,0,-3.0522213282,-1.4056980777,-4.4722439702 F,0,-3.3021257328,-0.4649969425,-2.5474017881 F,0,-0.4508609114,-0.67378732,-4.5618206392 F,0,-1.8685702879,0.9531454913,-4.5941691009</p>
<p>C₄F₈Fe(CO)₄ (14-9S) M06-L/cc-pVTZ C,0,3.9765363738,0.2397400891,1.7068987891 C,0,3.7187301724,-0.2454953796,-1.1397888448 C,0,2.9112041396,-1.866149724,0.6714957293 C,0,2.5686571299,1.7238990716,0.0957536928 Fe,0,2.7514409894,-0.0623680323,0.3910078359 O,0,3.1430490188,-2.9736428775,0.8069056877 O,0,4.2758356536,-0.360178634,-2.1315722627 O,0,4.7029074413,0.4333863752,2.5682679919 O,0,2.4716314168,2.8433899346,-0.090084865 C,0,-1.7185822929,-2.9217241764,-0.3480912005 C,0,-0.5225871015,-1.9468732203,-0.4973259916 C,0,-0.0506001136,-1.2591556664,0.8125456063 C,0,0.9238284516,-0.1078672803,0.5345626336 F,0,-0.8785376477,-1.0039704734,-1.3860902095 F,0,-1.8804549278,-3.5832751151,-1.4908008772 F,0,0.5127470985,-2.644343812,-1.0023637978 F,0,-1.1424840664,-0.8129039332,1.469422816 F,0,0.5279678076,-2.2025702847,1.5841699725 F,0,0.1261701953,0.9555936798,0.3336386744 F,0,-2.8366887256,-2.260249248,-0.082376101 F,0,-1.4904527234,-3.7989596132,0.6234983007</p>	

Complete Gaussian 09 reference

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