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# Binuclear Methylaminobis(difluorophosphine) Iron Carbonyls: Phosphorus-Nitrogen Bond Cleavage in Preference to Iron-Iron Multiple Bond Formation

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## Supporting Information

**Table S1.** The vibrational frequencies for the $CH_3N(PF_2)_2Fe_2(CO)_n$ ($n$ = 8, 7, 6, 5) structures at the B3LYP/DZP and BP86/DZP levels.

**Table S2.** The vibrational frequencies for the $[CH_3N(PF_2)_2]_2Fe_2(CO)_n$ ($n$ = 6, 5, 4, 3) structures at the B3LYP/DZP and BP86/DZP levels.

**Table S3.** The Cartesian coordinates of the optimized $CH_3N(PF_2)_2Fe_2(CO)_n$ ($n$ = 8, 7, 6, 5) structures at the B3LYP/DZP and BP86/DZP levels.

**Table S4.** The Cartesian coordinates of the optimized $[CH_3N(PF_2)_2]_2Fe_2(CO)_n$ ($n$ = 6, 5, 4, 3) structures at the B3LYP/DZP and BP86/DZP levels.

Complete Gaussian 03 reference (Reference 27).

**Table S1.** The vibrational frequencies (in $cm^{-1}$) and infrared intensities (in km/mol, given in parentheses) of the $CH_3N(PF_2)_2Fe_2(CO)_n$ (n = 8, 7, 6, 5) isomers at the B3LYP/DZP and BP86/DZP levels.

| Structure | B3LYP/DZP | BP86/DZP |
|---|---|---|
| $[CH_3N(PF_2)_2]Fe_2(CO)_8$ **(18-1S)** | 6 (0), 11 (0), 24 (1), 34 (0), 40 (0), 45 (0), 53 (0), 54 (0), 61 (0), 75 (0), 83 (0), 89 (0), 92 (0), 97 (0), 98 (0), 100 (0), 101 (0), 105 (0), 123 (1), 127 (0), 149 (0), 155 (0), 183 (0), 212 (0), 213 (1), 246 (5), 262 (0), 269 (1), 305 (19), 361 (27), 365 (105), 373 (4), 373 (0), 395 (2), 406 (6), 421 (38), 432 (2), 434 (0), 439 (2), 441 (34), 444 (14), 445 (2), 465 (88), 469 (9), 472 (71), 480 (12), 481 (4), 518 (4), 521 (25), 529 (2), 572 (0), 573 (0), 611 (8), 614 (165), 618 (22), 651 (70), 656 (357), 659 (126), 665 (15), 796 (208), 831 (20), 850 (931), 858 (320), 868 (321), 1099 (106), 1141 (2), 1199 (133), 1461 (5), 1494 (7), 1503 (27), 2053 (66), 2057 (2110), 2078 (631), 2079 (228), 2082 (100), 2086 (2520), 2140 (670), 2149 (18), 3069 (21), 3152 (8), 3162 (3) | 2i (0), 8 (0), 24 (1), 32 (0), 39 (0), 40 (0), 52 (0), 54 (0), 60 (0), 72 (0), 82 (0), 85 (0), 88 (0), 93 (0), 93 (0), 97 (0), 98 (0), 101 (0), 112 (0), 125 (0), 132 (0), 150 (0), 179 (0), 205 (0), 212 (1), 247 (9), 259 (0), 261 (0), 298 (16), 347 (11), 358 (92), 374 (2), 376 (0), 379 (0), 395 (3), 408 (30), 435 (15), 436 (48), 442 (55), 447 (0), 453 (50), 459 (8), 460 (4), 481 (1), 483 (26), 487 (5), 489 (0), 511 (4), 521 (1), 522 (3), 554 (0), 555 (0), 603 (10), 618 (95), 619 (82), 651 (110), 652 (380), 655 (115), 663 (21), 770 (184), 801 (151), 817 (753), 822 (317), 841 (253), 1063 (85), 1100 (5), 1151 (105), 1390 (11), 1440 (4), 1457 (16), 1980 (40), 1983 (1668), 1996 (70), 1999 (1626), 2002 (877), 2003 (432), 2060 (671), 2070 (26), 2982 (23), 3068 (7), 3082 (1) |
| $[CH_3N(PF_2)_2]Fe_2(CO)_8$ **(18-2S)** | 7 (0), 16 (0), 28 (0), 32 (0), 34 (1), 44 (0), 53 (0), 64 (0), 68 (0), 75 (0), 81 (0), 85 (0), 95 (0), 98 (0), 100 (0), 102 (0), 105 (0), 109 (0), 113 (1), 121 (1), 147 (0), 172 (1), 203 (1), 209 (0), 224 (0), 234 (1), 254 (4), 283 (0), 310 (22), 344 (15), 371 (57), 373 (0), 373 (2), 399 (11), 403 (3), 410 (8), 430 (0), 432 (9), 434 (15), 438 (10), 449 (2), 455 (3), 465 (35), 470 (7), 474 (3), 480 (17), 491 (8), 505 (236), 517 (2), 520 (32), 523 (58), 572 (0), 613 (82), 614 (118), 628 (20), 632 (80), 644 (184), 656 (175), 666 (56), 827 (45), 833 (2), 843 (249), 847 (195), 882 (942), 1058 (304), 1142 (4), 1204 (58), 1454 (3), 1494 (5), 1509 (10), 2052 (940), 2055 (830), 2058 (1423), 2079 (378), 2083 (366), 2087 (1612), 2137 (573), 2149 (169), 3080 (24), 3167 (4), 3178 (0) | 6 (0), 10 (0), 25 (0), 33 (0), 38 (1), 44 (0), 53 (0), 60 (0), 65 (0), 74 (0), 80 (0), 83 (0), 92 (0), 94 (0), 96 (0), 99 (0), 100 (0), 106 (0), 115 (1), 124 (1), 145 (0), 169 (0), 199 (0), 206 (1), 221 (0), 243 (1), 255 (6), 273 (1), 305 (18), 336 (10), 361 (60), 366 (0), 376 (0), 391 (7), 400 (2), 403 (6), 420 (7), 435 (15), 441 (1), 445 (17), 451 (8), 458 (51), 459 (1), 480 (6), 480 (8), 488 (24), 493 (13), 499 (192), 520 (1), 521 (5), 524 (3), 555 (0), 615 (36), 618 (93), 622 (112), 632 (78), 643 (218), 652 (129), 662 (68), 794 (28), 804 (23), 814 (230), 818 (196), 843 (897), 1028 (253), 1101 (2), 1157 (43), 1398 (4), 1440 (4), 1456 (9), 1975 (740), 1979 (773), 1984 (1051), 1998 (311), 2002 (1388), 2005 (349), 2056 (519), 2069 (175), 2996 (27), 3084 (1), 3097 (4) |

| | | |
|---|---|---|
| $[CH_3N(PF_2)_2]Fe_2(CO)_7$ **(17-1S)** | 4 (0), 48 (0), 49 (1), 52 (0), 68 (0), 70 (0), 70 (0), 76 (0), 79 (0), 88 (0), 96 (0), 97 (0), 103 (1), 113 (0), 121 (0), 128 (0), 139 (0), 155 (2), 190 (4), 195 (0), 197 (0), 204 (0), 239 (1), 255 (0), 263 (1), 279 (20), 298 (19), 300 (0), 360 (6), 389 (1), 399 (171), 419 (0), 420 (2), 424 (5), 425 (5), 428 (3), 439 (12), 452 (0), 453 (0), 457 (7), 484 (0), 485 (35), 496 (3), 512 (85), 514 (48), 517 (0), 579 (15), 602 (0), 614 (80), 634 (179), 638 (22), 648 (98), 669 (182), 697 (144), 818 (149), 820 (12), 832 (217), 840 (390), 904 (224), 1099 (348), 1140 (86), 1211 (28), 1458 (0), 1493 (15), 1496 (15), 1916 (445), 2059 (0), 2067 (640), 2076 (268), 2091 (2282), 2101 (1239), 2148 (233), 3077 (27), 3167 (6), 3171 (2) | 21 (0), 44 (1), 47 (1), 51 (0), 58 (0), 68 (0), 69 (0), 74 (0), 80 (0), 85 (0), 94 (0), 95 (0), 101 (0), 107 (0), 114 (0), 120 (0), 139 (1), 144 (1), 188 (0), 191 (0), 196 (3), 202 (0), 234 (3), 246 (1), 256 (0), 284 (5), 285 (6), 300 (10), 354 (3), 395 (0), 402 (26), 405 (92), 418 (4), 422 (1), 427 (11), 442 (0), 446 (1), 446 (0), 447 (0), 455 (2), 479 (1), 488 (57), 508 (0), 514 (47), 517 (16), 534 (1), 568 (9), 590 (1), 605 (99), 626 (166), 629 (21), 645 (61), 667 (191), 679 (155), 786 (113), 791 (21), 805 (198), 812 (357), 864 (248), 1066 (235), 1099 (102), 1160 (24), 1402 (1), 1440 (14), 1445 (15), 1855 (377), 1972 (46), 1987 (469), 1997 (159), 2001 (1888), 2027 (1070), 2064 (229), 3001 (27), 3091 (5), 3098 (2) |
| $[CH_3N(PF_2)_2]Fe_2(CO)_7$ **(17-2T)** | 14 (0), 30 (0), 38 (0), 39 (1), 46 (1), 47 (1), 53 (0), 62 (0), 63 (0), 73 (0), 76 (0), 79 (0), 81 (0), 86 (0), 95 (1), 98 (0), 103 (0), 104 (0), 133 (0), 170 (2), 192 (0), 216 (0), 228 (1), 241 (1), 257 (4), 280 (12), 292 (2), 298 (10), 327 (0), 361 (9), 362 (22), 371 (12), 372 (0), 377 (9), 397 (11), 426 (8), 428 (3), 428 (7), 444 (1), 449 (8), 459 (31), 462 (27), 467 (13), 477 (40), 486 (20), 503 (10), 509 (74), 514 (0), 517 (47), 567 (4), 606 (69), 641 (142), 650 (91), 685 (130), 809 (26), 815 (94), 826 (167), 831 (358), 914 (262), 1054 (400), 1134 (21), 1213 (25), 1458 (0), 1495 (12), 1499 (15), 2041 (653), 2048 (1195), 2056 (437), 2084 (425), 2091 (1941), 2102 (542), 2146 (293), 3086 (25), 3177 (5), 3182 (1) | 14 (0), 36 (0), 43 (1), 44 (0), 49 (0), 50 (0), 56 (0), 62 (0), 67 (0), 71 (0), 75 (0), 81 (0), 84 (0), 88 (0), 96 (0), 98 (0), 101 (0), 105 (1), 131 (0), 160 (2), 196 (0), 209 (0), 234 (0), 247 (3), 254 (6), 275 (5), 286 (1), 289 (8), 347 (6), 348 (0), 362 (31), 373 (0), 373 (2), 399 (15), 407 (4), 411 (1), 437 (3), 438 (1), 449 (10), 453 (3), 466 (18), 472 (22), 483 (1), 486 (1), 491 (4), 515 (1), 533 (29), 537 (36), 542 (95), 548 (2), 605 (66), 636 (162), 642 (66), 675 (134), 784 (31), 786 (85), 799 (163), 803 (350), 875 (229), 1030 (303), 1093 (27), 1164 (23), 1402 (1), 1441 (13), 1446 (15), 1946 (657), 1962 (505), 1981 (241), 1999 (975), 2006 (457), 2007 (1424), 2065 (301), 3007 (25), 3101 (5), 3103 (1) |
| $[CH_3N(PF_2)_2]Fe_2(CO)_7$ **(17-3S)** | 13 (0), 20 (0), 47 (1), 51 (0), 67 (0), 67 (0), 77 (0), 83 (0), 87 (0), 89 (0), 92 (1), 97 (0), 99 (0), 99 (0), 109 (1), 114 (1), 117 (0), 161 (3), 162 (1), 170 (3), 170 (0), 192 (2), 200 (2), 219 (7), 225 (0), 236 (1), 266 (9), 270 (0), 364 (3), 380 (79), 395 (0), 398 (18), 401 (1), 414 (10), 417 (3), 419 (0), 429 (11), 433 (43), 442 (0), 449 (38), 455 (9), 461 (107), 488 (21), 489 (0), 502 (15), 504 (4), 531 (7), 584 (81), 600 (51), 600 (52), 619 (142), 621 (33), 624 (188), 629 (10), 750 (86), 773 (376), 784 (124), 785 (64), 916 (166), 1105 (83), 1122 (0), 1251 (70), 1466 (4), 1484 (14), 1506 (5), 2027 (1171), 2040 (546), 2087 (1464), 2132 (591), 2137 (1064), 2141 (393), 2183 (481), 3043 (48), 3118 (10), 3128 (11) | 8 (0), 22 (0), 41 (2), 50 (0), 62 (0), 63 (0), 71 (0), 79 (0), 79 (0), 84 (0), 87 (1), 92 (0), 94 (0), 96 (0), 102 (1), 108 (0), 110 (0), 146 (10), 154 (0), 160 (2), 162 (0), 193 (1), 195 (1), 216 (3), 217 (1), 230 (1), 265 (15), 271 (1), 335 (2), 364 (75), 383 (1), 390 (2), 407 (2), 407 (19), 420 (0), 421 (51), 427 (1), 430 (2), 437 (0), 454 (8), 465 (46), 471 (25), 491 (3), 499 (12), 508 (5), 508 (7), 519 (6), 562 (48), 601 (53), 602 (35), 618 (34), 618 (112), 623 (213), 632 (28), 739 (65), 754 (248), 760 (120), 763 (163), 893 (139), 1054 (71), 1077 (0), 1196 (50), 1409 (4), 1426 (15), 1451 (6), 1952 (941), 1965 (380), 2013 (1347), 2029 (557), 2032 (1022), 2040 (372), 2089 (368), 2967 (47), 3047 (7), 3055 (10) |

| | | |
|---|---|---|
| $[CH_3N(PF_2)_2]Fe_2(CO)_6$ **(16-1S)** | 35 (0), 41 (0), 52 (0), 56 (0), 72 (0), 74 (0), 79 (0), 81 (0), 90 (0), 94 (0), 96 (0), 99 (0), 102 (0), 104 (0), 123 (0), 142 (0), 149 (0), 181 (1), 184 (1), 206 (4), 212 (1), 222 (4), 229 (1), 250 (2), 271 (4), 308 (1), 373 (4), 383 (3), 404 (6), 414 (3), 420 (1), 429 (4), 438 (4), 449 (1), 453 (1), 467 (10), 468 (23), 477 (19), 499 (3), 500 (19), 514 (22), 526 (11), 575 (69), 580 (93), 594 (2), 604 (37), 612 (48), 629 (152), 630 (220), 786 (156), 805 (55), 833 (196), 851 (290), 888 (226), 1125 (3), 1139 (30), 1288 (105), 1459 (4), 1484 (13), 1502 (8), 2075 (42), 2080 (94), 2091 (839), 2098 (1216), 2109 (2063), 2151 (429), 3029 (58), 3097 (18), 3114 (10) | 34 (0), 38 (0), 51 (0), 53 (0), 70 (0), 71 (0), 77 (0), 78 (0), 89 (0), 92 (0), 93 (0), 95 (0), 99 (0), 101 (0), 126 (0), 138 (0), 147 (0), 177 (1), 181 (1), 203 (2), 204 (2), 219 (1), 230 (1), 242 (3), 270 (3), 304 (2), 349 (4), 381 (10), 394 (9), 403 (4), 415 (3), 429 (4), 450 (0), 455 (2), 459 (4), 473 (41), 479 (0), 485 (3), 504 (5), 511 (0), 513 (10), 525 (5), 565 (42), 588 (42), 589 (34), 607 (13), 611 (68), 626 (221), 632 (107), 755 (142), 778 (47), 809 (182), 822 (289), 859 (197), 1081 (7), 1094 (16), 1246 (88), 1401 (3), 1428 (15), 1450 (9), 1985 (219), 1990 (75), 2002 (721), 2008 (922), 2029 (1496), 2063 (385), 2957 (54), 3030 (15), 3047 (8) |
| $[CH_3N(PF_2)_2]Fe_2(CO)_6$ **(16-2S)** | 14 (0), 45 (1), 46 (0), 60 (0), 60 (2), 65 (0), 78 (0), 85 (0), 88 (0), 99 (0), 101 (0), 108 (0), 110 (0), 143 (3), 149 (1), 182 (0), 196 (1), 211 (1), 219 (7), 226 (0), 250 (4), 253 (0), 268 (1), 277 (1), 284 (1), 308 (20), 344 (5), 371 (7), 391 (2), 393 (18), 411 (2), 426 (5), 440 (1), 448 (3), 450 (22), 461 (6), 471 (9), 471 (23), 474 (1), 487 (37), 504 (5), 542 (8), 552 (6), 565 (98), 596 (18), 600 (96), 607 (123), 620 (72), 699 (131), 821 (164), 830 (51), 839 (221), 857 (375), 901 (195), 1105 (269), 1142 (109), 1211 (29), 1460 (0), 1489 (16), 1496 (17), 1876 (946), 1925 (176), 2082 (0), 2087 (1481), 2097 (2281), 2132 (384), 3076 (23), 3165 (6), 3169 (3), | 8 (0), 44 (0), 45 (0), 56 (2), 57 (0), 66 (0), 76 (0), 83 (0), 86 (0), 95 (0), 98 (0), 107 (0), 109 (0), 141 (1), 141 (1), 182 (0), 203 (0), 207 (1), 218 (8), 233 (0), 243 (4), 244 (0), 273 (2), 276 (0), 283 (2), 305 (14), 360 (12), 372 (16), 392 (1), 397 (2), 403 (5), 414 (3), 434 (8), 438 (0), 448 (2), 454 (7), 473 (13), 479 (5), 490 (11), 494 (0), 508 (3), 545 (2), 553 (12), 571 (89), 594 (0), 595 (15), 602 (225), 611 (56), 680 (120), 790 (114), 800 (26), 808 (197), 825 (363), 864 (213), 1069 (170), 1104 (121), 1163 (26), 1405 (0), 1437 (18), 1445 (17), 1824 (610), 1857 (180), 1991 (4), 1996 (1263), 2015 (1688), 2041 (347), 3000 (23), 3091 (6), 3095 (2), |
| $[CH_3N(PF_2)_2]Fe_2(CO)_6$ **(16-3T)** | 8 (0), 24 (0), 45 (1), 53 (0), 58 (2), 58 (0), 64 (0), 64 (0), 66 (1), 77 (0), 85 (0), 97 (0), 97 (1), 105 (0), 116 (7), 156 (2), 164 (1), 170 (4), 176 (0), 200 (0), 231 (8), 234 (3), 257 (1), 261 (1), 287 (0), 289 (30), 322 (60), 328 (0), 379 (2), 382 (69), 403 (7), 416 (16), 421 (5), 425 (3), 427 (18), 436 (10), 438 (1), 459 (23), 468 (19), 469 (18), 474 (3), 502 (38), 512 (18), 520 (9), 544 (3), 596 (64), 623 (241), 651 (152), 693 (135), 806 (43), 814 (171), 833 (152), 841 (334), 905 (237), 1108 (386), 1132 (0), 1222 (48), 1459 (0), 1482 (12), 1508 (17), 1940 (414), 2032 (803), 2076 (1347), 2088 (576), 2092 (1490), 2141 (293), 3077 (27), 3164 (6), 3173 (3) | 12 (0), 18 (0), 36 (0), 45 (1), 55 (0), 57 (0), 62 (0), 68 (0), 72 (0), 80 (0), 84 (0), 93 (0), 96 (0), 101 (0), 120 (1), 147 (2), 173 (0), 178 (0), 183 (2), 197 (0), 234 (4), 243 (0), 255 (1), 268 (1), 278 (1), 295 (15), 338 (0), 343 (4), 375 (0), 383 (72), 397 (4), 419 (11), 424 (15), 427 (6), 436 (1), 448 (0), 453 (1), 468 (15), 473 (6), 488 (13), 499 (18), 505 (45), 513 (1), 531 (8), 548 (24), 592 (68), 615 (217), 643 (111), 679 (135), 782 (38), 785 (135), 805 (170), 813 (309), 868 (232), 1078 (279), 1090 (15), 1171 (46), 1403 (1), 1431 (13), 1455 (18), 1841 (346), 1950 (547), 1983 (1098), 1999 (1251), 2005 (573), 2054 (296), 3001 (26), 3091 (5), 3099 (2) |
| $[CH_3N(PF_2)_2]Fe_2(CO)_6$ **(16-4T)** | 12 (0), 20 (0), 31 (0), 34 (0), 68 (0), 73 (0), 75 (0), 77 (0), 80 (0), 87 (0), 93 (0), 94 (0), 97 (0), 104 (1), 134 (0), 150 (0), 166 (0), 172 (1), 184 (1), 200 (4), 206 (3), 223 (4), 228 (2), 239 (0), 259 (2), 275 (7), 327 (3), 361 (2), 374 (6), 381 (6), 393 (1), 396 (5), 403 (0), 412 (3), 426 (4), 429 (7), 430 (2), 455 (62), 473 (36), 478 (21), 484 (3), 491 (9), 535 (43), 552 (43), 564 (39), 567 (42), 586 (31), 597 (53), 605 (138), 790 (133), 798 (129), 814 (157), 821 (109), 885 (256), 1094 (112), 1115 (1), 1206 (40), 1454 (4), 1494 (13), 1505 (7), 2058 (701), 2077 (563), 2090 (838), 2093 (902), 2117 (1682), 2143 (277), 3042 (46), 3115 (15), 3132 (9) | 11 (0), 19 (0), 28 (0), 32 (0), 66 (0), 73 (0), 76 (0), 77 (0), 82 (0), 87 (0), 90 (0), 92 (0), 96 (0), 102 (0), 119 (0), 143 (1), 165 (0), 170 (0), 187 (0), 201 (2), 209 (4), 229 (2), 237 (2), 243 (0), 253 (2), 281 (4), 335 (2), 364 (4), 370 (8), 377 (6), 392 (7), 398 (6), 415 (1), 425 (18), 443 (0), 450 (2), 470 (11), 473 (15), 479 (2), 487 (2), 499 (15), 508 (9), 546 (47), 559 (37), 570 (15), 573 (42), 580 (32), 599 (61), 602 (193), 765 (134), 771 (44), 787 (195), 802 (102), 845 (264), 1044 (50), 1065 (1), 1144 (13), 1394 (5), 1435 (13), 1449 (5), 1969 (584), 1979 (491), 1998 (783), 1999 (646), 2020 (1607), 2048 (375), 2969 (34), 3046 (11), 3065 (6) |

| | | |
|---|---|---|
| $[CH_3N(PF_2)_2]Fe_2(CO)_5$ **(15-1S )** | 34 (0), 42 (0), 47 (0), 66 (0), 69 (0), 75 (0), 83 (0), 87 (0), 90 (0), 93 (0), 97 (0), 102 (0), 105 (0), 146 (0), 152 (1), 172 (1), 186 (1), 206 (0), 211 (5), 219 (0), 239 (0), 251 (4), 293 (7), 318 (5), 396 (7), 402 (11), 410 (1), 411 (2), 428 (6), 449 (4), 452 (2), 462 (1), 471 (10), 480 (50), 494 (7), 498 (5), 523 (25), 540 (44), 574 (21), 583 (88), 602 (53), 618 (52), 628 (120), 643 (100), 797 (61), 817 (52), 840 (155), 847 (388), 875 (317), 1121 (2), 1147 (30), 1219 (67), 1451 (5), 1490 (17), 1493 (9), 2059 (246), 2073 (921), 2085 (539), 2093 (2049), 2134 (577), 3038 (48), 3106 (13), 3140 (9) | 32 (0), 41 (1), 43 (0), 61 (0), 66 (0), 72 (0), 80 (0), 85 (0), 89 (0), 91 (0), 94 (0), 98 (0), 101 (0), 140 (0), 147 (1), 169 (0), 181 (1), 204 (1), 211 (3), 214 (1), 242 (0), 248 (3), 292 (6), 315 (4), 384 (3), 391 (16), 400 (3), 404 (4), 426 (11), 455 (3), 459 (0), 467 (9), 470 (44), 479 (7), 502 (9), 520 (2), 525 (5), 557 (20), 575 (35), 585 (56), 597 (26), 616 (44), 623 (165), 645 (53), 763 (52), 792 (19), 810 (181), 821 (394), 843 (259), 1075 (1), 1104 (15), 1169 (51), 1392 (4), 1435 (16), 1439 (12), 1963 (379), 1990 (677), 2000 (302), 2004 (1516), 2048 (602), 2966 (39), 3036 (9), 3077 (6) |
| $[CH_3N(PF_2)_2]Fe_2(CO)_5$ **(15-2S)** | 8 (0), 16 (0), 39 (0), 58 (1), 61 (0), 66 (0), 75 (0), 76 (0), 80 (0), 84 (0), 87 (0), 97 (0), 119 (3), 128 (1), 135 (2), 178 (0), 208 (2), 221 (4), 241 (1), 247 (1), 257 (6), 274 (2), 294 (0), 339 (7), 379 (1), 384 (10), 394 (44), 407 (6), 414 (2), 428 (18), 447 (6), 450 (11), 457 (12), 465 (6), 479 (2), 490 (2), 504 (29), 520 (10), 540 (84), 560 (42), 582 (61), 593 (98), 623 (70), 699 (105), 806 (188), 819 (76), 839 (211), 853 (264), 889 (284), 1128 (31), 1146 (299), 1215 (54), 1456 (0), 1481 (13), 1504 (18), 2002 (573), 2060 (227), 2068 (1498), 2081 (2106), 2115 (346), 3071 (29), 3155 (7), 3171 (3) | 17 (0), 32 (0), 48 (1), 61 (0), 64 (0), 67 (0), 76 (0), 81 (0), 83 (0), 84 (0), 91 (0), 96 (1), 116 (2), 119 (1), 143 (0), 179 (0), 201 (2), 216 (3), 233 (3), 241 (1), 247 (5), 283 (9), 287 (1), 340 (7), 359 (0), 368 (22), 386 (5), 395 (5), 424 (5), 432 (8), 442 (11), 462 (8), 475 (7), 485 (3), 490 (2), 505 (20), 521 (6), 528 (16), 556 (17), 574 (49), 609 (58), 611 (40), 657 (122), 693 (108), 770 (162), 794 (68), 811 (166), 820 (241), 860 (230), 1086 (22), 1119 (196), 1174 (74), 1403 (1), 1430 (12), 1450 (18), 1786 (283), 1971 (342), 1979 (1130), 2000 (1768), 2023 (134), 2997 (26), 3085 (7), 3094 (3) |
| $[CH_3N(PF_2)_2]Fe_2(CO)_5$ **(15-3T)** | 19 (0), 34 (0), 40 (0), 47 (0), 54 (0), 66 (0), 71 (0), 75 (0), 80 (0), 84 (0), 90 (0), 99 (0), 103 (0), 132 (1), 138 (1), 145 (1), 170 (1), 181 (1), 188 (4), 201 (6), 220 (1), 239 (3), 267 (5), 290 (2), 330 (3), 343 (1), 379 (1), 392 (6), 401 (16), 413 (12), 418 (5), 428 (1), 432 (5), 446 (2), 460 (15), 474 (9), 482 (81), 496 (3), 521 (24), 525 (19), 575 (67), 604 (32), 610 (35), 624 (212), 788 (112), 803 (59), 838 (125), 842 (338), 879 (341), 1117 (1), 1145 (28), 1220 (169), 1452 (8), 1493 (6), 1496 (16), 2042 (396), 2067 (1429), 2092 (1294), 2094 (608), 2139 (783), 3034 (63), 3101 (16), 3130 (9) | 22 (0), 37 (0), 42 (0), 44 (0), 59 (1), 69 (0), 72 (0), 79 (0), 83 (0), 86 (0), 90 (0), 97 (0), 101 (0), 127 (1), 136 (0), 146 (1), 167 (1), 180 (0), 192 (0), 200 (7), 230 (1), 239 (3), 276 (4), 294 (3), 348 (2), 359 (2), 375 (2), 393 (5), 394 (7), 411 (2), 437 (11), 450 (0), 453 (6), 466 (38), 473 (11), 486 (3), 496 (8), 519 (13), 527 (16), 556 (48), 579 (33), 601 (13), 605 (38), 623 (183), 757 (86), 780 (35), 806 (197), 813 (285), 846 (313), 1066 (0), 1104 (12), 1165 (117), 1394 (8), 1437 (7), 1440 (18), 1950 (381), 1979 (1032), 2002 (1035), 2005 (487), 2053 (696), 2961 (48), 3033 (12), 3064 (6) |
| $[CH_3N(PF_2)_2]Fe_2(CO)_5$ **(15-4S)** | 36 (0), 45 (0), 54 (0), 59 (0), 73 (0), 76 (0), 79 (0), 79 (0), 90 (0), 91 (0), 96 (0), 96 (0), 131 (1), 136 (1), 154 (0), 169 (1), 180 (2), 199 (3), 210 (1), 216 (2), 231 (3), 242 (2), 271 (8), 318 (4), 369 (5), 383 (2), 397 (5), 413 (4), 417 (2), 428 (2), 436 (2), 453 (2), 463 (7), 470 (9), 477 (22), 498 (11), 513 (29), 533 (8), 540 (55), 563 (95), 580 (89), 591 (27), 606 (55), 629 (170), 785 (132), 807 (46), 822 (241), 854 (274), 884 (213), 1124 (7), 1138 (21), 1288 (105), 1458 (3), 1485 (13), 1503 (6), 2065 (160), 2074 (724), 2085 (881), 2095 (2154), 2135 (420), 3029 (57), 3099 (17), 3115 (11) | 31 (0), 39 (0), 53 (1), 56 (0), 69 (0), 74 (0), 77 (0), 77 (0), 87 (0), 88 (0), 91 (0), 92 (0), 114 (0), 129 (0), 136 (0), 166 (1), 177 (3), 194 (2), 201 (2), 210 (1), 224 (1), 246 (2), 272 (6), 315 (3), 340 (6), 381 (7), 388 (5), 408 (2), 411 (7), 423 (1), 448 (2), 459 (4), 468 (16), 479 (3), 487 (5), 504 (4), 511 (11), 536 (9), 556 (27), 562 (46), 581 (28), 590 (75), 606 (73), 629 (135), 754 (102), 779 (48), 794 (236), 827 (258), 851 (175), 1076 (13), 1095 (7), 1251 (65), 1400 (3), 1427 (15), 1447 (7), 1971 (372), 1982 (555), 1992 (684), 2005 (1625), 2044 (420), 2956 (52), 3030 (14), 3049 (8) |

**Table S2.** The vibrational frequencies (in $cm^{-1}$) and infrared intensities (in km/mol, given in parentheses) of the $[CH_3N(PF_2)_2]_2Fe_2(CO)_n$ (n = 6, 5, 4, 3) isomers at the B3LYP/DZP and BP86/DZP levels.

| Structure | B3LYP/DZP | BP86/DZP |
|---|---|---|
| $[CH_3N(PF_2)_2]_2Fe_2(CO)_6$ **(26-1S)** | 13 (0), 16 (0), 20 (0), 38 (0), 41 (0), 45 (2), 46 (0), 63 (0), 69 (0), 76 (0), 78 (0), 92 (0), 92 (0), 94 (0), 97 (0), 102 (0), 103 (0), 104 (0), 110 (0), 114 (0), 131 (0), 156 (1), 174 (0), 186 (0), 188 (3), 196 (0), 211 (0), 217 (0), 240 (0), 251 (0), 258 (5), 261 (0), 288 (40), 293 (0), 298 (0), 301 (0), 311 (0), 313 (17), 317 (0), 328 (5), 357 (0), 371 (64), 398 (0), 404 (0), 420 (12), 422 (0), 435 (5), 437 (0), 439 (0), 447 (0), 448 (10), 472 (0), 472 (24), 477 (0), 478 (0), 496 (0), 499 (0), 521 (260), 538 (0), 545 (22), 588 (0), 590 (119), 613 (362), 615 (0), 640 (0), 646 (75), 687 (320), 698 (0), 808 (0), 814 (2), 816 (0), 818 (184), 820 (765), 824 (0), 828 (385), 836 (0), 911 (0), 933 (611), 1035 (812), 1043 (0), 1133 (34), 1133 (0), 1213 (0), 1214 (54), 1459 (1), 1459 (0), 1494 (21), 1494 (0), 1502 (29), 1502 (0), 2052 (0), 2068 (1172), 2074 (0), 2076 (2368), 2110 (737), 2126 (0), 3090 (51), 3090 (0), 3181 (0), 3181 (9), 3186 (2), 3186 (0) | 11 (0), 12 (0), 25 (0), 28 (0), 41 (2), 42 (0), 43 (0), 62 (0), 70 (0), 74 (0), 74 (0), 90 (0), 91 (0), 92 (0), 94 (0), 99 (0), 101 (0), 101 (0), 107 (0), 114 (0), 127 (0), 153 (1), 168 (0), 178 (3), 187 (0), 202 (0), 208 (0), 214 (0), 234 (0), 247 (3), 250 (1), 251 (0), 280 (39), 289 (0), 289 (0), 292 (0), 301 (13), 305 (0), 313 (0), 338 (1), 346 (0), 356 (55), 388 (1), 400 (0), 405 (0), 408 (10), 412 (0), 425 (15), 446 (0), 457 (3), 460 (0), 465 (16), 472 (0), 473 (2), 480 (0), 482 (0), 484 (0), 509 (231), 539 (0), 542 (0), 592 (0), 596 (108), 608 (0), 613 (342), 631 (0), 637 (46), 677 (324), 686 (0), 778 (0), 786 (5), 789 (0), 789 (162), 790 (761), 796 (0), 801 (358), 806 (0), 874 (0), 895 (591), 1006 (637), 1012 (0), 1091 (35), 1091 (0), 1164 (0), 1164 (43), 1403 (1), 1403 (0), 1441 (20), 1441 (0), 1449 (32), 1449 (0), 1966 (0), 1990 (1924), 1990 (973), 1997 (0), 2029 (655), 2045 (0), 3012 (51), 3012 (0), 3107 (0), 3107 (9), 3109 (2), 3109 (0) |
| $[CH_3N(PF_2)_2]_2Fe_2(CO)_6$ **(26-2S)** | 19 (0), 33 (0), 42 (0), 56 (0), 57 (4), 73 (0), 74 (0), 75 (0), 75 (0), 75 (0), 88 (0), 92 (0), 92 (0), 92 (1), 101 (0), 104 (0), 111 (1), 133 (1), 139 (0), 157 (0), 162 (1), 186 (0), 193 (2), 196 (0), 201 (0), 206 (0), 213 (0), 240 (4), 243 (0), 246 (2), 262 (9), 263 (0), 275 (0), 285 (7), 286 (45), 291 (1), 295 (0), 297 (0), 308 (20), 310 (0), 332 (0), 354 (0), 384 (0), 399 (38), 406 (0), 419 (110), 423 (24), 427 (0), 434 (0), 434 (13), 444 (9), 460 (0), 464 (0), 465 (0), 465 (0), 470 (0), 477 (0), 478 (32), 523 (0), 547 (0), 552 (93), 553 (83), 574 (0), 612 (0), 631 (79), 669 (546), 703 (305), 712 (0), 823 (0), 827 (1), 827 (0), 835 (2), 836 (219), 839 (403), 845 (648), 860 (0), 915 (0), 923 (345), 1083 (806), 1090 (1), 1138 (73), 1139 (0), 1211 (0), 1212 (46), 1461 (0), 1461 (1), 1495 (0), 1495 (27), 1499 (7), 1499 (21), 1774 (586), 1785 (2), 2089 (1), 2093 (1467), 2112 (2066), 2131 (0), 3084 (51), 3084 (1), 3175 (0), 3175 (8), 3179 (0), 3179 (3) | 15 (0), 28 (0), 39 (0), 52 (0), 54 (4), 71 (1), 73 (0), 73 (0), 84 (0), 84 (0), 85 (0), 90 (0), 90 (0), 90 (0), 98 (0), 102 (0), 109 (0), 127 (2), 134 (0), 149 (0), 152 (2), 183 (0), 191 (0), 191 (0), 197 (0), 199 (0), 207 (0), 234 (4), 238 (2), 239 (0), 251 (7), 253 (0), 262 (0), 273 (7), 277 (43), 284 (0), 287 (0), 296 (0), 309 (0), 313 (9), 325 (0), 351 (0), 369 (0), 386 (71), 400 (0), 403 (0), 408 (22), 422 (15), 434 (0), 437 (29), 444 (0), 447 (0), 448 (0), 453 (2), 459 (21), 460 (0), 463 (0), 468 (0), 512 (0), 531 (0), 549 (37), 553 (84), 570 (0), 591 (0), 621 (88), 638 (546), 685 (309), 693 (0), 791 (0), 794 (0), 796 (2), 803 (153), 803 (4), 807 (354), 812 (634), 827 (0), 871 (0), 879 (378), 1055 (643), 1062 (1), 1098 (104), 1099 (0), 1160 (0), 1160 (37), 1406 (0), 1407 (0), 1445 (0), 1445 (26), 1447 (8), 1447 (21), 1744 (473), 1752 (3), 1992 (0), 1997 (1286), 2023 (1630), 2037 (0), 3006 (57), 3006 (1), 3099 (0), 3099 (8), 3102 (3), 3102 (0) |
| $[CH_3N(PF_2)_2]_2Fe_2(CO)_6$ **(26-3T)** | 14 (0), 29 (0), 35 (0), 36 (2), 43 (0), 48 (0), 51 (1), 59 (1), 64 (0), 64 (0), 69 (0), 76 (0), 77 (0), 83 (0), 86 (0), 88 (0), 91 (1), 95 (0), 99 (0), 100 (0), 109 (1), 112 (0), 116 (1), 140 (5), 144 (0), 161 (0), 164 (3), 181 (0), 186 (2), 204 (0), 237 (0), 252 (29), 253 (0), 257 (7), 261 (4), 264 (0), 276 (0), 284 (7), 285 (8), 291 (5), 301 (2), 307 (1), 351 (42), 356 (1), 360 (10), 371 (52), 384 (1), 387 (2), 421 (1), 423 (21), 430 (0), 430 (22), 432 (0), 437 (2), 437 (8), 457 (10), 463 (0), 471 (0), 478 (7), 485 (2), 490 (98), 500 (8), 534 (0), 568 (66), 581 (202), 627 (38), 679 (278), 685 (1), 807 (205), 808 (0), 810 (109), 815 (235), 829 (491), 834 (13), 840 (304), 846 (24), 902 (25), 916 (408), 1060 (747), 1066 (1), 1133 (42), 1133 (0), 1210 (3), 1210 (46), 1458 (1), 1458 (0), 1495 (19), 1495 (6), 1498 (24), 1498 (4), 2021 (267), 2033 (534), 2060 (2127), 2065 (3), 2079 (1324), 2113 (196), 3083 (51), 3083 (1), 3171 (0), 3171 (10), 3184 (1), 3184 (2) | 13 (0), 26 (0), 32 (0), 33 (1), 40 (1), 49 (0), 52 (0), 61 (0), 64 (0), 68 (0), 75 (0), 77 (0), 81 (0), 84 (0), 86 (0), 89 (0), 91 (0), 95 (0), 96 (0), 99 (0), 107 (0), 115 (0), 123 (1), 146 (1), 147 (1), 152 (1), 176 (0), 183 (0), 196 (0), 218 (2), 221 (0), 228 (15), 240 (0), 244 (1), 258 (8), 268 (7), 275 (5), 281 (9), 290 (2), 308 (2), 311 (0), 347 (9), 350 (12), 360 (28), 371 (2), 378 (1), 390 (12), 399 (6), 405 (4), 412 (7), 426 (5), 431 (12), 438 (16), 444 (3), 455 (10), 456 (10), 466 (1), 468 (4), 472 (12), 489 (7), 514 (18), 522 (2), 547 (82), 572 (46), 579 (189), 613 (34), 661 (224), 668 (27), 740 (213), 774 (132), 777 (159), 785 (90), 794 (419), 803 (81), 810 (218), 814 (11), 856 (90), 867 (349), 1038 (428), 1045 (117), 1089 (24), 1091 (18), 1157 (18), 1160 (25), 1402 (1), 1403 (0), 1438 (12), 1440 (14), 1445 (15), 1447 (16), 1925 (640), 1945 (43), 1979 (1287), 1985 (820), 1995 (852), 2032 (196), 3004 (31), 3004 (24), 3092 (6), 3095 (4), 3101 (2), 3109 (1), |

| | | |
|---|---|---|
| $[CH_3N(PF_2)_2]_2Fe_2(CO)_5$ **(25-1S)** | 14 (0), 34 (0), 45 (2), 46 (0), 46 (0), 51 (0), 51 (2), 59 (0), 70 (0), 83 (0), 86 (0), 97 (0), 99 (0), 103 (0), 114 (0), 115 (0), 127 (0), 131 (0), 149 (0), 151 (2), 182 (0), 194 (0), 196 (1), 203 (0), 206 (0), 210 (0), 241 (0), 243 (4), 254 (0), 261 (11), 266 (0), 271 (7), 281 (31), 294 (0), 311 (0), 312 (3), 318 (0), 335 (15), 380 (0), 382 (27), 390 (0), 401 (88), 428 (1), 431 (75), 434 (9), 448 (1), 449 (40), 461 (1), 471 (0), 479 (0), 480 (6), 483 (6), 486 (0), 523 (8), 526 (23), 553 (12), 570 (254), 572 (94), 577 (0), 605 (107), 616 (179), 706 (250), 715 (0), 830 (0), 833 (1), 833 (0), 840 (308), 842 (1), 846 (407), 851 (701), 868 (0), 923 (0), 935 (410), 1103 (634), 1109 (3), 1143 (201), 1146 (3), 1217 (0), 1218 (70), 1461 (0), 1461 (0), 1492 (9), 1492 (21), 1496 (0), 1496 (30), 1863 (498), 2039 (55), 2057 (1438), 2071 (1685), 2102 (194), 3079 (48), 3079 (1), 3170 (0), 3170 (10), 3173 (0), 3173 (3) | 13 (0), 28 (0), 40 (1), 48 (3), 49 (0), 57 (0), 66 (0), 66 (0), 70 (0), 83 (0), 85 (0), 92 (0), 96 (0), 102 (0), 112 (0), 113 (0), 125 (1), 126 (0), 142 (0), 143 (2), 185 (0), 191 (0), 197 (0), 203 (0), 205 (0), 210 (0), 236 (0), 239 (1), 242 (0), 252 (7), 258 (0), 263 (5), 276 (36), 286 (0), 303 (4), 312 (0), 315 (0), 345 (4), 375 (0), 382 (9), 383 (0), 396 (66), 403 (0), 410 (12), 428 (61), 434 (0), 438 (33), 455 (0), 461 (5), 470 (0), 473 (0), 481 (1), 488 (3), 509 (4), 533 (98), 552 (27), 565 (136), 566 (0), 584 (57), 595 (105), 612 (182), 690 (247), 699 (0), 797 (0), 799 (0), 802 (8), 807 (241), 810 (4), 814 (374), 817 (692), 835 (0), 883 (0), 895 (424), 1070 (412), 1074 (2), 1105 (266), 1108 (3), 1167 (0), 1168 (62), 1405 (1), 1405 (0), 1440 (11), 1440 (20), 1445 (0), 1445 (30), 1804 (419), 1961 (101), 1977 (1100), 1993 (1323), 2018 (219), 3002 (50), 3002 (1), 3095 (1), 3095 (10), 3098 (0), 309 |
| $[CH_3N(PF_2)_2]_2Fe_2(CO)_5$ **(25-2T)** | 13 (0), 16 (0), 38 (0), 39 (0), 39 (1), 45 (2), 46 (0), 56 (0), 61 (0), 68 (0), 68 (0), 76 (0), 76 (0), 82 (0), 90 (0), 91 (0), 97 (0), 108 (1), 114 (0), 127 (0), 150 (0), 164 (2), 166 (0), 172 (1), 193 (0), 199 (0), 210 (0), 234 (0), 258 (4), 259 (0), 263 (0), 273 (44), 283 (4), 285 (10), 292 (6), 294 (5), 308 (1), 316 (10), 335 (1), 369 (0), 375 (0), 386 (51), 418 (41), 423 (24), 424 (1), 426 (0), 439 (5), 440 (5), 442 (6), 453 (28), 457 (0), 474 (0), 474 (5), 480 (1), 487 (23), 493 (51), 519 (2), 529 (15), 567 (78), 574 (253), 611 (43), 688 (326), 695 (1), 811 (113), 816 (119), 819 (126), 828 (202), 842 (324), 845 (169), 848 (293), 858 (38), 907 (42), 923 (462), 1073 (755), 1079 (4), 1136 (52), 1136 (1), 1214 (8), 1214 (56), 1458 (0), 1458 (0), 1492 (4), 1492 (23), 1500 (5), 1500 (25), 2020 (77), 2036 (1878), 2053 (220), 2073 (1499), 2103 (189), 3083 (51), 3083 (2), 3171 (0), 3171 (9), 3181 (0), 3181 (3) | 13 (0), 18 (0), 37 (1), 41 (2), 42 (0), 58 (0), 62 (0), 68 (0), 69 (0), 70 (0), 70 (0), 77 (0), 78 (0), 86 (0), 88 (0), 89 (0), 96 (0), 110 (1), 113 (0), 131 (0), 145 (0), 153 (2), 171 (1), 176 (0), 194 (0), 199 (0), 209 (0), 231 (0), 247 (3), 249 (1), 259 (5), 266 (29), 269 (3), 280 (1), 289 (2), 296 (5), 302 (2), 327 (5), 349 (2), 357 (0), 359 (0), 376 (52), 400 (1), 411 (15), 411 (34), 422 (10), 435 (6), 439 (1), 453 (1), 460 (1), 462 (0), 467 (8), 474 (6), 489 (12), 492 (50), 503 (20), 507 (9), 553 (38), 570 (199), 573 (60), 597 (39), 674 (302), 680 (3), 777 (127), 783 (120), 786 (107), 794 (172), 809 (433), 814 (44), 818 (263), 825 (22), 865 (61), 879 (451), 1048 (562), 1054 (3), 1095 (74), 1095 (1), 1162 (16), 1163 (48), 1402 (1), 1402 (0), 1440 (6), 1440 (22), 1448 (4), 1448 (25), 1944 (59), 1958 (1428), 1971 (105), 1986 (1417), 2017 (168), 3004 (56), 3004 (2), 3095 (0), 3095 (9), 3104 (0), 3104 (3) |

| | | |
|---|---|---|
| $[CH_3N(PF_2)_2]_2Fe_2(CO)_4$ **(24-1S)** | 31 (0), 40 (0), 54 (2), 55 (0), 71 (0), 72 (0), 76 (0), 80 (0), 81 (0), 84 (0), 87 (0), 92 (0), 97 (0), 114 (0), 126 (0), 133 (0), 141 (0), 148 (0), 154 (1), 165 (0), 176 (3), 184 (0), 194 (1), 200 (2), 216 (1), 226 (2), 238 (4), 244 (4), 255 (1), 263 (2), 268 (2), 277 (3), 305 (7), 306 (5), 316 (12), 358 (1), 377 (4), 386 (3), 394 (27), 408 (6), 423 (5), 436 (7), 447 (7), 456 (12), 459 (8), 467 (14), 484 (3), 494 (5), 505 (9), 507 (6), 539 (68), 557 (33), 567 (35), 578 (136), 585 (21), 590 (49), 608 (219), 702 (97), 786 (186), 802 (37), 808 (51), 832 (47), 835 (178), 846 (563), 852 (135), 867 (364), 888 (110), 918 (222), 1099 (308), 1127 (3), 1139 (29), 1142 (82), 1216 (33), 1290 (104), 1460 (4), 1461 (0), 1483 (12), 1490 (15), 1497 (16), 1503 (7), 2069 (76), 2081 (1048), 2095 (1774), 2122 (352), 3028 (62), 3079 (23), 3097 (18), 3113 (10), 3170 (5), 3172 (2) | 27 (0), 36 (0), 49 (2), 51 (0), 62 (0), 70 (0), 73 (0), 78 (0), 79 (0), 83 (0), 87 (0), 92 (0), 95 (0), 112 (0), 125 (1), 130 (0), 139 (0), 146 (1), 149 (0), 162 (0), 176 (1), 185 (1), 191 (1), 200 (2), 210 (1), 224 (2), 233 (2), 238 (6), 246 (0), 254 (1), 264 (2), 274 (5), 299 (6), 306 (1), 312 (11), 347 (3), 359 (1), 374 (8), 390 (34), 399 (7), 409 (3), 415 (6), 439 (13), 453 (6), 456 (9), 482 (2), 489 (9), 496 (2), 498 (1), 507 (25), 547 (38), 562 (28), 564 (23), 574 (41), 581 (33), 588 (16), 602 (257), 686 (94), 756 (163), 775 (33), 782 (37), 800 (32), 801 (151), 816 (548), 820 (126), 836 (340), 859 (93), 879 (253), 1066 (202), 1083 (7), 1093 (14), 1103 (110), 1166 (31), 1250 (86), 1402 (3), 1404 (1), 1426 (14), 1438 (15), 1445 (16), 1451 (9), 1979 (196), 1991 (806), 2010 (1369), 2031 (293), 2956 (58), 3002 (24), 3029 (14), 3045 (8), 3095 (5), 3098 (2) |
| $[CH_3N(PF_2)_2]_2Fe_2(CO)_4$ **(24-2S)** | 33 (0), 34 (1), 44 (0), 56 (0), 57 (3), 63 (0), 64 (0), 70 (0), 90 (0), 90 (0), 99 (0), 103 (0), 104 (0), 110 (0), 115 (0), 136 (0), 147 (0), 149 (1), 164 (1), 171 (0), 185 (1), 190 (0), 204 (1), 217 (1), 224 (2), 240 (1), 254 (12), 265 (6), 266 (1), 270 (1), 275 (2), 284 (10), 293 (1), 297 (11), 321 (2), 334 (15), 353 (5), 381 (1), 382 (18), 414 (46), 425 (16), 436 (8), 442 (33), 459 (8), 461 (18), 470 (6), 487 (1), 508 (2), 508 (6), 530 (31), 534 (6), 566 (163), 570 (7), 580 (52), 596 (43), 626 (45), 690 (270), 699 (3), 812 (63), 823 (133), 826 (35), 834 (354), 845 (183), 848 (428), 850 (353), 867 (4), 897 (45), 903 (339), 1107 (629), 1114 (15), 1140 (136), 1142 (3), 1214 (31), 1214 (46), 1458 (0), 1459 (0), 1491 (0), 1491 (26), 1502 (3), 1502 (25), 1900 (447), 1944 (465), 2063 (2193), 2078 (22), 3076 (62), 3076 (0), 3163 (1), 3163 (10), 3175 (0), 3175 (3) | 32 (0), 33 (1), 44 (0), 52 (0), 54 (2), 64 (0), 66 (0), 70 (0), 86 (0), 92 (0), 96 (0), 104 (0), 106 (0), 107 (1), 122 (0), 130 (0), 135 (0), 137 (1), 162 (2), 176 (0), 180 (0), 187 (0), 200 (1), 211 (0), 227 (0), 238 (1), 245 (7), 254 (3), 257 (1), 264 (19), 265 (2), 285 (3), 288 (0), 295 (8), 317 (1), 335 (6), 350 (5), 366 (1), 366 (5), 389 (60), 400 (0), 408 (18), 423 (41), 444 (6), 450 (8), 460 (10), 466 (1), 488 (2), 497 (7), 516 (16), 540 (8), 562 (98), 565 (3), 583 (42), 589 (4), 613 (28), 675 (261), 683 (1), 783 (36), 794 (163), 795 (13), 799 (217), 811 (126), 815 (536), 816 (340), 835 (12), 859 (22), 864 (352), 1075 (371), 1079 (5), 1105 (280), 1108 (5), 1163 (29), 1163 (34), 1403 (1), 1403 (0), 1442 (2), 1442 (26), 1448 (3), 1448 (25), 1832 (370), 1876 (341), 1976 (1668), 1990 (114), 2999 (68), 2999 (0), 3087 (2), 3087 (10), 3098 (0), 3098 (3) |
| $[CH_3N(PF_2)_2]_2Fe_2(CO)_4$ **(24-3T)** | 22 (0), 30 (1), 33 (0), 39 (1), 45 (0), 49 (0), 60 (0), 63 (2), 64 (0), 67 (0), 79 (0), 89 (1), 94 (0), 95 (0), 101 (0), 118 (0), 119 (0), 146 (0), 147 (3), 150 (1), 173 (1), 180 (0), 190 (0), 190 (0), 221 (1), 242 (0), 247 (5), 251 (11), 261 (4), 262 (0), 273 (1), 288 (2), 289 (1), 291 (3), 304 (1), 322 (27), 370 (0), 372 (14), 383 (32), 420 (1), 421 (10), 430 (1), 433 (47), 435 (8), 450 (2), 452 (13), 468 (3), 469 (11), 484 (35), 485 (9), 489 (1), 496 (22), 521 (5), 573 (68), 589 (256), 628 (33), 676 (251), 683 (6), 790 (62), 802 (99), 805 (204), 824 (307), 830 (413), 841 (134), 845 (353), 852 (32), 890 (79), 903 (368), 1104 (555), 1110 (59), 1135 (110), 1136 (26), 1204 (0), 1204 (47), 1458 (0), 1459 (0), 1488 (5), 1488 (19), 1497 (5), 1497 (27), 2033 (566), 2059 (1595), 2078 (405), 2119 (562), 3073 (58), 3073 (5), 3156 (0), 3156 (16), 3177 (0), 3177 (3) | 16 (0), 32 (0), 37 (2), 42 (0), 52 (0), 56 (0), 58 (1), 63 (0), 66 (0), 66 (0), 77 (0), 85 (0), 88 (0), 96 (0), 105 (0), 114 (0), 136 (0), 138 (2), 158 (1), 158 (0), 179 (1), 184 (0), 188 (0), 196 (1), 232 (0), 238 (1), 241 (0), 243 (14), 252 (1), 254 (7), 271 (0), 285 (2), 293 (6), 293 (6), 315 (0), 338 (5), 338 (8), 359 (0), 382 (67), 398 (1), 399 (0), 408 (8), 422 (27), 430 (8), 448 (4), 448 (3), 457 (2), 485 (8), 488 (14), 491 (11), 502 (12), 502 (1), 537 (68), 563 (47), 587 (189), 591 (48), 669 (210), 676 (10), 766 (18), 777 (120), 781 (106), 797 (230), 807 (516), 812 (0), 817 (222), 827 (132), 855 (82), 866 (372), 1073 (275), 1076 (27), 1103 (241), 1105 (35), 1158 (0), 1158 (42), 1401 (1), 1401 (0), 1440 (15), 1440 (16), 1446 (0), 1446 (28), 1821 (377), 1961 (1363), 1975 (635), 2014 (509), 2997 (55), 2997 (7), 3083 (0), 3083 (13), 3101 (0), 3101 (2) |

| | | |
|---|---|---|
| $[CH_3N(PF_2)_2]_2Fe_2(CO)_3$ **(23-1S)** | 35 (0), 36 (0), 55 (1), 57 (1), 64 (0), 72 (0), 76 (0), 77 (0), 84 (0), 86 (0), 93 (0), 95 (0), 116 (0), 127 (0), 141 (1), 150 (0), 151 (1), 157 (0), 171 (2), 182 (0), 188 (0), 193 (1), 209 (2), 232 (5), 236 (4), 249 (1), 258 (1), 264 (2), 278 (3), 294 (10), 305 (3), 319 (6), 320 (16), 359 (1), 385 (12), 403 (20), 409 (14), 418 (3), 428 (11), 436 (11), 454 (14), 465 (6), 483 (4), 500 (14), 507 (15), 520 (18), 530 (46), 551 (58), 557 (49), 586 (85), 593 (98), 624 (83), 701 (105), 790 (66), 811 (44), 821 (17), 826 (113), 832 (230), 841 (378), 850 (163), 858 (650), 878 (59), 912 (233), 1106 (287), 1120 (2), 1140 (98), 1146 (20), 1216 (24), 1221 (76), 1450 (6), 1462 (0), 1487 (13), 1488 (16), 1493 (9), 1499 (17), 2067 (896), 2071 (1328), 2103 (562), 3036 (53), 3077 (25), 3103 (13), 3139 (9), 3164 (6), 3173 (3) | 32 (0), 35 (0), 48 (0), 53 (2), 58 (1), 70 (0), 73 (0), 75 (0), 80 (0), 85 (0), 90 (0), 94 (0), 115 (0), 123 (0), 137 (1), 140 (0), 147 (1), 156 (0), 170 (2), 183 (0), 187 (0), 192 (1), 206 (2), 228 (5), 235 (6), 242 (1), 250 (0), 255 (1), 274 (6), 291 (7), 305 (2), 314 (6), 318 (14), 354 (0), 371 (13), 392 (6), 396 (25), 409 (12), 414 (4), 424 (16), 438 (12), 459 (6), 491 (5), 492 (6), 505 (34), 532 (9), 543 (23), 560 (54), 564 (25), 582 (21), 589 (105), 608 (92), 684 (94), 755 (48), 782 (16), 789 (133), 794 (8), 799 (188), 809 (297), 817 (187), 824 (627), 844 (68), 874 (258), 1073 (126), 1073 (46), 1101 (132), 1102 (7), 1168 (17), 1170 (63), 1390 (4), 1406 (0), 1431 (15), 1436 (13), 1438 (13), 1447 (17), 1973 (968), 1984 (686), 2017 (590), 2963 (42), 3000 (26), 3032 (10), 3075 (7), 3090 (6), 3097 (3) |
| $[CH_3N(PF_2)_2]_2Fe_2(CO)_3$ **(23-2T)** | 31 (4), 46 (0), 51 (0), 55 (1), 57 (0), 65 (2), 70 (0), 72 (0), 80 (0), 84 (0), 90 (0), 110 (1), 118 (0), 124 (1), 126 (0), 144 (1), 152 (1), 154 (13), 168 (1), 179 (0), 180 (12), 183 (0), 197 (0), 215 (6), 220 (8), 225 (2), 246 (3), 254 (1), 263 (0), 267 (0), 279 (9), 286 (2), 304 (0), 315 (18), 333 (3), 375 (1), 390 (15), 391 (8), 404 (5), 414 (9), 435 (6), 440 (37), 448 (23), 478 (8), 482 (6), 496 (19), 520 (56), 528 (93), 537 (112), 557 (9), 575 (44), 597 (87), 687 (104), 786 (74), 802 (51), 811 (25), 822 (109), 831 (300), 838 (167), 843 (225), 862 (610), 879 (53), 901 (282), 1092 (328), 1120 (1), 1134 (49), 1140 (49), 1211 (24), 1242 (83), 1457 (7), 1460 (0), 1484 (10), 1494 (14), 1498 (13), 1503 (6), 1914 (624), 2076 (1555), 2097 (498), 3034 (58), 3079 (26), 3104 (17), 3116 (11), 3169 (5), 3174 (1) | 44 (0), 49 (0), 52 (0), 57 (0), 63 (2), 67 (0), 70 (1), 72 (0), 75 (0), 82 (0), 88 (0), 114 (0), 116 (0), 123 (0), 127 (1), 142 (1), 149 (0), 167 (1), 169 (0), 182 (1), 186 (0), 201 (1), 214 (1), 221 (9), 228 (1), 245 (1), 251 (0), 255 (0), 265 (2), 279 (19), 287 (12), 293 (0), 306 (1), 319 (15), 340 (1), 357 (3), 376 (17), 390 (5), 400 (1), 405 (7), 409 (4), 435 (12), 441 (26), 462 (1), 480 (1), 490 (16), 515 (30), 537 (70), 547 (43), 550 (37), 564 (38), 580 (121), 672 (97), 745 (51), 775 (40), 785 (17), 789 (49), 802 (323), 804 (57), 808 (256), 826 (686), 844 (39), 860 (285), 1067 (214), 1072 (1), 1093 (29), 1103 (97), 1160 (20), 1181 (46), 1399 (9), 1405 (0), 1427 (11), 1442 (14), 1447 (13), 1448 (5), 1808 (424), 1981 (1364), 1997 (412), 2961 (47), 3000 (30), 3035 (14), 3049 (7), 3091 (5), 3096 (1) |
| $[CH_3N(PF_2)_2]_2Fe_2(CO)_3$ **(23-3T)** | 3 (0), 20 (0), 34 (1), 44 (0), 45 (2), 49 (0), 50 (2), 62 (0), 78 (1), 83 (0), 84 (0), 92 (0), 97 (0), 110 (0), 117 (1), 139 (0), 145 (3), 156 (0), 161 (1), 163 (1), 179 (1), 192 (0), 212 (1), 237 (1), 256 (9), 259 (0), 263 (0), 266 (17), 267 (5), 283 (1), 292 (3), 298 (5), 312 (0), 322 (40), 370 (9), 376 (0), 394 (75), 424 (4), 430 (0), 431 (14), 444 (5), 445 (35), 456 (31), 482 (2), 487 (0), 507 (9), 526 (72), 533 (19), 543 (48), 556 (24), 581 (86), 698 (268), 707 (10), 807 (21), 815 (55), 815 (84), 821 (326), 827 (44), 834 (666), 835 (385), 856 (84), 902 (7), 912 (306), 1112 (631), 1118 (21), 1136 (137), 1138 (17), 1215 (19), 1216 (63), 1456 (1), 1456 (0), 1485 (5), 1485 (22), 1503 (5), 1503 (30), 1920 (422), 2050 (2221), 2066 (191), 3076 (56), 3076 (5), 3163 (0), 3163 (12), 3175 (0), 3175 (3) | 7 (0), 23 (0), 37 (2), 39 (0), 40 (0), 46 (0), 47 (2), 61 (0), 77 (0), 85 (0), 88 (0), 91 (0), 107 (1), 110 (0), 115 (0), 129 (0), 133 (3), 154 (0), 158 (1), 169 (0), 184 (0), 201 (0), 214 (0), 238 (0), 246 (3), 250 (2), 255 (1), 256 (2), 260 (29), 270 (4), 289 (4), 301 (0), 302 (2), 328 (15), 360 (9), 362 (0), 388 (68), 406 (2), 413 (12), 420 (28), 433 (14), 434 (1), 439 (20), 469 (1), 472 (3), 513 (20), 536 (24), 540 (45), 541 (6), 561 (33), 583 (48), 680 (245), 687 (10), 773 (4), 785 (9), 786 (35), 788 (316), 792 (98), 801 (653), 802 (361), 824 (66), 859 (2), 867 (300), 1075 (293), 1078 (9), 1104 (322), 1107 (20), 1160 (4), 1160 (40), 1397 (1), 1397 (0), 1439 (9), 1439 (21), 1446 (2), 1446 (27), 1841 (307), 1965 (1793), 1981 (194), 2998 (62), 2998 (5), 3087 (0), 3087 (12), 3098 (0), 3098 (2) |

**Table S3.** The Cartesian coordinates of the optimized $[CH_3N(PF_2)_2]Fe_2(CO)_n$ (n = 8, 7, 6, 5) structures at the B3LYP/DZP and BP86/DZP levels.

$[CH_3N(PF_2)_2]Fe_2(CO)_8$ (**18-1S**) $C_1$ B3LYP
0 1
N,0,0.0060435775,0.0648931976,-0.0250348376
P,0,1.5074096765,-0.7540722228,0.1116640203
P,0,-1.5064156595,-0.6479192921,-0.4016087034
C,0,0.0450856946,1.5454248903,0.143903248
H,0,0.5142784222,1.8156715008,1.0943816873
H,0,0.5869326222,2.0218637469,-0.6789043715
H,0,-0.98207031,1.9170624481,0.1518046286
Fe,0,3.4197862825,0.2520975645,-0.0035537662
Fe,0,-3.4217816993,0.2291913874,0.1188710726
F,0,-1.3193673791,-1.0244462891,-1.942978123
F,0,-1.2360215185,-2.1015617192,0.1904351678
F,0,1.2676783562,-1.6333867934,1.4218508912
F,0,1.264546469,-1.9126572288,-0.9550007277
C,0,3.2749608301,0.4374512395,-1.8042008533
C,0,3.6740082936,0.1420738575,1.7934389025
C,0,3.5982439879,2.0421243719,0.1268992754
C,0,-3.7014684651,1.9554324275,0.5614144035
C,0,-3.7747743517,0.6660698568,-1.6113330462
C,0,-3.149188284,-0.1321365499,1.8784480278
O,0,3.2079023522,0.5715324105,-2.9486443315
O,0,3.7302119749,3.190649739,0.2077353853
O,0,3.8606884224,0.0888864451,2.9303851046
O,0,-3.0001410828,-0.346224575,3.0025564583
O,0,-3.9077889276,3.0587012774,0.8506786418
O,0,-4.0240419854,0.9579730178,-2.698774156
C,0,-4.753170687,-0.9870522805,0.0786836522
C,0,4.7984041923,-0.8853947613,-0.2497431246
O,0,-5.6257503997,-1.7461239421,0.0588830605
O,0,5.6995438405,-1.5937565662,-0.4061268951

$[CH_3N(PF_2)_2]Fe_2(CO)_8$ (**18-1S**) $C_1$ BP86
0 1
N,0,0.0052150136,-0.1208792428,0.2429596722
P,0,1.5528315505,-0.8653600634,0.0542887717
P,0,-1.475838092,-0.6008506671,-0.4924117377
C,0,-0.0369873063,0.9528359983,1.2810175235
H,0,0.1198844858,0.5392554446,2.2930205347
H,0,0.7341939075,1.7103172699,1.0655337283
H,0,-1.0293216026,1.4302372604,1.2453238724
Fe,0,3.3850641064,0.2688701228,0.0817972849
Fe,0,-3.3931902909,0.2299001901,0.0648618961
F,0,-1.1003465303,-0.4938448614,-2.0534992264
F,0,-1.3577545312,-2.2026678317,-0.3735774538
F,0,1.4559179026,-2.0860513498,1.1050818034
F,0,1.2557163894,-1.7042491158,-1.280879654
C,0,2.9828717343,1.0143537719,-1.5081865357
C,0,3.8659639706,-0.3949313192,1.6870266501
C,0,3.539963861,1.9180710315,0.7692746926
C,0,-3.6945073808,1.647995965,1.1215703686
C,0,-3.3816106691,1.3511384064,-1.3471876629
C,0,-3.4691840603,-0.8198275295,1.526819991
O,0,2.7498495697,1.5164544417,-2.537809172
O,0,3.6679863676,2.9970473581,1.2110848494
O,0,4.2043099261,-0.8049697572,2.7274757462
O,0,-3.5465766874,-1.4865352753,2.4841296999
O,0,-3.9247952975,2.5703954656,1.8086968184
O,0,-3.4051298717,2.0904833051,-2.2515016148
C,0,-4.7455951204,-0.6895872866,-0.6711445996
C,0,4.7635276671,-0.5925005934,-0.6786107122
O,0,-5.6493706435,-1.2690256206,-1.137919225
O,0,5.6793617295,-1.1338207201,-1.1672342036

$[CH_3N(PF_2)_2]Fe_2(CO)_8$ (**18-2S**) $C_1$ B3LYP
0 1
N,0,-0.1051305984,1.2064902955,0.0778994522
P,0,1.5963079256,1.2961784228,-0.0274639813
P,0,-1.0805575229,-0.1925658689,-0.0564871543
C,0,-0.7981659207,2.5280822233,0.2200210154
H,0,-0.4558034252,3.2158909066,-0.5583121138
H,0,-1.8713462119,2.3705370182,0.1033179784
H,0,-0.6011095787,2.9542571349,1.2072527428
Fe,0,3.0426703,-0.3382859549,0.0112331851
Fe,0,-3.2459872689,-0.1910715764,0.0135977575
F,0,-0.4433049752,-0.8618667847,-1.3593250743
F,0,-0.3718157924,-1.1466657583,1.0073587859
F,0,1.7373299723,2.2815357502,-1.2738325616
F,0,1.8414201263,2.3975437908,1.0990026001
C,0,2.465549117,-0.8728456968,1.6420709712
C,0,2.4931316896,-0.9876936692,-1.5882224439
C,0,4.2546203179,-1.67054905,0.0726605592
C,0,-4.3187179155,1.2505318167,0.1890966663
C,0,-3.3696567382,0.0005437148,-1.7912657068
C,0,-3.2473905447,-0.3462878034,1.8260025946
O,0,2.1649220273,-1.2367857615,2.6996568523
O,0,5.0306479851,-2.5240243587,0.1137019541
O,0,2.2235834371,-1.4313553086,-2.6229477468
O,0,-3.279726875,-0.4415976614,2.9747986495
O,0,-5.0319264811,2.1567704372,0.3007221746
O,0,-3.4790356517,0.1243308327,-2.9325520564
C,0,-3.8961545425,-1.8679435353,-0.1260905513
C,0,4.3781872804,0.8799445351,-0.0406711128
O,0,-4.3413898631,-2.9314387421,-0.2141546018

$[CH_3N(PF_2)_2]Fe_2(CO)_8$ (**18-2S**) $C_1$ BP86
0 1
N,0,-0.0985145061,1.1846707006,0.1383429491
P,0,1.610407084,1.2921731411,-0.0251080346
P,0,-1.0821608526,-0.1905948407,-0.1939390043
C,0,-0.799470714,2.4972626372,0.3439811262
H,0,-0.520092136,3.2119251209,-0.4479213187
H,0,-1.8843618514,2.3143343248,0.2945066956
H,0,-0.5454324125,2.9077265779,1.3334819283
Fe,0,3.030591944,-0.3324808222,0.0219462667
Fe,0,-3.2272626774,-0.1931907742,0.0415828973
F,0,-0.5327171855,-0.6217453397,-1.647985035
F,0,-0.3007852143,-1.3185566575,0.6425030214
F,0,1.7201711426,2.2713638623,-1.2989188738
F,0,1.8700888874,2.4173188951,1.095258659
C,0,2.431947195,-0.8289301317,1.6451709909
C,0,2.4945223148,-1.0028257056,-1.5618858612
C,0,4.2151203448,-1.6656278347,0.1237371154
C,0,-4.288281614,1.2048964775,0.4165643436
C,0,-3.4890338113,0.1486944948,-1.7097063478
C,0,-3.0785975607,-0.4842833677,1.8144975597
O,0,2.1043084126,-1.176971487,2.7159307895
O,0,4.9908635235,-2.5376479328,0.1932262264
O,0,2.2357312111,-1.4762903811,-2.6020499216
O,0,-3.0167108673,-0.670307104,2.9663112605
O,0,-5.0095702833,2.0964538001,0.6613256636
O,0,-3.6928537691,0.3713531668,-2.8381802783
C,0,-3.897995199,-1.8429609163,-0.1769590148
C,0,4.3717649358,0.8636583739,-0.0597684749
O,0,-4.3659779316,-2.9066383043,-0.3145672134

O,0,5.2750145301,1.6118947211,-0.0715047827

$[CH_3N(PF_2)_2]Fe_2(CO)_7$ (**17-1S**) $C_{2v}$ B3LYP
0 1
N,0,0.0237562606,2.3378086492,0.
P,0,0.0112313718,1.4557718546,1.4459980542
P,0,0.0112313718,1.4557718546,-1.4459980542
C,0,-0.0132374747,3.8278016748,0.
H,0,-1.0468809745,4.1862384613,0.
H,0,0.5077328681,4.2006241546,0.8861011969
H,0,0.5077328681,4.2006241546,-0.8861011969
Fe,0,-0.0031219774,-0.7121981119,1.3544273242
Fe,0,-0.0031219774,-0.7121981119,-1.3544273242
F,0,1.2005144551,2.1907555028,-2.2268893366
F,0,-1.1728268046,2.211176478,-2.2150710144
F,0,-1.1728268046,2.211176478,2.2150710144
F,0,1.2005144551,2.1907555028,2.2268893366
C,0,1.814060927,-0.8057099042,1.4506053293
C,0,-1.8212720211,-0.7813520489,1.4506689842
C,0,-0.0087629277,-1.530903504,2.9374741279
C,0,-0.0087629277,-1.530903504,-2.9374741279
C,0,1.814060927,-0.8057099042,-1.4506053293
C,0,-1.8212720211,-0.7813520489,-1.4506689842
O,0,2.956152552,-0.8880450155,1.5913523334
O,0,-0.0122943396,-2.0510493653,3.9712416949
O,0,-2.9643703031,-0.8483579347,1.5917647391
O,0,-2.9643703031,-0.8483579347,-1.5917647391
O,0,-0.0122943396,-2.0510493653,-3.9712416949
O,0,2.956152552,-0.8880450155,-1.5913523334
C,0,-0.0129675348,-2.1678411784,0.
O,0,-0.0211661878,-3.3463517679,0.

$[CH_3N(PF_2)_2]Fe_2(CO)_7$ (**17-2T**) $C_1$ B3LYP
0 3
N,0,0.2541559625,2.1281955134,-0.0127447455
P,0,1.7107967364,1.2272205078,-0.019592337
P,0,-1.2909138,1.4511209102,-0.026524147
C,0,0.3582844075,3.6234330014,0.0526668681
H,0,0.3996445831,3.9552587851,1.0936000532
H,0,1.2599504257,3.9420000915,-0.4751583085
H,0,-0.5046430237,4.0707647061,-0.4459568651
Fe,0,1.8947678225,-0.9538056587,0.0031449178
Fe,0,-1.9084230823,-0.6428261049,0.013537376
F,0,-1.9312729144,2.2728276131,-1.2439791848
F,0,-1.9548841181,2.3288711426,1.1374755731
F,0,2.466774367,2.0273913553,1.1480955892
F,0,2.453046348,1.9916795744,-1.2203530847
C,0,1.6117556491,-1.3463138179,-1.8033081218
C,0,1.6322480561,-1.3053331115,1.8208602985
C,0,3.7419322155,-0.9900459601,-0.0063250748
C,0,-3.7105570381,-0.634422963,0.0265626268
C,0,-1.857216063,-0.710727474,-1.8057385434
C,0,-1.830208706,-0.6446578366,1.8324566826
O,0,1.5059850555,-1.5744945008,-2.9309015128
O,0,4.8974504191,-1.0579803663,-0.0115559154
O,0,1.5400394693,-1.5085398324,2.9544777582
O,0,-1.7969950288,-0.6736622637,2.9846042912
O,0,-4.8658900991,-0.6691433018,0.0358236826
O,0,-1.8408706794,-0.7824546516,-2.9562135341
C,0,-1.174982989,-2.2985757313,0.0375016912
O,0,-0.7995759342,-3.3940548896,0.0540228586

O,0,5.2882094852,1.5927318445,-0.1094756059

$[CH_3N(PF_2)_2]Fe_2(CO)_7$ (**17-1S**) $C_1$ BP86
0 1
N,0,-0.0063033765,2.3329857673,-0.0206113803
P,0,1.4324570151,1.4368655887,-0.2222352724
P,0,-1.4402281436,1.4376763384,0.2077978983
C,0,0.0082715748,3.8262667328,0.0090531478
H,0,0.2725982537,4.1916173947,1.0148514021
H,0,0.7401018606,4.1957729233,-0.7277927271
H,0,-0.9877542361,4.2010941463,-0.2754624269
Fe,0,1.3338720333,-0.7107262238,0.0237413244
Fe,0,-1.333426075,-0.7129310776,-0.0150189104
F,0,-2.4322942973,2.2691804744,-0.7614974239
F,0,-1.9867591245,2.0853411435,1.5827806154
F,0,2.409034415,2.2900058793,0.7436094966
F,0,1.9859254398,2.067877148,-1.6023159477
C,0,1.6165507444,-1.0520641402,-1.7320074017
C,0,1.2396988072,-0.5567851082,1.8194390769
C,0,2.9168486228,-1.4613563531,0.2903466276
C,0,-2.9143729621,-1.4703304861,-0.2742772376
C,0,-1.2388227671,-0.5754238994,-1.8121428933
C,0,-1.61567077,-1.0349669279,1.7444147774
O,0,1.8915807134,-1.3022262324,-2.8394001621
O,0,3.9692724723,-1.942731347,0.4738967886
O,0,1.270317219,-0.4722337552,2.9859630394
O,0,-1.8905729058,-1.2731239862,2.854502423
O,0,-3.9653824129,-1.9564483327,-0.4533199258
O,0,-1.2688996901,-0.5015577586,-2.9793386535
C,0,0.0007552083,-2.1772099827,0.0121477376
O,0,0.0018653623,-3.3682581643,0.018607324

$[CH_3N(PF_2)_2]Fe_2(CO)_7$ (**17-2T**) $C_1$ BP86
0 3
N,0,0.2605950421,2.1479709918,-0.0141273343
P,0,1.7075792473,1.2061921488,-0.0215192428
P,0,-1.2858267324,1.4578403515,-0.0125180224
C,0,0.3767347772,3.6442400485,0.0416852322
H,0,0.4607439328,3.9838676297,1.0863478781
H,0,1.2664366495,3.9540764844,-0.5285383757
H,0,-0.5090397338,4.0971779291,-0.4306033566
Fe,0,1.7646130725,-0.9241171043,0.0069644004
Fe,0,-1.8190293583,-0.6534145751,0.0136279197
F,0,-1.964798717,2.282178981,-1.2259023104
F,0,-1.9640693089,2.3190203941,1.174540256
F,0,2.4907363468,1.9959275354,1.1540049969
F,0,2.4678763294,1.9549364686,-1.2390745263
C,0,1.523934987,-1.2672268882,-1.7817466935
C,0,1.5374567601,-1.2193355758,1.8059695736
C,0,3.5609819804,-1.0708450127,0.0021000151
C,0,-3.6118233188,-0.7079804212,0.0186881501
C,0,-1.7804316849,-0.7009151345,-1.7922004776
C,0,-1.7703221173,-0.6556505794,1.8195682865
O,0,1.4859203148,-1.4658095464,-2.9366140346
O,0,4.7270647412,-1.2001543066,-0.0003708318
O,0,1.5087277093,-1.3874256895,2.9660241044
O,0,-1.7785653561,-0.6847921227,2.9863880454
O,0,-4.7790355868,-0.7855218918,0.0221385352
O,0,-1.7949125734,-0.7598697249,-2.9577328814
C,0,-1.0846926032,-2.3052186047,0.0326869887
O,0,-0.7364567582,-3.4234270481,0.046692597

$[CH_3N(PF_2)_2]Fe_2(CO)_7$ (**17-3S**) $C_s$ B3LYP
0 1
N,0,-0.8750214433,1.7096009623,0.
P,0,0.702350493,1.6797928379,0.
P,0,-0.4486361164,-1.3181034901,0.
C,0,-1.5567577571,3.0278397035,0.
H,0,-0.8502618914,3.8680373704,0.
H,0,-2.1918568544,3.1166392194,-0.8883442527
H,0,-2.1918568544,3.1166392194,0.8883442527
Fe,0,1.8025387505,-0.3188059136,0.
Fe,0,-2.0870329348,-0.0028089557,0.
F,0,-0.2746914031,-2.4265700969,-1.1787138751
F,0,-0.2746914031,-2.4265700969,1.1787138751
F,0,1.2990875358,2.6120838152,-1.1745386867
F,0,1.2990875358,2.6120838152,1.1745386867
C,0,1.6247244131,-0.3328489651,1.8320406599
C,0,1.6247244131,-0.3328489651,-1.8320406599
C,0,2.4469844367,-2.0356827645,0.
C,0,-2.6518967267,0.5054541288,-1.645754799
C,0,-2.6518967267,0.5054541288,1.645754799
O,0,1.5330667932,-0.3386390657,2.9743390894
O,0,2.8665461264,-3.1030136878,0.
O,0,1.5330667932,-0.3386390657,-2.9743390894
O,0,-3.002622858,0.8450327931,2.6991904912
O,0,-3.002622858,0.8450327931,-2.6991904912
C,0,-3.2935900694,-1.3097034956,0.
C,0,3.4501369624,0.5270505426,0.
O,0,-4.0988594985,-2.1442531892,0.
O,0,4.4909599019,1.0094323522,0.

$[CH_3N(PF_2)_2]Fe_2(CO)_6$ (**16-1S**) $C_1$ B3LYP
0 1
N,0,-0.9177733533,1.6626474831,-0.4412092772
P,0,0.6372369377,1.7580206719,-0.1308817589
P,0,-0.0972435783,-0.8572393701,-1.3846097562
C,0,-1.8245859259,2.7426338249,-0.830873701
H,0,-1.2658734535,3.6176375506,-1.1864047695
H,0,-2.4748824785,2.4084188968,-1.6490252603
H,0,-2.4595905733,3.0582293497,0.0086059476
Fe,0,1.351141308,-0.329296935,0.1579281902
Fe,0,-1.4110890465,-0.2330586239,0.2194505237
F,0,-0.1480621236,-0.1587767723,-2.8192179946
F,0,-0.1010939094,-2.3714641105,-1.9106110285
F,0,1.3369205645,2.6887442576,-1.2326644167
F,0,0.9427845902,2.7693972014,1.0864629351
C,0,1.6447188263,0.0334908778,1.917887652
C,0,2.9128774691,-0.0633003472,-0.6874134433
C,0,1.6558812923,-2.0886872359,0.4665957752
C,0,-3.0275318803,-0.1881917779,-0.5688048265
C,0,-1.6990592991,0.5073095648,1.8842602596
O,0,1.8421277278,0.2263666693,3.0378547716
O,0,1.8856725546,-3.1975391402,0.6826243444
O,0,3.9149747339,0.0998919499,-1.235365277
O,0,-1.8948205469,1.0001718175,2.9061747614
O,0,-4.0607855772,-0.1726804,-1.0820214737
C,0,-1.6091650535,-1.9094059589,0.8449484045
O,0,-1.750734273,-2.9768322835,1.2602108513

$[CH_3N(PF_2)_2]Fe_2(CO)_7$ (**17-3S**) $C_s$ BP86
0 1
N,0,-1.7054283218,0.8739932911,0.
P,0,-1.6678314079,-0.7247151611,0.
P,0,1.3247265197,0.499387573,0.
C,0,-3.0380829304,1.538838306,0.
H,0,-3.8712597283,0.8113495006,0.
H,0,-3.1351659931,2.1768196076,0.8958355756
H,0,-3.1351659931,2.1768196076,-0.8958355756
Fe,0,0.3262001325,-1.8200402591,0.
Fe,0,-0.0376539706,2.0867702372,0.
F,0,2.435098595,0.3558870213,1.1922752883
F,0,2.435098595,0.3558870213,-1.1922752883
F,0,-2.6168542004,-1.3113899787,1.1847789051
F,0,-2.6168542004,-1.3113899787,-1.1847789051
C,0,0.3430003567,-1.6284085807,-1.810155311
C,0,0.3430003567,-1.6284085807,1.810155311
C,0,2.0280460328,-2.4363354085,0.
C,0,-0.4841258911,2.5928930352,1.6721118454
C,0,-0.4841258911,2.5928930352,-1.6721118454
O,0,0.3505919242,-1.5395053349,-2.9690275192
O,0,3.1089035305,-2.866816864,0.
O,0,0.3505919242,-1.5395053349,2.9690275192
O,0,-0.7695186707,2.932707473,-2.7598566639
O,0,-0.7695186707,2.932707473,2.7598566639
C,0,1.1866879588,3.3513103697,0.
C,0,-0.4865450084,-3.4587260745,0.
O,0,1.9831931998,4.2149193686,0.
O,0,-0.9356981528,-4.5323520638,0.

$[CH_3N(PF_2)_2]\ Fe_2(CO)_6$ (**16-1S**) $C_1$ BP86
0 1
N,0,-0.9111839602,1.668580889,-0.4796556978
P,0,0.646602981,1.7487190627,-0.1093567972
P,0,-0.1064500763,-0.854547796,-1.389369442
C,0,-1.8244169573,2.7525919764,-0.8538657433
H,0,-1.260843158,3.6129040101,-1.2600851635
H,0,-2.5165171365,2.3987849975,-1.6394266674
H,0,-2.4227865086,3.1006900863,0.0098738581
Fe,0,1.3432816832,-0.3382181257,0.1542178128
Fe,0,-1.4057798483,-0.2071531517,0.222538488
F,0,-0.1469570893,-0.1475360164,-2.835463624
F,0,-0.1381217318,-2.378315394,-1.9216524054
F,0,1.3870696385,2.7016186497,-1.1854612865
F,0,0.9333318185,2.7398424375,1.1472887416
C,0,1.6364536206,-0.0094227632,1.9067437145
C,0,2.8951020467,-0.0599723039,-0.6787348366
C,0,1.6716770277,-2.0814402665,0.4307873117
C,0,-3.0119365345,-0.2158138986,-0.5498495775
C,0,-1.7290744042,0.5344965316,1.853608096
O,0,1.8416152787,0.1546951135,3.0448281574
O,0,1.9400658682,-3.2005087793,0.6312673426
O,0,3.9143069688,0.1096665321,-1.2256877164
O,0,-1.9688940484,1.0172312423,2.8888265426
O,0,-4.0688685508,-0.254190402,-1.0505286579
C,0,-1.5838245127,-1.8481047959,0.8760232316
O,0,-1.7318074831,-2.9181106757,1.3270357519

$[CH_3N(PF_2)_2]Fe_2(CO)_6$ (**16-2S**) $C_s$ B3LYP
0 1
N,0,0.2837884862,2.1976675479,0.
P,0,0.2137036246,1.3059895741,1.4397422529
P,0,0.2137036246,1.3059895741,-1.4397422529
C,0,0.3720421271,3.6840534966,0.
H,0,-0.6266907817,4.13085176,0.
H,0,0.9232271087,4.0119102155,0.8857840327
H,0,0.9232271087,4.0119102155,-0.8857840327
Fe,0,-0.1219193962,-0.7959092813,1.2082452639
Fe,0,-0.1219193962,-0.7959092813,-1.2082452639
F,0,1.5508498385,1.7833081427,-2.1697926258
F,0,-0.7625707244,2.237664762,-2.294344208
F,0,-0.7625707244,2.237664762,2.294344208
F,0,1.5508498385,1.7833081427,2.1697926258
C,0,1.2618930625,-1.3718513954,2.2283015938
C,0,-1.3075954371,-1.1510507819,2.5157664043
C,0,1.2618930625,-1.3718513954,-2.2283015938
C,0,-1.3075954371,-1.1510507819,-2.5157664043
O,0,2.1187898669,-1.7342189614,2.9103911776
O,0,-2.0837383444,-1.3940831965,3.3344185476
O,0,-2.0837383444,-1.3940831965,-3.3344185476
O,0,2.1187898669,-1.7342189614,-2.9103911776
C,0,0.5108529443,-2.2161085086,0.
O,0,0.9990175391,-3.2890028021,0.
C,0,-1.5626716789,-0.2182962901,0.
O,0,-2.6739969523,0.1791648444,0.

$[CH_3N(PF_2)_2]Fe_2(CO)_6$ (**16-3T**) $C_s$ B3LYP
0 3
N,0,-2.243596951,-0.2190329749,0.
P,0,-1.4936252733,1.2735043109,0.
P,0,-1.2175630459,-1.5967195665,0.
C,0,-3.7263378993,-0.3590785645,0.
H,0,-4.0459194176,-0.8993242664,0.896033172
H,0,-4.1867146216,0.6322100294,0.
H,0,-4.0459194176,-0.8993242664,-0.896033172
Fe,0,0.690213788,1.3804803239,0.
Fe,0,0.9619695736,-1.2958436103,0.
F,0,-1.9283843656,-2.416315025,-1.183809787
F,0,-1.9283843656,-2.416315025,1.183809787
F,0,-2.2644737071,2.0196706318,1.1856111082
F,0,-2.2644737071,2.0196706318,-1.1856111082
C,0,0.7023001762,1.3114707666,-1.826179587
C,0,1.1957165864,3.1035354313,0.
C,0,1.3842442669,-2.3814727451,-1.4424244401
C,0,1.3842442669,-2.3814727451,1.4424244401
O,0,0.7342354418,1.2917117937,-2.9777762523
O,0,1.5343423328,4.2077089822,0.
O,0,1.6564192146,-3.0659409187,2.3356790713
O,0,1.6564192146,-3.0659409187,-2.3356790713
C,0,2.2507219251,0.3648358148,0.
O,0,3.4093111559,0.1774557254,0.
C,0,0.7023001762,1.3114707666,1.826179587
O,0,0.7342354418,1.2917117937,2.9777762523

$[CH_3N(PF_2)_2]Fe_2(CO)_6$ (**16-2S**) $C_s$ BP86
0 1
N,0,0.3271304335,2.1868797387,0.
P,0,0.2304848145,1.2840204877,1.4461200163
P,0,0.2304848145,1.2840204877,-1.4461200163
C,0,0.4434516204,3.67421303,0.
H,0,-0.5535600217,4.1446005088,0.
H,0,1.0064893868,3.9923229999,0.8923475364
H,0,1.0064893868,3.9923229999,-0.8923475364
Fe,0,-0.1359164143,-0.7993169812,1.2104817131
Fe,0,-0.1359164143,-0.7993169812,-1.2104817131
F,0,1.5774754432,1.7482858978,-2.1990645343
F,0,-0.7536486032,2.2303859182,-2.3040449656
F,0,-0.7536486032,2.2303859182,2.3040449656
F,0,1.5774754432,1.7482858978,2.1990645343
C,0,1.215915853,-1.3901086932,2.2444937121
C,0,-1.3105413875,-1.0880311937,2.5205817312
C,0,1.215915853,-1.3901086932,-2.2444937121
C,0,-1.3105413875,-1.0880311937,-2.5205817312
O,0,2.0568448837,-1.7688404629,2.9628221402
O,0,-2.0918536242,-1.3008388222,3.3649942798
O,0,-2.0918536242,-1.3008388222,-3.3649942798
O,0,2.0568448837,-1.7688404629,-2.9628221402
C,0,0.5400159111,-2.2043653639,0.
O,0,1.0324265631,-3.2884429093,0.
C,0,-1.5642666806,-0.2075056498,0.
O,0,-2.6879794681,0.1970173823,0.

$[CH_3N(PF_2)_2]Fe_2(CO)_6$ (**16-3T**) $C_1$ BP86
0 3
N,0,-2.2446416824,-0.1046404529,-0.0091620667
P,0,-1.4283420051,1.3660204754,-0.1346895902
P,0,-1.2415508653,-1.4988602315,0.1376489241
C,0,-3.7333834232,-0.2040527422,0.0021408729
H,0,-4.0769008236,-0.587032296,0.9773429239
H,0,-4.1644361277,0.7961005003,-0.1626690983
H,0,-4.0662451198,-0.8745991022,-0.8067043375
Fe,0,0.7296219245,1.3168901729,0.0019847316
Fe,0,0.898672042,-1.2944767611,-0.0135710216
F,0,-2.0289093751,-2.4694920576,-0.8906445156
F,0,-1.8922201235,-2.1427325386,1.4739438226
F,0,-2.2410466386,2.265389398,0.9310494474
F,0,-2.112286349,2.0150682942,-1.4434256556
C,0,0.8512745993,1.2881680528,-1.8055609045
C,0,1.3469076412,2.9905147425,0.1015379011
C,0,1.1439425208,-2.325018114,-1.4846406122
C,0,1.341072903,-2.4796947055,1.2788013062
O,0,0.956295644,1.2961042348,-2.9682679967
O,0,1.7580143481,4.0836849596,0.168069473
O,0,1.6341783313,-3.27364196,2.0915958146
O,0,1.3137259682,-3.0213758479,-2.4135692683
C,0,2.2531785271,0.2124456194,0.0355089883
O,0,3.4321301077,0.0471509085,0.0390018592
C,0,0.6186395749,1.1658299256,1.8042861906
O,0,0.5724494012,1.1038855255,2.9699928118

$[CH_3N(PF_2)_2]Fe_2(CO)_6$ (**16-4T**) $C_1$ B3LYP
0 3
N,0,0.8930135085,1.5774708873,0.3036458594
P,0,-0.6957345609,1.6819413959,0.0489649723
P,0,0.0982580407,-1.145807534,0.5644881035
C,0,1.6234191266,2.8182158962,0.6653391315
H,0,0.956976884,3.5767565221,1.0925663021
H,0,2.3823055578,2.5815620575,1.4185760441
H,0,2.1216389318,3.2553821173,-0.20974058
Fe,0,-1.8292375352,-0.2602456676,-0.2358268114
Fe,0,1.94033544,-0.0943214258,-0.196386011
F,0,0.0878448609,-1.1254920633,2.1739844309
F,0,0.1564103435,-2.7451218564,0.3906425662
F,0,-1.3104711299,2.6080035968,1.2095893314
F,0,-0.9525313462,2.7710067148,-1.1123108169
C,0,-3.1094735727,0.5828486415,-1.2341749915
C,0,-2.7505675219,-0.2789649882,1.3725934509
C,0,-2.3444944553,-1.8993941368,-0.8461789722
C,0,2.9914634019,-0.7577428739,1.1854599752
C,0,3.2997206442,0.8792894204,-0.947586247
O,0,-3.9342033348,1.0875025721,-1.860606376
O,0,-2.6986143942,-2.9273973693,-1.2284553845
O,0,-3.3118269929,-0.3019133492,2.3775616417
O,0,4.1750072273,1.4509269112,-1.4341076755
O,0,3.6430681978,-1.1631668067,2.0466826827
C,0,2.1569125891,-1.3939819927,-1.4516904439
O,0,2.2928114792,-2.2153168348,-2.2547532063

$[CH_3N(PF_2)_2]Fe_2(CO)_5$ (**15-1S**) $C_1$ B3LYP
0 1
N,0,-0.9792099332,1.6883908079,-0.2507545615
P,0,0.635746567,1.7076895886,-0.2361543688
P,0,-0.0720555981,-1.0342670709,-1.4034737068
C,0,-1.8249953498,2.8282575392,-0.6335764647
H,0,-1.4899781245,3.747593726,-0.1356446454
H,0,-1.8044891149,2.9954975435,-1.7188123499
H,0,-2.857213284,2.635918148,-0.3260480064
Fe,0,1.3846974316,-0.3586811425,0.0600120218
Fe,0,-1.3498266493,-0.1776048801,0.0172910721
F,0,-0.1732005162,-0.4652049816,-2.8947908885
F,0,-0.1419473126,-2.5842859946,-1.7870449405
F,0,1.1405846354,2.5196584897,-1.5233327698
F,0,1.1148356757,2.8030038318,0.8286643383
C,0,1.4858741672,0.0037068779,1.8326092272
C,0,2.9642072753,-0.0504678596,-0.7489805023
C,0,1.770005568,-2.0852862524,0.4309891925
C,0,-2.9889919842,-0.1946876852,-0.686236165
O,0,1.5500136984,0.1878479645,2.9717572996
O,0,2.0501570599,-3.1746291945,0.6868518925
O,0,3.9788102253,0.1394292577,-1.2662080727
O,0,-4.0263743805,-0.2496100573,-1.1933075556
C,0,-1.6048787599,-1.7080425401,0.9307304578
O,0,-1.7850462968,-2.6541111157,1.570516496

$[CH_3N(PF_2)_2]Fe_2(CO)_6$ (**16-4T**) $C_1$ BP86
0 3
N,0,-0.9147589597,1.6107521087,-0.0512646156
P,0,0.7052127935,1.6268067279,0.2049944876
P,0,-0.1315314341,-0.9920972523,-0.8889509735
C,0,-1.6113948656,2.9237808717,-0.1241771726
H,0,-0.9151746364,3.746807083,-0.3661782884
H,0,-2.3749053347,2.8784232527,-0.9190992768
H,0,-2.110222429,3.1589853205,0.8343471629
Fe,0,1.7325985136,-0.3553594291,0.1696610712
Fe,0,-1.9396056214,-0.1061427497,0.0724527387
F,0,-0.0850234195,-0.6098504287,-2.4626765279
F,0,-0.2345641531,-2.5955544235,-1.0796542694
F,0,1.3379708249,2.7230189349,-0.8057442919
F,0,0.9676772385,2.522191663,1.5339012095
C,0,2.9220829321,0.1989130208,1.4165206124
C,0,2.7567103144,-0.1213181047,-1.2924238657
C,0,2.1527934061,-2.0788985609,0.4886491645
C,0,-2.9736295071,-0.6276639106,-1.3115058026
C,0,-3.3355937957,0.6665001795,0.9259803733
O,0,3.715668331,0.5234811713,2.2094673623
O,0,2.4728723103,-3.1834292034,0.694137574
O,0,3.4371475977,0.0102768466,-2.2329277797
O,0,-4.2698876923,1.1051974622,1.4762374249
O,0,-3.6760171818,-0.9858520531,-2.1773101436
C,0,-2.0647567275,-1.5391937174,1.1508709551
O,0,-2.1811025041,-2.4728918092,1.8502478714

$[CH_3N(PF_2)_2]Fe_2(CO)_5$ (**15-1S**) $C_1$ BP86
0 1
N,0,-1.0627778107,1.7765408863,0.3808054096
P,0,0.5467745968,1.7602000977,0.0940489359
P,0,-0.3879269911,-0.8449767239,-1.2325042531
C,0,-1.9240616293,2.967601501,0.2772494552
H,0,-1.5014233897,3.8026867723,0.8670861514
H,0,-2.0301728188,3.299297932,-0.7729094121
H,0,-2.9208863684,2.7283475121,0.6812460083
Fe,0,1.2680771976,-0.3209093988,0.0716326887
Fe,0,-1.4207582167,-0.0980083826,0.4203334447
F,0,-0.6845560759,-0.1309609847,-2.6499543433
F,0,-0.5669405713,-2.3596739,-1.7490615102
F,0,0.8360141167,2.6708899803,-1.2105219573
F,0,1.2469338927,2.7564090679,1.1526601126
C,0,1.5550916716,-0.177409285,1.8434388788
C,0,2.73402266,0.0774619223,-0.8754512985
C,0,1.7015442696,-2.055700837,0.1829819273
C,0,-3.1242566526,-0.0468602935,-0.0182703082
O,0,1.7437638511,-0.1405534889,2.9977853655
O,0,2.0335177608,-3.1727196526,0.2705697565
O,0,3.6986235504,0.3269723885,-1.4883878819
O,0,-4.2458982129,-0.0646117402,-0.3653761443
C,0,-1.5987769725,-1.6861031627,1.1844676353
O,0,-1.7397325563,-2.7019407721,1.7556115205

$[CH_3N(PF_2)_2]Fe_2(CO)_5$ (**15-2S**) $C_s$ B3LYP
0 1
N,0,-0.7974618363,2.0068375796,-0.1581522016
P,0,0.7063878624,1.4721710002,0.4409935652
P,0,-1.6943492519,0.6614237076,-0.6290435155
C,0,-1.269934364,3.4115206273,-0.1542600322
H,0,-1.4007892325,3.7686994219,0.8728597157
H,0,-0.5458056575,4.0429911399,-0.677181076
H,0,-2.2308676723,3.4672520191,-0.672661512
Fe,0,1.3680116226,-0.460888432,-0.1660500753
Fe,0,-0.7627137879,-1.017132601,0.2332350139
F,0,-1.936229168,0.8574014329,-2.1910834025
F,0,-3.1670808586,1.1095893265,-0.203954273
F,0,0.6368924199,1.8790200381,1.9849874388
F,0,1.5796158527,2.7472848438,0.0082535206
C,0,2.2851888956,0.0081349905,-1.6404581137
C,0,2.8181953903,-0.6624930144,0.8737058075
C,0,-2.0533032128,-2.21428893,-0.1805637217
C,0,-1.182536928,-0.9963683817,1.9709322317
O,0,2.8146661628,0.2856372591,-2.6305652837
O,0,3.7115021277,-0.8375720029,1.587117311
O,0,-1.4556478108,-0.9231755198,3.0930034242
O,0,-2.8248079388,-3.0257558817,-0.4648806329
C,0,0.9637811425,-2.1925437576,-0.6197550357
O,0,0.9333698624,-3.2961523424,-0.9895108753

$[CH_3N(PF_2)_2]Fe_2(CO)_5$ (**15-3T**) $C_1$ B3LYP
0 3
N,0,-0.4085201026,2.1202765941,0.0468887297
P,0,1.0742704893,1.5387200633,-0.0611732605
P,0,-0.6134494648,-0.6873883874,-1.319911236
C,0,-0.770758484,3.5466493692,-0.0099823772
H,0,-0.300753194,4.0488164716,-0.8660719533
H,0,-1.8561604446,3.6390619523,-0.1203471819
H,0,-0.4748793544,4.0713540479,0.9086019813
Fe,0,1.0101873048,-0.7090679219,0.0990222463
Fe,0,-1.5421574867,0.4686885569,0.3080625536
F,0,-0.4709025567,0.0411638859,-2.7353058111
F,0,-1.1846419796,-2.0721761434,-1.8811415875
F,0,1.8215365372,2.1700673698,-1.3345127592
F,0,2.0276220784,2.2596078341,1.0146162089
C,0,1.5597026272,-0.5311895627,1.83396627
C,0,2.4800840808,-0.9569903464,-0.9004968692
C,0,0.7220154026,-2.4757076047,0.3874507964
C,0,-3.2466014487,0.0072343167,-0.2228490409
O,0,1.915309237,-0.466384595,2.9283245633
O,0,0.5639926811,-3.5989250673,0.5904676638
O,0,3.4212635837,-1.1288442017,-1.5452883284
O,0,-4.323889216,-0.2642357201,-0.5442816988
C,0,-1.678082408,-0.3434387276,1.9969514526
O,0,-1.7886034478,-0.8155878848,3.0459328549

$[CH_3N(PF_2)_2]Fe_2(CO)_5$ (**15-2S**) $C_s$ BP86
0 1
N,0,-0.6769781706,1.9859501945,-0.0076281599
P,0,0.9258188359,1.6432826479,0.4021648847
P,0,-1.3345995123,0.5244711183,-0.6045315987
C,0,-1.3712355602,3.2967592178,0.0509484694
H,0,-2.1552150885,3.2855078295,0.8257980479
H,0,-0.627781257,4.0736483477,0.2927222699
H,0,-1.8168314881,3.5322709613,-0.9299473276
Fe,0,1.4148077227,-0.3465250811,-0.1964959798
Fe,0,-0.8407263656,-1.3751092947,0.1212584279
F,0,-1.4153175087,0.7518113444,-2.1996875425
F,0,-2.8888677813,0.901187307,-0.3327891474
F,0,1.0412555392,2.1092400775,1.9383113438
F,0,1.7035031093,2.9205731245,-0.1975807297
C,0,2.085572964,-0.0085183308,-1.8084626651
C,0,2.9768494137,-0.4471648503,0.642516154
C,0,-2.3566173691,-2.1838703787,-0.3920933138
C,0,-1.3312195769,-1.1558738837,1.7989083875
O,0,2.51691485,0.1592744087,-2.8854454618
O,0,4.0081902748,-0.5623618069,1.1875819408
O,0,-1.6434635071,-0.9664670684,2.9144942737
O,0,-3.3243436247,-2.7526338966,-0.7265860612
C,0,0.9861981982,-2.0741467702,-0.1375436204
O,0,0.6201695217,-3.2197126949,-0.0689443143

$[CH_3N(PF_2)_2]Fe_2(CO)_5$ (**15-3T**) $C_1$ BP86
0 3
N,0,-0.997271808,1.7747656401,-0.368098948
P,0,0.6028987443,1.72364918,-0.1323677087
P,0,-0.004273154,-0.8209847773,-1.7029498679
C,0,-1.8231021219,2.9943512418,-0.4617601315
H,0,-1.5506009347,3.5918674291,-1.3522394452
H,0,-2.8833607196,2.7043299751,-0.5531777135
H,0,-1.7128491526,3.6270726115,0.4393257504
Fe,0,1.2379392626,-0.4123897682,0.0273040645
Fe,0,-1.5381014344,-0.1268894876,-0.3444045322
F,0,0.2298040173,-0.0215095509,-3.0870200327
F,0,0.0109896928,-2.3020843228,-2.3408176711
F,0,1.354309395,2.6588627724,-1.2201543731
F,0,0.9799553408,2.6574384921,1.1363612434
C,0,1.4041495813,-0.1755429101,1.8176084372
C,0,2.856926561,-0.1399552183,-0.6683578692
C,0,1.4766255696,-2.175028435,0.267747089
C,0,-2.7496788706,-1.1913655842,-1.1153054611
O,0,1.5471106556,-0.0755504,2.9720554496
O,0,1.6646268005,-3.3125532056,0.4524176718
O,0,3.9230045153,0.018511742,-1.1215423548
O,0,-3.576382466,-1.8700239217,-1.6009709466
C,0,-1.6748010071,-1.0022469521,1.2413001283
O,0,-1.8011934673,-1.6046095503,2.2401042213

$[CH_3N(PF_2)_2]Fe_2(CO)_5$ (**15-4S**) $C_1$ B3LYP
0 1
N,0,0.352602069,-0.995170115,-1.376733914
P,0,-1.1442465589,-1.0120848531,-0.8466802237
P,0,0.2628887437,1.6119687022,-0.5021150468
C,0,0.9257543055,-1.6990595018,-2.523751022
H,0,0.1427314535,-2.0076771339,-3.2281498479
H,0,1.6148374446,-1.0348600423,-3.0598534293
H,0,1.481244174,-2.5936399846,-2.2097548285
Fe,0,-1.2560892747,0.5294152354,0.6410515425
Fe,0,1.3552604323,-0.1075688578,0.2110649579
F,0,0.2119212597,2.0237630319,-2.042875438
F,0,0.5565329552,3.0737306916,0.1014408297
F,0,-2.1478663579,-0.9795209329,-2.093648335
F,0,-1.6010671296,-2.4753502685,-0.3538798527
C,0,-1.6289973836,-0.6481227373,1.991284906
C,0,-2.848072402,1.222948693,0.1674679084
C,0,2.9314048644,-0.0124984033,-0.6614093884
C,0,1.4056794875,-1.7445186029,1.0463599643
O,0,-1.864044493,-1.3652238746,2.8645088
O,0,-3.8693295543,1.6461789558,-0.1673893135
O,0,1.4520976837,-2.7808873862,1.5487064641
O,0,3.9433548513,0.0650614102,-1.211324015
C,0,1.9192172366,0.7355960499,1.6902727407
O,0,2.2800877115,1.2666012364,2.6515431755

$[CH_3N(PF_2)_2]Fe_2(CO)_5$ (**15-4S**) $C_1$ BP86
0 1
N,0,0.4303626433,-0.7901563835,-1.5191917897
P,0,-1.0562786464,-0.9473115909,-0.9426454118
P,0,0.2302242926,1.6542081097,-0.3571343922
C,0,1.0453421723,-1.3020503709,-2.7443430845
H,0,0.2743247593,-1.4976946593,-3.5124480039
H,0,1.7483995704,-0.5511439538,-3.1474513303
H,0,1.6031577408,-2.2395555622,-2.5551456149
Fe,0,-1.2697372852,0.4331497109,0.648528631
Fe,0,1.3353959931,-0.1250622973,0.2184853463
F,0,0.2312592764,2.2168165383,-1.863947892
F,0,0.4885895601,3.0643974082,0.4000448923
F,0,-2.1025509431,-0.8651978477,-2.1708105001
F,0,-1.4151476843,-2.4838761602,-0.5652172951
C,0,-1.7399029499,-0.8305005024,1.849004633
C,0,-2.8435632169,1.1466145483,0.224529162
C,0,2.9540877718,0.1790320042,-0.4853116719
C,0,1.5016804609,-1.8358548074,0.8041331604
O,0,-2.0504474792,-1.6206535357,2.6546388186
O,0,-3.8833340662,1.5795510771,-0.1007152703
O,0,1.6469768149,-2.9319060871,1.1806654448
O,0,4.0201789607,0.3972395242,-0.9155224155
C,0,1.7068593461,0.5008318784,1.8344496917
O,0,1.9582475372,0.8931909297,2.9104221996

**Table S4.** The Cartesian coordinates of the optimized $[CH_3N(PF_2)_2]_2Fe_2(CO)_n$ (n = 6, 5, 4, 3) structures at the B3LYP/DZP and BP86/DZP levels.

$[CH_3N(PF_2)_2]_2Fe_2(CO)_6$ (**26-1S**) $C_{2h}$ B3LYP
0 1
C,0,0.,0.,3.8915309632
O,0,0.,0.,5.0489826377
Fe,0,0.,0.,2.1024390427
P,0,-0.0269963108,2.0713429183,1.5175786817
P,0,0.0269963108,-2.0713429183,1.5175786817
C,0,-1.808434341,-0.0265945771,1.9656926912
C,0,1.808434341,0.0265945771,1.9656926912
O,0,-2.9617146026,-0.04481677,1.8882476495
O,0,2.9617146026,0.04481677,1.8882476495
F,0,1.1342948896,2.9319168748,2.2103433288
F,0,-1.2503827619,2.8841089449,2.1607377079
F,0,1.2503827619,-2.8841089449,2.1607377079
F,0,-1.1342948896,-2.9319168748,2.2103433288
O,0,-2.9617146026,-0.04481677,-1.8882476495
C,0,-1.808434341,-0.0265945771,-1.9656926912
Fe,0,0.,0.,-2.1024390427
P,0,-0.0269963108,2.0713429183,-1.5175786817
P,0,0.0269963108,-2.0713429183,-1.5175786817
C,0,1.808434341,0.0265945771,-1.9656926912
C,0,0.,0.,-3.8915309632
F,0,-1.2503827619,2.8841089449,-2.1607377079
F,0,1.1342948896,2.9319168748,-2.2103433288
F,0,-1.1342948896,-2.9319168748,-2.2103433288
F,0,1.2503827619,-2.8841089449,-2.1607377079
O,0,2.9617146026,0.04481677,-1.8882476495
O,0,0.,0.,-5.0489826377
H,0,-0.4111710863,4.7280078793,0.8841603918
C,0,0.0959377204,4.3362805091,0.
H,0,-0.4111710863,4.7280078793,-0.8841603918
H,0,1.1424245298,4.6516834146,0.
N,0,0.0085145304,2.8348919752,0.
H,0,0.4111710863,-4.7280078793,-0.8841603918
C,0,-0.0959377204,-4.3362805091,0.
H,0,-1.1424245298,-4.6516834146,0.
H,0,0.4111710863,-4.7280078793,0.8841603918
N,0,-0.0085145304,-2.8348919752,0.

$[CH_3N(PF_2)_2]_2Fe_2(CO)_6$ (**26-2S**) $C_{2v}$ B3LYP
0 1
Fe,0,-1.622074,0.,-0.00612309
Fe,0,1.622074,0.,-0.00612309
P,0,1.475913,2.15622515,-0.0038111
P,0,-1.475913,2.15622515,-0.0038111
P,0,-1.475913,-2.15622515,-0.0038111
P,0,1.475913,-2.15622515,-0.0038111
F,0,2.225493,2.93082915,-1.1826071
F,0,2.21887,2.93366716,1.1770129
F,0,-2.21887,2.93366716,1.1770129
F,0,-2.225493,2.93082915,-1.1826071
F,0,-2.225493,-2.93082915,-1.1826071
F,0,-2.21887,-2.93366716,1.1770129
F,0,2.225493,-2.93082915,-1.1826071
F,0,2.21887,-2.93366716,1.1770129
C,0,2.831856,0.,-1.39050609
C,0,-2.831856,0.,-1.39050609
O,0,3.55765,0.,-2.28465809
O,0,-3.55765,0.,-2.28465809
N,0,0.,-2.97470585,-0.00281508
N,0,0.,2.97470585,-0.00281508
H,0,-0.885509,4.85520515,-0.43825611
C,0,0.,4.46936715,0.07248489
H,0,0.,4.79492616,1.11641989
H,0,0.885509,4.85520515,-0.43825611
H,0,0.,-4.79492616,1.11641989
C,0,0.,-4.46936715,0.07248489
H,0,-0.885509,-4.85520515,-0.43825611
H,0,0.885509,-4.85520515,-0.43825611
C,0,-2.832741,0.,1.37670891
C,0,2.832741,0.,1.37670891
O,0,-3.559352,0.,2.27033191
O,0,3.559352,0.,2.27033191
C,0,0.,0.,1.28694591
O,0,0.,0.,2.48662791
C,0,0.,0.,-1.29901509
O,0,0.,0.,-2.49844709

$[CH_3N(PF_2)_2]_2Fe_2(CO)_6$ (**26-1S**) $C_{2h}$ BP86
0 1
C,0,0.,0.,3.8463266398
O,0,0.,0.,5.0177809107
Fe,0,0.,0.,2.0623472528
P,0,-0.0277298789,2.0688591572,1.5263575538
P,0,0.0277298789,-2.0688591572,1.5263575538
C,0,-1.7898194331,-0.0277970588,1.8798958661
C,0,1.7898194331,0.0277970588,1.8798958661
O,0,-2.9574531555,-0.0472989411,1.7861494553
O,0,2.9574531555,0.0472989411,1.7861494553
F,0,1.1429685046,2.9344681337,2.2299550064
F,0,-1.2640970243,2.8854443582,2.1758021877
F,0,1.2640970243,-2.8854443582,2.1758021877
F,0,-1.1429685046,-2.9344681337,2.2299550064
O,0,-2.9574531555,-0.0472989411,-1.7861494553
C,0,-1.7898194331,-0.0277970588,-1.8798958661
Fe,0,0.,0.,-2.0623472528
P,0,-0.0277298789,2.0688591572,-1.5263575538
P,0,0.0277298789,-2.0688591572,-1.5263575538
C,0,1.7898194331,0.0277970588,-1.8798958661
C,0,0.,0.,-3.8463266398
F,0,-1.2640970243,2.8854443582,-2.1758021877
F,0,1.1429685046,2.9344681337,-2.2299550064
F,0,-1.1429685046,-2.9344681337,-2.2299550064
F,0,1.2640970243,-2.8854443582,-2.1758021877
O,0,2.9574531555,0.0472989411,-1.7861494553
O,0,0.,0.,-5.0177809107
H,0,-0.4136437494,4.7368892273,0.8910435039
C,0,0.0993498337,4.3439313121,0.
H,0,-0.4136437494,4.7368892273,-0.8910435039
H,0,1.1536103929,4.662017609,0.
N,0,0.0112032746,2.8393508681,0.
H,0,0.4136437494,-4.7368892273,-0.8910435039
C,0,-0.0993498337,-4.3439313121,0.
H,0,-1.1536103929,-4.662017609,0.
H,0,0.4136437494,-4.7368892273,0.8910435039
N,0,-0.0112032746,-2.8393508681,0.

$[CH_3N(PF_2)_2]_2Fe_2(CO)_6$ (**26-2S**) $C_{2v}$ BP86
0 1
Fe,0,0.,1.6203503488,0.0091907037
Fe,0,0.,-1.6203503488,0.0091907037
P,0,-2.1554727438,-1.4833031246,0.005822214
P,0,-2.1554727438,1.4833031246,0.005822214
P,0,2.1554727438,1.4833031246,0.005822214
P,0,2.1554727438,-1.4833031246,0.005822214
F,0,-2.9365856067,-2.2429416798,1.1952094195
F,0,-2.9377795379,-2.2366122149,-1.186292398
F,0,-2.9377795379,2.2366122149,-1.186292398
F,0,-2.9365856067,2.2429416798,1.1952094195
F,0,2.9365856067,2.2429416798,1.1952094195
F,0,2.9377795379,2.2366122149,-1.186292398
F,0,2.9365856067,-2.2429416798,1.1952094195
F,0,2.9377795379,-2.2366122149,-1.186292398
C,0,0.,-2.8398270236,1.365874324
C,0,0.,2.8398270236,1.365874324
O,0,0.,-3.607985092,2.2450952088
O,0,0.,3.607985092,2.2450952088
N,0,2.9872700424,0.,0.0055719046
N,0,-2.9872700424,0.,0.0055719046
H,0,-4.8706605342,0.8926219758,0.4492081764
C,0,-4.4840367841,0.,-0.0672466147
H,0,-4.8151282434,0.,-1.1181792975
H,0,-4.8706605342,-0.8926219758,0.4492081764
H,0,4.8151282434,0.,-1.1181792975
C,0,4.4840367841,0.,-0.0672466147
H,0,4.8706605342,0.8926219758,0.4492081764
H,0,4.8706605342,-0.8926219758,0.4492081764
C,0,0.,2.8418640619,-1.3452089131
C,0,0.,-2.8418640619,-1.3452089131
O,0,0.,3.6118092972,-2.2229881887
O,0,0.,-3.6118092972,-2.2229881887
C,0,0.,0.,-1.2822562299
O,0,0.,0.,-2.4888443802
C,0,0.,0.,1.3004407002
O,0,0.,0.,2.5067902572

$[CH_3N(PF_2)_2]_2Fe_2(CO)_6$ (**26-3T**) $C_2$ B3LYP
0 3
C,0,0.,0.,3.627519
O,0,0.,0.,4.787065
Fe,0,0.,0.,1.783041
P,0,0.290294,2.322302,1.413672
P,0,-0.290294,-2.322302,1.413672
C,0,-1.924602,0.277558,1.724242
C,0,1.924602,-0.277558,1.724242
O,0,-3.049279,0.402181,1.960275
O,0,3.049279,-0.402181,1.960275
F,0,1.657196,3.086032,1.777138
F,0,-0.650262,3.268244,2.308241
F,0,0.650262,-3.268244,2.308241
F,0,-1.657196,-3.086032,1.777138
O,0,-2.897896,-0.438021,-1.280958
C,0,-1.763649,-0.260121,-1.428397
Fe,0,0.,0.,-1.760517
P,0,-0.290087,2.137397,-1.503028
P,0,0.290087,-2.137397,-1.503028
C,0,1.763649,0.260121,-1.428397
C,0,0.,0.,-3.567084
F,0,-1.72118,2.682833,-1.952969
F,0,0.559627,3.012873,-2.535725
F,0,-0.559627,-3.012873,-2.535725
F,0,1.72118,-2.682833,-1.952969
O,0,2.897896,0.438021,-1.280958
O,0,0.,0.,-4.722513
H,0,-0.264464,4.971188,0.737661
C,0,-0.016589,4.538742,-0.23387
H,0,-0.781049,4.849483,-0.951126
H,0,0.965219,4.892844,-0.559637
N,0,-0.018206,3.044895,-0.113633
H,0,0.781049,-4.849483,-0.951126
C,0,0.016589,-4.538742,-0.23387
H,0,-0.965219,-4.892844,-0.559637
H,0,0.264464,-4.971188,0.737661
N,0,0.018206,-3.044895,-0.113633

$[CH_3N(PF_2)_2]_2Fe_2(CO)_5$ (**25-1S**) $C_{2v}$ B3LYP
0 1
Fe,0,0.,-1.3632838971,-0.0244111491
Fe,0,0.,1.3632838971,-0.0244111491
P,0,2.1550522305,1.4352030962,-0.0651387649
P,0,2.1550522305,-1.4352030962,-0.0651387649
P,0,-2.1550522305,-1.4352030962,-0.0651387649
P,0,-2.1550522305,1.4352030962,-0.0651387649
F,0,2.8942553387,2.1986550599,1.1245928993
F,0,2.8760792793,2.2510803276,-1.229690722
F,0,2.8760792793,-2.2510803276,-1.229690722
F,0,2.8942553387,-2.1986550599,1.1245928993
F,0,-2.8942553387,-2.1986550599,1.1245928993
F,0,-2.8760792793,-2.2510803276,-1.229690722
F,0,-2.8942553387,2.1986550599,1.1245928993
F,0,-2.8760792793,2.2510803276,-1.229690722
C,0,0.,1.6247390039,1.7801951814
C,0,0.,-1.6247390039,1.7801951814
O,0,0.,1.8191241669,2.921307355
O,0,0.,-1.8191241669,2.921307355
N,0,-3.0336315035,0.,-0.1218789582
N,0,3.0336315035,0.,-0.1218789582
H,0,4.9229082266,-0.8861868275,0.2407764558
C,0,4.5187359834,0.,-0.2557162712
H,0,4.8077252042,0.,-1.3106427302
H,0,4.9229082266,0.8861868275,0.2407764558
H,0,-4.8077252042,0.,-1.3106427302
C,0,-4.5187359834,0.,-0.2557162712
H,0,-4.9229082266,-0.8861868275,0.2407764558
H,0,-4.9229082266,0.8861868275,0.2407764558
C,0,0.,-2.8732088022,-0.9678741341
C,0,0.,2.8732088022,-0.9678741341
O,0,0.,-3.8676550208,-1.5633441668
O,0,0.,3.8676550208,-1.5633441668
C,0,0.,0.,-1.4784586965
O,0,0.,0.,-2.6651093184

$[CH_3N(PF_2)_2]_2Fe_2(CO)_6$ (**26-3T**) $C_1$ BP86
0 3
C,0,-0.0547693643,0.0509117842,3.5026668366
O,0,-0.0259368535,0.0390516513,4.6757674673
Fe,0,-0.0869062872,0.0973004949,1.7062233211
P,0,0.4281932488,2.2046838455,1.428042728
P,0,-0.5808087752,-2.2711320075,1.3155360807
C,0,-1.914592648,0.5346285072,1.6593356671
C,0,1.685436751,-0.4669925136,1.5622671979
O,0,-3.0044867631,0.90082235,1.8936929261
O,0,2.8354172937,-0.6517811226,1.718736097
F,0,1.9261982013,2.7744626734,1.6583333548
F,0,-0.2876592185,3.2626737773,2.4266871977
F,0,0.2887367205,-3.1272409357,2.3843389571
F,0,-1.9432724497,-3.1543985645,1.5158457242
O,0,-2.9575254618,-0.652947327,-1.2158538374
C,0,-1.8233571894,-0.3984918643,-1.3588496883
Fe,0,-0.0919054855,-0.0174481315,-1.7016567741
P,0,-0.4729979674,2.0931526697,-1.395958501
P,0,0.3515949078,-2.1272607882,-1.5016795496
C,0,1.6599778989,0.3459477489,-1.4534714617
C,0,-0.1566770528,0.0155139082,-3.5005596229
F,0,-2.0011957026,2.5727812907,-1.5684704036
F,0,0.1313567721,3.0230892544,-2.5679502695
F,0,-0.3592776894,-3.0455421261,-2.622605243
F,0,1.8580291395,-2.5682172317,-1.8588291982
O,0,2.8010657064,0.5938688479,-1.3695677023
O,0,-0.2004242294,0.0380134789,-4.669140256
H,0,0.2456817421,4.9162633969,0.8236624819
C,0,0.1341811065,4.4899191322,-0.1847173931
H,0,-0.7984204722,4.8815428579,-0.623768904
H,0,0.9960042574,4.7789798746,-0.8068513222
N,0,0.0559771363,2.996671231,-0.0663618115
H,0,1.3167174103,-4.7101977462,0.3262391966
C,0,0.3254424079,-4.5094092003,-0.1108192966
H,0,0.2832620452,-4.8961838269,-1.1411975452
H,0,-0.4547315267,-5.0162553772,0.4799922391
N,0,0.045672391,-3.0367800116,-0.1185996931

$[CH_3N(PF_2)_2]_2Fe_2(CO)_5$ (**25-1S**) $C_{2v}$ BP86
0 1
Fe,0,0.,-1.3505471487,-0.014343195
Fe,0,0.,1.3505471487,-0.014343195
P,0,2.1358667282,1.4378548342,-0.0813920502
P,0,2.1358667282,-1.4378548342,-0.0813920502
P,0,-2.1358667282,-1.4378548342,-0.0813920502
P,0,-2.1358667282,1.4378548342,-0.0813920502
F,0,2.8873056511,2.2378756994,1.0969549102
F,0,2.8458259997,2.2471765701,-1.2787793426
F,0,2.8458259997,-2.2471765701,-1.2787793426
F,0,2.8873056511,-2.2378756994,1.0969549102
F,0,-2.8873056511,-2.2378756994,1.0969549102
F,0,-2.8458259997,-2.2471765701,-1.2787793426
F,0,-2.8873056511,2.2378756994,1.0969549102
F,0,-2.8458259997,2.2471765701,-1.2787793426
C,0,0.,1.6074913354,1.7822458266
C,0,0.,-1.6074913354,1.7822458266
O,0,0.,1.8003788452,2.9378544768
O,0,0.,-1.8003788452,2.9378544768
N,0,-3.0345890009,0.,-0.119649416
N,0,3.0345890009,0.,-0.119649416
H,0,4.9292294673,-0.8930985304,0.2350634755
C,0,4.5209132081,0.,-0.2645928804
H,0,4.8072574126,0.,-1.3288730472
H,0,4.9292294673,0.8930985304,0.2350634755
H,0,-4.8072574126,0.,-1.3288730472
C,0,-4.5209132081,0.,-0.2645928804
H,0,-4.9292294673,-0.8930985304,0.2350634755
H,0,-4.9292294673,0.8930985304,0.2350634755
C,0,0.,-2.8895258751,-0.8906194663
C,0,0.,2.8895258751,-0.8906194663
O,0,0.,-3.9247455929,-1.4453924662
O,0,0.,3.9247455929,-1.4453924662
C,0,0.,0.,-1.473687879
O,0,0.,0.,-2.6730065021

$[CH_3N(PF_2)_2]_2Fe_2(CO)_5$ (**25-2T**) $C_s$ B3LYP
0 3
Fe,0,-1.6248674378,-0.0060370199,0.
Fe,0,1.785062434,0.0396128312,0.
P,0,1.4217575172,-0.1925503038,2.1855519202
P,0,-1.535503951,0.003145282,2.157975547
P,0,-1.535503951,0.003145282,-2.157975547
P,0,1.4217575172,-0.1925503038,-2.1855519202
F,0,2.2374476363,0.8216879101,3.1174607303
F,0,1.9750630756,-1.5210896538,2.8938629593
F,0,-2.3854635362,-1.1259267971,2.8947006272
F,0,-2.237434928,1.2392903812,2.8772200581
F,0,-2.237434928,1.2392903812,-2.8772200581
F,0,-2.3854635362,-1.1259267971,-2.8947006272
F,0,2.2374476363,0.8216879101,-3.1174607303
F,0,1.9750630756,-1.5210896538,-2.8938629593
C,0,2.3071180603,1.8040508792,0.
C,0,-1.0950915329,1.7265512872,0.
O,0,2.6637405689,2.9070476686,0.
O,0,-0.8404459734,2.8573458408,0.
N,0,-0.0918759392,-0.0928362579,-2.9963029577
N,0,-0.0918759392,-0.0928362579,2.9963029577
H,0,-1.0081573217,0.3314127952,4.8688013693
C,0,-0.1306416774,-0.198198388,4.4888783934
H,0,-0.1690459741,-1.2472217257,4.7958612174
H,0,0.7616300913,0.2788176508,4.9003605244
H,0,-0.1690459741,-1.2472217257,-4.7958612174
C,0,-0.1306416774,-0.198198388,-4.4888783934
H,0,-1.0081573217,0.3314127952,-4.8688013693
H,0,0.7616300913,0.2788176508,-4.9003605244
C,0,-3.4330000418,-0.0389919706,0.
C,0,3.4769195587,-0.7035918409,0.
O,0,-4.5892402189,-0.0632752343,0.
O,0,4.5435658414,-1.1578859339,0.
C,0,-1.0097798276,-1.7055456162,0.
O,0,-0.6721750081,-2.8167399473,0.

$[CH_3N(PF_2)_2]_2Fe_2(CO)_5$ (**25-2T**) $C_s$ BP86
0 3
Fe,0,-1.5709329696,-0.0173921097,0.0000000168
Fe,0,1.735754708,0.0042914688,-0.0000000186
P,0,1.4062938653,-0.2067712915,2.1471551691
P,0,-1.5465398044,-0.0027228725,2.1442596209
P,0,-1.5465398504,-0.0027228725,-2.1442595877
P,0,1.4062938193,-0.2067712915,-2.1471551993
F,0,2.2603612575,0.8026168521,3.0776047758
F,0,1.9519268896,-1.5578460795,2.8566664177
F,0,-2.4059972873,-1.1513453794,2.8717307653
F,0,-2.2888271311,1.2354707585,2.8515499094
F,0,-2.2888271922,1.2354707585,-2.8515498604
F,0,-2.4059973489,-1.1513453794,-2.8717307138
F,0,2.2603611916,0.8026168521,-3.0776048242
F,0,1.9519268284,-1.5578460795,-2.8566664595
C,0,2.2752656816,1.7189906845,-0.0000000244
C,0,-1.0260544392,1.7046357607,0.000000011
O,0,2.6705673224,2.8251263703,-0.0000000286
O,0,-0.779219515,2.8515798633,0.0000000084
N,0,-0.1025320076,-0.0699950584,-2.9980233228
N,0,-0.1025319434,-0.0699950584,2.998023325
H,0,-1.0068042925,0.4021165024,4.8727012231
C,0,-0.1320513307,-0.1504152252,4.4935228771
H,0,-0.179809031,-1.2009431595,4.8233714141
H,0,0.7770397624,0.3281650129,4.8894052055
H,0,-0.1798091344,-1.2009431595,-4.8233714102
C,0,-0.132051427,-0.1504152252,-4.4935228743
H,0,-1.006804397,0.4021165024,-4.8727012016
H,0,0.7770396576,0.3281650129,-4.8894052222
C,0,-3.3689315229,-0.0577650807,0.0000000361
C,0,3.3956128429,-0.7049311923,-0.0000000364
O,0,-4.5402714284,-0.0855351846,0.0000000487
O,0,4.489855667,-1.1324309027,-0.0000000481
C,0,-0.9324151573,-1.7053545058,0.00000001
O,0,-0.5972959928,-2.831876353,0.0000000064

$[CH_3N(PF_2)_2]_2Fe_2(CO)_4$ (**24-1S**) $C_1$ B3LYP
0 1
Fe,0,0.2988078371,1.3910280398,0.0583351738
Fe,0,0.3525362227,-1.3171106545,0.0671446793
P,0,-1.7933949068,-1.5009898126,0.0481981813
P,0,-1.8385793557,1.3911178158,0.2731271554
P,0,0.2666770101,0.0492570674,-1.6411747734
P,0,2.4095170787,-0.5448043615,0.2816416446
F,0,-2.4713042205,-2.3566832529,1.2116279766
F,0,-2.5479748432,-2.2395719385,-1.1434546809
F,0,-2.724281621,2.2957113647,-0.6976460169
F,0,-2.4497633533,1.9763543486,1.6276576683
F,0,1.3808730363,0.1001167599,-2.7832018178
F,0,-0.9959956841,-0.0468270695,-2.639311121
F,0,3.1198703596,-0.7930289728,1.7064082741
F,0,3.605534737,-1.2077504906,-0.5566447466
C,0,0.3514342494,-1.6382128437,1.8496854667
O,0,0.3547347974,-1.854019971,2.9842448067
N,0,2.3246707647,1.0033504482,-0.0685073766
N,0,-2.6847381089,-0.0697930127,0.1432175559
H,0,-4.5687358581,0.7565978402,0.6551577565
C,0,-4.1749480258,-0.084828766,0.0788262043
H,0,-4.5137599252,-0.0141022788,-0.9588079181
H,0,-4.5442934796,-1.0100619147,0.5292289321
H,0,3.2634002015,2.5626814014,-1.1284120664
C,0,3.4163625663,1.9627789795,-0.2223348163
H,0,3.4765603661,2.6443473919,0.637462608
H,0,4.3810160725,1.4488227251,-0.3214518949
C,0,0.4293925462,3.0152972463,-0.6904745914
C,0,0.7605505469,-2.9000652344,-0.6668336226
O,0,0.5260265834,4.055376547,-1.1843347658
O,0,1.0365690428,-3.9140023949,-1.1466291659
C,0,0.5825975277,1.73958424,1.8353199007
O,0,0.8303310558,1.9739469997,2.9364131381

$[CH_3N(PF_2)_2]_2Fe_2(CO)_4$ (**24-1S**) $C_1$ BP86
0 1
Fe,0,0.3059441394,1.3821997309,0.0521801256
Fe,0,0.3479461003,-1.3158445073,0.061596347
P,0,-1.7789342487,-1.5121003932,0.0283551691
P,0,-1.8019128016,1.385777419,0.2774708899
P,0,0.2775075409,0.043392225,-1.6506351443
P,0,2.394042671,-0.5546380249,0.2973619759
F,0,-2.4697654073,-2.4113325529,1.1721231059
F,0,-2.526731138,-2.2328746759,-1.1998119085
F,0,-2.6934642179,2.3002833399,-0.7063051736
F,0,-2.4164206059,1.9904808432,1.6406670534
F,0,1.4117225651,0.0809891581,-2.7935481041
F,0,-0.983604926,-0.0359015724,-2.6713574102
F,0,3.0865649326,-0.7873677366,1.7491921776
F,0,3.6068687755,-1.2470012296,-0.5204446388
C,0,0.3275934711,-1.6381424308,1.8298808328
O,0,0.3123061118,-1.8633887815,2.9778571313
N,0,2.329372978,0.9992488568,-0.0959965052
N,0,-2.6777082853,-0.0766568889,0.159705318
H,0,-4.5526256253,0.7451642474,0.7370709454
C,0,-4.1708386107,-0.0781838842,0.1122106241
H,0,-4.5262197834,0.0414710224,-0.9242153685
H,0,-4.5422136336,-1.0277471683,0.5298716666
H,0,3.2479987634,2.606119362,-1.110958304
C,0,3.4157500569,1.9727492496,-0.2208447356
H,0,3.4810259637,2.6278649203,0.6689448757
H,0,4.3855614935,1.4565963826,-0.3484422466
C,0,0.4004644867,2.9906133156,-0.6964182063
C,0,0.7547960417,-2.8919840083,-0.6586655427
O,0,0.4627387642,4.0499918664,-1.1942671082
O,0,1.0342982119,-3.9241810303,-1.1353894828
C,0,0.5890982024,1.7625013289,1.798233615
O,0,0.8285312334,2.0364178635,2.9090557741

$[CH_3N(PF_2)_2]_2Fe_2(CO)_4$ (**24-2S**) $C_s$ B3LYP
0 1
Fe,0,1.2003202379,0.2314778149,0.
Fe,0,-1.3722011961,0.2277020125,0.
P,0,-1.3517868568,0.2556076341,2.2116378295
P,0,1.4547001992,-0.3914853867,2.0261313509
P,0,1.4547001992,-0.3914853867,-2.0261313509
P,0,-1.3517868568,0.2556076341,-2.2116378295
F,0,-2.4611823796,-0.599639959,2.9674106426
F,0,-1.6859868774,1.6383233887,2.9306123723
F,0,2.4639880233,0.4264884328,2.9586019625
F,0,1.9575798088,-1.83253367,2.5105820753
F,0,1.9575798088,-1.83253367,-2.5105820753
F,0,2.4639880233,0.4264884328,-2.9586019625
F,0,-2.4611823796,-0.599639959,-2.9674106426
F,0,-1.6859868774,1.6383233887,-2.9306123723
C,0,-0.3230711099,-1.267240975,0.
C,0,2.8381283008,0.9315833624,0.
O,0,-0.3323591444,-2.4498527698,0.
O,0,3.893399817,1.4105245921,0.
N,0,0.0335970959,-0.2790642576,-2.9825620312
N,0,0.0335970959,-0.2790642576,2.9825620312
H,0,0.6706893744,-1.4357496721,4.6330916236
C,0,0.0795538839,-0.5342376048,4.4486640725
H,0,0.526588184,0.3168270856,4.9717310859
H,0,-0.9336899957,-0.7039154295,4.8211838811
H,0,0.526588184,0.3168270856,-4.9717310859
C,0,0.0795538839,-0.5342376048,-4.4486640725
H,0,0.6706893744,-1.4357496721,-4.6330916236
H,0,-0.9336899957,-0.7039154295,-4.8211838811
C,0,0.3155202932,1.7501788261,0.
C,0,-3.0546220709,-0.3445486289,0.
O,0,-0.1900511448,2.8129061432,0.
O,0,-4.1328327708,-0.7685921272,0.

$[CH_3N(PF_2)_2]_2Fe_2(CO)_4$ (**24-3T**) $C_s$ B3LYP
0 3
N,0,0.4841041194,-0.3210050345,-2.8413845967
N,0,0.4841041194,-0.3210050345,2.8413845967
C,0,0.8998419861,-0.3968062194,-4.2695272249
H,0,0.1777142686,0.1283464198,-4.9029922592
H,0,1.895001413,0.0379759863,-4.4024255769
H,0,0.9185266208,-1.447178081,-4.5689059483
H,0,0.1777142686,0.1283464198,4.9029922592
C,0,0.8998419861,-0.3968062194,4.2695272249
H,0,0.9185266208,-1.447178081,4.5689059483
H,0,1.895001413,0.0379759863,4.4024255769
P,0,0.3956879533,-1.7240854196,1.8184068193
P,0,-0.0271893661,1.1187731325,2.1715583286
P,0,0.3956879533,-1.7240854196,-1.8184068193
P,0,-0.0271893661,1.1187731325,-2.1715583286
C,0,-2.0853563036,-2.164941008,0.
C,0,1.672797772,0.9162353946,0.
O,0,-3.0229872113,-2.8511218837,0.
O,0,2.7995047158,0.65495337,0.
Fe,0,-0.5983820642,-1.1007266299,0.
Fe,0,-0.0723135745,1.4203611841,0.
F,0,0.9096593133,2.1388703437,2.9661250547
F,0,-1.3677963265,1.4684904769,2.9611831921
F,0,-0.2609878134,-2.7349569928,2.8810502378
F,0,1.893356632,-2.2675675557,2.0411728519
F,0,1.893356632,-2.2675675557,-2.0411728519
F,0,-0.2609878134,-2.7349569928,-2.8810502378
F,0,0.9096593133,2.1388703437,-2.9661250547
F,0,-1.3677963265,1.4684904769,-2.9611831921
C,0,0.066917069,3.2219112948,0.
C,0,-1.8881849062,1.2469150773,0.
O,0,0.1487988329,4.3728154885,0.
O,0,-3.045089171,1.2563479757,0.

$[CH_3N(PF_2)_2]_2Fe_2(CO)_4$ (**24-2S**) $C_s$ BP86
0 1
Fe,0,1.2053336995,0.1865501727,0.
Fe,0,-1.3355793246,0.2046887347,0.
P,0,-1.355812096,0.251527913,2.1793520204
P,0,1.4551070022,-0.3754569108,2.0416629828
P,0,1.4551070022,-0.3754569108,-2.0416629828
P,0,-1.355812096,0.251527913,-2.1793520204
F,0,-2.4778978009,-0.6129532877,2.9387481719
F,0,-1.7207525162,1.6535830938,2.8839195234
F,0,2.4692647784,0.4719418207,2.9657105399
F,0,1.9870901828,-1.8209483676,2.5307059009
F,0,1.9870901828,-1.8209483676,-2.5307059009
F,0,2.4692647784,0.4719418207,-2.9657105399
F,0,-2.4778978009,-0.6129532877,-2.9387481719
F,0,-1.7207525162,1.6535830938,-2.8839195234
C,0,-0.2915427027,-1.3025022418,0.
C,0,2.8456715723,0.8504828187,0.
O,0,-0.3075453398,-2.498147253,0.
O,0,3.9263094987,1.3115833361,0.
N,0,0.0273150239,-0.2681325405,-2.9982743158
N,0,0.0273150239,-0.2681325405,2.9982743158
H,0,0.6956624702,-1.381052764,4.674866486
C,0,0.0530539431,-0.5093293786,4.4691325998
H,0,0.4393747841,0.3757457623,5.0017007622
H,0,-0.9658640902,-0.7393809332,4.8186470201
H,0,0.4393747841,0.3757457623,-5.0017007622
C,0,0.0530539431,-0.5093293786,-4.4691325998
H,0,0.6956624702,-1.381052764,-4.674866486
H,0,-0.9658640902,-0.7393809332,-4.8186470201
C,0,0.3123866206,1.7117731165,0.
C,0,-3.0064139534,-0.3550491816,0.
O,0,-0.1033437645,2.8276320877,0.
O,0,-4.1090651108,-0.7631435979,0.

$[CH_3N(PF_2)_2]_2Fe_2(CO)_4$ (**24-3T**) $C_s$ BP86
0 3
N,0,0.2577338473,-0.4783660696,2.8246033988
N,0,0.2577338473,-0.4783660696,-2.8246033988
C,0,0.3686906149,-0.9167445194,4.2448106397
H,0,-0.2538758266,-0.2685332652,4.8838481872
H,0,0.0492599842,-1.9666506383,4.3542898771
H,0,1.4178778179,-0.8114012647,4.5620989093
H,0,-0.2538758266,-0.2685332652,-4.8838481872
C,0,0.3686906149,-0.9167445194,-4.2448106397
H,0,1.4178778179,-0.8114012647,-4.5620989093
H,0,0.0492599842,-1.9666506383,-4.3542898771
P,0,1.5851994675,-0.4409333796,-1.7058815762
P,0,-1.2053555264,0.0156451417,-2.1520772692
P,0,1.5851994675,-0.4409333796,1.7058815762
P,0,-1.2053555264,0.0156451417,2.1520772692
C,0,2.5974881745,1.8754579353,0.
C,0,-1.2463871366,-1.6878420244,0.
O,0,3.5399845697,2.5782796227,0.
O,0,-1.2210692016,-2.859873541,0.
Fe,0,1.178868233,0.7815593799,0.
Fe,0,-1.3401182439,0.1175656376,0.
F,0,-2.2273144255,-0.9873128983,-2.8846905092
F,0,-1.5968075776,1.316113503,-3.0141333584
F,0,2.7496724931,-0.0566933355,-2.7660233285
F,0,1.9669994883,-2.0139251985,-1.645047367
F,0,1.9669994883,-2.0139251985,1.645047367
F,0,2.7496724931,-0.0566933355,2.7660233285
F,0,-2.2273144255,-0.9873128983,2.8846905092
F,0,-1.5968075776,1.316113503,3.0141333584
C,0,-3.0662929227,0.5692791474,0.
C,0,-0.5507878644,1.8396482889,0.
O,0,-4.2012881901,0.8603027225,0.
O,0,-0.6324107971,3.0298843114,0.

$[CH_3N(PF_2)_2]_2Fe_2(CO)_3$ (**23-1S**) $C_1$ B3LYP
0 1
Fe,0,-0.4324967263,1.4157311096,-0.2075835477
Fe,0,-0.3433325153,-1.2499783272,0.0066783819
P,0,1.8018951272,-1.3722288314,0.1159978166
P,0,1.681401379,1.4215049327,-0.5903844888
P,0,-0.3191279174,0.2998196448,1.5533284768
P,0,-2.3487985347,-0.5006361901,-0.5026799889
F,0,2.5368679965,-2.3887788195,-0.8697170798
F,0,2.5543685178,-1.8646325322,1.4297544542
F,0,2.6376484038,2.547097558,0.0159980895
F,0,2.0788890852,1.6799878872,-2.1189078667
F,0,-1.4959100304,0.4796266445,2.6204583012
F,0,0.8923676966,0.3933483504,2.6036418488
F,0,-3.0241923737,-1.0774517315,-1.8362281846
F,0,-3.5794568152,-0.8758719694,0.4575277372
C,0,-0.204689145,-1.7131606199,-1.7318190544
O,0,-0.1154461415,-2.0146366074,-2.8449579321
N,0,-2.2794518536,1.1085098862,-0.6305290816
N,0,2.6270915485,0.0590968297,-0.2206321622
H,0,4.4541103907,0.7109938199,-1.0830299057
C,0,4.1153112403,0.133085633,-0.2181325137
H,0,4.4731069033,0.5996008525,0.7042527728
H,0,4.5237408145,-0.8774583297,-0.2998660284
H,0,-3.9658707247,2.0779834136,0.2413617616
C,0,-3.4436443274,1.9987870951,-0.721736134
H,0,-3.1155978463,2.9969279428,-1.0273653811
H,0,-4.1565746984,1.631896962,-1.472063114
C,0,-0.5569784241,3.1276940704,0.2670722821
C,0,-0.7959864256,-2.7568352737,0.8757497926
O,0,-0.6318123562,4.2198335088,0.644686867
O,0,-1.1008080751,-3.7203871797,1.4363855719

$[CH_3N(PF_2)_2]_2Fe_2(CO)_3$ (**23-1S**) $C_1$ BP86
0 1
Fe,0,-0.4473198993,1.3980922704,-0.16330624
Fe,0,-0.3423586953,-1.2531675231,0.0247657666
P,0,1.789768353,-1.3813379167,0.1245609573
P,0,1.6288307145,1.4244016909,-0.5571139607
P,0,-0.3082420084,0.2866833217,1.5834324716
P,0,-2.3281863162,-0.5039341043,-0.4875883477
F,0,2.5274466529,-2.4216216388,-0.8588886572
F,0,2.546138374,-1.8734986983,1.4559057242
F,0,2.5944386301,2.556064178,0.0660373491
F,0,2.0138404747,1.7240073832,-2.1005673457
F,0,-1.4908527358,0.4575840502,2.6695233414
F,0,0.910224832,0.3912141824,2.6445179207
F,0,-3.0207933288,-1.1047111728,-1.8175681944
F,0,-3.5605707001,-0.8452654742,0.5068079835
C,0,-0.1966587201,-1.7064355884,-1.7026950842
O,0,-0.1007618496,-2.0092223187,-2.8306380708
N,0,-2.2600662903,1.1225383987,-0.6678628178
N,0,2.6131851209,0.0546982306,-0.2350641811
H,0,4.4170676342,0.7248758422,-1.147120714
C,0,4.1023142954,0.1429600837,-0.2652281038
H,0,4.4805643485,0.6193235243,0.6539555568
H,0,4.5202489805,-0.8724900959,-0.3547283861
H,0,-4.0018525997,2.0535596835,0.1576666934
C,0,-3.4244586858,2.0140936237,-0.7855749797
H,0,-3.0777492477,3.0292787653,-1.0376966932
H,0,-4.097016423,1.6645312851,-1.5919284436
C,0,-0.5413902839,3.0906035691,0.3050426981
C,0,-0.7901877666,-2.7568563048,0.8810999081
O,0,-0.5904738662,4.2022258345,0.6875589811
O,0,-1.0985048216,-3.7387253519,1.4399565585

$[CH_3N(PF_2)_2]_2Fe_2(CO)_3$ (**23-2T**) $C_1$ B3LYP
0 3
Fe,0,-0.3022117371,1.3453804224,-0.0539057879
Fe,0,-0.4236863347,-1.2437792979,-0.273189532
P,0,1.7329962354,-1.553169584,-0.3011298254
P,0,1.8523764335,1.4048743694,-0.2042997956
P,0,-0.3623122351,-0.0100481242,1.6196333925
P,0,-2.5032733849,-0.4661381191,-0.6532798481
F,0,2.4171016255,-2.3292505816,-1.5163852457
F,0,2.4474070051,-2.3998214713,0.8411168008
F,0,2.7130989057,2.0991589278,0.9455153736
F,0,2.6000899457,2.1519884978,-1.4048843571
F,0,-1.610074295,-0.1426373554,2.6172358871
F,0,0.7699630294,-0.380900458,2.7048017861
F,0,-3.2756216603,-0.8244927167,-2.0148377429
F,0,-3.7180615566,-0.9140649788,0.2928428544
C,0,-0.107589358,0.0172466919,-1.6630837376
O,0,0.0410627372,0.2430328633,-2.8098534748
N,0,-2.2674000434,1.1204925431,-0.5357211136
N,0,2.6271291593,-0.1198823181,-0.2797923967
H,0,4.5126871379,0.6765118188,-0.8328458335
C,0,4.1188421726,-0.1810461235,-0.2810841473
H,0,4.502429118,-0.1725486941,0.7433643305
H,0,4.4438774029,-1.0919622946,-0.7906109618
H,0,-3.4853733744,2.5389107237,0.4745256262
C,0,-3.3391018666,2.1253263218,-0.5322144465
H,0,-3.0813970966,2.9469826493,-1.2111748423
H,0,-4.2950928759,1.7023563672,-0.8663175631
C,0,-0.46993314,2.9993439964,0.6162418921
C,0,-0.8908966846,-2.7602667894,0.5995087109
O,0,-0.5888594903,4.0600457417,1.0613440427
O,0,-1.202088549,-3.7294736654,1.1436031321

$[CH_3N(PF_2)_2]_2Fe_2(CO)_3$ (**23-2T**) $C_1$ BP86
0 3
Fe,0,-0.3022932965,1.3214105689,-0.071475148
Fe,0,-0.4286467488,-1.2431488882,-0.1925422769
P,0,1.6993946221,-1.5515749746,-0.2562961204
P,0,1.8188375061,1.4069677206,-0.1880352002
P,0,-0.374025733,-0.0215711255,1.5922402411
P,0,-2.4705759387,-0.4849635309,-0.649738892
F,0,2.3636383001,-2.3560138789,-1.4868946887
F,0,2.4424521396,-2.3948562275,0.8941407726
F,0,2.670625513,2.1224437401,0.9769921196
F,0,2.5611580516,2.1817685314,-1.3960045641
F,0,-1.6156764761,-0.0221643564,2.6289312976
F,0,0.7794468969,-0.2096683592,2.7182065791
F,0,-3.206883998,-0.8754989614,-2.0398382381
F,0,-3.7291913873,-0.8940449693,0.2797761718
C,0,-0.09372787,0.0858486025,-1.5966871385
O,0,0.0634942848,0.1157633975,-2.7831875941
N,0,-2.2481145002,1.1322120871,-0.5571861922
N,0,2.6173112732,-0.1144734037,-0.2748723914
H,0,4.4903946553,0.6999721414,-0.8648576231
C,0,4.10895568,-0.1735170983,-0.3120667778
H,0,4.5231716542,-0.1809851148,0.7096523433
H,0,4.4228259546,-1.0831101532,-0.8491277871
H,0,-3.4274699608,2.5734871325,0.4765418776
C,0,-3.3239899028,2.1347549634,-0.5339967657
H,0,-3.0935908006,2.9467840632,-1.2467275234
H,0,-4.2966964064,1.6932917925,-0.8187810238
C,0,-0.4491063527,2.9440409855,0.6484070315
C,0,-0.8951374418,-2.8131364402,0.5254639145
O,0,-0.5377817736,4.0153732968,1.1187249481
O,0,-1.2127107184,-3.8432221788,0.9843618254

$[CH_3N(PF_2)_2]_2Fe_2(CO)_3$ (**23-3T**) $C_s$ B3LYP
0 3
Fe,0,0.,1.3813434559,0.3010073683
Fe,0,0.,-1.3858416227,0.2229659596
P,0,-2.1718034312,-1.3634758591,-0.0248307822
P,0,-2.0472598296,1.4433518287,-0.4196886358
P,0,2.0472598296,1.4433518287,-0.4196886358
P,0,2.1718034312,-1.3634758591,-0.0248307822
F,0,-3.0854549962,-2.0559385067,1.0860657688
F,0,-2.6830936481,-2.265839697,-1.2424605231
F,0,-2.2952628366,1.8680339837,-1.9455123299
F,0,-3.080055971,2.5003171967,0.1975861297
F,0,3.080055971,2.5003171967,0.1975861297
F,0,2.2952628366,1.8680339837,-1.9455123299
F,0,3.0854549962,-2.0559385067,1.0860657688
F,0,2.6830936481,-2.265839697,-1.2424605231
C,0,0.,0.3374375404,1.740910088
O,0,0.,-0.317888333,2.7208500685
N,0,3.0240500341,0.0571955684,-0.2943179272
N,0,-3.0240500341,0.0571955684,-0.2943179272
H,0,-4.9405699714,0.9095787745,-0.0078965666
C,0,-4.4891586769,0.076431338,-0.5529208867
H,0,-4.6865251805,0.1804072006,-1.6247057656
H,0,-4.9292797562,-0.8569965616,-0.1923370962
H,0,4.6865251805,0.1804072006,-1.6247057656
C,0,4.4891586769,0.076431338,-0.5529208867
H,0,4.9405699714,0.9095787745,-0.0078965666
H,0,4.9292797562,-0.8569965616,-0.1923370962
C,0,0.,2.9817517598,1.0802910574
C,0,0.,-3.1705013789,0.3284633396
O,0,0.,3.9896039288,1.6555715424
O,0,0.,-4.3265932598,0.4314424483

$[CH_3N(PF_2)_2]_2Fe_2(CO)_3$ (**23-3T**) $C_s$ BP86
0 3
Fe,0,0.,1.3342966183,0.2372808894
Fe,0,0.,-1.365500072,0.2528120424
P,0,-2.1353874788,-1.3610930235,-0.0703124599
P,0,-2.0534103786,1.4543992671,-0.3887543616
P,0,2.0534103786,1.4543992671,-0.3887543616
P,0,2.1353874788,-1.3610930235,-0.0703124599
F,0,-3.0878867702,-2.1503410576,0.9652187484
F,0,-2.5721321556,-2.2091440468,-1.3748679543
F,0,-2.3682039242,1.9584443963,-1.8949266371
F,0,-3.0475075438,2.5028580508,0.3330851529
F,0,3.0475075438,2.5028580508,0.3330851529
F,0,2.3682039242,1.9584443963,-1.8949266371
F,0,3.0878867702,-2.1503410576,0.9652187484
F,0,2.5721321556,-2.2091440468,-1.3748679543
C,0,0.,0.3058198807,1.6717644315
O,0,0.,-0.2913438579,2.7076342522
N,0,3.0362702131,0.0599872805,-0.2797203576
N,0,-3.0362702131,0.0599872805,-0.2797203576
H,0,-4.932652098,0.9942747617,-0.1240233259
C,0,-4.5046060792,0.063325313,-0.5290847831
H,0,-4.7180543735,-0.0090946068,-1.6088849253
H,0,-4.9603117453,-0.7900806413,-0.0015135241
H,0,4.7180543735,-0.0090946068,-1.6088849253
C,0,4.5046060792,0.063325313,-0.5290847831
H,0,4.932652098,0.9942747617,-0.1240233259
H,0,4.9603117453,-0.7900806413,-0.0015135241
C,0,0.,2.9355029569,0.9864596769
C,0,0.,-3.1353448048,0.417186021
O,0,0.,3.9671972596,1.5509634415
O,0,0.,-4.3024053863,0.5640957477

**Complete Gaussian 03 reference (Reference 27)**

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