# Effect of Metal Complexation on the Equilibrium Between Methylphosphepine and Methylphosphanorcaradiene and Their Benzo Analogues

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## Supporting Information

**Tables S1-S48.** Harmonic vibrational frequencies (in $cm^{-1}$) and infrared intensities (in parentheses, in km/mol) for the structures of $C_6H_6PCH_3$, $C_{10}H_8PCH_3$, $(C_6H_6PCH_3)Fe(CO)_3$, $(C_6H_6PCH_3)Co(C_5H_5)$, $(C_{10}H_8PCH_3)Fe(CO)_3$, and $(C_{10}H_8PCH_3)Co(C_5H_5)$.

**Table S49.** Cartesian coordinates for the structures of $C_6H_6PCH_3$, $C_{10}H_8PCH_3$, $(C_6H_6PCH_3)Fe(CO)_3$, $(C_6H_6PCH_3)Co(C_5H_5)$, $(C_{10}H_8PCH_3)Fe(CO)_3$ and $(C_{10}H_8PCH_3)Co(C_5H_5)$.

**Tables S50 - S55.** The total energies (E, in hartree), relative energies (ΔE, in kcal/mol), and the number of imaginary vibrational frequencies (Nimg) for $C_6H_6PCH_3$, $C_{10}H_8PCH_3$, $(C_6H_6PCH_3)Fe(CO)_3$, $(C_6H_6PCH_3)Co(C_5H_5)$, $(C_{10}H_8PCH_3)Fe(CO)_3$ and $(C_{10}H_8PCH_3)Co(C_5H_5)$.

**Table S56.** Harmonic ν(CO) vibrational frequencies (in $cm^{-1}$) predicted for the isomers of $(C_6H_6PCH_3)Fe(CO)_3$ by the BP86 method.

**Table S57.** Harmonic ν(CO) vibrational frequencies (in $cm^{-1}$) predicted for the isomers of $(C_{10}H_8PCH_3)Fe(CO)_3$ by the BP86 method.

**Figures S1-S2.** The higher-lying $(C_{10}H_8PCH_3)Fe(CO)_3$ and $(C_{10}H_8PCH_3)Co(C_5H_5)$ structures.

**Complete Gaussian reference 42.**

**Table S1.** Harmonic vibrational frequencies (in $cm^{-1}$) and infrared intensities (in parentheses, in km/mol) for the structure **1-1** of $C_6H_6PCH_3$ with $C_s$ symmetry.

| BP86 | | B3LYP | | M06-L | |
|---|---|---|---|---|---|
| 32 | (0) | 44 | (0) | 124 | (0) |
| 175 | (0) | 180 | (0) | 196 | (0) |
| 181 | (0) | 184 | (0) | 197 | (0) |
| 280 | (1) | 292 | (1) | 291 | (1) |
| 294 | (2) | 302 | (1) | 311 | (2) |
| 398 | (4) | 414 | (4) | 418 | (3) |
| 478 | (3) | 495 | (3) | 521 | (2) |
| 483 | (6) | 500 | (5) | 535 | (6) |
| 541 | (2) | 558 | (2) | 562 | (2) |
| 582 | (3) | 602 | (3) | 607 | (3) |
| 654 | (3) | 680 | (3) | 696 | (4) |
| 674 | (30) | 691 | (26) | 718 | (48) |
| 718 | (74) | 746 | (82) | 751 | (45) |
| 774 | (0) | 807 | (0) | 801 | (0) |
| 834 | (1) | 855 | (0) | 864 | (3) |
| 843 | (5) | 877 | (4) | 871 | (1) |
| 875 | (9) | 912 | (9) | 896 | (10) |
| 913 | (0) | 959 | (3) | 949 | (0) |
| 924 | (0) | 962 | (0) | 961 | (1) |
| 930 | (2) | 968 | (1) | 969 | (1) |
| 944 | (2) | 973 | (1) | 990 | (0) |
| 952 | (0) | 981 | (0) | 991 | (2) |
| 968 | (6) | 998 | (5) | 1005 | (6) |
| 1032 | (2) | 1070 | (3) | 1072 | (3) |
| 1105 | (11) | 1136 | (14) | 1144 | (11) |
| 1146 | (1) | 1186 | (1) | 1175 | (2) |
| 1155 | (1) | 1193 | (1) | 1189 | (1) |
| 1279 | (4) | 1332 | (5) | 1310 | (4) |
| 1288 | (1) | 1337 | (1) | 1334 | (1) |
| 1291 | (19) | 1338 | (18) | 1346 | (14) |
| 1368 | (11) | 1412 | (12) | 1422 | (6) |
| 1400 | (17) | 1452 | (1) | 1434 | (17) |
| 1405 | (2) | 1456 | (15) | 1449 | (10) |
| 1414 | (16) | 1465 | (15) | 1466 | (8) |
| 1541 | (1) | 1595 | (1) | 1616 | (2) |
| 1612 | (0) | 1670 | (0) | 1687 | (0) |
| 2968 | (21) | 3046 | (19) | 3046 | (37) |
| 3056 | (6) | 3135 | (6) | 3148 | (7) |
| 3068 | (2) | 3136 | (2) | 3150 | (8) |
| 3073 | (3) | 3146 | (3) | 3160 | (23) |
| 3082 | (11) | 3156 | (11) | 3166 | (4) |
| 3101 | (2) | 3177 | (1) | 3185 | (5) |
| 3107 | (5) | 3183 | (4) | 3191 | (9) |
| 3121 | (33) | 3197 | (32) | 3206 | (63) |
| 3132 | (16) | 3208 | (16) | 3218 | (31) |

**Table S2.** Harmonic vibrational frequencies (in $cm^{-1}$) and infrared intensities (in parentheses, in km/mol) for the structure 1-2 of $C_6H_6PCH_3$ with $C_s$ symmetry.

| BP86 | | B3LYP | | M06-L | |
|---|---|---|---|---|---|
| 80 | (0) | 91 | (0) | 82 | (0) |
| 144 | (1) | 154 | (0) | 152 | (1) |
| 145 | (0) | 154 | (1) | 157 | (0) |
| 226 | (0) | 234 | (0) | 240 | (0) |
| 256 | (1) | 265 | (1) | 269 | (1) |
| 372 | (4) | 386 | (4) | 389 | (4) |
| 480 | (1) | 499 | (1) | 514 | (0) |
| 505 | (14) | 524 | (13) | 549 | (14) |
| 545 | (5) | 562 | (5) | 567 | (5) |
| 581 | (4) | 600 | (4) | 607 | (5) |
| 661 | (11) | 682 | (11) | 704 | (12) |
| 670 | (5) | 695 | (6) | 714 | (7) |
| 718 | (94) | 747 | (96) | 750 | (79) |
| 767 | (0) | 800 | (0) | 797 | (0) |
| 825 | (0) | 845 | (0) | 859 | (0) |
| 850 | (3) | 884 | (3) | 880 | (2) |
| 860 | (3) | 891 | (3) | 890 | (2) |
| 916 | (2) | 954 | (0) | 954 | (2) |
| 918 | (2) | 964 | (0) | 956 | (0) |
| 932 | (0) | 966 | (2) | 970 | (0) |
| 939 | (1) | 971 | (10) | 974 | (2) |
| 940 | (12) | 980 | (1) | 984 | (8) |
| 956 | (4) | 984 | (5) | 993 | (4) |
| 1023 | (0) | 1059 | (2) | 1064 | (1) |
| 1097 | (13) | 1125 | (15) | 1136 | (14) |
| 1148 | (1) | 1185 | (1) | 1179 | (1) |
| 1158 | (2) | 1194 | (2) | 1195 | (2) |
| 1275 | (8) | 1325 | (9) | 1316 | (5) |
| 1283 | (1) | 1329 | (1) | 1328 | (0) |
| 1293 | (4) | 1338 | (3) | 1342 | (4) |
| 1359 | (7) | 1403 | (6) | 1410 | (4) |
| 1402 | (1) | 1446 | (1) | 1452 | (4) |
| 1414 | (6) | 1462 | (6) | 1454 | (1) |
| 1423 | (11) | 1471 | (10) | 1463 | (11) |
| 1557 | (1) | 1612 | (1) | 1623 | (1) |
| 1623 | 0 | 1681 | (0) | 1689 | (0) |
| 2969 | (23) | 3040 | (21) | 3033 | (45) |
| 3059 | (10) | 3125 | (11) | 3133 | (9) |
| 3064 | (9) | 3132 | (10) | 3141 | (18) |
| 3069 | (3) | 3145 | (3) | 3142 | (17) |
| 3077 | (18) | 3153 | (18) | 3144 | (30) |
| 3101 | (1) | 3177 | (1) | 3174 | (3) |
| 3107 | (3) | 3183 | (3) | 3180 | (7) |
| 3122 | (36) | 3198 | (35) | 3196 | (67) |
| 3132 | (21) | 3209 | (20) | 3207 | (39) |

**Table S3.** Harmonic vibrational frequencies (in $cm^{-1}$) and infrared intensities (in parentheses, in km/mol) for the structure 1-3 of $C_6H_6PCH_3$ with $C_s$ symmetry.

| BP86 | | B3LYP | | M06-L | |
|---|---|---|---|---|---|
| 101 | (0) | 105 | (0) | 105 | (0) |
| 172 | (0) | 182 | (0) | 155 | (0) |
| 191 | (0) | 200 | (0) | 205 | (0) |
| 250 | (2) | 256 | (2) | 255 | (2) |
| 260 | (3) | 277 | (2) | 275 | (2) |
| 270 | (1) | 284 | (1) | 284 | (1) |
| 351 | (0) | 363 | (0) | 360 | (0) |
| 392 | (2) | 411 | (2) | 410 | (1) |
| 515 | (4) | 537 | (4) | 539 | (3) |
| 584 | (9) | 602 | (6) | 614 | (14) |
| 633 | (126) | 659 | (127) | 662 | (103) |
| 673 | (1) | 691 | (0) | 709 | (0) |
| 683 | (25) | 705 | (24) | 729 | (26) |
| 702 | (18) | 733 | (18) | 734 | (17) |
| 717 | (7) | 740 | (13) | 755 | (6) |
| 788 | (1) | 815 | (1) | 822 | (1) |
| 834 | (3) | 864 | (2) | 864 | (3) |
| 883 | (1) | 911 | (1) | 918 | (18) |
| 892 | (23) | 927 | (26) | 926 | (3) |
| 907 | (4) | 939 | (5) | 937 | (2) |
| 913 | (1) | 960 | (0) | 953 | (0) |
| 917 | (0) | 969 | (0) | 962 | (0) |
| 948 | (0) | 996 | (0) | 991 | (0) |
| 994 | (3) | 1017 | (2) | 1033 | (2) |
| 1144 | (0) | 1189 | (0) | 1181 | (0) |
| 1160 | (0) | 1204 | (0) | 1195 | (0) |
| 1210 | (1) | 1251 | (1) | 1250 | (1) |
| 1282 | (9) | 1335 | (9) | 1320 | (6) |
| 1291 | (6) | 1346 | (4) | 1341 | (5) |
| 1323 | (2) | 1376 | (1) | 1375 | (1) |
| 1404 | (0) | 1451 | (0) | 1456 | (10) |
| 1421 | (10) | 1469 | (9) | 1460 | (0) |
| 1421 | (8) | 1470 | (8) | 1463 | (6) |
| 1543 | (2) | 1600 | (2) | 1625 | (2) |
| 1576 | (5) | 1633 | (4) | 1655 | (7) |
| 1590 | (0) | 1652 | (0) | 1667 | (1) |
| 2975 | (21) | 3046 | (19) | 3045 | (41) |
| 3058 | (3) | 3135 | (7) | 3140 | (1) |
| 3059 | (2) | 3136 | (13) | 3141 | (6) |
| 3069 | (11) | 3137 | (1) | 3154 | (20) |
| 3071 | (5) | 3138 | (1) | 3157 | (2) |
| 3074 | (0) | 3151 | (0) | 3163 | (28) |
| 3083 | (17) | 3161 | (16) | 3164 | (1) |
| 3086 | (40) | 3164 | (38) | 3167 | (88) |
| 3096 | (32) | 3175 | (31) | 3182 | (61) |

**Table S4**. Harmonic vibrational frequencies (in $cm^{-1}$) and infrared intensities (in parentheses, in km/mol) for the structure 1-4 of $C_6H_6PCH_3$ with $C_s$ symmetry.

| BP86 | | B3LYP | | M06-L | |
|---|---|---|---|---|---|
| 123 | (0) | 120 | (0) | 151 | (0) |
| 170 | (1) | 178 | (0) | 179 | (0) |
| 188 | (0) | 199 | (0) | 193 | (0) |
| 225 | (0) | 233 | (0) | 240 | (0) |
| 261 | (1) | 277 | (0) | 272 | (0) |
| 307 | (3) | 322 | (3) | 317 | (3) |
| 373 | (1) | 384 | (1) | 385 | (1) |
| 406 | (1) | 424 | (0) | 423 | (1) |
| 554 | (2) | 573 | (3) | 573 | (2) |
| 596 | (19) | 610 | (20) | 632 | (25) |
| 635 | (52) | 657 | (44) | 665 | (69) |
| 661 | (0) | 680 | (0) | 705 | (0) |
| 666 | (77) | 687 | (86) | 715 | (34) |
| 719 | (6) | 742 | (9) | 758 | (10) |
| 736 | (18) | 765 | (17) | 764 | (17) |
| 811 | (1) | 838 | (1) | 844 | (1) |
| 852 | (1) | 885 | (1) | 881 | (2) |
| 875 | (7) | 906 | (7) | 902 | (3) |
| 888 | (21) | 914 | (4) | 909 | (26) |
| 900 | (8) | 926 | (26) | 937 | (2) |
| 933 | (1) | 986 | (1) | 969 | (1) |
| 945 | (0) | 997 | (0) | 987 | (0) |
| 960 | (0) | 1009 | (0) | 999 | (0) |
| 1012 | (0) | 1034 | (0) | 1049 | (0) |
| 1180 | (0) | 1225 | (0) | 1219 | (0) |
| 1199 | (0) | 1243 | (0) | 1236 | (1) |
| 1224 | (3) | 1266 | (3) | 1262 | (3) |
| 1273 | (9) | 1326 | (8) | 1311 | (7) |
| 1313 | (4) | 1369 | (3) | 1363 | (4) |
| 1340 | (16) | 1394 | (16) | 1391 | (12) |
| 1409 | (9) | 1459 | (9) | 1448 | (8) |
| 1414 | (4) | 1462 | (3) | 1453 | (4) |
| 1421 | (2) | 1470 | (3) | 1472 | (0) |
| 1519 | (14) | 1574 | (16) | 1589 | (16) |
| 1578 | (0) | 1635 | (0) | 1650 | (1) |
| 1587 | (2) | 1651 | (3) | 1660 | (3) |
| 2978 | (19) | 3050 | (18) | 3060 | (38) |
| 3042 | (17) | 3124 | (15) | 3132 | (31) |
| 3043 | (5) | 3125 | (4) | 3133 | (12) |
| 3066 | (6) | 3132 | (7) | 3163 | (10) |
| 3076 | (1) | 3153 | (0) | 3169 | (11) |
| 3083 | (16) | 3158 | (8) | 3177 | (19) |
| 3083 | (41) | 3160 | (12) | 3178 | (32) |
| 3087 | (6) | 3162 | (43) | 3179 | (66) |
| 3097 | (31) | 3176 | (30) | 3186 | (41) |

**Table S5.** Harmonic vibrational frequencies (in $cm^{-1}$) and infrared intensities (in parentheses, in km/mol) for the structure 2-1 of $C_6H_6PCH_3$ with $C_s$ symmetry.

| BP86 | | B3LYP | | M06-L | |
|---|---|---|---|---|---|
| 40 | (0) | 44 | (0) | 36 | (0) |
| 117 | (0) | 123 | (0) | 119 | (0) |
| 168 | (1) | 174 | (1) | 169 | (0) |
| 170 | (0) | 178 | (0) | 170 | (1) |
| 181 | (0) | 189 | (0) | 188 | (0) |
| 241 | (6) | 253 | (6) | 248 | (6) |
| 267 | (3) | 279 | (1) | 271 | (0) |
| 269 | (1) | 280 | (3) | 277 | (3) |
| 385 | (0) | 402 | (0) | 398 | (0) |
| 390 | (3) | 408 | (3) | 402 | (3) |
| 418 | (0) | 432 | (0) | 432 | (0) |
| 505 | (22) | 526 | (22) | 523 | (19) |
| 520 | (0) | 540 | (0) | 536 | (0) |
| 538 | (5) | 554 | (6) | 559 | (5) |
| 595 | (3) | 613 | (2) | 630 | (4) |
| 636 | (0) | 655 | (0) | 660 | (1) |
| 654 | (3) | 680 | (4) | 682 | (2) |
| 662 | (7) | 685 | (6) | 688 | (9) |
| 680 | (35) | 703 | (31) | 710 | (20) |
| 693 | (5) | 719 | (9) | 732 | (0) |
| 702 | (0) | 725 | (0) | 740 | (18) |
| 739 | (49) | 765 | (41) | 768 | (41) |
| 763 | (2) | 796 | (2) | 790 | (2) |
| 773 | (84) | 802 | (94) | 803 | (66) |
| 839 | (2) | 868 | (1) | 871 | (2) |
| 857 | (0) | 893 | (0) | 889 | (0) |
| 891 | (25) | 924 | (26) | 918 | (22) |
| 897 | (6) | 929 | (8) | 924 | (5) |
| 914 | (0) | 963 | (2) | 951 | (0) |
| 924 | (0) | 973 | (3) | 960 | (4) |
| 924 | (5) | 976 | (0) | 962 | (0) |
| 947 | (0) | 994 | (0) | 982 | (0) |
| 1037 | (7) | 1066 | (6) | 1068 | (7) |
| 1087 | (4) | 1121 | (3) | 1121 | (4) |
| 1141 | (2) | 1177 | (2) | 1173 | (0) |
| 1145 | (0) | 1179 | (0) | 1177 | (1) |
| 1153 | (3) | 1189 | (2) | 1186 | (2) |
| 1197 | (0) | 1230 | (0) | 1232 | (0) |
| 1212 | (0) | 1253 | (0) | 1253 | (0) |
| 1256 | (2) | 1299 | (2) | 1293 | (3) |
| 1282 | (5) | 1334 | (6) | 1320 | (4) |
| 1329 | (7) | 1363 | (2) | 1375 | (7) |
| 1345 | (1) | 1381 | (5) | 1389 | (2) |
| 1358 | (1) | 1398 | (1) | 1395 | (2) |
| 1406 | (8) | 1455 | (8) | 1455 | (6) |
| 1420 | (10) | 1468 | (10) | 1456 | (10) |
| 1420 | (8) | 1469 | (8) | 1459 | (6) |
| 1469 | (11) | 1518 | (12) | 1521 | (7) |
| 1551 | (1) | 1601 | (1) | 1608 | (0) |
| 1590 | (0) | 1642 | 0 | 1651 | (0) |
| 1597 | (4) | 1656 | (3) | 1674 | (6) |
| 1602 | (8) | 1659 | (10) | 1677 | (12) |
| 2977 | (26) | 3047 | (23) | 3051 | (49) |
| 3056 | (4) | 3135 | (8) | 3148 | (2) |
| 3057 | (2) | 3137 | (2) | 3148 | (7) |
| 3071 | (3) | 3138 | (0) | 3161 | (16) |
| 3074 | (9) | 3141 | (10) | 3169 | (0) |
| 3083 | (31) | 3162 | (28) | 3172 | (75) |
| 3083 | (7) | 3162 | (6) | 3172 | (15) |

| | | | | | |
|---|---|---|---|---|---|
| 3098 | (12) | 3178 | (9) | 3176 | (32) |
| 3102 | (1) | 3182 | (1) | 3180 | (1) |
| 3119 | (18) | 3197 | (19) | 3200 | (36) |
| 3135 | (25) | 3212 | (22) | 3217 | (52) |

**Table S6.** Harmonic vibrational frequencies (in $cm^{-1}$) and infrared intensities (in parentheses, in km/mol) for the structure 2-2 of $C_6H_6PCH_3$ with $C_s$ symmetry.

| BP86 | | B3LYP | | M06-L | |
|---|---|---|---|---|---|
| 58 | (0) | 60 | (0) | 77 | (0) |
| 104 | (0) | 109 | (0) | 106 | (0) |
| 161 | (2) | 168 | (2) | 177 | (0) |
| 182 | (0) | 191 | (0) | 201 | (3) |
| 204 | (0) | 213 | (0) | 220 | (0) |
| 237 | (3) | 250 | (2) | 255 | (2) |
| 257 | (0) | 269 | (0) | 261 | (0) |
| 305 | (3) | 318 | (3) | 323 | (3) |
| 379 | (0) | 397 | (0) | 393 | (0) |
| 392 | (2) | 411 | (3) | 406 | (1) |
| 415 | (1) | 428 | (1) | 430 | (1) |
| 487 | (25) | 508 | (24) | 511 | (23) |
| 531 | (1) | 550 | (3) | 547 | (1) |
| 534 | (3) | 551 | (1) | 558 | (2) |
| 613 | (7) | 630 | (8) | 651 | (14) |
| 635 | (0) | 654 | (0) | 663 | (0) |
| 652 | (11) | 674 | (11) | 695 | (8) |
| 668 | (7) | 689 | (9) | 699 | (3) |
| 680 | (6) | 705 | (7) | 707 | (6) |
| 698 | (0) | 723 | (0) | 730 | (0) |
| 703 | (4) | 733 | (4) | 737 | (6) |
| 749 | (70) | 776 | (60) | 783 | (67) |
| 773 | (4) | 805 | (3) | 801 | (4) |
| 782 | (63) | 810 | (76) | 818 | (47) |
| 846 | (0) | 879 | (0) | 880 | (0) |
| 866 | (0) | 899 | (0) | 895 | (8) |
| 874 | (12) | 908 | (14) | 902 | (2) |
| 892 | (41) | 927 | (41) | 926 | (37) |
| 924 | (4) | 968 | (4) | 962 | (3) |
| 941 | (0) | 993 | (0) | 978 | (0) |
| 946 | (0) | 994 | (0) | 987 | (0) |
| 955 | (0) | 1005 | (0) | 994 | (0) |
| 1037 | (7) | 1066 | (6) | 1068 | (7) |
| 1095 | (4) | 1129 | (3) | 1130 | (4) |
| 1147 | (0) | 1182 | (0) | 1179 | (0) |
| 1154 | (3) | 1188 | (3) | 1192 | (2) |
| 1164 | (3) | 1195 | (2) | 1201 | (2) |
| 1205 | (0) | 1243 | (1) | 1235 | (0) |
| 1218 | (1) | 1261 | (1) | 1258 | (1) |
| 1267 | (4) | 1310 | (3) | 1300 | (5) |
| 1272 | (5) | 1327 | (6) | 1322 | (3) |
| 1340 | (3) | 1374 | (2) | 1385 | (4) |
| 1353 | (4) | 1394 | (2) | 1399 | (3) |
| 1367 | (3) | 1407 | (5) | 1404 | (1) |
| 1405 | (4) | 1454 | (5) | 1453 | (8) |
| 1412 | (10) | 1462 | (9) | 1454 | (0) |
| 1416 | (5) | 1466 | (5) | 1458 | (6) |
| 1467 | (6) | 1517 | (6) | 1519 | (4) |
| 1540 | (13) | 1592 | (13) | 1600 | (8) |
| 1589 | (39) | 1642 | (1) | 1654 | (0) |
| 1591 | (1) | 1647 | (45) | 1661 | (52) |
| 1601 | (0) | 1659 | (0) | 1678 | (0) |
| 2977 | (18) | 3049 | (17) | 3057 | (31) |
| 3039 | (17) | 3124 | (12) | 3129 | (34) |
| 3040 | (4) | 3124 | (3) | 3130 | (11) |
| 3067 | (6) | 3133 | (7) | 3164 | (11) |
| 3082 | (34) | 3153 | (10) | 3171 | (18) |
| 3083 | (11) | 3161 | (34) | 3173 | (55) |
| 3084 | (8) | 3161 | (10) | 3174 | (21) |

| | | | | | |
|---|---|---|---|---|---|
| 3100 | (10) | 3179 | (7) | 3178 | (27) |
| 3104 | (1) | 3184 | (1) | 3182 | (2) |
| 3121 | (17) | 3198 | (18) | 3200 | (37) |
| 3136 | (22) | 3213 | (20) | 3216 | (48) |

**Table S7.** Harmonic vibrational frequencies (in $cm^{-1}$) and infrared intensities (in parentheses, in km/mol) for the structure 2-3 of $C_6H_6PCH_3$ with $C_s$ symmetry.

| BP86 | | B3LYP | | M06-L | |
|---|---|---|---|---|---|
| 74 | (0) | 74 | (0) | 85 | (0) |
| 94 | (0) | 96 | (0) | 101 | (0) |
| 130 | (0) | 133 | (0) | 169 | (0) |
| 204 | (0) | 212 | (0) | 242 | (2) |
| 216 | (3) | 222 | (2) | 276 | (1) |
| 292 | (4) | 301 | (3) | 314 | (2) |
| 294 | (3) | 303 | (3) | 333 | (3) |
| 378 | (0) | 393 | (0) | 392 | (0) |
| 382 | (1) | 394 | (1) | 402 | (1) |
| 425 | (13) | 441 | (12) | 443 | (12) |
| 471 | (0) | 487 | (1) | 491 | (1) |
| 483 | (23) | 498 | (27) | 529 | (1) |
| 498 | (2) | 514 | (2) | 533 | (17) |
| 523 | (7) | 539 | (5) | 547 | (17) |
| 596 | (1) | 620 | (1) | 622 | (2) |
| 600 | (2) | 621 | (2) | 649 | (2) |
| 678 | (6) | 693 | (6) | 727 | (3) |
| 710 | (14) | 729 | (4) | 739 | (14) |
| 724 | (13) | 750 | (24) | 754 | (9) |
| 731 | (0) | 757 | (0) | 756 | (1) |
| 735 | (0) | 761 | (0) | 764 | (0) |
| 790 | (0) | 826 | (0) | 820 | (0) |
| 818 | (73) | 858 | (65) | 847 | (63) |
| 835 | (1) | 872 | (3) | 860 | (1) |
| 847 | (0) | 877 | (8) | 881 | (5) |
| 847 | (5) | 884 | (3) | 885 | (0) |
| 876 | (11) | 911 | (0) | 917 | (0) |
| 881 | (0) | 912 | (13) | 926 | (9) |
| 929 | (2) | 978 | (2) | 966 | (1) |
| 941 | (0) | 989 | (0) | 976 | (0) |
| 960 | (8) | 993 | (2) | 1000 | (3) |
| 962 | (2) | 997 | (8) | 1010 | (8) |
| 986 | (7) | 1003 | (7) | 1020 | (6) |
| 1057 | (1) | 1091 | (0) | 1093 | (0) |
| 1120 | (7) | 1153 | (11) | 1153 | (8) |
| 1128 | (8) | 1165 | (8) | 1165 | (8) |
| 1142 | (0) | 1177 | (0) | 1173 | (1) |
| 1195 | (4) | 1228 | (4) | 1237 | (2) |
| 1202 | (0) | 1238 | (0) | 1241 | (0) |
| 1256 | (2) | 1302 | (2) | 1293 | (2) |
| 1276 | (2) | 1323 | (10) | 1328 | (1) |
| 1285 | (16) | 1332 | (8) | 1337 | (13) |
| 1335 | (15) | 1380 | (16) | 1384 | (11) |
| 1365 | (1) | 1408 | (1) | 1415 | (3) |
| 1387 | (2) | 1430 | (2) | 1440 | (1) |
| 1401 | (21) | 1455 | (19) | 1461 | (18) |
| 1414 | (19) | 1466 | (17) | 1462 | (18) |
| 1432 | (0) | 1473 | (0) | 1493 | (2) |
| 1503 | (1) | 1553 | (1) | 1566 | (0) |
| 1527 | (2) | 1580 | (3) | 1596 | (2) |
| 1569 | (2) | 1627 | (2) | 1637 | (1) |
| 1620 | (2) | 1680 | (2) | 1693 | (1) |
| 2969 | (19) | 3045 | (18) | 3042 | (32) |
| 3058 | (6) | 3134 | (7) | 3143 | (9) |
| 3067 | (1) | 3134 | (2) | 3157 | (4) |
| 3077 | (2) | 3151 | (2) | 3165 | (2) |
| 3085 | (12) | 3160 | (12) | 3173 | (23) |
| 3098 | (1) | 3176 | (0) | 3174 | (13) |
| 3102 | (0) | 3181 | (0) | 3179 | (1) |

| | | | | | |
|---|---|---|---|---|---|
| 3104 | (18) | 3182 | (14) | 3189 | (52) |
| 3107 | (3) | 3185 | (3) | 3192 | (8) |
| 3119 | (30) | 3197 | (30) | 3196 | (48) |
| 3132 | (25) | 3210 | (23) | 3210 | (52) |

**Table S8.** Harmonic vibrational frequencies (in $cm^{-1}$) and infrared intensities (in parentheses, in km/mol) for the structure 2-4 of $C_6H_6PCH_3$ with $C_s$ symmetry.

| BP86 | | B3LYP | | M06-L | |
|---|---|---|---|---|---|
| 41 | (0) | 64 | (0) | 46 | (1) |
| 83 | (1) | 87 | (1) | 87 | (1) |
| 110 | (0) | 114 | (0) | 111 | (0) |
| 153 | (1) | 159 | (1) | 163 | (1) |
| 211 | (2) | 218 | (2) | 216 | (2) |
| 245 | (0) | 253 | (0) | 258 | (0) |
| 279 | (2) | 288 | (2) | 289 | (2) |
| 362 | (1) | 376 | (1) | 377 | (0) |
| 366 | (0) | 379 | (0) | 379 | (1) |
| 421 | (17) | 438 | (17) | 437 | (15) |
| 469 | (2) | 484 | (3) | 488 | (3) |
| 505 | (2) | 522 | (2) | 528 | (1) |
| 507 | (35) | 527 | (37) | 542 | (0) |
| 521 | (3) | 537 | (1) | 556 | (41) |
| 600 | (2) | 620 | (2) | 624 | (3) |
| 616 | (1) | 643 | (2) | 672 | (3) |
| 662 | (15) | 682 | (15) | 716 | (17) |
| 709 | (11) | 727 | (3) | 736 | (9) |
| 721 | (8) | 746 | (20) | 750 | (5) |
| 727 | (0) | 755 | (0) | 753 | (0) |
| 733 | (1) | 758 | (1) | 760 | (1) |
| 783 | (0) | 820 | (0) | 813 | (0) |
| 814 | (86) | 858 | (85) | 844 | (69) |
| 832 | (0) | 866 | (1) | 859 | (0) |
| 839 | (2) | 870 | (0) | 875 | (2) |
| 857 | (0) | 892 | (0) | 885 | (0) |
| 860 | (1) | 895 | (0) | 893 | (0) |
| 882 | (2) | 911 | (3) | 917 | (3) |
| 931 | (2) | 979 | (1) | 968 | (1) |
| 942 | (0) | 982 | (6) | 977 | (0) |
| 948 | (5) | 988 | (0) | 981 | (7) |
| 954 | (15) | 995 | (16) | 997 | (13) |
| 982 | (9) | 999 | (7) | 1016 | (8) |
| 1059 | (1) | 1090 | (0) | 1092 | (1) |
| 1112 | (13) | 1144 | (16) | 1145 | (13) |
| 1128 | (6) | 1164 | (7) | 1165 | (7) |
| 1141 | (0) | 1177 | (0) | 1171 | (0) |
| 1193 | (2) | 1226 | (3) | 1235 | (0) |
| 1199 | (0) | 1234 | (0) | 1238 | (0) |
| 1255 | (1) | 1302 | (1) | 1292 | (1) |
| 1272 | (5) | 1320 | (5) | 1316 | (3) |
| 1288 | (4) | 1338 | (4) | 1334 | (3) |
| 1326 | (11) | 1371 | (10) | 1374 | (8) |
| 1360 | (0) | 1404 | (0) | 1409 | (0) |
| 1384 | (2) | 1428 | (2) | 1437 | (2) |
| 1413 | (6) | 1462 | (6) | 1452 | (4) |
| 1423 | (10) | 1470 | (0) | 1464 | (10) |
| 1429 | (1) | 1472 | (11) | 1489 | (2) |
| 1515 | (2) | 1568 | (1) | 1583 | (1) |
| 1532 | (2) | 1586 | (2) | 1604 | (2) |
| 1576 | (1) | 1636 | (1) | 1648 | (1) |
| 1622 | (3) | 1684 | (3) | 1699 | (2) |
| 2968 | (27) | 3040 | (26) | 3045 | (54) |
| 3057 | (10) | 3125 | (11) | 3149 | (8) |
| 3064 | (8) | 3133 | (9) | 3152 | (15) |
| 3069 | (3) | 3148 | (3) | 3156 | (15) |
| 3077 | (21) | 3156 | (21) | 3158 | (38) |
| 3099 | (1) | 3177 | (0) | 3176 | (16) |

| | | | | | |
|---|---|---|---|---|---|
| 3103 | (0) | 3181 | (0) | 3180 | (0) |
| 3105 | (17) | 3184 | (13) | 3187 | (45) |
| 3108 | (2) | 3186 | (2) | 3189 | (4) |
| 3120 | (32) | 3198 | (32) | 3199 | (54) |
| 3132 | (28) | 3210 | (25) | 3213 | (55) |

**Table S9.** Harmonic vibrational frequencies (in $cm^{-1}$) and infrared intensities (in parentheses, in km/mol) for the structure 1Fe-1 of $(C_6H_6PCH_3)Fe(CO)_3$ with $C_s$ symmetry.

| BP86 | | B3LYP | | M06-L | |
|---|---|---|---|---|---|
| 41 | (0) | 45 | (0) | 46 | (0) |
| 68 | (0) | 71 | (0) | 71 | (0) |
| 75 | (0) | 76 | (0) | 74 | (0) |
| 84 | (1) | 86 | (0) | 84 | (1) |
| 90 | 0 | 95 | (0) | 92 | (0) |
| 91 | (0) | 95 | (0) | 95 | (0) |
| 109 | (0) | 114 | (0) | 130 | (0) |
| 138 | (2) | 143 | (2) | 140 | (2) |
| 162 | (1) | 168 | (1) | 168 | (1) |
| 194 | (1) | 202 | (0) | 211 | (0) |
| 219 | (3) | 226 | (1) | 235 | (1) |
| 257 | (1) | 266 | (1) | 265 | (1) |
| 330 | (4) | 330 | (5) | 346 | (4) |
| 389 | (18) | 387 | (9) | 389 | (6) |
| 402 | (0) | 409 | (0) | 407 | (1) |
| 436 | (20) | 438 | (41) | 447 | (38) |
| 459 | (10) | 463 | (8) | 457 | (0) |
| 469 | (1) | 466 | (0) | 462 | (5) |
| 502 | (1) | 493 | (3) | 489 | (1) |
| 507 | (0) | 503 | (0) | 496 | (3) |
| 523 | (8) | 526 | (17) | 510 | (23) |
| 553 | (7) | 561 | (70) | 553 | (65) |
| 557 | (3) | 575 | (3) | 573 | (6) |
| 563 | (39) | 578 | (8) | 576 | (9) |
| 600 | (8) | 614 | (31) | 617 | (53) |
| 604 | (11) | 624 | (5) | 633 | (113) |
| 631 | (106) | 632 | (130) | 647 | (5) |
| 633 | (76) | 641 | (40) | 660 | (26) |
| 642 | (12) | 667 | (9) | 683 | (7) |
| 668 | (13) | 688 | (12) | 727 | (18) |
| 819 | (1) | 851 | (0) | 843 | (1) |
| 829 | (12) | 859 | (18) | 855 | (14) |
| 848 | (6) | 864 | (2) | 878 | (4) |
| 856 | (2) | 889 | (1) | 881 | (2) |
| 858 | (4) | 890 | (2) | 883 | (2) |
| 893 | (8) | 925 | (12) | 922 | (5) |
| 903 | (8) | 944 | (8) | 930 | (11) |
| 909 | (3) | 948 | (0) | 944 | (3) |
| 947 | (6) | 984 | (10) | 979 | (12) |
| 949 | (11) | 993 | (6) | 986 | (7) |
| 1006 | (10) | 1034 | (17) | 1043 | (17) |
| 1014 | (3) | 1059 | (4) | 1058 | (3) |
| 1081 | (4) | 1113 | (8) | 1115 | (6) |
| 1113 | (3) | 1147 | (4) | 1145 | (3) |
| 1131 | (0) | 1168 | (0) | 1163 | (1) |
| 1264 | (0) | 1312 | (0) | 1307 | (0) |
| 1280 | (8) | 1325 | (4) | 1318 | (6) |
| 1292 | (9) | 1335 | (7) | 1347 | (6) |
| 1314 | (11) | 1360 | (9) | 1361 | (7) |
| 1371 | (6) | 1418 | (2) | 1418 | (3) |
| 1412 | (7) | 1462 | (6) | 1451 | (5) |
| 1419 | (10) | 1468 | (9) | 1460 | (9) |
| 1422 | (0) | 1474 | (1) | 1472 | (1) |
| 1442 | (2) | 1484 | (8) | 1486 | (4) |
| 1959 | (707) | 2048 | (951) | 2037 | (849) |
| 1966 | (826) | 2049 | (833) | 2040 | (979) |
| 2018 | (827) | 2100 | (1061) | 2097 | (962) |
| 2969 | (19) | 3041 | (19) | 3048 | (45) |
| 3062 | (7) | 3128 | (9) | 3157 | (17) |

| | | | | | |
|---|---|---|---|---|---|
| 3064 | (8) | 3132 | (9) | 3164 | (4) |
| 3090 | (1) | 3161 | (1) | 3166 | (14) |
| 3097 | (6) | 3169 | (8) | 3173 | (14) |
| 3110 | (13) | 3182 | (15) | 3196 | (34) |
| 3112 | (1) | 3184 | (1) | 3197 | (2) |
| 3133 | (4) | 3209 | (3) | 3221 | (14) |
| 3146 | (6) | 3222 | (6) | 3235 | (20) |

**Table S10.** Harmonic vibrational frequencies (in $cm^{-1}$) and infrared intensities (in parentheses, in km/mol) for the structure 1Fe-2 of $(C_6H_6PCH_3)Fe(CO)_3$ with $C_1$ symmetry.

| BP86 | | B3LYP | | M06-L | |
|---|---|---|---|---|---|
| 35 | (0) | 38 | (0) | 38 | (0) |
| 64 | (0) | 65 | (0) | 64 | (0) |
| 75 | (0) | 76 | (0) | 75 | (0) |
| 83 | (0) | 87 | (0) | 82 | (0) |
| 90 | (0) | 93 | (0) | 93 | (0) |
| 95 | (0) | 99 | (0) | 95 | (0) |
| 121 | (2) | 128 | (1) | 127 | (1) |
| 144 | (0) | 149 | (0) | 145 | (0) |
| 153 | (4) | 157 | (2) | 153 | (3) |
| 197 | (0) | 199 | (0) | 197 | (0) |
| 216 | (1) | 223 | (1) | 217 | (1) |
| 277 | (2) | 287 | (3) | 284 | (3) |
| 292 | (3) | 303 | (3) | 300 | (2) |
| 308 | (5) | 308 | (6) | 321 | (5) |
| 370 | (2) | 379 | (1) | 378 | (1) |
| 380 | (1) | 391 | (1) | 386 | (1) |
| 394 | (2) | 402 | (1) | 395 | (1) |
| 434 | (7) | 442 | (8) | 438 | (7) |
| 465 | (4) | 467 | (1) | 459 | (1) |
| 490 | (1) | 478 | (8) | 465 | (4) |
| 493 | (10) | 503 | (10) | 489 | (16) |
| 503 | (9) | 508 | (13) | 508 | (4) |
| 523 | (1) | 519 | (2) | 521 | (22) |
| 542 | (13) | 553 | (17) | 546 | (16) |
| 578 | (58) | 576 | (66) | 568 | (62) |
| 599 | (4) | 604 | (78) | 595 | (77) |
| 606 | (87) | 617 | (25) | 618 | (129) |
| 617 | (133) | 625 | (151) | 626 | (45) |
| 652 | (54) | 685 | (67) | 675 | (43) |
| 719 | (5) | 738 | (2) | 742 | (4) |
| 736 | (14) | 762 | (32) | 756 | (12) |
| 747 | (20) | 770 | (9) | 776 | (13) |
| 759 | (20) | 792 | (20) | 793 | (31) |
| 790 | (3) | 812 | (2) | 827 | (10) |
| 833 | (3) | 862 | (7) | 860 | (4) |
| 850 | (2) | 869 | (1) | 878 | (2) |
| 883 | (23) | 917 | (25) | 900 | (21) |
| 895 | (4) | 931 | (4) | 912 | (4) |
| 925 | (1) | 970 | (18) | 963 | (7) |
| 943 | (13) | 985 | (14) | 976 | (20) |
| 949 | (13) | 994 | (2) | 982 | (1) |
| 994 | (0) | 1014 | (2) | 1021 | (1) |
| 1119 | (1) | 1157 | (2) | 1148 | (2) |
| 1178 | (5) | 1219 | (5) | 1211 | (6) |
| 1236 | (7) | 1276 | (8) | 1271 | (7) |
| 1278 | (7) | 1323 | (15) | 1315 | (10) |
| 1287 | (17) | 1341 | (18) | 1322 | (17) |
| 1327 | (16) | 1379 | (16) | 1374 | (15) |
| 1398 | (7) | 1440 | (31) | 1442 | (10) |
| 1410 | (11) | 1461 | (9) | 1446 | (6) |
| 1415 | (6) | 1463 | (7) | 1452 | (8) |
| 1438 | (18) | 1476 | (25) | 1493 | (28) |
| 1514 | (78) | 1559 | (93) | 1575 | (99) |
| 1566 | (22) | 1630 | (31) | 1634 | (34) |
| 1943 | (715) | 2026 | (871) | 2015 | (876) |
| 1958 | (793) | 2044 | (931) | 2033 | (928) |
| 2007 | (838) | 2089 | (1080) | 2083 | (1001) |
| 2993 | (3) | 3063 | (3) | 3072 | (13) |
| 3070 | (3) | 3143 | (3) | 3160 | (7) |

| | | | | | |
|---|---|---|---|---|---|
| 3077 | (6) | 3151 | (5) | 3164 | (9) |
| 3086 | (11) | 3152 | (3) | 3175 | (23) |
| 3088 | (2) | 3160 | (13) | 3184 | (5) |
| 3100 | (5) | 3168 | (1) | 3187 | (23) |
| 3102 | (2) | 3176 | (8) | 3196 | (3) |
| 3110 | (22) | 3187 | (25) | 3198 | (17) |
| 3123 | (1) | 3198 | (1) | 3200 | (43) |

**Table S11.** Harmonic vibrational frequencies (in $cm^{-1}$) and infrared intensities (in parentheses, in km/mol) for the structure 1Fe-3 of $(C_6H_6PCH_3)Fe(CO)_3$ with $C_1$ symmetry.

| BP86 | | B3LYP | | M06-L | |
|---|---|---|---|---|---|
| 40 | (0) | 45 | (0) | 44 | (0) |
| 70 | (0) | 73 | (0) | 70 | (0) |
| 78 | (0) | 84 | (0) | 76 | (0) |
| 83 | (1) | 87 | (0) | 83 | (0) |
| 93 | (0) | 98 | (0) | 92 | (0) |
| 98 | (0) | 102 | (0) | 101 | (0) |
| 119 | (1) | 125 | (1) | 120 | (1) |
| 155 | (1) | 161 | (1) | 154 | (1) |
| 169 | (0) | 176 | (0) | 166 | (0) |
| 208 | (6) | 219 | (3) | 213 | (4) |
| 233 | (0) | 245 | (0) | 243 | (0) |
| 263 | (1) | 273 | (1) | 274 | (1) |
| 306 | (2) | 313 | (2) | 322 | (2) |
| 351 | (1) | 360 | (2) | 356 | (1) |
| 380 | (11) | 385 | (3) | 380 | (3) |
| 402 | (1) | 410 | (5) | 405 | (2) |
| 408 | (3) | 414 | (5) | 419 | (6) |
| 456 | (11) | 460 | (7) | 451 | (2) |
| 469 | (1) | 463 | (2) | 455 | (5) |
| 474 | (3) | 487 | (6) | 479 | (14) |
| 506 | (3) | 493 | (7) | 483 | (4) |
| 509 | (0) | 509 | (7) | 496 | (15) |
| 520 | (3) | 521 | (12) | 505 | (10) |
| 543 | (7) | 557 | (23) | 551 | (39) |
| 566 | (52) | 572 | (47) | 577 | (29) |
| 612 | (90) | 613 | (79) | 608 | (61) |
| 618 | (40) | 622 | (100) | 617 | (112) |
| 629 | (46) | 638 | (21) | 650 | (9) |
| 678 | (38) | 699 | (11) | 700 | (29) |
| 686 | (20) | 704 | (24) | 723 | (25) |
| 696 | (11) | 717 | (27) | 742 | (3) |
| 731 | (17) | 753 | (18) | 756 | (16) |
| 803 | (7) | 831 | (7) | 826 | (8) |
| 846 | (3) | 865 | (2) | 873 | (3) |
| 855 | (9) | 890 | (10) | 878 | (6) |
| 879 | (11) | 915 | (13) | 898 | (11) |
| 893 | (7) | 923 | (8) | 916 | (6) |
| 901 | (1) | 945 | (1) | 928 | (1) |
| 905 | (5) | 953 | (3) | 936 | (6) |
| 923 | (3) | 970 | (1) | 957 | (1) |
| 960 | (1) | 1005 | (1) | 995 | (1) |
| 1041 | (1) | 1073 | (3) | 1076 | (3) |
| 1122 | (1) | 1156 | (3) | 1155 | (2) |
| 1159 | (1) | 1199 | (1) | 1192 | (1) |
| 1221 | (3) | 1259 | (4) | 1255 | (3) |
| 1276 | (11) | 1327 | (10) | 1314 | (9) |
| 1282 | (3) | 1333 | (5) | 1324 | (3) |
| 1337 | (1) | 1388 | (1) | 1385 | (0) |
| 1362 | (2) | 1411 | (2) | 1410 | (0) |
| 1414 | (12) | 1464 | (11) | 1449 | (12) |
| 1420 | (7) | 1469 | (2) | 1456 | (5) |
| 1423 | (1) | 1470 | (8) | 1477 | (2) |
| 1457 | (3) | 1501 | (10) | 1503 | (7) |
| 1575 | (3) | 1637 | (5) | 1641 | (6) |
| 1962 | (649) | 2055 | (755) | 2037 | (777) |
| 1971 | (766) | 2059 | (870) | 2048 | (901) |
| 2021 | (763) | 2105 | (990) | 2099 | (903) |
| 2983 | (19) | 3051 | (19) | 3056 | (38) |

| | | | | | |
|---|---|---|---|---|---|
| 3050 | (3) | 3118 | (5) | 3116 | (10) |
| 3065 | (5) | 3136 | (9) | 3150 | (5) |
| 3073 | (5) | 3138 | (3) | 3165 | (29) |
| 3084 | (10) | 3153 | (6) | 3167 | (7) |
| 3088 | (5) | 3155 | (12) | 3174 | (9) |
| 3100 | (11) | 3173 | (16) | 3182 | (12) |
| 3103 | (8) | 3179 | (6) | 3187 | (40) |
| 3117 | (16) | 3194 | (16) | 3203 | (35) |

**Table S12.** Harmonic vibrational frequencies (in $cm^{-1}$) and infrared intensities (in parentheses, in km/mol) for the structure 1Fe-4 of $(C_6H_6PCH_3)Fe(CO)_3$ with $C_1$ symmetry.

| BP86 | | B3LYP | | M06-L | |
|---|---|---|---|---|---|
| 48 | (1) | 51 | (1) | 54 | (1) |
| 71 | (0) | 73 | (0) | 71 | (0) |
| 73 | (0) | 77 | (0) | 79 | (0) |
| 85 | (0) | 87 | (0) | 88 | (0) |
| 87 | (0) | 90 | (0) | 90 | (0) |
| 90 | (0) | 94 | (0) | 92 | (0) |
| 127 | (0) | 147 | (0) | 147 | (0) |
| 148 | (0) | 154 | (0) | 195 | (1) |
| 173 | (1) | 179 | (0) | 226 | (0) |
| 212 | (5) | 218 | (3) | 231 | (2) |
| 229 | (1) | 233 | (1) | 249 | (0) |
| 287 | (2) | 294 | (3) | 311 | (2) |
| 343 | (6) | 347 | (8) | 358 | (6) |
| 389 | (16) | 388 | (8) | 390 | (6) |
| 399 | (0) | 405 | (0) | 405 | (0) |
| 449 | (11) | 448 | (33) | 452 | (26) |
| 455 | (13) | 459 | (11) | 455 | (0) |
| 466 | (1) | 464 | (0) | 461 | (6) |
| 497 | (1) | 497 | (1) | 492 | (1) |
| 508 | (0) | 498 | (0) | 500 | (12) |
| 523 | (10) | 524 | (21) | 508 | (20) |
| 539 | (2) | 558 | (69) | 549 | (67) |
| 547 | (1) | 560 | (3) | 564 | (6) |
| 562 | (40) | 569 | (1) | 586 | (10) |
| 578 | (14) | 594 | (28) | 601 | (28) |
| 587 | (11) | 608 | (3) | 628 | (105) |
| 624 | (57) | 626 | (81) | 632 | (46) |
| 630 | (109) | 631 | (84) | 635 | (1) |
| 634 | (9) | 656 | (5) | 667 | (5) |
| 682 | (10) | 702 | (8) | 738 | (9) |
| 814 | (7) | 846 | (5) | 831 | (4) |
| 832 | (12) | 857 | (16) | 857 | (14) |
| 848 | (0) | 867 | (0) | 870 | (0) |
| 849 | (5) | 878 | (1) | 881 | (4) |
| 870 | (5) | 906 | (7) | 904 | (4) |
| 892 | (0) | 923 | (0) | 922 | (0) |
| 904 | (2) | 945 | (2) | 929 | (3) |
| 916 | (1) | 954 | (0) | 949 | (0) |
| 954 | (1) | 998 | (1) | 992 | (1) |
| 965 | (9) | 1000 | (9) | 1004 | (9) |
| 1008 | (9) | 1036 | (15) | 1044 | (16) |
| 1034 | (6) | 1081 | (6) | 1082 | (6) |
| 1091 | (8) | 1123 | (14) | 1125 | (10) |
| 1120 | (3) | 1155 | (4) | 1155 | (3) |
| 1145 | (2) | 1183 | (2) | 1180 | (3) |
| 1274 | (0) | 1323 | (0) | 1313 | (4) |
| 1274 | (7) | 1327 | (6) | 1316 | (0) |
| 1300 | (16) | 1338 | (10) | 1354 | (11) |
| 1324 | (16) | 1369 | (16) | 1371 | (12) |
| 1378 | (3) | 1426 | (2) | 1425 | (1) |
| 1408 | (24) | 1461 | (19) | 1453 | (22) |
| 1414 | (17) | 1468 | (16) | 1465 | (16) |
| 1433 | (0) | 1486 | (0) | 1484 | (0) |
| 1446 | (3) | 1489 | (12) | 1494 | (7) |
| 1959 | (702) | 2048 | (831) | 2041 | (835) |
| 1966 | (814) | 2049 | (945) | 2046 | (976) |
| 2018 | (854) | 2100 | (1091) | 2101 | (974) |
| 2979 | (14) | 3052 | (15) | 3053 | (31) |

| | | | | | |
|---|---|---|---|---|---|
| 3069 | (5) | 3137 | (7) | 3161 | (3) |
| 3078 | (5) | 3149 | (6) | 3165 | (13) |
| 3080 | (2) | 3151 | (3) | 3165 | (10) |
| 3089 | (3) | 3160 | (5) | 3170 | (10) |
| 3110 | (11) | 3183 | (13) | 3189 | (31) |
| 3112 | (2) | 3185 | (2) | 3191 | (4) |
| 3131 | (3) | 3207 | (3) | 3211 | (14) |
| 3143 | (4) | 3220 | (4) | 3225 | (15) |

**Table S13**. Harmonic vibrational frequencies (in $cm^{-1}$) and infrared intensities (in parentheses, in km/mol) for the structure 1Fe-5 of $(C_6H_6PCH_3)Fe(CO)_3$ with $C_1$ symmetry.

| BP86 | | B3LYP | | M06-L | |
|---|---|---|---|---|---|
| 46 | (0) | 48 | (0) | 46 | (0) |
| 64 | (0) | 65 | (0) | 62 | (0) |
| 79 | (0) | 81 | (0) | 74 | (0) |
| 87 | (0) | 86 | (0) | 82 | (0) |
| 90 | (0) | 94 | (0) | 86 | (0) |
| 91 | (0) | 94 | (0) | 87 | (0) |
| 161 | (0) | 163 | (0) | 164 | (0) |
| 169 | (0) | 167 | (0) | 178 | (0) |
| 181 | (0) | 187 | (0) | 201 | (0) |
| 242 | (1) | 248 | (0) | 244 | (0) |
| 247 | (0) | 249 | (1) | 247 | (0) |
| 295 | (0) | 291 | (1) | 294 | (0) |
| 303 | (1) | 317 | (1) | 309 | (1) |
| 317 | (7) | 319 | (8) | 325 | (6) |
| 383 | (14) | 381 | (16) | 393 | (12) |
| 420 | (3) | 424 | (3) | 417 | (3) |
| 440 | (0) | 445 | (0) | 451 | (12) |
| 452 | (1) | 463 | (13) | 453 | (3) |
| 465 | (6) | 468 | (1) | 459 | (2) |
| 468 | (7) | 471 | (2) | 473 | (2) |
| 484 | (17) | 482 | (5) | 485 | (0) |
| 493 | (3) | 501 | (19) | 496 | (28) |
| 512 | (3) | 513 | (3) | 505 | (8) |
| 524 | (5) | 518 | (16) | 512 | (3) |
| 564 | (23) | 560 | (47) | 553 | (49) |
| 604 | (33) | 613 | (29) | 617 | (64) |
| 625 | (58) | 622 | (62) | 622 | (40) |
| 634 | (88) | 635 | (94) | 633 | (90) |
| 640 | (0) | 664 | (3) | 660 | (4) |
| 668 | (53) | 697 | (53) | 686 | (46) |
| 712 | (49) | 739 | (48) | 742 | (42) |
| 749 | (60) | 769 | (58) | 780 | (37) |
| 774 | (8) | 795 | (2) | 815 | (20) |
| 802 | (11) | 833 | (9) | 826 | (7) |
| 814 | (7) | 833 | (9) | 842 | (9) |
| 861 | (9) | 889 | (24) | 881 | (26) |
| 892 | (2) | 923 | (45) | 913 | (49) |
| 893 | (41) | 937 | (23) | 925 | (10) |
| 904 | (24) | 938 | (1) | 932 | (15) |
| 912 | (32) | 959 | (25) | 948 | (26) |
| 948 | (0) | 988 | (0) | 984 | (0) |
| 996 | (0) | 1029 | (0) | 1033 | (0) |
| 1067 | (12) | 1107 | (16) | 1099 | (15) |
| 1087 | (1) | 1129 | (1) | 1118 | (1) |
| 1141 | (4) | 1180 | (8) | 1175 | (6) |
| 1260 | (0) | 1313 | (0) | 1309 | (0) |
| 1274 | (35) | 1328 | (34) | 1319 | (28) |
| 1287 | (5) | 1340 | (3) | 1327 | (6) |
| 1314 | (12) | 1368 | (25) | 1368 | (17) |
| 1340 | (1) | 1391 | (1) | 1394 | (0) |
| 1408 | (12) | 1458 | (11) | 1445 | (11) |
| 1412 | (6) | 1460 | (6) | 1448 | (5) |
| 1544 | (47) | 1600 | (53) | 1611 | (62) |
| 1554 | (3) | 1607 | (3) | 1622 | (6) |
| 1944 | (922) | 2025 | (1082) | 2016 | (1080) |
| 1955 | (562) | 2040 | (667) | 2030 | (706) |
| 2010 | (706) | 2090 | (901) | 2086 | (812) |
| 2987 | (3) | 3056 | (4) | 3058 | (13) |
| 3071 | (5) | 3147 | (3) | 3153 | (2) |

| | | | | | |
|---|---|---|---|---|---|
| 3072 | (14) | 3148 | (3) | 3157 | (23) |
| 3083 | (2) | 3150 | (13) | 3166 | (32) |
| 3086 | (9) | 3155 | (1) | 3170 | (8) |
| 3092 | (1) | 3161 | (12) | 3176 | (58) |
| 3098 | (23) | 3173 | (25) | 3178 | (5) |
| 3128 | (5) | 3204 | (6) | 3209 | (18) |
| 3129 | (6) | 3204 | (5) | 3212 | (19) |

**Table S14**. Harmonic vibrational frequencies (in $cm^{-1}$) and infrared intensities (in parentheses, in km/mol) for the structure 1Fe-6 of $(C_6H_6PCH_3)Fe(CO)_3$ with $C_1$ symmetry.

| BP86 | | B3LYP | | M06-L | |
|---|---|---|---|---|---|
| 44 | (1) | 49 | (1) | 44 | (1) |
| 58 | (1) | 60 | (1) | 56 | (0) |
| 78 | (0) | 81 | (0) | 76 | (0) |
| 79 | (0) | 83 | (0) | 78 | (0) |
| 88 | (0) | 91 | (0) | 87 | (0) |
| 95 | (0) | 98 | (0) | 93 | (0) |
| 113 | (0) | 118 | (0) | 110 | (0) |
| 154 | (0) | 160 | (0) | 153 | (0) |
| 182 | (0) | 190 | (0) | 196 | (0) |
| 196 | (1) | 204 | (0) | 213 | (0) |
| 210 | (2) | 219 | (1) | 215 | (1) |
| 277 | (3) | 293 | (2) | 293 | (1) |
| 307 | (1) | 320 | (2) | 319 | (1) |
| 354 | (3) | 364 | (1) | 362 | (1) |
| 381 | (4) | 381 | (1) | 382 | (1) |
| 403 | (3) | 410 | (5) | 408 | (2) |
| 412 | (5) | 422 | (7) | 425 | (8) |
| 452 | (12) | 457 | (10) | 451 | (6) |
| 465 | (4) | 462 | (1) | 453 | (2) |
| 472 | (1) | 481 | (11) | 476 | (13) |
| 501 | (1) | 487 | (7) | 481 | (10) |
| 505 | (1) | 506 | (2) | 496 | (7) |
| 519 | (9) | 519 | (20) | 504 | (17) |
| 539 | (4) | 551 | (23) | 547 | (36) |
| 575 | (45) | 578 | (44) | 582 | (26) |
| 616 | (46) | 615 | (60) | 612 | (53) |
| 617 | (83) | 623 | (115) | 621 | (114) |
| 631 | (45) | 641 | (16) | 655 | (10) |
| 662 | (14) | 680 | (13) | 706 | (5) |
| 679 | (25) | 701 | (10) | 708 | (32) |
| 698 | (26) | 723 | (39) | 729 | (18) |
| 741 | (21) | 764 | (20) | 766 | (19) |
| 797 | (8) | 825 | (7) | 820 | (8) |
| 848 | (14) | 872 | (10) | 878 | (11) |
| 857 | (4) | 888 | (9) | 882 | (6) |
| 872 | (8) | 902 | (13) | 898 | (5) |
| 886 | (18) | 920 | (19) | 912 | (16) |
| 907 | (3) | 951 | (1) | 934 | (2) |
| 920 | (5) | 966 | (2) | 953 | (3) |
| 930 | (5) | 979 | (5) | 970 | (6) |
| 961 | (1) | 1009 | (1) | 1001 | (2) |
| 1044 | (6) | 1076 | (10) | 1079 | (10) |
| 1128 | (3) | 1161 | (4) | 1161 | (4) |
| 1164 | (1) | 1204 | (3) | 1196 | (1) |
| 1215 | (2) | 1255 | (2) | 1252 | (2) |
| 1271 | (2) | 1323 | (4) | 1307 | (2) |
| 1294 | (6) | 1344 | (9) | 1336 | (7) |
| 1341 | (2) | 1390 | (4) | 1388 | (1) |
| 1366 | (2) | 1413 | (7) | 1412 | (4) |
| 1414 | (12) | 1463 | (11) | 1452 | (4) |
| 1417 | (6) | 1465 | (3) | 1453 | (11) |
| 1421 | (1) | 1468 | (3) | 1474 | (1) |
| 1464 | (8) | 1508 | (21) | 1510 | (16) |
| 1590 | (2) | 1653 | (6) | 1674 | (6) |
| 1963 | (638) | 2057 | (751) | 2044 | (762) |
| 1979 | (806) | 2067 | (930) | 2061 | (970) |
| 2027 | (744) | 2112 | (945) | 2111 | (867) |
| 2974 | (27) | 3043 | (26) | 3045 | (52) |
| 3039 | (3) | 3111 | (5) | 3118 | (11) |

| | | | | | |
|---|---|---|---|---|---|
| 3054 | (8) | 3129 | (8) | 3148 | (6) |
| 3068 | (6) | 3132 | (8) | 3160 | (21) |
| 3077 | (10) | 3142 | (11) | 3161 | (14) |
| 3078 | (8) | 3150 | (12) | 3164 | (20) |
| 3090 | (11) | 3165 | (18) | 3179 | (25) |
| 3092 | (14) | 3169 | (10) | 3181 | (42) |
| 3109 | (17) | 3187 | (17) | 3201 | (38) |

**Table S15.** Harmonic vibrational frequencies (in $cm^{-1}$) and infrared intensities (in parentheses, in km/mol) for the structure 1Fe-7 of $(C_6H_6PCH_3)Fe(CO)_3$ with $C_s$ symmetry.

| BP86 | | B3LYP | | M06-L | |
|---|---|---|---|---|---|
| 27 | (0) | 17*i* | (0) | 11 | (0) |
| 79 | (0) | 81 | (0) | 78 | (0) |
| 80 | (0) | 84 | (0) | 78 | (0) |
| 85 | (0) | 87 | (0) | 80 | (0) |
| 100 | (0) | 103 | (0) | 97 | (0) |
| 116 | (0) | 117 | (0) | 114 | (0) |
| 146 | (2) | 149 | (2) | 149 | (2) |
| 173 | (1) | 175 | (3) | 177 | (1) |
| 198 | (0) | 193 | (1) | 200 | (0) |
| 222 | (2) | 226 | (3) | 230 | (1) |
| 258 | (3) | 228 | (1) | 241 | (5) |
| 262 | (3) | 257 | (6) | 267 | (4) |
| 290 | (2) | 295 | (1) | 299 | (1) |
| 294 | (2) | 306 | (0) | 301 | (1) |
| 375 | (12) | 364 | (14) | 371 | (13) |
| 386 | (0) | 388 | (0) | 392 | (0) |
| 437 | (0) | 439 | (0) | 443 | (5) |
| 437 | (5) | 440 | (4) | 451 | (0) |
| 472 | (7) | 472 | (0) | 473 | (4) |
| 478 | (0) | 475 | (3) | 476 | (0) |
| 495 | (3) | 486 | (23) | 496 | (20) |
| 505 | (9) | 498 | (4) | 504 | (2) |
| 525 | (7) | 521 | (19) | 509 | (17) |
| 557 | (5) | 550 | (53) | 551 | (55) |
| 567 | (39) | 578 | (0) | 583 | (0) |
| 575 | (21) | 591 | (34) | 594 | (41) |
| 622 | (96) | 625 | (85) | 630 | (86) |
| 638 | (32) | 640 | (31) | 643 | (26) |
| 671 | (28) | 694 | (29) | 704 | (24) |
| 683 | (0) | 704 | (1) | 711 | (1) |
| 693 | (0) | 714 | (0) | 728 | (1) |
| 753 | (26) | 779 | (22) | 782 | (21) |
| 780 | (11) | 803 | (11) | 797 | (11) |
| 815 | (0) | 833 | (0) | 831 | (1) |
| 821 | (9) | 848 | (3) | 841 | (3) |
| 888 | (11) | 922 | (10) | 914 | (10) |
| 893 | (0) | 927 | (2) | 917 | (1) |
| 901 | (1) | 939 | (10) | 935 | (1) |
| 918 | (3) | 942 | (2) | 941 | (4) |
| 938 | (1) | 972 | (1) | 966 | (2) |
| 946 | (5) | 983 | (5) | 974 | (8) |
| 958 | (0) | 1001 | (1) | 983 | (1) |
| 1108 | (4) | 1150 | (7) | 1143 | (5) |
| 1111 | (0) | 1154 | (0) | 1144 | (0) |
| 1122 | (1) | 1166 | (1) | 1158 | (2) |
| 1250 | (4) | 1307 | (5) | 1294 | (4) |
| 1274 | (8) | 1328 | (10) | 1308 | (7) |
| 1291 | (4) | 1346 | (4) | 1336 | (4) |
| 1327 | (3) | 1384 | (3) | 1379 | (1) |
| 1384 | (4) | 1452 | (9) | 1445 | (4) |
| 1387 | (6) | 1453 | (9) | 1447 | (9) |
| 1416 | (10) | 1464 | (10) | 1451 | (12) |
| 1422 | (3) | 1471 | (3) | 1456 | (1) |
| 1638 | (8) | 1691 | (7) | 1706 | (11) |
| 1950 | (610) | 2031 | (740) | 2029 | (710) |
| 1970 | (758) | 2044 | (916) | 2047 | (896) |
| 2013 | (750) | 2090 | (898) | 2094 | (827) |
| 2970 | (18) | 3042 | (16) | 3023 | (36) |

| | | | | | |
|---|---|---|---|---|---|
| 3066 | (7) | 3134 | (5) | 3136 | (13) |
| 3070 | (5) | 3135 | (7) | 3142 | (0) |
| 3078 | (0) | 3157 | (1) | 3142 | (5) |
| 3078 | (1) | 3158 | (1) | 3154 | (10) |
| 3088 | (0) | 3167 | (1) | 3158 | (12) |
| 3095 | (18) | 3177 | (12) | 3158 | (8) |
| 3095 | (6) | 3178 | (7) | 3162 | (37) |
| 3112 | (20) | 3190 | (17) | 3184 | (46) |

**Table S16.** Harmonic vibrational frequencies (in $cm^{-1}$) and infrared intensities (in parentheses, in km/mol) for the structure 1Fe-8 of $(C_6H_6PCH_3)Fe(CO)_3$ with $C_s$ symmetry.

| BP86 | | B3LYP | | M06-L | |
|---|---|---|---|---|---|
| 28 | (0) | 13*i* | (0) | 24 | (0) |
| 80 | (0) | 83 | (0) | 82 | (0) |
| 82 | (0) | 87 | (0) | 84 | (0) |
| 90 | (0) | 92 | (0) | 87 | (0) |
| 102 | (0) | 105 | (0) | 93 | (0) |
| 106 | (0) | 109 | (0) | 102 | (0) |
| 132 | (0) | 141 | (0) | 112 | (0) |
| 159 | (0) | 167 | (0) | 162 | (0) |
| 173 | (1) | 178 | (1) | 168 | (1) |
| 223 | (3) | 218 | (5) | 222 | (3) |
| 244 | (0) | 228 | (2) | 244 | (5) |
| 257 | (3) | 247 | (1) | 249 | (0) |
| 294 | (5) | 289 | (7) | 299 | (5) |
| 320 | (0) | 332 | (0) | 325 | (0) |
| 385 | (7) | 379 | (8) | 383 | (8) |
| 391 | (1) | 394 | (0) | 393 | (0) |
| 427 | (0) | 429 | (0) | 435 | 0 |
| 436 | (7) | 440 | (8) | 437 | (10) |
| 477 | (1) | 472 | (12) | 464 | (10) |
| 480 | (1) | 473 | (0) | 467 | (1) |
| 499 | (2) | 498 | (11) | 488 | (14) |
| 511 | (6) | 503 | (2) | 504 | 0 |
| 530 | (9) | 527 | (17) | 514 | (12) |
| 560 | (24) | 549 | (54) | 538 | (57) |
| 572 | (23) | 589 | (2) | 594 | (94) |
| 577 | (46) | 591 | (76) | 594 | (1) |
| 624 | (111) | 628 | (79) | 632 | (66) |
| 630 | (27) | 634 | (32) | 641 | (18) |
| 645 | (13) | 663 | (24) | 682 | (22) |
| 665 | (0) | 688 | (0) | 707 | (0) |
| 693 | (11) | 714 | (10) | 734 | (18) |
| 755 | (38) | 780 | (30) | 779 | (32) |
| 784 | (9) | 812 | (9) | 803 | (8) |
| 838 | (4) | 860 | (5) | 852 | (2) |
| 845 | (1) | 878 | (1) | 865 | (1) |
| 865 | (14) | 894 | (5) | 883 | (12) |
| 867 | (10) | 904 | (16) | 884 | (3) |
| 903 | (0) | 941 | (1) | 935 | (0) |
| 923 | (15) | 944 | (19) | 953 | (20) |
| 937 | (1) | 973 | (1) | 971 | (2) |
| 956 | (0) | 999 | (0) | 983 | (3) |
| 970 | (1) | 1017 | (1) | 993 | (1) |
| 1120 | (5) | 1163 | (9) | 1156 | (8) |
| 1142 | (0) | 1186 | (1) | 1179 | (0) |
| 1144 | (3) | 1188 | (5) | 1181 | (6) |
| 1258 | (12) | 1316 | (14) | 1293 | (10) |
| 1271 | (4) | 1327 | (5) | 1320 | (5) |
| 1307 | (3) | 1364 | (4) | 1358 | (3) |
| 1330 | (4) | 1388 | (3) | 1382 | (1) |
| 1387 | (2) | 1451 | (4) | 1437 | (19) |
| 1388 | (19) | 1452 | (24) | 1445 | (3) |
| 1404 | (4) | 1458 | (8) | 1446 | (10) |
| 1421 | (5) | 1471 | (6) | 1457 | (5) |
| 1651 | (7) | 1705 | (6) | 1729 | (9) |
| 1961 | (592) | 2044 | (711) | 2037 | (705) |
| 1977 | (768) | 2052 | (918) | 2053 | (931) |
| 2020 | (802) | 2098 | (974) | 2100 | (897) |
| 2973 | (21) | 3044 | (20) | 3052 | (43) |

| | | | | | |
|---|---|---|---|---|---|
| 3054 | (6) | 3119 | (7) | 3150 | (11) |
| 3060 | (7) | 3141 | (6) | 3150 | (9) |
| 3061 | (4) | 3142 | (3) | 3156 | (10) |
| 3083 | (1) | 3163 | (1) | 3167 | (25) |
| 3087 | (7) | 3170 | (17) | 3170 | (11) |
| 3087 | (20) | 3170 | (8) | 3176 | (33) |
| 3101 | (6) | 3174 | (5) | 3182 | (8) |
| 3108 | (19) | 3186 | (17) | 3199 | (46) |

**Table S17.** Harmonic vibrational frequencies (in $cm^{-1}$) and infrared intensities (in parentheses, in km/mol) for the structure 1Co-1 of $(C_6H_6PCH_3)Co(C_5H_5)$ with $C_1$ symmetry.

| BP86 | | B3LYP | | M06-L | |
|---|---|---|---|---|---|
| 34 | (0) | 14 | (0) | 68 | (0) |
| 68 | (0) | 61 | (0) | 75 | (0) |
| 91 | (0) | 92 | (0) | 90 | (0) |
| 158 | (2) | 158 | (1) | 163 | (1) |
| 170 | (0) | 176 | (1) | 169 | (1) |
| 172 | (1) | 180 | (0) | 180 | (1) |
| 209 | (4) | 216 | (3) | 217 | (3) |
| 231 | (0) | 240 | (0) | 247 | (0) |
| 278 | (0) | 288 | (0) | 292 | (0) |
| 301 | (0) | 298 | (0) | 320 | (0) |
| 335 | (1) | 332 | (5) | 345 | (2) |
| 350 | (2) | 344 | (1) | 385 | (1) |
| 373 | (6) | 354 | (4) | 406 | (5) |
| 391 | (4) | 392 | (5) | 427 | (5) |
| 417 | (9) | 424 | (5) | 458 | (7) |
| 468 | (10) | 479 | (14) | 485 | (11) |
| 497 | (9) | 501 | (4) | 511 | (9) |
| 540 | (7) | 560 | (5) | 566 | (6) |
| 559 | (1) | 587 | (0) | 595 | (1) |
| 562 | (1) | 591 | (3) | 601 | (3) |
| 610 | (8) | 630 | (6) | 642 | (7) |
| 671 | (32) | 694 | (10) | 697 | (25) |
| 678 | (24) | 700 | (22) | 717 | (23) |
| 687 | (7) | 710 | (28) | 730 | (6) |
| 727 | (12) | 751 | (13) | 751 | (11) |
| 772 | (10) | 805 | (11) | 795 | (5) |
| 784 | (39) | 812 | (60) | 814 | (22) |
| 792 | (5) | 822 | (7) | 818 | (12) |
| 800 | (2) | 836 | (3) | 827 | (1) |
| 804 | (3) | 840 | (1) | 832 | (5) |
| 812 | (3) | 845 | (2) | 840 | (4) |
| 843 | (9) | 869 | (3) | 873 | (6) |
| 850 | (6) | 879 | (13) | 880 | (7) |
| 855 | (0) | 897 | (1) | 888 | (0) |
| 855 | (0) | 905 | (0) | 892 | (1) |
| 871 | (12) | 909 | (16) | 897 | (14) |
| 876 | (1) | 913 | (6) | 905 | (2) |
| 888 | (10) | 927 | (4) | 910 | (3) |
| 891 | (0) | 937 | (1) | 927 | (3) |
| 913 | (2) | 965 | (1) | 956 | (1) |
| 949 | (2) | 989 | (3) | 985 | (2) |
| 981 | (9) | 1013 | (11) | 1025 | (8) |
| 988 | (12) | 1024 | (12) | 1029 | (11) |
| 1032 | (1) | 1065 | (1) | 1070 | (1) |
| 1032 | (2) | 1066 | (4) | 1071 | (2) |
| 1034 | (2) | 1068 | (3) | 1073 | (4) |
| 1101 | (12) | 1135 | (8) | 1140 | (17) |
| 1109 | (2) | 1149 | (3) | 1149 | (2) |
| 1147 | (1) | 1191 | (1) | 1186 | (1) |
| 1211 | (3) | 1253 | (4) | 1249 | (3) |
| 1219 | (0) | 1271 | (0) | 1261 | (0) |
| 1265 | (9) | 1319 | (9) | 1303 | (6) |
| 1272 | (2) | 1325 | (3) | 1318 | (2) |
| 1333 | (1) | 1384 | (2) | 1382 | (0) |
| 1350 | (1) | 1394 | (1) | 1405 | (1) |
| 1351 | (1) | 1395 | (1) | 1408 | (1) |
| 1362 | (0) | 1411 | (2) | 1416 | (0) |
| 1394 | (3) | 1450 | (3) | 1448 | (9) |
| 1403 | (1) | 1461 | (1) | 1453 | (2) |

| | | | | | |
|---|---|---|---|---|---|
| 1412 | (10) | 1463 | (8) | 1455 | (7) |
| 1419 | (7) | 1468 | (6) | 1459 | (0) |
| 1422 | (2) | 1471 | (9) | 1478 | (2) |
| 1437 | (4) | 1484 | (10) | 1492 | (8) |
| 1564 | (7) | 1628 | (10) | 1643 | (13) |
| 2974 | (25) | 3043 | (23) | 3040 | (42) |
| 3021 | (10) | 3099 | (9) | 3094 | (19) |
| 3040 | (9) | 3120 | (9) | 3132 | (9) |
| 3059 | (27) | 3132 | (11) | 3147 | (28) |
| 3068 | (7) | 3138 | (8) | 3148 | (17) |
| 3074 | (9) | 3139 | (26) | 3156 | (35) |
| 3078 | (12) | 3162 | (7) | 3160 | (11) |
| 3092 | (40) | 3167 | (26) | 3171 | (88) |
| 3094 | (15) | 3179 | (27) | 3174 | (37) |
| 3159 | (0) | 3238 | (0) | 3231 | (1) |
| 3163 | (1) | 3242 | (1) | 3235 | (2) |
| 3173 | (7) | 3253 | (3) | 3247 | (22) |
| 3177 | (5) | 3256 | (3) | 3257 | (21) |
| 3188 | (2) | 3268 | (1) | 3265 | (7) |

**Table S18.** Harmonic vibrational frequencies (in $cm^{-1}$) and infrared intensities (in parentheses, in km/mol) for the structure 1Co-2 of $(C_6H_6PCH_3)Co(C_5H_5)$ with $C_s$ symmetry.

| BP86 | | B3LYP | | M06-L | |
|---|---|---|---|---|---|
| 40 | (0) | 19 | (0) | 34 | (0) |
| 77 | (0) | 74 | (0) | 74 | (0) |
| 101 | (0) | 112 | (0) | 120 | (0) |
| 123 | (0) | 127 | (0) | 135 | (0) |
| 158 | (2) | 159 | (2) | 160 | (3) |
| 163 | (1) | 168 | (1) | 171 | (1) |
| 210 | (1) | 212 | (1) | 224 | (1) |
| 218 | (0) | 224 | (0) | 235 | (0) |
| 257 | (1) | 262 | (1) | 267 | (0) |
| 337 | (1) | 323 | (5) | 349 | (2) |
| 353 | (1) | 341 | (1) | 380 | (1) |
| 372 | (6) | 357 | (4) | 402 | (4) |
| 387 | (10) | 374 | (11) | 424 | (10) |
| 448 | (18) | 444 | (12) | 476 | (10) |
| 493 | (14) | 498 | (16) | 515 | (18) |
| 537 | (2) | 564 | (3) | 562 | (4) |
| 555 | (8) | 578 | (4) | 585 | (6) |
| 558 | (1) | 582 | (2) | 585 | (2) |
| 568 | (3) | 595 | (3) | 604 | (3) |
| 582 | (0) | 608 | (0) | 627 | (1) |
| 604 | (4) | 626 | (5) | 647 | (10) |
| 629 | (5) | 656 | (6) | 667 | (5) |
| 662 | (18) | 683 | (16) | 721 | (21) |
| 759 | (12) | 789 | (4) | 769 | (1) |
| 781 | (34) | 803 | (64) | 794 | (26) |
| 791 | (1) | 824 | (1) | 811 | (1) |
| 800 | (0) | 835 | (5) | 822 | (0) |
| 800 | (4) | 837 | (0) | 823 | (9) |
| 815 | (3) | 849 | (8) | 839 | (3) |
| 818 | (6) | 849 | (3) | 841 | (4) |
| 842 | (1) | 861 | (2) | 863 | (0) |
| 843 | (3) | 876 | (0) | 868 | (4) |
| 848 | (4) | 880 | (3) | 875 | (3) |
| 851 | (0) | 900 | (0) | 881 | (0) |
| 855 | (1) | 900 | (2) | 883 | (1) |
| 868 | (4) | 916 | (10) | 896 | (4) |
| 880 | (10) | 922 | (9) | 911 | (12) |
| 894 | (11) | 927 | (4) | 932 | (7) |
| 936 | (5) | 977 | (7) | 972 | (6) |
| 941 | (8) | 980 | (6) | 972 | (8) |
| 977 | (11) | 1010 | (12) | 1011 | (9) |
| 989 | (15) | 1022 | (17) | 1027 | (13) |
| 1002 | (22) | 1030 | (30) | 1037 | (29) |
| 1004 | (2) | 1049 | (3) | 1045 | (2) |
| 1030 | 0 | 1063 | (0) | 1063 | (0) |
| 1031 | (0) | 1065 | (0) | 1065 | (0) |
| 1064 | (3) | 1100 | (8) | 1102 | (6) |
| 1100 | (13) | 1133 | (9) | 1136 | (4) |
| 1100 | (4) | 1139 | (5) | 1138 | (18) |
| 1120 | (0) | 1157 | (0) | 1153 | (0) |
| 1218 | (0) | 1269 | (0) | 1254 | (0) |
| 1257 | (0) | 1305 | (0) | 1299 | (0) |
| 1275 | (7) | 1319 | (4) | 1315 | (6) |
| 1287 | (6) | 1329 | (6) | 1341 | (5) |
| 1304 | (7) | 1352 | (6) | 1351 | (4) |
| 1346 | (0) | 1389 | (0) | 1399 | (0) |
| 1353 | (1) | 1394 | (1) | 1406 | (0) |
| 1367 | (0) | 1416 | (0) | 1415 | (1) |

| | | | | | |
|---|---|---|---|---|---|
| 1388 | (3) | 1443 | (3) | 1440 | (1) |
| 1408 | (0) | 1462 | (1) | 1455 | (4) |
| 1413 | (5) | 1463 | (5) | 1459 | (0) |
| 1418 | (5) | 1466 | (3) | 1462 | (7) |
| 1419 | (2) | 1470 | (15) | 1470 | (2) |
| 1422 | (6) | 1476 | (1) | 1470 | (4) |
| 2965 | (28) | 3038 | (26) | 3043 | (59) |
| 3057 | (9) | 3125 | (11) | 3145 | (1) |
| 3059 | (11) | 3128 | (12) | 3152 | (19) |
| 3075 | (0) | 3151 | (0) | 3153 | (16) |
| 3081 | (9) | 3158 | (12) | 3154 | (21) |
| 3088 | (27) | 3167 | (26) | 3165 | (60) |
| 3093 | (10) | 3171 | (7) | 3168 | (11) |
| 3109 | (15) | 3193 | (9) | 3195 | (26) |
| 3122 | (18) | 3208 | (13) | 3210 | (38) |
| 3158 | (0) | 3237 | (0) | 3229 | (0) |
| 3159 | (1) | 3239 | (0) | 3234 | (0) |
| 3170 | (9) | 3250 | (6) | 3248 | (24) |
| 3177 | (6) | 3255 | (4) | 3249 | (32) |
| 3186 | (3) | 3265 | (1) | 3261 | (9) |

**Table S19**. Harmonic vibrational frequencies (in $cm^{-1}$) and infrared intensities (in parentheses, in km/mol) for the structure 1Co-3 of $(C_6H_6PCH_3)Co(C_5H_5)$ with $C_s$ symmetry.

| BP86 | | B3LYP | | M06-L | |
|---|---|---|---|---|---|
| 21 | (0) | 13*i* | (0) | 22 | (0) |
| 86 | (0) | 85 | (0) | 79 | (0) |
| 97 | (0) | 98 | (0) | 98 | (0) |
| 132 | (0) | 150 | (0) | 148 | (0) |
| 173 | (0) | 177 | (0) | 186 | (0) |
| 173 | (0) | 177 | (0) | 191 | (0) |
| 219 | (2) | 219 | (1) | 231 | (1) |
| 253 | (0) | 257 | (0) | 271 | (0) |
| 283 | (1) | 287 | (1) | 305 | (1) |
| 342 | (2) | 334 | (5) | 350 | (3) |
| 359 | (1) | 350 | (1) | 386 | (0) |
| 371 | (7) | 352 | (5) | 405 | (6) |
| 383 | (12) | 373 | (13) | 421 | (13) |
| 442 | (12) | 438 | (8) | 465 | (7) |
| 507 | (12) | 513 | (13) | 535 | (12) |
| 521 | (1) | 548 | (2) | 551 | (2) |
| 535 | (15) | 557 | (11) | 578 | (14) |
| 556 | (1) | 581 | (2) | 587 | (2) |
| 563 | (0) | 591 | (0) | 594 | (4) |
| 564 | (3) | 594 | (3) | 609 | (0) |
| 590 | (1) | 609 | (1) | 615 | (3) |
| 621 | (2) | 646 | (2) | 657 | (2) |
| 682 | (8) | 701 | (7) | 731 | (9) |
| 750 | (2) | 786 | (5) | 777 | (2) |
| 769 | (43) | 801 | (62) | 804 | (29) |
| 795 | (0) | 825 | (0) | 816 | (1) |
| 800 | (0) | 837 | (0) | 823 | (0) |
| 802 | (3) | 837 | (3) | 827 | (5) |
| 815 | (11) | 847 | (10) | 840 | (8) |
| 825 | (6) | 853 | (8) | 852 | (7) |
| 842 | (0) | 863 | (1) | 868 | (1) |
| 845 | (5) | 871 | (1) | 874 | (3) |
| 855 | (0) | 899 | (0) | 877 | (2) |
| 857 | (2) | 901 | (6) | 882 | (0) |
| 867 | (7) | 903 | (4) | 893 | (5) |
| 870 | (0) | 913 | (0) | 896 | (0) |
| 883 | (0) | 922 | (1) | 910 | (1) |
| 893 | (1) | 931 | (1) | 933 | (1) |
| 942 | (0) | 984 | (0) | 980 | (1) |
| 954 | (7) | 989 | (7) | 985 | (6) |
| 974 | (10) | 1009 | (11) | 1016 | (9) |
| 990 | (14) | 1023 | (16) | 1026 | (13) |
| 1003 | (22) | 1032 | (28) | 1040 | (28) |
| 1020 | (5) | 1063 | (1) | 1064 | (4) |
| 1030 | (0) | 1065 | (0) | 1066 | (0) |
| 1031 | (0) | 1069 | (5) | 1067 | (1) |
| 1074 | (6) | 1110 | (15) | 1110 | (9) |
| 1100 | (13) | 1133 | (9) | 1138 | (18) |
| 1108 | (4) | 1145 | (6) | 1144 | (4) |
| 1136 | (1) | 1174 | (2) | 1172 | (3) |
| 1218 | (0) | 1270 | (0) | 1257 | (0) |
| 1267 | (0) | 1318 | (0) | 1312 | (0) |
| 1270 | (6) | 1323 | (5) | 1313 | (4) |
| 1295 | (12) | 1335 | (8) | 1352 | (9) |
| 1314 | (11) | 1362 | (11) | 1363 | (8) |
| 1343 | (0) | 1388 | (0) | 1398 | (0) |
| 1353 | (2) | 1394 | (2) | 1406 | (1) |
| 1371 | (0) | 1422 | (2) | 1420 | (2) |

| | | | | | |
|---|---|---|---|---|---|
| 1384 | (3) | 1442 | (3) | 1439 | (17) |
| 1408 | (18) | 1461 | (13) | 1440 | (2) |
| 1409 | (3) | 1462 | (1) | 1458 | (15) |
| 1412 | (15) | 1465 | (15) | 1459 | (0) |
| 1426 | (4) | 1471 | (20) | 1477 | (6) |
| 1426 | (0) | 1484 | (0) | 1479 | (0) |
| 2977 | (21) | 3050 | (19) | 3048 | (40) |
| 3067 | (6) | 3136 | (8) | 3150 | (0) |
| 3069 | (1) | 3143 | (2) | 3157 | (15) |
| 3077 | (6) | 3148 | (7) | 3158 | (7) |
| 3078 | (7) | 3153 | (9) | 3162 | (7) |
| 3088 | (25) | 3168 | (24) | 3165 | (49) |
| 3091 | (7) | 3171 | (5) | 3170 | (22) |
| 3107 | (15) | 3192 | (10) | 3183 | (37) |
| 3120 | (14) | 3206 | (10) | 3197 | (27) |
| 3157 | (0) | 3236 | (0) | 3230 | (2) |
| 3159 | (1) | 3238 | (0) | 3232 | (3) |
| 3169 | (9) | 3249 | (6) | 3245 | (28) |
| 3176 | (6) | 3254 | (3) | 3256 | (20) |
| 3186 | (2) | 3265 | (1) | 3269 | (10) |

**Table S20.** Harmonic vibrational frequencies (in $cm^{-1}$) and infrared intensities (in parentheses, in km/mol) for the structure 1Co-4 of $(C_6H_6PCH_3)Co(C_5H_5)$ with $C_1$ symmetry.

| BP86 | | B3LYP | | M06-L | |
|---|---|---|---|---|---|
| 40 | (0) | 27 | (0) | 45 | (0) |
| 51 | (2) | 53 | (2) | 48 | (2) |
| 89 | (1) | 87 | (1) | 85 | (1) |
| 141 | (0) | 145 | (0) | 145 | (0) |
| 176 | (1) | 180 | (0) | 180 | (1) |
| 189 | (0) | 197 | (0) | 189 | (0) |
| 204 | (1) | 207 | (1) | 214 | (1) |
| 210 | (1) | 218 | (1) | 219 | (1) |
| 292 | (0) | 295 | (0) | 305 | (0) |
| 309 | (0) | 317 | (1) | 323 | (0) |
| 330 | (1) | 328 | (2) | 340 | (2) |
| 350 | (4) | 343 | (3) | 379 | (2) |
| 373 | (4) | 356 | (3) | 404 | (3) |
| 393 | (3) | 397 | (3) | 430 | (3) |
| 439 | (7) | 441 | (6) | 476 | (6) |
| 464 | (10) | 473 | (14) | 483 | (11) |
| 484 | (6) | 490 | (1) | 500 | (7) |
| 545 | (6) | 562 | (4) | 570 | (5) |
| 562 | (3) | 587 | (3) | 594 | (3) |
| 567 | (1) | 595 | (3) | 608 | (4) |
| 615 | (3) | 633 | (4) | 649 | (3) |
| 656 | (13) | 676 | (14) | 703 | (22) |
| 674 | (15) | 696 | (5) | 710 | (17) |
| 692 | (28) | 719 | (40) | 723 | (14) |
| 740 | (14) | 762 | (15) | 765 | (12) |
| 767 | (7) | 799 | (23) | 787 | (3) |
| 781 | (43) | 813 | (49) | 805 | (33) |
| 787 | (4) | 818 | (4) | 810 | (3) |
| 802 | (1) | 838 | (1) | 824 | (0) |
| 806 | (1) | 841 | (1) | 833 | (4) |
| 815 | (6) | 846 | (6) | 838 | (6) |
| 842 | (16) | 873 | (9) | 869 | (10) |
| 850 | (10) | 875 | (21) | 876 | (14) |
| 860 | (1) | 900 | (11) | 889 | (1) |
| 865 | (4) | 904 | (2) | 892 | (3) |
| 871 | (7) | 907 | (2) | 898 | (4) |
| 880 | (11) | 916 | (17) | 907 | (7) |
| 886 | (10) | 928 | (4) | 913 | (13) |
| 909 | (4) | 954 | (2) | 943 | (3) |
| 924 | (6) | 978 | (4) | 966 | (6) |
| 962 | (0) | 1002 | (0) | 998 | (1) |
| 979 | (8) | 1014 | (9) | 1017 | (7) |
| 991 | (14) | 1024 | (15) | 1028 | (12) |
| 1032 | (8) | 1065 | (15) | 1065 | (1) |
| 1033 | (2) | 1067 | (1) | 1068 | (7) |
| 1035 | (5) | 1068 | (5) | 1070 | (13) |
| 1101 | (11) | 1135 | (8) | 1141 | (16) |
| 1117 | (3) | 1155 | (5) | 1154 | (3) |
| 1152 | (1) | 1196 | (2) | 1186 | (1) |
| 1205 | (2) | 1247 | (3) | 1239 | (3) |
| 1219 | (0) | 1271 | (0) | 1257 | (0) |
| 1265 | (2) | 1319 | (4) | 1302 | (2) |
| 1283 | (5) | 1336 | (9) | 1327 | (6) |
| 1336 | (2) | 1386 | (4) | 1381 | (1) |
| 1348 | (1) | 1392 | (3) | 1403 | (1) |
| 1352 | (1) | 1396 | (1) | 1405 | (5) |
| 1363 | (3) | 1412 | (11) | 1415 | (3) |
| 1390 | (4) | 1448 | (4) | 1445 | (2) |

| | | | | | |
|---|---|---|---|---|---|
| 1408 | (1) | 1462 | (1) | 1451 | (9) |
| 1415 | (11) | 1464 | (10) | 1451 | (4) |
| 1417 | (3) | 1466 | (3) | 1460 | (0) |
| 1419 | (2) | 1469 | (4) | 1472 | (1) |
| 1440 | (9) | 1487 | (21) | 1494 | (15) |
| 1584 | (4) | 1647 | (9) | 1661 | (11) |
| 2970 | (37) | 3040 | (33) | 3042 | (65) |
| 3013 | (10) | 3096 | (9) | 3086 | (18) |
| 3032 | (12) | 3113 | (11) | 3119 | (15) |
| 3051 | (28) | 3128 | (11) | 3137 | (46) |
| 3063 | (8) | 3132 | (25) | 3142 | (38) |
| 3066 | (16) | 3139 | (13) | 3155 | (22) |
| 3074 | (10) | 3153 | (9) | 3159 | (18) |
| 3082 | (37) | 3159 | (29) | 3170 | (55) |
| 3084 | (24) | 3172 | (27) | 3176 | (54) |
| 3160 | (0) | 3238 | (0) | 3235 | (0) |
| 3164 | (1) | 3244 | (1) | 3240 | (2) |
| 3174 | (6) | 3254 | (3) | 3253 | (23) |
| 3179 | (4) | 3257 | (2) | 3256 | (18) |
| 3190 | (1) | 3269 | (1) | 3268 | (7) |

**Table S21.** Harmonic vibrational frequencies (in $cm^{-1}$) and infrared intensities (in parentheses, in km/mol) for the structure 1Co-5 of $(C_6H_6PCH_3)Co(C_5H_5)$ with $C_1$ symmetry.

| BP86 | | B3LYP | | M06-L | |
|---|---|---|---|---|---|
| 23 | (0) | 25 | (0) | 43 | (0) |
| 71 | (1) | 74 | (0) | 66 | (1) |
| 105 | (1) | 105 | (1) | 104 | (1) |
| 107 | (3) | 121 | (1) | 109 | (4) |
| 151 | (1) | 160 | (1) | 157 | (1) |
| 163 | (5) | 169 | (5) | 165 | (6) |
| 200 | (0) | 202 | (0) | 210 | (0) |
| 218 | (2) | 220 | (1) | 224 | (2) |
| 263 | (1) | 262 | (0) | 272 | (1) |
| 289 | (4) | 301 | (5) | 297 | (5) |
| 312 | (3) | 320 | (1) | 332 | (3) |
| 345 | (0) | 333 | (6) | 367 | (0) |
| 361 | (7) | 344 | (1) | 382 | (2) |
| 373 | (3) | 375 | (7) | 410 | (10) |
| 383 | (15) | 396 | (6) | 423 | (13) |
| 468 | (4) | 465 | (4) | 487 | (4) |
| 504 | (9) | 518 | (2) | 527 | (26) |
| 536 | (45) | 556 | (47) | 560 | (31) |
| 556 | (4) | 585 | (2) | 593 | (4) |
| 558 | (0) | 588 | (1) | 596 | (1) |
| 592 | (7) | 612 | (6) | 619 | (9) |
| 629 | (65) | 673 | (77) | 658 | (56) |
| 716 | (16) | 737 | (2) | 732 | (5) |
| 721 | (18) | 748 | (21) | 749 | (8) |
| 734 | (7) | 757 | (19) | 756 | (13) |
| 741 | (24) | 774 | (16) | 781 | (27) |
| 764 | (2) | 798 | (2) | 784 | (3) |
| 773 | (38) | 805 | (53) | 802 | (22) |
| 785 | (5) | 810 | (17) | 814 | (9) |
| 796 | (8) | 831 | (5) | 823 | (13) |
| 801 | (4) | 836 | (4) | 828 | (8) |
| 805 | (1) | 840 | (1) | 833 | (3) |
| 828 | (3) | 859 | (6) | 857 | (6) |
| 842 | (1) | 865 | (1) | 870 | (1) |
| 845 | (4) | 886 | (20) | 875 | (4) |
| 847 | (3) | 890 | (0) | 878 | (2) |
| 856 | (6) | 898 | (1) | 881 | (6) |
| 876 | (17) | 912 | (14) | 904 | (15) |
| 907 | (0) | 962 | (14) | 946 | (0) |
| 926 | (2) | 974 | (16) | 961 | (4) |
| 936 | (21) | 986 | (1) | 969 | (21) |
| 974 | (11) | 1006 | (10) | 1014 | (7) |
| 986 | (10) | 1007 | (5) | 1017 | (4) |
| 989 | (5) | 1023 | (14) | 1024 | (13) |
| 1029 | (0) | 1063 | (0) | 1064 | (1) |
| 1032 | (0) | 1065 | (0) | 1068 | (0) |
| 1097 | (13) | 1132 | (10) | 1130 | (1) |
| 1099 | (1) | 1139 | (2) | 1137 | (21) |
| 1165 | (6) | 1208 | (7) | 1198 | (7) |
| 1217 | (0) | 1266 | (11) | 1256 | (0) |
| 1227 | (9) | 1269 | (0) | 1264 | (8) |
| 1262 | (5) | 1309 | (17) | 1302 | (11) |
| 1277 | (13) | 1334 | (14) | 1319 | (11) |
| 1317 | (20) | 1373 | (18) | 1363 | (20) |
| 1345 | (1) | 1389 | (1) | 1399 | (3) |
| 1348 | (0) | 1392 | (2) | 1404 | (1) |
| 1386 | (2) | 1433 | (37) | 1441 | (6) |
| 1393 | (4) | 1443 | (2) | 1442 | (1) |

| | | | | | |
|---|---|---|---|---|---|
| 1403 | (1) | 1462 | (1) | 1452 | (5) |
| 1413 | (9) | 1464 | (8) | 1454 | (9) |
| 1417 | (6) | 1466 | (7) | 1455 | (0) |
| 1438 | (14) | 1477 | (22) | 1494 | (28) |
| 1496 | (80) | 1542 | (104) | 1549 | (107) |
| 1541 | (17) | 1615 | (27) | 1604 | (27) |
| 2988 | (8) | 3058 | (8) | 3064 | (23) |
| 3047 | (5) | 3125 | (5) | 3134 | (10) |
| 3063 | (16) | 3140 | (9) | 3149 | (17) |
| 3069 | (17) | 3145 | (21) | 3153 | (34) |
| 3080 | (4) | 3145 | (6) | 3164 | (29) |
| 3092 | (18) | 3161 | (2) | 3172 | (9) |
| 3095 | (6) | 3168 | (16) | 3174 | (33) |
| 3096 | (8) | 3177 | (26) | 3188 | (9) |
| 3101 | (29) | 3178 | (16) | 3188 | (67) |
| 3156 | (0) | 3236 | (0) | 3222 | (2) |
| 3161 | (1) | 3239 | (1) | 3234 | (8) |
| 3171 | (9) | 3250 | (5) | 3247 | (20) |
| 3175 | (7) | 3254 | (5) | 3248 | (27) |
| 3187 | (3) | 3265 | (2) | 3266 | (11) |

**Table S22**. Harmonic vibrational frequencies (in $cm^{-1}$) and infrared intensities (in parentheses, in km/mol) for the structure 1Co-6 of $(C_6H_6PCH_3)Co(C_5H_5)$ with $C_1$ symmetry.

| BP86 | | B3LYP | | M06-L | |
|---|---|---|---|---|---|
| 32 | (0) | 31 | (0) | 34 | (0) |
| 91 | (1) | 94 | (1) | 96 | (1) |
| 108 | (0) | 102 | (0) | 101 | (0) |
| 160 | (0) | 171 | (0) | 127 | (0) |
| 187 | (0) | 186 | (0) | 187 | (0) |
| 193 | (1) | 194 | (0) | 193 | (1) |
| 225 | (0) | 225 | (1) | 232 | (0) |
| 259 | (0) | 252 | (0) | 265 | (0) |
| 273 | (1) | 268 | (1) | 280 | (2) |
| 302 | (1) | 302 | (4) | 309 | (1) |
| 331 | (1) | 315 | (0) | 335 | (3) |
| 333 | (6) | 321 | (1) | 364 | (6) |
| 370 | (5) | 359 | (9) | 382 | (4) |
| 396 | (5) | 374 | (2) | 432 | (5) |
| 447 | (16) | 451 | (7) | 463 | (13) |
| 454 | (4) | 463 | (3) | 475 | (5) |
| 477 | (1) | 490 | (4) | 490 | (2) |
| 485 | (17) | 502 | (16) | 504 | (16) |
| 557 | (0) | 585 | (0) | 589 | (0) |
| 563 | (1) | 590 | (1) | 601 | (1) |
| 591 | (7) | 607 | (7) | 621 | (8) |
| 630 | (11) | 657 | (10) | 655 | (13) |
| 667 | (33) | 694 | (35) | 688 | (27) |
| 704 | (46) | 735 | (44) | 738 | (40) |
| 742 | (49) | 762 | (43) | 777 | (1) |
| 755 | (1) | 783 | (2) | 781 | (30) |
| 756 | (6) | 788 | (17) | 801 | (27) |
| 774 | (41) | 797 | (56) | 809 | (13) |
| 788 | (5) | 821 | (15) | 814 | (2) |
| 798 | (12) | 822 | (4) | 820 | (20) |
| 803 | (5) | 827 | (6) | 827 | (5) |
| 809 | (4) | 837 | (1) | 834 | (2) |
| 813 | (7) | 843 | (1) | 837 | (12) |
| 847 | (0) | 876 | (42) | 872 | (0) |
| 850 | (3) | 883 | (0) | 877 | (23) |
| 854 | (21) | 892 | (3) | 883 | (18) |
| 883 | (53) | 921 | (48) | 911 | (62) |
| 883 | (0) | 928 | (24) | 914 | (16) |
| 892 | (23) | 932 | (0) | 928 | (6) |
| 905 | (46) | 957 | (33) | 948 | (31) |
| 944 | (0) | 983 | (1) | 975 | (1) |
| 966 | (11) | 1000 | (13) | 1005 | (10) |
| 986 | (1) | 1013 | (0) | 1023 | (0) |
| 995 | (12) | 1028 | (14) | 1035 | (11) |
| 1032 | (0) | 1065 | (0) | 1066 | (0) |
| 1032 | (0) | 1066 | (0) | 1067 | (0) |
| 1056 | (16) | 1100 | (19) | 1094 | (17) |
| 1077 | (1) | 1123 | (1) | 1115 | (1) |
| 1099 | (9) | 1134 | (5) | 1139 | (13) |
| 1123 | (3) | 1166 | (7) | 1160 | (4) |
| 1218 | (0) | 1269 | (0) | 1257 | (0) |
| 1253 | (0) | 1309 | (0) | 1301 | (0) |
| 1263 | (32) | 1323 | (34) | 1309 | (27) |
| 1274 | (8) | 1335 | (7) | 1314 | (6) |
| 1294 | (5) | 1351 | (19) | 1349 | (12) |
| 1329 | (1) | 1380 | (2) | 1380 | (0) |
| 1348 | (0) | 1392 | (0) | 1406 | (0) |
| 1353 | (4) | 1396 | (6) | 1410 | (5) |
| 1388 | (4) | 1445 | (3) | 1442 | (2) |

| | | | | | |
|---|---|---|---|---|---|
| 1411 | (8) | 1462 | (5) | 1447 | (8) |
| 1412 | (4) | 1462 | (8) | 1449 | (3) |
| 1419 | (1) | 1473 | (1) | 1471 | (0) |
| 1532 | (36) | 1589 | (40) | 1603 | (48) |
| 1542 | (8) | 1596 | (7) | 1613 | (12) |
| 2982 | (9) | 3053 | (8) | 3057 | (25) |
| 3041 | (1) | 3126 | (0) | 3119 | (0) |
| 3050 | (23) | 3134 | (22) | 3126 | (35) |
| 3061 | (25) | 3142 | (6) | 3136 | (49) |
| 3066 | (52) | 3142 | (25) | 3143 | (103) |
| 3076 | (5) | 3150 | (46) | 3166 | (12) |
| 3087 | (4) | 3151 | (4) | 3179 | (10) |
| 3113 | (13) | 3193 | (11) | 3192 | (26) |
| 3114 | (18) | 3194 | (13) | 3193 | (43) |
| 3155 | (1) | 3233 | (1) | 3227 | (1) |
| 3158 | (1) | 3234 | (1) | 3231 | (0) |
| 3168 | (9) | 3245 | (7) | 3244 | (29) |
| 3177 | (7) | 3255 | (5) | 3249 | (26) |
| 3185 | (3) | 3263 | (2) | 3260 | (10) |

**Table S23**. Harmonic vibrational frequencies (in $cm^{-1}$) and infrared intensities (in parentheses, in km/mol) for the structure 1Co-7 of $(C_6H_6PCH_3)Co(C_5H_5)$ with $C_1$ symmetry.

| BP86 | | B3LYP | | M06-L | |
|---|---|---|---|---|---|
| 29 | (0) | 25 | (0) | 34 | (0) |
| 97 | (0) | 98 | (0) | 102 | (0) |
| 145 | (2) | 149 | (2) | 152 | (2) |
| 160 | (1) | 161 | (0) | 159 | (1) |
| 173 | (0) | 177 | (0) | 174 | (0) |
| 197 | (0) | 202 | (0) | 219 | (0) |
| 226 | (2) | 230 | (1) | 237 | (2) |
| 251 | (1) | 247 | (4) | 258 | (2) |
| 269 | (0) | 282 | (0) | 287 | (0) |
| 299 | (1) | 298 | (1) | 313 | (0) |
| 338 | (3) | 327 | (1) | 369 | (1) |
| 351 | (8) | 340 | (5) | 380 | (6) |
| 371 | (1) | 343 | (10) | 388 | (2) |
| 378 | (5) | 362 | (2) | 398 | (10) |
| 435 | (10) | 421 | (7) | 454 | (9) |
| 472 | (2) | 479 | (2) | 514 | (3) |
| 494 | (7) | 503 | (7) | 520 | (8) |
| 547 | (1) | 569 | (1) | 577 | (1) |
| 557 | (1) | 585 | (1) | 592 | (1) |
| 562 | (1) | 587 | (1) | 594 | (1) |
| 586 | (1) | 607 | (3) | 628 | (2) |
| 669 | (3) | 691 | (3) | 707 | (4) |
| 670 | (41) | 692 | (39) | 710 | (32) |
| 687 | (1) | 709 | (1) | 733 | (3) |
| 748 | (3) | 777 | (8) | 765 | (4) |
| 752 | (11) | 779 | (8) | 778 | (7) |
| 761 | (14) | 789 | (10) | 790 | (16) |
| 773 | (34) | 802 | (58) | 803 | (27) |
| 784 | (26) | 815 | (26) | 815 | (19) |
| 787 | (4) | 826 | (0) | 816 | (0) |
| 805 | (0) | 838 | (0) | 827 | (0) |
| 807 | (2) | 842 | (0) | 830 | (1) |
| 823 | (11) | 851 | (9) | 844 | (10) |
| 859 | (2) | 900 | (0) | 883 | (5) |
| 861 | (3) | 904 | (3) | 888 | (0) |
| 875 | (3) | 915 | (3) | 902 | (2) |
| 879 | (4) | 918 | (4) | 914 | (5) |
| 892 | (1) | 933 | (2) | 929 | (1) |
| 908 | (2) | 944 | (10) | 944 | (1) |
| 924 | (0) | 952 | (19) | 958 | (1) |
| 926 | (19) | 969 | (0) | 961 | (22) |
| 936 | (2) | 972 | (2) | 971 | (3) |
| 974 | (8) | 1008 | (11) | 1011 | (8) |
| 998 | (13) | 1030 | (14) | 1034 | (11) |
| 1032 | (0) | 1066 | (0) | 1064 | (0) |
| 1036 | (0) | 1067 | (0) | 1071 | (0) |
| 1097 | (5) | 1138 | (4) | 1129 | (4) |
| 1100 | (0) | 1141 | (12) | 1131 | (2) |
| 1105 | (8) | 1144 | (1) | 1143 | (14) |
| 1111 | (1) | 1156 | (2) | 1146 | (0) |
| 1220 | (0) | 1272 | (0) | 1257 | (0) |
| 1238 | (3) | 1296 | (5) | 1287 | (4) |
| 1263 | (4) | 1321 | (7) | 1307 | (5) |
| 1278 | (8) | 1334 | (8) | 1323 | (6) |
| 1318 | (3) | 1378 | (3) | 1369 | (1) |
| 1350 | (0) | 1394 | (0) | 1404 | (0) |
| 1358 | (2) | 1401 | (2) | 1413 | (2) |
| 1367 | (11) | 1432 | (22) | 1424 | (17) |

| | | | | | |
|---|---|---|---|---|---|
| 1373 | (7) | 1437 | (11) | 1432 | (10) |
| 1387 | (5) | 1444 | (4) | 1438 | (2) |
| 1416 | (8) | 1464 | (8) | 1451 | (8) |
| 1422 | (4) | 1472 | (4) | 1463 | (2) |
| 1425 | (1) | 1475 | (1) | 1473 | (0) |
| 1629 | (9) | 1683 | (6) | 1708 | (12) |
| 2965 | (27) | 3040 | (22) | 3035 | (48) |
| 3042 | (10) | 3131 | (12) | 3120 | (18) |
| 3044 | (10) | 3131 | (13) | 3122 | (18) |
| 3060 | (8) | 3132 | (3) | 3138 | (51) |
| 3061 | (18) | 3133 | (2) | 3141 | (22) |
| 3065 | (12) | 3151 | (4) | 3145 | (19) |
| 3067 | (16) | 3155 | (17) | 3159 | (28) |
| 3072 | (21) | 3156 | (28) | 3163 | (17) |
| 3095 | (45) | 3177 | (37) | 3184 | (85) |
| 3154 | (1) | 3233 | (1) | 3222 | (2) |
| 3157 | (2) | 3235 | (2) | 3229 | (8) |
| 3171 | (4) | 3249 | (3) | 3247 | (16) |
| 3181 | (4) | 3258 | (3) | 3249 | (16) |
| 3188 | (2) | 3266 | (1) | 3265 | (10) |

**Table S24.** Harmonic vibrational frequencies (in $cm^{-1}$) and infrared intensities (in parentheses, in km/mol) for the structure **1Co-8** of $(C_6H_6PCH_3)Co(C_5H_5)$ with $C_s$ symmetry.

| BP86 | | B3LYP | | M06-L | |
|---|---|---|---|---|---|
| 7 | (0) | 20 | (0) | 28 | (0) |
| 97 | (1) | 97 | (1) | 95 | (1) |
| 130 | (1) | 134 | (1) | 108 | (0) |
| 141 | (0) | 145 | (0) | 140 | (0) |
| 176 | (1) | 180 | (1) | 175 | (1) |
| 187 | (0) | 191 | (0) | 191 | (0) |
| 214 | (2) | 217 | (2) | 217 | (2) |
| 252 | (3) | 253 | (3) | 258 | (4) |
| 291 | (0) | 288 | (3) | 306 | (1) |
| 295 | (0) | 295 | (2) | 308 | (1) |
| 351 | (5) | 341 | (8) | 380 | (0) |
| 357 | (11) | 343 | (8) | 381 | (9) |
| 378 | (4) | 354 | (2) | 403 | (1) |
| 386 | (1) | 381 | (1) | 405 | (10) |
| 441 | (10) | 424 | (6) | 466 | (8) |
| 463 | (2) | 470 | (2) | 500 | (1) |
| 490 | (9) | 501 | (11) | 519 | (12) |
| 557 | (0) | 581 | (1) | 585 | (0) |
| 560 | (2) | 588 | (2) | 597 | (2) |
| 570 | (1) | 591 | (1) | 597 | (2) |
| 589 | (3) | 609 | (6) | 627 | (5) |
| 633 | (45) | 658 | (48) | 680 | (40) |
| 661 | (1) | 681 | (1) | 703 | (2) |
| 699 | (7) | 719 | (7) | 735 | (11) |
| 754 | (15) | 783 | (19) | 771 | (6) |
| 761 | (22) | 793 | (14) | 786 | (24) |
| 770 | (7) | 796 | (7) | 791 | (5) |
| 783 | (49) | 809 | (69) | 804 | (36) |
| 803 | (1) | 837 | (0) | 825 | (0) |
| 809 | (1) | 838 | (1) | 833 | (2) |
| 820 | (1) | 843 | (0) | 834 | (1) |
| 822 | (1) | 849 | (3) | 837 | (3) |
| 842 | (10) | 869 | (6) | 858 | (8) |
| 847 | (7) | 881 | (3) | 868 | (1) |
| 858 | (18) | 898 | (21) | 876 | (13) |
| 866 | (0) | 904 | (0) | 888 | (0) |
| 867 | (5) | 909 | (4) | 888 | (5) |
| 897 | (0) | 936 | (2) | 930 | (1) |
| 923 | (6) | 953 | (33) | 950 | (4) |
| 933 | (1) | 969 | (1) | 964 | (0) |
| 934 | (21) | 973 | (1) | 972 | (33) |
| 942 | (0) | 984 | (0) | 973 | (2) |
| 975 | (7) | 1009 | (10) | 1015 | (7) |
| 998 | (12) | 1030 | (13) | 1033 | (10) |
| 1034 | (0) | 1066 | (0) | 1067 | (0) |
| 1034 | (0) | 1068 | (0) | 1070 | (0) |
| 1106 | (8) | 1138 | (5) | 1144 | (14) |
| 1110 | (7) | 1153 | (15) | 1147 | (7) |
| 1131 | (0) | 1176 | (1) | 1167 | (0) |
| 1133 | (5) | 1179 | (8) | 1170 | (8) |
| 1221 | (0) | 1272 | (0) | 1258 | (0) |
| 1252 | (12) | 1311 | (13) | 1289 | (10) |
| 1262 | (4) | 1319 | (6) | 1309 | (5) |
| 1294 | (5) | 1352 | (8) | 1343 | (6) |
| 1319 | (3) | 1380 | (2) | 1370 | (1) |
| 1352 | (0) | 1395 | (1) | 1405 | (1) |
| 1360 | (3) | 1401 | (1) | 1414 | (3) |
| 1372 | (24) | 1436 | (44) | 1428 | (36) |

| | | | | | |
|---|---|---|---|---|---|
| 1377 | (4) | 1438 | (7) | 1436 | (6) |
| 1389 | (5) | 1445 | (4) | 1442 | (2) |
| 1405 | (4) | 1456 | (3) | 1442 | (2) |
| 1423 | (1) | 1473 | (1) | 1460 | (4) |
| 1423 | (5) | 1474 | (5) | 1471 | (0) |
| 1638 | (6) | 1692 | (4) | 1718 | (9) |
| 2972 | (31) | 3044 | (28) | 3050 | (57) |
| 3023 | (25) | 3116 | (17) | 3108 | (42) |
| 3024 | (15) | 3117 | (12) | 3110 | (26) |
| 3053 | (7) | 3119 | (8) | 3145 | (48) |
| 3063 | (21) | 3149 | (1) | 3146 | (18) |
| 3064 | (13) | 3154 | (35) | 3153 | (12) |
| 3068 | (26) | 3155 | (15) | 3156 | (41) |
| 3091 | (41) | 3172 | (5) | 3179 | (10) |
| 3098 | (7) | 3174 | (36) | 3181 | (81) |
| 3160 | (1) | 3237 | (1) | 3230 | (1) |
| 3161 | (2) | 3239 | (1) | 3233 | (7) |
| 3173 | (4) | 3251 | (3) | 3250 | (16) |
| 3184 | (3) | 3261 | (2) | 3255 | (12) |
| 3191 | (1) | 3268 | (1) | 3267 | (9) |

**Table S25**. Harmonic vibrational frequencies (in $cm^{-1}$) and infrared intensities (in parentheses, in km/mol) for the structure **2Fe-1** of $(C_{10}H_8PCH_3)Fe(CO)_3$ with $C_1$ symmetry.

| BP86 | | B3LYP | | M06-L | |
|---|---|---|---|---|---|
| 27 | (0) | 31 | (0) | 27 | (0) |
| 46 | (0) | 49 | (0) | 43 | (0) |
| 61 | (0) | 63 | (0) | 64 | (0) |
| 72 | (0) | 73 | (0) | 73 | (0) |
| 80 | (0) | 83 | (0) | 81 | (0) |
| 91 | (0) | 94 | (1) | 94 | (0) |
| 96 | (0) | 100 | (0) | 97 | (1) |
| 112 | (0) | 116 | (0) | 114 | (0) |
| 128 | (0) | 135 | (0) | 160 | (1) |
| 161 | (2) | 167 | (1) | 167 | (0) |
| 180 | (1) | 183 | (1) | 189 | (1) |
| 207 | (1) | 213 | (1) | 224 | (0) |
| 219 | (1) | 224 | (1) | 231 | (1) |
| 270 | (4) | 278 | (5) | 276 | (3) |
| 275 | (4) | 284 | (1) | 281 | (3) |
| 322 | (6) | 324 | (14) | 332 | (9) |
| 347 | (4) | 351 | (6) | 357 | (3) |
| 384 | (5) | 393 | (4) | 393 | (3) |
| 397 | (1) | 404 | (0) | 400 | (0) |
| 406 | (4) | 422 | (3) | 418 | (3) |
| 431 | (10) | 440 | (10) | 440 | (8) |
| 469 | (6) | 469 | (10) | 460 | (6) |
| 471 | (4) | 472 | (3) | 465 | (0) |
| 493 | (4) | 495 | (6) | 487 | (21) |
| 503 | (34) | 507 | (24) | 503 | (9) |
| 513 | (14) | 515 | (5) | 505 | (5) |
| 520 | (0) | 532 | (35) | 528 | (35) |
| 540 | (8) | 555 | (39) | 551 | (41) |
| 555 | (27) | 568 | (26) | 567 | (37) |
| 581 | (45) | 578 | (44) | 576 | (41) |
| 604 | (12) | 613 | (78) | 605 | (77) |
| 612 | (54) | 624 | (1) | 625 | (16) |
| 622 | (87) | 631 | (88) | 633 | (66) |
| 652 | (5) | 672 | (5) | 676 | (5) |
| 661 | (18) | 685 | (10) | 681 | (15) |
| 675 | (12) | 702 | (15) | 700 | (9) |
| 729 | (19) | 758 | (15) | 744 | (22) |
| 739 | (25) | 762 | (29) | 759 | (20) |
| 742 | (40) | 768 | (43) | 770 | (20) |
| 750 | (30) | 774 | (23) | 782 | (32) |
| 756 | (37) | 788 | (44) | 789 | (41) |
| 800 | (4) | 820 | (5) | 838 | (11) |
| 841 | (1) | 873 | (1) | 868 | (1) |
| 848 | (1) | 881 | (3) | 878 | (1) |
| 883 | (27) | 916 | (30) | 905 | (21) |
| 903 | (10) | 939 | (11) | 928 | (11) |
| 917 | (2) | 962 | (2) | 950 | (1) |
| 937 | (2) | 978 | (18) | 973 | (10) |
| 946 | (17) | 990 | (8) | 980 | (14) |
| 950 | (6) | 995 | (0) | 983 | (1) |
| 1034 | (5) | 1063 | (5) | 1064 | (5) |
| 1064 | (4) | 1099 | (3) | 1090 | (5) |
| 1111 | (2) | 1145 | (3) | 1144 | (2) |
| 1143 | (2) | 1177 | (3) | 1174 | (0) |
| 1157 | (4) | 1194 | (7) | 1187 | (5) |
| 1182 | (4) | 1213 | (5) | 1215 | (6) |
| 1213 | (8) | 1253 | (9) | 1252 | (9) |
| 1248 | (8) | 1292 | (6) | 1285 | (10) |
| 1285 | (14) | 1336 | (11) | 1327 | (8) |

| | | | | | |
|---|---|---|---|---|---|
| 1297 | (9) | 1342 | (21) | 1330 | (17) |
| 1355 | (5) | 1378 | (4) | 1398 | (5) |
| 1369 | (5) | 1410 | (5) | 1411 | (3) |
| 1384 | (1) | 1432 | (3) | 1429 | (3) |
| 1409 | (8) | 1459 | (7) | 1452 | (4) |
| 1414 | (7) | 1463 | (8) | 1454 | (8) |
| 1429 | (24) | 1474 | (40) | 1481 | (27) |
| 1461 | (16) | 1512 | (16) | 1512 | (17) |
| 1535 | (21) | 1587 | (19) | 1595 | (21) |
| 1582 | (71) | 1642 | (73) | 1653 | (71) |
| 1594 | (13) | 1645 | (20) | 1656 | (35) |
| 1940 | (697) | 2022 | (879) | 2016 | (866) |
| 1955 | (788) | 2039 | (929) | 2031 | (938) |
| 2003 | (825) | 2084 | (1037) | 2082 | (927) |
| 2993 | (3) | 3062 | (3) | 3067 | (13) |
| 3066 | (8) | 3146 | (7) | 3142 | (17) |
| 3069 | (4) | 3149 | (2) | 3148 | (12) |
| 3087 | (2) | 3151 | (2) | 3176 | (15) |
| 3097 | (4) | 3167 | (1) | 3177 | (15) |
| 3101 | (11) | 3174 | (6) | 3177 | (21) |
| 3102 | (5) | 3181 | (12) | 3180 | (10) |
| 3106 | (0) | 3186 | (2) | 3181 | (4) |
| 3115 | (2) | 3193 | (2) | 3192 | (4) |
| 3123 | (14) | 3200 | (16) | 3206 | (27) |
| 3139 | (22) | 3216 | (20) | 3222 | (49) |

**Table S26.** Harmonic vibrational frequencies (in $cm^{-1}$) and infrared intensities (in parentheses, in km/mol) for the structure **2Fe-2** of $(C_{10}H_8PCH_3)Fe(CO)_3$ with $C_s$ symmetry.

| BP86 | | B3LYP | | M06-L | |
|---|---|---|---|---|---|
| 34 | (0) | 37 | (0) | 40 | (0) |
| 69 | (0) | 72 | (0) | 72 | (0) |
| 73 | (0) | 76 | (0) | 74 | (1) |
| 74 | (2) | 77 | (1) | 74 | (0) |
| 80 | (0) | 82 | (0) | 81 | (0) |
| 91 | 0 | 95 | (0) | 93 | (0) |
| 92 | (0) | 97 | (0) | 96 | (0) |
| 120 | (0) | 121 | (0) | 141 | (0) |
| 133 | (1) | 139 | (1) | 149 | (1) |
| 154 | (1) | 159 | (0) | 160 | (3) |
| 158 | (4) | 164 | (3) | 180 | (0) |
| 207 | (0) | 215 | (0) | 218 | (0) |
| 229 | (2) | 237 | (1) | 241 | (1) |
| 238 | (0) | 245 | (0) | 246 | (0) |
| 315 | (2) | 323 | (2) | 323 | (2) |
| 333 | (1) | 345 | (1) | 338 | (1) |
| 377 | (1) | 387 | (1) | 388 | (1) |
| 411 | (0) | 420 | (0) | 418 | (0) |
| 425 | (12) | 433 | (6) | 428 | (2) |
| 462 | (11) | 461 | (0) | 455 | (1) |
| 463 | (0) | 465 | (33) | 457 | (30) |
| 466 | (12) | 466 | (5) | 464 | (2) |
| 500 | (1) | 498 | (0) | 491 | (6) |
| 500 | (3) | 502 | (2) | 497 | (3) |
| 507 | (1) | 520 | (5) | 520 | (10) |
| 515 | (19) | 531 | (14) | 522 | (4) |
| 531 | (5) | 537 | (16) | 536 | (24) |
| 537 | (6) | 556 | (18) | 553 | (29) |
| 574 | (45) | 574 | (42) | 571 | (26) |
| 580 | (1) | 602 | (7) | 601 | (15) |
| 603 | (11) | 608 | (49) | 608 | (58) |
| 621 | (97) | 624 | (109) | 625 | (101) |
| 621 | (1) | 642 | (46) | 655 | (31) |
| 631 | (76) | 650 | (2) | 677 | (2) |
| 668 | (15) | 687 | (14) | 716 | (18) |
| 717 | (2) | 746 | (2) | 746 | (2) |
| 731 | (2) | 758 | (0) | 757 | (1) |
| 739 | (49) | 765 | (26) | 763 | (40) |
| 753 | (19) | 779 | (41) | 782 | (16) |
| 826 | (0) | 859 | (0) | 855 | (0) |
| 845 | (0) | 878 | (0) | 873 | (6) |
| 847 | (7) | 881 | (8) | 874 | (0) |
| 869 | (7) | 892 | (3) | 897 | (7) |
| 870 | (6) | 903 | (6) | 899 | (3) |
| 911 | (7) | 948 | (12) | 937 | (11) |
| 914 | (7) | 949 | (8) | 940 | (9) |
| 930 | (1) | 975 | (1) | 962 | (1) |
| 953 | (12) | 987 | (12) | 988 | (0) |
| 954 | (0) | 997 | (9) | 988 | (12) |
| 955 | (10) | 999 | (0) | 1006 | (8) |
| 1002 | (6) | 1026 | (6) | 1035 | (6) |
| 1016 | (1) | 1053 | (4) | 1050 | (2) |
| 1103 | (6) | 1130 | (10) | 1135 | (8) |
| 1116 | (4) | 1152 | (4) | 1155 | (4) |
| 1145 | (1) | 1180 | (0) | 1178 | (1) |
| 1187 | (7) | 1217 | (7) | 1227 | (11) |
| 1204 | (0) | 1243 | 0 | 1243 | (0) |
| 1210 | (5) | 1249 | (4) | 1250 | (5) |
| 1271 | (4) | 1308 | (2) | 1314 | (5) |

| | | | | | |
|---|---|---|---|---|---|
| 1280 | (7) | 1321 | (6) | 1325 | (5) |
| 1282 | (8) | 1331 | (7) | 1329 | (6) |
| 1335 | (0) | 1381 | (0) | 1383 | (0) |
| 1360 | (4) | 1395 | (3) | 1413 | (5) |
| 1381 | (1) | 1415 | (0) | 1432 | (0) |
| 1414 | (6) | 1463 | (6) | 1452 | (4) |
| 1420 | (11) | 1469 | (10) | 1463 | (10) |
| 1447 | (10) | 1487 | (14) | 1498 | (9) |
| 1455 | (5) | 1500 | (7) | 1513 | (4) |
| 1521 | (4) | 1568 | (4) | 1584 | (5) |
| 1604 | (1) | 1657 | (1) | 1670 | (0) |
| 1961 | (656) | 2048 | (829) | 2042 | (781) |
| 1963 | (719) | 2054 | (763) | 2043 | (869) |
| 2017 | (906) | 2101 | (1167) | 2099 | (1031) |
| 2969 | (21) | 3040 | (22) | 3041 | (48) |
| 3062 | (7) | 3128 | (9) | 3151 | (16) |
| 3065 | (8) | 3132 | (9) | 3154 | (14) |
| 3087 | (0) | 3157 | (1) | 3159 | (0) |
| 3092 | (5) | 3162 | (5) | 3166 | (14) |
| 3098 | (19) | 3168 | (22) | 3177 | (55) |
| 3102 | (3) | 3173 | (5) | 3179 | (4) |
| 3109 | (0) | 3184 | (0) | 3186 | (7) |
| 3114 | (1) | 3190 | (1) | 3189 | (1) |
| 3126 | (14) | 3202 | (13) | 3209 | (30) |
| 3137 | (17) | 3213 | (16) | 3223 | (43) |

**Table S27**. Harmonic vibrational frequencies (in $cm^{-1}$) and infrared intensities (in parentheses, in km/mol) for the structure **2Fe-3** of $(C_{10}H_8PCH_3)Fe(CO)_3$ with $C_s$ symmetry.

| BP86 | | B3LYP | | M06-L | |
|---|---|---|---|---|---|
| 27 | (0) | 14 | (0) | 17 | (0) |
| 61 | (0) | 63 | (0) | 58 | (0) |
| 76 | (0) | 80 | (0) | 74 | (0) |
| 78 | (0) | 81 | (0) | 77 | (1) |
| 85 | (0) | 87 | (0) | 80 | (0) |
| 94 | (0) | 97 | (0) | 93 | (0) |
| 100 | (0) | 103 | (0) | 96 | (0) |
| 124 | (0) | 129 | (0) | 126 | (0) |
| 156 | (2) | 160 | (2) | 159 | (2) |
| 163 | (1) | 167 | (2) | 171 | (1) |
| 186 | (0) | 185 | (0) | 199 | (0) |
| 230 | (1) | 211 | (2) | 224 | (2) |
| 237 | (2) | 236 | (2) | 242 | (2) |
| 259 | (4) | 263 | (3) | 269 | (4) |
| 266 | (3) | 277 | (4) | 277 | (3) |
| 336 | (6) | 325 | (6) | 334 | (6) |
| 376 | (15) | 376 | (26) | 378 | (21) |
| 379 | (0) | 394 | (0) | 395 | (0) |
| 394 | (0) | 396 | (0) | 401 | (0) |
| 426 | (10) | 428 | (4) | 429 | (5) |
| 443 | (12) | 449 | (13) | 451 | (17) |
| 470 | (2) | 468 | (2) | 470 | (2) |
| 476 | (1) | 482 | (22) | 475 | (15) |
| 499 | (3) | 482 | (3) | 486 | (4) |
| 501 | (1) | 505 | (1) | 503 | (13) |
| 507 | (6) | 511 | (7) | 507 | (0) |
| 527 | (10) | 530 | (17) | 527 | (8) |
| 548 | (0) | 557 | (47) | 557 | (48) |
| 563 | (12) | 568 | (1) | 569 | (0) |
| 570 | (41) | 577 | (17) | 585 | (18) |
| 591 | (6) | 608 | (19) | 609 | (28) |
| 625 | (2) | 630 | (90) | 633 | (83) |
| 627 | (103) | 645 | (47) | 651 | (46) |
| 641 | (54) | 647 | (1) | 652 | (1) |
| 677 | (5) | 699 | (6) | 707 | (5) |
| 679 | (1) | 703 | (1) | 708 | (1) |
| 691 | (8) | 712 | (7) | 728 | (8) |
| 733 | (47) | 761 | (48) | 759 | (39) |
| 747 | (0) | 775 | (0) | 774 | (0) |
| 767 | (7) | 793 | (8) | 794 | (3) |
| 806 | (8) | 823 | (4) | 818 | (4) |
| 831 | (0) | 850 | (15) | 846 | (17) |
| 831 | (12) | 861 | (0) | 860 | (0) |
| 859 | (0) | 894 | (0) | 885 | (0) |
| 887 | (10) | 922 | (13) | 914 | (10) |
| 892 | (1) | 925 | (2) | 918 | (1) |
| 916 | (3) | 959 | (3) | 947 | (2) |
| 938 | (1) | 980 | (2) | 963 | (1) |
| 944 | (0) | 989 | (0) | 972 | (1) |
| 950 | (1) | 994 | (1) | 983 | (0) |
| 1022 | (3) | 1051 | (3) | 1058 | (3) |
| 1061 | (1) | 1099 | (2) | 1097 | (1) |
| 1100 | (5) | 1141 | (7) | 1132 | (5) |
| 1107 | (2) | 1143 | (1) | 1144 | (2) |
| 1144 | (0) | 1177 | (0) | 1174 | (0) |
| 1181 | (4) | 1221 | (4) | 1219 | (5) |
| 1198 | (0) | 1233 | (0) | 1235 | (1) |
| 1234 | (3) | 1278 | (4) | 1273 | (4) |
| 1271 | (3) | 1327 | (7) | 1310 | (5) |

| | | | | | |
|---|---|---|---|---|---|
| 1273 | (6) | 1330 | (3) | 1318 | (3) |
| 1298 | (11) | 1347 | (2) | 1343 | (12) |
| 1349 | (2) | 1359 | (15) | 1394 | (4) |
| 1369 | (7) | 1427 | (10) | 1423 | (7) |
| 1404 | (4) | 1462 | (2) | 1452 | (7) |
| 1415 | (10) | 1466 | (15) | 1455 | (2) |
| 1418 | (3) | 1467 | (3) | 1462 | (8) |
| 1443 | (1) | 1498 | (0) | 1501 | (0) |
| 1474 | (20) | 1523 | (26) | 1531 | (17) |
| 1579 | (4) | 1627 | (4) | 1643 | (5) |
| 1590 | (1) | 1644 | (1) | 1657 | (1) |
| 1951 | (603) | 2032 | (729) | 2029 | (701) |
| 1971 | (756) | 2046 | (934) | 2048 | (904) |
| 2013 | (849) | 2091 | (1000) | 2093 | (922) |
| 2969 | (19) | 3042 | (18) | 3023 | (40) |
| 3066 | (6) | 3135 | (5) | 3137 | (14) |
| 3070 | (4) | 3136 | (7) | 3139 | (5) |
| 3079 | (1) | 3159 | (1) | 3139 | (3) |
| 3079 | (0) | 3159 | (1) | 3156 | (19) |
| 3095 | (8) | 3178 | (4) | 3158 | (9) |
| 3097 | (5) | 3180 | (5) | 3159 | (18) |
| 3104 | (4) | 3181 | (4) | 3170 | (17) |
| 3108 | (1) | 3186 | (2) | 3173 | (1) |
| 3121 | (16) | 3198 | (15) | 3191 | (35) |
| 3136 | (25) | 3213 | (22) | 3207 | (54) |

**Table S28.** Harmonic vibrational frequencies (in $cm^{-1}$) and infrared intensities (in parentheses, in km/mol) for the structure **2Fe-4** of $(C_{10}H_8PCH_3)Fe(CO)_3$ with $C_s$ symmetry.

| BP86 | | B3LYP | | M06-L | |
|---|---|---|---|---|---|
| 25 | (0) | 13 | (0) | 13 | (0) |
| 61 | (0) | 63 | (0) | 60 | (0) |
| 77 | (0) | 80 | (0) | 77 | (0) |
| 84 | (0) | 88 | (0) | 83 | (0) |
| 92 | (0) | 95 | (0) | 92 | (0) |
| 96 | (0) | 99 | (0) | 92 | (0) |
| 101 | (0) | 105 | (0) | 99 | (0) |
| 109 | (0) | 116 | (0) | 114 | (0) |
| 131 | (0) | 140 | (0) | 137 | (0) |
| 174 | (0) | 176 | (0) | 177 | (0) |
| 176 | (1) | 180 | (1) | 178 | (0) |
| 223 | (3) | 221 | (2) | 232 | (2) |
| 234 | (1) | 229 | (2) | 232 | (2) |
| 243 | (3) | 241 | (3) | 248 | (2) |
| 301 | (5) | 315 | (5) | 310 | (5) |
| 340 | (5) | 329 | (5) | 328 | (6) |
| 383 | (14) | 379 | (19) | 386 | (16) |
| 388 | (0) | 395 | (0) | 393 | (0) |
| 400 | (0) | 411 | (0) | 405 | (0) |
| 422 | (4) | 428 | (5) | 424 | (3) |
| 447 | (10) | 454 | (5) | 452 | (8) |
| 458 | (0) | 461 | (2) | 459 | (2) |
| 479 | (1) | 478 | (1) | 469 | (25) |
| 495 | (9) | 481 | (34) | 482 | (2) |
| 504 | (1) | 510 | (1) | 494 | (16) |
| 512 | (3) | 512 | (6) | 508 | (1) |
| 530 | (11) | 535 | (16) | 532 | (9) |
| 547 | (0) | 556 | (46) | 546 | (49) |
| 560 | (16) | 569 | (6) | 569 | (3) |
| 571 | (44) | 573 | (26) | 579 | (29) |
| 594 | (26) | 607 | (53) | 610 | (61) |
| 627 | (99) | 633 | (75) | 632 | (69) |
| 629 | (1) | 640 | (42) | 654 | (32) |
| 633 | (40) | 650 | (1) | 654 | (1) |
| 661 | (12) | 679 | (4) | 687 | (2) |
| 676 | (0) | 701 | (1) | 710 | (0) |
| 689 | (14) | 709 | (15) | 723 | (17) |
| 737 | (62) | 765 | (67) | 767 | (55) |
| 745 | (0) | 775 | (0) | 773 | (0) |
| 788 | (6) | 814 | (7) | 816 | (8) |
| 832 | (2) | 859 | (2) | 850 | (2) |
| 845 | (0) | 869 | (16) | 862 | (20) |
| 847 | (14) | 875 | (0) | 868 | (1) |
| 851 | (8) | 881 | (3) | 874 | (1) |
| 864 | (0) | 900 | (0) | 894 | (0) |
| 877 | (28) | 915 | (29) | 895 | (25) |
| 916 | (5) | 959 | (5) | 949 | (3) |
| 946 | (0) | 991 | (0) | 982 | (1) |
| 957 | (1) | 1002 | (1) | 982 | (0) |
| 968 | (1) | 1016 | (1) | 995 | (1) |
| 1022 | (2) | 1051 | (2) | 1053 | (2) |
| 1072 | (1) | 1108 | (2) | 1107 | (2) |
| 1114 | (3) | 1150 | (2) | 1147 | (2) |
| 1125 | (10) | 1165 | (14) | 1157 | (13) |
| 1143 | (0) | 1177 | (0) | 1173 | (0) |
| 1192 | (4) | 1234 | (4) | 1229 | (5) |
| 1203 | (0) | 1241 | (0) | 1240 | (1) |
| 1237 | (4) | 1280 | (5) | 1272 | (5) |
| 1267 | (8) | 1323 | (9) | 1301 | (5) |

| | | | | | |
|---|---|---|---|---|---|
| 1294 | (1) | 1352 | (2) | 1342 | (2) |
| 1314 | (4) | 1352 | (2) | 1361 | (5) |
| 1349 | (3) | 1372 | (10) | 1378 | (7) |
| 1367 | (3) | 1424 | (6) | 1415 | (4) |
| 1404 | (18) | 1456 | (13) | 1445 | (12) |
| 1410 | (2) | 1467 | (4) | 1453 | (3) |
| 1415 | (4) | 1467 | (14) | 1459 | (13) |
| 1443 | (1) | 1497 | (1) | 1496 | (0) |
| 1478 | (19) | 1527 | (25) | 1530 | (17) |
| 1582 | (5) | 1631 | (4) | 1633 | (6) |
| 1588 | (1) | 1642 | (1) | 1649 | (1) |
| 1961 | (585) | 2046 | (701) | 2040 | (701) |
| 1978 | (753) | 2054 | (913) | 2049 | (879) |
| 2020 | (918) | 2098 | (1104) | 2097 | (1071) |
| 2974 | (17) | 3045 | (18) | 3052 | (35) |
| 3054 | (5) | 3120 | (6) | 3146 | (15) |
| 3063 | (5) | 3144 | (4) | 3146 | (8) |
| 3064 | (3) | 3145 | (2) | 3155 | (8) |
| 3090 | (11) | 3172 | (5) | 3168 | (32) |
| 3091 | (7) | 3173 | (8) | 3169 | (12) |
| 3100 | (4) | 3174 | (6) | 3179 | (5) |
| 3104 | (4) | 3181 | (3) | 3180 | (14) |
| 3109 | (1) | 3186 | (1) | 3184 | (1) |
| 3122 | (15) | 3198 | (14) | 3200 | (35) |
| 3136 | (23) | 3213 | (21) | 3216 | (50) |

**Table S29.** Harmonic vibrational frequencies (in $cm^{-1}$) and infrared intensities (in parentheses, in km/mol) for the structure **2Fe-5** of $(C_{10}H_8PCH_3)Fe(CO)_3$ with $C_1$ symmetry.

| BP86 | | B3LYP | | M06-L | |
|---|---|---|---|---|---|
| 32 | (0) | 38 | (0) | 37 | (0) |
| 70 | (0) | 74 | (0) | 73 | (0) |
| 73 | (0) | 76 | (0) | 77 | (0) |
| 80 | (0) | 83 | (0) | 80 | (0) |
| 80 | (0) | 85 | (0) | 87 | (0) |
| 88 | (0) | 92 | (0) | 92 | (0) |
| 99 | (0) | 103 | (0) | 105 | (0) |
| 99 | (0) | 110 | (0) | 108 | (0) |
| 133 | (0) | 147 | (0) | 164 | (0) |
| 156 | (0) | 163 | (0) | 186 | (2) |
| 176 | (4) | 181 | (3) | 236 | (1) |
| 204 | (2) | 212 | (1) | 245 | (0) |
| 236 | (0) | 245 | (0) | 284 | (0) |
| 291 | (2) | 300 | (2) | 316 | (3) |
| 319 | (2) | 328 | (1) | 333 | (1) |
| 325 | (1) | 337 | (2) | 333 | (0) |
| 385 | (2) | 395 | (2) | 393 | (2) |
| 408 | (0) | 418 | (0) | 421 | (0) |
| 421 | (15) | 428 | (14) | 430 | (5) |
| 459 | (8) | 458 | (24) | 449 | (23) |
| 462 | (7) | 460 | (0) | 453 | (1) |
| 463 | (0) | 462 | (3) | 461 | (2) |
| 488 | (1) | 500 | (0) | 491 | (3) |
| 500 | (2) | 501 | (2) | 503 | (3) |
| 502 | (0) | 508 | (4) | 508 | (3) |
| 524 | (15) | 532 | (10) | 514 | (18) |
| 531 | (12) | 544 | (24) | 552 | (44) |
| 536 | (6) | 556 | (22) | 553 | (20) |
| 546 | (4) | 567 | (5) | 568 | (13) |
| 571 | (43) | 570 | (39) | 592 | (11) |
| 588 | (1) | 605 | (42) | 601 | (38) |
| 594 | (10) | 617 | (1) | 620 | (91) |
| 620 | (73) | 618 | (88) | 633 | (49) |
| 622 | (85) | 633 | (60) | 644 | (1) |
| 682 | (9) | 701 | (8) | 731 | (8) |
| 717 | (1) | 745 | (1) | 750 | (1) |
| 727 | (1) | 756 | (0) | 756 | (0) |
| 737 | (50) | 763 | (27) | 763 | (44) |
| 752 | (19) | 779 | (42) | 782 | (15) |
| 823 | (3) | 854 | (3) | 850 | (1) |
| 827 | (5) | 861 | (4) | 857 | (5) |
| 857 | (15) | 885 | (13) | 886 | (0) |
| 859 | (0) | 892 | (0) | 894 | (16) |
| 881 | (0) | 911 | (3) | 923 | (1) |
| 905 | (2) | 941 | (7) | 936 | (5) |
| 909 | (3) | 943 | (3) | 937 | (3) |
| 929 | (1) | 975 | (1) | 961 | (1) |
| 952 | (0) | 998 | (0) | 986 | (0) |
| 969 | (9) | 1005 | (9) | 1007 | (10) |
| 974 | (3) | 1010 | (2) | 1024 | (2) |
| 1001 | (5) | 1024 | (6) | 1032 | (5) |
| 1038 | (4) | 1082 | (5) | 1078 | (5) |
| 1118 | (7) | 1154 | (18) | 1154 | (7) |
| 1124 | (9) | 1155 | (7) | 1159 | (12) |
| 1146 | (1) | 1182 | (0) | 1176 | (1) |
| 1189 | (5) | 1222 | (6) | 1229 | (8) |
| 1204 | (0) | 1244 | (0) | 1241 | (0) |
| 1215 | (5) | 1256 | (4) | 1256 | (4) |
| 1275 | (3) | 1321 | (5) | 1323 | (2) |

| | | | | | |
|---|---|---|---|---|---|
| 1286 | (15) | 1329 | (5) | 1341 | (11) |
| 1296 | (11) | 1341 | (10) | 1342 | (9) |
| 1339 | (0) | 1386 | (0) | 1385 | (0) |
| 1368 | (2) | 1404 | (3) | 1420 | (3) |
| 1383 | (0) | 1422 | (0) | 1432 | (1) |
| 1411 | (24) | 1465 | (21) | 1466 | (20) |
| 1421 | (18) | 1474 | (17) | 1486 | (17) |
| 1447 | (10) | 1488 | (16) | 1498 | (10) |
| 1457 | (6) | 1503 | (7) | 1512 | (4) |
| 1519 | (4) | 1566 | (5) | 1580 | (5) |
| 1604 | (1) | 1658 | (1) | 1670 | (0) |
| 1961 | (648) | 2050 | (820) | 2044 | (850) |
| 1964 | (710) | 2054 | (755) | 2045 | (770) |
| 2016 | (937) | 2101 | (1206) | 2100 | (1081) |
| 2985 | (12) | 3058 | (13) | 3059 | (25) |
| 3071 | (6) | 3139 | (8) | 3156 | (0) |
| 3076 | (1) | 3146 | (1) | 3163 | (15) |
| 3084 | (4) | 3155 | (6) | 3163 | (4) |
| 3089 | (4) | 3160 | (5) | 3169 | (53) |
| 3097 | (18) | 3168 | (21) | 3174 | (9) |
| 3099 | (1) | 3171 | (1) | 3176 | (9) |
| 3108 | (1) | 3183 | (1) | 3184 | (6) |
| 3112 | (1) | 3188 | (0) | 3188 | (1) |
| 3125 | (13) | 3202 | (12) | 3206 | (28) |
| 3137 | (16) | 3214 | (15) | 3220 | (37) |

**Table S30.** Harmonic vibrational frequencies (in $cm^{-1}$) and infrared intensities (in parentheses, in km/mol) for the structure **2Fe-6** of $(C_{10}H_8PCH_3)Fe(CO)_3$ with $C_1$ symmetry.

| BP86 | | B3LYP | | M06-L | |
|---|---|---|---|---|---|
| 34 | (0) | 38 | (0) | 42 | (0) |
| 49 | (0) | 51 | (0) | 49 | (0) |
| 56 | (0) | 53 | (0) | 50 | (0) |
| 76 | (0) | 75 | (0) | 74 | (0) |
| 81 | (1) | 82 | (0) | 78 | (0) |
| 84 | (0) | 84 | (0) | 86 | (0) |
| 86 | (0) | 90 | (0) | 89 | (0) |
| 105 | (0) | 109 | (1) | 108 | (1) |
| 131 | (0) | 133 | (0) | 138 | (0) |
| 147 | (1) | 153 | (1) | 155 | (1) |
| 197 | (0) | 198 | (0) | 224 | (0) |
| 254 | (6) | 262 | (3) | 289 | (0) |
| 268 | (1) | 276 | (1) | 290 | (7) |
| 297 | (10) | 305 | (22) | 321 | (5) |
| 298 | (29) | 309 | (7) | 324 | (21) |
| 374 | (7) | 381 | (3) | 384 | (3) |
| 382 | (1) | 394 | (1) | 396 | (1) |
| 397 | (0) | 407 | (4) | 411 | (0) |
| 400 | (5) | 408 | (1) | 414 | (2) |
| 429 | (3) | 441 | (15) | 442 | (10) |
| 454 | (6) | 458 | (6) | 462 | 0 |
| 458 | (1) | 461 | (0) | 462 | (3) |
| 483 | (0) | 488 | (8) | 485 | (6) |
| 494 | (15) | 488 | (11) | 485 | (2) |
| 507 | (0) | 517 | (13) | 505 | (26) |
| 514 | (20) | 519 | (18) | 518 | (0) |
| 520 | (6) | 525 | (15) | 532 | (22) |
| 526 | (3) | 544 | (8) | 557 | (53) |
| 554 | (14) | 559 | (50) | 572 | (17) |
| 584 | (45) | 598 | (36) | 608 | (27) |
| 589 | (7) | 610 | (22) | 610 | (26) |
| 608 | (8) | 621 | (97) | 621 | (87) |
| 622 | (79) | 630 | (51) | 628 | (91) |
| 626 | (120) | 630 | (45) | 652 | (0) |
| 677 | (8) | 696 | (8) | 716 | (9) |
| 706 | (0) | 736 | (0) | 738 | (1) |
| 736 | (0) | 752 | (7) | 763 | (8) |
| 737 | (9) | 760 | (0) | 763 | (0) |
| 801 | (0) | 838 | (0) | 825 | (0) |
| 819 | (14) | 855 | (14) | 845 | (13) |
| 838 | (23) | 868 | (18) | 862 | (20) |
| 851 | (3) | 885 | (9) | 878 | (2) |
| 860 | (1) | 887 | (10) | 887 | (1) |
| 862 | (2) | 893 | (1) | 891 | (0) |
| 879 | (15) | 911 | (15) | 908 | (15) |
| 887 | (0) | 927 | (0) | 913 | (0) |
| 905 | (5) | 948 | (5) | 935 | (6) |
| 933 | (0) | 978 | (0) | 971 | (0) |
| 954 | (7) | 990 | (4) | 991 | (4) |
| 961 | (3) | 1005 | (2) | 1008 | (2) |
| 1019 | (1) | 1051 | (1) | 1055 | (2) |
| 1034 | (2) | 1068 | (2) | 1066 | (2) |
| 1059 | (3) | 1093 | (6) | 1093 | (4) |
| 1089 | (0) | 1123 | (0) | 1118 | (0) |
| 1124 | (13) | 1155 | (21) | 1157 | (16) |
| 1178 | (0) | 1211 | (0) | 1216 | (1) |
| 1186 | (1) | 1219 | (2) | 1223 | (2) |
| 1246 | (3) | 1291 | (3) | 1283 | (3) |
| 1276 | (3) | 1327 | (3) | 1316 | (2) |

| | | | | | |
|---|---|---|---|---|---|
| 1298 | (14) | 1340 | (10) | 1349 | (9) |
| 1310 | (5) | 1358 | (6) | 1353 | (2) |
| 1331 | (9) | 1374 | (9) | 1380 | (9) |
| 1355 | (3) | 1390 | (1) | 1406 | (1) |
| 1398 | (3) | 1442 | (7) | 1445 | (9) |
| 1405 | (17) | 1457 | (16) | 1445 | (15) |
| 1415 | (20) | 1467 | (10) | 1454 | (15) |
| 1419 | (2) | 1469 | (5) | 1472 | (1) |
| 1446 | (5) | 1489 | (10) | 1502 | (8) |
| 1576 | (6) | 1633 | (0) | 1643 | (2) |
| 1625 | (1) | 1690 | (1) | 1697 | (1) |
| 1961 | (674) | 2052 | (795) | 2045 | (788) |
| 1974 | (789) | 2061 | (946) | 2056 | (929) |
| 2021 | (990) | 2105 | (1215) | 2106 | (1087) |
| 2970 | (22) | 3045 | (20) | 3034 | (39) |
| 3059 | (6) | 3134 | (7) | 3136 | (9) |
| 3069 | (2) | 3135 | (3) | 3147 | (2) |
| 3078 | (1) | 3147 | (3) | 3153 | (6) |
| 3086 | (9) | 3157 | (11) | 3155 | (23) |
| 3105 | (10) | 3179 | (3) | 3164 | (37) |
| 3107 | (2) | 3181 | (2) | 3166 | (2) |
| 3107 | (16) | 3182 | (22) | 3172 | (40) |
| 3109 | (3) | 3184 | (3) | 3175 | (4) |
| 3134 | (3) | 3210 | (2) | 3199 | (9) |
| 3146 | (8) | 3223 | (8) | 3213 | (23) |

**Table S31**. Harmonic vibrational frequencies (in $cm^{-1}$) and infrared intensities (in parentheses, in km/mol) for the structure **2Fe-7** of $(C_{10}H_8PCH_3)Fe(CO)_3$ with $C_1$ symmetry.

| BP86 | | B3LYP | | M06-L | |
|---|---|---|---|---|---|
| 32 | (0) | 36 | (0) | 39 | (0) |
| 46 | (1) | 47 | (1) | 44 | (1) |
| 65 | (0) | 67 | (0) | 68 | (0) |
| 77 | (0) | 80 | (0) | 81 | (1) |
| 80 | (1) | 83 | (1) | 82 | (0) |
| 85 | (0) | 89 | (0) | 86 | (0) |
| 96 | (0) | 100 | (0) | 104 | (2) |
| 102 | (1) | 106 | (1) | 126 | (0) |
| 128 | (1) | 132 | (0) | 134 | (1) |
| 147 | (0) | 153 | (0) | 149 | (0) |
| 153 | (0) | 158 | (0) | 179 | (0) |
| 218 | (6) | 226 | (3) | 232 | (4) |
| 264 | (3) | 274 | (2) | 287 | (0) |
| 280 | (2) | 290 | (3) | 297 | (4) |
| 287 | (32) | 298 | (21) | 311 | (21) |
| 358 | (2) | 369 | (1) | 377 | (1) |
| 375 | (2) | 386 | (3) | 385 | (3) |
| 391 | (8) | 394 | (3) | 396 | (2) |
| 395 | (0) | 406 | (0) | 404 | (0) |
| 426 | (3) | 438 | (16) | 436 | (13) |
| 452 | (4) | 458 | (5) | 452 | (0) |
| 455 | (0) | 460 | (0) | 456 | (2) |
| 482 | (1) | 486 | (0) | 477 | (2) |
| 495 | (13) | 489 | (17) | 483 | (10) |
| 507 | (0) | 517 | (0) | 499 | (22) |
| 516 | (17) | 519 | (19) | 515 | (2) |
| 519 | (8) | 525 | (21) | 533 | (27) |
| 554 | (12) | 561 | (55) | 554 | (56) |
| 558 | (23) | 574 | (22) | 594 | (16) |
| 587 | (12) | 608 | (35) | 611 | (97) |
| 596 | (49) | 608 | (30) | 620 | (40) |
| 620 | (90) | 621 | (95) | 621 | (25) |
| 623 | (112) | 629 | (95) | 626 | (88) |
| 625 | (1) | 651 | (3) | 678 | (3) |
| 663 | (19) | 683 | (17) | 714 | (21) |
| 704 | (0) | 734 | (0) | 739 | (1) |
| 735 | (11) | 750 | (8) | 765 | (0) |
| 736 | (0) | 760 | (1) | 765 | (9) |
| 796 | (0) | 833 | (0) | 826 | (0) |
| 816 | (18) | 853 | (14) | 846 | (16) |
| 837 | (27) | 867 | (16) | 868 | (21) |
| 848 | (1) | 876 | (21) | 883 | (1) |
| 858 | (3) | 893 | (0) | 885 | (0) |
| 861 | (5) | 895 | (3) | 895 | (3) |
| 864 | (2) | 896 | (5) | 896 | (3) |
| 888 | (1) | 927 | (0) | 917 | (0) |
| 906 | (6) | 948 | (6) | 936 | (7) |
| 934 | (3) | 977 | (3) | 975 | (1) |
| 940 | (5) | 978 | (5) | 976 | (6) |
| 949 | (7) | 997 | (6) | 995 | (6) |
| 1020 | (1) | 1050 | (1) | 1054 | (3) |
| 1035 | (2) | 1067 | (2) | 1069 | (3) |
| 1057 | (2) | 1089 | (4) | 1094 | (2) |
| 1092 | (0) | 1125 | (0) | 1119 | (0) |
| 1116 | (18) | 1147 | (24) | 1156 | (21) |
| 1179 | (1) | 1210 | (1) | 1221 | (1) |
| 1185 | (1) | 1218 | (1) | 1228 | (1) |
| 1246 | (2) | 1290 | (2) | 1287 | (2) |
| 1277 | (6) | 1328 | (5) | 1318 | (5) |

| | | | | | |
|---|---|---|---|---|---|
| 1294 | (3) | 1339 | (1) | 1351 | (1) |
| 1309 | (7) | 1354 | (7) | 1357 | (3) |
| 1321 | (2) | 1366 | (1) | 1375 | (4) |
| 1356 | (3) | 1389 | (1) | 1415 | (0) |
| 1394 | (1) | 1438 | (4) | 1448 | (2) |
| 1412 | (5) | 1462 | (6) | 1451 | (4) |
| 1420 | (2) | 1469 | (1) | 1466 | (9) |
| 1422 | (11) | 1471 | (10) | 1475 | (0) |
| 1447 | (5) | 1489 | (11) | 1497 | (9) |
| 1589 | (6) | 1647 | (0) | 1668 | (1) |
| 1634 | (0) | 1699 | (1) | 1716 | (1) |
| 1959 | (673) | 2051 | (796) | 2037 | (806) |
| 1972 | (792) | 2059 | (956) | 2052 | (1009) |
| 2019 | (1016) | 2103 | (1240) | 2100 | (1101) |
| 2969 | (28) | 3040 | (27) | 3038 | (60) |
| 3060 | (9) | 3126 | (10) | 3148 | (18) |
| 3065 | (9) | 3132 | (10) | 3150 | (17) |
| 3076 | (1) | 3149 | (2) | 3154 | (3) |
| 3083 | (19) | 3157 | (21) | 3161 | (35) |
| 3106 | (9) | 3180 | (0) | 3191 | (77) |
| 3108 | (0) | 3182 | (0) | 3193 | (0) |
| 3108 | (18) | 3183 | (26) | 3193 | (3) |
| 3110 | (2) | 3185 | (3) | 3194 | (1) |
| 3135 | (3) | 3211 | (2) | 3219 | (12) |
| 3147 | (9) | 3224 | (8) | 3233 | (28) |

**Table S32**. Harmonic vibrational frequencies (in $cm^{-1}$) and infrared intensities (in parentheses, in km/mol) for the structure **2Fe-8** of $(C_{10}H_8PCH_3)Fe(CO)_3$ with $C_1$ symmetry.

| BP86 | | B3LYP | | M06-L | |
|---|---|---|---|---|---|
| 34 | (0) | 36 | (0) | 42 | (0) |
| 68 | (0) | 69 | (0) | 69 | (0) |
| 77 | (0) | 81 | (0) | 80 | (0) |
| 80 | (0) | 81 | (0) | 81 | (0) |
| 83 | (1) | 86 | (0) | 92 | (0) |
| 94 | (0) | 94 | (1) | 97 | (0) |
| 97 | (1) | 100 | (0) | 103 | (0) |
| 119 | (0) | 121 | (0) | 126 | (1) |
| 131 | (2) | 135 | (1) | 134 | (1) |
| 151 | (3) | 157 | (2) | 157 | (2) |
| 159 | (0) | 169 | (0) | 191 | (0) |
| 199 | (4) | 208 | (2) | 213 | (3) |
| 216 | (0) | 224 | (0) | 226 | (0) |
| 242 | (2) | 249 | (2) | 250 | (2) |
| 273 | (1) | 282 | (0) | 282 | (0) |
| 295 | (1) | 302 | (2) | 303 | (1) |
| 368 | (15) | 376 | (12) | 375 | (9) |
| 390 | (1) | 397 | (4) | 397 | (4) |
| 406 | (2) | 417 | (2) | 417 | (3) |
| 408 | (3) | 427 | (5) | 425 | (5) |
| 433 | (5) | 436 | (8) | 434 | (4) |
| 443 | (1) | 454 | (2) | 452 | (4) |
| 462 | (4) | 461 | (1) | 456 | (3) |
| 481 | (7) | 480 | (7) | 467 | (7) |
| 495 | (3) | 491 | (10) | 482 | (10) |
| 506 | (1) | 498 | (4) | 485 | (4) |
| 512 | (2) | 521 | (9) | 514 | (2) |
| 529 | (1) | 548 | (1) | 544 | (18) |
| 555 | (4) | 556 | (42) | 553 | (35) |
| 571 | (53) | 577 | (32) | 582 | (21) |
| 591 | (65) | 593 | (71) | 589 | (71) |
| 611 | (47) | 615 | (73) | 614 | (75) |
| 623 | (29) | 638 | (12) | 649 | (3) |
| 640 | (11) | 663 | (7) | 666 | (8) |
| 654 | (5) | 676 | (8) | 684 | (7) |
| 668 | (16) | 694 | (12) | 696 | (13) |
| 689 | (20) | 706 | (21) | 722 | (24) |
| 696 | (12) | 713 | (6) | 734 | (6) |
| 721 | (6) | 752 | (6) | 753 | (8) |
| 741 | (87) | 768 | (54) | 767 | (74) |
| 752 | (16) | 777 | (56) | 779 | (13) |
| 813 | (0) | 850 | (0) | 841 | (0) |
| 837 | (1) | 865 | (1) | 869 | (1) |
| 866 | (5) | 896 | (3) | 876 | (2) |
| 879 | (8) | 913 | (10) | 909 | (7) |
| 897 | (5) | 927 | (9) | 921 | (6) |
| 912 | (3) | 965 | (1) | 958 | (1) |
| 926 | (6) | 973 | (5) | 960 | (4) |
| 935 | (4) | 982 | (3) | 976 | (5) |
| 945 | (0) | 992 | (1) | 978 | (1) |
| 1014 | (7) | 1038 | (7) | 1049 | (7) |
| 1087 | (2) | 1123 | (2) | 1129 | (3) |
| 1122 | (2) | 1151 | (2) | 1165 | (4) |
| 1136 | (1) | 1171 | (2) | 1173 | (1) |
| 1146 | (0) | 1185 | (1) | 1180 | (0) |
| 1180 | (0) | 1216 | (1) | 1219 | (1) |
| 1197 | (1) | 1238 | (2) | 1239 | (2) |
| 1244 | (11) | 1287 | (10) | 1284 | (11) |
| 1278 | (12) | 1331 | (12) | 1314 | (9) |

| | | | | | |
|---|---|---|---|---|---|
| 1300 | (3) | 1350 | (4) | 1347 | (3) |
| 1347 | (2) | 1389 | (3) | 1396 | (2) |
| 1364 | (2) | 1410 | (1) | 1413 | (2) |
| 1370 | (1) | 1420 | (0) | 1423 | (2) |
| 1414 | (11) | 1463 | (10) | 1452 | (8) |
| 1420 | (6) | 1469 | (6) | 1458 | (8) |
| 1433 | (11) | 1481 | (16) | 1486 | (9) |
| 1450 | (7) | 1491 | (14) | 1504 | (7) |
| 1514 | (2) | 1559 | (4) | 1576 | (3) |
| 1586 | (1) | 1647 | (2) | 1657 | (3) |
| 1609 | (3) | 1662 | (5) | 1678 | (3) |
| 1957 | (572) | 2048 | (791) | 2040 | (810) |
| 1964 | (656) | 2054 | (684) | 2041 | (640) |
| 2013 | (833) | 2097 | (1055) | 2094 | (981) |
| 2981 | (22) | 3050 | (22) | 3056 | (43) |
| 3048 | (4) | 3115 | (6) | 3112 | (12) |
| 3063 | (7) | 3136 | (8) | 3137 | (16) |
| 3073 | (5) | 3142 | (3) | 3167 | (9) |
| 3086 | (5) | 3150 | (7) | 3174 | (11) |
| 3097 | (11) | 3170 | (12) | 3176 | (28) |
| 3099 | (5) | 3179 | (5) | 3180 | (23) |
| 3105 | (5) | 3184 | (6) | 3182 | (10) |
| 3110 | (1) | 3189 | (1) | 3193 | (5) |
| 3127 | (14) | 3204 | (15) | 3215 | (26) |
| 3140 | (16) | 3217 | (15) | 3230 | (38) |

**Table S33**. Harmonic vibrational frequencies (in $cm^{-1}$) and infrared intensities (in parentheses, in km/mol) for the structure **2Fe-9** of $(C_{10}H_8PCH_3)Fe(CO)_3$ with $C_1$ symmetry.

| BP86 | | B3LYP | | M06-L | |
|---|---|---|---|---|---|
| 34 | (0) | 37 | (0) | 40 | (0) |
| 56 | (2) | 51 | (1) | 43 | (2) |
| 75 | (0) | 76 | (0) | 73 | (0) |
| 77 | (0) | 81 | (0) | 76 | (0) |
| 82 | (0) | 85 | (0) | 83 | (0) |
| 91 | (0) | 93 | (0) | 91 | (0) |
| 99 | (1) | 101 | (0) | 98 | (0) |
| 111 | (1) | 112 | (1) | 117 | (2) |
| 139 | (2) | 144 | (1) | 140 | (1) |
| 156 | (0) | 161 | (0) | 160 | (0) |
| 176 | (1) | 181 | (0) | 181 | (0) |
| 192 | (1) | 200 | (1) | 197 | (1) |
| 199 | (0) | 202 | (0) | 233 | (0) |
| 241 | (2) | 243 | (1) | 245 | (2) |
| 283 | (1) | 299 | (1) | 291 | (1) |
| 292 | (2) | 304 | (2) | 300 | (1) |
| 367 | (6) | 373 | (6) | 370 | (5) |
| 391 | (2) | 401 | (2) | 397 | (2) |
| 397 | (2) | 407 | (5) | 405 | (4) |
| 414 | (7) | 428 | (14) | 427 | (15) |
| 435 | (6) | 438 | (6) | 433 | (3) |
| 442 | (1) | 452 | (3) | 446 | (3) |
| 464 | (3) | 463 | (2) | 458 | (2) |
| 470 | (5) | 479 | (10) | 467 | (16) |
| 488 | (3) | 481 | (8) | 475 | (4) |
| 505 | (1) | 494 | (1) | 480 | (4) |
| 512 | (6) | 512 | (14) | 499 | (5) |
| 522 | (1) | 542 | (0) | 538 | (8) |
| 555 | (4) | 555 | (46) | 549 | (49) |
| 573 | (62) | 577 | (43) | 582 | (36) |
| 597 | (61) | 597 | (65) | 594 | (62) |
| 614 | (10) | 621 | (64) | 621 | (59) |
| 620 | (56) | 637 | (5) | 643 | (7) |
| 643 | (8) | 668 | (5) | 666 | (9) |
| 649 | (10) | 671 | (9) | 676 | (5) |
| 666 | (17) | 685 | (20) | 700 | (7) |
| 680 | (10) | 703 | (11) | 709 | (21) |
| 694 | (13) | 716 | (3) | 722 | (11) |
| 720 | (21) | 750 | (29) | 747 | (17) |
| 736 | (71) | 765 | (61) | 755 | (64) |
| 769 | (25) | 795 | (36) | 793 | (20) |
| 811 | (1) | 847 | (0) | 835 | (0) |
| 845 | (3) | 875 | (2) | 875 | (3) |
| 862 | (12) | 893 | (14) | 887 | (7) |
| 874 | (10) | 905 | (14) | 897 | (12) |
| 888 | (16) | 918 | (17) | 912 | (14) |
| 922 | (5) | 971 | (8) | 955 | (4) |
| 924 | (7) | 976 | (2) | 962 | (2) |
| 931 | (2) | 980 | (2) | 968 | (6) |
| 945 | (1) | 991 | (1) | 974 | (1) |
| 1011 | (8) | 1036 | (7) | 1046 | (7) |
| 1087 | (2) | 1122 | (2) | 1127 | (3) |
| 1123 | (5) | 1152 | (4) | 1166 | (8) |
| 1141 | (4) | 1176 | (8) | 1174 | (2) |
| 1145 | (1) | 1185 | (1) | 1180 | (3) |
| 1184 | (1) | 1222 | (1) | 1224 | (1) |
| 1195 | (1) | 1237 | (2) | 1235 | (2) |
| 1247 | (10) | 1292 | (9) | 1286 | (9) |

| | | | | | |
|---|---|---|---|---|---|
| 1272 | (3) | 1322 | (4) | 1305 | (3) |
| 1317 | (4) | 1365 | (10) | 1362 | (7) |
| 1351 | (2) | 1397 | (4) | 1397 | (2) |
| 1366 | (3) | 1412 | (4) | 1415 | (4) |
| 1372 | (0) | 1421 | (1) | 1427 | (2) |
| 1415 | (12) | 1463 | (10) | 1454 | (11) |
| 1418 | (6) | 1466 | (5) | 1457 | (4) |
| 1433 | (16) | 1483 | (23) | 1486 | (16) |
| 1455 | (10) | 1494 | (22) | 1509 | (14) |
| 1515 | (1) | 1560 | (2) | 1578 | (2) |
| 1595 | (1) | 1657 | (2) | 1676 | (2) |
| 1607 | (4) | 1662 | (7) | 1678 | (6) |
| 1958 | (537) | 2050 | (722) | 2041 | (606) |
| 1971 | (707) | 2059 | (785) | 2051 | (884) |
| 2017 | (843) | 2101 | (1064) | 2099 | (980) |
| 2975 | (28) | 3043 | (26) | 3048 | (54) |
| 3035 | (4) | 3108 | (5) | 3121 | (11) |
| 3052 | (8) | 3132 | (9) | 3136 | (18) |
| 3069 | (6) | 3134 | (4) | 3163 | (17) |
| 3079 | (9) | 3142 | (11) | 3166 | (12) |
| 3086 | (18) | 3162 | (16) | 3168 | (33) |
| 3087 | (5) | 3170 | (7) | 3175 | (25) |
| 3105 | (4) | 3183 | (4) | 3182 | (17) |
| 3109 | (1) | 3187 | (0) | 3185 | (1) |
| 3127 | (13) | 3204 | (14) | 3213 | (25) |
| 3140 | (16) | 3217 | (14) | 3228 | (38) |

**Table S34.** Harmonic vibrational frequencies (in $cm^{-1}$) and infrared intensities (in parentheses, in km/mol) for the structure **2Fe-10** of $(C_{10}H_8PCH_3)Fe(CO)_3$ with $C_1$ symmetry.

| BP86 | | B3LYP | | M06-L | |
|---|---|---|---|---|---|
| 37 | (0) | 42 | (0) | 41 | (0) |
| 61 | (0) | 64 | (0) | 59 | (0) |
| 72 | (0) | 74 | (0) | 71 | (0) |
| 74 | (1) | 77 | (1) | 75 | (1) |
| 79 | (0) | 81 | (0) | 81 | (0) |
| 85 | (0) | 92 | (0) | 92 | (0) |
| 91 | (0) | 96 | (0) | 94 | (0) |
| 95 | (0) | 102 | (0) | 125 | (0) |
| 132 | (0) | 139 | (0) | 137 | (0) |
| 151 | (1) | 157 | (1) | 158 | (1) |
| 165 | (0) | 171 | (0) | 172 | (0) |
| 237 | (0) | 245 | (2) | 259 | (1) |
| 258 | (0) | 267 | (1) | 271 | (1) |
| 262 | (0) | 268 | (1) | 275 | (0) |
| 281 | (2) | 292 | (2) | 293 | (2) |
| 329 | (0) | 340 | (0) | 344 | (0) |
| 397 | (0) | 406 | (0) | 402 | (0) |
| 398 | (5) | 414 | (2) | 413 | (2) |
| 426 | (0) | 432 | (1) | 428 | (2) |
| 458 | (21) | 459 | (5) | 453 | (7) |
| 468 | (3) | 471 | (0) | 467 | (3) |
| 468 | (0) | 471 | (3) | 468 | (0) |
| 491 | (4) | 481 | (31) | 494 | (11) |
| 504 | (0) | 500 | (9) | 498 | (25) |
| 510 | (7) | 523 | (2) | 529 | (0) |
| 511 | (5) | 529 | (9) | 531 | (9) |
| 534 | (9) | 542 | (7) | 561 | (17) |
| 558 | (11) | 575 | (44) | 569 | (37) |
| 564 | (3) | 576 | (17) | 587 | (12) |
| 573 | (35) | 587 | (0) | 588 | (1) |
| 597 | (1) | 611 | (82) | 609 | (75) |
| 614 | (80) | 615 | (26) | 616 | (16) |
| 628 | (8) | 636 | (98) | 641 | (110) |
| 632 | (114) | 649 | (3) | 675 | (3) |
| 662 | (12) | 682 | (15) | 714 | (19) |
| 697 | (7) | 723 | (5) | 722 | (6) |
| 722 | (4) | 747 | (4) | 763 | (0) |
| 735 | (47) | 765 | (53) | 767 | (44) |
| 762 | (0) | 793 | (0) | 790 | (0) |
| 780 | (2) | 807 | (2) | 816 | (1) |
| 837 | (0) | 868 | (0) | 867 | (0) |
| 852 | (1) | 885 | (1) | 879 | (0) |
| 865 | (3) | 901 | (5) | 889 | (1) |
| 875 | (2) | 910 | (1) | 902 | (0) |
| 891 | (16) | 933 | (21) | 918 | (26) |
| 911 | (4) | 954 | (6) | 944 | (2) |
| 914 | (1) | 960 | (2) | 948 | (3) |
| 942 | (0) | 985 | (4) | 974 | (3) |
| 947 | (4) | 986 | (0) | 982 | (0) |
| 964 | (12) | 1006 | (10) | 996 | (11) |
| 1012 | (5) | 1039 | (4) | 1045 | (5) |
| 1031 | (2) | 1066 | (10) | 1065 | (1) |
| 1037 | (6) | 1067 | (3) | 1072 | (7) |
| 1091 | (4) | 1123 | (4) | 1127 | (3) |
| 1141 | (0) | 1174 | (0) | 1173 | (0) |
| 1164 | (5) | 1201 | (4) | 1206 | (4) |
| 1187 | (0) | 1224 | (0) | 1225 | (1) |
| 1195 | (2) | 1238 | (6) | 1243 | (5) |
| 1218 | (2) | 1257 | (2) | 1258 | (3) |

| | | | | | |
|---|---|---|---|---|---|
| 1243 | (2) | 1293 | (1) | 1293 | (1) |
| 1280 | (7) | 1322 | (2) | 1321 | (9) |
| 1295 | (5) | 1339 | (8) | 1341 | (1) |
| 1310 | (0) | 1355 | (0) | 1358 | (0) |
| 1373 | (5) | 1386 | (6) | 1411 | (6) |
| 1413 | (6) | 1463 | (5) | 1453 | (4) |
| 1420 | (11) | 1469 | (11) | 1463 | (10) |
| 1436 | (4) | 1484 | (5) | 1491 | (2) |
| 1458 | (13) | 1505 | (19) | 1509 | (9) |
| 1575 | (0) | 1625 | (1) | 1630 | (1) |
| 1591 | (0) | 1644 | (0) | 1655 | (0) |
| 1954 | (696) | 2049 | (818) | 2036 | (835) |
| 1966 | (812) | 2056 | (895) | 2049 | (973) |
| 2020 | (861) | 2105 | (1149) | 2105 | (1008) |
| 2971 | (15) | 3042 | (15) | 3049 | (37) |
| 3065 | (5) | 3130 | (7) | 3159 | (15) |
| 3068 | (7) | 3134 | (8) | 3169 | (26) |
| 3097 | (8) | 3164 | (12) | 3169 | (19) |
| 3099 | (1) | 3166 | (0) | 3170 | (1) |
| 3102 | (5) | 3177 | (4) | 3177 | (19) |
| 3107 | (1) | 3183 | (1) | 3181 | (0) |
| 3119 | (19) | 3194 | (20) | 3199 | (38) |
| 3124 | (1) | 3199 | (1) | 3202 | (5) |
| 3127 | (2) | 3202 | (2) | 3206 | (5) |
| 3134 | (28) | 3209 | (27) | 3215 | (61) |

**Table S35**. Harmonic vibrational frequencies (in $cm^{-1}$) and infrared intensities (in parentheses, in km/mol) for the structure **2Fe-11** of $(C_{10}H_8PCH_3)Fe(CO)_3$ with $C_1$ symmetry.

| BP86 | | B3LYP | | M06-L | |
|---|---|---|---|---|---|
| 36 | (0) | 38 | (0) | 36 | (0) |
| 38 | (0) | 38 | (0) | 43 | (0) |
| 62 | (0) | 64 | (0) | 66 | (0) |
| 75 | (0) | 76 | (0) | 76 | (0) |
| 77 | (0) | 79 | (0) | 77 | (0) |
| 82 | (0) | 84 | (0) | 82 | (0) |
| 95 | (0) | 98 | (0) | 95 | (0) |
| 129 | (1) | 134 | (0) | 128 | (0) |
| 137 | (1) | 139 | (0) | 141 | (0) |
| 165 | (1) | 172 | (1) | 176 | (1) |
| 176 | 0 | 182 | (0) | 198 | (2) |
| 186 | (4) | 189 | (3) | 206 | (0) |
| 240 | (0) | 247 | (0) | 248 | (1) |
| 252 | (1) | 264 | (2) | 265 | (1) |
| 300 | (2) | 298 | (3) | 317 | (1) |
| 304 | (3) | 298 | (5) | 319 | (2) |
| 351 | (13) | 355 | (20) | 358 | (15) |
| 385 | (0) | 400 | (1) | 392 | (1) |
| 397 | (1) | 402 | (0) | 401 | (0) |
| 409 | (3) | 411 | (8) | 414 | (4) |
| 445 | (0) | 453 | (0) | 449 | (0) |
| 457 | (6) | 457 | (0) | 453 | (1) |
| 471 | (1) | 469 | (0) | 465 | (28) |
| 479 | (39) | 470 | (40) | 467 | (1) |
| 491 | (0) | 490 | (0) | 490 | (1) |
| 504 | (20) | 517 | (41) | 501 | (34) |
| 519 | (9) | 528 | (9) | 529 | (13) |
| 526 | (3) | 536 | (21) | 536 | (30) |
| 536 | (12) | 544 | (0) | 540 | (18) |
| 567 | (54) | 555 | (71) | 552 | (51) |
| 596 | (8) | 613 | (9) | 621 | (28) |
| 611 | (8) | 621 | (79) | 622 | (71) |
| 623 | (78) | 628 | (68) | 632 | (60) |
| 631 | (60) | 640 | (7) | 644 | (7) |
| 649 | (5) | 665 | (3) | 685 | (4) |
| 671 | (83) | 691 | (57) | 699 | (66) |
| 680 | (33) | 704 | (31) | 724 | (32) |
| 703 | (4) | 725 | (2) | 739 | (2) |
| 708 | (22) | 732 | (36) | 752 | (26) |
| 753 | (2) | 789 | (2) | 784 | (2) |
| 783 | (9) | 807 | (11) | 817 | (6) |
| 819 | (4) | 848 | (2) | 843 | (2) |
| 841 | (16) | 868 | (20) | 865 | (17) |
| 877 | (3) | 914 | (2) | 905 | (0) |
| 883 | (1) | 925 | (21) | 922 | (16) |
| 892 | (3) | 930 | (4) | 922 | (3) |
| 894 | (17) | 938 | (1) | 925 | (1) |
| 905 | (1) | 951 | (3) | 935 | (3) |
| 911 | (3) | 958 | (0) | 951 | (0) |
| 942 | (0) | 986 | (0) | 973 | (0) |
| 1022 | (2) | 1059 | (2) | 1056 | (2) |
| 1034 | (2) | 1064 | (4) | 1068 | (4) |
| 1081 | (0) | 1113 | (1) | 1112 | (1) |
| 1100 | (1) | 1139 | (2) | 1136 | (1) |
| 1128 | (0) | 1164 | (1) | 1162 | (0) |
| 1156 | (1) | 1196 | (1) | 1196 | (2) |
| 1164 | (0) | 1204 | (0) | 1205 | (0) |
| 1211 | (10) | 1250 | (9) | 1252 | (9) |
| 1284 | (8) | 1335 | (8) | 1321 | (5) |

| | | | | | |
|---|---|---|---|---|---|
| 1295 | (0) | 1352 | (0) | 1339 | (0) |
| 1320 | (2) | 1366 | (13) | 1370 | (4) |
| 1330 | (3) | 1383 | (2) | 1383 | (6) |
| 1335 | (10) | 1387 | (8) | 1387 | (9) |
| 1418 | (1) | 1468 | (10) | 1461 | (12) |
| 1421 | (8) | 1469 | (7) | 1462 | (6) |
| 1421 | (11) | 1474 | (0) | 1478 | (0) |
| 1436 | (3) | 1484 | (7) | 1484 | (5) |
| 1525 | (12) | 1582 | (14) | 1596 | (16) |
| 1563 | (5) | 1628 | (6) | 1638 | (3) |
| 1563 | (0) | 1628 | (1) | 1648 | (10) |
| 1960 | (697) | 2049 | (822) | 2035 | (831) |
| 1973 | (844) | 2055 | (1005) | 2048 | (1058) |
| 2021 | (851) | 2102 | (1067) | 2099 | (930) |
| 2976 | (25) | 3046 | (23) | 3047 | (51) |
| 3054 | (7) | 3131 | (9) | 3125 | (23) |
| 3054 | (0) | 3132 | (1) | 3126 | (3) |
| 3070 | (10) | 3137 | (4) | 3154 | (18) |
| 3072 | (3) | 3137 | (11) | 3164 | (13) |
| 3086 | (19) | 3164 | (19) | 3165 | (19) |
| 3087 | (8) | 3164 | (7) | 3167 | (37) |
| 3107 | (11) | 3182 | (12) | 3171 | (29) |
| 3108 | (1) | 3184 | (0) | 3172 | (1) |
| 3136 | (2) | 3213 | (2) | 3214 | (8) |
| 3149 | (7) | 3227 | (7) | 3229 | (23) |

**Table S36.** Harmonic vibrational frequencies (in $cm^{-1}$) and infrared intensities (in parentheses, in km/mol) for the structure **2Fe-12** of $(C_{10}H_8PCH_3)Fe(CO)_3$ with $C_s$ symmetry.

| BP86 | | B3LYP | | M06-L | |
|---|---|---|---|---|---|
| 36 | (0) | 42 | (0) | 43 | (0) |
| 64 | (0) | 67 | (0) | 54 | (0) |
| 71 | (0) | 74 | (0) | 72 | (0) |
| 77 | (0) | 79 | (0) | 78 | (0) |
| 84 | (0) | 88 | (0) | 83 | (0) |
| 87 | (0) | 91 | (0) | 87 | (0) |
| 94 | (0) | 99 | (0) | 97 | (0) |
| 99 | (0) | 103 | (0) | 102 | (0) |
| 141 | (0) | 152 | (0) | 159 | (0) |
| 155 | (0) | 163 | (0) | 189 | (0) |
| 177 | (1) | 182 | (1) | 253 | (0) |
| 221 | (1) | 226 | (0) | 279 | (1) |
| 271 | (0) | 279 | (1) | 309 | (0) |
| 283 | (1) | 293 | (4) | 309 | (1) |
| 296 | (1) | 307 | (1) | 320 | (2) |
| 350 | (0) | 363 | (0) | 369 | (0) |
| 399 | (1) | 407 | (1) | 403 | (1) |
| 405 | (5) | 419 | (4) | 423 | (2) |
| 422 | (0) | 431 | (0) | 429 | (0) |
| 461 | (6) | 455 | (5) | 448 | (5) |
| 462 | (0) | 464 | (0) | 461 | (0) |
| 469 | (12) | 467 | (4) | 462 | (6) |
| 489 | (11) | 483 | (31) | 488 | (11) |
| 495 | (4) | 493 | (9) | 498 | (27) |
| 500 | (0) | 517 | (2) | 519 | (3) |
| 508 | (3) | 521 | (1) | 525 | (3) |
| 526 | (5) | 536 | (4) | 552 | (17) |
| 544 | (9) | 559 | (15) | 562 | (41) |
| 557 | (6) | 568 | (43) | 575 | (3) |
| 567 | (23) | 581 | (2) | 586 | (1) |
| 593 | (17) | 608 | (79) | 608 | (69) |
| 598 | (4) | 614 | (57) | 615 | (44) |
| 613 | (85) | 615 | (6) | 632 | (80) |
| 623 | (92) | 631 | (60) | 640 | (4) |
| 651 | (4) | 667 | (2) | 702 | (2) |
| 697 | (6) | 720 | (4) | 723 | (4) |
| 723 | (5) | 744 | (8) | 759 | (3) |
| 736 | (57) | 766 | (62) | 770 | (51) |
| 757 | (0) | 790 | (0) | 790 | (0) |
| 783 | (3) | 808 | (4) | 821 | (5) |
| 825 | (4) | 856 | (3) | 856 | (3) |
| 836 | (0) | 871 | (1) | 864 | (1) |
| 865 | (0) | 900 | (0) | 892 | (0) |
| 873 | (13) | 913 | (15) | 909 | (12) |
| 893 | (7) | 931 | (11) | 932 | (9) |
| 910 | (3) | 952 | (3) | 939 | (2) |
| 912 | (0) | 955 | (0) | 940 | (0) |
| 940 | (0) | 985 | (0) | 979 | (0) |
| 964 | (7) | 995 | (8) | 996 | (8) |
| 975 | (3) | 1007 | (2) | 1017 | (4) |
| 1013 | (4) | 1041 | (3) | 1046 | (4) |
| 1050 | (6) | 1087 | (14) | 1082 | (6) |
| 1053 | (8) | 1092 | (5) | 1092 | (12) |
| 1092 | (9) | 1125 | (10) | 1132 | (8) |
| 1141 | (0) | 1173 | (0) | 1174 | (0) |
| 1173 | (5) | 1209 | (4) | 1217 | (4) |
| 1190 | (0) | 1227 | (0) | 1230 | (1) |
| 1203 | (1) | 1246 | (3) | 1248 | (1) |
| 1218 | (0) | 1256 | (0) | 1260 | (1) |

| | | | | | |
|---|---|---|---|---|---|
| 1250 | (4) | 1298 | (3) | 1296 | (3) |
| 1281 | (5) | 1333 | (0) | 1326 | (3) |
| 1303 | (0) | 1336 | (6) | 1355 | (1) |
| 1316 | (0) | 1361 | (0) | 1369 | (0) |
| 1373 | (4) | 1387 | (3) | 1418 | (5) |
| 1407 | (28) | 1461 | (24) | 1468 | (26) |
| 1407 | (19) | 1463 | (17) | 1475 | (18) |
| 1437 | (5) | 1485 | (6) | 1498 | (3) |
| 1457 | (14) | 1504 | (20) | 1511 | (10) |
| 1573 | (0) | 1623 | (0) | 1633 | (0) |
| 1587 | (0) | 1640 | (0) | 1656 | (0) |
| 1955 | (689) | 2051 | (811) | 2043 | (828) |
| 1966 | (800) | 2056 | (885) | 2049 | (921) |
| 2019 | (914) | 2105 | (1224) | 2105 | (1133) |
| 2983 | (9) | 3057 | (11) | 3058 | (22) |
| 3074 | (2) | 3146 | (3) | 3160 | (5) |
| 3097 | (6) | 3164 | (10) | 3169 | (35) |
| 3098 | (1) | 3166 | (1) | 3170 | (2) |
| 3100 | (8) | 3175 | (6) | 3176 | (22) |
| 3104 | (1) | 3180 | (1) | 3179 | (0) |
| 3108 | (2) | 3183 | (3) | 3193 | (4) |
| 3119 | (16) | 3191 | (1) | 3197 | (6) |
| 3121 | (2) | 3194 | (18) | 3201 | (4) |
| 3124 | (2) | 3194 | (3) | 3203 | (31) |
| 3134 | (25) | 3209 | (25) | 3220 | (58) |

**Table S37**. Harmonic vibrational frequencies (in $cm^{-1}$) and infrared intensities (in parentheses, in km/mol) for the structure **2Fe-13** of $(C_{10}H_8PCH_3)Fe(CO)_3$ with $C_s$ symmetry.

| BP86 | | B3LYP | | M06-L | |
|---|---|---|---|---|---|
| 38 | (0) | 40 | (0) | 40 | (0) |
| 47 | (0) | 45 | (0) | 41 | (0) |
| 58 | (0) | 60 | (0) | 56 | (0) |
| 77 | (0) | 78 | (0) | 73 | (0) |
| 78 | (1) | 79 | (0) | 74 | (1) |
| 83 | (0) | 85 | (0) | 85 | (0) |
| 99 | (0) | 101 | (0) | 101 | (0) |
| 124 | (0) | 129 | (0) | 120 | 0 |
| 142 | (0) | 143 | (0) | 145 | (0) |
| 190 | (0) | 195 | (0) | 162 | (0) |
| 199 | (1) | 206 | (0) | 209 | (0) |
| 214 | (7) | 222 | (4) | 229 | (4) |
| 230 | (0) | 238 | (1) | 241 | (1) |
| 234 | (0) | 240 | (0) | 244 | (0) |
| 314 | (3) | 308 | (3) | 327 | (3) |
| 326 | (6) | 322 | (9) | 338 | (3) |
| 368 | (0) | 379 | (6) | 376 | (3) |
| 368 | (2) | 387 | (0) | 383 | (0) |
| 399 | (0) | 402 | (0) | 398 | (1) |
| 410 | (3) | 411 | (6) | 414 | (2) |
| 448 | (0) | 454 | (0) | 450 | (0) |
| 458 | (5) | 457 | (0) | 454 | (1) |
| 474 | (0) | 471 | (1) | 465 | (31) |
| 481 | (32) | 471 | (37) | 469 | (3) |
| 493 | (0) | 493 | (0) | 494 | (1) |
| 500 | (11) | 514 | (31) | 501 | (34) |
| 518 | (9) | 526 | (3) | 522 | (10) |
| 536 | (10) | 533 | (24) | 538 | (21) |
| 542 | (0) | 555 | (42) | 549 | (48) |
| 569 | (53) | 562 | (25) | 564 | (15) |
| 610 | (42) | 618 | (82) | 624 | (100) |
| 627 | (65) | 625 | (41) | 628 | (35) |
| 632 | (71) | 635 | (59) | 646 | (54) |
| 648 | (32) | 666 | (3) | 677 | (6) |
| 649 | (8) | 671 | (32) | 686 | (3) |
| 652 | (0) | 675 | (5) | 689 | (23) |
| 680 | (19) | 697 | (18) | 708 | (9) |
| 698 | (5) | 722 | (3) | 732 | (2) |
| 724 | (59) | 752 | (58) | 755 | (55) |
| 770 | (4) | 805 | (4) | 798 | (3) |
| 793 | (1) | 817 | (3) | 824 | (0) |
| 828 | (2) | 858 | (1) | 854 | (1) |
| 844 | (18) | 872 | (21) | 870 | (18) |
| 869 | (4) | 902 | (5) | 891 | (3) |
| 892 | (47) | 922 | (46) | 908 | (44) |
| 894 | (2) | 928 | (1) | 917 | (1) |
| 906 | (0) | 951 | (1) | 939 | (1) |
| 917 | (3) | 969 | (4) | 948 | (4) |
| 935 | (0) | 986 | (0) | 973 | (0) |
| 944 | (0) | 992 | (1) | 981 | (0) |
| 1024 | (2) | 1061 | (3) | 1059 | (3) |
| 1036 | (1) | 1065 | (2) | 1069 | (3) |
| 1080 | (0) | 1113 | (0) | 1109 | (0) |
| 1118 | (2) | 1155 | (4) | 1156 | (2) |
| 1144 | (2) | 1172 | (3) | 1184 | (2) |
| 1172 | (0) | 1209 | (0) | 1212 | (0) |
| 1188 | (2) | 1234 | (1) | 1222 | (2) |
| 1241 | (16) | 1283 | (14) | 1280 | (17) |
| 1272 | (8) | 1324 | (8) | 1305 | (6) |

| | | | | | |
|---|---|---|---|---|---|
| 1308 | (0) | 1363 | (0) | 1352 | (0) |
| 1322 | (5) | 1367 | (20) | 1376 | (9) |
| 1346 | (6) | 1400 | (4) | 1396 | (22) |
| 1346 | (22) | 1402 | (19) | 1398 | (6) |
| 1411 | (8) | 1460 | (8) | 1444 | (7) |
| 1416 | (5) | 1468 | (5) | 1456 | (3) |
| 1420 | (0) | 1474 | (0) | 1476 | (0) |
| 1436 | (2) | 1485 | (7) | 1484 | (4) |
| 1509 | (41) | 1560 | (54) | 1574 | (51) |
| 1557 | (1) | 1622 | (5) | 1624 | (7) |
| 1566 | (1) | 1627 | (1) | 1643 | (4) |
| 1963 | (690) | 2053 | (813) | 2046 | (824) |
| 1977 | (829) | 2060 | (983) | 2050 | (931) |
| 2025 | (832) | 2106 | (1048) | 2105 | (1027) |
| 2978 | (18) | 3050 | (18) | 3048 | (35) |
| 3033 | (19) | 3115 | (17) | 3118 | (43) |
| 3034 | (2) | 3116 | (2) | 3119 | (6) |
| 3067 | (5) | 3133 | (6) | 3159 | (9) |
| 3084 | (10) | 3155 | (11) | 3162 | (14) |
| 3086 | (19) | 3163 | (22) | 3172 | (41) |
| 3087 | (8) | 3163 | (8) | 3173 | (21) |
| 3106 | (10) | 3183 | (12) | 3187 | (29) |
| 3107 | (1) | 3184 | (0) | 3189 | (1) |
| 3136 | (2) | 3213 | (2) | 3216 | (11) |
| 3149 | (6) | 3226 | (6) | 3230 | (21) |

**Table S38**. Harmonic vibrational frequencies (in $cm^{-1}$) and infrared intensities (in parentheses, in km/mol) for the structure **2Co-1** of $(C_{10}H_8PCH_3)Co(C_5H_5)$ with $C_1$ symmetry.

| BP86 | | B3LYP | | M06-L | |
|---|---|---|---|---|---|
| 33 | (0) | 24 | (0) | 24 | (0) |
| 61 | (1) | 63 | (0) | 58 | (0) |
| 97 | (0) | 95 | (0) | 99 | (0) |
| 101 | (0) | 107 | (0) | 107 | (0) |
| 149 | (1) | 152 | (0) | 155 | (1) |
| 171 | (0) | 175 | (0) | 179 | (0) |
| 181 | (2) | 184 | (0) | 187 | (2) |
| 184 | (0) | 184 | (2) | 211 | (0) |
| 234 | (1) | 229 | (2) | 242 | (1) |
| 264 | (4) | 266 | (0) | 271 | (0) |
| 268 | (0) | 275 | (3) | 274 | (5) |
| 272 | (2) | 276 | (3) | 284 | (1) |
| 342 | (4) | 333 | (4) | 373 | (8) |
| 350 | (9) | 335 | (8) | 380 | (3) |
| 376 | (0) | 368 | (3) | 394 | (1) |
| 384 | (0) | 386 | (11) | 401 | (0) |
| 405 | (5) | 403 | (1) | 423 | (5) |
| 419 | (8) | 412 | (5) | 428 | (12) |
| 469 | (12) | 460 | (12) | 482 | (11) |
| 496 | (2) | 510 | (0) | 522 | (1) |
| 501 | (1) | 514 | (4) | 533 | (2) |
| 548 | (1) | 567 | (1) | 570 | (1) |
| 558 | (0) | 583 | (0) | 588 | (0) |
| 559 | (1) | 588 | (2) | 597 | (1) |
| 581 | (15) | 600 | (14) | 610 | (15) |
| 604 | (5) | 623 | (2) | 645 | (2) |
| 619 | (0) | 642 | (0) | 650 | (0) |
| 671 | (2) | 695 | (3) | 703 | (3) |
| 674 | (12) | 697 | (14) | 714 | (7) |
| 692 | (2) | 712 | (2) | 737 | (10) |
| 732 | (51) | 760 | (51) | 756 | (43) |
| 744 | (0) | 769 | (0) | 766 | (0) |
| 755 | (5) | 783 | (4) | 778 | (1) |
| 769 | (10) | 794 | (1) | 785 | (0) |
| 776 | (3) | 795 | (6) | 796 | (3) |
| 780 | (56) | 805 | (84) | 807 | (43) |
| 804 | (0) | 829 | (29) | 826 | (1) |
| 806 | (14) | 837 | (1) | 828 | (29) |
| 811 | (15) | 843 | (0) | 835 | (6) |
| 817 | (8) | 847 | (6) | 838 | (7) |
| 829 | (1) | 859 | (0) | 859 | (0) |
| 853 | (2) | 890 | (0) | 882 | (3) |
| 855 | (0) | 898 | (0) | 883 | (0) |
| 858 | (0) | 898 | (2) | 885 | (0) |
| 882 | (2) | 918 | (2) | 910 | (1) |
| 884 | (11) | 920 | (13) | 918 | (14) |
| 910 | (4) | 955 | (4) | 944 | (4) |
| 919 | (0) | 957 | (2) | 947 | (1) |
| 920 | (2) | 958 | (0) | 950 | (1) |
| 940 | (0) | 987 | (0) | 975 | (0) |
| 974 | (7) | 1007 | (9) | 1013 | (6) |
| 998 | (12) | 1030 | (13) | 1033 | (11) |
| 1019 | (4) | 1048 | (3) | 1048 | (4) |
| 1032 | 0 | 1065 | (0) | 1066 | (0) |
| 1037 | (0) | 1068 | (0) | 1073 | (0) |
| 1050 | (1) | 1090 | (2) | 1085 | (2) |
| 1079 | (7) | 1123 | (13) | 1112 | (10) |
| 1100 | (3) | 1136 | (1) | 1131 | (1) |

| | | | | | |
|---|---|---|---|---|---|
| 1105 | (7) | 1138 | (4) | 1143 | (11) |
| 1140 | (1) | 1174 | (1) | 1166 | (1) |
| 1179 | (4) | 1219 | (4) | 1214 | (4) |
| 1194 | (1) | 1231 | (0) | 1229 | (2) |
| 1220 | (0) | 1270 | (4) | 1258 | (0) |
| 1226 | (3) | 1271 | (0) | 1260 | (5) |
| 1255 | (3) | 1315 | (4) | 1308 | (3) |
| 1265 | (3) | 1322 | (4) | 1310 | (3) |
| 1282 | (14) | 1337 | (9) | 1332 | (13) |
| 1343 | (5) | 1353 | (19) | 1374 | (11) |
| 1350 | (2) | 1394 | (1) | 1400 | (7) |
| 1354 | (4) | 1401 | (3) | 1408 | (2) |
| 1363 | (6) | 1414 | (10) | 1413 | (4) |
| 1387 | (4) | 1444 | (3) | 1438 | (11) |
| 1389 | (6) | 1447 | (15) | 1440 | (2) |
| 1416 | (8) | 1465 | (9) | 1456 | (2) |
| 1418 | (4) | 1467 | (4) | 1456 | (8) |
| 1424 | (2) | 1474 | (1) | 1471 | (0) |
| 1437 | (1) | 1491 | (0) | 1486 | (0) |
| 1469 | (22) | 1518 | (26) | 1518 | (19) |
| 1576 | (3) | 1625 | (3) | 1626 | (5) |
| 1587 | (0) | 1641 | (1) | 1644 | (0) |
| 2965 | (29) | 3039 | (24) | 3042 | (52) |
| 3046 | (5) | 3131 | (9) | 3129 | (15) |
| 3047 | (6) | 3132 | (8) | 3129 | (3) |
| 3060 | (6) | 3136 | (2) | 3144 | (69) |
| 3064 | (13) | 3136 | (4) | 3146 | (21) |
| 3067 | (19) | 3156 | (20) | 3152 | (17) |
| 3068 | (23) | 3158 | (16) | 3169 | (15) |
| 3097 | (5) | 3175 | (4) | 3172 | (21) |
| 3102 | (1) | 3181 | (1) | 3176 | (1) |
| 3115 | (23) | 3193 | (21) | 3193 | (45) |
| 3130 | (34) | 3208 | (29) | 3210 | (67) |
| 3154 | (1) | 3233 | (0) | 3226 | (0) |
| 3156 | (3) | 3235 | (2) | 3232 | (9) |
| 3172 | (3) | 3249 | (3) | 3248 | (17) |
| 3182 | (4) | 3259 | (3) | 3251 | (17) |
| 3189 | (2) | 3267 | (1) | 3267 | (11) |

**Table S39**. Harmonic vibrational frequencies (in $cm^{-1}$) and infrared intensities (in parentheses, in km/mol) for the structure **2Co-2** of $(C_{10}H_8PCH_3)Co(C_5H_5)$ with $C_1$ symmetry.

| BP86 | | B3LYP | | M06-L | |
|---|---|---|---|---|---|
| 20 | (0) | 24 | (0) | 20 | (0) |
| 55 | (0) | 59 | (0) | 60 | (0) |
| 94 | (0) | 97 | (0) | 99 | (0) |
| 102 | (0) | 108 | (0) | 104 | (0) |
| 129 | (1) | 131 | (0) | 120 | (0) |
| 142 | (0) | 149 | (0) | 146 | (0) |
| 191 | (0) | 196 | (0) | 197 | (0) |
| 192 | (0) | 197 | (0) | 206 | (2) |
| 214 | (2) | 215 | (3) | 226 | (1) |
| 244 | (2) | 246 | (2) | 257 | (2) |
| 269 | (0) | 266 | (0) | 276 | (0) |
| 297 | (6) | 309 | (6) | 307 | (7) |
| 351 | (4) | 340 | (5) | 378 | (4) |
| 355 | (12) | 341 | (10) | 381 | (6) |
| 376 | (1) | 368 | (2) | 386 | (4) |
| 403 | (6) | 380 | (8) | 415 | (1) |
| 405 | (1) | 416 | (6) | 419 | (9) |
| 409 | (6) | 420 | (1) | 424 | (5) |
| 459 | (11) | 455 | (9) | 472 | (9) |
| 488 | (0) | 498 | (0) | 518 | (2) |
| 494 | (2) | 512 | (6) | 519 | (1) |
| 546 | (2) | 566 | (2) | 569 | (2) |
| 556 | (5) | 582 | (0) | 586 | (5) |
| 556 | (0) | 583 | (10) | 591 | (0) |
| 575 | (15) | 596 | (12) | 604 | (16) |
| 609 | (6) | 629 | (2) | 642 | (3) |
| 627 | (0) | 648 | (0) | 654 | (0) |
| 646 | (7) | 671 | (11) | 678 | (9) |
| 673 | (1) | 695 | (1) | 703 | (1) |
| 693 | (9) | 713 | (10) | 724 | (12) |
| 733 | (65) | 762 | (69) | 760 | (55) |
| 744 | (0) | 772 | (0) | 774 | (0) |
| 752 | (17) | 790 | (22) | 783 | (9) |
| 784 | (36) | 812 | (36) | 812 | (26) |
| 789 | (8) | 814 | (26) | 814 | (9) |
| 803 | (1) | 822 | (0) | 818 | (1) |
| 805 | (0) | 838 | (0) | 827 | (0) |
| 807 | (3) | 840 | (10) | 829 | (9) |
| 826 | (24) | 847 | (20) | 842 | (29) |
| 832 | (0) | 861 | (8) | 856 | (8) |
| 836 | (9) | 865 | (0) | 863 | (0) |
| 848 | (5) | 881 | (3) | 866 | (2) |
| 860 | (0) | 897 | (0) | 890 | (5) |
| 866 | (9) | 907 | (30) | 891 | (0) |
| 868 | (0) | 907 | (0) | 896 | (0) |
| 870 | (26) | 908 | (5) | 897 | (26) |
| 909 | (5) | 954 | (5) | 943 | (4) |
| 925 | (3) | 968 | (1) | 952 | (0) |
| 927 | (0) | 973 | (0) | 954 | (4) |
| 940 | (0) | 987 | (0) | 976 | (0) |
| 974 | (7) | 1009 | (9) | 1014 | (6) |
| 999 | (12) | 1031 | (13) | 1035 | (10) |
| 1019 | (4) | 1048 | (3) | 1055 | (3) |
| 1034 | (0) | 1067 | (0) | 1068 | (0) |
| 1035 | (0) | 1067 | (0) | 1070 | (0) |
| 1067 | (1) | 1105 | (2) | 1104 | (2) |
| 1105 | (5) | 1138 | (5) | 1144 | (2) |
| 1108 | (3) | 1144 | (1) | 1145 | (17) |

| | | | | | |
|---|---|---|---|---|---|
| 1112 | (15) | 1153 | (24) | 1146 | (12) |
| 1140 | (0) | 1174 | (1) | 1171 | (0) |
| 1192 | (4) | 1234 | (5) | 1230 | (4) |
| 1202 | (1) | 1240 | (0) | 1240 | (2) |
| 1221 | (0) | 1272 | (5) | 1257 | (0) |
| 1229 | (4) | 1273 | (0) | 1267 | (5) |
| 1260 | (7) | 1317 | (8) | 1303 | (5) |
| 1283 | (2) | 1341 | (3) | 1327 | (3) |
| 1302 | (5) | 1349 | (4) | 1346 | (8) |
| 1344 | (7) | 1362 | (19) | 1393 | (12) |
| 1351 | (1) | 1395 | (1) | 1404 | (4) |
| 1356 | (2) | 1400 | (2) | 1412 | (1) |
| 1362 | (5) | 1413 | (7) | 1418 | (3) |
| 1387 | (5) | 1445 | (4) | 1442 | (2) |
| 1395 | (20) | 1451 | (37) | 1444 | (22) |
| 1408 | (1) | 1459 | (0) | 1451 | (6) |
| 1420 | (4) | 1470 | (4) | 1455 | (2) |
| 1422 | (2) | 1472 | (1) | 1474 | (0) |
| 1439 | (1) | 1492 | (0) | 1496 | (0) |
| 1472 | (20) | 1522 | (24) | 1531 | (18) |
| 1578 | (3) | 1627 | (3) | 1644 | (5) |
| 1585 | (0) | 1639 | (1) | 1654 | (0) |
| 2973 | (25) | 3044 | (24) | 3041 | (46) |
| 3028 | (19) | 3120 | (19) | 3088 | (37) |
| 3030 | (11) | 3120 | (0) | 3090 | (22) |
| 3055 | (7) | 3122 | (9) | 3134 | (41) |
| 3073 | (28) | 3160 | (20) | 3136 | (29) |
| 3073 | (16) | 3161 | (16) | 3140 | (17) |
| 3096 | (5) | 3169 | (5) | 3163 | (19) |
| 3097 | (5) | 3176 | (4) | 3167 | (1) |
| 3102 | (1) | 3181 | (1) | 3172 | (8) |
| 3115 | (21) | 3194 | (19) | 3185 | (42) |
| 3130 | (32) | 3209 | (27) | 3201 | (63) |
| 3160 | (1) | 3238 | (1) | 3222 | (3) |
| 3161 | (2) | 3239 | (1) | 3225 | (5) |
| 3174 | (4) | 3252 | (3) | 3241 | (15) |
| 3184 | (2) | 3261 | (1) | 3253 | (14) |
| 3191 | (1) | 3268 | (1) | 3260 | (6) |

**Table S40**. Harmonic vibrational frequencies (in $cm^{-1}$) and infrared intensities (in parentheses, in km/mol) for the structure **2Co-3** of $(C_{10}H_8PCH_3)Co(C_5H_5)$ with $C_1$ symmetry.

| BP86 | | B3LYP | | M06-L | |
|---|---|---|---|---|---|
| 40 | (0) | 31 | (0) | 45 | (0) |
| 48 | (0) | 51 | (0) | 65 | (0) |
| 69 | (0) | 69 | (0) | 74 | (0) |
| 102 | (1) | 102 | (1) | 99 | (1) |
| 125 | (1) | 129 | (0) | 132 | (0) |
| 147 | (1) | 150 | (0) | 150 | (1) |
| 162 | (3) | 167 | (2) | 171 | (3) |
| 183 | (1) | 185 | (1) | 189 | (0) |
| 212 | (3) | 217 | (2) | 222 | (4) |
| 225 | (2) | 232 | (2) | 236 | (2) |
| 261 | (0) | 264 | (0) | 270 | (0) |
| 277 | (8) | 281 | (8) | 287 | (9) |
| 313 | (0) | 309 | (2) | 327 | (0) |
| 350 | (2) | 330 | (7) | 375 | (0) |
| 366 | (2) | 351 | (1) | 389 | (1) |
| 376 | (9) | 372 | (5) | 414 | (6) |
| 380 | (8) | 391 | (4) | 417 | (4) |
| 406 | (5) | 423 | (3) | 425 | (13) |
| 454 | (1) | 456 | (1) | 477 | (2) |
| 491 | (17) | 502 | (11) | 511 | (19) |
| 509 | (24) | 532 | (30) | 534 | (19) |
| 541 | (7) | 563 | (2) | 563 | (5) |
| 555 | (1) | 578 | (1) | 591 | (3) |
| 561 | (2) | 591 | (2) | 593 | (1) |
| 567 | (2) | 593 | (3) | 600 | (1) |
| 600 | (11) | 619 | (7) | 625 | (12) |
| 646 | (1) | 668 | (1) | 673 | (1) |
| 651 | (12) | 680 | (7) | 679 | (9) |
| 671 | (15) | 698 | (17) | 701 | (15) |
| 716 | (2) | 744 | (3) | 741 | (2) |
| 727 | (45) | 752 | (41) | 759 | (23) |
| 733 | (52) | 762 | (41) | 762 | (16) |
| 740 | (7) | 766 | (8) | 775 | (39) |
| 751 | (35) | 787 | (45) | 780 | (9) |
| 755 | (5) | 793 | (17) | 783 | (33) |
| 771 | (37) | 806 | (48) | 801 | (24) |
| 792 | (2) | 816 | (8) | 822 | (4) |
| 801 | (16) | 829 | (7) | 830 | (21) |
| 806 | (6) | 837 | (3) | 835 | (9) |
| 809 | (1) | 841 | (1) | 837 | (3) |
| 832 | (2) | 868 | (6) | 866 | (4) |
| 842 | (2) | 873 | (8) | 873 | (3) |
| 847 | (1) | 887 | (3) | 880 | (2) |
| 854 | (5) | 895 | (2) | 885 | (5) |
| 866 | (17) | 897 | (15) | 890 | (11) |
| 881 | (20) | 918 | (19) | 905 | (21) |
| 906 | (0) | 957 | (2) | 950 | (1) |
| 926 | (3) | 963 | (23) | 960 | (15) |
| 934 | (18) | 983 | (5) | 972 | (6) |
| 939 | (1) | 989 | (1) | 979 | (0) |
| 972 | (9) | 1004 | (12) | 1015 | (8) |
| 988 | (13) | 1025 | (12) | 1030 | (11) |
| 1028 | (3) | 1058 | (9) | 1063 | (6) |
| 1030 | (1) | 1064 | (1) | 1068 | (2) |
| 1030 | (6) | 1065 | (0) | 1069 | (0) |
| 1054 | (5) | 1088 | (4) | 1088 | (8) |
| 1097 | (14) | 1132 | (10) | 1137 | (21) |
| 1105 | (2) | 1139 | (2) | 1143 | (2) |

| | | | | | |
|---|---|---|---|---|---|
| 1138 | (2) | 1173 | (4) | 1177 | (1) |
| 1149 | (3) | 1188 | (6) | 1185 | (3) |
| 1170 | (7) | 1201 | (9) | 1210 | (9) |
| 1205 | (7) | 1245 | (8) | 1248 | (8) |
| 1216 | (0) | 1270 | (0) | 1260 | (0) |
| 1239 | (11) | 1283 | (11) | 1281 | (12) |
| 1275 | (11) | 1323 | (15) | 1313 | (8) |
| 1283 | (7) | 1335 | (14) | 1320 | (9) |
| 1344 | (2) | 1375 | (2) | 1394 | (5) |
| 1350 | (1) | 1389 | (0) | 1402 | (1) |
| 1353 | (7) | 1393 | (2) | 1408 | (1) |
| 1366 | (1) | 1406 | (4) | 1414 | (3) |
| 1379 | (1) | 1426 | (4) | 1428 | (3) |
| 1383 | (3) | 1442 | (2) | 1440 | (1) |
| 1406 | (1) | 1462 | (12) | 1451 | (6) |
| 1413 | (8) | 1465 | (27) | 1452 | (7) |
| 1416 | (10) | 1465 | (0) | 1462 | (0) |
| 1424 | (26) | 1468 | (29) | 1481 | (29) |
| 1456 | (20) | 1508 | (20) | 1515 | (24) |
| 1525 | (24) | 1581 | (19) | 1591 | (25) |
| 1572 | (46) | 1635 | (51) | 1649 | (56) |
| 1592 | (17) | 1643 | (25) | 1659 | (28) |
| 2986 | (9) | 3057 | (9) | 3059 | (27) |
| 3034 | (15) | 3121 | (12) | 3113 | (27) |
| 3060 | (4) | 3142 | (2) | 3145 | (5) |
| 3079 | (4) | 3144 | (5) | 3150 | (30) |
| 3082 | (13) | 3159 | (2) | 3167 | (44) |
| 3086 | (12) | 3166 | (13) | 3168 | (22) |
| 3093 | (16) | 3169 | (8) | 3171 | (10) |
| 3095 | (5) | 3174 | (15) | 3174 | (14) |
| 3097 | (4) | 3179 | (5) | 3182 | (10) |
| 3116 | (20) | 3194 | (21) | 3197 | (35) |
| 3134 | (28) | 3211 | (26) | 3216 | (62) |
| 3155 | (0) | 3233 | (0) | 3229 | (2) |
| 3160 | (2) | 3237 | (1) | 3234 | (3) |
| 3169 | (10) | 3249 | (5) | 3247 | (28) |
| 3175 | (8) | 3253 | (5) | 3257 | (27) |
| 3188 | (2) | 3264 | (1) | 3266 | (9) |

**Table S41**. Harmonic vibrational frequencies (in $cm^{-1}$) and infrared intensities (in parentheses, in km/mol) for the structure **2Co-4** of $(C_{10}H_8PCH_3)Co(C_5H_5)$ with $C_s$ symmetry.

| BP86 | | B3LYP | | M06-L | |
|---|---|---|---|---|---|
| 41 | (0) | 35 | (0) | 44 | (0) |
| 70 | (1) | 71 | (0) | 71 | (0) |
| 80 | (0) | 78 | (1) | 89 | (0) |
| 103 | (0) | 104 | (0) | 110 | (0) |
| 120 | (0) | 121 | 0 | 136 | (0) |
| 128 | (1) | 134 | (0) | 147 | (1) |
| 151 | (1) | 157 | (1) | 175 | (0) |
| 175 | (3) | 181 | (2) | 185 | (4) |
| 214 | (1) | 215 | (0) | 229 | (1) |
| 231 | (0) | 239 | (0) | 247 | (0) |
| 243 | (0) | 250 | (0) | 255 | (0) |
| 302 | (2) | 299 | (3) | 317 | (2) |
| 326 | (1) | 337 | (2) | 336 | (0) |
| 354 | (7) | 338 | (6) | 387 | (2) |
| 382 | (4) | 372 | (4) | 414 | (17) |
| 386 | (13) | 389 | (11) | 422 | (3) |
| 414 | (4) | 417 | (2) | 454 | (7) |
| 450 | (5) | 458 | (4) | 475 | (1) |
| 483 | (0) | 499 | (1) | 504 | (0) |
| 499 | (1) | 520 | (2) | 519 | (1) |
| 509 | (22) | 530 | (24) | 541 | (20) |
| 535 | (0) | 557 | (0) | 565 | (0) |
| 557 | (7) | 584 | (8) | 594 | (9) |
| 565 | (1) | 594 | (1) | 603 | (1) |
| 572 | (5) | 599 | (4) | 610 | (6) |
| 599 | (1) | 629 | (2) | 644 | (15) |
| 611 | (10) | 634 | (8) | 658 | (2) |
| 663 | (19) | 684 | (17) | 715 | (21) |
| 703 | (0) | 736 | (1) | 737 | (1) |
| 725 | (2) | 753 | (2) | 750 | (2) |
| 729 | (57) | 758 | (40) | 757 | (47) |
| 753 | (16) | 780 | (36) | 783 | (14) |
| 778 | (23) | 808 | (52) | 797 | (4) |
| 778 | (4) | 814 | (19) | 802 | (9) |
| 781 | (27) | 815 | (4) | 808 | (28) |
| 803 | (0) | 838 | (0) | 826 | (0) |
| 806 | (2) | 841 | (1) | 835 | (3) |
| 814 | (0) | 850 | (0) | 842 | (0) |
| 837 | (0) | 874 | (0) | 862 | (9) |
| 839 | (8) | 874 | (10) | 864 | (0) |
| 841 | (0) | 888 | (0) | 869 | (0) |
| 856 | (1) | 892 | (1) | 889 | (2) |
| 862 | (4) | 899 | (4) | 898 | (5) |
| 868 | (6) | 902 | (1) | 901 | (6) |
| 884 | (6) | 917 | (11) | 906 | (4) |
| 893 | (8) | 929 | (7) | 924 | (10) |
| 920 | (0) | 970 | (0) | 954 | (0) |
| 939 | (0) | 983 | (13) | 978 | (0) |
| 945 | (11) | 989 | (9) | 983 | (14) |
| 949 | (12) | 989 | (2) | 990 | (9) |
| 977 | (13) | 1010 | (14) | 1017 | (12) |
| 989 | (8) | 1018 | (5) | 1027 | (0) |
| 994 | (8) | 1024 | (11) | 1028 | (14) |
| 1008 | (1) | 1044 | (3) | 1037 | (0) |
| 1031 | (0) | 1064 | (0) | 1067 | (0) |
| 1034 | (0) | 1068 | (0) | 1073 | (0) |
| 1099 | (3) | 1129 | (13) | 1127 | (9) |
| 1099 | (18) | 1134 | (9) | 1138 | (19) |

| | | | | | |
|---|---|---|---|---|---|
| 1112 | (5) | 1150 | (5) | 1154 | (4) |
| 1140 | (1) | 1177 | (0) | 1175 | (0) |
| 1185 | (7) | 1217 | (8) | 1226 | (11) |
| 1201 | (0) | 1241 | (0) | 1240 | (1) |
| 1204 | (3) | 1247 | (2) | 1245 | (2) |
| 1219 | (0) | 1271 | (0) | 1259 | (0) |
| 1272 | (3) | 1314 | (1) | 1315 | (4) |
| 1281 | (4) | 1327 | (4) | 1321 | (3) |
| 1282 | (8) | 1331 | (8) | 1334 | (6) |
| 1333 | (0) | 1381 | (0) | 1384 | 0 |
| 1348 | (0) | 1389 | (5) | 1402 | 0 |
| 1349 | (0) | 1390 | (0) | 1404 | (0) |
| 1352 | (4) | 1393 | (1) | 1408 | (4) |
| 1376 | (2) | 1417 | (1) | 1427 | (2) |
| 1395 | (1) | 1450 | (1) | 1448 | (0) |
| 1405 | (2) | 1461 | (2) | 1454 | (4) |
| 1414 | (6) | 1463 | (6) | 1456 | (1) |
| 1420 | (10) | 1469 | (9) | 1463 | (9) |
| 1448 | (5) | 1487 | (11) | 1501 | (6) |
| 1456 | (4) | 1503 | (6) | 1517 | (3) |
| 1509 | (0) | 1558 | (1) | 1574 | (1) |
| 1598 | (0) | 1655 | (0) | 1666 | (0) |
| 2965 | (30) | 3037 | (29) | 3045 | (64) |
| 3057 | (9) | 3124 | (11) | 3142 | (27) |
| 3059 | (10) | 3127 | (11) | 3145 | (7) |
| 3071 | (12) | 3148 | (9) | 3154 | (20) |
| 3074 | (5) | 3151 | (6) | 3155 | (51) |
| 3084 | (23) | 3160 | (25) | 3160 | (17) |
| 3092 | (14) | 3167 | (13) | 3164 | (26) |
| 3099 | (1) | 3178 | (0) | 3178 | (13) |
| 3105 | (1) | 3184 | (1) | 3181 | (1) |
| 3118 | (23) | 3197 | (21) | 3201 | (42) |
| 3130 | (27) | 3208 | (24) | 3216 | (57) |
| 3160 | (0) | 3238 | (0) | 3235 | (0) |
| 3161 | (0) | 3240 | (0) | 3236 | (1) |
| 3173 | (6) | 3252 | (4) | 3251 | (25) |
| 3176 | (6) | 3254 | (4) | 3254 | (23) |
| 3186 | (3) | 3265 | (2) | 3265 | (10) |

**Table S42**. Harmonic vibrational frequencies (in $cm^{-1}$) and infrared intensities (in parentheses, in km/mol) for the structure **2Co-5** of $(C_{10}H_8PCH_3)Co(C_5H_5)$ with $C_1$ symmetry.

| BP86 | | B3LYP | | M06-L | |
|---|---|---|---|---|---|
| 6 | (0) | 22 | (0) | 32 | (0) |
| 45 | (0) | 39 | (0) | 42 | (0) |
| 63 | (0) | 49 | (0) | 49 | (0) |
| 81 | (0) | 78 | (0) | 102 | (1) |
| 98 | (1) | 97 | (1) | 127 | (0) |
| 164 | (1) | 165 | (0) | 178 | (3) |
| 168 | (3) | 173 | (2) | 182 | (1) |
| 198 | (0) | 205 | (0) | 248 | (0) |
| 251 | (2) | 250 | (1) | 287 | (3) |
| 284 | (1) | 291 | (3) | 304 | (1) |
| 292 | (12) | 291 | (9) | 329 | (7) |
| 313 | (2) | 315 | (2) | 343 | (2) |
| 347 | (2) | 347 | (0) | 363 | (4) |
| 364 | (2) | 356 | (7) | 397 | (0) |
| 371 | (9) | 365 | (10) | 404 | (4) |
| 390 | (4) | 401 | (5) | 417 | (10) |
| 392 | (16) | 401 | (1) | 423 | (13) |
| 418 | (11) | 431 | (10) | 442 | (9) |
| 472 | (4) | 478 | (2) | 484 | (4) |
| 473 | (0) | 494 | (0) | 495 | (0) |
| 516 | (21) | 533 | (34) | 560 | (26) |
| 547 | (14) | 558 | (11) | 576 | (18) |
| 556 | (1) | 582 | (9) | 590 | (3) |
| 565 | (2) | 587 | (1) | 593 | (7) |
| 565 | (8) | 593 | (2) | 603 | (2) |
| 589 | (0) | 612 | (0) | 608 | (0) |
| 593 | (0) | 620 | (0) | 644 | (1) |
| 679 | (8) | 695 | (8) | 732 | (0) |
| 699 | (0) | 732 | (0) | 735 | (10) |
| 734 | (1) | 752 | (4) | 761 | (0) |
| 736 | (7) | 758 | (0) | 766 | (6) |
| 758 | (3) | 794 | (5) | 776 | (3) |
| 774 | (48) | 807 | (69) | 800 | (32) |
| 786 | (1) | 825 | (1) | 811 | (1) |
| 799 | (0) | 838 | (0) | 821 | (0) |
| 801 | (4) | 838 | (3) | 828 | (6) |
| 805 | (8) | 842 | (4) | 831 | (4) |
| 806 | (4) | 844 | (5) | 833 | (6) |
| 822 | (20) | 858 | (30) | 845 | (17) |
| 847 | (3) | 880 | (1) | 870 | (0) |
| 851 | (0) | 882 | (4) | 873 | (3) |
| 853 | (2) | 885 | (0) | 884 | (0) |
| 854 | (2) | 899 | (1) | 888 | (2) |
| 855 | (1) | 902 | (1) | 889 | (2) |
| 865 | (1) | 908 | (17) | 893 | (2) |
| 878 | (15) | 908 | (4) | 914 | (3) |
| 891 | (5) | 930 | (4) | 919 | (15) |
| 922 | (0) | 964 | (0) | 957 | (0) |
| 950 | (6) | 987 | (4) | 981 | (5) |
| 955 | (4) | 999 | (4) | 1000 | (4) |
| 978 | (8) | 1011 | (9) | 1016 | (7) |
| 989 | (12) | 1023 | (14) | 1024 | (10) |
| 1014 | (6) | 1046 | (6) | 1047 | (8) |
| 1029 | (3) | 1063 | (1) | 1061 | (3) |
| 1031 | (0) | 1065 | (0) | 1064 | (0) |
| 1033 | (1) | 1068 | (2) | 1066 | (1) |
| 1054 | (3) | 1090 | (7) | 1088 | (4) |
| 1080 | (0) | 1116 | (0) | 1109 | (0) |

| | | | | | |
|---|---|---|---|---|---|
| 1100 | (15) | 1134 | (10) | 1140 | (21) |
| 1120 | (14) | 1153 | (23) | 1153 | (17) |
| 1179 | (1) | 1212 | (1) | 1222 | (1) |
| 1185 | (1) | 1219 | (3) | 1229 | (4) |
| 1219 | (0) | 1271 | (0) | 1254 | (0) |
| 1242 | (3) | 1288 | (3) | 1284 | (3) |
| 1272 | (4) | 1326 | (3) | 1317 | (2) |
| 1296 | (7) | 1339 | (7) | 1350 | (6) |
| 1304 | (4) | 1353 | (5) | 1350 | (2) |
| 1325 | (9) | 1371 | (10) | 1375 | (9) |
| 1345 | (0) | 1388 | (7) | 1402 | (0) |
| 1347 | (1) | 1390 | (0) | 1405 | (1) |
| 1366 | (0) | 1403 | (7) | 1425 | (2) |
| 1387 | (4) | 1439 | (5) | 1442 | (1) |
| 1393 | (2) | 1444 | (3) | 1446 | (11) |
| 1401 | (17) | 1455 | (16) | 1450 | (11) |
| 1407 | (1) | 1462 | (1) | 1459 | (0) |
| 1417 | (19) | 1466 | (18) | 1464 | (18) |
| 1422 | (2) | 1474 | (0) | 1477 | (0) |
| 1434 | (4) | 1478 | (10) | 1489 | (5) |
| 1565 | (2) | 1624 | (6) | 1639 | (4) |
| 1612 | (1) | 1679 | (1) | 1689 | (2) |
| 2966 | (29) | 3043 | (25) | 3046 | (47) |
| 3054 | (6) | 3131 | (7) | 3149 | (2) |
| 3066 | (3) | 3134 | (4) | 3150 | (11) |
| 3069 | (2) | 3142 | (3) | 3159 | (34) |
| 3079 | (16) | 3152 | (18) | 3161 | (6) |
| 3084 | (16) | 3166 | (10) | 3163 | (39) |
| 3085 | (3) | 3167 | (3) | 3167 | (14) |
| 3099 | (27) | 3176 | (28) | 3186 | (46) |
| 3102 | (3) | 3178 | (3) | 3190 | (15) |
| 3113 | (9) | 3197 | (6) | 3192 | (17) |
| 3126 | (24) | 3211 | (17) | 3207 | (49) |
| 3159 | (0) | 3238 | (0) | 3231 | (1) |
| 3161 | (1) | 3241 | (1) | 3232 | (1) |
| 3171 | (7) | 3251 | (4) | 3247 | (26) |
| 3178 | (5) | 3257 | (3) | 3250 | (19) |
| 3187 | (2) | 3267 | (1) | 3261 | (13) |

**Table S43**. Harmonic vibrational frequencies (in $cm^{-1}$) and infrared intensities (in parentheses, in km/mol) for the structure **2Co-6** of $(C_{10}H_8PCH_3)Co(C_5H_5)$ with $C_1$ symmetry.

| BP86 | | B3LYP | | M06-L | |
|---|---|---|---|---|---|
| 28 | (0) | 26 | (0) | 34 | (0) |
| 73 | (0) | 75 | (0) | 71 | (0) |
| 85 | (0) | 90 | (0) | 77 | (0) |
| 87 | (0) | 91 | (0) | 92 | (0) |
| 114 | (0) | 123 | (0) | 122 | (0) |
| 132 | (0) | 148 | (0) | 169 | (0) |
| 166 | (0) | 172 | (0) | 210 | (1) |
| 179 | (1) | 183 | (1) | 226 | (2) |
| 214 | (2) | 219 | (1) | 236 | (0) |
| 256 | (0) | 265 | (0) | 275 | (0) |
| 278 | (1) | 277 | (0) | 316 | (0) |
| 308 | (2) | 313 | (3) | 322 | (3) |
| 319 | (2) | 329 | (2) | 330 | (0) |
| 358 | (4) | 333 | (9) | 387 | (2) |
| 369 | (2) | 371 | (4) | 399 | (3) |
| 399 | (14) | 393 | (9) | 431 | (14) |
| 415 | (4) | 419 | (3) | 444 | (4) |
| 439 | (4) | 441 | (3) | 465 | (2) |
| 487 | (0) | 506 | (3) | 507 | (0) |
| 489 | (0) | 507 | (1) | 508 | (1) |
| 520 | (29) | 541 | (24) | 555 | (20) |
| 531 | (1) | 551 | (7) | 561 | (1) |
| 531 | (2) | 554 | (0) | 575 | (13) |
| 556 | (1) | 588 | (1) | 591 | (1) |
| 563 | (3) | 593 | (1) | 606 | (4) |
| 566 | (1) | 598 | (0) | 614 | (1) |
| 604 | (7) | 627 | (5) | 627 | (6) |
| 677 | (7) | 695 | (7) | 728 | (7) |
| 705 | (0) | 737 | (0) | 738 | (0) |
| 722 | (2) | 751 | (1) | 747 | (1) |
| 727 | (60) | 756 | (40) | 753 | (55) |
| 752 | (15) | 779 | (36) | 777 | (5) |
| 754 | (5) | 807 | (38) | 781 | (7) |
| 770 | (35) | 821 | (32) | 800 | (24) |
| 800 | (4) | 821 | (3) | 826 | (4) |
| 803 | (0) | 837 | (0) | 827 | (0) |
| 806 | (5) | 841 | (1) | 834 | (8) |
| 812 | (0) | 848 | (1) | 839 | (1) |
| 821 | (8) | 856 | (7) | 848 | (6) |
| 850 | (11) | 880 | (12) | 877 | (0) |
| 851 | (2) | 885 | (0) | 882 | (15) |
| 853 | (3) | 897 | (0) | 886 | (1) |
| 857 | (0) | 900 | (2) | 891 | (1) |
| 877 | (1) | 908 | (1) | 910 | (1) |
| 893 | (3) | 914 | (10) | 925 | (4) |
| 895 | (2) | 924 | (2) | 928 | (3) |
| 920 | (0) | 970 | (0) | 952 | (0) |
| 940 | (0) | 989 | (0) | 973 | (0) |
| 959 | (7) | 998 | (7) | 994 | (9) |
| 961 | (4) | 1001 | (3) | 1010 | (3) |
| 978 | (10) | 1009 | (14) | 1017 | (10) |
| 987 | (12) | 1016 | (5) | 1024 | (6) |
| 991 | (7) | 1025 | (10) | 1026 | (10) |
| 1024 | (2) | 1065 | (0) | 1061 | (2) |

| | | | | | |
|---|---|---|---|---|---|
| 1031 | (1) | 1067 | (0) | 1066 | (1) |
| 1034 | (0) | 1071 | (5) | 1069 | (1) |
| 1099 | (13) | 1134 | (9) | 1138 | (19) |
| 1114 | (7) | 1147 | (21) | 1151 | (7) |
| 1115 | (10) | 1153 | (8) | 1153 | (13) |
| 1141 | (1) | 1178 | (0) | 1171 | (2) |
| 1185 | (6) | 1219 | (8) | 1225 | (9) |
| 1199 | (0) | 1240 | (0) | 1237 | (0) |
| 1209 | (3) | 1253 | (2) | 1250 | (2) |
| 1219 | (0) | 1271 | 0 | 1257 | (0) |
| 1269 | (3) | 1321 | (3) | 1312 | (2) |
| 1287 | (12) | 1327 | (5) | 1340 | (6) |
| 1292 | (8) | 1338 | (8) | 1344 | (8) |
| 1334 | (0) | 1385 | (0) | 1382 | (0) |
| 1343 | (0) | 1390 | (0) | 1399 | (0) |
| 1351 | (1) | 1392 | (1) | 1407 | (1) |
| 1359 | (7) | 1397 | (9) | 1415 | (8) |
| 1377 | (1) | 1422 | (2) | 1427 | (1) |
| 1391 | (3) | 1449 | (2) | 1446 | (1) |
| 1405 | (1) | 1463 | (2) | 1456 | (1) |
| 1411 | (22) | 1465 | (18) | 1458 | (18) |
| 1417 | (17) | 1470 | (16) | 1475 | (16) |
| 1448 | (4) | 1488 | (13) | 1503 | (5) |
| 1457 | (4) | 1506 | (6) | 1515 | (3) |
| 1508 | (1) | 1557 | (2) | 1571 | (1) |
| 1598 | (1) | 1656 | (0) | 1666 | (0) |
| 2982 | (16) | 3055 | (16) | 3058 | (30) |
| 3066 | (0) | 3136 | (8) | 3141 | (12) |
| 3069 | (6) | 3141 | (1) | 3146 | (4) |
| 3073 | (6) | 3149 | (9) | 3154 | (64) |
| 3079 | (33) | 3155 | (4) | 3161 | (12) |
| 3085 | (6) | 3158 | (34) | 3163 | (26) |
| 3085 | (9) | 3162 | (7) | 3175 | (13) |
| 3098 | (2) | 3177 | (1) | 3176 | (5) |
| 3103 | (1) | 3182 | (0) | 3180 | (1) |
| 3117 | (22) | 3196 | (20) | 3197 | (42) |
| 3130 | (25) | 3209 | (22) | 3211 | (50) |
| 3160 | (1) | 3238 | (0) | 3233 | (0) |
| 3161 | (0) | 3240 | (0) | 3238 | (0) |
| 3172 | (7) | 3252 | (4) | 3252 | (20) |
| 3177 | (4) | 3255 | (3) | 3253 | (23) |
| 3186 | (3) | 3266 | (2) | 3266 | (12) |

**Table S44**. Harmonic vibrational frequencies (in $cm^{-1}$) and infrared intensities (in parentheses, in km/mol) for the structure **2Co-7** of $(C_{10}H_8PCH_3)Co(C_5H_5)$ with $C_1$ symmetry.

| BP86 | | B3LYP | | M06-L | |
|---|---|---|---|---|---|
| 28 | (0) | 21 | (0) | 28 | (0) |
| 47 | (1) | 47 | (0) | 44 | (0) |
| 70 | (0) | 72 | (0) | 67 | (0) |
| 92 | (1) | 96 | (3) | 95 | (3) |
| 94 | (2) | 99 | (0) | 133 | (1) |
| 147 | (1) | 151 | (1) | 165 | (1) |
| 170 | (2) | 173 | (1) | 173 | (2) |
| 172 | (1) | 174 | (1) | 179 | (0) |
| 217 | (2) | 224 | (2) | 231 | (2) |
| 272 | (1) | 274 | (7) | 285 | (1) |
| 277 | (8) | 283 | (1) | 293 | (7) |
| 300 | (1) | 300 | (1) | 322 | (1) |
| 349 | (3) | 348 | (0) | 359 | (5) |
| 354 | (0) | 358 | (6) | 376 | (1) |
| 369 | (7) | 363 | (8) | 397 | (0) |
| 379 | (16) | 377 | (6) | 412 | (10) |
| 385 | (3) | 393 | (2) | 415 | (10) |
| 413 | (12) | 425 | (11) | 431 | (13) |
| 472 | (1) | 479 | (1) | 481 | (2) |
| 474 | (3) | 492 | (2) | 491 | (1) |
| 542 | (30) | 553 | (28) | 563 | (26) |
| 550 | (12) | 571 | (25) | 591 | (0) |
| 557 | (1) | 584 | (4) | 593 | (20) |
| 568 | (1) | 595 | (6) | 594 | (12) |
| 576 | (9) | 596 | (3) | 603 | (2) |
| 586 | (1) | 610 | (1) | 611 | (10) |
| 617 | (2) | 646 | (3) | 670 | (3) |
| 661 | (20) | 681 | (18) | 706 | (19) |
| 698 | (0) | 730 | (0) | 729 | (1) |
| 733 | (7) | 749 | (5) | 760 | (1) |
| 733 | (2) | 758 | (1) | 763 | (6) |
| 764 | (3) | 798 | (13) | 778 | (6) |
| 779 | (49) | 811 | (61) | 808 | (30) |
| 780 | (1) | 821 | (0) | 809 | (2) |
| 800 | (12) | 837 | (2) | 825 | (0) |
| 802 | (1) | 839 | (1) | 828 | (7) |
| 804 | (4) | 841 | (5) | 830 | (6) |
| 807 | (5) | 842 | (7) | 831 | (10) |
| 824 | (22) | 858 | (35) | 853 | (16) |
| 845 | (0) | 870 | (3) | 876 | (0) |
| 852 | (2) | 885 | (0) | 882 | (0) |
| 855 | (1) | 890 | (3) | 885 | (1) |
| 857 | (2) | 894 | (4) | 887 | (1) |
| 859 | (6) | 900 | (0) | 889 | (1) |
| 860 | (1) | 904 | (1) | 893 | (5) |
| 867 | (1) | 909 | (0) | 898 | (2) |
| 896 | (4) | 935 | (4) | 922 | (3) |
| 926 | (1) | 968 | (1) | 962 | (0) |
| 941 | (5) | 978 | (6) | 976 | (7) |
| 948 | (10) | 994 | (10) | 995 | (8) |
| 976 | (8) | 1011 | (9) | 1014 | (7) |
| 989 | (12) | 1023 | (14) | 1025 | (10) |
| 1014 | (6) | 1046 | (6) | 1047 | (9) |
| 1030 | (2) | 1064 | (2) | 1063 | (2) |
| 1031 | (0) | 1065 | (0) | 1065 | (0) |
| 1033 | (1) | 1067 | (1) | 1068 | (3) |
| 1054 | (2) | 1088 | (5) | 1091 | (2) |
| 1083 | (0) | 1119 | (0) | 1112 | (0) |

| | | | | | |
|---|---|---|---|---|---|
| 1100 | (16) | 1134 | (11) | 1139 | (23) |
| 1113 | (19) | 1145 | (26) | 1150 | (22) |
| 1181 | (2) | 1213 | (2) | 1222 | (2) |
| 1185 | (0) | 1219 | (2) | 1228 | (2) |
| 1218 | (0) | 1271 | (0) | 1254 | (0) |
| 1242 | (2) | 1287 | (2) | 1283 | (3) |
| 1274 | (5) | 1325 | (4) | 1315 | (6) |
| 1292 | (1) | 1337 | (1) | 1348 | (0) |
| 1304 | (6) | 1350 | (7) | 1351 | (2) |
| 1316 | (2) | 1362 | (2) | 1368 | (4) |
| 1345 | (0) | 1387 | (8) | 1398 | (0) |
| 1347 | (1) | 1390 | (0) | 1404 | (1) |
| 1368 | (1) | 1402 | (7) | 1425 | (2) |
| 1387 | (3) | 1437 | (2) | 1441 | (1) |
| 1391 | (1) | 1444 | (3) | 1445 | (3) |
| 1407 | (1) | 1461 | (1) | 1452 | (4) |
| 1413 | (5) | 1463 | (6) | 1458 | (0) |
| 1422 | (9) | 1471 | (8) | 1466 | (9) |
| 1423 | (1) | 1474 | (0) | 1478 | (0) |
| 1434 | (3) | 1477 | (10) | 1487 | (5) |
| 1577 | (2) | 1638 | (8) | 1652 | (7) |
| 1621 | (1) | 1688 | (1) | 1699 | (2) |
| 2965 | (37) | 3038 | (33) | 3045 | (74) |
| 3056 | (11) | 3123 | (12) | 3135 | (7) |
| 3059 | (10) | 3128 | (11) | 3144 | (46) |
| 3064 | (2) | 3140 | (3) | 3155 | (20) |
| 3072 | (30) | 3149 | (29) | 3156 | (19) |
| 3085 | (17) | 3166 | (12) | 3163 | (35) |
| 3086 | (3) | 3167 | (3) | 3169 | (21) |
| 3100 | (27) | 3177 | (27) | 3183 | (47) |
| 3102 | (1) | 3180 | (2) | 3186 | (6) |
| 3114 | (9) | 3197 | (7) | 3196 | (20) |
| 3127 | (27) | 3212 | (18) | 3211 | (55) |
| 3159 | (0) | 3238 | (0) | 3233 | (2) |
| 3162 | (1) | 3241 | (0) | 3236 | (1) |
| 3172 | (8) | 3252 | (5) | 3250 | (25) |
| 3178 | (6) | 3256 | (3) | 3257 | (21) |
| 3188 | (2) | 3267 | (1) | 3266 | (14) |

**Table S45**. Harmonic vibrational frequencies (in $cm^{-1}$) and infrared intensities (in parentheses, in km/mol) for the structure **2Co-8** of $(C_{10}H_8PCH_3)Co(C_5H_5)$ with $C_1$ symmetry.

| BP86 | | B3LYP | | M06-L | |
|---|---|---|---|---|---|
| 15 | (0) | 11 | (0) | 40 | (0) |
| 63 | (0) | 62 | (0) | 62 | (0) |
| 78 | (0) | 76 | (0) | 75 | (0) |
| 106 | (0) | 103 | (0) | 112 | (0) |
| 121 | (0) | 121 | (0) | 131 | (0) |
| 160 | (1) | 164 | (2) | 170 | (2) |
| 171 | (4) | 175 | (2) | 177 | (4) |
| 177 | (0) | 184 | (0) | 188 | (0) |
| 202 | (3) | 209 | (2) | 210 | (2) |
| 221 | (0) | 228 | (0) | 234 | (0) |
| 254 | (1) | 252 | (1) | 265 | (1) |
| 267 | (0) | 273 | (0) | 278 | (0) |
| 292 | (1) | 297 | (2) | 302 | (1) |
| 345 | (3) | 335 | (4) | 366 | (2) |
| 362 | (6) | 347 | (1) | 397 | (7) |
| 371 | (4) | 363 | (6) | 402 | (2) |
| 394 | (13) | 402 | (12) | 424 | (9) |
| 413 | (1) | 429 | (1) | 434 | (2) |
| 433 | (4) | 443 | (3) | 454 | (5) |
| 469 | (10) | 480 | (4) | 484 | (8) |
| 487 | (2) | 505 | (7) | 501 | (4) |
| 521 | (2) | 544 | (2) | 545 | (2) |
| 553 | (1) | 579 | (0) | 584 | (4) |
| 558 | (0) | 580 | (8) | 588 | (3) |
| 564 | (6) | 589 | (0) | 594 | (2) |
| 612 | (2) | 632 | (1) | 642 | (0) |
| 631 | (4) | 656 | (3) | 656 | (4) |
| 649 | (13) | 675 | (14) | 676 | (14) |
| 667 | (8) | 691 | (4) | 693 | (8) |
| 682 | (27) | 701 | (29) | 713 | (22) |
| 687 | (9) | 706 | (6) | 729 | (9) |
| 713 | (3) | 747 | (4) | 742 | (5) |
| 736 | (92) | 765 | (74) | 762 | (75) |
| 747 | (19) | 771 | (47) | 769 | (18) |
| 766 | (3) | 800 | (4) | 791 | (7) |
| 778 | (50) | 809 | (70) | 808 | (29) |
| 799 | (1) | 836 | (2) | 825 | (3) |
| 802 | (0) | 838 | (1) | 828 | (3) |
| 804 | (2) | 839 | (0) | 831 | (2) |
| 811 | (3) | 847 | (4) | 835 | (3) |
| 833 | (4) | 861 | (4) | 858 | (7) |
| 845 | (5) | 883 | (4) | 865 | (2) |
| 850 | (2) | 901 | (1) | 878 | (3) |
| 853 | (2) | 905 | (0) | 889 | (2) |
| 872 | (9) | 908 | (16) | 897 | (8) |
| 889 | (4) | 921 | (9) | 915 | (4) |
| 905 | (7) | 949 | (7) | 939 | (11) |
| 909 | (4) | 962 | (0) | 947 | (0) |
| 921 | (1) | 970 | (1) | 957 | (0) |
| 933 | (1) | 981 | (1) | 970 | (1) |
| 974 | (8) | 1006 | (9) | 1012 | (7) |
| 991 | (12) | 1028 | (12) | 1031 | (10) |
| 1009 | (9) | 1034 | (8) | 1045 | (9) |
| 1030 | (0) | 1063 | (0) | 1064 | (0) |
| 1033 | (0) | 1067 | (0) | 1070 | (0) |
| 1081 | (4) | 1118 | (5) | 1121 | (5) |
| 1101 | (11) | 1136 | (7) | 1140 | (16) |
| 1117 | (2) | 1147 | (2) | 1159 | (4) |

| | | | | | |
|---|---|---|---|---|---|
| 1128 | (1) | 1167 | (3) | 1169 | (0) |
| 1139 | (1) | 1180 | (2) | 1177 | (1) |
| 1176 | (0) | 1214 | (1) | 1214 | (0) |
| 1193 | (2) | 1236 | (3) | 1237 | (3) |
| 1218 | (0) | 1271 | (0) | 1257 | (0) |
| 1235 | (9) | 1282 | (9) | 1275 | (9) |
| 1268 | (10) | 1321 | (11) | 1304 | (7) |
| 1292 | (1) | 1344 | (4) | 1340 | (2) |
| 1339 | (9) | 1383 | (12) | 1391 | (4) |
| 1344 | (0) | 1389 | (0) | 1398 | (0) |
| 1352 | (1) | 1395 | (1) | 1406 | (4) |
| 1358 | (3) | 1407 | (3) | 1407 | (8) |
| 1361 | (3) | 1415 | (1) | 1414 | (3) |
| 1387 | (3) | 1443 | (2) | 1439 | (1) |
| 1411 | (2) | 1462 | (8) | 1451 | (9) |
| 1413 | (9) | 1469 | (1) | 1457 | (7) |
| 1421 | (7) | 1470 | (7) | 1464 | (0) |
| 1427 | (7) | 1478 | (16) | 1483 | (6) |
| 1448 | (3) | 1490 | (11) | 1504 | (4) |
| 1510 | (3) | 1555 | (7) | 1576 | (5) |
| 1579 | (6) | 1642 | (8) | 1652 | (11) |
| 1604 | (3) | 1659 | (6) | 1675 | (4) |
| 2974 | (29) | 3043 | (26) | 3044 | (51) |
| 3022 | (11) | 3100 | (11) | 3098 | (20) |
| 3044 | (12) | 3129 | (10) | 3139 | (50) |
| 3069 | (6) | 3133 | (8) | 3140 | (10) |
| 3070 | (20) | 3139 | (11) | 3157 | (19) |
| 3074 | (9) | 3160 | (15) | 3163 | (12) |
| 3089 | (1) | 3164 | (11) | 3173 | (9) |
| 3091 | (20) | 3173 | (10) | 3177 | (45) |
| 3100 | (1) | 3180 | (0) | 3193 | (1) |
| 3117 | (20) | 3196 | (21) | 3209 | (42) |
| 3131 | (25) | 3210 | (21) | 3222 | (51) |
| 3160 | (1) | 3240 | (1) | 3231 | (3) |
| 3166 | (0) | 3244 | (0) | 3234 | (2) |
| 3174 | (6) | 3253 | (3) | 3247 | (20) |
| 3182 | (3) | 3260 | (2) | 3257 | (16) |
| 3191 | (2) | 3269 | (1) | 3266 | (9) |

**Table S46**. Harmonic vibrational frequencies (in $cm^{-1}$) and infrared intensities (in parentheses, in km/mol) for the structure **2Co-9** of $(C_{10}H_8PCH_3)Co(C_5H_5)$ with $C_1$ symmetry.

| BP86 | | B3LYP | | M06-L | |
|---|---|---|---|---|---|
| 36 | (0) | 25 | (0) | 53 | (2) |
| 49 | (2) | 49 | (2) | 56 | (0) |
| 79 | (0) | 77 | (0) | 74 | (0) |
| 108 | (0) | 106 | (0) | 108 | (0) |
| 123 | (0) | 121 | (1) | 128 | (0) |
| 147 | (0) | 153 | (0) | 153 | (0) |
| 175 | (0) | 178 | (0) | 182 | (0) |
| 182 | (0) | 188 | (0) | 192 | (1) |
| 187 | (0) | 191 | (0) | 213 | (0) |
| 204 | (1) | 208 | (0) | 217 | (0) |
| 256 | (1) | 251 | (2) | 262 | (1) |
| 284 | (1) | 297 | (2) | 295 | (1) |
| 295 | (2) | 304 | (2) | 304 | (1) |
| 337 | (0) | 325 | (1) | 351 | (0) |
| 346 | (6) | 339 | (3) | 379 | (5) |
| 371 | (5) | 358 | (6) | 401 | (3) |
| 397 | (3) | 410 | (3) | 414 | (2) |
| 426 | (5) | 434 | (3) | 443 | (3) |
| 433 | (6) | 441 | (7) | 459 | (6) |
| 463 | (11) | 477 | (5) | 481 | (8) |
| 483 | (3) | 497 | (7) | 494 | (7) |
| 519 | (0) | 542 | (1) | 544 | (0) |
| 554 | (2) | 580 | (9) | 586 | (2) |
| 561 | (0) | 583 | (0) | 587 | (6) |
| 566 | (5) | 590 | (0) | 594 | (0) |
| 611 | (1) | 633 | (1) | 640 | (2) |
| 637 | (4) | 663 | (4) | 663 | (4) |
| 645 | (11) | 669 | (8) | 673 | (9) |
| 659 | (15) | 681 | (22) | 702 | (5) |
| 677 | (7) | 702 | (9) | 710 | (24) |
| 684 | (10) | 706 | (2) | 716 | (5) |
| 714 | (22) | 745 | (31) | 742 | (25) |
| 733 | (69) | 762 | (61) | 756 | (56) |
| 762 | (8) | 791 | (38) | 778 | (4) |
| 767 | (30) | 801 | (35) | 791 | (20) |
| 780 | (47) | 817 | (48) | 799 | (42) |
| 801 | (1) | 837 | (3) | 822 | (1) |
| 803 | (1) | 838 | (2) | 828 | (4) |
| 804 | (3) | 840 | (2) | 831 | (0) |
| 816 | (4) | 850 | (4) | 839 | (3) |
| 840 | (13) | 871 | (10) | 867 | (12) |
| 852 | (12) | 886 | (17) | 879 | (2) |
| 855 | (0) | 900 | (10) | 883 | (1) |
| 859 | (3) | 906 | (4) | 887 | (16) |
| 864 | (13) | 906 | (5) | 891 | (7) |
| 880 | (15) | 916 | (17) | 909 | (14) |
| 905 | (9) | 950 | (7) | 940 | (9) |
| 918 | (2) | 968 | (1) | 954 | (1) |
| 924 | (2) | 979 | (1) | 965 | (0) |
| 934 | (1) | 983 | (2) | 968 | (4) |
| 971 | (8) | 1005 | (9) | 1012 | (7) |
| 996 | (12) | 1030 | (13) | 1033 | (10) |
| 1007 | (9) | 1033 | (8) | 1041 | (9) |
| 1031 | (0) | 1065 | (1) | 1066 | (0) |
| 1033 | (1) | 1068 | (0) | 1068 | (1) |
| 1081 | (4) | 1118 | (4) | 1122 | (6) |
| 1102 | (9) | 1136 | (6) | 1140 | (14) |
| 1118 | (5) | 1149 | (4) | 1161 | (8) |

| | | | | | |
|---|---|---|---|---|---|
| 1133 | (4) | 1172 | (10) | 1170 | (1) |
| 1140 | (2) | 1180 | (2) | 1175 | (3) |
| 1181 | (1) | 1221 | (1) | 1220 | (1) |
| 1192 | (3) | 1236 | (4) | 1233 | (5) |
| 1219 | (0) | 1273 | (0) | 1258 | (0) |
| 1238 | (7) | 1285 | (7) | 1280 | (7) |
| 1263 | (3) | 1318 | (4) | 1302 | (3) |
| 1312 | (4) | 1360 | (12) | 1357 | (8) |
| 1343 | (5) | 1388 | (6) | 1394 | (8) |
| 1346 | (4) | 1390 | (7) | 1400 | (1) |
| 1354 | (0) | 1396 | (2) | 1409 | (0) |
| 1359 | (4) | 1407 | (6) | 1414 | (7) |
| 1363 | (4) | 1418 | (2) | 1416 | (8) |
| 1387 | (4) | 1444 | (3) | 1442 | (2) |
| 1413 | (10) | 1461 | (10) | 1452 | (10) |
| 1416 | (1) | 1466 | (4) | 1457 | (3) |
| 1417 | (5) | 1471 | (1) | 1467 | (0) |
| 1428 | (12) | 1479 | (23) | 1481 | (13) |
| 1450 | (6) | 1492 | (20) | 1505 | (10) |
| 1510 | (1) | 1556 | (4) | 1574 | (3) |
| 1593 | (4) | 1655 | (7) | 1670 | (7) |
| 1602 | (4) | 1659 | (8) | 1673 | (7) |
| 2970 | (37) | 3040 | (33) | 3041 | (64) |
| 3012 | (10) | 3096 | (10) | 3083 | (19) |
| 3035 | (15) | 3121 | (11) | 3123 | (27) |
| 3059 | (20) | 3128 | (10) | 3132 | (39) |
| 3063 | (9) | 3140 | (13) | 3154 | (22) |
| 3074 | (11) | 3152 | (17) | 3160 | (21) |
| 3081 | (15) | 3157 | (17) | 3163 | (28) |
| 3089 | (8) | 3171 | (7) | 3168 | (24) |
| 3099 | (1) | 3179 | (0) | 3182 | (6) |
| 3116 | (19) | 3196 | (19) | 3203 | (36) |
| 3131 | (25) | 3209 | (21) | 3221 | (51) |
| 3160 | (1) | 3240 | (1) | 3231 | (0) |
| 3167 | (0) | 3245 | (0) | 3238 | (2) |
| 3175 | (5) | 3254 | (3) | 3251 | (15) |
| 3183 | (2) | 3261 | (1) | 3252 | (19) |
| 3192 | (1) | 3270 | (1) | 3265 | (8) |

**Table S47**. Harmonic vibrational frequencies (in $cm^{-1}$) and infrared intensities (in parentheses, in km/mol) for the structure **2Co-10** of $(C_{10}H_8PCH_3)Co(C_5H_5)$ with $C_1$ symmetry.

| BP86 | | B3LYP | | M06-L | |
|---|---|---|---|---|---|
| 25 | (0) | 24 | (0) | 33 | (0) |
| 36 | (0) | 41 | (0) | 39 | (0) |
| 72 | (0) | 75 | (0) | 73 | (0) |
| 76 | (0) | 79 | (0) | 80 | (1) |
| 158 | (2) | 159 | (1) | 164 | (2) |
| 163 | (1) | 165 | (1) | 168 | (1) |
| 169 | (0) | 176 | (0) | 181 | (0) |
| 180 | (0) | 186 | (0) | 196 | (2) |
| 187 | (2) | 189 | (1) | 210 | (0) |
| 247 | (1) | 255 | (1) | 255 | (1) |
| 250 | (1) | 257 | (1) | 262 | (1) |
| 277 | (1) | 273 | (3) | 291 | (1) |
| 333 | (1) | 318 | (1) | 343 | (16) |
| 336 | (10) | 331 | (13) | 355 | (0) |
| 359 | (2) | 345 | (10) | 385 | (1) |
| 372 | (7) | 359 | (7) | 394 | (0) |
| 381 | (1) | 393 | (4) | 409 | (5) |
| 391 | (1) | 399 | (0) | 415 | (1) |
| 453 | (2) | 460 | (11) | 473 | (8) |
| 463 | (18) | 462 | (2) | 474 | (8) |
| 499 | (25) | 524 | (33) | 519 | (30) |
| 515 | (7) | 534 | (6) | 531 | (7) |
| 551 | (3) | 564 | (8) | 578 | (4) |
| 560 | (8) | 578 | (2) | 586 | (4) |
| 569 | (1) | 598 | (1) | 606 | (2) |
| 596 | (12) | 613 | (10) | 628 | (19) |
| 600 | (8) | 633 | (7) | 629 | (7) |
| 645 | (0) | 663 | (1) | 677 | (1) |
| 664 | (65) | 686 | (46) | 689 | (55) |
| 678 | (42) | 703 | (37) | 720 | (32) |
| 701 | (2) | 725 | (1) | 732 | (0) |
| 706 | (22) | 731 | (36) | 751 | (27) |
| 748 | (3) | 783 | (11) | 765 | (3) |
| 750 | (5) | 784 | (7) | 776 | (3) |
| 771 | (47) | 803 | (71) | 792 | (34) |
| 782 | (13) | 805 | (8) | 813 | (9) |
| 797 | (0) | 831 | (0) | 817 | (1) |
| 800 | (0) | 836 | (0) | 821 | (0) |
| 804 | (2) | 840 | (2) | 830 | (6) |
| 816 | (7) | 849 | (9) | 839 | (4) |
| 821 | (5) | 853 | (5) | 845 | (4) |
| 851 | (0) | 893 | (0) | 868 | (0) |
| 854 | (1) | 898 | (0) | 884 | (1) |
| 858 | (3) | 903 | (2) | 890 | (3) |
| 874 | (3) | 921 | (6) | 911 | (0) |
| 886 | (5) | 923 | (22) | 915 | (4) |
| 889 | (23) | 926 | (2) | 918 | (23) |
| 891 | (2) | 939 | (5) | 921 | (5) |
| 897 | (0) | 955 | (0) | 938 | (0) |
| 924 | (0) | 966 | (0) | 958 | (0) |
| 974 | (9) | 1008 | (10) | 1013 | (7) |
| 992 | (15) | 1026 | (17) | 1027 | (13) |
| 1014 | (3) | 1055 | (3) | 1050 | (4) |
| 1026 | (9) | 1058 | (11) | 1059 | (12) |
| 1030 | (0) | 1064 | (1) | 1063 | (1) |
| 1032 | (0) | 1066 | (0) | 1065 | (1) |
| 1066 | (0) | 1104 | (4) | 1096 | (2) |
| 1097 | (1) | 1134 | (8) | 1133 | (1) |

| | | | | | |
|---|---|---|---|---|---|
| 1101 | (12) | 1137 | (2) | 1140 | (18) |
| 1129 | (0) | 1166 | (0) | 1163 | (0) |
| 1158 | (1) | 1197 | (0) | 1196 | (1) |
| 1164 | (0) | 1205 | (0) | 1205 | (0) |
| 1209 | (11) | 1250 | (10) | 1248 | (11) |
| 1218 | (0) | 1270 | (0) | 1254 | (0) |
| 1279 | (8) | 1332 | (8) | 1322 | (6) |
| 1290 | (0) | 1349 | (0) | 1334 | (1) |
| 1312 | (8) | 1361 | (23) | 1368 | (11) |
| 1328 | (8) | 1382 | (3) | 1381 | (6) |
| 1328 | (4) | 1382 | (4) | 1382 | (7) |
| 1342 | (0) | 1387 | (1) | 1399 | (1) |
| 1357 | (3) | 1397 | (2) | 1412 | (3) |
| 1384 | (3) | 1442 | (3) | 1440 | (1) |
| 1411 | (1) | 1467 | (11) | 1460 | (6) |
| 1415 | (1) | 1468 | (1) | 1461 | (10) |
| 1416 | (1) | 1469 | (3) | 1465 | (0) |
| 1419 | (10) | 1470 | (7) | 1467 | (1) |
| 1421 | (7) | 1472 | (1) | 1471 | (0) |
| 1520 | (23) | 1576 | (18) | 1586 | (22) |
| 1559 | (4) | 1625 | (12) | 1634 | (16) |
| 1563 | (10) | 1628 | (9) | 1644 | (15) |
| 2974 | (29) | 3045 | (26) | 3046 | (55) |
| 3045 | (12) | 3125 | (11) | 3126 | (24) |
| 3046 | (0) | 3126 | (0) | 3127 | (7) |
| 3068 | (12) | 3136 | (13) | 3152 | (20) |
| 3071 | (3) | 3136 | (5) | 3157 | (36) |
| 3080 | (1) | 3159 | (19) | 3159 | (15) |
| 3080 | (10) | 3160 | (9) | 3161 | (24) |
| 3081 | (50) | 3167 | (25) | 3162 | (27) |
| 3082 | (3) | 3168 | (2) | 3164 | (40) |
| 3116 | (7) | 3201 | (5) | 3194 | (20) |
| 3129 | (18) | 3215 | (12) | 3209 | (42) |
| 3158 | (1) | 3236 | (0) | 3229 | (2) |
| 3159 | (1) | 3238 | (1) | 3230 | (2) |
| 3170 | (7) | 3249 | (5) | 3245 | (27) |
| 3178 | (5) | 3256 | (3) | 3251 | (20) |
| 3187 | (2) | 3266 | (1) | 3261 | (11) |

**Table S48**. Harmonic vibrational frequencies (in $cm^{-1}$) and infrared intensities (in parentheses, in km/mol) for the structure **2Co-11** of $(C_{10}H_8PCH_3)Co(C_5H_5)$ with $C_s$ symmetry.

| BP86 | | B3LYP | | M06-L | |
|---|---|---|---|---|---|
| 27 | (0) | 19 | (0) | 16 | (0) |
| 49 | (0) | 48 | (0) | 44 | (0) |
| 66 | (0) | 67 | (0) | 69 | (0) |
| 85 | (1) | 84 | (1) | 93 | (1) |
| 162 | (0) | 159 | (0) | 162 | (0) |
| 163 | (1) | 164 | (1) | 174 | (1) |
| 189 | (0) | 192 | (0) | 191 | (1) |
| 204 | (1) | 213 | (0) | 215 | (0) |
| 214 | (2) | 216 | (1) | 230 | (2) |
| 227 | (1) | 239 | (1) | 245 | (0) |
| 237 | (0) | 246 | (0) | 246 | (1) |
| 299 | (1) | 285 | (7) | 308 | (1) |
| 339 | (0) | 327 | (0) | 358 | (0) |
| 351 | (5) | 338 | (3) | 367 | (4) |
| 361 | (2) | 362 | (9) | 377 | (1) |
| 369 | (2) | 375 | (8) | 391 | (2) |
| 380 | (8) | 386 | (1) | 408 | (8) |
| 398 | (1) | 399 | (2) | 419 | (1) |
| 456 | (1) | 462 | (11) | 476 | (2) |
| 468 | (15) | 465 | (1) | 481 | (11) |
| 492 | (17) | 515 | (25) | 516 | (23) |
| 528 | (2) | 547 | (3) | 551 | (2) |
| 554 | (1) | 561 | (5) | 584 | (1) |
| 556 | (9) | 579 | (1) | 590 | (7) |
| 572 | (3) | 597 | (2) | 600 | (3) |
| 614 | (25) | 630 | (25) | 644 | (34) |
| 641 | (5) | 662 | (0) | 670 | (5) |
| 646 | (2) | 670 | (6) | 678 | (0) |
| 647 | (29) | 671 | (31) | 683 | (25) |
| 675 | (17) | 694 | (15) | 702 | (8) |
| 698 | (1) | 724 | (1) | 729 | (1) |
| 719 | (62) | 751 | (61) | 750 | (58) |
| 753 | (2) | 784 | (11) | 773 | (2) |
| 763 | (6) | 800 | (6) | 794 | (5) |
| 773 | (49) | 803 | (68) | 798 | (34) |
| 789 | (1) | 815 | (2) | 822 | (1) |
| 800 | (0) | 835 | (0) | 822 | (0) |
| 806 | (3) | 837 | (0) | 829 | (1) |
| 809 | (0) | 841 | (1) | 830 | (4) |
| 823 | (9) | 855 | (12) | 847 | (8) |
| 830 | (3) | 860 | (2) | 855 | (2) |
| 859 | (0) | 898 | (0) | 879 | (0) |
| 863 | (1) | 900 | (2) | 887 | (0) |
| 866 | (4) | 904 | (3) | 888 | (3) |
| 868 | (5) | 904 | (3) | 891 | (3) |
| 887 | (47) | 921 | (46) | 909 | (43) |
| 894 | (1) | 931 | (2) | 923 | (1) |
| 911 | (6) | 969 | (7) | 949 | (7) |
| 928 | (0) | 969 | (0) | 964 | (0) |
| 934 | (0) | 990 | (1) | 973 | (1) |
| 975 | (8) | 1008 | (10) | 1014 | (7) |

| | | | | | |
|---|---|---|---|---|---|
| 993 | (14) | 1026 | (16) | 1030 | (12) |
| 1017 | (4) | 1056 | (4) | 1051 | (5) |
| 1027 | (7) | 1060 | (8) | 1065 | (4) |
| 1031 | (1) | 1064 | (1) | 1065 | (7) |
| 1033 | (0) | 1066 | (0) | 1067 | (0) |
| 1067 | (0) | 1103 | (1) | 1097 | (0) |
| 1101 | (12) | 1134 | (8) | 1143 | (17) |
| 1116 | (2) | 1154 | (3) | 1153 | (1) |
| 1145 | (2) | 1175 | (1) | 1183 | (2) |
| 1167 | (0) | 1208 | (1) | 1208 | (0) |
| 1186 | (1) | 1234 | (1) | 1221 | (1) |
| 1219 | (0) | 1271 | (0) | 1256 | (0) |
| 1238 | (17) | 1283 | (15) | 1277 | (18) |
| 1267 | (8) | 1323 | (8) | 1303 | (6) |
| 1300 | (0) | 1357 | (0) | 1342 | (0) |
| 1312 | (17) | 1362 | (36) | 1368 | (21) |
| 1342 | (6) | 1387 | (0) | 1392 | (5) |
| 1343 | (0) | 1397 | (3) | 1393 | (26) |
| 1345 | (25) | 1398 | (4) | 1402 | (0) |
| 1358 | (2) | 1402 | (19) | 1416 | (2) |
| 1385 | (4) | 1442 | (3) | 1441 | (1) |
| 1408 | (8) | 1458 | (8) | 1445 | (7) |
| 1410 | (4) | 1468 | (1) | 1454 | (3) |
| 1414 | (1) | 1468 | (6) | 1467 | (0) |
| 1416 | (0) | 1469 | (3) | 1469 | (1) |
| 1419 | (3) | 1472 | (0) | 1470 | (1) |
| 1506 | (65) | 1557 | (69) | 1570 | (75) |
| 1550 | (6) | 1616 | (20) | 1616 | (12) |
| 1562 | (4) | 1625 | (3) | 1632 | (8) |
| 2976 | (21) | 3048 | (21) | 3040 | (40) |
| 3025 | (25) | 3110 | (21) | 3090 | (53) |
| 3026 | (2) | 3111 | (1) | 3092 | (6) |
| 3065 | (6) | 3131 | (7) | 3139 | (44) |
| 3080 | (6) | 3153 | (11) | 3140 | (3) |
| 3081 | (13) | 3159 | (24) | 3148 | (9) |
| 3081 | (43) | 3160 | (9) | 3151 | (50) |
| 3082 | (5) | 3168 | (23) | 3152 | (27) |
| 3083 | (4) | 3169 | (3) | 3155 | (11) |
| 3116 | (7) | 3201 | (5) | 3183 | (16) |
| 3130 | (16) | 3216 | (10) | 3198 | (36) |
| 3160 | (0) | 3237 | (0) | 3226 | (2) |
| 3161 | (1) | 3239 | (1) | 3226 | (2) |
| 3171 | (7) | 3249 | (5) | 3241 | (22) |
| 3179 | (4) | 3257 | (2) | 3250 | (18) |
| 3189 | (1) | 3266 | (1) | 3258 | (8) |

**Table S49**. Cartesian coordinates for the structures of $C_6H_6PCH_3$, $C_{10}H_8PCH_3$, $(C_6H_6PCH_3)Fe(CO)_3$, $(C_6H_6PCH_3)Co(C_5H_5)$, $(C_{10}H_8PCH_3)Fe(CO)_3$ and $(C_{10}H_8PCH_3)Co(C_5H_5)$.

$C_6H_6PCH_3$

**1-1**($C_s$) / BP86

| | | | |
|---|---|---|---|
| C | -0.81853300 | 1.65956900 | 0.72937100 |
| C | -0.81853300 | 0.48012200 | 1.43376100 |
| C | -0.81853300 | 0.48012200 | -1.43376100 |
| C | -0.81853300 | 1.65956900 | -0.72937100 |
| H | -0.90544200 | 2.61445300 | 1.26227500 |
| H | -0.93426500 | 0.48712800 | 2.52508100 |
| H | -0.93426500 | 0.48712800 | -2.52508100 |
| H | -0.90544200 | 2.61445300 | -1.26227500 |
| C | -0.67956600 | -0.82571300 | 0.76806400 |
| H | -1.16944500 | -1.67188700 | 1.26780300 |
| C | -0.67956600 | -0.82571300 | -0.76806400 |
| H | -1.16944500 | -1.67188700 | -1.26780300 |
| P | 0.99046300 | -1.39343400 | 0.00000000 |
| C | 2.03101700 | 0.14954100 | 0.00000000 |
| H | 3.08723900 | -0.17242500 | 0.00000000 |
| H | 1.84380300 | 0.77478400 | 0.89085800 |
| H | 1.84380300 | 0.77478400 | -0.89085800 |

**1-1**($C_s$) / B3LYP

| | | | |
|---|---|---|---|
| C | -0.80388900 | 1.67142900 | 0.72883200 |
| C | -0.80388900 | 0.50337500 | 1.42788700 |
| C | -0.80388900 | 0.50337500 | -1.42788700 |
| C | -0.80388900 | 1.67142900 | -0.72883200 |
| H | -0.88040900 | 2.62078200 | 1.25572400 |
| H | -0.90637400 | 0.51189900 | 2.51198700 |
| H | -0.90637400 | 0.51189900 | -2.51198700 |
| H | -0.88040900 | 2.62078200 | -1.25572400 |
| C | -0.68605600 | -0.80433100 | 0.76326000 |
| H | -1.19800500 | -1.62811700 | 1.25961300 |
| C | -0.68605600 | -0.80433100 | -0.76326000 |
| H | -1.19800500 | -1.62811700 | -1.25961300 |
| P | 0.95613200 | -1.41103300 | 0.00000000 |
| C | 2.04853300 | 0.09070100 | 0.00000000 |
| H | 3.08469700 | -0.26655700 | 0.00000000 |
| H | 1.88885000 | 0.71652000 | 0.88463300 |
| H | 1.88885000 | 0.71652000 | -0.88463300 |

**1-1**($C_s$) / M06-L

| | | | |
|---|---|---|---|
| C | -0.80419400 | 1.63213300 | 0.72336100 |
| C | -0.80419400 | 0.46515600 | 1.41914400 |
| C | -0.80419400 | 0.46515600 | -1.41914400 |
| C | -0.80419400 | 1.63213300 | -0.72336100 |
| H | -0.89334400 | 2.57647500 | 1.25178000 |
| H | -0.91760600 | 0.47165900 | 2.49937500 |
| H | -0.91760600 | 0.47165900 | -2.49937500 |
| H | -0.89334400 | 2.57647500 | -1.25178000 |
| C | -0.65990500 | -0.82884000 | 0.75976700 |
| H | -1.14461200 | -1.66847800 | 1.25164700 |
| C | -0.65990500 | -0.82884000 | -0.75976700 |
| H | -1.14461200 | -1.66847800 | -1.25164700 |
| P | 0.98060600 | -1.36871700 | 0.00000000 |
| C | 1.97363200 | 0.17733400 | 0.00000000 |
| H | 3.02842200 | -0.10579100 | 0.00000000 |
| H | 1.77567100 | 0.79592000 | 0.88050700 |
| H | 1.77567100 | 0.79592000 | -0.88050700 |

**1-2**($C_s$) / BP86

| | | | |
|---|---|---|---|
| C | -0.10073400 | -2.22142900 | 0.73204800 |
| C | 0.28250200 | -1.11286900 | 1.43769600 |
| C | 0.28250200 | -1.11286900 | -1.43769600 |
| C | -0.10073400 | -2.22142900 | -0.73204800 |
| H | -0.33959300 | -3.15174200 | 1.26191000 |
| H | 0.38053200 | -1.15391900 | 2.52976000 |
| H | 0.38053200 | -1.15391900 | -2.52976000 |
| H | -0.33959300 | -3.15174200 | -1.26191000 |
| C | 0.58707400 | 0.17251000 | 0.76954400 |
| H | 1.33063600 | 0.80465500 | 1.27383900 |
| C | 0.58707400 | 0.17251000 | -0.76954400 |
| H | 1.33063600 | 0.80465500 | -1.27383900 |
| P | -0.82910200 | 1.19515100 | 0.00000000 |
| C | 0.00000000 | 2.88192700 | 0.00000000 |
| H | -0.31769500 | 3.44931300 | -0.89302100 |
| H | -0.31769500 | 3.44931300 | 0.89302100 |
| H | 1.10255200 | 2.82612200 | 0.00000000 |

**1-2**($C_s$) / B3LYP

| | | | |
|---|---|---|---|
| C | 0.55335200 | -2.14605300 | -0.73175500 |
| C | -0.03624100 | -1.14449500 | -1.43197100 |
| C | -0.03624100 | -1.14449500 | 1.43197100 |
| C | 0.55335200 | -2.14605300 | 0.73175500 |
| H | 0.97728900 | -3.00075000 | -1.25563100 |
| H | -0.11173400 | -1.19846300 | -2.51675300 |
| H | -0.11173400 | -1.19846300 | 2.51675300 |
| H | 0.97728900 | -3.00075000 | 1.25563100 |
| C | -0.60437600 | 0.04735000 | -0.76491700 |
| H | -1.46312700 | 0.49514900 | -1.26438500 |
| C | -0.60437600 | 0.04735000 | 0.76491700 |
| H | -1.46312700 | 0.49514900 | 1.26438500 |
| P | 0.55335200 | 1.33747400 | 0.00000000 |
| C | -0.59832100 | 2.81232500 | 0.00000000 |
| H | -0.40520100 | 3.42853600 | 0.88616300 |
| H | -0.40520100 | 3.42853600 | -0.88616300 |
| H | -1.65775400 | 2.53343500 | 0.00000000 |

**1-2**($C_s$) / M06-L

| | | | |
|---|---|---|---|
| C | 0.39670700 | -2.16057800 | 0.72574000 |
| C | 0.51671800 | -1.00613900 | 1.42276200 |
| C | 0.51671800 | -1.00613900 | -1.42276200 |
| C | 0.39670700 | -2.16057800 | -0.72574000 |
| H | 0.37599500 | -3.11001000 | 1.25206000 |
| H | 0.61688000 | -1.02333600 | 2.50399900 |
| H | 0.61688000 | -1.02333600 | -2.50399900 |
| H | 0.37599500 | -3.11001000 | -1.25206000 |
| C | 0.51671800 | 0.30301000 | 0.76061100 |
| H | 1.09111800 | 1.08382500 | 1.25524000 |
| C | 0.51671800 | 0.30301000 | -0.76061100 |
| H | 1.09111800 | 1.08382500 | -1.25524000 |
| P | -1.06551500 | 0.96339800 | 0.00000000 |
| C | -0.62087900 | 2.76237100 | 0.00000000 |
| H | -1.04061400 | 3.25310000 | -0.88204800 |
| H | -1.04061400 | 3.25310000 | 0.88204800 |
| H | 0.45951000 | 2.93211800 | 0.00000000 |

**1-3**($C_s$) / BP86

| | | | |
|---|---|---|---|
| C | 0.21103400 | -2.10204400 | 0.69021700 |
| C | 0.21103400 | -2.10204400 | -0.69021700 |
| C | -0.32633100 | -1.07290400 | -1.57729700 |
| C | -0.32633100 | -1.07290400 | 1.57729700 |
| C | -0.32633100 | 0.27884400 | -1.36494100 |
| C | -0.32633100 | 0.27884400 | 1.36494100 |
| H | 0.52861200 | -3.03421400 | 1.18017900 |
| H | 0.52861200 | -3.03421400 | -1.18017900 |
| H | -0.78764300 | -1.44521500 | -2.50540900 |
| H | -0.78764300 | -1.44521500 | 2.50540900 |
| H | -0.85461800 | 0.92954400 | -2.07810900 |
| H | -0.85461800 | 0.92954400 | 2.07810900 |
| P | 0.62022100 | 1.06015700 | 0.00000000 |
| C | -0.15205600 | 2.76218400 | 0.00000000 |
| H | 0.19592000 | 3.31685900 | 0.88870500 |
| H | 0.19592000 | 3.31685900 | -0.88870500 |
| H | -1.25598900 | 2.74384900 | 0.00000000 |

**1-3**($C_s$) / B3LYP

| | | | |
|---|---|---|---|
| C | -0.23695600 | -2.09636600 | 0.68328300 |
| C | -0.23695600 | -2.09636600 | -0.68328300 |
| C | -0.53185000 | -0.97717700 | -1.57639600 |
| C | -0.53185000 | -0.97717700 | 1.57639600 |
| C | -0.23695600 | 0.33076300 | -1.37307300 |
| C | -0.23695600 | 0.33076300 | 1.37307300 |
| H | -0.11566100 | -3.06484000 | 1.17118700 |
| H | -0.11566100 | -3.06484000 | -1.17118700 |
| H | -1.05310800 | -1.24521900 | -2.49825900 |
| H | -1.05310800 | -1.24521900 | 2.49825900 |
| H | -0.58930400 | 1.06529600 | -2.09974800 |
| H | -0.58930400 | 1.06529600 | 2.09974800 |
| P | 0.82225600 | 0.91604000 | 0.00000000 |
| C | 0.38342200 | 2.72472500 | 0.00000000 |
| H | 0.82383200 | 3.20245400 | 0.88239600 |
| H | 0.82383200 | 3.20245400 | -0.88239600 |
| H | -0.69674900 | 2.90904200 | 0.00000000 |

**1-3**($C_s$) / M06-L

| | | | |
|---|---|---|---|
| C | -0.25205000 | -2.07090000 | 0.68217200 |
| C | -0.25205000 | -2.07090000 | -0.68217200 |
| C | -0.56017700 | -0.95885300 | -1.56052200 |
| C | -0.56017700 | -0.95885300 | 1.56052200 |
| C | -0.25205000 | 0.34242100 | -1.35387600 |
| C | -0.25205000 | 0.34242100 | 1.35387600 |
| H | -0.13600000 | -3.03885500 | 1.16682100 |
| H | -0.13600000 | -3.03885500 | -1.16682100 |
| H | -1.10317000 | -1.21630800 | -2.46997300 |
| H | -1.10317000 | -1.21630800 | 2.46997300 |
| H | -0.61713600 | 1.08911800 | -2.05942700 |
| H | -0.61713600 | 1.08911800 | 2.05942700 |
| P | 0.83343200 | 0.88231700 | 0.00000000 |
| C | 0.46155300 | 2.68824800 | 0.00000000 |
| H | 0.91172700 | 3.15518200 | 0.87886200 |
| H | 0.91172700 | 3.15518200 | -0.87886200 |
| H | -0.61031800 | 2.90548400 | 0.00000000 |

**1-4**($C_s$) / BP86

| | | | |
|---|---|---|---|
| C | -0.84568000 | 1.65422000 | 0.69192000 |
| C | -0.84568000 | 1.65422000 | -0.69192000 |
| C | -0.84568000 | 0.51333600 | -1.58850000 |
| C | -0.84568000 | 0.51333600 | 1.58850000 |
| C | -0.34973600 | -0.75202200 | -1.38485000 |
| C | -0.34973600 | -0.75202200 | 1.38485000 |
| H | -1.00423300 | 2.62971100 | 1.17447800 |
| H | -1.00423300 | 2.62971100 | -1.17447800 |
| H | -1.33317900 | 0.70157700 | -2.55994000 |
| H | -1.33317900 | 0.70157700 | 2.55994000 |
| H | -0.58062900 | -1.50282700 | -2.15507900 |
| H | -0.58062900 | -1.50282700 | 2.15507900 |
| P | 0.70405000 | -1.35707100 | 0.00000000 |
| C | 2.09522200 | -0.10821200 | 0.00000000 |
| H | 2.71912400 | -0.28927900 | -0.89313800 |
| H | 1.75891400 | 0.94058200 | 0.00000000 |
| H | 2.71912400 | -0.28927900 | 0.89313800 |

**1-4**($C_s$) / B3LYP

| | | | |
|---|---|---|---|
| C | -0.83504000 | 1.66614700 | 0.68477400 |
| C | -0.83504000 | 1.66614700 | -0.68477400 |
| C | -0.83504000 | 0.52989100 | -1.58895500 |
| C | -0.83504000 | 0.52989100 | 1.58895500 |
| C | -0.34406400 | -0.72519600 | -1.39583000 |
| C | -0.34406400 | -0.72519600 | 1.39583000 |
| H | -0.97351600 | 2.63620100 | 1.16462400 |
| H | -0.97351600 | 2.63620100 | -1.16462400 |
| H | -1.31410400 | 0.72786200 | -2.55228100 |
| H | -1.31410400 | 0.72786200 | 2.55228100 |
| H | -0.55189200 | -1.45490400 | -2.18019700 |
| H | -0.55189200 | -1.45490400 | 2.18019700 |
| P | 0.66383200 | -1.36362300 | 0.00000000 |
| C | 2.10632700 | -0.18448800 | 0.00000000 |
| H | 2.71815800 | -0.38827500 | -0.88652900 |
| H | 1.81699000 | 0.86940600 | 0.00000000 |
| H | 2.71815800 | -0.38827500 | 0.88652900 |

**1-4**($C_s$) / M06-L

| | | | |
|---|---|---|---|
| C | -0.84529700 | 1.61642100 | 0.68403500 |
| C | -0.84529700 | 1.61642100 | -0.68403500 |
| C | -0.84529700 | 0.48190300 | -1.57040800 |
| C | -0.84529700 | 0.48190300 | 1.57040800 |
| C | -0.33787800 | -0.76328800 | -1.36969400 |
| C | -0.33787800 | -0.76328800 | 1.36969400 |
| H | -1.00294400 | 2.58161200 | 1.16183400 |
| H | -1.00294400 | 2.58161200 | -1.16183400 |
| H | -1.34200200 | 0.65969300 | -2.52633400 |
| H | -1.34200200 | 0.65969300 | 2.52633400 |
| H | -0.56271700 | -1.50978200 | -2.13043000 |
| H | -0.56271700 | -1.50978200 | 2.13043000 |
| P | 0.72654700 | -1.32714500 | 0.00000000 |
| C | 2.04173600 | -0.03479800 | 0.00000000 |
| H | 2.67021800 | -0.17930400 | -0.88238700 |
| H | 1.66792200 | 0.99107600 | 0.00000000 |
| H | 2.67021800 | -0.17930400 | 0.88238700 |

$C_{10}H_8PCH_3$

**2-1**($C_s$) / BP86

| | | | |
|---|---|---|---|
| C | -0.18723000 | -1.00751000 | 0.71839400 |
| C | -0.18723000 | -1.00751000 | -0.71839400 |
| C | -0.48217500 | 0.15262200 | -1.58476200 |
| C | -0.23742900 | 1.47824200 | -1.38930800 |
| C | -0.23742900 | 1.47824200 | 1.38930800 |
| C | -0.48217500 | 0.15262200 | 1.58476200 |
| C | 0.01889100 | -2.24320100 | 1.39118400 |
| C | 0.26584000 | -3.44261700 | 0.70550000 |
| C | 0.26584000 | -3.44261700 | -0.70550000 |
| C | 0.01889100 | -2.24320100 | -1.39118400 |
| P | 0.69020800 | 2.22172300 | 0.00000000 |
| C | -0.04596000 | 3.94053500 | 0.00000000 |
| H | -0.93434300 | -0.12188200 | -2.55047900 |
| H | -0.53789900 | 2.17225800 | -2.18866500 |
| H | -0.53789900 | 2.17225800 | 2.18866500 |
| H | -0.93434300 | -0.12188200 | 2.55047900 |
| H | -0.01288100 | -2.24722100 | 2.48877100 |
| H | 0.43893700 | -4.37075800 | 1.26307700 |
| H | 0.43893700 | -4.37075800 | -1.26307700 |
| H | -0.01288100 | -2.24722100 | -2.48877100 |
| H | -1.14940100 | 3.94143400 | 0.00000000 |
| H | 0.31482200 | 4.48713500 | -0.88865000 |
| H | 0.31482200 | 4.48713500 | 0.88865000 |

**2-1**($C_s$) / B3LYP

| | | | |
|---|---|---|---|
| C | -0.19348300 | -1.00373000 | 0.71334400 |
| C | -0.19348300 | -1.00373000 | -0.71334400 |
| C | -0.48860600 | 0.15587900 | -1.57956700 |
| C | -0.23385500 | 1.46835900 | -1.38790500 |
| C | -0.23385500 | 1.46835900 | 1.38790500 |
| C | -0.48860600 | 0.15587900 | 1.57956700 |
| C | 0.01969000 | -2.23030700 | 1.38368100 |
| C | 0.26974500 | -3.42187200 | 0.70163600 |
| C | 0.26974500 | -3.42187200 | -0.70163600 |
| C | 0.01969000 | -2.23030700 | -1.38368100 |
| P | 0.69097900 | 2.20680200 | 0.00000000 |
| C | -0.04247100 | 3.91820900 | 0.00000000 |
| H | -0.94800600 | -0.11688800 | -2.53182800 |
| H | -0.53005700 | 2.15759600 | -2.18084400 |
| H | -0.53005700 | 2.15759600 | 2.18084400 |
| H | -0.94800600 | -0.11688800 | 2.53182800 |
| H | -0.00871300 | -2.23524600 | 2.47233400 |
| H | 0.44655500 | -4.34195200 | 1.25467400 |
| H | 0.44655500 | -4.34195200 | -1.25467400 |
| H | -0.00871300 | -2.23524600 | -2.47233400 |
| H | -1.13780200 | 3.91780900 | 0.00000000 |
| H | 0.31324800 | 4.46197200 | -0.88239800 |
| H | 0.31324800 | 4.46197200 | 0.88239800 |

**2-1**($C_s$) / M06-L

| | | | |
|---|---|---|---|
| C | -0.19131100 | -0.99595300 | 0.71145900 |
| C | -0.19131100 | -0.99595300 | -0.71145900 |
| C | -0.49138000 | 0.15550700 | -1.56745300 |
| C | -0.23985700 | 1.46549000 | -1.37427500 |
| C | -0.23985700 | 1.46549000 | 1.37427500 |
| C | -0.49138000 | 0.15550700 | 1.56745300 |
| C | 0.01884900 | -2.21884500 | 1.37752600 |
| C | 0.27331100 | -3.40426700 | 0.69869900 |
| C | 0.27331100 | -3.40426700 | -0.69869900 |
| C | 0.01884900 | -2.21884500 | -1.37752600 |
| P | 0.68879900 | 2.19172500 | 0.00000000 |
| C | -0.02958400 | 3.89063000 | 0.00000000 |
| H | -0.94990700 | -0.11699000 | -2.51905500 |
| H | -0.53910300 | 2.15568700 | -2.16336000 |
| H | -0.53910300 | 2.15568700 | 2.16336000 |
| H | -0.94990700 | -0.11699000 | 2.51905500 |
| H | -0.01687300 | -2.22010800 | 2.46473400 |
| H | 0.45072700 | -4.32190200 | 1.25087700 |
| H | 0.45072700 | -4.32190200 | -1.25087700 |
| H | -0.01687300 | -2.22010800 | -2.46473400 |
| H | -1.12274800 | 3.89142900 | 0.00000000 |
| H | 0.32161100 | 4.43618100 | -0.87879800 |
| H | 0.32161100 | 4.43618100 | 0.87879800 |

**2-2**($C_s$) / BP86

| | | | |
|---|---|---|---|
| C | 0.28358400 | -0.82047400 | -0.71939500 |
| C | 0.28358400 | -0.82047400 | 0.71939500 |
| C | 0.71103200 | 0.28631000 | 1.58876400 |
| C | 0.68960600 | 1.63807200 | 1.40087500 |
| C | 0.68960600 | 1.63807200 | -1.40087500 |
| C | 0.71103200 | 0.28631000 | -1.58876400 |
| C | -0.05721500 | -2.03010000 | -1.39137500 |
| C | -0.44065200 | -3.19037000 | -0.70666200 |
| C | -0.44065200 | -3.19037000 | 0.70666200 |
| C | -0.05721500 | -2.03010000 | 1.39137500 |
| P | 0.00000000 | 2.61446700 | 0.00000000 |
| C | -1.78392200 | 2.03708200 | 0.00000000 |
| H | 1.09214400 | -0.05776400 | 2.56489200 |
| H | 1.11657900 | 2.24700200 | 2.21116700 |
| H | 1.11657900 | 2.24700200 | -2.21116700 |
| H | 1.09214400 | -0.05776400 | -2.56489200 |
| H | -0.02474400 | -2.03885600 | -2.48876700 |
| H | -0.71839100 | -4.09317300 | -1.26345700 |
| H | -0.71839100 | -4.09317300 | 1.26345700 |
| H | -0.02474400 | -2.03885600 | 2.48876700 |
| H | -2.28353800 | 2.45191600 | -0.89325000 |
| H | -2.28353800 | 2.45191600 | 0.89325000 |
| H | -1.89699000 | 0.94097000 | 0.00000000 |

**2-2**($C_s$) / B3LYP

| | | | |
|---|---|---|---|
| C | 0.29021000 | -0.82366000 | -0.71404300 |
| C | 0.29021000 | -0.82366000 | 0.71404300 |
| C | 0.70676000 | 0.28543100 | 1.58553600 |
| C | 0.67002900 | 1.62601100 | 1.40319700 |
| C | 0.67002900 | 1.62601100 | -1.40319700 |
| C | 0.70676000 | 0.28543100 | -1.58553600 |
| C | -0.04871600 | -2.02549800 | -1.38342100 |
| C | -0.42592900 | -3.18100100 | -0.70258700 |
| C | -0.42592900 | -3.18100100 | 0.70258700 |
| C | -0.04871600 | -2.02549800 | 1.38342100 |
| P | 0.00000000 | 2.60014300 | 0.00000000 |
| C | -1.78720200 | 2.06039100 | 0.00000000 |
| H | 1.08714500 | -0.05560200 | 2.55224800 |
| H | 1.07570200 | 2.23105300 | 2.21536600 |
| H | 1.07570200 | 2.23105300 | -2.21536600 |
| H | 1.08714500 | -0.05560200 | -2.55224800 |
| H | -0.01936800 | -2.03485200 | -2.47185800 |
| H | -0.69963900 | -4.07724100 | -1.25520900 |
| H | -0.69963900 | -4.07724100 | 1.25520900 |
| H | -0.01936800 | -2.03485200 | 2.47185800 |
| H | -2.27723000 | 2.47933100 | -0.88654300 |
| H | -2.27723000 | 2.47933100 | 0.88654300 |
| H | -1.91837900 | 0.97477000 | 0.00000000 |

**2-2**($C_s$) / M06-L

| | | | |
|---|---|---|---|
| C | 0.32260500 | 0.77999200 | 0.71257100 |
| C | 0.32260500 | 0.77999200 | -0.71257100 |
| C | 0.72903700 | -0.32963800 | -1.56843400 |
| C | 0.64996300 | -1.66493300 | -1.38011800 |
| C | 0.64996300 | -1.66493300 | 1.38011800 |
| C | 0.72903700 | -0.32963800 | 1.56843400 |
| C | 0.00508900 | 1.98326400 | 1.37829200 |
| C | -0.36191000 | 3.13589000 | 0.69996600 |
| C | -0.36191000 | 3.13589000 | -0.69996600 |
| C | 0.00508900 | 1.98326400 | -1.37829200 |
| P | -0.13124900 | -2.56610600 | 0.00000000 |
| C | -1.81509500 | -1.80316900 | 0.00000000 |
| H | 1.13997000 | 0.00052900 | -2.52548100 |
| H | 1.06866500 | -2.28874500 | -2.16830900 |
| H | 1.06866500 | -2.28874500 | 2.16830900 |
| H | 1.13997000 | 0.00052900 | 2.52548100 |
| H | 0.04174400 | 1.98840600 | 2.46528200 |
| H | -0.62543300 | 4.03277100 | 1.25136600 |
| H | -0.62543300 | 4.03277100 | -1.25136600 |
| H | 0.04174400 | 1.98840600 | -2.46528200 |
| H | -2.35839500 | -2.14988600 | 0.88255700 |
| H | -2.35839500 | -2.14988600 | -0.88255700 |
| H | -1.81119700 | -0.71045800 | 0.00000000 |

**2-3**($C_s$) / BP86

| | | | |
|---|---|---|---|
| C | -0.31822700 | 0.76765200 | 0.74003300 |
| C | -0.31822700 | 0.76765200 | -0.74003300 |
| C | -0.72126700 | -0.36959200 | -1.43136700 |
| C | -0.99041500 | -1.64266600 | -0.77212100 |
| C | -0.99041500 | -1.64266600 | 0.77212100 |
| C | -0.72126700 | -0.36959200 | 1.43136700 |
| C | 0.00467200 | 2.00495700 | 1.42600700 |
| C | 0.31610300 | 3.15009100 | 0.72518900 |
| C | 0.31610300 | 3.15009100 | -0.72518900 |
| C | 0.00467200 | 2.00495700 | -1.42600700 |
| P | 0.43296900 | -2.70117100 | 0.00000000 |
| C | 1.89729900 | -1.55485500 | 0.00000000 |
| H | -0.85583600 | -0.31692600 | -2.51953400 |
| H | -1.70790700 | -2.30594200 | -1.27234500 |
| H | -1.70790700 | -2.30594200 | 1.27234500 |
| H | -0.85583600 | -0.31692600 | 2.51953400 |
| H | 0.00000000 | 2.00786700 | 2.52381900 |
| H | 0.56141300 | 4.07552800 | 1.26017900 |
| H | 0.56141300 | 4.07552800 | -1.26017900 |
| H | 0.00000000 | 2.00786700 | -2.52381900 |
| H | 1.91803000 | -0.90431600 | 0.89198200 |
| H | 2.80001000 | -2.19103800 | 0.00000000 |
| H | 1.91803000 | -0.90431600 | -0.89198200 |

**2-3**($C_s$) / B3LYP

| | | | |
|---|---|---|---|
| C | -0.31514400 | 0.77118100 | 0.73765300 |
| C | -0.31514400 | 0.77118100 | -0.73765300 |
| C | -0.70688300 | -0.35613400 | -1.42440100 |
| C | -0.98865700 | -1.62602600 | -0.76633600 |
| C | -0.98865700 | -1.62602600 | 0.76633600 |
| C | -0.70688300 | -0.35613400 | 1.42440100 |
| C | 0.01006300 | 2.00883900 | 1.42084800 |
| C | 0.31935700 | 3.14219200 | 0.72504100 |
| C | 0.31935700 | 3.14219200 | -0.72504100 |
| C | 0.01006300 | 2.00883900 | -1.42084800 |
| P | 0.40691100 | -2.70333400 | 0.00000000 |
| C | 1.89504300 | -1.59560900 | 0.00000000 |
| H | -0.82669300 | -0.30819200 | -2.50568000 |
| H | -1.71360400 | -2.26803500 | -1.26475200 |
| H | -1.71360400 | -2.26803500 | 1.26475200 |
| H | -0.82669300 | -0.30819200 | 2.50568000 |
| H | 0.00553900 | 2.01252700 | 2.50980800 |
| H | 0.56390600 | 4.06146900 | 1.25344900 |
| H | 0.56390600 | 4.06146900 | -1.25344900 |
| H | 0.00553900 | 2.01252700 | -2.50980800 |
| H | 1.93367700 | -0.95200700 | 0.88547200 |
| H | 2.77558500 | -2.24847900 | 0.00000000 |
| H | 1.93367700 | -0.95200700 | -0.88547200 |

**2-3**($C_s$) / M06-L

| | | | |
|---|---|---|---|
| C | -0.32079100 | 0.74635600 | 0.73340800 |
| C | -0.32079100 | 0.74635600 | -0.73340800 |
| C | -0.71395100 | -0.38075000 | -1.41713300 |
| C | -0.96327700 | -1.64670800 | -0.76375600 |
| C | -0.96327700 | -1.64670800 | 0.76375600 |
| C | -0.71395100 | -0.38075000 | 1.41713300 |
| C | -0.00524800 | 1.97596000 | 1.41226100 |
| C | 0.30137600 | 3.10930400 | 0.71938500 |
| C | 0.30137600 | 3.10930400 | -0.71938500 |
| C | -0.00524800 | 1.97596000 | -1.41226100 |
| P | 0.44952800 | -2.65412100 | 0.00000000 |
| C | 1.85781400 | -1.47419600 | 0.00000000 |
| H | -0.84521100 | -0.32801100 | -2.49507900 |
| H | -1.66797000 | -2.31237500 | -1.25555200 |
| H | -1.66797000 | -2.31237500 | 1.25555200 |
| H | -0.84521100 | -0.32801100 | 2.49507900 |
| H | -0.01099700 | 1.97680100 | 2.49955600 |
| H | 0.54218800 | 4.02521400 | 1.25030800 |
| H | 0.54218800 | 4.02521400 | -1.25030800 |
| H | -0.01099700 | 1.97680100 | -2.49955600 |
| H | 1.85969500 | -0.82644400 | 0.88174400 |
| H | 2.77748700 | -2.06332200 | 0.00000000 |
| H | 1.85969500 | -0.82644400 | -0.88174400 |

**2-4**($C_s$) / BP86

| | | | |
|---|---|---|---|
| C | 0.17376200 | -1.04153200 | 0.74218300 |
| C | 0.17376200 | -1.04153200 | -0.74218300 |
| C | 0.48866600 | 0.11619400 | -1.43426500 |
| C | 0.65814000 | 1.41424800 | -0.77364100 |
| C | 0.65814000 | 1.41424800 | 0.77364100 |
| C | 0.48866600 | 0.11619400 | 1.43426500 |
| C | -0.07052500 | -2.29957300 | 1.42738300 |
| C | -0.31065500 | -3.45978600 | 0.72648000 |
| C | -0.31065500 | -3.45978600 | -0.72648000 |
| C | -0.07052500 | -2.29957300 | -1.42738300 |
| P | -0.85614500 | 2.30711900 | 0.00000000 |
| C | -0.17352400 | 4.05815000 | 0.00000000 |
| H | 0.62382100 | 0.07619900 | -2.52265500 |
| H | 1.32594200 | 2.12406300 | -1.28016800 |
| H | 1.32594200 | 2.12406300 | 1.28016800 |
| H | 0.62382100 | 0.07619900 | 2.52265500 |
| H | -0.06971800 | -2.30199100 | 2.52513700 |
| H | -0.50185500 | -4.39850400 | 1.26041100 |
| H | -0.50185500 | -4.39850400 | -1.26041100 |
| H | -0.06971800 | -2.30199100 | -2.52513700 |
| H | -0.53773500 | 4.59605700 | 0.89352500 |
| H | 0.92976000 | 4.09806300 | 0.00000000 |
| H | -0.53773500 | 4.59605700 | -0.89352500 |

**2-4**($C_s$) / B3LYP

| | | | |
|---|---|---|---|
| C | 0.17196800 | -1.03653400 | 0.74021700 |
| C | 0.17196800 | -1.03653400 | -0.74021700 |
| C | 0.47287000 | 0.11130700 | -1.42777800 |
| C | 0.65233200 | 1.40787300 | -0.76779400 |
| C | 0.65233200 | 1.40787300 | 0.76779400 |
| C | 0.47287000 | 0.11130700 | 1.42777800 |
| C | -0.07019100 | -2.29651600 | 1.42241100 |
| C | -0.30369000 | -3.44574700 | 0.72646800 |
| C | -0.30369000 | -3.44574700 | -0.72646800 |
| C | -0.07019100 | -2.29651600 | -1.42241100 |
| P | -0.84459400 | 2.30481100 | 0.00000000 |
| C | -0.16600800 | 4.04892500 | 0.00000000 |
| H | 0.58956400 | 0.07574600 | -2.50965200 |
| H | 1.32587100 | 2.10076700 | -1.27080500 |
| H | 1.32587100 | 2.10076700 | 1.27080500 |
| H | 0.58956400 | 0.07574600 | 2.50965200 |
| H | -0.06907900 | -2.29980100 | 2.51133600 |
| H | -0.49002500 | -4.37918800 | 1.25378900 |
| H | -0.49002500 | -4.37918800 | -1.25378900 |
| H | -0.06907900 | -2.29980100 | -2.51133600 |
| H | -0.52799000 | 4.58309000 | 0.88653400 |
| H | 0.92881000 | 4.08847200 | 0.00000000 |
| H | -0.52799000 | 4.58309000 | -0.88653400 |

**2-4**($C_s$) / M06-L

| | | | |
|---|---|---|---|
| C | 0.16391100 | -1.02716900 | 0.73550800 |
| C | 0.16391100 | -1.02716900 | -0.73550800 |
| C | 0.47073700 | 0.11954500 | -1.41995100 |
| C | 0.63504700 | 1.40707400 | -0.76470400 |
| C | 0.63504700 | 1.40707400 | 0.76470400 |
| C | 0.47073700 | 0.11954500 | 1.41995100 |
| C | -0.06712000 | -2.27828400 | 1.41368500 |
| C | -0.29308400 | -3.42820000 | 0.72071500 |
| C | -0.29308400 | -3.42820000 | -0.72071500 |
| C | -0.06712000 | -2.27828400 | -1.41368500 |
| P | -0.84788900 | 2.28459300 | 0.00000000 |
| C | -0.14741200 | 4.00051000 | 0.00000000 |
| H | 0.59988300 | 0.07883400 | -2.49847400 |
| H | 1.29945700 | 2.11200400 | -1.26103800 |
| H | 1.29945700 | 2.11200400 | 1.26103800 |
| H | 0.59988300 | 0.07883400 | 2.49847400 |
| H | -0.06457300 | -2.27878700 | 2.50087300 |
| H | -0.47220400 | -4.35909300 | 1.25013400 |
| H | -0.47220400 | -4.35909300 | -1.25013400 |
| H | -0.06457300 | -2.27878700 | -2.50087300 |
| H | -0.49114300 | 4.54677700 | 0.88231300 |
| H | 0.94607200 | 4.01296100 | 0.00000000 |
| H | -0.49114300 | 4.54677700 | -0.88231300 |

$(C_6H_6PCH_3)Fe(CO)_3$

**1Fe-1**($C_s$) / BP86

| | | | |
|---|---|---|---|
| C | -0.35968700 | 0.55026200 | 1.33042500 |
| C | -0.35968700 | 0.55026200 | -1.33042500 |
| C | -1.56443200 | 0.04388100 | -0.71542400 |
| C | -1.56443200 | 0.04388100 | 0.71542400 |
| H | -0.25178900 | 0.39765000 | 2.41136500 |
| H | -0.25178900 | 0.39765000 | -2.41136500 |
| H | -2.38525000 | -0.39830800 | -1.28921200 |
| H | -2.38525000 | -0.39830800 | 1.28921200 |
| C | 0.34563000 | 1.74576600 | 0.75286600 |
| H | 1.26831800 | 2.04686200 | 1.26459600 |
| C | 0.34563000 | 1.74576600 | -0.75286600 |
| H | 1.26831800 | 2.04686200 | -1.26459600 |
| P | -0.68065400 | 3.15928800 | 0.00000000 |
| Fe | -0.02457200 | -1.14419800 | 0.00000000 |
| C | -0.20612100 | -2.37354400 | 1.27426900 |
| C | -0.20612100 | -2.37354400 | -1.27426900 |
| C | 1.74688400 | -0.94259100 | 0.00000000 |
| O | -0.30645600 | -3.18301300 | 2.12036600 |
| O | -0.30645600 | -3.18301300 | -2.12036600 |
| O | 2.91287300 | -0.80268400 | 0.00000000 |
| C | 0.59639100 | 4.53104300 | 0.00000000 |
| H | 0.45326200 | 5.16604400 | -0.89231600 |
| H | 0.45326200 | 5.16604400 | 0.89231600 |
| H | 1.63556600 | 4.15790200 | 0.00000000 |

**1Fe-1**($C_s$) / B3LYP

| | | | |
|---|---|---|---|
| C | -0.38086900 | 0.53785800 | 1.32754500 |
| C | -0.38086900 | 0.53785800 | -1.32754500 |
| C | -1.57141500 | 0.03271000 | -0.71106300 |
| C | -1.57141500 | 0.03271000 | 0.71106300 |
| H | -0.28622200 | 0.40024000 | 2.40322700 |
| H | -0.28622200 | 0.40024000 | -2.40322700 |
| H | -2.38377100 | -0.41471900 | -1.27656500 |
| H | -2.38377100 | -0.41471900 | 1.27656500 |
| C | 0.32422000 | 1.73337800 | 0.75082600 |
| H | 1.24445300 | 2.01928500 | 1.25745400 |
| C | 0.32422000 | 1.73337800 | -0.75082600 |
| H | 1.24445300 | 2.01928500 | -1.25745400 |
| P | -0.67585800 | 3.14649700 | 0.00000000 |
| Fe | -0.01756600 | -1.14676700 | 0.00000000 |
| C | -0.19412900 | -2.37454700 | 1.29883100 |
| C | -0.19412900 | -2.37454700 | -1.29883100 |
| C | 1.75792300 | -0.92204500 | 0.00000000 |
| O | -0.29440300 | -3.14539400 | 2.15848300 |
| O | -0.29440300 | -3.14539400 | -2.15848300 |
| O | 2.90608500 | -0.76125500 | 0.00000000 |
| C | 0.60766800 | 4.50236800 | 0.00000000 |
| H | 0.47241400 | 5.13417400 | -0.88572400 |
| H | 0.47241400 | 5.13417400 | 0.88572400 |
| H | 1.63538300 | 4.12214200 | 0.00000000 |

**1Fe-1**($C_s$) / M06-L

| | | | |
|---|---|---|---|
| C | -0.36924700 | 0.51699700 | 1.31363500 |
| C | -0.36924700 | 0.51699700 | -1.31363500 |
| C | -1.56787200 | 0.01366500 | -0.70888200 |
| C | -1.56787200 | 0.01366500 | 0.70888200 |
| H | -0.26409000 | 0.36922300 | 2.38532200 |
| H | -0.26409000 | 0.36922300 | -2.38532200 |
| H | -2.37034400 | -0.44246000 | -1.27746400 |
| H | -2.37034400 | -0.44246000 | 1.27746400 |
| C | 0.30951600 | 1.71789700 | 0.74568300 |
| H | 1.22665700 | 2.02109600 | 1.24555300 |
| C | 0.30951600 | 1.71789700 | -0.74568300 |
| H | 1.22665700 | 2.02109600 | -1.24555300 |
| P | -0.70208300 | 3.09824800 | 0.00000000 |
| Fe | -0.01519700 | -1.13687600 | 0.00000000 |
| C | -0.17267800 | -2.36483200 | 1.29497400 |
| C | -0.17267800 | -2.36483200 | -1.29497400 |
| C | 1.75142200 | -0.85055700 | 0.00000000 |
| O | -0.26264800 | -3.14168200 | 2.15474700 |
| O | -0.26264800 | -3.14168200 | -2.15474700 |
| O | 2.88720100 | -0.60529700 | 0.00000000 |
| C | 0.57399100 | 4.43561500 | 0.00000000 |
| H | 0.45116700 | 5.06976500 | -0.88157500 |
| H | 0.45116700 | 5.06976500 | 0.88157500 |
| H | 1.59524700 | 4.04401800 | 0.00000000 |

**1Fe-2**($C_1$) / BP86

| | | | |
|---|---|---|---|
| C | 1.40638800 | -1.99276200 | -0.70401200 |
| C | 2.58899100 | -1.75188300 | -0.00658500 |
| C | 3.19203700 | -0.52024700 | 0.42264000 |
| C | 0.45556300 | -1.14534700 | -1.40523700 |
| C | 2.67177400 | 0.76063700 | 0.39729300 |
| C | 0.43981400 | 0.29078500 | -1.56045400 |
| H | 1.15830600 | -3.05989900 | -0.80680700 |
| H | 3.13105700 | -2.65556700 | 0.30109300 |
| H | 4.18939800 | -0.62227200 | 0.87550500 |
| H | -0.13389300 | -1.69006300 | -2.15598200 |
| H | 3.24785600 | 1.58196700 | 0.84494400 |
| H | 0.11884900 | 0.78183900 | -2.48575900 |
| P | 1.02125500 | 1.16106300 | -0.12769100 |
| Fe | -0.82255100 | -0.10399500 | 0.02648000 |
| C | 0.95642800 | 2.97801800 | -0.35107300 |
| H | -0.00060000 | 3.25075700 | -0.82284700 |
| H | 1.01319500 | 3.47605000 | 0.63110800 |
| H | 1.79550200 | 3.31877700 | -0.98036400 |
| C | -1.85630300 | 1.30995100 | 0.30059400 |
| C | -2.14382500 | -1.09889400 | -0.62739400 |
| C | -0.73299100 | -0.86881300 | 1.64101000 |
| O | -2.59701100 | 2.20817200 | 0.48708400 |
| O | -3.03660500 | -1.73331900 | -1.05650800 |
| O | -0.65631100 | -1.33264600 | 2.71758800 |

**1Fe-2**($C_1$) / B3LYP

| | | | |
|---|---|---|---|
| C | 1.45104600 | -1.97550800 | -0.68837700 |
| C | 2.62205200 | -1.71716900 | -0.00904600 |
| C | 3.21179200 | -0.46910000 | 0.40199800 |
| C | 0.46385600 | -1.14128800 | -1.35779500 |
| C | 2.67299300 | 0.78798200 | 0.38550300 |
| C | 0.43497200 | 0.28519300 | -1.53088100 |
| H | 1.22648200 | -3.03825600 | -0.79800300 |
| H | 3.18311000 | -2.60049600 | 0.29275000 |
| H | 4.21711200 | -0.55304500 | 0.81885200 |
| H | -0.10444700 | -1.69594700 | -2.10499400 |
| H | 3.25355600 | 1.61700100 | 0.79009100 |
| H | 0.13717000 | 0.75776400 | -2.46333500 |
| P | 1.00540400 | 1.16365400 | -0.10890500 |
| Fe | -0.83834600 | -0.10484300 | 0.04029300 |
| C | 0.94747700 | 2.97158100 | -0.36739900 |
| H | -0.01233700 | 3.24440200 | -0.81402700 |
| H | 1.03841800 | 3.48813500 | 0.59359900 |
| H | 1.76261400 | 3.29293600 | -1.02369000 |
| C | -1.86115300 | 1.31258800 | 0.38666400 |
| C | -2.17133400 | -1.04162600 | -0.70231100 |
| C | -0.74881300 | -0.97717200 | 1.61450600 |
| O | -2.56177900 | 2.21176600 | 0.61889500 |
| O | -3.03704200 | -1.63424700 | -1.19757700 |
| O | -0.66656100 | -1.50930100 | 2.64087400 |

**1Fe-2**($C_1$) / M06-L

| | | | |
|---|---|---|---|
| C | 1.39998500 | -1.94995200 | -0.70137100 |
| C | 2.57231400 | -1.69504800 | -0.02256800 |
| C | 3.16965800 | -0.46256300 | 0.37742500 |
| C | 0.43003500 | -1.13012900 | -1.38402200 |
| C | 2.64225100 | 0.79875800 | 0.34230900 |
| C | 0.39422000 | 0.29711400 | -1.55234200 |
| H | 1.16665600 | -3.01075800 | -0.78926800 |
| H | 3.11735100 | -2.58208900 | 0.28807600 |
| H | 4.16675100 | -0.55110200 | 0.80612700 |
| H | -0.15865200 | -1.68622700 | -2.11153100 |
| H | 3.21269200 | 1.62492900 | 0.76198600 |
| H | 0.07376900 | 0.77160900 | -2.47476200 |
| P | 0.98795500 | 1.15909200 | -0.14493000 |
| Fe | -0.82207000 | -0.11460900 | 0.03843500 |
| C | 0.87253500 | 2.95340100 | -0.35703800 |
| H | -0.07311200 | 3.19999100 | -0.84067200 |
| H | 0.89627900 | 3.44970700 | 0.61450700 |
| H | 1.70106300 | 3.32362800 | -0.96360500 |
| C | -1.81137600 | 1.31004000 | 0.42884800 |
| C | -2.17594400 | -1.04927900 | -0.66239000 |
| C | -0.66947600 | -0.98601800 | 1.60737000 |
| O | -2.48240900 | 2.23045700 | 0.68197400 |
| O | -3.06234600 | -1.63981000 | -1.12985900 |
| O | -0.51693200 | -1.52367000 | 2.62619200 |

**1Fe-3**($C_1$) / BP86

| | | | |
|---|---|---|---|
| C | 0.38136600 | -1.32315000 | -1.50147400 |
| C | -0.04270400 | -1.91780400 | -0.24371000 |
| C | -1.37536400 | -2.07030400 | 0.36762500 |
| C | -0.01188800 | -0.00764600 | -1.88803800 |
| C | -2.47182400 | -1.25728800 | 0.31684100 |
| C | -0.88372800 | 0.74993000 | -1.00820100 |
| H | 1.15853100 | -1.82926600 | -2.08777000 |
| H | 0.61743300 | -2.74661200 | 0.04823700 |
| H | -1.46008500 | -2.97563100 | 0.98691800 |
| H | 0.45776600 | 0.44700000 | -2.76913900 |
| H | -3.37706000 | -1.57071700 | 0.85519300 |
| H | -0.87802100 | 1.83043400 | -1.22515900 |
| P | -2.61229100 | 0.26104700 | -0.63315600 |
| Fe | 0.92247700 | 0.04799300 | -0.04177200 |
| C | 2.50144700 | -0.71915800 | 0.28507300 |
| C | 1.69962700 | 1.62684500 | -0.32181700 |
| C | 0.36781300 | 0.29478200 | 1.63241800 |
| O | -0.01210800 | 0.44792900 | 2.73149200 |
| O | 3.54949800 | -1.19820600 | 0.51155400 |
| O | 2.23239800 | 2.66074300 | -0.48516200 |
| C | -3.12098800 | 1.48684700 | 0.67902900 |
| H | -3.19125000 | 2.49235500 | 0.22945500 |
| H | -4.12605900 | 1.21473100 | 1.04546400 |
| H | -2.42212600 | 1.51213000 | 1.53066500 |

**1Fe-3**($C_1$) / B3LYP

| | | | |
|---|---|---|---|
| C | 0.39172700 | -1.30211500 | -1.51642300 |
| C | -0.01042600 | -1.90079400 | -0.26528600 |
| C | -1.34521000 | -2.07137200 | 0.34283400 |
| C | -0.00947600 | 0.00360700 | -1.88832100 |
| C | -2.43910200 | -1.27618300 | 0.29606100 |
| C | -0.87424600 | 0.74908400 | -1.00566100 |
| H | 1.16542700 | -1.79101500 | -2.10580400 |
| H | 0.64011000 | -2.73348600 | 0.00431100 |
| H | -1.42134200 | -2.97958000 | 0.94353900 |
| H | 0.45282800 | 0.46176200 | -2.76081800 |
| H | -3.33313600 | -1.60367400 | 0.82761300 |
| H | -0.88211000 | 1.81929200 | -1.23014400 |
| P | -2.60382700 | 0.25187300 | -0.63698900 |
| Fe | 0.91922400 | 0.05738800 | -0.03367400 |
| C | 2.51753800 | -0.71456100 | 0.27840600 |
| C | 1.66169000 | 1.67337500 | -0.30157400 |
| C | 0.35463800 | 0.26993500 | 1.65232100 |
| O | -0.02769000 | 0.39499300 | 2.73744500 |
| O | 3.54152500 | -1.21290700 | 0.48684500 |
| O | 2.13300400 | 2.71787500 | -0.46695300 |
| C | -3.08448300 | 1.44731400 | 0.70555300 |
| H | -3.15106500 | 2.45663200 | 0.28396500 |
| H | -4.08028200 | 1.17888900 | 1.07620900 |
| H | -2.38344200 | 1.45156400 | 1.54531800 |

**1Fe-3**($C_1$) / M06-L

| | | | |
|---|---|---|---|
| C | 0.41845300 | -1.24989000 | -1.54281300 |
| C | 0.00223800 | -1.88173900 | -0.31473600 |
| C | -1.31887200 | -2.06708800 | 0.28586600 |
| C | 0.01786200 | 0.06235000 | -1.88199700 |
| C | -2.41164800 | -1.27222000 | 0.26252200 |
| C | -0.86297900 | 0.76380100 | -0.98247400 |
| H | 1.20979100 | -1.71585100 | -2.12378800 |
| H | 0.66503700 | -2.70586000 | -0.05494400 |
| H | -1.38914600 | -2.97818800 | 0.87867600 |
| H | 0.49227200 | 0.55427400 | -2.72679200 |
| H | -3.29854100 | -1.60700600 | 0.79674600 |
| H | -0.87004700 | 1.84258000 | -1.16026100 |
| P | -2.57522400 | 0.25300300 | -0.64285500 |
| Fe | 0.91077700 | 0.06188200 | -0.03022200 |
| C | 2.50162800 | -0.71450700 | 0.28060600 |
| C | 1.64694200 | 1.68274500 | -0.24720100 |
| C | 0.31175700 | 0.21929200 | 1.65083500 |
| O | -0.11850000 | 0.29637600 | 2.72569500 |
| O | 3.52614700 | -1.22059800 | 0.48737900 |
| O | 2.12214100 | 2.73370300 | -0.38291600 |
| C | -3.06352400 | 1.41609600 | 0.70038000 |
| H | -3.15480900 | 2.42708900 | 0.29729700 |
| H | -4.04387300 | 1.12673600 | 1.08529400 |
| H | -2.35197600 | 1.42337600 | 1.52916200 |

**1Fe-4**($C_s$) / BP86

| | | | |
|---|---|---|---|
| C | -0.06020600 | 0.69521200 | 1.33502100 |
| C | -0.06020600 | 0.69521200 | -1.33502100 |
| C | -1.33304400 | 0.42207800 | -0.71563700 |
| C | -1.33304400 | 0.42207800 | 0.71563700 |
| H | 0.01292300 | 0.52243900 | 2.41590900 |
| H | 0.01292300 | 0.52243900 | -2.41590900 |
| H | -2.22187300 | 0.14100400 | -1.28983300 |
| H | -2.22187300 | 0.14100400 | 1.28983300 |
| C | 0.90989600 | 1.67894200 | 0.75240000 |
| H | 1.88554400 | 1.70131500 | 1.25508200 |
| C | 0.90989600 | 1.67894200 | -0.75240000 |
| H | 1.88554400 | 1.70131500 | -1.25508200 |
| P | 0.46370700 | 3.38184400 | 0.00000000 |
| C | -1.40215900 | 3.48221800 | 0.00000000 |
| H | -1.65737800 | 4.55655800 | 0.00000000 |
| H | -1.84968900 | 3.01831500 | -0.89479300 |
| H | -1.84968900 | 3.01831500 | 0.89479300 |
| Fe | -0.06779100 | -1.05571400 | 0.00000000 |
| C | -0.50073400 | -2.22453900 | 1.26768200 |
| C | -0.50073400 | -2.22453900 | -1.26768200 |
| C | 1.71088600 | -1.23880100 | 0.00000000 |
| O | -0.76559000 | -2.99616200 | 2.11375100 |
| O | -0.76559000 | -2.99616200 | -2.11375100 |
| O | 2.87708100 | -1.37300600 | 0.00000000 |

**1Fe-4**($C_s$) / B3LYP

| | | | |
|---|---|---|---|
| C | -0.07848400 | 0.68659400 | 1.33273800 |
| C | -0.07848400 | 0.68659400 | -1.33273800 |
| C | -1.33705400 | 0.41751800 | -0.71155800 |
| C | -1.33705400 | 0.41751800 | 0.71155800 |
| H | -0.01569400 | 0.53124100 | 2.40833900 |
| H | -0.01569400 | 0.53124100 | -2.40833900 |
| H | -2.22020200 | 0.13478100 | -1.27723100 |
| H | -2.22020200 | 0.13478100 | 1.27723100 |
| C | 0.89604700 | 1.66532700 | 0.75023900 |
| H | 1.86456800 | 1.67324700 | 1.24878900 |
| C | 0.89604700 | 1.66532700 | -0.75023900 |
| H | 1.86456800 | 1.67324700 | -1.24878900 |
| P | 0.47286500 | 3.35737100 | 0.00000000 |
| C | -1.38495500 | 3.49286900 | 0.00000000 |
| H | -1.61997100 | 4.56330100 | 0.00000000 |
| H | -1.83767200 | 3.04108700 | -0.88793200 |
| H | -1.83767200 | 3.04108700 | 0.88793200 |
| Fe | -0.06502200 | -1.06265300 | 0.00000000 |
| C | -0.49920200 | -2.22899700 | 1.29305500 |
| C | -0.49920200 | -2.22899700 | -1.29305500 |
| C | 1.72191400 | -1.23014200 | 0.00000000 |
| O | -0.76032700 | -2.96133300 | 2.15269700 |
| O | -0.76032700 | -2.96133300 | -2.15269700 |
| O | 2.87541900 | -1.34199200 | 0.00000000 |

**1Fe-4**($C_s$) / M06-L

| | | | |
|---|---|---|---|
| C | -0.07682900 | 0.66703100 | 1.31855600 |
| C | -0.07682900 | 0.66703100 | -1.31855600 |
| C | -1.34193900 | 0.39575100 | -0.70908200 |
| C | -1.34193900 | 0.39575100 | 0.70908200 |
| H | -0.00653900 | 0.50093900 | 2.39048100 |
| H | -0.00653900 | 0.50093900 | -2.39048100 |
| H | -2.21621000 | 0.10192000 | -1.27904300 |
| H | -2.21621000 | 0.10192000 | 1.27904300 |
| C | 0.87695300 | 1.65644200 | 0.74525300 |
| H | 1.84599900 | 1.67655600 | 1.23896700 |
| C | 0.87695300 | 1.65644200 | -0.74525300 |
| H | 1.84599900 | 1.67655600 | -1.23896700 |
| P | 0.42856900 | 3.31945900 | 0.00000000 |
| C | -1.41455900 | 3.38618800 | 0.00000000 |
| H | -1.69647300 | 4.44156300 | 0.00000000 |
| H | -1.85434400 | 2.92022000 | -0.88495300 |
| H | -1.85434400 | 2.92022000 | 0.88495300 |
| Fe | -0.06041400 | -1.04781200 | 0.00000000 |
| C | -0.47257600 | -2.22086800 | 1.28695200 |
| C | -0.47257600 | -2.22086800 | -1.28695200 |
| C | 1.73337000 | -1.14913700 | 0.00000000 |
| O | -0.72469300 | -2.96485900 | 2.14355500 |
| O | -0.72469300 | -2.96485900 | -2.14355500 |
| O | 2.89447400 | -1.16930600 | 0.00000000 |

**1Fe-5**($C_1$) / BP86

| | | | |
|---|---|---|---|
| C | -0.01473900 | -1.75606300 | 0.74588800 |
| C | -0.01474200 | -1.75600900 | -0.74601200 |
| C | -1.24642700 | -1.60537500 | -1.56273200 |
| C | -1.24641300 | -1.60547500 | 1.56263100 |
| C | -2.10759000 | -0.56250300 | -1.37770900 |
| C | -2.10757800 | -0.56258900 | 1.37768800 |
| H | 0.74645400 | -2.40348500 | 1.20003600 |
| H | 0.74645000 | -2.40339900 | -1.20020700 |
| H | -1.47509900 | -2.39293500 | -2.29684900 |
| H | -1.47507700 | -2.39307900 | 2.29670400 |
| H | -3.09593000 | -0.48829200 | -1.84677000 |
| H | -3.09590900 | -0.48840500 | 1.84677200 |
| P | -1.50172000 | 0.46140700 | 0.00000000 |
| Fe | 0.73161300 | 0.04494700 | 0.00000000 |
| C | 0.97525400 | 1.03597600 | 1.46427700 |
| C | 0.97523900 | 1.03608700 | -1.46420800 |
| C | 2.42164000 | -0.50401400 | 0.00000000 |
| O | 1.14031900 | 1.69523900 | 2.42572400 |
| O | 3.53814600 | -0.87033100 | 0.00000000 |
| O | 1.14028900 | 1.69542600 | -2.42560500 |
| C | -2.30439400 | 2.10803300 | 0.00000000 |
| H | -1.98720100 | 2.66694700 | 0.89600900 |
| H | -1.98722100 | 2.66699900 | -0.89583800 |
| H | -3.40413100 | 2.01484100 | 0.00000000 |

**1Fe-5**($C_1$) / B3LYP

| | | | |
|---|---|---|---|
| C | -0.03611400 | -1.74390500 | -0.73848500 |
| C | -0.03612600 | -1.74402800 | 0.73819000 |
| C | 1.19139900 | -1.61950900 | 1.56212600 |
| C | 1.19142700 | -1.61925500 | -1.56237600 |
| C | 2.07877600 | -0.61279400 | 1.37910000 |
| C | 2.07880200 | -0.61257000 | -1.37917700 |
| H | -0.80348000 | -2.37011600 | -1.19110400 |
| H | -0.80350000 | -2.37031600 | 1.19069200 |
| H | 1.38287200 | -2.39733700 | 2.30411300 |
| H | 1.38291700 | -2.39696800 | -2.30448000 |
| H | 3.04706100 | -0.55973700 | 1.87208100 |
| H | 3.04709800 | -0.55944200 | -1.87212900 |
| P | 1.53203700 | 0.42879000 | 0.00000000 |
| Fe | -0.74202900 | 0.07701600 | 0.00000000 |
| C | -0.96831400 | 1.07607500 | -1.47571200 |
| C | -0.96836800 | 1.07579200 | 1.47589000 |
| C | -2.44845000 | -0.47577200 | 0.00000000 |
| O | -1.10287100 | 1.72692100 | -2.42888700 |
| O | -3.54352200 | -0.85508600 | -0.00011500 |
| O | -1.10298100 | 1.72644400 | 2.42919000 |
| C | 2.44612500 | 2.01106400 | 0.00020000 |
| H | 2.17524900 | 2.59004400 | -0.88852700 |
| H | 2.17522100 | 2.58986600 | 0.88903400 |
| H | 3.52882200 | 1.84290900 | 0.00020000 |

**1Fe-5**($C_1$) / M06-L

| | | | |
|---|---|---|---|
| C | 0.06561000 | -1.76579600 | 0.64762200 |
| C | 0.06966000 | -1.68746400 | -0.83276000 |
| C | -1.15543100 | -1.54900600 | -1.63568400 |
| C | -1.16246700 | -1.71200600 | 1.45612400 |
| C | -2.04824900 | -0.56015000 | -1.40732900 |
| C | -2.05403600 | -0.70346400 | 1.32889300 |
| H | 0.83902100 | -2.41133100 | 1.05894900 |
| H | 0.84505000 | -2.28663800 | -1.30579300 |
| H | -1.34980800 | -2.29851600 | -2.40281400 |
| H | -1.35940400 | -2.53711200 | 2.14073000 |
| H | -3.02716700 | -0.50657600 | -1.87482700 |
| H | -3.03450100 | -0.69775000 | 1.79661700 |
| P | -1.50382800 | 0.39670900 | 0.01558600 |
| Fe | 0.74569300 | 0.07532600 | 0.00516600 |
| C | 0.90512500 | 0.99198000 | 1.53814300 |
| C | 0.91410800 | 1.17101700 | -1.40424200 |
| C | 2.45850400 | -0.43763900 | -0.02748700 |
| O | 0.96011000 | 1.58499000 | 2.53966700 |
| O | 3.56317700 | -0.79712500 | -0.05368100 |
| O | 0.97629400 | 1.88759900 | -2.32111900 |
| C | -2.35536900 | 1.99230000 | 0.09670200 |
| H | -2.05745100 | 2.51700800 | 1.00629100 |
| H | -2.06717300 | 2.60057200 | -0.76243200 |
| H | -3.44053900 | 1.86887300 | 0.09634700 |

**1Fe-6**($C_1$) / BP86

| | | | |
|---|---|---|---|
| C | 0.05208300 | -0.59837800 | -1.80158400 |
| C | -0.15225100 | -1.64986600 | -0.82083300 |
| C | -1.41700600 | -2.06844000 | -0.17673300 |
| C | -0.35302700 | 0.74318300 | -1.54352500 |
| C | -2.43845800 | -1.30783000 | 0.30810100 |
| C | -0.92464200 | 1.09311100 | -0.25985000 |
| H | 0.66390400 | -0.79828200 | -2.69074900 |
| H | 0.50164200 | -2.51416400 | -1.00528600 |
| H | -1.51530500 | -3.16148800 | -0.08561900 |
| H | -0.04323400 | 1.52577300 | -2.24942600 |
| H | -3.30616000 | -1.83365400 | 0.73253800 |
| H | -0.85258900 | 2.17332600 | -0.05106100 |
| P | -2.41366900 | 0.47162200 | 0.62318500 |
| Fe | 0.95248400 | 0.07394900 | -0.05668000 |
| C | 2.50776500 | -0.73433100 | -0.37712900 |
| C | 1.79555000 | 1.63466900 | 0.15387700 |
| C | 0.73013600 | -0.40105200 | 1.65080200 |
| O | 0.58996000 | -0.72186600 | 2.76836700 |
| O | 3.54240800 | -1.25525100 | -0.56974000 |
| O | 2.36471200 | 2.64870600 | 0.31500800 |
| C | -3.76959600 | 1.06521600 | -0.53189500 |
| H | -4.73979300 | 0.68525100 | -0.16592300 |
| H | -3.80960500 | 2.16804600 | -0.50418800 |
| H | -3.61836600 | 0.72777900 | -1.57085100 |

**1Fe-6**($C_1$) / B3LYP

| | | | |
|---|---|---|---|
| C | 0.03637200 | -0.57476400 | -1.79871900 |
| C | -0.13538200 | -1.62539000 | -0.82427400 |
| C | -1.39126500 | -2.05435500 | -0.16499700 |
| C | -0.36589900 | 0.75311400 | -1.52564000 |
| C | -2.39908700 | -1.31218600 | 0.34160300 |
| C | -0.91809600 | 1.09359800 | -0.23985200 |
| H | 0.63132500 | -0.76105300 | -2.69154600 |
| H | 0.49878000 | -2.48646900 | -1.03916200 |
| H | -1.48502400 | -3.14030300 | -0.09129900 |
| H | -0.06906900 | 1.53299600 | -2.22648200 |
| H | -3.24780700 | -1.84591800 | 0.77207000 |
| H | -0.85683800 | 2.16669800 | -0.03727100 |
| P | -2.41563600 | 0.47348900 | 0.62531800 |
| Fe | 0.95523000 | 0.07735900 | -0.04913200 |
| C | 2.51660300 | -0.74816600 | -0.39870700 |
| C | 1.78167200 | 1.66669600 | 0.16593700 |
| C | 0.74119600 | -0.40888900 | 1.66568500 |
| O | 0.59741500 | -0.73395000 | 2.76547500 |
| O | 3.51574200 | -1.29051300 | -0.61690200 |
| O | 2.29961800 | 2.68996900 | 0.32044500 |
| C | -3.74746900 | 1.00129000 | -0.57624200 |
| H | -4.71377700 | 0.61516400 | -0.23111400 |
| H | -3.81074500 | 2.09544300 | -0.58533500 |
| H | -3.56235300 | 0.64004400 | -1.59310600 |

**1Fe-6**($C_1$) / M06-L

| | | | |
|---|---|---|---|
| C | 0.03597300 | -0.57662000 | -1.78641800 |
| C | -0.14093300 | -1.61921300 | -0.80675200 |
| C | -1.38770200 | -2.03932200 | -0.15425900 |
| C | -0.36315800 | 0.74968800 | -1.51470900 |
| C | -2.39287700 | -1.29337700 | 0.34649300 |
| C | -0.90502000 | 1.08118700 | -0.22357700 |
| H | 0.63674400 | -0.76738900 | -2.67227200 |
| H | 0.50317900 | -2.47420000 | -1.00892900 |
| H | -1.48481100 | -3.12236500 | -0.07254900 |
| H | -0.06256800 | 1.53153600 | -2.20940700 |
| H | -3.24123300 | -1.82512600 | 0.77491100 |
| H | -0.82952500 | 2.15207600 | -0.01640200 |
| P | -2.39258800 | 0.47571900 | 0.63796300 |
| Fe | 0.94705100 | 0.07563700 | -0.05689200 |
| C | 2.50109200 | -0.74553100 | -0.41638300 |
| C | 1.77441200 | 1.65887300 | 0.15552300 |
| C | 0.72287400 | -0.42005900 | 1.65575700 |
| O | 0.54653200 | -0.75688700 | 2.74994900 |
| O | 3.50366600 | -1.28451000 | -0.64544700 |
| O | 2.29951100 | 2.68256900 | 0.30915000 |
| C | -3.69851700 | 1.01617400 | -0.55905600 |
| H | -4.67063200 | 0.64061200 | -0.22992500 |
| H | -3.75347300 | 2.10735100 | -0.57165300 |
| H | -3.50672200 | 0.65498400 | -1.57294600 |

**1Fe-7**($C_s$) / BP86

| | | | |
|---|---|---|---|
| C | 2.48153400 | 0.63388900 | 0.67652000 |
| C | 2.48153400 | 0.63388900 | -0.67652000 |
| C | 1.21931500 | 0.29016500 | -1.40736700 |
| C | 1.21931500 | 0.29016500 | 1.40736700 |
| C | 0.05523300 | 1.10532100 | -1.27077200 |
| C | 0.05523300 | 1.10532100 | 1.27077200 |
| H | 3.36611200 | 0.92377000 | 1.26022600 |
| H | 3.36611200 | 0.92377000 | -1.26022600 |
| H | 1.31871700 | -0.29818400 | -2.33020800 |
| H | 1.31871700 | -0.29818400 | 2.33020800 |
| H | -0.69147400 | 1.12732300 | -2.07574600 |
| H | -0.69147400 | 1.12732300 | 2.07574600 |
| P | 0.01183200 | 2.45787900 | 0.00000000 |
| Fe | -0.16249600 | -0.63410400 | 0.00000000 |
| C | -1.35289300 | -1.13515400 | 1.21156100 |
| C | -1.35289300 | -1.13515400 | -1.21156100 |
| C | 0.94343300 | -2.04562600 | 0.00000000 |
| O | -2.12455000 | -1.48936700 | 2.02657900 |
| O | -2.12455000 | -1.48936700 | -2.02657900 |
| O | 1.63321500 | -2.99374000 | 0.00000000 |
| C | -1.82164000 | 2.79527400 | 0.00000000 |
| H | -2.07805600 | 3.39697600 | 0.88949600 |
| H | -2.07805600 | 3.39697600 | -0.88949600 |
| H | -2.42509900 | 1.87000800 | 0.00000000 |

**1Fe-7**($C_s$) / B3LYP

| | | | |
|---|---|---|---|
| C | 2.48056800 | 0.60653200 | 0.67173400 |
| C | 2.48056800 | 0.60653200 | -0.67173400 |
| C | 1.22014800 | 0.30830100 | -1.41673800 |
| C | 1.22014800 | 0.30830100 | 1.41673800 |
| C | 0.07779300 | 1.12082300 | -1.27745200 |
| C | 0.07779300 | 1.12082300 | 1.27745200 |
| H | 3.37496700 | 0.85032900 | 1.24503600 |
| H | 3.37496700 | 0.85032900 | -1.24503600 |
| H | 1.31663500 | -0.27564900 | -2.33212100 |
| H | 1.31663500 | -0.27564900 | 2.33212100 |
| H | -0.66740600 | 1.14057500 | -2.07115100 |
| H | -0.66740600 | 1.14057500 | 2.07115100 |
| P | 0.02259500 | 2.45359200 | 0.00000000 |
| Fe | -0.17209200 | -0.64464600 | 0.00000000 |
| C | -1.36964900 | -1.13066600 | 1.23484600 |
| C | -1.36964900 | -1.13066600 | -1.23484600 |
| C | 0.93235000 | -2.06576500 | 0.00000000 |
| O | -2.12114200 | -1.45907900 | 2.05724000 |
| O | -2.12114200 | -1.45907900 | -2.05724000 |
| O | 1.60509200 | -3.00887900 | 0.00000000 |
| C | -1.80071800 | 2.79932800 | 0.00000000 |
| H | -2.05282800 | 3.39795100 | 0.88280400 |
| H | -2.05282800 | 3.39795100 | -0.88280400 |
| H | -2.40585200 | 1.88554200 | 0.00000000 |

**1Fe-7**($C_s$) / M06-L

| | | | |
|---|---|---|---|
| C | -0.46445900 | 2.49754200 | 0.66998100 |
| C | -0.46460800 | 2.49762400 | -0.66975100 |
| C | -0.21231400 | 1.22858900 | -1.39650700 |
| C | -0.21196300 | 1.22843100 | 1.39653700 |
| C | -1.09244900 | 0.13188000 | -1.26189500 |
| C | -1.09215300 | 0.13170400 | 1.26205000 |
| H | -0.68598600 | 3.39381900 | 1.24464000 |
| H | -0.68625900 | 3.39395900 | -1.24426900 |
| H | 0.38112800 | 1.28385800 | -2.30752500 |
| H | 0.38160200 | 1.28367700 | 2.30747700 |
| H | -1.14864300 | -0.61171300 | -2.05495100 |
| H | -1.14824900 | -0.61189300 | 2.05511000 |
| P | -2.42409600 | 0.14116200 | 0.00024000 |
| Fe | 0.61895000 | -0.20041500 | 0.00000000 |
| C | 1.02396600 | -1.42541300 | 1.22729000 |
| C | 1.02310500 | -1.42594400 | -1.22717600 |
| C | 2.08795300 | 0.84671100 | -0.00052500 |
| O | 1.28730900 | -2.20730800 | 2.04898200 |
| O | 1.28594800 | -2.20818800 | -2.04870400 |
| O | 3.03692600 | 1.51458300 | -0.00077600 |
| C | -2.78086100 | -1.66472200 | 0.00013100 |
| H | -3.37246100 | -1.92621300 | 0.88005500 |
| H | -3.37263800 | -1.92607600 | -0.87971500 |
| H | -1.85851900 | -2.25715000 | 0.00000000 |

**1Fe-8**($C_s$) / BP86

| | | | |
|---|---|---|---|
| C | 1.92465000 | 1.43732700 | 0.67505900 |
| C | 1.92465000 | 1.43732700 | -0.67505900 |
| C | 0.88718700 | 0.64355600 | -1.40515800 |
| C | 0.88718700 | 0.64355600 | 1.40515800 |
| C | -0.51257300 | 0.92242600 | -1.31028600 |
| C | -0.51257300 | 0.92242600 | 1.31028600 |
| H | 2.64011100 | 2.02954700 | 1.26259000 |
| H | 2.64011100 | 2.02954700 | -1.26259000 |
| H | 1.22059000 | 0.14594100 | -2.32879400 |
| H | 1.22059000 | 0.14594100 | 2.32879400 |
| H | -1.14400300 | 0.61757900 | -2.15573100 |
| H | -1.14400300 | 0.61757900 | 2.15573100 |
| P | -1.38277300 | 1.89172400 | 0.00000000 |
| Fe | -0.04169400 | -0.73959300 | 0.00000000 |
| C | -0.93456300 | -1.67303600 | 1.21379100 |
| C | -0.93456300 | -1.67303600 | -1.21379100 |
| C | 1.52430800 | -1.60763200 | 0.00000000 |
| O | -1.50121600 | -2.30705600 | 2.02494300 |
| O | -1.50121600 | -2.30705600 | -2.02494300 |
| O | 2.52811300 | -2.21286300 | 0.00000000 |
| C | -0.63049000 | 3.60796900 | 0.00000000 |
| H | -1.01070100 | 4.14177600 | -0.89030900 |
| H | -1.01070100 | 4.14177600 | 0.89030900 |
| H | 0.46887700 | 3.63436200 | 0.00000000 |

**1Fe-8**($C_s$) / B3LYP

| | | | |
|---|---|---|---|
| C | 1.92709900 | 1.41807000 | 0.67020100 |
| C | 1.92709900 | 1.41807000 | -0.67020100 |
| C | 0.87703500 | 0.66289800 | -1.41415800 |
| C | 0.87703500 | 0.66289800 | 1.41415800 |
| C | -0.50322300 | 0.94233000 | -1.31190400 |
| C | -0.50322300 | 0.94233000 | 1.31190400 |
| H | 2.66369600 | 1.97752900 | 1.24726300 |
| H | 2.66369600 | 1.97752900 | -1.24726300 |
| H | 1.20603800 | 0.17470400 | -2.33364700 |
| H | 1.20603800 | 0.17470400 | 2.33364700 |
| H | -1.13446200 | 0.63687000 | -2.14504100 |
| H | -1.13446200 | 0.63687000 | 2.14504100 |
| P | -1.36756200 | 1.89821400 | 0.00000000 |
| Fe | -0.04513300 | -0.75374500 | 0.00000000 |
| C | -0.94803100 | -1.68044500 | 1.23776100 |
| C | -0.94803100 | -1.68044500 | -1.23776100 |
| C | 1.52632000 | -1.62519500 | 0.00000000 |
| O | -1.50413800 | -2.28452600 | 2.05655500 |
| O | -1.50413800 | -2.28452600 | -2.05655500 |
| O | 2.51564900 | -2.22721900 | 0.00000000 |
| C | -0.61942800 | 3.60705600 | 0.00000000 |
| H | -0.99492100 | 4.13807400 | -0.88387700 |
| H | -0.99492100 | 4.13807400 | 0.88387700 |
| H | 0.47129100 | 3.63456700 | 0.00000000 |

**1Fe-8**($C_s$) / M06-L

| | | | |
|---|---|---|---|
| C | 1.88562200 | 1.43318000 | 0.66865000 |
| C | 1.88562200 | 1.43318000 | -0.66865000 |
| C | 0.86258700 | 0.64678400 | -1.39735400 |
| C | 0.86258700 | 0.64678400 | 1.39735400 |
| C | -0.52496100 | 0.91108800 | -1.30061400 |
| C | -0.52496100 | 0.91108800 | 1.30061400 |
| H | 2.59434100 | 2.02374500 | 1.24563900 |
| H | 2.59434100 | 2.02374500 | -1.24563900 |
| H | 1.19519400 | 0.15063600 | -2.31001400 |
| H | 1.19519400 | 0.15063600 | 2.31001400 |
| H | -1.14849400 | 0.58507900 | -2.13060300 |
| H | -1.14849400 | 0.58507900 | 2.13060300 |
| P | -1.38795700 | 1.85611800 | 0.00000000 |
| Fe | -0.04356900 | -0.74197800 | 0.00000000 |
| C | -0.92525400 | -1.68301900 | 1.23101300 |
| C | -0.92525400 | -1.68301900 | -1.23101300 |
| C | 1.56211300 | -1.55626000 | 0.00000000 |
| O | -1.47741700 | -2.29593300 | 2.05002300 |
| O | -1.47741700 | -2.29593300 | -2.05002300 |
| O | 2.59277800 | -2.08837500 | 0.00000000 |
| C | -0.63752500 | 3.54623200 | 0.00000000 |
| H | -1.00463400 | 4.08319800 | -0.87927600 |
| H | -1.00463400 | 4.08319800 | 0.87927600 |
| H | 0.45231000 | 3.57004300 | 0.00000000 |

$(C_6H_6PCH_3)Co(C_5H_5)$

**1Co-1**($C_1$) / BP86

| | | | |
|---|---|---|---|
| C | -0.17565900 | -1.76988800 | 1.01412400 |
| C | 0.15634200 | -1.86437500 | -0.40035900 |
| C | 1.41810900 | -1.69119300 | -1.13549800 |
| C | 0.17976200 | -0.61003900 | 1.78217600 |
| C | 2.46633500 | -0.83932000 | -0.91521300 |
| C | 0.89312300 | 0.45945900 | 1.10786100 |
| H | -0.87455500 | -2.49751700 | 1.44914700 |
| H | -0.50018900 | -2.58554500 | -0.91215200 |
| H | 1.49149400 | -2.33388600 | -2.02735400 |
| H | -0.24213200 | -0.48886400 | 2.78942900 |
| H | 3.32615100 | -0.88116100 | -1.59879000 |
| H | 0.80786300 | 1.42651700 | 1.63427500 |
| P | 2.60410600 | 0.31831600 | 0.45657300 |
| C | -2.93943500 | -0.13063700 | -0.03820700 |
| C | -2.28548300 | -0.14288600 | -1.32495600 |
| C | -1.46335300 | 1.04130700 | -1.43685200 |
| C | -1.60258800 | 1.77268600 | -0.19871500 |
| H | -2.81299400 | 1.34907000 | 1.66867900 |
| H | -3.61757200 | -0.89745300 | 0.34358100 |
| H | -2.38055700 | -0.92445100 | -2.08228700 |
| H | -0.84336000 | 1.32033300 | -2.29060400 |
| H | -1.09058700 | 2.70386600 | 0.05367400 |
| C | -2.51640800 | 1.05360300 | 0.65951900 |
| Co | -0.83547700 | -0.11189200 | 0.15533900 |
| C | 2.80769800 | 1.93251300 | -0.46780500 |
| H | 2.86075100 | 2.76659000 | 0.25379800 |
| H | 3.76075100 | 1.91136400 | -1.02459800 |
| H | 1.98057300 | 2.11010600 | -1.17600200 |

**1Co-1**($C_1$) / B3LYP

| | | | |
|---|---|---|---|
| C | -0.11690300 | -1.82232700 | 0.96037400 |
| C | 0.18896400 | -1.85600900 | -0.44949300 |
| C | 1.44270200 | -1.63200900 | -1.18874600 |
| C | 0.22341700 | -0.69588400 | 1.76215000 |
| C | 2.46395300 | -0.77367400 | -0.94995500 |
| C | 0.90203400 | 0.40971400 | 1.13680900 |
| H | -0.80553500 | -2.56078100 | 1.36944800 |
| H | -0.44881100 | -2.56916700 | -0.97594200 |
| H | 1.52233500 | -2.24580500 | -2.08939400 |
| H | -0.20511200 | -0.61898800 | 2.76092500 |
| H | 3.30997800 | -0.77754500 | -1.63842900 |
| H | 0.79929900 | 1.34048800 | 1.70466200 |
| P | 2.60288600 | 0.34720700 | 0.45274600 |
| C | -2.96365600 | 0.04016400 | 0.19712200 |
| C | -2.48520200 | -0.23046200 | -1.12039900 |
| C | -1.59895700 | 0.83270000 | -1.51330500 |
| C | -1.51391500 | 1.74165000 | -0.41580400 |
| H | -2.48357000 | 1.71348600 | 1.61517000 |
| H | -3.63460500 | -0.58772600 | 0.77194900 |
| H | -2.74065300 | -1.09412100 | -1.72353200 |
| H | -1.07645700 | 0.91392200 | -2.45843700 |
| H | -0.90818500 | 2.63900200 | -0.37915200 |
| C | -2.34982600 | 1.24878400 | 0.64514800 |
| Co | -0.81516900 | -0.14071500 | 0.15932100 |
| C | 2.70702500 | 1.98379500 | -0.43476600 |
| H | 2.72744100 | 2.79802400 | 0.29902400 |
| H | 3.64404800 | 2.02616400 | -1.00162300 |
| H | 1.86828800 | 2.13558400 | -1.12233500 |

**1Co-1**($C_1$) / M06-L

| | | | |
|---|---|---|---|
| C | -0.18222300 | -1.78182300 | 0.99735200 |
| C | 0.14949000 | -1.84848300 | -0.40557600 |
| C | 1.40142000 | -1.65916600 | -1.13184200 |
| C | 0.16637300 | -0.64390900 | 1.77605300 |
| C | 2.43004300 | -0.80794700 | -0.90817300 |
| C | 0.87585700 | 0.42260300 | 1.12093600 |
| H | -0.88600800 | -2.50198000 | 1.40913700 |
| H | -0.50019200 | -2.55461800 | -0.92548400 |
| H | 1.47568100 | -2.28126100 | -2.02486500 |
| H | -0.26679200 | -0.53228200 | 2.76815000 |
| H | 3.27419700 | -0.83153700 | -1.59507600 |
| H | 0.77897500 | 1.37515000 | 1.65376400 |
| P | 2.56728800 | 0.32649400 | 0.46350500 |
| C | -2.89837700 | -0.07544600 | -0.02478700 |
| C | -2.25936000 | -0.14375000 | -1.29960600 |
| C | -1.40001600 | 0.99425400 | -1.44437300 |
| C | -1.50946900 | 1.75675600 | -0.24006900 |
| H | -2.70326600 | 1.42574700 | 1.62919400 |
| H | -3.59157200 | -0.80140300 | 0.37768000 |
| H | -2.37463300 | -0.94057300 | -2.02216500 |
| H | -0.77442700 | 1.22164300 | -2.29640500 |
| H | -0.95165300 | 2.65499800 | -0.00963600 |
| C | -2.43131100 | 1.09940900 | 0.63439000 |
| Co | -0.82131100 | -0.12487200 | 0.15664500 |
| C | 2.67005500 | 1.92926800 | -0.44911300 |
| H | 2.68007900 | 2.76103200 | 0.26024700 |
| H | 3.60096000 | 1.97151700 | -1.01928100 |
| H | 1.82986400 | 2.05711000 | -1.13840300 |

**1Co-2**($C_s$) / BP86

| | | | |
|---|---|---|---|
| C | 0.51753600 | 0.32080700 | -1.31750900 |
| C | 0.51753600 | 0.32080700 | 1.31750900 |
| C | 1.45211200 | -0.60784400 | 0.72061500 |
| C | 1.45211200 | -0.60784400 | -0.72061500 |
| H | 0.33323400 | 0.21130500 | -2.39483500 |
| H | 0.33323400 | 0.21130500 | 2.39483500 |
| H | 2.02495700 | -1.34095100 | 1.30039600 |
| H | 2.02495700 | -1.34095100 | -1.30039600 |
| C | 0.31758800 | 1.70174100 | -0.75324600 |
| H | -0.42235000 | 2.32678600 | -1.27001700 |
| C | 0.31758800 | 1.70174100 | 0.75324600 |
| H | -0.42235000 | 2.32678600 | 1.27001700 |
| C | -1.08640900 | -2.87361100 | -0.71649800 |
| C | -1.88344000 | -1.74904600 | -1.16019400 |
| C | -2.40919800 | -1.06516900 | 0.00000000 |
| C | -1.88344000 | -1.74904600 | 1.16019400 |
| H | -0.55681800 | -3.57625500 | 1.36391500 |
| H | -0.55681800 | -3.57625500 | -1.36391500 |
| H | -2.06052300 | -1.46788400 | -2.20121300 |
| H | -3.06779300 | -0.19479300 | 0.00000000 |
| H | -2.06052300 | -1.46788400 | 2.20121300 |
| C | -1.08640900 | -2.87361100 | 0.71649800 |
| P | 1.79427300 | 2.64353600 | 0.00000000 |
| C | 1.10417300 | 4.39067200 | 0.00000000 |
| H | 1.46612200 | 4.93177900 | 0.89262300 |
| H | 1.46612200 | 4.93177900 | -0.89262300 |
| H | 0.00000000 | 4.41901900 | 0.00000000 |
| Co | -0.34792800 | -1.01867900 | 0.00000000 |

**1Co-2**($C_s$) / B3LYP

| | | | |
|---|---|---|---|
| C | -0.53825900 | -0.35223300 | 1.31750400 |
| C | -0.52912300 | -0.36394500 | -1.31801600 |
| C | -0.11767900 | -1.59265000 | -0.70903600 |
| C | -0.12263900 | -1.58629100 | 0.72233600 |
| H | -0.36909500 | -0.24081100 | 2.38791700 |
| H | -0.35253400 | -0.26203800 | -2.38817800 |
| H | 0.30323500 | -2.42130500 | -1.27299700 |
| H | 0.29432100 | -2.40989300 | 1.29654200 |
| C | -1.66974600 | 0.45389100 | 0.74358700 |
| H | -1.87364300 | 1.39653200 | 1.24948000 |
| C | -1.66453400 | 0.44722100 | -0.75914700 |
| H | -1.86487500 | 1.38532900 | -1.27479300 |
| P | -3.17414900 | -0.40842000 | -0.00919700 |
| C | -4.39963300 | 1.00452200 | -0.01971700 |
| H | -3.91859100 | 1.98940400 | -0.02238800 |
| H | -5.03890600 | 0.93027700 | -0.90758900 |
| H | -5.04509200 | 0.93810300 | 0.86429200 |
| C | 2.41915300 | 0.92721200 | 1.15596500 |
| C | 2.04083000 | 1.68605500 | 0.00000000 |
| C | 2.42676200 | 0.91769100 | -1.14711800 |
| C | 3.08421100 | -0.27781000 | -0.70024800 |
| H | 3.47536100 | -1.04639600 | 1.36997100 |
| H | 2.24174200 | 1.21242700 | 2.18666600 |
| H | 1.54470300 | 2.64868800 | -0.00562200 |
| H | 2.25617400 | 1.19435500 | -2.18129600 |
| H | 3.48426800 | -1.05762300 | -1.33778500 |
| C | 3.07954000 | -0.27190000 | 0.72337200 |
| Co | 1.05266100 | -0.15116000 | 0.00432900 |

**1Co-2**($C_s$) / M06-L

| | | | |
|---|---|---|---|
| C | -0.31785900 | 0.50600000 | 1.30042000 |
| C | -0.31785900 | 0.50600000 | -1.30042000 |
| C | -1.56262300 | 0.10109400 | -0.71411800 |
| C | -1.56262300 | 0.10109400 | 0.71411800 |
| H | -0.20153500 | 0.32560100 | 2.36759700 |
| H | -0.20153500 | 0.32560100 | -2.36759700 |
| H | -2.38919300 | -0.30686400 | -1.28784800 |
| H | -2.38919300 | -0.30686400 | 1.28784800 |
| C | 0.45802600 | 1.65444700 | 0.74583000 |
| H | 1.39152500 | 1.88861900 | 1.25324900 |
| C | 0.45802600 | 1.65444700 | -0.74583000 |
| H | 1.39152500 | 1.88861900 | -1.25324900 |
| C | -0.29060300 | -3.01685900 | 0.71052000 |
| C | 0.90823800 | -2.36822600 | 1.14858200 |
| C | 1.67230500 | -1.98449400 | 0.00000000 |
| C | 0.90823800 | -2.36822600 | -1.14858200 |
| H | -1.06966800 | -3.40597100 | -1.35201800 |
| H | -1.06966800 | -3.40597100 | 1.35201800 |
| H | 1.18066500 | -2.18113500 | 2.17906800 |
| H | 2.63490400 | -1.49243300 | 0.00000000 |
| H | 1.18066500 | -2.18113500 | -2.17906800 |
| C | -0.29060300 | -3.01685900 | -0.71052000 |
| P | -0.43379600 | 3.11942300 | 0.00000000 |
| C | 0.95956700 | 4.33995200 | 0.00000000 |
| H | 0.89786600 | 4.98304200 | -0.88186100 |
| H | 0.89786600 | 4.98304200 | 0.88186100 |
| H | 1.94064700 | 3.85530900 | 0.00000000 |
| Co | -0.14153000 | -1.05226000 | 0.00000000 |

**1Co-3**($C_s$) / BP86

| | | | |
|---|---|---|---|
| C | -0.02469200 | 0.63503100 | 1.32388100 |
| C | -0.02469200 | 0.63503100 | -1.32388100 |
| C | -1.32443400 | 0.44873100 | -0.72076400 |
| C | -1.32443400 | 0.44873100 | 0.72076400 |
| H | 0.05119300 | 0.43696600 | 2.40163000 |
| H | 0.05119300 | 0.43696600 | -2.40163000 |
| H | -2.22271000 | 0.20381700 | -1.29969500 |
| H | -2.22271000 | 0.20381700 | 1.29969500 |
| C | 1.01530100 | 1.55520900 | 0.75212500 |
| H | 1.98824500 | 1.50803000 | 1.25944000 |
| C | 1.01530100 | 1.55520900 | -0.75212500 |
| H | 1.98824500 | 1.50803000 | -1.25944000 |
| P | 0.69867100 | 3.29375400 | 0.00000000 |
| C | -1.15629500 | 3.52068700 | 0.00000000 |
| H | -1.34275300 | 4.60931200 | 0.00000000 |
| H | -1.62984400 | 3.08092900 | -0.89363300 |
| H | -1.62984400 | 3.08092900 | 0.89363300 |
| C | 0.62845500 | -2.48202700 | 1.15887600 |
| C | 1.46361100 | -2.26263100 | 0.00000000 |
| C | 0.62845500 | -2.48202700 | -1.15887600 |
| C | -0.68863800 | -2.89457500 | -0.71561600 |
| H | -1.53581800 | -3.13073000 | 1.36373500 |
| H | 0.93892000 | -2.36556100 | 2.20011700 |
| H | 2.51594200 | -1.97291100 | 0.00000000 |
| H | 0.93892000 | -2.36556100 | -2.20011700 |
| H | -1.53581800 | -3.13073000 | -1.36373500 |
| C | -0.68863800 | -2.89457500 | 0.71561600 |
| Co | -0.14626000 | -0.97060700 | 0.00000000 |

**1Co-3**($C_s$) / B3LYP

| | | | |
|---|---|---|---|
| C | -0.04843700 | 0.65529300 | 1.32410000 |
| C | -0.04843700 | 0.65529300 | -1.32410000 |
| C | -1.32930900 | 0.47341100 | -0.71601800 |
| C | -1.32930900 | 0.47341100 | 0.71601800 |
| H | 0.01894700 | 0.46652800 | 2.39484500 |
| H | 0.01894700 | 0.46652800 | -2.39484500 |
| H | -2.21929600 | 0.21526300 | -1.28460600 |
| H | -2.21929600 | 0.21526300 | 1.28460600 |
| C | 1.00328900 | 1.55739100 | 0.75023600 |
| H | 1.96778100 | 1.48877600 | 1.25268400 |
| C | 1.00328900 | 1.55739100 | -0.75023600 |
| H | 1.96778100 | 1.48877600 | -1.25268400 |
| P | 0.71918700 | 3.28378000 | 0.00000000 |
| C | -1.12293700 | 3.55599000 | 0.00000000 |
| H | -1.28257900 | 4.64046300 | 0.00000000 |
| H | -1.60419300 | 3.13278500 | -0.88703000 |
| H | -1.60419300 | 3.13278500 | 0.88703000 |
| C | 0.62805700 | -2.51447200 | 1.15058700 |
| C | 1.45389900 | -2.29476700 | 0.00000000 |
| C | 0.62805700 | -2.51447200 | -1.15058700 |
| C | -0.67656400 | -2.92602700 | -0.71112500 |
| H | -1.51681500 | -3.16215100 | 1.35378100 |
| H | 0.93722700 | -2.39977600 | 2.18327800 |
| H | 2.49629900 | -2.00098100 | 0.00000000 |
| H | 0.93722700 | -2.39977600 | -2.18327800 |
| H | -1.51681500 | -3.16215100 | -1.35378100 |
| C | -0.67656400 | -2.92602700 | 0.71112500 |
| Co | -0.15107500 | -0.95901900 | 0.00000000 |

**1Co-3**($C_s$) / M06-L

| | | | |
|---|---|---|---|
| C | -0.03257500 | 0.62347800 | 1.30716400 |
| C | -0.03257500 | 0.62347800 | -1.30716400 |
| C | -1.32476900 | 0.45046500 | -0.71405800 |
| C | -1.32476900 | 0.45046500 | 0.71405800 |
| H | 0.04129600 | 0.42532900 | 2.37492100 |
| H | 0.04129600 | 0.42532900 | -2.37492100 |
| H | -2.21240900 | 0.20416700 | -1.28883000 |
| H | -2.21240900 | 0.20416700 | 1.28883000 |
| C | 1.00276300 | 1.53587200 | 0.74490700 |
| H | 1.96795300 | 1.47611200 | 1.24334400 |
| C | 1.00276300 | 1.53587200 | -0.74490700 |
| H | 1.96795300 | 1.47611200 | -1.24334400 |
| P | 0.69775500 | 3.23621200 | 0.00000000 |
| C | -1.13446400 | 3.44352600 | 0.00000000 |
| H | -1.33905800 | 4.51684500 | 0.00000000 |
| H | -1.60483000 | 3.00613900 | -0.88391500 |
| H | -1.60483000 | 3.00613900 | 0.88391500 |
| C | 0.63261100 | -2.43926500 | 1.14766300 |
| C | 1.45656800 | -2.20754100 | 0.00000000 |
| C | 0.63261100 | -2.43926500 | -1.14766300 |
| C | -0.66680800 | -2.85624900 | -0.70976400 |
| H | -1.50470700 | -3.09412400 | 1.35095500 |
| H | 0.93421600 | -2.30559100 | 2.17846800 |
| H | 2.49359900 | -1.90265900 | 0.00000000 |
| H | 0.93421600 | -2.30559100 | -2.17846800 |
| H | -1.50470700 | -3.09412400 | -1.35095500 |
| C | -0.66680800 | -2.85624900 | 0.70976400 |
| Co | -0.15300800 | -0.95440600 | 0.00000000 |

**1Co-4**($C_1$) / BP86

| | | | |
|---|---|---|---|
| C | -0.08320900 | 0.99454900 | 1.62123800 |
| C | -0.19359900 | 1.77324300 | 0.39765600 |
| C | -1.38354500 | 2.01343300 | -0.44555900 |
| C | -0.45931000 | -0.39046300 | 1.63312700 |
| C | -2.34603300 | 1.13848300 | -0.85652500 |
| C | -0.88823700 | -1.01749000 | 0.39806100 |
| H | 0.45633800 | 1.40269100 | 2.48762900 |
| H | 0.45992700 | 2.66006400 | 0.42310900 |
| H | -1.47526100 | 3.05628800 | -0.79215400 |
| H | -0.19900100 | -0.99645800 | 2.51353600 |
| H | -3.16712300 | 1.53336700 | -1.47302400 |
| H | -0.74365000 | -2.11224700 | 0.41840400 |
| P | -2.27420500 | -0.66684300 | -0.75400200 |
| C | -3.76122800 | -1.01842000 | 0.34282200 |
| H | -4.68446100 | -0.74439000 | -0.19832500 |
| H | -3.80472800 | -2.10073800 | 0.55700300 |
| H | -3.71810600 | -0.45853600 | 1.29232500 |
| C | 2.96664100 | 0.14241900 | 0.41965500 |
| C | 2.50301100 | 0.79919000 | -0.78221200 |
| C | 1.83799400 | -0.17628900 | -1.61644900 |
| C | 1.87166100 | -1.43087600 | -0.89995500 |
| H | 2.75807300 | -2.00234900 | 1.10506900 |
| H | 3.49842700 | 0.62128300 | 1.24519700 |
| H | 2.62583300 | 1.85906200 | -1.01669000 |
| H | 1.38149000 | 0.00240500 | -2.59135100 |
| H | 1.41779700 | -2.36549000 | -1.23742800 |
| C | 2.58138800 | -1.23841500 | 0.34443000 |
| Co | 0.86793800 | 0.00413000 | 0.19403700 |

**1Co-4**($C_1$) / B3LYP

| | | | |
|---|---|---|---|
| C | -0.12825400 | 0.98459000 | 1.62615100 |
| C | -0.21823600 | 1.76109800 | 0.41414300 |
| C | -1.39300400 | 1.98737100 | -0.45535100 |
| C | -0.48601900 | -0.39243700 | 1.62997700 |
| C | -2.32724400 | 1.11184700 | -0.88848300 |
| C | -0.89410100 | -1.02469200 | 0.40288600 |
| H | 0.40704700 | 1.38305000 | 2.48780700 |
| H | 0.41396900 | 2.65103200 | 0.45722700 |
| H | -1.48998700 | 3.02328100 | -0.79228100 |
| H | -0.21583100 | -0.98987900 | 2.50148800 |
| H | -3.12838700 | 1.50006000 | -1.51982900 |
| H | -0.74245100 | -2.10859800 | 0.43288000 |
| P | -2.28276400 | -0.69152200 | -0.74565800 |
| C | -3.75598300 | -0.97895900 | 0.37348600 |
| H | -4.67535800 | -0.70865800 | -0.15965600 |
| H | -3.81600300 | -2.04450600 | 0.62376900 |
| H | -3.69340200 | -0.39396000 | 1.29709400 |
| C | 2.99246700 | 0.14213100 | 0.40770900 |
| C | 2.52945000 | 0.80532700 | -0.77529400 |
| C | 1.87393000 | -0.15612000 | -1.61363600 |
| C | 1.90967200 | -1.40877800 | -0.91932100 |
| H | 2.78650400 | -1.99379200 | 1.06587300 |
| H | 3.51608400 | 0.60962400 | 1.23360400 |
| H | 2.64759400 | 1.85967300 | -0.99625300 |
| H | 1.41971700 | 0.03214600 | -2.57826100 |
| H | 1.46564300 | -2.33436200 | -1.26637300 |
| C | 2.61002100 | -1.22851000 | 0.31899200 |
| Co | 0.85444900 | 0.01001900 | 0.19519400 |

**1Co-4**($C_1$) / M06-L

| | | | |
|---|---|---|---|
| C | -0.08810700 | 0.94283000 | 1.62721200 |
| C | -0.18961500 | 1.73554600 | 0.42584400 |
| C | -1.36864200 | 1.98705600 | -0.40922000 |
| C | -0.45328300 | -0.43053000 | 1.60363200 |
| C | -2.31620600 | 1.12889300 | -0.84131900 |
| C | -0.86912400 | -1.01974700 | 0.35776100 |
| H | 0.45136300 | 1.32611200 | 2.49176100 |
| H | 0.45579600 | 2.61465500 | 0.47354500 |
| H | -1.46327300 | 3.02752300 | -0.72737900 |
| H | -0.18797200 | -1.05188800 | 2.45846000 |
| H | -3.12392000 | 1.53729400 | -1.44774400 |
| H | -0.71366000 | -2.10392100 | 0.35493200 |
| P | -2.26703400 | -0.66333200 | -0.74988400 |
| C | -3.69444700 | -0.97308000 | 0.39303700 |
| H | -4.62912300 | -0.68756800 | -0.09706500 |
| H | -3.75428600 | -2.03942400 | 0.62521500 |
| H | -3.59943900 | -0.40961200 | 1.32540500 |
| C | 2.93310000 | 0.11533900 | 0.41850700 |
| C | 2.48371600 | 0.82014500 | -0.74109500 |
| C | 1.81618200 | -0.10177100 | -1.61108300 |
| C | 1.84305000 | -1.37552000 | -0.96022000 |
| H | 2.69891300 | -2.03519800 | 1.00415300 |
| H | 3.45600900 | 0.54989200 | 1.25984200 |
| H | 2.59873000 | 1.88150200 | -0.91641100 |
| H | 1.35918700 | 0.12391600 | -2.56417300 |
| H | 1.37337200 | -2.27771400 | -1.32929900 |
| C | 2.53821700 | -1.24572700 | 0.28271800 |
| Co | 0.86202900 | -0.00022900 | 0.18749500 |

**1Co-5**($C_1$) / BP86

| | | | |
|---|---|---|---|
| **C** | **-1.16503200** | **-2.07226300** | **0.43870300** |
| C | -2.31957600 | -1.94340500 | -0.35090200 |
| C | -3.05663400 | -0.78591700 | -0.76109500 |
| C | -0.44141700 | -1.18663600 | 1.33112900 |
| C | -2.70549500 | 0.55239900 | -0.63163000 |
| C | -0.62080100 | 0.23847100 | 1.51344100 |
| H | -0.76243800 | -3.09763000 | 0.46238700 |
| H | -2.68305700 | -2.88814100 | -0.77775200 |
| H | -3.98879100 | -0.99275500 | -1.30829500 |
| H | 0.15133000 | -1.69977100 | 2.10385400 |
| H | -3.32621500 | 1.32272900 | -1.10984100 |
| H | -0.42180500 | 0.74393800 | 2.46675100 |
| P | -1.12919800 | 1.05098100 | 0.02027700 |
| C | -1.19235300 | 2.87664300 | 0.23294600 |
| H | -0.27953100 | 3.20470300 | 0.75548500 |
| H | -1.22473800 | 3.36735500 | -0.75448200 |
| H | -2.08102000 | 3.17838700 | 0.81272700 |
| C | 2.54783600 | -1.05110300 | 0.27251200 |
| C | 2.09519800 | -1.12452000 | -1.09632400 |
| C | 1.92178300 | 0.22714000 | -1.56426900 |
| C | 2.31795300 | 1.13899100 | -0.50226300 |
| H | 3.02715800 | 0.71914500 | 1.60528300 |
| H | 2.74823300 | -1.90211500 | 0.92797100 |
| H | 1.88046800 | -2.03396800 | -1.66083300 |
| H | 1.56015000 | 0.51778600 | -2.55327000 |
| H | 2.32629600 | 2.22958100 | -0.56308200 |
| C | 2.69480100 | 0.34305000 | 0.63465000 |
| Co | 0.72423600 | -0.06337200 | 0.08102000 |

**1Co-5**($C_1$) / B3LYP

| | | | |
|---|---|---|---|
| C | -1.30207800 | -2.08090400 | 0.41959600 |
| C | -2.43609200 | -1.90176000 | -0.35354100 |
| C | -3.12901500 | -0.70351700 | -0.74805300 |
| C | -0.49118200 | -1.20429600 | 1.24583000 |
| C | -2.72439000 | 0.60124900 | -0.63316800 |
| C | -0.63460800 | 0.21289100 | 1.46564300 |
| H | -0.96289200 | -3.11889800 | 0.46645900 |
| H | -2.85670600 | -2.81800100 | -0.76722600 |
| H | -4.08251600 | -0.87111200 | -1.25330500 |
| H | 0.08424800 | -1.73829800 | 2.00465500 |
| H | -3.34661000 | 1.38984300 | -1.05714100 |
| H | -0.47314100 | 0.68256900 | 2.43372700 |
| P | -1.12043700 | 1.06074000 | -0.00648300 |
| C | -1.18150200 | 2.87133800 | 0.26871900 |
| H | -0.25877700 | 3.18610800 | 0.76451700 |
| H | -1.25222000 | 3.39297900 | -0.69163200 |
| H | -2.04134100 | 3.15037900 | 0.88677700 |
| C | 2.61031400 | -0.93642200 | 0.44708400 |
| C | 2.21300200 | -1.22980800 | -0.90334700 |
| C | 2.02835900 | 0.01249700 | -1.57343300 |
| C | 2.35127700 | 1.07837100 | -0.65375200 |
| H | 3.01191800 | 1.01337200 | 1.49011700 |
| H | 2.81036000 | -1.66698900 | 1.22252700 |
| H | 2.04351500 | -2.21448800 | -1.32184200 |
| H | 1.69432000 | 0.13954900 | -2.59653900 |
| H | 2.32366800 | 2.13844000 | -0.87746900 |
| C | 2.72616400 | 0.48555900 | 0.58762900 |
| Co | 0.73819400 | -0.06695300 | 0.07327300 |

**1Co-5**($C_1$) / M06-L

| | | | |
|---|---|---|---|
| C | -1.15029300 | -2.04240500 | 0.45930800 |
| C | -2.29576900 | -1.93265400 | -0.31819300 |
| C | -3.04467400 | -0.79432600 | -0.72357900 |
| C | -0.42886900 | -1.14976400 | 1.32532500 |
| C | -2.70284300 | 0.53151700 | -0.61196900 |
| C | -0.60903500 | 0.26824900 | 1.48797400 |
| H | -0.74195400 | -3.05420000 | 0.48884500 |
| H | -2.64534200 | -2.87417000 | -0.73520200 |
| H | -3.97481400 | -1.01336100 | -1.24736900 |
| H | 0.16978200 | -1.64681100 | 2.08980600 |
| H | -3.33134100 | 1.28668600 | -1.08082900 |
| H | -0.42157200 | 0.78177500 | 2.42768500 |
| P | -1.12730300 | 1.03420700 | -0.00340800 |
| C | -1.18950900 | 2.84180800 | 0.17211700 |
| H | -0.27448700 | 3.18771400 | 0.65524600 |
| H | -1.25648300 | 3.31221300 | -0.81076100 |
| H | -2.05207800 | 3.15179800 | 0.76559800 |
| C | 2.49833000 | -1.08537200 | 0.23635900 |
| C | 2.06087900 | -1.08416600 | -1.12456400 |
| C | 1.93152300 | 0.28006900 | -1.52560300 |
| C | 2.32895000 | 1.12311300 | -0.42969600 |
| H | 2.98727400 | 0.58976700 | 1.64628200 |
| H | 2.65477800 | -1.96175800 | 0.85186900 |
| H | 1.82815600 | -1.95178100 | -1.72584500 |
| H | 1.57917500 | 0.62232300 | -2.48920900 |
| H | 2.35804100 | 2.20466500 | -0.43681300 |
| C | 2.67238000 | 0.27171100 | 0.66123600 |
| Co | 0.72607400 | -0.05609800 | 0.07405600 |

**1Co-6**($C_1$) / BP86

| | | | |
|---|---|---|---|
| C | 1.46226000 | -0.89826500 | 0.75559100 |
| C | 1.46226000 | -0.89826500 | -0.75559100 |
| C | 0.71758600 | -1.89692700 | -1.56177500 |
| C | 0.71758600 | -1.89692700 | 1.56177500 |
| C | -0.62350900 | -2.08730500 | -1.36834600 |
| C | -0.62350900 | -2.08730500 | 1.36834600 |
| H | 2.41351600 | -0.56732800 | 1.19981700 |
| H | 2.41351600 | -0.56732800 | -1.19981700 |
| H | 1.27510000 | -2.51869400 | -2.28019800 |
| H | 1.27510000 | -2.51869400 | 2.28019800 |
| H | -1.19896000 | -2.90376300 | -1.82324100 |
| H | -1.19896000 | -2.90376300 | 1.82324100 |
| P | -1.16149600 | -1.00347900 | 0.00000000 |
| C | -2.99951400 | -0.89226900 | 0.00000000 |
| H | -3.33768700 | -0.34689500 | 0.89688800 |
| H | -3.33768700 | -0.34689500 | -0.89688800 |
| H | -3.45514500 | -1.89799000 | 0.00000000 |
| Co | 0.34475200 | 0.55188500 | 0.00000000 |
| C | 0.73360100 | 2.25343700 | 1.17692200 |
| C | 1.57828700 | 2.21297000 | 0.00000000 |
| C | 0.73360100 | 2.25343700 | -1.17692200 |
| C | -0.62351600 | 2.26203300 | -0.73189100 |
| H | -1.51073100 | 2.27241100 | 1.36925100 |
| H | 1.07323300 | 2.24198800 | 2.21466300 |
| H | 2.67078900 | 2.17389400 | 0.00000000 |
| H | 1.07323300 | 2.24198800 | -2.21466300 |
| H | -1.51073100 | 2.27241100 | -1.36925100 |
| C | -0.62351600 | 2.26203300 | 0.73189100 |

**1Co-6**($C_1$) / B3LYP

| | | | |
|---|---|---|---|
| C | -1.71302500 | -0.14859200 | -0.74593600 |
| C | -1.71302500 | -0.14859200 | 0.74593600 |
| C | -1.48873800 | -1.36225800 | 1.56462700 |
| C | -1.48873800 | -1.36225800 | -1.56462700 |
| C | -0.39561500 | -2.14458300 | 1.37507100 |
| C | -0.39561500 | -2.14458300 | -1.37507100 |
| H | -2.40059800 | 0.57265500 | -1.19082000 |
| H | -2.40059800 | 0.57265500 | 1.19082000 |
| H | -2.24529400 | -1.63714700 | 2.30354700 |
| H | -2.24529400 | -1.63714700 | -2.30354700 |
| H | -0.24701500 | -3.10506700 | 1.86530700 |
| H | -0.24701500 | -3.10506700 | -1.86530700 |
| P | 0.58131100 | -1.47280600 | 0.00000000 |
| C | 2.23811100 | -2.25819900 | 0.00000000 |
| H | 2.79475900 | -1.94469500 | -0.88918400 |
| H | 2.79475900 | -1.94469500 | 0.88918400 |
| H | 2.15822500 | -3.35117300 | 0.00000000 |
| Co | -0.05838400 | 0.64456400 | 0.00000000 |
| C | 0.37743500 | 2.39680000 | -1.16646100 |
| C | -0.39561500 | 2.72255600 | 0.00000000 |
| C | 0.37743500 | 2.39680000 | 1.16646100 |
| C | 1.58121900 | 1.79325000 | 0.72580100 |
| H | 2.37425500 | 1.41121300 | -1.35841100 |
| H | 0.06840200 | 2.53439400 | -2.19586400 |
| H | -1.38083200 | 3.17585100 | 0.00000000 |
| H | 0.06840200 | 2.53439400 | 2.19586400 |
| H | 2.37425500 | 1.41121300 | 1.35841100 |
| C | 1.58121900 | 1.79325000 | -0.72580100 |

**1Co-6**($C_1$) / M06-L

| | | | |
|---|---|---|---|
| C | 1.65919200 | -0.34785500 | 0.74898200 |
| C | 1.65919200 | -0.34785500 | -0.74898200 |
| C | 1.30451600 | -1.53166200 | -1.54374000 |
| C | 1.30451600 | -1.53166200 | 1.54374000 |
| C | 0.11773500 | -2.15752600 | -1.35689100 |
| C | 0.11773500 | -2.15752600 | 1.35689100 |
| H | 2.43809000 | 0.27977300 | 1.18553900 |
| H | 2.43809000 | 0.27977300 | -1.18553900 |
| H | 2.03368200 | -1.92592100 | -2.25317800 |
| H | 2.03368200 | -1.92592100 | 2.25317800 |
| H | -0.13888100 | -3.11375300 | -1.80707600 |
| H | -0.13888100 | -3.11375300 | 1.80707600 |
| P | -0.74652600 | -1.33940900 | 0.00000000 |
| C | -2.49354800 | -1.84455900 | 0.00000000 |
| H | -2.99317000 | -1.44695600 | 0.88571700 |
| H | -2.99317000 | -1.44695600 | -0.88571700 |
| H | -2.59465800 | -2.93274300 | 0.00000000 |
| Co | 0.13280800 | 0.64044500 | 0.00000000 |
| C | -0.06838600 | 2.35279600 | 1.16510000 |
| C | 0.73479100 | 2.59180600 | 0.00000000 |
| C | -0.06838600 | 2.35279600 | -1.16510000 |
| C | -1.33584000 | 1.90498300 | -0.72406700 |
| H | -2.16468800 | 1.60867700 | 1.35376500 |
| H | 0.25583500 | 2.44484300 | 2.19256700 |
| H | 1.77090400 | 2.90624300 | 0.00000000 |
| H | 0.25583500 | 2.44484300 | -2.19256700 |
| H | -2.16468800 | 1.60867700 | -1.35376500 |
| C | -1.33584000 | 1.90498300 | 0.72406700 |

**1Co-7**($C_1$) / BP86

| | | | |
|---|---|---|---|
| C | 1.08459500 | 2.32213000 | -0.67339100 |
| C | 1.08254500 | 2.32140700 | 0.68184200 |
| C | 0.46609800 | 1.14868900 | 1.37673500 |
| C | 0.46782800 | 1.15102000 | -1.37065000 |
| C | 1.01649700 | -0.17651400 | 1.25824800 |
| C | 1.01789200 | -0.17577800 | -1.25543500 |
| H | 1.55042900 | 3.12658900 | -1.26132400 |
| H | 1.54607500 | 3.12564100 | 1.27185800 |
| H | -0.11168600 | 1.36401800 | 2.28946300 |
| H | -0.10888800 | 1.36955200 | -2.28355100 |
| H | 0.83891700 | -0.91506000 | 2.05420600 |
| H | 0.84119600 | -0.91182200 | -2.05426900 |
| P | 2.34660100 | -0.50219800 | 0.00171500 |
| C | 2.28056200 | -2.36871400 | 0.00224800 |
| H | 2.81019800 | -2.75366500 | -0.88688000 |
| H | 2.80638200 | -2.75268600 | 0.89408100 |
| H | 1.24250400 | -2.74736700 | 0.00031500 |
| Co | -0.54850700 | 0.03057400 | -0.00207800 |
| C | -2.52531600 | 0.50183900 | -0.62858000 |
| C | -2.49849700 | 0.37907500 | 0.78952000 |
| C | -2.02571100 | -0.95607200 | 1.11447600 |
| C | -1.80011200 | -1.67710600 | -0.10646200 |
| H | -1.94051200 | -0.97077000 | -2.25112500 |
| H | -2.80875900 | 1.39003000 | -1.19680000 |
| H | -2.75538400 | 1.15826000 | 1.51032400 |
| H | -1.87671300 | -1.34407600 | 2.12557900 |
| H | -1.47229100 | -2.71400400 | -0.20006600 |
| C | -2.05818100 | -0.75617200 | -1.18545800 |

**1Co-7**($C_1$) / B3LYP

| | | | |
|---|---|---|---|
| C | 1.12685400 | 2.30424000 | -0.67058500 |
| C | 1.12621800 | 2.30405200 | 0.67477400 |
| C | 0.52547200 | 1.13933300 | 1.38663400 |
| C | 0.52499400 | 1.14035800 | -1.38281500 |
| C | 1.04060900 | -0.17765000 | 1.26436900 |
| C | 1.03995000 | -0.17773500 | -1.26259700 |
| H | 1.56846200 | 3.11695300 | -1.24894200 |
| H | 1.56695100 | 3.11668400 | 1.25387500 |
| H | -0.05209900 | 1.36465400 | 2.28528600 |
| H | -0.05259800 | 1.36735200 | -2.28122800 |
| H | 0.83640000 | -0.90841400 | 2.04764100 |
| H | 0.83511800 | -0.90756500 | -2.04677400 |
| P | 2.33786800 | -0.54923000 | 0.00039000 |
| C | 2.22912600 | -2.40542800 | 0.00140400 |
| H | 2.74689000 | -2.79886900 | -0.88097700 |
| H | 2.74389000 | -2.79750500 | 0.88616400 |
| H | 1.19365300 | -2.76489600 | -0.00001400 |
| Co | -0.53803400 | 0.04780900 | -0.00120400 |
| C | -2.53813000 | 0.52439500 | -0.62803000 |
| C | -2.50757700 | 0.41071500 | 0.78332700 |
| C | -2.06889900 | -0.92349600 | 1.11035800 |
| C | -1.87326800 | -1.64969900 | -0.09964700 |
| H | -2.00107900 | -0.96077500 | -2.23026600 |
| H | -2.80471600 | 1.40715600 | -1.19659600 |
| H | -2.74829800 | 1.19135100 | 1.49512100 |
| H | -1.93178800 | -1.31070900 | 2.11403600 |
| H | -1.55995800 | -2.68281600 | -0.18861000 |
| C | -2.10567200 | -0.73658600 | -1.17420100 |

**1Co-7**($C_1$) / M06-L

| | | | |
|---|---|---|---|
| C | 1.12451900 | 2.28416700 | -0.66898000 |
| C | 1.12261900 | 2.28526800 | 0.67259000 |
| C | 0.48439700 | 1.14067300 | 1.36471000 |
| C | 0.48523900 | 1.13960400 | -1.35994600 |
| C | 1.00739000 | -0.17994600 | 1.25283700 |
| C | 1.00716800 | -0.18231900 | -1.24826700 |
| H | 1.60559800 | 3.06969300 | -1.25004800 |
| H | 1.60167900 | 3.07212800 | 1.25350700 |
| H | -0.09666000 | 1.36552800 | 2.26109900 |
| H | -0.09759900 | 1.36537000 | -2.25531200 |
| H | 0.80430600 | -0.91202800 | 2.03593000 |
| H | 0.80075600 | -0.91539200 | -2.03009500 |
| P | 2.30216800 | -0.54552100 | 0.00231600 |
| C | 2.14260000 | -2.38205800 | 0.00579200 |
| H | 2.63545500 | -2.80113300 | -0.87480600 |
| H | 2.63791400 | -2.79749300 | 0.88674800 |
| H | 1.09179800 | -2.69434200 | 0.00808400 |
| Co | -0.54183900 | 0.04420900 | -0.00042800 |
| C | -2.48518900 | 0.52768700 | -0.62140800 |
| C | -2.45829200 | 0.40090100 | 0.78402500 |
| C | -1.99713800 | -0.92366200 | 1.10081100 |
| C | -1.77807300 | -1.63576800 | -0.11168200 |
| H | -1.89953800 | -0.92127100 | -2.23258300 |
| H | -2.75116900 | 1.41295700 | -1.18201200 |
| H | -2.69473900 | 1.17495600 | 1.50144100 |
| H | -1.83913300 | -1.30794000 | 2.10070100 |
| H | -1.45027000 | -2.66164900 | -0.20805800 |
| C | -2.03045500 | -0.71791400 | -1.17677900 |

**1Co-8**($C_s$) / BP86

| | | | |
|---|---|---|---|
| C | 1.96044400 | 1.36286600 | 0.67648100 |
| C | 1.96044400 | 1.36286600 | -0.67648100 |
| C | 0.90610100 | 0.56374200 | -1.37064000 |
| C | 0.90610100 | 0.56374200 | 1.37064000 |
| C | -0.50536900 | 0.84804000 | -1.28919900 |
| C | -0.50536900 | 0.84804000 | 1.28919900 |
| H | 2.68486200 | 1.94121700 | 1.26900100 |
| H | 2.68486200 | 1.94121700 | -1.26900100 |
| H | 1.23211500 | 0.03957200 | -2.28519000 |
| H | 1.23211500 | 0.03957200 | 2.28519000 |
| H | -1.13724800 | 0.49445300 | -2.11719400 |
| H | -1.13724800 | 0.49445300 | 2.11719400 |
| Co | -0.01325400 | -0.64435900 | 0.00000000 |
| C | 0.75976600 | -2.48193900 | 0.71243400 |
| C | 0.75976600 | -2.48193900 | -0.71243400 |
| C | -0.60870700 | -2.27100800 | -1.15435800 |
| C | -1.46275900 | -2.18596100 | 0.00000000 |
| H | -0.93068500 | -2.19193000 | 2.19587800 |
| H | 1.63297500 | -2.58977500 | 1.35901500 |
| H | 1.63297500 | -2.58977500 | -1.35901500 |
| H | -0.93068500 | -2.19193000 | -2.19587800 |
| H | -2.54363100 | -2.03510000 | 0.00000000 |
| C | -0.60870700 | -2.27100800 | 1.15435800 |
| P | -1.36319400 | 1.84983900 | 0.00000000 |
| C | -0.59363700 | 3.56297100 | 0.00000000 |
| H | 0.50619600 | 3.57306700 | 0.00000000 |
| H | -0.96463400 | 4.10129600 | -0.89143900 |
| H | -0.96463400 | 4.10129600 | 0.89143900 |

**1Co-8**($C_s$) / B3LYP

| | | | |
|---|---|---|---|
| C | -1.95173400 | -1.36977700 | 0.67150700 |
| C | -1.95173400 | -1.36977700 | -0.67150700 |
| C | -0.89157100 | -0.60044000 | -1.38044500 |
| C | -0.89157100 | -0.60044000 | 1.38044500 |
| C | 0.50172800 | -0.87206400 | -1.29045400 |
| C | 0.50172800 | -0.87206400 | 1.29045400 |
| H | -2.69279800 | -1.91927600 | 1.25403900 |
| H | -2.69279800 | -1.91927600 | -1.25403900 |
| H | -1.21729600 | -0.07733400 | -2.28365000 |
| H | -1.21729600 | -0.07733400 | 2.28365000 |
| H | 1.13041300 | -0.50765100 | -2.10315400 |
| H | 1.13041300 | -0.50765100 | 2.10315400 |
| Co | 0.00836400 | 0.63723200 | 0.00000000 |
| C | -0.75928200 | 2.49932400 | 0.70879000 |
| C | -0.75928200 | 2.49932400 | -0.70879000 |
| C | 0.60132000 | 2.30959500 | -1.14623200 |
| C | 1.44804400 | 2.24452100 | 0.00000000 |
| H | 0.92474800 | 2.24000700 | 2.17886000 |
| H | -1.62612300 | 2.59940100 | 1.35078000 |
| H | -1.62612300 | 2.59940100 | -1.35078000 |
| H | 0.92474800 | 2.24000700 | -2.17886000 |
| H | 2.52197900 | 2.10411900 | 0.00000000 |
| C | 0.60132000 | 2.30959500 | 1.14623200 |
| P | 1.36085300 | -1.85752600 | 0.00000000 |
| C | 0.60636700 | -3.56649300 | 0.00000000 |
| H | -0.48458800 | -3.58598700 | 0.00000000 |
| H | 0.97704600 | -4.09930900 | -0.88474600 |
| H | 0.97704600 | -4.09930900 | 0.88474600 |

**1Co-8**($C_s$) / M06-L

| | | | |
|---|---|---|---|
| C | 1.93307300 | 1.36308600 | 0.66968400 |
| C | 1.93307300 | 1.36308600 | -0.66968400 |
| C | 0.89702900 | 0.56415300 | -1.36063600 |
| C | 0.89702900 | 0.56415300 | 1.36063600 |
| C | -0.50234800 | 0.83758400 | -1.28326600 |
| C | -0.50234800 | 0.83758400 | 1.28326600 |
| H | 2.64456700 | 1.94615600 | 1.25358900 |
| H | 2.64456700 | 1.94615600 | -1.25358900 |
| H | 1.22392900 | 0.03350000 | -2.25938900 |
| H | 1.22392900 | 0.03350000 | 2.25938900 |
| H | -1.12390400 | 0.46548200 | -2.09803300 |
| H | -1.12390400 | 0.46548200 | 2.09803300 |
| Co | -0.01251800 | -0.63966200 | 0.00000000 |
| C | 0.75909600 | -2.44577400 | 0.70615500 |
| C | 0.75909600 | -2.44577400 | -0.70615500 |
| C | -0.59522800 | -2.23893600 | -1.14348400 |
| C | -1.44239900 | -2.15615000 | 0.00000000 |
| H | -0.91148100 | -2.14791300 | 2.17496600 |
| H | 1.62521600 | -2.53684500 | 1.34700900 |
| H | 1.62521600 | -2.53684500 | -1.34700900 |
| H | -0.91148100 | -2.14791300 | -2.17496600 |
| H | -2.51178000 | -2.00183600 | 0.00000000 |
| C | -0.59522800 | -2.23893600 | 1.14348400 |
| P | -1.35467400 | 1.80933300 | 0.00000000 |
| C | -0.59566200 | 3.49935200 | 0.00000000 |
| H | 0.49461500 | 3.51318800 | 0.00000000 |
| H | -0.95625400 | 4.03910300 | -0.88044900 |
| H | -0.95625400 | 4.03910300 | 0.88044900 |

$(C_{10}H_8PCH_3)Fe(CO)_3$

**2Fe-1**($C_1$) / BP86

| | | | |
|---|---|---|---|
| C | 1.79247300 | -0.24678500 | -0.63595300 |
| C | 2.37251700 | 0.90894200 | 0.01346700 |
| C | 1.73965900 | 2.18664200 | 0.33378500 |
| C | 0.45856900 | -0.41447100 | -1.26058000 |
| C | 0.44139600 | 2.61805200 | 0.26943700 |
| C | -0.59648300 | 0.51887500 | -1.56592000 |
| H | 2.44668400 | 2.92654300 | 0.73789200 |
| H | 0.46909400 | -1.27122000 | -1.94925400 |
| H | 0.20913700 | 3.62730700 | 0.63652500 |
| H | -1.14305100 | 0.50374300 | -2.51551300 |
| P | -0.95492100 | 1.63103200 | -0.24043700 |
| Fe | -1.24559100 | -0.54483300 | 0.08987100 |
| C | -2.31279800 | 2.79760400 | -0.63090400 |
| H | -3.13178500 | 2.24227600 | -1.11463300 |
| H | -2.69958500 | 3.24373000 | 0.30052200 |
| H | -1.95734700 | 3.59988000 | -1.29881400 |
| C | -2.99058300 | -0.36985000 | 0.35788100 |
| C | -1.41361100 | -2.22145900 | -0.46696900 |
| C | -0.56018100 | -0.86301300 | 1.71115100 |
| O | -4.15228600 | -0.29682500 | 0.54923000 |
| O | -1.53570000 | -3.33099400 | -0.84038200 |
| O | -0.12581400 | -1.04781500 | 2.78733100 |
| C | 3.73617400 | 0.83278300 | 0.43759900 |
| H | 4.17396000 | 1.72138300 | 0.91077300 |
| C | 2.62451300 | -1.39944900 | -0.76729600 |
| H | 2.19632400 | -2.28705300 | -1.25020000 |
| C | 4.52234600 | -0.31299700 | 0.29208500 |
| H | 5.56041100 | -0.32400000 | 0.64288500 |
| C | 3.94674200 | -1.45253900 | -0.31399300 |
| H | 4.53134200 | -2.37134500 | -0.44245800 |

**2Fe-1**($C_1$) / B3LYP

| | | | |
|---|---|---|---|
| C | 1.78927900 | -0.24470600 | -0.62607700 |
| C | 2.37521500 | 0.90059700 | 0.01132900 |
| C | 1.75287700 | 2.18969800 | 0.31545800 |
| C | 0.44695900 | -0.40606200 | -1.23854700 |
| C | 0.46792700 | 2.62117900 | 0.26144200 |
| C | -0.59340000 | 0.53025600 | -1.53915900 |
| H | 2.46584400 | 2.92687700 | 0.68750900 |
| H | 0.46062100 | -1.24575900 | -1.93326900 |
| H | 0.25236400 | 3.63628800 | 0.59516300 |
| H | -1.12557400 | 0.53012500 | -2.48687600 |
| P | -0.94043800 | 1.63454500 | -0.21363200 |
| Fe | -1.25702700 | -0.54617500 | 0.09986200 |
| C | -2.27083400 | 2.81776400 | -0.62568000 |
| H | -3.10236600 | 2.27631200 | -1.08491300 |
| H | -2.63699600 | 3.29809500 | 0.28754300 |
| H | -1.90817900 | 3.58765100 | -1.31422800 |
| C | -3.00074400 | -0.34076700 | 0.41489100 |
| C | -1.47288700 | -2.20350600 | -0.53437900 |
| C | -0.52359000 | -0.94112100 | 1.69500600 |
| O | -4.13814800 | -0.22841800 | 0.63495700 |
| O | -1.60766700 | -3.27379000 | -0.96341700 |
| O | -0.05654100 | -1.17260900 | 2.73088000 |
| C | 3.72959800 | 0.81829900 | 0.43394900 |
| H | 4.17244800 | 1.69749500 | 0.89892000 |
| C | 2.60816600 | -1.39627400 | -0.75740000 |
| H | 2.17925400 | -2.27542500 | -1.23467100 |
| C | 4.50386700 | -0.32746200 | 0.29260000 |
| H | 5.53396900 | -0.34448200 | 0.64017500 |
| C | 3.92400200 | -1.45688100 | -0.30854900 |
| H | 4.49812400 | -2.37233200 | -0.43595100 |

**2Fe-1**($C_1$) / M06-L

| | | | |
|---|---|---|---|
| C | 1.75260500 | -0.20621600 | -0.62468200 |
| C | 2.31017500 | 0.94949500 | 0.01267000 |
| C | 1.67141800 | 2.22096000 | 0.29546400 |
| C | 0.43997100 | -0.39208200 | -1.26146800 |
| C | 0.38033000 | 2.62660700 | 0.22653500 |
| C | -0.62914700 | 0.51315600 | -1.56442300 |
| H | 2.36921600 | 2.96826000 | 0.67354500 |
| H | 0.47638000 | -1.24077100 | -1.94463500 |
| H | 0.13602700 | 3.63211300 | 0.56367600 |
| H | -1.16255800 | 0.49932400 | -2.51020600 |
| P | -0.98189900 | 1.59980100 | -0.24200000 |
| Fe | -1.21762600 | -0.56639400 | 0.07802300 |
| C | -2.37496300 | 2.70283800 | -0.59254300 |
| H | -3.16328600 | 2.13530600 | -1.08780000 |
| H | -2.77987200 | 3.10272200 | 0.33849800 |
| H | -2.06600000 | 3.53309700 | -1.23010000 |
| C | -2.95132900 | -0.37847500 | 0.44070900 |
| C | -1.39745000 | -2.22990700 | -0.54129700 |
| C | -0.40625100 | -0.91977400 | 1.64502900 |
| O | -4.08800600 | -0.25675400 | 0.67630900 |
| O | -1.50128000 | -3.30978900 | -0.96330600 |
| O | 0.15440300 | -1.10823100 | 2.64588400 |
| C | 3.65046600 | 0.88121700 | 0.46643100 |
| H | 4.06929800 | 1.77475400 | 0.92416900 |
| C | 2.57536600 | -1.35405700 | -0.70148100 |
| H | 2.15494000 | -2.24154400 | -1.16968900 |
| C | 4.42986200 | -0.25746200 | 0.37001800 |
| H | 5.44859700 | -0.26118000 | 0.74231400 |
| C | 3.87124600 | -1.39967000 | -0.21544400 |
| H | 4.44929900 | -2.31443500 | -0.30255500 |

**2Fe-2**($C_s$) / BP86

| | | | |
|---|---|---|---|
| C | 0.06895700 | 1.07995600 | 0.72794400 |
| C | 0.06895700 | 1.07995600 | -0.72794400 |
| C | 0.63330500 | -0.12663900 | -1.31826700 |
| C | 1.91809300 | -0.67527000 | -0.75386800 |
| C | 1.91809300 | -0.67527000 | 0.75386800 |
| C | 0.63330500 | -0.12663900 | 1.31826700 |
| C | -0.53655600 | 2.18068100 | 1.42759500 |
| C | -1.07812700 | 3.24332500 | 0.71712200 |
| C | -1.07812700 | 3.24332500 | -0.71712200 |
| C | -0.53655600 | 2.18068100 | -1.42759500 |
| P | 3.20291800 | 0.50914000 | 0.00000000 |
| C | 4.71562500 | -0.59857600 | 0.00000000 |
| H | 0.48999900 | -0.24953300 | -2.39989900 |
| H | 2.32266500 | -1.55702800 | -1.26638700 |
| H | 2.32266500 | -1.55702800 | 1.26638700 |
| H | 0.48999900 | -0.24953300 | 2.39989900 |
| H | -0.53125200 | 2.18162200 | 2.52436600 |
| H | -1.51470300 | 4.09408600 | 1.25386400 |
| H | -1.51470300 | 4.09408600 | -1.25386400 |
| H | -0.53125200 | 2.18162200 | -2.52436600 |
| H | 5.32895700 | -0.38121200 | 0.89250000 |
| H | 4.46788900 | -1.67454500 | 0.00000000 |
| H | 5.32895700 | -0.38121200 | -0.89250000 |
| Fe | -0.97138600 | -0.64979700 | 0.00000000 |
| C | -2.20594400 | -0.67674300 | -1.29595400 |
| C | -2.20594400 | -0.67674300 | 1.29595400 |
| C | -0.53655600 | -2.36252600 | 0.00000000 |
| O | -3.01232600 | -0.73641200 | -2.14748500 |
| O | -3.01232600 | -0.73641200 | 2.14748500 |
| O | -0.24015100 | -3.49964100 | 0.00000000 |

**2Fe-2**($C_s$) / B3LYP

| | | | |
|---|---|---|---|
| C | -1.08428300 | -0.01154900 | 0.72207600 |
| C | -1.08428300 | -0.01154900 | -0.72207600 |
| C | 0.07652500 | 0.62413800 | -1.31272200 |
| C | 0.53522300 | 1.94494200 | -0.75128500 |
| C | 0.53522300 | 1.94494200 | 0.75128500 |
| C | 0.07652500 | 0.62413800 | 1.31272200 |
| C | -2.13914000 | -0.68727900 | 1.41865500 |
| C | -3.15529600 | -1.29656100 | 0.71492600 |
| C | -3.15529600 | -1.29656100 | -0.71492600 |
| C | -2.13914000 | -0.68727900 | -1.41865500 |
| P | -0.70893200 | 3.15091400 | 0.00000000 |
| C | 0.30219500 | 4.72131000 | 0.00000000 |
| H | 0.19002000 | 0.50420700 | -2.38976700 |
| H | 1.38658800 | 2.39428000 | -1.25974500 |
| H | 1.38658800 | 2.39428000 | 1.25974500 |
| H | 0.19002000 | 0.50420700 | 2.38976700 |
| H | -2.14203800 | -0.68037600 | 2.50680000 |
| H | -3.96882700 | -1.78517300 | 1.24715300 |
| H | -3.96882700 | -1.78517300 | -1.24715300 |
| H | -2.14203800 | -0.68037600 | -2.50680000 |
| H | 0.05191500 | 5.31685800 | 0.88585100 |
| H | 1.38259400 | 4.53834400 | 0.00000000 |
| H | 0.05191500 | 5.31685800 | -0.88585100 |
| Fe | 0.72078900 | -0.92526700 | 0.00000000 |
| C | 0.82109400 | -2.15183500 | -1.32333900 |
| C | 0.82109400 | -2.15183500 | 1.32333900 |
| C | 2.40457400 | -0.36490800 | 0.00000000 |
| O | 0.91268000 | -2.91372200 | -2.19016200 |
| O | 0.91268000 | -2.91372200 | 2.19016200 |
| O | 3.49782200 | 0.02177000 | 0.00000000 |

**2Fe-2**($C_s$) / M06-L

| | | | |
|---|---|---|---|
| C | -1.07422900 | -0.04554500 | 0.72096300 |
| C | -1.07422900 | -0.04554500 | -0.72096300 |
| C | 0.06096100 | 0.63513100 | -1.30296900 |
| C | 0.45970700 | 1.96396600 | -0.74682000 |
| C | 0.45970700 | 1.96396600 | 0.74682000 |
| C | 0.06096100 | 0.63513100 | 1.30296900 |
| C | -2.07062900 | -0.79437500 | 1.41393500 |
| C | -3.03661900 | -1.47295200 | 0.71083800 |
| C | -3.03661900 | -1.47295200 | -0.71083800 |
| C | -2.07062900 | -0.79437500 | -1.41393500 |
| P | -0.82694700 | 3.09404000 | 0.00000000 |
| C | 0.13207600 | 4.67588900 | 0.00000000 |
| H | 0.18708800 | 0.51079700 | -2.37733500 |
| H | 1.28937200 | 2.45686700 | -1.24820000 |
| H | 1.28937200 | 2.45686700 | 1.24820000 |
| H | 0.18708800 | 0.51079700 | 2.37733500 |
| H | -2.06584500 | -0.79512100 | 2.50050100 |
| H | -3.80746400 | -2.02146000 | 1.24251400 |
| H | -3.80746400 | -2.02146000 | -1.24251400 |
| H | -2.06584500 | -0.79512100 | -2.50050100 |
| H | -0.12387100 | 5.26853800 | 0.88152400 |
| H | 1.21329600 | 4.51166900 | 0.00000000 |
| H | -0.12387100 | 5.26853800 | -0.88152400 |
| Fe | 0.74212900 | -0.88365000 | 0.00000000 |
| C | 0.87794600 | -2.10293200 | -1.32131200 |
| C | 0.87794600 | -2.10293200 | 1.32131200 |
| C | 2.38894900 | -0.22513000 | 0.00000000 |
| O | 0.97810600 | -2.86164600 | -2.19467500 |
| O | 0.97810600 | -2.86164600 | 2.19467500 |
| O | 3.44443600 | 0.26195500 | 0.00000000 |

**2Fe-3**($C_s$) / BP86

| | | | |
|---|---|---|---|
| C | 1.08668300 | -0.39794100 | 1.26216800 |
| C | 1.08668300 | -0.39794100 | -1.26216800 |
| C | 0.00086300 | 0.51352300 | -1.41205600 |
| C | -0.03608000 | 1.83539800 | -0.70845900 |
| C | -0.03608000 | 1.83539800 | 0.70845900 |
| C | 0.00086300 | 0.51352300 | 1.41205600 |
| C | -0.09480700 | 3.05494600 | 1.41035000 |
| C | -0.14851300 | 4.27637800 | 0.70447700 |
| C | -0.14851300 | 4.27637800 | -0.70447700 |
| C | -0.09480700 | 3.05494600 | -1.41035000 |
| H | 1.29978700 | -1.10889300 | 2.07121600 |
| H | 1.29978700 | -1.10889300 | -2.07121600 |
| H | -0.57959900 | 0.44753400 | -2.34281200 |
| H | -0.57959900 | 0.44753400 | 2.34281200 |
| H | -0.11058300 | 3.05180900 | 2.50759800 |
| H | -0.20462700 | 5.22376200 | 1.25375700 |
| H | -0.20462700 | 5.22376200 | -1.25375700 |
| H | -0.11058300 | 3.05180900 | -2.50759800 |
| Fe | -0.54308200 | -1.05692100 | 0.00000000 |
| C | -0.71662600 | -2.33227100 | -1.21625800 |
| C | -2.19776500 | -0.36518900 | 0.00000000 |
| C | -0.71662600 | -2.33227100 | 1.21625800 |
| O | -0.85862000 | -3.16907600 | -2.03144800 |
| O | -3.29554400 | 0.04604500 | 0.00000000 |
| O | -0.85862000 | -3.16907600 | 2.03144800 |
| P | 2.41320700 | -0.09951100 | 0.00000000 |
| C | 3.19544800 | -1.79070600 | 0.00000000 |
| H | 3.84164200 | -1.89054900 | -0.88954400 |
| H | 3.84164200 | -1.89054900 | 0.88954400 |
| H | 2.44671500 | -2.60289600 | 0.00000000 |

**2Fe-3**($C_s$) / B3LYP

| | | | |
|---|---|---|---|
| C | 1.10096900 | -0.39517400 | 1.26943000 |
| C | 1.10096900 | -0.39517400 | -1.26943000 |
| C | 0.04099200 | 0.51814300 | -1.42014800 |
| C | -0.00516700 | 1.82971900 | -0.70468000 |
| C | -0.00516700 | 1.82971900 | 0.70468000 |
| C | 0.04099200 | 0.51814300 | 1.42014800 |
| C | -0.07820300 | 3.04315700 | 1.40088700 |
| C | -0.14494500 | 4.25765800 | 0.70068200 |
| C | -0.14494500 | 4.25765800 | -0.70068200 |
| C | -0.07820300 | 3.04315700 | -1.40088700 |
| H | 1.29695600 | -1.11068500 | 2.06609500 |
| H | 1.29695600 | -1.11068500 | -2.06609500 |
| H | -0.53727900 | 0.46256300 | -2.34231900 |
| H | -0.53727900 | 0.46256300 | 2.34231900 |
| H | -0.09262100 | 3.04060100 | 2.48944500 |
| H | -0.20839400 | 5.19684800 | 1.24624300 |
| H | -0.20839400 | 5.19684800 | -1.24624300 |
| H | -0.09262100 | 3.04060100 | -2.48944500 |
| Fe | -0.55940900 | -1.05302000 | 0.00000000 |
| C | -0.74663800 | -2.32776300 | 1.23831300 |
| C | -0.74663800 | -2.32776300 | -1.23831300 |
| C | -2.20572900 | -0.32611700 | 0.00000000 |
| O | -3.28392600 | 0.09681000 | 0.00000000 |
| O | -0.88736600 | -3.13540900 | 2.06078000 |
| O | -0.88736600 | -3.13540900 | -2.06078000 |
| P | 2.41586900 | -0.13780000 | 0.00000000 |
| C | 3.17325900 | -1.83108600 | 0.00000000 |
| H | 3.81358900 | -1.93882900 | -0.88286200 |
| H | 3.81358900 | -1.93882900 | 0.88286200 |
| H | 2.42208900 | -2.62907500 | 0.00000000 |

**2Fe-3**($C_s$) / M06-L

| | | | |
|---|---|---|---|
| C | 0.42165300 | 1.07334300 | 1.25327900 |
| C | 0.42163400 | 1.07339700 | -1.25325600 |
| C | -0.50754700 | 0.02240300 | -1.40242100 |
| C | -1.81731500 | 0.01222900 | -0.70234800 |
| C | -1.81730800 | 0.01220200 | 0.70234500 |
| C | -0.50753300 | 0.02234100 | 1.40240500 |
| C | -3.02753900 | -0.03070000 | 1.39632100 |
| C | -4.23733200 | -0.06651700 | 0.69770900 |
| C | -4.23733900 | -0.06649000 | -0.69769500 |
| C | -3.02755100 | -0.03064600 | -1.39631700 |
| H | 1.14157300 | 1.25529200 | 2.04889800 |
| H | 1.14156400 | 1.25536200 | -2.04886100 |
| H | -0.45434600 | -0.55620900 | -2.32375100 |
| H | -0.45432600 | -0.55630700 | 2.32371100 |
| H | -3.02296800 | -0.04970000 | 2.48298600 |
| H | -5.17552900 | -0.10908400 | 1.24164900 |
| H | -5.17554000 | -0.10903500 | -1.24162900 |
| H | -3.02299200 | -0.04960500 | -2.48298200 |
| Fe | 1.03516400 | -0.56333000 | 0.00000000 |
| C | 2.30719100 | -0.75766500 | -1.23082800 |
| C | 0.24736100 | -2.18637900 | 0.00000000 |
| C | 2.30711400 | -0.75780200 | 1.23084800 |
| O | 3.12199000 | -0.88736200 | -2.05231100 |
| O | -0.25781900 | -3.23085300 | -0.00011700 |
| O | 3.12185800 | -0.88757800 | 2.05237400 |
| P | 0.18880700 | 2.39024600 | 0.00000000 |
| C | 1.90893900 | 3.04425900 | 0.00000000 |
| H | 2.06778400 | 3.67101500 | -0.87998700 |
| H | 2.06779900 | 3.67094700 | 0.88012400 |
| H | 2.64581400 | 2.23269700 | 0.00000000 |

**2Fe-4**($C_s$) / BP86

| | | | |
|---|---|---|---|
| C | 1.16989100 | -0.34553400 | 1.29998600 |
| C | 1.16989100 | -0.34553400 | -1.29998600 |
| C | -0.06123100 | 0.36962500 | -1.41288900 |
| C | -0.35553900 | 1.65568800 | -0.70731900 |
| C | -0.35553900 | 1.65568800 | 0.70731900 |
| C | -0.06123100 | 0.36962500 | 1.41288900 |
| C | -0.65870500 | 2.83762700 | 1.40990000 |
| C | -0.95204700 | 4.02576700 | 0.70430600 |
| C | -0.95204700 | 4.02576700 | -0.70430600 |
| C | -0.65870500 | 2.83762700 | -1.40990000 |
| H | 1.44533700 | -0.98912700 | 2.14588800 |
| H | 1.44533700 | -0.98912700 | -2.14588800 |
| H | -0.62389200 | 0.21319300 | -2.34577700 |
| H | -0.62389200 | 0.21319300 | 2.34577700 |
| H | -0.67641000 | 2.83058400 | 2.50712200 |
| H | -1.19630900 | 4.94259400 | 1.25393100 |
| H | -1.19630900 | 4.94259400 | -1.25393100 |
| H | -0.67641000 | 2.83058400 | -2.50712200 |
| P | 2.46691600 | -0.17008000 | 0.00000000 |
| Fe | -0.29019300 | -1.27938100 | 0.00000000 |
| C | -0.23676200 | -2.56587100 | -1.21768700 |
| C | -2.04024400 | -0.90143100 | 0.00000000 |
| C | -0.23676200 | -2.56587100 | 1.21768700 |
| O | -0.23042200 | -3.41617600 | -2.02871600 |
| O | -3.19452700 | -0.69840200 | 0.00000000 |
| O | -0.23042200 | -3.41617600 | 2.02871600 |
| C | 2.98023100 | 1.63149500 | 0.00000000 |
| H | 3.61312800 | 1.80080600 | 0.89043400 |
| H | 3.61312800 | 1.80080600 | -0.89043400 |
| H | 2.15333300 | 2.35701200 | 0.00000000 |

**2Fe-4**($C_s$) / B3LYP

| | | | |
|---|---|---|---|
| C | 1.18115800 | -0.33230300 | 1.30279100 |
| C | 1.18115800 | -0.33230300 | -1.30279100 |
| C | -0.03080200 | 0.37976500 | -1.41969300 |
| C | -0.34067500 | 1.65217100 | -0.70343800 |
| C | -0.34067500 | 1.65217100 | 0.70343800 |
| C | -0.03080200 | 0.37976500 | 1.41969300 |
| C | -0.66016900 | 2.82398100 | 1.40044200 |
| C | -0.96972300 | 4.00155600 | 0.70046600 |
| C | -0.96972300 | 4.00155600 | -0.70046600 |
| C | -0.66016900 | 2.82398100 | -1.40044200 |
| H | 1.45012100 | -0.97951000 | 2.13580500 |
| H | 1.45012100 | -0.97951000 | -2.13580500 |
| H | -0.58775900 | 0.23144400 | -2.34653700 |
| H | -0.58775900 | 0.23144400 | 2.34653700 |
| H | -0.67584500 | 2.81788400 | 2.48898600 |
| H | -1.22280000 | 4.90797800 | 1.24637500 |
| H | -1.22280000 | 4.90797800 | -1.24637500 |
| H | -0.67584500 | 2.81788400 | -2.48898600 |
| P | 2.46589900 | -0.17557600 | 0.00000000 |
| Fe | -0.30016200 | -1.28244300 | 0.00000000 |
| C | -0.24984000 | -2.57122100 | -1.24106900 |
| C | -2.05209900 | -0.88529800 | 0.00000000 |
| C | -0.24984000 | -2.57122100 | 1.24106900 |
| O | -0.24103800 | -3.39171400 | -2.06017900 |
| O | -3.19098500 | -0.67647200 | 0.00000000 |
| O | -0.24103800 | -3.39171400 | 2.06017900 |
| C | 2.99774500 | 1.61217000 | 0.00000000 |
| H | 3.62696700 | 1.77543800 | 0.88404900 |
| H | 3.62696700 | 1.77543800 | -0.88404900 |
| H | 2.18559500 | 2.34127500 | 0.00000000 |

**2Fe-4**($C_s$) / M06-L

| | | | |
|---|---|---|---|
| C | 1.16448200 | -0.34943900 | 1.28926200 |
| C | 1.16448200 | -0.34943900 | -1.28926200 |
| C | -0.05846000 | 0.35199500 | -1.40232300 |
| C | -0.35161600 | 1.62526200 | -0.70117900 |
| C | -0.35161600 | 1.62526200 | 0.70117900 |
| C | -0.05846000 | 0.35199500 | 1.40232300 |
| C | -0.63777200 | 2.80055100 | 1.39623000 |
| C | -0.91024600 | 3.98083000 | 0.69751600 |
| C | -0.91024600 | 3.98083000 | -0.69751600 |
| C | -0.63777200 | 2.80055100 | -1.39623000 |
| H | 1.43122500 | -1.00132900 | 2.11822600 |
| H | 1.43122500 | -1.00132900 | -2.11822600 |
| H | -0.61750000 | 0.19242300 | -2.32571000 |
| H | -0.61750000 | 0.19242300 | 2.32571000 |
| H | -0.65354700 | 2.79246800 | 2.48307100 |
| H | -1.13746000 | 4.89207300 | 1.24177100 |
| H | -1.13746000 | 4.89207300 | -1.24177100 |
| H | -0.65354700 | 2.79246800 | -2.48307100 |
| P | 2.43766600 | -0.15458800 | 0.00000000 |
| Fe | -0.28859900 | -1.28402700 | 0.00000000 |
| C | -0.23958500 | -2.56731800 | -1.23611400 |
| C | -2.03615700 | -0.85208400 | 0.00000000 |
| C | -0.23958500 | -2.56731800 | 1.23611400 |
| O | -0.22470100 | -3.38831000 | -2.05856300 |
| O | -3.16430700 | -0.58245300 | 0.00000000 |
| O | -0.22470100 | -3.38831000 | 2.05856300 |
| C | 2.89040600 | 1.63840200 | 0.00000000 |
| H | 3.51120800 | 1.83284700 | 0.87920800 |
| H | 3.51120800 | 1.83284700 | -0.87920800 |
| H | 2.05328000 | 2.33867600 | 0.00000000 |

**2Fe-5**($C_1$) / BP86

| | | | |
|---|---|---|---|
| C | 0.50939500 | 0.81904300 | 0.72765700 |
| C | 0.50939100 | 0.81904100 | -0.72766400 |
| C | 0.61068000 | -0.50337200 | -1.32325400 |
| C | 1.54733400 | -1.53121000 | -0.75361200 |
| C | 1.54733600 | -1.53121000 | 0.75361100 |
| C | 0.61068600 | -0.50336500 | 1.32325200 |
| C | 0.32756600 | 2.06486100 | 1.42743500 |
| C | 0.19627100 | 3.24980000 | 0.71792100 |
| C | 0.19626800 | 3.24979700 | -0.71793700 |
| C | 0.32755900 | 2.06485500 | -1.42744700 |
| P | 3.27910600 | -1.22170300 | 0.00000100 |
| H | 0.42847800 | -0.56256700 | -2.40450400 |
| H | 1.49472200 | -2.50680300 | -1.25486000 |
| H | 1.49471800 | -2.50680100 | 1.25486100 |
| H | 0.42848800 | -0.56255700 | 2.40450300 |
| H | 0.32685400 | 2.06312900 | 2.52444900 |
| H | 0.08394000 | 4.19932100 | 1.25470300 |
| H | 0.08393500 | 4.19931700 | -1.25472200 |
| H | 0.32684200 | 2.06311900 | -2.52446100 |
| Fe | -1.09665300 | -0.39246400 | 0.00000300 |
| C | -2.25364000 | 0.05157200 | -1.28945400 |
| C | -2.25363200 | 0.05158000 | 1.28946500 |
| C | -1.35620600 | -2.14610800 | 0.00000100 |
| O | -3.02340800 | 0.30449900 | -2.13940700 |
| O | -3.02339500 | 0.30451300 | 2.13942000 |
| O | -1.54211400 | -3.30589600 | -0.00000400 |
| C | 3.55425100 | 0.62830300 | 0.00000300 |
| H | 3.14073600 | 1.12076400 | -0.89478500 |
| H | 3.14073900 | 1.12076600 | 0.89479100 |
| H | 4.64872900 | 0.77548400 | 0.00000100 |

**2Fe-5**($C_1$) / B3LYP

| | | | |
|---|---|---|---|
| C | 0.49980400 | 0.82374600 | 0.72202600 |
| C | 0.49980300 | 0.82374600 | -0.72202700 |
| C | 0.59919400 | -0.48852500 | -1.31845400 |
| C | 1.54031100 | -1.51387500 | -0.75112000 |
| C | 1.54031100 | -1.51387700 | 0.75111700 |
| C | 0.59919500 | -0.48852600 | 1.31845200 |
| C | 0.31535600 | 2.06611000 | 1.41857000 |
| C | 0.18025700 | 3.24228700 | 0.71597900 |
| C | 0.18025600 | 3.24228700 | -0.71597900 |
| C | 0.31535500 | 2.06611100 | -1.41857100 |
| P | 3.25838500 | -1.21635000 | 0.00000000 |
| H | 0.43842900 | -0.53811100 | -2.39500000 |
| H | 1.48091700 | -2.48108800 | -1.24943900 |
| H | 1.48091300 | -2.48109100 | 1.24943400 |
| H | 0.43843100 | -0.53811300 | 2.39499800 |
| H | 0.31754600 | 2.06525200 | 2.50695400 |
| H | 0.06699200 | 4.18444300 | 1.24814400 |
| H | 0.06699100 | 4.18444300 | -1.24814400 |
| H | 0.31754400 | 2.06525300 | -2.50695500 |
| Fe | -1.10030100 | -0.40129500 | 0.00000000 |
| C | -2.25154500 | 0.04799500 | -1.31695700 |
| C | -2.25153900 | 0.04798100 | 1.31696600 |
| C | -1.34730700 | -2.16431200 | -0.00000800 |
| O | -2.97765000 | 0.30192500 | -2.18215800 |
| O | -2.97764200 | 0.30190100 | 2.18217200 |
| O | -1.50658700 | -3.31241200 | -0.00001400 |
| C | 3.55790800 | 0.62417000 | 0.00000300 |
| H | 3.15466500 | 1.11865500 | -0.88794900 |
| H | 3.15465600 | 1.11865500 | 0.88795100 |
| H | 4.64584200 | 0.75740800 | 0.00000800 |

**2Fe-5**($C_1$) / M06-L

| | | | |
|---|---|---|---|
| C | -0.83365100 | 0.46198200 | 0.72077500 |
| C | -0.83365100 | 0.46198200 | -0.72077500 |
| C | 0.47275600 | 0.62432400 | -1.30878900 |
| C | 1.44179800 | 1.60849300 | -0.74630600 |
| C | 1.44179800 | 1.60849300 | 0.74630600 |
| C | 0.47275600 | 0.62432400 | 1.30878900 |
| C | -2.05363000 | 0.19432300 | 1.41409400 |
| C | -3.21486600 | -0.01324200 | 0.71194200 |
| C | -3.21486600 | -0.01324200 | -0.71194200 |
| C | -2.05363000 | 0.19432300 | -1.41409400 |
| P | 1.03886200 | 3.28236400 | 0.00000000 |
| H | 0.53334400 | 0.45513300 | -2.38278800 |
| H | 2.41177200 | 1.60382600 | -1.23931100 |
| H | 2.41177200 | 1.60382600 | 1.23931100 |
| H | 0.53334400 | 0.45513300 | 2.38278800 |
| H | -2.04862800 | 0.18817700 | 2.50091200 |
| H | -4.14442900 | -0.19037500 | 1.24348100 |
| H | -4.14442900 | -0.19037500 | -1.24348100 |
| H | -2.04862800 | 0.18817700 | -2.50091200 |
| Fe | 0.44906100 | -1.06457800 | 0.00000000 |
| C | 0.04506700 | -2.22806200 | -1.31407800 |
| C | 0.04506700 | -2.22806200 | 1.31407800 |
| C | 2.22497300 | -1.19478900 | 0.00000000 |
| O | -0.19385100 | -2.95862900 | -2.18448900 |
| O | -0.19385100 | -2.95862900 | 2.18448900 |
| O | 3.38601600 | -1.23871700 | 0.00000000 |
| C | -0.80321800 | 3.42106100 | 0.00000000 |
| H | -1.26594600 | 2.97915800 | -0.88525400 |
| H | -1.26594600 | 2.97915800 | 0.88525400 |
| H | -1.03748300 | 4.48811400 | 0.00000000 |

**2Fe-6**($C_1$) / BP86

| | | | |
|---|---|---|---|
| C | 0.98201600 | -0.15761100 | -0.71860800 |
| C | 0.98101900 | 0.03254900 | 0.73912500 |
| C | 1.99901400 | 0.71427600 | 1.35967500 |
| C | 3.18975600 | 1.16373100 | 0.62136900 |
| C | 3.18997200 | 0.96866100 | -0.89342700 |
| C | 2.00004800 | 0.34297700 | -1.49245200 |
| C | -0.23970200 | -0.79021900 | -1.24775600 |
| C | -0.91439200 | -1.81582300 | -0.48276800 |
| C | -0.91599300 | -1.63027900 | 0.93471900 |
| C | -0.24232900 | -0.44213400 | 1.41105800 |
| P | 4.54368000 | -0.06792900 | 0.00924700 |
| C | 3.74407300 | -1.73731700 | 0.21934800 |
| H | 1.93614600 | 0.94403600 | 2.43102100 |
| H | 3.66647600 | 2.07642300 | 1.00205400 |
| H | 3.66426800 | 1.75584100 | -1.49393500 |
| H | 1.93790700 | 0.29044400 | -2.58697600 |
| H | -0.36586800 | -0.80583500 | -2.33770400 |
| H | -1.45588500 | -2.64152400 | -0.95532700 |
| H | -1.45887800 | -2.30680500 | 1.60240700 |
| H | -0.36969900 | -0.17733300 | 2.46834200 |
| H | 3.13713300 | -2.01760000 | -0.65942600 |
| H | 4.55844600 | -2.47285600 | 0.34071200 |
| H | 3.09129900 | -1.77609800 | 1.10916800 |
| Fe | -1.89499200 | -0.06316500 | 0.00827900 |
| C | -3.13743400 | -0.25999600 | -1.25079500 |
| C | -1.50182700 | 1.66617100 | -0.22274500 |
| C | -3.13651000 | 0.08137400 | 1.27554500 |
| O | -3.95642600 | -0.37267200 | -2.08565900 |
| O | -1.24069700 | 2.79853700 | -0.37396300 |
| O | -3.95450700 | 0.19593400 | 2.11111900 |

**2Fe-6**($C_1$) / B3LYP

| | | | |
|---|---|---|---|
| C | 0.96734300 | 0.66221400 | 0.30561700 |
| C | 0.96271400 | -0.61104700 | -0.42403500 |
| C | 1.97522700 | -1.50668000 | -0.27226200 |
| C | 3.16615500 | -1.19757400 | 0.53372600 |
| C | 3.17102000 | 0.11896100 | 1.29473400 |
| C | 1.98383400 | 0.98031500 | 1.14986500 |
| C | -0.25636100 | 1.46498100 | 0.12015000 |
| C | -0.91204900 | 1.47848100 | -1.15655600 |
| C | -0.91770200 | 0.24513300 | -1.86174000 |
| C | -0.26587400 | -0.85225700 | -1.20431400 |
| P | 4.53072500 | 0.02054400 | -0.04041700 |
| C | 3.78062500 | 0.89688300 | -1.49725300 |
| H | 1.91691900 | -2.48662600 | -0.74328100 |
| H | 3.62282100 | -2.05295600 | 1.03004500 |
| H | 3.61417600 | 0.10902200 | 2.29009700 |
| H | 1.93138400 | 1.88351300 | 1.75574600 |
| H | -0.36916000 | 2.34463100 | 0.75162400 |
| H | -1.44902200 | 2.34637300 | -1.52825400 |
| H | -1.45902800 | 0.12871400 | -2.79613300 |
| H | -0.38478700 | -1.84206100 | -1.64181400 |
| H | 3.37866200 | 1.87529200 | -1.21173200 |
| H | 4.58053400 | 1.04751900 | -2.23122600 |
| H | 2.97581100 | 0.32067100 | -1.96573900 |
| Fe | -1.89666400 | 0.02931100 | -0.04889900 |
| C | -3.13408900 | 1.17488700 | 0.57120300 |
| C | -1.48755900 | -0.83916500 | 1.47043200 |
| C | -3.14020800 | -1.08204500 | -0.71694900 |
| O | -3.91095200 | 1.92532700 | 0.98968500 |
| O | -1.21370100 | -1.39731600 | 2.44566900 |
| O | -3.92089400 | -1.82086700 | -1.14878000 |

**2Fe-6**($C_1$) / M06-L

| | | | |
|---|---|---|---|
| C | -0.96049900 | -0.72866900 | -0.07120200 |
| C | -0.96050300 | 0.72869200 | -0.07083300 |
| C | -1.96526100 | 1.42424500 | 0.52390200 |
| C | -3.15349200 | 0.75601800 | 1.04311100 |
| C | -3.15348900 | -0.75657000 | 1.04271900 |
| C | -1.96525700 | -1.42452900 | 0.52317600 |
| C | 0.26129200 | -1.32331300 | -0.61469400 |
| C | 0.92310900 | -0.70748200 | -1.72954500 |
| C | 0.92310500 | 0.70835300 | -1.72918800 |
| C | 0.26128400 | 1.32361800 | -0.61402600 |
| P | -4.45345000 | 0.00000000 | -0.10578300 |
| C | -3.60620300 | 0.00047200 | -1.73905900 |
| H | -1.89976000 | 2.50524000 | 0.61658400 |
| H | -3.63583000 | 1.24082400 | 1.88785200 |
| H | -3.63584100 | -1.24181400 | 1.88720100 |
| H | -1.89975500 | -2.50557200 | 0.61530300 |
| H | 0.38514300 | -2.39675300 | -0.49219400 |
| H | 1.47238000 | -1.27712700 | -2.47023900 |
| H | 1.47237000 | 1.27837700 | -2.46959500 |
| H | 0.38512900 | 2.39699600 | -0.49098400 |
| H | -2.97371600 | -0.88174700 | -1.87760500 |
| H | -4.37702800 | 0.00056000 | -2.51260000 |
| H | -2.97391000 | 0.88289000 | -1.87721600 |
| Fe | 1.86661600 | 0.00000000 | -0.05199000 |
| C | 3.10633200 | -1.29322500 | -0.06084800 |
| C | 1.39900000 | -0.00042100 | 1.68461700 |
| C | 3.10633400 | 1.29325900 | -0.06019600 |
| O | 3.89427500 | -2.14707500 | -0.05990700 |
| O | 1.04345100 | -0.00069800 | 2.78802600 |
| O | 3.89427800 | 2.14710600 | -0.05882200 |

**2Fe-7**($C_1$) / BP86

| | | | |
|---|---|---|---|
| C | 0.82736200 | 0.73760700 | -0.29588500 |
| C | 0.82736200 | -0.73759800 | -0.29591100 |
| C | 1.89559800 | -1.44128900 | 0.19306900 |
| C | 3.13909900 | -0.76505000 | 0.61938900 |
| C | 3.13909900 | 0.76502900 | 0.61941500 |
| C | 1.89559800 | 1.44128200 | 0.19311700 |
| C | -0.43940200 | 1.34226500 | -0.74137800 |
| C | -1.21452200 | 0.71482600 | -1.78813300 |
| C | -1.21452200 | -0.71476700 | -1.78815800 |
| C | -0.43940000 | -1.34224400 | -0.74142700 |
| P | 4.29892500 | 0.00001200 | -0.69682900 |
| C | 5.90325200 | -0.00000300 | 0.27918100 |
| H | 1.84777300 | -2.53434200 | 0.27740100 |
| H | 3.69764400 | -1.26248900 | 1.42347600 |
| H | 3.69764300 | 1.26244200 | 1.42351800 |
| H | 1.84777300 | 2.53433200 | 0.27748700 |
| H | -0.55349400 | 2.42538500 | -0.60765200 |
| H | -1.82407600 | 1.28955900 | -2.49255900 |
| H | -1.82407300 | -1.28947700 | -2.49260600 |
| H | -0.55348700 | -2.42536800 | -0.60773900 |
| H | 6.49666000 | 0.89302000 | 0.01359900 |
| H | 5.74794200 | -0.00003900 | 1.37223800 |
| H | 6.49667600 | -0.89299800 | 0.01354100 |
| Fe | -2.03570700 | -0.00000200 | -0.03009400 |
| C | -3.27397500 | 1.27523000 | 0.05741000 |
| C | -1.48174000 | -0.00004000 | 1.66957000 |
| C | -3.27399300 | -1.27521900 | 0.05736700 |
| O | -4.09101000 | 2.11638100 | 0.13417300 |
| O | -1.11436800 | -0.00006700 | 2.78277000 |
| O | -4.09104500 | -2.11635500 | 0.13411000 |

**2Fe-7**($C_1$) / B3LYP

| | | | |
|---|---|---|---|
| C | 0.81638600 | 0.73624700 | -0.29241600 |
| C | 0.81638800 | -0.73624500 | -0.29244200 |
| C | 1.87890300 | -1.43568100 | 0.17790400 |
| C | 3.12345900 | -0.76187000 | 0.60553400 |
| C | 3.12345900 | 0.76184600 | 0.60556700 |
| C | 1.87890000 | 1.43566800 | 0.17795400 |
| C | -0.45526100 | 1.33554500 | -0.73646800 |
| C | -1.20942600 | 0.71038300 | -1.78502300 |
| C | -1.20942300 | -0.71033300 | -1.78504800 |
| C | -0.45525200 | -1.33553300 | -0.73652200 |
| P | 4.28107600 | 0.00002100 | -0.69150900 |
| C | 5.87917200 | -0.00000600 | 0.28052800 |
| H | 1.83623100 | -2.52105700 | 0.25154100 |
| H | 3.66475400 | -1.25471300 | 1.41241000 |
| H | 3.66473800 | 1.25466100 | 1.41247100 |
| H | 1.83622600 | 2.52104200 | 0.25162800 |
| H | -0.56021400 | 2.41249000 | -0.61661600 |
| H | -1.81523700 | 1.27708300 | -2.48605100 |
| H | -1.81523900 | -1.27701300 | -2.48608900 |
| H | -0.56021300 | -2.41248000 | -0.61669900 |
| H | 6.46887100 | 0.88619700 | 0.01762300 |
| H | 5.72415600 | -0.00000800 | 1.36513200 |
| H | 6.46884800 | -0.88622200 | 0.01761500 |
| Fe | -2.03205200 | -0.00000100 | -0.02026600 |
| C | -3.26913900 | 1.29940000 | 0.06302600 |
| C | -1.46156200 | -0.00003800 | 1.68290000 |
| C | -3.26916000 | -1.29938900 | 0.06299200 |
| O | -4.04706500 | 2.15574600 | 0.12477100 |
| O | -1.08337700 | -0.00005800 | 2.77621200 |
| O | -4.04710500 | -2.15571700 | 0.12472600 |

**2Fe-7**($C_1$) / M06-L

| | | | |
|---|---|---|---|
| C | -0.78777800 | -0.35344200 | 0.73118300 |
| C | -0.78777800 | -0.35344200 | -0.73118300 |
| C | -1.85868900 | 0.09990400 | -1.42698500 |
| C | -3.10762900 | 0.47397600 | -0.75735400 |
| C | -3.10762900 | 0.47397600 | 0.75735400 |
| C | -1.85868900 | 0.09990400 | 1.42698500 |
| C | 0.49290100 | -0.73209800 | 1.32645100 |
| C | 1.30630700 | -1.73865000 | 0.70806900 |
| C | 1.30630700 | -1.73865000 | -0.70806900 |
| C | 0.49290100 | -0.73209800 | -1.32645100 |
| P | -4.20191800 | -0.85240700 | 0.00000000 |
| C | -5.80076300 | 0.08374800 | 0.00000000 |
| H | -1.80988800 | 0.19051400 | -2.50893000 |
| H | -3.68854300 | 1.25453800 | -1.24414300 |
| H | -3.68854300 | 1.25453800 | 1.24414300 |
| H | -1.80988800 | 0.19051400 | 2.50893000 |
| H | 0.59789500 | -0.59725500 | 2.40047600 |
| H | 1.95416700 | -2.39489000 | 1.27771000 |
| H | 1.95416700 | -2.39489000 | -1.27771000 |
| H | 0.59789500 | -0.59725500 | -2.40047600 |
| H | -6.39026800 | -0.17903500 | 0.88190600 |
| H | -5.65450200 | 1.16759100 | 0.00000000 |
| H | -6.39026800 | -0.17903500 | -0.88190600 |
| Fe | 2.01007300 | 0.05560200 | 0.00000000 |
| C | 3.23655600 | 0.21681500 | 1.29477100 |
| C | 1.30630700 | 1.71016300 | 0.00000000 |
| C | 3.23655600 | 0.21681500 | -1.29477100 |
| O | 4.01571800 | 0.32646100 | 2.14992400 |
| O | 0.80370900 | 2.75512800 | 0.00000000 |
| O | 4.01571800 | 0.32646100 | -2.14992400 |

**2Fe-8**($C_1$) / BP86

| | | | |
|---|---|---|---|
| C | -1.84822900 | -2.07572000 | 0.58347800 |
| C | -1.42119100 | 0.12653900 | -1.17584200 |
| C | -0.10376000 | -0.10883300 | -1.72851700 |
| C | 0.89022300 | -0.87749000 | -1.01829600 |
| C | 0.66351400 | -1.40142900 | 0.34615700 |
| C | -0.52894900 | -2.06343900 | 0.92868800 |
| C | 1.87973000 | -1.73758900 | 1.07708200 |
| C | 3.14059300 | -1.74434900 | 0.50976100 |
| C | 3.30164500 | -1.42424100 | -0.87987900 |
| C | 2.21153300 | -0.99040800 | -1.60585000 |
| H | -2.51993700 | -2.70292100 | 1.18583500 |
| H | -1.96743300 | 0.91690200 | -1.71534000 |
| H | 0.20274300 | 0.33853000 | -2.68246400 |
| H | -0.26436300 | -2.67163700 | 1.80646800 |
| H | 1.76227800 | -2.06925300 | 2.11660400 |
| H | 4.00957100 | -2.03786300 | 1.10973400 |
| H | 4.28755400 | -1.50241100 | -1.35254800 |
| H | 2.32355500 | -0.69638700 | -2.65687700 |
| Fe | 0.16880400 | 0.87443500 | 0.05052200 |
| C | -0.10150500 | 2.47241000 | -0.64106300 |
| C | 1.77591900 | 1.40865300 | 0.63064800 |
| C | -0.75396700 | 1.03418900 | 1.57755100 |
| O | -0.28050000 | 3.54797600 | -1.08201600 |
| O | 2.80456600 | 1.82201100 | 1.01602800 |
| O | -1.38096900 | 1.17890400 | 2.55922900 |
| P | -2.61237500 | -1.21303400 | -0.79205800 |
| C | -3.99175000 | -0.30396600 | 0.07698500 |
| H | -4.52858500 | 0.32535900 | -0.65360400 |
| H | -4.71053400 | -1.04212900 | 0.47337600 |
| H | -3.62573400 | 0.32491200 | 0.90477300 |

**2Fe-8**($C_1$) / B3LYP

| | | | |
|---|---|---|---|
| C | -1.76695100 | -2.11273900 | 0.57217300 |
| C | -1.40101100 | 0.08928700 | -1.18114500 |
| C | -0.07952100 | -0.10342900 | -1.71436200 |
| C | 0.92599000 | -0.85365400 | -1.01119400 |
| C | 0.72213600 | -1.39211300 | 0.33376000 |
| C | -0.46217700 | -2.06806300 | 0.92106900 |
| C | 1.93764000 | -1.71760100 | 1.05568100 |
| C | 3.19190900 | -1.67696600 | 0.49760200 |
| C | 3.34294600 | -1.32105800 | -0.87801200 |
| C | 2.24696900 | -0.91266400 | -1.59248200 |
| H | -2.41853000 | -2.74222800 | 1.17901900 |
| H | -1.96209300 | 0.84422700 | -1.73848100 |
| H | 0.21919800 | 0.34815800 | -2.65817600 |
| H | -0.18952600 | -2.65836000 | 1.79683300 |
| H | 1.82900100 | -2.07175900 | 2.07908700 |
| H | 4.06116000 | -1.95912200 | 1.08686400 |
| H | 4.32360700 | -1.35718800 | -1.34714500 |
| H | 2.35215500 | -0.59947600 | -2.62939100 |
| Fe | 0.12968100 | 0.89147500 | 0.06280900 |
| C | -0.25704800 | 2.48709100 | -0.61346400 |
| C | 1.75410700 | 1.48415900 | 0.59761200 |
| C | -0.77766400 | 0.99116200 | 1.61843400 |
| O | -0.53028400 | 3.52408200 | -1.05454700 |
| O | 2.77767400 | 1.89386800 | 0.94774300 |
| O | -1.38411700 | 1.09088900 | 2.59985300 |
| P | -2.55893500 | -1.28435000 | -0.80925900 |
| C | -3.94189700 | -0.40580100 | 0.07310800 |
| H | -4.48762600 | 0.21867800 | -0.64306600 |
| H | -4.64473900 | -1.15070500 | 0.46345600 |
| H | -3.58904900 | 0.21828000 | 0.89976800 |

**2Fe-8**($C_1$) / M06-L

| | | | |
|---|---|---|---|
| C | -1.80747100 | -2.06828700 | 0.52047700 |
| C | -1.39781200 | 0.13727600 | -1.17609100 |
| C | -0.08857400 | -0.06162900 | -1.73381100 |
| C | 0.90346700 | -0.83409500 | -1.04804500 |
| C | 0.68086100 | -1.38572200 | 0.28960900 |
| C | -0.50104800 | -2.05445800 | 0.85683700 |
| C | 1.88557300 | -1.69900400 | 1.02227200 |
| C | 3.14333700 | -1.63994400 | 0.48650500 |
| C | 3.31209400 | -1.27893200 | -0.87922800 |
| C | 2.22732400 | -0.88113800 | -1.60761200 |
| H | -2.46497900 | -2.69283500 | 1.12173000 |
| H | -1.94569400 | 0.92985500 | -1.69214500 |
| H | 0.21914200 | 0.41778500 | -2.66063200 |
| H | -0.23205400 | -2.65741900 | 1.72448100 |
| H | 1.75930300 | -2.06208700 | 2.03951500 |
| H | 4.00323500 | -1.91220300 | 1.08871600 |
| H | 4.29817600 | -1.30035600 | -1.33167500 |
| H | 2.34135300 | -0.55851200 | -2.63895400 |
| Fe | 0.14578800 | 0.85573800 | 0.07106200 |
| C | -0.21809900 | 2.47392200 | -0.54426600 |
| C | 1.78022100 | 1.39181800 | 0.61580500 |
| C | -0.75206500 | 0.89180400 | 1.63733500 |
| O | -0.47327600 | 3.53353500 | -0.94957600 |
| O | 2.82293400 | 1.76650100 | 0.96166800 |
| O | -1.36293700 | 0.92012700 | 2.62437400 |
| P | -2.57835000 | -1.20057000 | -0.82926600 |
| C | -3.90364800 | -0.29479000 | 0.07506600 |
| H | -4.45317800 | 0.34336500 | -0.62051500 |
| H | -4.61336100 | -1.01117900 | 0.49411400 |
| H | -3.50592300 | 0.32070900 | 0.88589600 |

**2Fe-9** ($C_s$) / BP86

| | | | |
|---|---|---|---|
| C | -2.21254500 | -1.45516700 | 1.07992000 |
| C | -1.50998900 | 0.53727000 | -0.86922200 |
| C | -0.44419700 | -0.13836400 | -1.57177500 |
| C | 0.45053200 | -1.06803800 | -0.92942700 |
| C | 0.32895900 | -1.40545300 | 0.50067600 |
| C | -0.90117200 | -1.78113200 | 1.24701700 |
| C | 1.52681400 | -1.98508900 | 1.09740000 |
| C | 2.64150200 | -2.35437900 | 0.36733800 |
| C | 2.64844800 | -2.19475100 | -1.05970300 |
| C | 1.59200300 | -1.55816200 | -1.67859800 |
| H | -2.92751200 | -1.94412400 | 1.75755700 |
| H | -1.88059600 | 1.41168900 | -1.42910500 |
| H | -0.20526700 | 0.13855500 | -2.60758000 |
| H | -0.68170600 | -2.48809400 | 2.06220400 |
| H | 1.49557400 | -2.20088300 | 2.17306500 |
| H | 3.49992100 | -2.81312300 | 0.87125700 |
| H | 3.49886400 | -2.55721600 | -1.64877100 |
| H | 1.60088300 | -1.38643000 | -2.76232100 |
| P | -2.91548000 | -0.09747400 | 0.12291700 |
| C | -3.88720700 | -1.02612700 | -1.18895700 |
| H | -4.73700500 | -1.54115400 | -0.70728800 |
| H | -4.29991800 | -0.29866200 | -1.90949700 |
| H | -3.27141100 | -1.76716700 | -1.72535600 |
| Fe | 0.39199100 | 0.88574100 | 0.01923700 |
| C | 0.47228400 | 2.43900400 | -0.81552900 |
| C | 2.14687300 | 1.01252200 | 0.32279600 |
| C | -0.21695200 | 1.39267400 | 1.63106600 |
| O | 0.52150000 | 3.48766800 | -1.34496100 |
| O | 3.29352500 | 1.15683400 | 0.52771500 |
| O | -0.61046400 | 1.77932200 | 2.66523700 |

**2Fe-9** ($C_s$) / B3LYP

| | | | |
|---|---|---|---|
| C | -2.17310100 | -1.43412100 | 1.11830600 |
| C | -1.50444400 | 0.51462700 | -0.87049900 |
| C | -0.43028900 | -0.14722900 | -1.55426500 |
| C | 0.46206000 | -1.06951500 | -0.91126200 |
| C | 0.35438400 | -1.40543000 | 0.50480600 |
| C | -0.87105100 | -1.75303000 | 1.27349200 |
| C | 1.54432300 | -1.99023300 | 1.09420400 |
| C | 2.65628800 | -2.34302700 | 0.36963900 |
| C | 2.66231700 | -2.16685800 | -1.04949800 |
| C | 1.60568900 | -1.54116600 | -1.65808000 |
| H | -2.86779700 | -1.89973300 | 1.81896600 |
| H | -1.88858600 | 1.36054600 | -1.44747700 |
| H | -0.19186800 | 0.11886900 | -2.58298800 |
| H | -0.64525600 | -2.43389500 | 2.09639600 |
| H | 1.51427200 | -2.21364000 | 2.15916400 |
| H | 3.50959800 | -2.79981100 | 0.86526600 |
| H | 3.50949800 | -2.51255000 | -1.63765200 |
| H | 1.61399500 | -1.36457600 | -2.73203500 |
| P | -2.91299700 | -0.14377100 | 0.09654300 |
| C | -3.78741500 | -1.17060600 | -1.19925100 |
| H | -4.61903600 | -1.70977100 | -0.73068700 |
| H | -4.20986000 | -0.50167400 | -1.95785500 |
| H | -3.12176400 | -1.89238400 | -1.68370800 |
| Fe | 0.37614400 | 0.91301700 | 0.02481100 |
| C | 0.38295900 | 2.48255400 | -0.81517200 |
| C | 2.15936800 | 1.05273200 | 0.28310200 |
| C | -0.22659300 | 1.40849900 | 1.65494700 |
| O | 0.35700900 | 3.50930200 | -1.35266400 |
| O | 3.29658200 | 1.17265200 | 0.45839000 |
| O | -0.61546200 | 1.77349100 | 2.68134500 |

**2Fe-9** ($C_s$) / M06-L

| | | | |
|---|---|---|---|
| C | -2.17064300 | -1.44029200 | 1.09196700 |
| C | -1.50377700 | 0.52196400 | -0.84727000 |
| C | -0.45094200 | -0.14254400 | -1.56167600 |
| C | 0.45119200 | -1.05285000 | -0.92928400 |
| C | 0.34427800 | -1.37286700 | 0.49193400 |
| C | -0.86837100 | -1.75018900 | 1.24285000 |
| C | 1.54637100 | -1.91061800 | 1.08751000 |
| C | 2.66763300 | -2.23406000 | 0.37326500 |
| C | 2.67372300 | -2.08084000 | -1.04242100 |
| C | 1.60357300 | -1.50279500 | -1.66370500 |
| H | -2.86054600 | -1.92719300 | 1.77963400 |
| H | -1.87750000 | 1.38510200 | -1.40490200 |
| H | -0.21750000 | 0.13665100 | -2.58802900 |
| H | -0.63394500 | -2.44280100 | 2.05318500 |
| H | 1.51338100 | -2.12482100 | 2.15310600 |
| H | 3.53090500 | -2.65432400 | 0.87822200 |
| H | 3.53225600 | -2.40491800 | -1.62113900 |
| H | 1.60696000 | -1.33881000 | -2.73795500 |
| P | -2.89924200 | -0.12805300 | 0.11775400 |
| C | -3.78465600 | -1.10218100 | -1.18606200 |
| H | -4.61453400 | -1.65058200 | -0.73378100 |
| H | -4.20588200 | -0.41646900 | -1.92499200 |
| H | -3.12580600 | -1.81311600 | -1.69183100 |
| Fe | 0.37448300 | 0.88016600 | 0.01955700 |
| C | 0.39333300 | 2.45123000 | -0.80440700 |
| C | 2.15101700 | 1.00116800 | 0.27752700 |
| C | -0.23365200 | 1.33821800 | 1.66118900 |
| O | 0.38045100 | 3.48439100 | -1.33679200 |
| O | 3.29500500 | 1.10757300 | 0.44268000 |
| O | -0.65173200 | 1.65149900 | 2.69601100 |

**2Fe-10** ($C_1$) / BP86

| | | | |
|---|---|---|---|
| C | 1.60624300 | -0.32087100 | -0.71263400 |
| C | 1.60624400 | -0.32086800 | 0.71264700 |
| C | 0.29741700 | 0.07380500 | 1.31173400 |
| C | -0.25026700 | 1.38063200 | 0.84119400 |
| C | -0.25028100 | 1.38062300 | -0.84120900 |
| C | 0.29741800 | 0.07379400 | -1.31173100 |
| C | 2.75933700 | -0.70220500 | -1.41783000 |
| C | 3.91574600 | -1.09767200 | -0.70439900 |
| C | 3.91574700 | -1.09766900 | 0.70441200 |
| C | 2.75933800 | -0.70220200 | 1.41784400 |
| P | 0.84600500 | 2.65046400 | -0.00002500 |
| H | 0.15197700 | -0.13687700 | 2.37896400 |
| H | -1.09782400 | 1.81719000 | 1.37870400 |
| H | -1.09784500 | 1.81715700 | -1.37872600 |
| H | 0.15199700 | -0.13690600 | -2.37896000 |
| H | 2.75691000 | -0.70871200 | -2.51520700 |
| H | 4.81239300 | -1.41496000 | -1.25041300 |
| H | 4.81239400 | -1.41495700 | 1.25042600 |
| H | 2.75691300 | -0.70870700 | 2.51522000 |
| Fe | -1.22331900 | -0.46502600 | -0.00000200 |
| C | -0.76310100 | -2.17011200 | -0.00000800 |
| C | -2.47155100 | -0.55056000 | -1.28966800 |
| C | -2.47151900 | -0.55051500 | 1.28969700 |
| O | -0.45501700 | -3.30197600 | -0.00001700 |
| O | -3.27888100 | -0.66415400 | -2.13575300 |
| O | -3.27881800 | -0.66406300 | 2.13581800 |
| C | -0.33857400 | 4.10436900 | -0.00002600 |
| H | -0.15020300 | 4.72584500 | -0.89333500 |
| H | -1.40177500 | 3.80702100 | 0.00000200 |
| H | -0.15016500 | 4.72588500 | 0.89324700 |

**2Fe-10** ($C_1$) / B3LYP

| | | | |
|---|---|---|---|
| C | 1.59309400 | -0.30682300 | -0.70843500 |
| C | 1.59309600 | -0.30682500 | 0.70843000 |
| C | 0.28206600 | 0.07655000 | 1.30444000 |
| C | -0.26577400 | 1.38155000 | 0.83243100 |
| C | -0.26577300 | 1.38155100 | -0.83241700 |
| C | 0.28206100 | 0.07655300 | -1.30444000 |
| C | 2.74288400 | -0.67620300 | -1.40921000 |
| C | 3.89704700 | -1.06009000 | -0.70047100 |
| C | 3.89705000 | -1.06008900 | 0.70045600 |
| C | 2.74288900 | -0.67620600 | 1.40920000 |
| P | 0.80914300 | 2.65915400 | 0.00001300 |
| H | 0.15843900 | -0.11334700 | 2.36998500 |
| H | -1.10974000 | 1.80587500 | 1.36772000 |
| H | -1.10973000 | 1.80589900 | -1.36770200 |
| H | 0.15844400 | -0.11332100 | -2.36999100 |
| H | 2.74208200 | -0.68100200 | -2.49800700 |
| H | 4.79027600 | -1.36443600 | -1.24249100 |
| H | 4.79028100 | -1.36443500 | 1.24247300 |
| H | 2.74209000 | -0.68100700 | 2.49799700 |
| Fe | -1.21835400 | -0.48592700 | -0.00000400 |
| C | -0.72897600 | -2.19267100 | -0.00001100 |
| C | -2.45758200 | -0.57778400 | -1.32482900 |
| C | -2.45757000 | -0.57782500 | 1.32483100 |
| O | -0.38900700 | -3.29897100 | -0.00001300 |
| O | -3.21829400 | -0.67820900 | -2.19200300 |
| O | -3.21827000 | -0.67828800 | 2.19201100 |
| C | -0.38378800 | 4.09684000 | 0.00001300 |
| H | -0.20274000 | 4.71624000 | -0.88625000 |
| H | -1.43639400 | 3.79265900 | 0.00001800 |
| H | -0.20273100 | 4.71623300 | 0.88628000 |

**2Fe-10** ($C_1$) / M06-L

| | | | |
|---|---|---|---|
| C | -0.25580600 | 1.59830600 | 0.70643000 |
| C | -0.25580600 | 1.59830600 | -0.70643000 |
| C | 0.08400200 | 0.28726700 | -1.29756700 |
| C | 1.35564300 | -0.30891700 | -0.81952000 |
| C | 1.35564300 | -0.30891700 | 0.81952000 |
| C | 0.08400200 | 0.28726700 | 1.29756700 |
| C | -0.59894700 | 2.75211000 | 1.40433900 |
| C | -0.95447600 | 3.90844800 | 0.69748100 |
| C | -0.95447600 | 3.90844800 | -0.69748100 |
| C | -0.59894700 | 2.75211000 | -1.40433900 |
| P | 2.65883100 | 0.72138100 | 0.00000000 |
| H | -0.10854200 | 0.15921900 | -2.36079500 |
| H | 1.75373200 | -1.16876900 | -1.34851800 |
| H | 1.75373200 | -1.16876900 | 1.34851800 |
| H | -0.10854200 | 0.15921900 | 2.36079500 |
| H | -0.60700600 | 2.74816300 | 2.49136800 |
| H | -1.24029900 | 4.80542100 | 1.23826700 |
| H | -1.24029900 | 4.80542100 | -1.23826700 |
| H | -0.60700600 | 2.74816300 | -2.49136800 |
| Fe | -0.50700500 | -1.20011700 | 0.00000000 |
| C | -2.18655800 | -0.63164000 | 0.00000000 |
| C | -0.63282000 | -2.43935500 | 1.31485100 |
| C | -0.63282000 | -2.43935500 | -1.31485100 |
| O | -3.26657200 | -0.20737700 | 0.00000000 |
| O | -0.75767000 | -3.20714800 | 2.17764500 |
| O | -0.75767000 | -3.20714800 | -2.17764500 |
| C | 4.02368900 | -0.52919900 | 0.00000000 |
| H | 4.65328900 | -0.39083900 | 0.88242400 |
| H | 3.65868600 | -1.55994700 | 0.00000000 |
| H | 4.65328900 | -0.39083900 | -0.88242400 |

**2Fe-11**($C_1$) / BP86

| | | | |
|---|---|---|---|
| C | 3.28036100 | 1.35419100 | 0.38022000 |
| C | 3.28036300 | -1.35418200 | 0.38024000 |
| C | 1.92835500 | -1.57455900 | 0.36370900 |
| C | 0.90628800 | -0.69760100 | -0.18401700 |
| C | 0.90628500 | 0.69760500 | -0.18402500 |
| C | 1.92835300 | 1.57457100 | 0.36368900 |
| C | -0.38288100 | 1.30508800 | -0.62714400 |
| C | -1.08173800 | 0.71167700 | -1.75063600 |
| C | -1.08173500 | -0.71169500 | -1.75062800 |
| C | -0.38287600 | -1.30509300 | -0.62713200 |
| H | 3.92523000 | 2.04390400 | 0.94455900 |
| H | 3.92523100 | -2.04388800 | 0.94458900 |
| H | 1.55138900 | -2.49929000 | 0.82897600 |
| H | 1.55138900 | 2.49930800 | 0.82894600 |
| H | -0.49416100 | 2.38694100 | -0.48120700 |
| H | -1.63493600 | 1.29731000 | -2.49149000 |
| H | -1.63493200 | -1.29733900 | -2.49147300 |
| H | -0.49415400 | -2.38694500 | -0.48118100 |
| P | 4.05331800 | 0.00000000 | -0.58541000 |
| Fe | -2.02030100 | 0.00000000 | -0.04109700 |
| C | -3.27929400 | 1.25752600 | -0.02716700 |
| C | -3.27934300 | -1.25748000 | -0.02723800 |
| C | -1.53663800 | 0.00000000 | 1.68331100 |
| O | -4.08716100 | 2.11022800 | 0.00081400 |
| O | -4.08724600 | -2.11015000 | 0.00069000 |
| O | -1.22764000 | 0.00000000 | 2.81380400 |
| C | 5.76876400 | 0.00000000 | 0.15340600 |
| H | 6.31579600 | -0.88889800 | -0.20570300 |
| H | 6.31581600 | 0.88887000 | -0.20575400 |
| H | 5.77217100 | 0.00000000 | 1.25741300 |

**2Fe-11**($C_1$) / B3LYP

| | | | |
|---|---|---|---|
| C | -0.29879400 | -3.26102600 | 1.36589900 |
| C | -0.29879400 | -3.26102600 | -1.36589900 |
| C | -0.30741700 | -1.92025700 | -1.57198200 |
| C | 0.21915600 | -0.88800900 | -0.69026900 |
| C | 0.21915600 | -0.88800900 | 0.69026900 |
| C | -0.30741700 | -1.92025700 | 1.57198200 |
| C | 0.65184900 | 0.39515600 | 1.30566900 |
| C | 1.74041100 | 1.11672800 | 0.70717800 |
| C | 1.74041100 | 1.11672800 | -0.70717800 |
| C | 0.65184900 | 0.39515600 | -1.30566900 |
| H | -0.82062200 | -3.90250000 | 2.07788300 |
| H | -0.82062200 | -3.90250000 | -2.07788300 |
| H | -0.76870800 | -1.54828900 | -2.49009700 |
| H | -0.76870800 | -1.54828900 | 2.49009700 |
| H | 0.52418200 | 0.48718900 | 2.38274000 |
| H | 2.46106300 | 1.68880100 | 1.28387700 |
| H | 2.46106300 | 1.68880100 | -1.28387700 |
| H | 0.52418200 | 0.48718900 | -2.38274000 |
| P | 0.62933000 | -4.04709600 | 0.00000000 |
| Fe | 0.00000000 | 2.01978800 | 0.00000000 |
| C | -0.03793400 | 3.27756300 | 1.28456200 |
| C | -0.03793400 | 3.27756300 | -1.28456200 |
| C | -1.71868100 | 1.48454200 | 0.00000000 |
| O | -0.07237300 | 4.04596400 | 2.15125000 |
| O | -0.07237300 | 4.04596400 | -2.15125000 |
| O | -2.82488900 | 1.14486800 | 0.00000000 |
| C | -0.15049500 | -5.73593600 | 0.00000000 |
| H | 0.18927100 | -6.28943800 | -0.88252300 |
| H | 0.18927100 | -6.28943800 | 0.88252300 |
| H | -1.24587900 | -5.70786600 | 0.00000000 |

**2Fe-11**($C_1$) / M06-L

| | | | |
|---|---|---|---|
| C | -1.69116100 | 2.77249200 | 1.34304100 |
| C | -1.69116100 | 2.77249200 | -1.34304100 |
| C | -0.87886100 | 1.70964800 | -1.55733800 |
| C | -0.70116000 | 0.56917400 | -0.69024300 |
| C | -0.70116000 | 0.56917400 | 0.69024300 |
| C | -0.87886100 | 1.70964800 | 1.55733800 |
| C | -0.25387300 | -0.70630400 | 1.29047200 |
| C | -0.70117200 | -1.94140800 | 0.70494300 |
| C | -0.70117200 | -1.94140800 | -0.70494300 |
| C | -0.25387300 | -0.70630400 | -1.29047200 |
| H | -1.64105700 | 3.62201800 | 2.02399200 |
| H | -1.64105700 | 3.62201800 | -2.02399200 |
| H | -0.27141100 | 1.69879600 | -2.46435200 |
| H | -0.27141100 | 1.69879600 | 2.46435200 |
| H | -0.07874300 | -0.70240600 | 2.36423300 |
| H | -0.92564700 | -2.82889500 | 1.28534000 |
| H | -0.92564700 | -2.82889500 | -1.28534000 |
| H | -0.07874300 | -0.70240600 | -2.36423300 |
| P | -2.91264700 | 2.78455400 | 0.00000000 |
| Fe | 1.20429000 | -1.59867100 | 0.00000000 |
| C | 2.00038400 | -2.56777400 | 1.27981500 |
| C | 2.00038400 | -2.56777400 | -1.27981500 |
| C | 2.20445600 | -0.09989800 | 0.00000000 |
| O | 2.49788200 | -3.16301200 | 2.14484100 |
| O | 2.49788200 | -3.16301200 | -2.14484100 |
| O | 2.80105300 | 0.89440200 | 0.00000000 |
| C | -3.36997600 | 4.57011400 | 0.00000000 |
| H | -3.97881200 | 4.79293900 | -0.87892700 |
| H | -3.97881200 | 4.79293900 | 0.87892700 |
| H | -2.50154400 | 5.23496600 | 0.00000000 |

**2Fe-12**($C_s$) / BP86

| | | | |
|---|---|---|---|
| C | -0.45794900 | 1.40133800 | 0.71290200 |
| C | -0.45794900 | 1.40133800 | -0.71290200 |
| C | 0.19466100 | 0.20746300 | -1.31487700 |
| C | 1.56270100 | -0.16704200 | -0.83166000 |
| C | 1.56270100 | -0.16704200 | 0.83166000 |
| C | 0.19466100 | 0.20746300 | 1.31487700 |
| C | -1.11869200 | 2.42189200 | 1.41680000 |
| C | -1.78326700 | 3.44883300 | 0.70470900 |
| C | -1.78326700 | 3.44883300 | -0.70470900 |
| C | -1.11869200 | 2.42189200 | -1.41680000 |
| P | 2.84823200 | 0.94106300 | 0.00000000 |
| C | 2.24595000 | 2.70450900 | 0.00000000 |
| H | 0.02048000 | 0.03438300 | -2.38481300 |
| H | 2.06914800 | -0.97362000 | -1.37006600 |
| H | 2.06914800 | -0.97362000 | 1.37006600 |
| H | 0.02048000 | 0.03438300 | 2.38481300 |
| H | -1.13499300 | 2.41098900 | 2.51424600 |
| H | -2.31256900 | 4.23846000 | 1.25149700 |
| H | -2.31256900 | 4.23846000 | -1.25149700 |
| H | -1.13499300 | 2.41098900 | -2.51424600 |
| H | 1.66101300 | 2.96731000 | 0.89423200 |
| H | 3.17653100 | 3.30220700 | 0.00000000 |
| H | 1.66101300 | 2.96731000 | -0.89423200 |
| Fe | -0.14042000 | -1.38428900 | 0.00000000 |
| C | -1.90024200 | -1.19462000 | 0.00000000 |
| C | -0.04327400 | -2.63758300 | 1.28408300 |
| C | -0.04327400 | -2.63758300 | -1.28408300 |
| O | -3.06781400 | -1.08072500 | 0.00000000 |
| O | -0.03982200 | -3.45587700 | 2.12690900 |
| O | -0.03982200 | -3.45587700 | -2.12690900 |

**2Fe-12**($C_s$) / B3LYP

| | | | |
|---|---|---|---|
| C | -0.46325900 | 1.38564400 | 0.70852000 |
| C | -0.46325900 | 1.38564400 | -0.70852000 |
| C | 0.18730100 | 0.19177000 | -1.30769600 |
| C | 1.55831500 | -0.16623900 | -0.82722500 |
| C | 1.55831500 | -0.16623900 | 0.82722500 |
| C | 0.18730100 | 0.19177000 | 1.30769600 |
| C | -1.11392100 | 2.40430300 | 1.40814500 |
| C | -1.76938600 | 3.42985900 | 0.70078300 |
| C | -1.76938600 | 3.42985900 | -0.70078300 |
| C | -1.11392100 | 2.40430300 | -1.40814500 |
| P | 2.83897600 | 0.92829000 | 0.00000000 |
| C | 2.25877100 | 2.69366100 | 0.00000000 |
| H | 0.02787400 | 0.03931700 | -2.37461800 |
| H | 2.05969300 | -0.96528800 | -1.36441700 |
| H | 2.05969300 | -0.96528800 | 1.36441700 |
| H | 0.02787400 | 0.03931700 | 2.37461800 |
| H | -1.12777600 | 2.39621200 | 2.49703000 |
| H | -2.28742400 | 4.21804900 | 1.24348300 |
| H | -2.28742400 | 4.21804900 | -1.24348300 |
| H | -1.12777600 | 2.39621200 | -2.49703000 |
| H | 1.68037300 | 2.95904200 | 0.88699800 |
| H | 3.18593600 | 3.28073800 | 0.00000000 |
| H | 1.68037300 | 2.95904200 | -0.88699800 |
| Fe | -0.14957700 | -1.38688400 | 0.00000000 |
| C | -1.91790800 | -1.19126200 | 0.00000000 |
| C | -0.04320800 | -2.63105600 | 1.32051200 |
| C | -0.04320800 | -2.63105600 | -1.32051200 |
| O | -3.06717100 | -1.05468700 | 0.00000000 |
| O | -0.02280900 | -3.39931500 | 2.18625200 |
| O | -0.02280900 | -3.39931500 | -2.18625200 |

**2Fe-12**($C_s$) / M06-L

| | | | |
|---|---|---|---|
| C | -0.42853000 | 1.38969000 | 0.70643300 |
| C | -0.42853000 | 1.38969000 | -0.70643300 |
| C | 0.19780500 | 0.19674200 | -1.30154100 |
| C | 1.54513700 | -0.20638100 | -0.81418300 |
| C | 1.54513700 | -0.20638100 | 0.81418300 |
| C | 0.19780500 | 0.19674200 | 1.30154100 |
| C | -1.06501600 | 2.41297900 | 1.40318000 |
| C | -1.69891100 | 3.44467100 | 0.69795700 |
| C | -1.69891100 | 3.44467100 | -0.69795700 |
| C | -1.06501600 | 2.41297900 | -1.40318000 |
| P | 2.83774300 | 0.85727100 | 0.00000000 |
| C | 2.25191000 | 2.60163800 | 0.00000000 |
| H | 0.03904000 | 0.03957800 | -2.36672200 |
| H | 2.02311700 | -1.02250800 | -1.34439100 |
| H | 2.02311700 | -1.02250800 | 1.34439100 |
| H | 0.03904000 | 0.03957800 | 2.36672200 |
| H | -1.07980700 | 2.40136700 | 2.49034800 |
| H | -2.20510800 | 4.23811600 | 1.23871700 |
| H | -2.20510800 | 4.23811600 | -1.23871700 |
| H | -1.07980700 | 2.40136700 | -2.49034800 |
| H | 1.67334700 | 2.87009800 | 0.88430700 |
| H | 3.16993700 | 3.19626900 | 0.00000000 |
| H | 1.67334700 | 2.87009800 | -0.88430700 |
| Fe | -0.16393500 | -1.37518500 | 0.00000000 |
| C | -1.92179400 | -1.11057400 | 0.00000000 |
| C | -0.08715200 | -2.62472900 | 1.30971000 |
| C | -0.08715200 | -2.62472900 | -1.30971000 |
| O | -3.06226700 | -0.89650300 | 0.00000000 |
| O | -0.08859400 | -3.40524000 | 2.16952700 |
| O | -0.08859400 | -3.40524000 | -2.16952700 |

**2Fe-13**($C_s$) / BP86

| | | | |
|---|---|---|---|
| C | 0.76527800 | 3.33598000 | 1.37247300 |
| C | 0.76527800 | 3.33598000 | -1.37247300 |
| C | 0.54610500 | 1.99362300 | -1.58175200 |
| C | -0.03609800 | 1.00971700 | -0.69923500 |
| C | -0.03609800 | 1.00971700 | 0.69923500 |
| C | 0.54610500 | 1.99362300 | 1.58175200 |
| C | -0.55081900 | -0.25485600 | 1.30372300 |
| C | -1.71602600 | -0.88439300 | 0.71171800 |
| C | -1.71602600 | -0.88439300 | -0.71171800 |
| C | -0.55081900 | -0.25485600 | -1.30372300 |
| H | 1.36935600 | 3.85957900 | 2.12754700 |
| H | 1.36935600 | 3.85957900 | -2.12754700 |
| H | 0.87494800 | 1.58691400 | -2.55354900 |
| H | 0.87494800 | 1.58691400 | 2.55354900 |
| H | -0.41037200 | -0.37535200 | 2.38535800 |
| H | -2.48854800 | -1.39213300 | 1.29771500 |
| H | -2.48854800 | -1.39213300 | -1.29771500 |
| H | -0.41037200 | -0.37535200 | -2.38535800 |
| P | 0.14144800 | 4.39046200 | 0.00000000 |
| C | -1.68510200 | 3.98688200 | 0.00000000 |
| H | -2.13882600 | 4.45129400 | 0.89328600 |
| H | -2.13882600 | 4.45129400 | -0.89328600 |
| H | -1.90971000 | 2.90841100 | 0.00000000 |
| Fe | -0.06351900 | -1.91752900 | 0.00000000 |
| C | -0.12289300 | -3.17492300 | 1.25874600 |
| C | -0.12289300 | -3.17492300 | -1.25874600 |
| C | 1.68829900 | -1.54202700 | 0.00000000 |
| O | -0.14359900 | -3.98270200 | 2.11103300 |
| O | -0.14359900 | -3.98270200 | -2.11103300 |
| O | 2.83477500 | -1.30223300 | 0.00000000 |

**2Fe-13**($C_s$) / B3LYP

| | | | |
|---|---|---|---|
| C | 0.74487600 | 3.30721900 | 1.38557400 |
| C | 0.74487600 | 3.30721900 | -1.38557400 |
| C | 0.53114900 | 1.97595500 | -1.58021300 |
| C | -0.04943100 | 0.99308100 | -0.69185500 |
| C | -0.04943100 | 0.99308100 | 0.69185500 |
| C | 0.53114900 | 1.97595500 | 1.58021300 |
| C | -0.57531200 | -0.25815500 | 1.30336900 |
| C | -1.72104600 | -0.88937000 | 0.70704600 |
| C | -1.72104600 | -0.88937000 | -0.70704600 |
| C | -0.57531200 | -0.25815500 | -1.30336900 |
| H | 1.31208500 | 3.82568100 | 2.15973800 |
| H | 1.31208500 | 3.82568100 | -2.15973800 |
| H | 0.85243800 | 1.56587700 | -2.54255600 |
| H | 0.85243800 | 1.56587700 | 2.54255600 |
| H | -0.45376200 | -0.36116300 | 2.38012500 |
| H | -2.48509700 | -1.40140800 | 1.28442800 |
| H | -2.48509700 | -1.40140800 | -1.28442800 |
| H | -0.45376200 | -0.36116300 | -2.38012500 |
| P | 0.17839800 | 4.36682300 | 0.00000000 |
| C | -1.65831900 | 4.04754800 | 0.00000000 |
| H | -2.09111900 | 4.52517200 | 0.88664900 |
| H | -2.09111900 | 4.52517200 | -0.88664900 |
| H | -1.92399700 | 2.98729700 | 0.00000000 |
| Fe | -0.05577600 | -1.92117300 | 0.00000000 |
| C | -0.11506000 | -3.17800300 | 1.28624400 |
| C | -0.11506000 | -3.17800300 | -1.28624400 |
| C | 1.70171700 | -1.52839100 | 0.00000000 |
| O | -0.14126300 | -3.94659100 | 2.15233800 |
| O | -0.14126300 | -3.94659100 | -2.15233800 |
| O | 2.83085000 | -1.27821000 | 0.00000000 |

**2Fe-13**($C_s$) / M06-L

| | | | |
|---|---|---|---|
| C | 0.74799300 | 3.29600600 | 1.36021200 |
| C | 0.74799300 | 3.29600600 | -1.36021200 |
| C | 0.54374700 | 1.96597500 | -1.56484000 |
| C | -0.03971300 | 0.98980700 | -0.69176500 |
| C | -0.03971300 | 0.98980700 | 0.69176500 |
| C | 0.54374700 | 1.96597500 | 1.56484000 |
| C | -0.54534400 | -0.26566500 | 1.28894700 |
| C | -1.70510600 | -0.88740800 | 0.70502300 |
| C | -1.70510600 | -0.88740800 | -0.70502300 |
| C | -0.54534400 | -0.26566500 | -1.28894700 |
| H | 1.34377900 | 3.81771700 | 2.10758400 |
| H | 1.34377900 | 3.81771700 | -2.10758400 |
| H | 0.88032900 | 1.55827000 | -2.52203900 |
| H | 0.88032900 | 1.55827000 | 2.52203900 |
| H | -0.41064300 | -0.37920200 | 2.36265000 |
| H | -2.46397900 | -1.39931900 | 1.28548100 |
| H | -2.46397900 | -1.39931900 | -1.28548100 |
| H | -0.41064300 | -0.37920200 | -2.36265000 |
| P | 0.10167800 | 4.32003000 | 0.00000000 |
| C | -1.68375000 | 3.85241800 | 0.00000000 |
| H | -2.15702300 | 4.29037900 | 0.88238600 |
| H | -2.15702300 | 4.29037900 | -0.88238600 |
| H | -1.87291800 | 2.77623500 | 0.00000000 |
| Fe | -0.05293300 | -1.89545700 | 0.00000000 |
| C | -0.10173100 | -3.14827000 | 1.28158500 |
| C | -0.10173100 | -3.14827000 | -1.28158500 |
| C | 1.69602600 | -1.45958300 | 0.00000000 |
| O | -0.12468400 | -3.92337600 | 2.14614800 |
| O | -0.12468400 | -3.92337600 | -2.14614800 |
| O | 2.80777700 | -1.13235500 | 0.00000000 |

$(C_{10}H_8PCH_3)Co(C_5H_5)$

**2Co-1**($C_1$) / BP86

| | | | |
|---|---|---|---|
| C | -1.79249400 | -0.21189100 | 0.70897800 |
| C | -1.79249400 | -0.21186900 | -0.70897300 |
| C | -0.46116300 | -0.08849900 | -1.38169300 |
| C | 0.38510800 | 1.06615400 | -1.24736700 |
| C | 0.38508800 | 1.06614500 | 1.24735900 |
| C | -0.46116300 | -0.08851600 | 1.38169700 |
| C | -3.00318500 | -0.37849300 | 1.41107000 |
| C | -4.21483100 | -0.54332700 | 0.70503000 |
| C | -4.21483200 | -0.54330200 | -0.70502900 |
| C | -3.00318900 | -0.37844400 | -1.41106600 |
| P | -0.01865300 | 2.37973800 | -0.00000300 |
| H | -0.34406400 | -0.67723700 | -2.30482000 |
| H | 1.10086300 | 1.30131500 | -2.04916100 |
| H | 1.10087200 | 1.30130600 | 2.04912700 |
| H | -0.34405100 | -0.67724900 | 2.30482600 |
| H | -2.99908500 | -0.39185800 | 2.50875200 |
| H | -5.15451500 | -0.68355400 | 1.25331400 |
| H | -5.15451800 | -0.68350900 | -1.25331500 |
| H | -2.99909100 | -0.39177300 | -2.50874800 |
| Co | 1.01780800 | -0.38935500 | -0.00001100 |
| C | 2.54922000 | -1.19764700 | -1.15511700 |
| H | 2.73546000 | -0.92533400 | -2.19743700 |
| C | 1.68754600 | -2.28013700 | -0.71185300 |
| H | 1.11342600 | -2.94757000 | -1.35781300 |
| C | 2.54932000 | -1.19754000 | 1.15506800 |
| H | 2.73564000 | -0.92513000 | 2.19734800 |
| C | 1.68760500 | -2.28006700 | 0.71197100 |
| H | 1.11353700 | -2.94743600 | 1.35804400 |
| C | 3.12263300 | -0.55778900 | -0.00007600 |
| H | 3.83539100 | 0.26878900 | -0.00014500 |
| C | 1.61605600 | 3.28229300 | 0.00003700 |
| H | 1.67415800 | 3.93285900 | -0.89026600 |
| H | 1.67412300 | 3.93280700 | 0.89038200 |
| H | 2.47548900 | 2.58766300 | 0.00004000 |

**2Co-1**($C_1$) / B3LYP

| | | | |
|---|---|---|---|
| C | -1.79729700 | -0.20436500 | 0.70488300 |
| C | -1.79729200 | -0.20437700 | -0.70487800 |
| C | -0.47911500 | -0.05506300 | -1.38988600 |
| C | 0.35435200 | 1.08423500 | -1.25539400 |
| C | 0.35433600 | 1.08425200 | 1.25539200 |
| C | -0.47912400 | -0.05503700 | 1.38990000 |
| C | -2.99843900 | -0.39569400 | 1.40198200 |
| C | -4.20012400 | -0.58233000 | 0.70128500 |
| C | -4.20011900 | -0.58234600 | -0.70128300 |
| C | -2.99843200 | -0.39572000 | -1.40197800 |
| P | -0.02239900 | 2.38553000 | -0.00001600 |
| H | -0.35542700 | -0.65073400 | -2.29589400 |
| H | 1.07495000 | 1.30708600 | -2.04283600 |
| H | 1.07496600 | 1.30709400 | 2.04280700 |
| H | -0.35543000 | -0.65072300 | 2.29589800 |
| H | -2.99468600 | -0.40811700 | 2.49084400 |
| H | -5.12972300 | -0.73669100 | 1.24576400 |
| H | -5.12971600 | -0.73671900 | -1.24576300 |
| H | -2.99467300 | -0.40816300 | -2.49083900 |
| Co | 1.00651500 | -0.37759000 | -0.00000900 |
| C | 2.57363900 | -1.21045500 | -1.14675600 |
| H | 2.76589700 | -0.94318900 | -2.18010400 |
| C | 1.71063100 | -2.27804200 | -0.70812000 |
| H | 1.14121700 | -2.93986500 | -1.34962400 |
| C | 2.57381800 | -1.21025500 | 1.14668600 |
| H | 2.76623300 | -0.94280800 | 2.17995800 |
| C | 1.71073300 | -2.27791000 | 0.70836200 |
| H | 1.14141900 | -2.93962300 | 1.35006900 |
| C | 3.15023300 | -0.58561100 | -0.00013100 |
| H | 3.85471400 | 0.23708400 | -0.00025400 |
| C | 1.60695100 | 3.28035800 | 0.00000500 |
| H | 1.66494800 | 3.92651400 | -0.88348600 |
| H | 1.66491200 | 3.92650300 | 0.88350600 |
| H | 2.46197600 | 2.59446200 | 0.00001100 |

**2Co-1**($C_1$) / M06-L

| | | | |
|---|---|---|---|
| C | 1.78334600 | -0.22119000 | -0.70247300 |
| C | 1.78334500 | -0.22118300 | 0.70247700 |
| C | 0.46282100 | -0.10128500 | 1.36839700 |
| C | -0.36592500 | 1.04892000 | 1.24053700 |
| C | -0.36592100 | 1.04891200 | -1.24054600 |
| C | 0.46282400 | -0.10129400 | -1.36839800 |
| C | 2.98510700 | -0.37175000 | -1.39764600 |
| C | 4.18625100 | -0.51742700 | -0.69829000 |
| C | 4.18625000 | -0.51741900 | 0.69830100 |
| C | 2.98510500 | -0.37173600 | 1.39765300 |
| P | 0.01756100 | 2.34487500 | 0.00000000 |
| H | 0.33692400 | -0.69337600 | 2.27750400 |
| H | -1.08506700 | 1.27554400 | 2.02937800 |
| H | -1.08505900 | 1.27553200 | -2.02939200 |
| H | 0.33693000 | -0.69338900 | -2.27750300 |
| H | 2.97992100 | -0.38619300 | -2.48499700 |
| H | 5.11870100 | -0.64223100 | -1.24095300 |
| H | 5.11869900 | -0.64221800 | 1.24096700 |
| H | 2.97991700 | -0.38616700 | 2.48500400 |
| Co | -1.01066600 | -0.38805400 | 0.00000000 |
| C | -2.53095400 | -1.15610000 | 1.14427200 |
| H | -2.69939500 | -0.87441700 | 2.17638700 |
| C | -1.69509000 | -2.24048000 | 0.70566300 |
| H | -1.12768400 | -2.90172600 | 1.34590700 |
| C | -2.53104900 | -1.15601500 | -1.14422200 |
| H | -2.69957500 | -0.87426000 | -2.17630300 |
| C | -1.69514700 | -2.24042400 | -0.70575800 |
| H | -1.12779000 | -2.90162000 | -1.34609800 |
| C | -3.08985300 | -0.51322500 | 0.00000000 |
| H | -3.77792100 | 0.32084700 | 0.00012900 |
| C | -1.62288800 | 3.18479900 | 0.00000000 |
| H | -1.71407300 | 3.82492900 | 0.88067200 |
| H | -1.71407000 | 3.82492100 | -0.88070800 |
| H | -2.44523300 | 2.45955200 | 0.00000000 |

**2Co-2**($C_1$) / BP86

| | | | |
|---|---|---|---|
| C | 1.57108400 | -0.50243300 | -0.70819800 |
| C | 1.57108400 | -0.50243100 | 0.70819900 |
| C | 0.29489000 | -0.11360100 | 1.38044100 |
| C | -0.34192100 | 1.17368500 | 1.27998900 |
| C | -0.34192100 | 1.17368000 | -1.27999200 |
| C | 0.29488900 | -0.11360700 | -1.38044100 |
| C | 2.71887100 | -0.92021600 | -1.41080300 |
| C | 3.87111800 | -1.33292100 | -0.70488300 |
| C | 3.87111800 | -1.33291900 | 0.70488500 |
| C | 2.71887200 | -0.92021100 | 1.41080300 |
| P | -0.04958300 | 2.46662900 | -0.00000400 |
| C | 1.78887100 | 2.84277000 | 0.00000100 |
| H | 0.07590800 | -0.67667700 | 2.30297100 |
| H | -1.00665000 | 1.46221000 | 2.10677900 |
| H | -1.00665100 | 1.46221000 | -2.10678000 |
| H | 0.07590700 | -0.67668600 | -2.30296900 |
| H | 2.71102800 | -0.93503500 | -2.50845200 |
| H | 4.76014400 | -1.66732500 | -1.25352600 |
| H | 4.76014500 | -1.66732200 | 1.25352700 |
| H | 2.71103000 | -0.93502700 | 2.50845300 |
| H | 2.44339000 | 1.95858500 | 0.00000200 |
| H | 2.01000300 | 3.45761300 | -0.89158500 |
| H | 2.00999600 | 3.45760800 | 0.89159200 |
| Co | -1.21948000 | -0.14014800 | 0.00000000 |
| C | -2.86508600 | -0.66727600 | 1.15508500 |
| H | -3.00062200 | -0.36443900 | 2.19650200 |
| C | -2.19358000 | -1.87761400 | 0.71276600 |
| H | -1.74396200 | -2.63464800 | 1.35846400 |
| C | -2.86508400 | -0.66728100 | -1.15508400 |
| H | -3.00061900 | -0.36444900 | -2.19650300 |
| C | -2.19357800 | -1.87761700 | -0.71275900 |
| H | -1.74396300 | -2.63465600 | -1.35845200 |
| C | -3.31979700 | 0.06067100 | -0.00000100 |
| H | -3.86436900 | 1.00652900 | -0.00000400 |

**2Co-2**($C_1$) / B3LYP

| | | | |
|---|---|---|---|
| C | 1.57187700 | -0.50702000 | -0.70400900 |
| C | 1.57188800 | -0.50699500 | 0.70402000 |
| C | 0.31457200 | -0.09064800 | 1.38720700 |
| C | -0.30354600 | 1.18404900 | 1.28278900 |
| C | -0.30355400 | 1.18401300 | -1.28279000 |
| C | 0.31455100 | -0.09069000 | -1.38718500 |
| C | 2.70523700 | -0.94569900 | -1.40177500 |
| C | 3.84356900 | -1.37678000 | -0.70109200 |
| C | 3.84358300 | -1.37675200 | 0.70109400 |
| C | 2.70526200 | -0.94564800 | 1.40178100 |
| P | -0.01142000 | 2.46389900 | -0.00001600 |
| C | 1.81847800 | 2.83545000 | -0.00003400 |
| H | 0.08710800 | -0.65371400 | 2.29565400 |
| H | -0.97163900 | 1.47167500 | 2.09431100 |
| H | -0.97167200 | 1.47162500 | -2.09429700 |
| H | 0.08706600 | -0.65377300 | -2.29561700 |
| H | 2.69816000 | -0.95910200 | -2.49061900 |
| H | 4.72013300 | -1.72201400 | -1.24588400 |
| H | 4.72015700 | -1.72196500 | 1.24588300 |
| H | 2.69820300 | -0.95901000 | 2.49062600 |
| H | 2.46856800 | 1.95884300 | -0.00002900 |
| H | 2.03970500 | 3.44528000 | -0.88493200 |
| H | 2.03972600 | 3.44530700 | 0.88484000 |
| Co | -1.21054600 | -0.12753900 | 0.00003000 |
| C | -2.89834900 | -0.65850300 | 1.14673900 |
| H | -3.03708300 | -0.35789000 | 2.17923000 |
| C | -2.23374700 | -1.86020000 | 0.70910800 |
| H | -1.79368000 | -2.61428900 | 1.35039800 |
| C | -2.89818700 | -0.65862400 | -1.14682800 |
| H | -3.03676800 | -0.35811200 | -2.17936900 |
| C | -2.23365100 | -1.86027800 | -0.70898400 |
| H | -1.79350100 | -2.61443900 | -1.35013100 |
| C | -3.35322600 | 0.05859100 | -0.00011300 |
| H | -3.88696100 | 1.00103900 | -0.00020000 |

**2Co-2**($C_1$) / M06-L

| | | | |
|---|---|---|---|
| C | -1.55148600 | -0.49983200 | 0.71916900 |
| C | -1.56026600 | -0.52664400 | -0.68348900 |
| C | -0.29807700 | -0.16199700 | -1.36547400 |
| C | 0.32217600 | 1.12015300 | -1.29907000 |
| C | 0.34022100 | 1.16722000 | 1.24831100 |
| C | -0.27922800 | -0.11240000 | 1.36881100 |
| C | -2.69382000 | -0.87253200 | 1.42995700 |
| C | -3.84858700 | -1.26471100 | 0.74514700 |
| C | -3.85729000 | -1.29176700 | -0.65080900 |
| C | -2.71138100 | -0.92659700 | -1.36477600 |
| P | 0.03258600 | 2.40920700 | -0.04627200 |
| C | -1.78868500 | 2.74812200 | -0.04118400 |
| H | -0.07970600 | -0.74303800 | -2.26559500 |
| H | 0.98405900 | 1.38589200 | -2.12264600 |
| H | 1.01637100 | 1.46093500 | 2.05105800 |
| H | -0.04442200 | -0.66390900 | 2.28367500 |
| H | -2.67827700 | -0.86571600 | 2.51724100 |
| H | -4.73377100 | -1.56133200 | 1.29976500 |
| H | -4.74934800 | -1.60931100 | -1.18236000 |
| H | -2.70970100 | -0.96169300 | -2.45163900 |
| H | -2.42929200 | 1.86530100 | -0.02039500 |
| H | -2.02039900 | 3.36861700 | 0.82905100 |
| H | -2.03138800 | 3.33512000 | -0.93143600 |
| Co | 1.21700500 | -0.14445400 | -0.00412200 |
| C | 2.94019700 | -0.51014500 | -1.08453600 |
| H | 3.13249200 | -0.10245300 | -2.06849100 |
| C | 2.26836300 | -1.75254600 | -0.81710800 |
| H | 1.87804500 | -2.43236000 | -1.56208000 |
| C | 2.75753400 | -0.73858100 | 1.18633900 |
| H | 2.79002700 | -0.52948700 | 2.24836400 |
| C | 2.16180300 | -1.90073700 | 0.58554500 |
| H | 1.68293800 | -2.71472700 | 1.11140500 |
| C | 3.27621100 | 0.10298300 | 0.15345600 |
| H | 3.77834500 | 1.05039600 | 0.28770300 |

**2Co-3**($C_1$) / BP86

| | | | |
|---|---|---|---|
| C | 1.71984700 | -0.30661900 | -0.57841100 |
| C | 2.37905700 | 0.75218600 | 0.16430800 |
| C | 1.85320100 | 2.05796900 | 0.55954000 |
| C | 0.41041000 | -0.30915800 | -1.26685300 |
| C | 0.59033800 | 2.59295300 | 0.52021000 |
| C | -0.54851300 | 0.74800100 | -1.51005600 |
| H | 2.61441000 | 2.70401600 | 1.02270300 |
| H | 0.36010600 | -1.12020300 | -2.01096800 |
| H | 0.43137200 | 3.58312100 | 0.97142700 |
| H | -1.05488500 | 0.88559400 | -2.47436800 |
| P | -0.85674700 | 1.71674000 | -0.06276900 |
| C | -2.14991600 | 2.99816100 | -0.33344400 |
| H | -3.00400700 | 2.52725400 | -0.84612400 |
| H | -2.49950200 | 3.39064500 | 0.63650400 |
| H | -1.76438500 | 3.83355000 | -0.94235700 |
| C | 3.71235800 | 0.52012400 | 0.62935000 |
| H | 4.21127600 | 1.33539600 | 1.17021000 |
| C | 2.45057200 | -1.52716000 | -0.74092000 |
| H | 1.96445400 | -2.33792700 | -1.29940200 |
| C | 4.39587700 | -0.68427500 | 0.44553000 |
| H | 5.41460700 | -0.81131300 | 0.82947700 |
| C | 3.74131100 | -1.73097100 | -0.24637200 |
| H | 4.24631700 | -2.69068300 | -0.41183900 |
| Co | -1.22576300 | -0.39065200 | -0.03961400 |
| C | -3.20212200 | -1.00577700 | 0.25840200 |
| H | -4.11039300 | -0.45309800 | 0.00867000 |
| C | -2.50987200 | -1.94077000 | -0.58645900 |
| H | -2.78500700 | -2.21731700 | -1.60731500 |
| C | -1.35427900 | -1.84644000 | 1.45708100 |
| H | -0.61996300 | -2.01933000 | 2.24564600 |
| C | -1.36957800 | -2.45174800 | 0.15200400 |
| H | -0.63793000 | -3.17011100 | -0.22502300 |
| C | -2.46860700 | -0.92667000 | 1.50782000 |
| H | -2.72016300 | -0.28192500 | 2.35350300 |

**2Co-3**($C_1$) / B3LYP

| | | | |
|---|---|---|---|
| C | 1.72240900 | -0.33794500 | -0.56933000 |
| C | 2.41909900 | 0.68835400 | 0.15992100 |
| C | 1.94883700 | 2.02643200 | 0.52843400 |
| C | 0.40512300 | -0.29117200 | -1.24558400 |
| C | 0.71656100 | 2.59541400 | 0.50467300 |
| C | -0.51288700 | 0.79150600 | -1.47755300 |
| H | 2.73996600 | 2.65447500 | 0.94150200 |
| H | 0.33799800 | -1.07865900 | -1.99894300 |
| H | 0.60840400 | 3.60597500 | 0.90058600 |
| H | -0.99721000 | 0.96750400 | -2.43626900 |
| P | -0.77202400 | 1.75336800 | -0.02324800 |
| C | -2.01011500 | 3.07647600 | -0.30281700 |
| H | -2.89230300 | 2.63638600 | -0.77669900 |
| H | -2.31535600 | 3.51245000 | 0.65441400 |
| H | -1.60970700 | 3.86989400 | -0.94270200 |
| C | 3.73216600 | 0.40933800 | 0.62827400 |
| H | 4.26103100 | 1.19969200 | 1.15905400 |
| C | 2.39729500 | -1.58027700 | -0.72579400 |
| H | 1.88345800 | -2.36869500 | -1.27343400 |
| C | 4.36242200 | -0.81740900 | 0.45469600 |
| H | 5.36626100 | -0.98285500 | 0.83894100 |
| C | 3.67164200 | -1.83264800 | -0.23027000 |
| H | 4.13295300 | -2.80580100 | -0.38805300 |
| Co | -1.23443900 | -0.35907100 | -0.04262700 |
| C | -3.08671000 | -1.39240400 | -0.36612500 |
| H | -3.78705900 | -1.19319100 | -1.16888900 |
| C | -1.96495300 | -2.28128600 | -0.42823800 |
| H | -1.68379700 | -2.88746700 | -1.28204500 |
| C | -1.96992600 | -1.32094300 | 1.67122000 |
| H | -1.69582500 | -1.04485800 | 2.68260500 |
| C | -1.29694300 | -2.26412200 | 0.84890700 |
| H | -0.41404400 | -2.83270900 | 1.11571300 |
| C | -3.07511200 | -0.77378800 | 0.91606400 |
| H | -3.77798500 | -0.03091000 | 1.27500000 |

**2Co-3**($C_1$) / M06-L

| | | | |
|---|---|---|---|
| C | 1.68642500 | -0.29585800 | -0.57593000 |
| C | 2.35515900 | 0.75258100 | 0.14334400 |
| C | 1.85610000 | 2.06837900 | 0.50073900 |
| C | 0.39077200 | -0.28652500 | -1.26359200 |
| C | 0.60933700 | 2.60235900 | 0.47200800 |
| C | -0.56446000 | 0.76335500 | -1.49407300 |
| H | 2.62929600 | 2.71134700 | 0.92329900 |
| H | 0.33780600 | -1.09307200 | -1.99960600 |
| H | 0.46682000 | 3.59884800 | 0.88816100 |
| H | -1.06768900 | 0.91116000 | -2.44737200 |
| P | -0.83572700 | 1.71288200 | -0.04947700 |
| C | -2.12728100 | 2.96990000 | -0.28989500 |
| H | -2.99059700 | 2.50112600 | -0.76438000 |
| H | -2.44575700 | 3.37481400 | 0.67261700 |
| H | -1.77200900 | 3.79239900 | -0.91464000 |
| C | 3.66473200 | 0.50267600 | 0.62241100 |
| H | 4.16941100 | 1.31469600 | 1.14172200 |
| C | 2.38088900 | -1.52650700 | -0.69845700 |
| H | 1.88181300 | -2.32761700 | -1.24038100 |
| C | 4.31338400 | -0.71136600 | 0.48038800 |
| H | 5.31358100 | -0.85235600 | 0.87662700 |
| C | 3.64671100 | -1.74873100 | -0.18612600 |
| H | 4.12277700 | -2.71578500 | -0.31883100 |
| Co | -1.20995700 | -0.38591600 | -0.03789000 |
| C | -3.15610500 | -1.01541400 | 0.25292200 |
| H | -4.05760300 | -0.46752200 | 0.01371400 |
| C | -2.46005700 | -1.91972700 | -0.60205300 |
| H | -2.72516700 | -2.17144800 | -1.62048000 |
| C | -1.31038000 | -1.84409500 | 1.41799600 |
| H | -0.57665900 | -2.01699700 | 2.19230100 |
| C | -1.32606100 | -2.42650400 | 0.11735300 |
| H | -0.58650100 | -3.11137300 | -0.27670800 |
| C | -2.42877600 | -0.95115700 | 1.48750400 |
| H | -2.67709800 | -0.32192800 | 2.33190400 |

**2Co-4**($C_s$) / BP86

| | | | |
|---|---|---|---|
| C | -1.04803600 | 0.07258700 | 0.73306800 |
| C | -1.04803600 | 0.07258700 | -0.73306800 |
| C | 0.17094300 | 0.62127400 | -1.30816500 |
| C | 0.76930500 | 1.88734300 | -0.75388900 |
| C | 0.76930500 | 1.88734300 | 0.75388900 |
| C | 0.17094300 | 0.62127400 | 1.30816500 |
| C | -2.13719300 | -0.56488900 | 1.42944900 |
| C | -3.18106000 | -1.14038300 | 0.71945200 |
| C | -3.18106000 | -1.14038300 | -0.71945200 |
| C | -2.13719300 | -0.56488900 | -1.42944900 |
| P | -0.35198900 | 3.23269900 | 0.00000000 |
| H | 0.32078300 | 0.44820700 | -2.38340300 |
| H | 1.66507800 | 2.25613600 | -1.27035400 |
| H | 1.66507800 | 2.25613600 | 1.27035400 |
| H | 0.32078300 | 0.44820700 | 2.38340300 |
| H | -2.14448300 | -0.55527800 | 2.52679800 |
| H | -4.02012000 | -1.60111600 | 1.25531700 |
| H | -4.02012000 | -1.60111600 | -1.25531700 |
| H | -2.14448300 | -0.55527800 | -2.52679800 |
| Co | 0.57787800 | -0.90121000 | 0.00000000 |
| C | 2.35874300 | -1.64221400 | -0.71900700 |
| H | 3.04849300 | -1.09161500 | -1.36226700 |
| C | 1.26716100 | -2.49112200 | -1.16449600 |
| H | 0.98587700 | -2.67880000 | -2.20331700 |
| C | 1.26716100 | -2.49112200 | 1.16449600 |
| H | 0.98587700 | -2.67880000 | 2.20331700 |
| C | 0.60967100 | -3.02050800 | 0.00000000 |
| H | -0.27312200 | -3.66409800 | 0.00000000 |
| C | 2.35874300 | -1.64221400 | 0.71900700 |
| H | 3.04849300 | -1.09161500 | 1.36226700 |
| C | 0.83190500 | 4.69082000 | 0.00000000 |
| H | 0.64866200 | 5.31557300 | -0.89257000 |
| H | 0.64866200 | 5.31557300 | 0.89257000 |
| H | 1.89384600 | 4.38706000 | 0.00000000 |

**2Co-4**($C_s$) / B3LYP

| | | | |
|---|---|---|---|
| C | -1.06540300 | 0.09834500 | 0.72641600 |
| C | -1.06540300 | 0.09834500 | -0.72641600 |
| C | 0.15096800 | 0.62236600 | -1.30508100 |
| C | 0.77140100 | 1.87655800 | -0.75171400 |
| C | 0.77140100 | 1.87655800 | 0.75171400 |
| C | 0.15096800 | 0.62236600 | 1.30508100 |
| C | -2.15731000 | -0.52698000 | 1.42034600 |
| C | -3.19830200 | -1.08972300 | 0.71721400 |
| C | -3.19830200 | -1.08972300 | -0.71721400 |
| C | -2.15731000 | -0.52698000 | -1.42034600 |
| P | -0.30250800 | 3.23978300 | 0.00000000 |
| H | 0.28445400 | 0.45714700 | -2.37457800 |
| H | 1.67143100 | 2.21531600 | -1.26298600 |
| H | 1.67143100 | 2.21531600 | 1.26298600 |
| H | 0.28445400 | 0.45714700 | 2.37457800 |
| H | -2.16434600 | -0.51639200 | 2.50883100 |
| H | -4.03598700 | -1.53766900 | 1.24845000 |
| H | -4.03598700 | -1.53766900 | -1.24845000 |
| H | -2.16434600 | -0.51639200 | -2.50883100 |
| Co | 0.56498500 | -0.89281800 | 0.00000000 |
| C | 2.34849500 | -1.68711400 | -0.71309500 |
| H | 3.03368100 | -1.14386000 | -1.35279100 |
| C | 1.26282400 | -2.52742200 | -1.15412700 |
| H | 0.98479600 | -2.71568600 | -2.18466900 |
| C | 1.26282400 | -2.52742200 | 1.15412700 |
| H | 0.98479600 | -2.71568600 | 2.18466900 |
| C | 0.61996600 | -3.06365200 | 0.00000000 |
| H | -0.25750300 | -3.70027400 | 0.00000000 |
| C | 2.34849500 | -1.68711400 | 0.71309500 |
| H | 3.03368100 | -1.14386000 | 1.35279100 |
| C | 0.91174400 | 4.66229100 | 0.00000000 |
| H | 0.74638500 | 5.28705600 | -0.88590600 |
| H | 0.74638500 | 5.28705600 | 0.88590600 |
| H | 1.95738800 | 4.33359500 | 0.00000000 |

**2Co-4**($C_s$) / M06-L

| | | | |
|---|---|---|---|
| C | -1.04312600 | 0.06611600 | 0.72603000 |
| C | -1.04312600 | 0.06611600 | -0.72603000 |
| C | 0.15789600 | 0.63089400 | -1.29390100 |
| C | 0.71689400 | 1.90320400 | -0.74666300 |
| C | 0.71689400 | 1.90320400 | 0.74666300 |
| C | 0.15789600 | 0.63089400 | 1.29390100 |
| C | -2.08782900 | -0.62452900 | 1.41529100 |
| C | -3.08846400 | -1.24969300 | 0.71309300 |
| C | -3.08846400 | -1.24969300 | -0.71309300 |
| C | -2.08782900 | -0.62452900 | -1.41529100 |
| P | -0.41186800 | 3.19558200 | 0.00000000 |
| H | 0.30386300 | 0.46375100 | -2.36128000 |
| H | 1.59824600 | 2.29082200 | -1.25336900 |
| H | 1.59824600 | 2.29082200 | 1.25336900 |
| H | 0.30386300 | 0.46375100 | 2.36128000 |
| H | -2.08997400 | -0.62161800 | 2.50238200 |
| H | -3.89018000 | -1.75345000 | 1.24429900 |
| H | -3.89018000 | -1.75345000 | -1.24429900 |
| H | -2.08997400 | -0.62161800 | -2.50238200 |
| Co | 0.58956400 | -0.86685700 | 0.00000000 |
| C | 2.35601000 | -1.58441300 | -0.71155300 |
| H | 3.02732800 | -1.02493400 | -1.34879100 |
| C | 1.27537800 | -2.42647200 | -1.15322800 |
| H | 0.99125000 | -2.60583700 | -2.18190600 |
| C | 1.27537800 | -2.42647200 | 1.15322800 |
| H | 0.99125000 | -2.60583700 | 2.18190600 |
| C | 0.62964600 | -2.95697000 | 0.00000000 |
| H | -0.25083900 | -3.58629600 | 0.00000000 |
| C | 2.35601000 | -1.58441300 | 0.71155300 |
| H | 3.02732800 | -1.02493400 | 1.34879100 |
| C | 0.74558200 | 4.64203800 | 0.00000000 |
| H | 0.56994900 | 5.26420000 | -0.88167500 |
| H | 0.56994900 | 5.26420000 | 0.88167500 |
| H | 1.79718500 | 4.34013800 | 0.00000000 |

**2Co-5**($C_1$) / BP86

| | | | |
|---|---|---|---|
| C | -0.88799900 | 0.06052000 | -0.74272200 |
| C | -0.89069700 | 0.08376900 | 0.73030300 |
| C | -1.87252700 | -0.56727100 | 1.44074000 |
| C | -3.01771200 | -1.21092400 | 0.77337500 |
| C | -3.01481100 | -1.23179300 | -0.75166800 |
| C | -1.86768300 | -0.61425500 | -1.43542500 |
| C | 0.30660400 | 0.66739400 | -1.34989700 |
| C | 0.95997800 | 1.81128500 | -0.74998800 |
| C | 0.95683600 | 1.83473700 | 0.68785000 |
| C | 0.30075900 | 0.71116700 | 1.32205700 |
| P | -4.45677200 | -0.18074200 | 0.00218400 |
| H | -1.81161300 | -0.62520700 | 2.53530400 |
| H | -3.42637300 | -2.09650100 | 1.27843800 |
| H | -3.43316900 | -2.12510900 | -1.23416800 |
| H | -1.80329800 | -0.70776900 | -2.52729700 |
| H | 0.45140200 | 0.51241800 | -2.42796400 |
| H | 1.50857600 | 2.55333800 | -1.34113400 |
| H | 1.50294800 | 2.59577600 | 1.25675700 |
| H | 0.44129500 | 0.59161900 | 2.40520700 |
| Co | 1.83387300 | 0.19853300 | -0.00297100 |
| C | 2.94711500 | -1.06604100 | 1.18061900 |
| H | 2.71845200 | -1.29489500 | 2.22430900 |
| C | 3.81071900 | 0.00303100 | 0.72206500 |
| H | 4.33877000 | 0.71630500 | 1.35900500 |
| C | 2.95346300 | -1.10339500 | -1.13958600 |
| H | 2.73119600 | -1.36667400 | -2.17651500 |
| C | 3.81482400 | -0.02024200 | -0.71117700 |
| H | 4.34712800 | 0.67161000 | -1.36792300 |
| C | 2.43554800 | -1.77488500 | 0.03030500 |
| H | 1.76188800 | -2.63363600 | 0.04212400 |
| C | -3.77510800 | 1.55275900 | -0.00178700 |
| H | -3.04088200 | 1.70724700 | -0.81253100 |
| H | -4.62659400 | 2.23991700 | -0.15036500 |
| H | -3.27859800 | 1.79715400 | 0.95383200 |

**2Co-5**($C_1$) / B3LYP

| | | | |
|---|---|---|---|
| C | -0.89394000 | 0.07316100 | -0.73341200 |
| C | -0.89436100 | 0.07681800 | 0.73615900 |
| C | -1.86561000 | -0.57470500 | 1.43456000 |
| C | -3.00632800 | -1.21895700 | 0.76277300 |
| C | -3.00557100 | -1.22324600 | -0.75599300 |
| C | -1.86428000 | -0.58174000 | -1.42964000 |
| C | 0.29568400 | 0.70083500 | -1.32994900 |
| C | 0.92517300 | 1.83350900 | -0.71658100 |
| C | 0.92536800 | 1.83679000 | 0.71183400 |
| C | 0.29567200 | 0.70648800 | 1.33016500 |
| P | -4.45342900 | -0.21946100 | -0.00088500 |
| H | -1.80737700 | -0.64176800 | 2.51996800 |
| H | -3.39274900 | -2.11067000 | 1.25565600 |
| H | -3.39036000 | -2.11812100 | -1.24444000 |
| H | -1.80488200 | -0.65374400 | -2.51469000 |
| H | 0.43776500 | 0.56810500 | -2.40199500 |
| H | 1.47507800 | 2.57621400 | -1.28867300 |
| H | 1.47405900 | 2.58274400 | 1.28084700 |
| H | 0.43681200 | 0.57881600 | 2.40291900 |
| Co | 1.82691600 | 0.21265200 | 0.00161500 |
| C | 3.05180400 | -0.99295100 | 1.18219100 |
| H | 2.89160600 | -1.15624200 | 2.24184100 |
| C | 3.88224200 | 0.02742300 | 0.61030800 |
| H | 4.44615600 | 0.77042000 | 1.16210000 |
| C | 2.91132900 | -1.17829600 | -1.10939700 |
| H | 2.62640800 | -1.50321300 | -2.10342100 |
| C | 3.78843400 | -0.07958200 | -0.80663000 |
| H | 4.27351700 | 0.56284900 | -1.53227100 |
| C | 2.47326700 | -1.76521800 | 0.11917100 |
| H | 1.80603200 | -2.61127400 | 0.22734500 |
| C | -3.82752000 | 1.52991800 | -0.00721600 |
| H | -3.23136800 | 1.74844100 | -0.89994700 |
| H | -4.70389000 | 2.18812800 | 0.00320500 |
| H | -3.21030100 | 1.74816700 | 0.87114500 |

**2Co-5**($C_1$) / M06-L

| | | | |
|---|---|---|---|
| C | 0.87081500 | 0.08444100 | 0.73967900 |
| C | 0.88475300 | 0.07908600 | -0.72008000 |
| C | 1.85159000 | -0.59434000 | -1.40288800 |
| C | 2.98634000 | -1.20990100 | -0.72083200 |
| C | 2.97363000 | -1.20004900 | 0.78903300 |
| C | 1.82618100 | -0.58183400 | 1.44557600 |
| C | -0.32018900 | 0.69910200 | 1.31663800 |
| C | -0.95835800 | 1.82598000 | 0.69848900 |
| C | -0.94378500 | 1.82234400 | -0.72608400 |
| C | -0.29396000 | 0.69104300 | -1.32437400 |
| P | 4.37517800 | -0.16733200 | 0.03701800 |
| H | 1.79361700 | -0.67833300 | -2.48546300 |
| H | 3.40123600 | -2.09583000 | -1.19610800 |
| H | 3.38533600 | -2.07770900 | 1.28196700 |
| H | 1.74877900 | -0.65713100 | 2.52757000 |
| H | -0.47592200 | 0.56354700 | 2.38602300 |
| H | -1.51587600 | 2.56502800 | 1.26507600 |
| H | -1.48778200 | 2.55941600 | -1.30803300 |
| H | -0.42733100 | 0.54940500 | -2.39596600 |
| Co | -1.80556000 | 0.20339500 | -0.01777300 |
| C | -2.93106400 | -1.00917500 | -1.19893500 |
| H | -2.74124600 | -1.16538100 | -2.25273900 |
| C | -3.78668100 | -0.00300100 | -0.64722400 |
| H | -4.35470600 | 0.72439100 | -1.21105400 |
| C | -2.81892600 | -1.17466800 | 1.08998800 |
| H | -2.52664600 | -1.47257600 | 2.08825600 |
| C | -3.71191200 | -0.09933500 | 0.76890600 |
| H | -4.21577800 | 0.53853000 | 1.48247100 |
| C | -2.34690500 | -1.75873300 | -0.12490500 |
| H | -1.65062900 | -2.58056200 | -0.21695300 |
| C | 3.65744300 | 1.52631500 | 0.00892600 |
| H | 2.99414900 | 1.70999200 | 0.86022600 |
| H | 4.48293400 | 2.24053700 | 0.04918400 |
| H | 3.07847500 | 1.71134100 | -0.90132900 |

**2Co-6**($C_1$) / BP86

| | | | |
|---|---|---|---|
| C | -0.50389800 | 0.77641300 | -0.73248800 |
| C | -0.50265100 | 0.77510200 | 0.73216600 |
| C | -0.55572900 | -0.55530900 | 1.31447100 |
| C | -1.43210100 | -1.63859700 | 0.75207700 |
| C | -1.43383900 | -1.63709200 | -0.75350400 |
| C | -0.55797300 | -0.55339500 | -1.31647500 |
| C | -0.33112700 | 2.02868900 | -1.42932800 |
| C | -0.19879800 | 3.21240100 | -0.71942900 |
| C | -0.19621400 | 3.21109700 | 0.72115700 |
| C | -0.32667600 | 2.02648500 | 1.42991000 |
| P | -3.18813800 | -1.43003800 | 0.00131000 |
| H | -0.34553000 | -0.61936300 | 2.39158100 |
| H | -1.32575500 | -2.60807500 | 1.25726000 |
| H | -1.32908200 | -2.60575400 | -1.26053100 |
| H | -0.35151100 | -0.61654200 | -2.39428900 |
| H | -0.33939400 | 2.03148100 | -2.52689200 |
| H | -0.09180700 | 4.16398700 | -1.25456600 |
| H | -0.08705400 | 4.16181300 | 1.25740500 |
| H | -0.33159200 | 2.02817800 | 2.52751400 |
| C | -3.54607100 | 0.40525100 | 0.00401300 |
| H | -3.14712400 | 0.91224100 | 0.89756700 |
| H | -3.15009500 | 0.91424700 | -0.88972400 |
| H | -4.64573600 | 0.50908200 | 0.00596800 |
| Co | 1.01932600 | -0.34699600 | -0.00254800 |
| C | 2.51493400 | -1.22177800 | 1.11322100 |
| H | 2.37533400 | -1.64544900 | 2.11052500 |
| C | 2.91184400 | 0.13864300 | 0.82421400 |
| H | 3.10585800 | 0.91921000 | 1.56324700 |
| C | 2.58079000 | -0.96841700 | -1.19641500 |
| H | 2.50166300 | -1.16941400 | -2.26753400 |
| C | 2.95560000 | 0.29198700 | -0.60260100 |
| H | 3.18135900 | 1.21310300 | -1.14467300 |
| C | 2.32691000 | -1.92415500 | -0.13542400 |
| H | 2.05071300 | -2.97324700 | -0.25708600 |

**2Co-6**($C_1$) / B3LYP

| | | | |
|---|---|---|---|
| C | 0.52742200 | 0.78359700 | 0.72615900 |
| C | 0.52742600 | 0.78361000 | -0.72616800 |
| C | 0.56954800 | -0.53314900 | -1.31228000 |
| C | 1.43271900 | -1.62594400 | -0.75101200 |
| C | 1.43271200 | -1.62596300 | 0.75099200 |
| C | 0.56958300 | -0.53314900 | 1.31227200 |
| C | 0.34214100 | 2.03072100 | 1.42033300 |
| C | 0.19979100 | 3.20471900 | 0.71817400 |
| C | 0.19980700 | 3.20472800 | -0.71817900 |
| C | 0.34215000 | 2.03073200 | -1.42034200 |
| P | 3.17292300 | -1.45153600 | 0.00000000 |
| H | 0.36653600 | -0.58990200 | -2.38188700 |
| H | 1.30738700 | -2.58477700 | -1.25351500 |
| H | 1.30735400 | -2.58479100 | 1.25349400 |
| H | 0.36656200 | -0.58989000 | 2.38187900 |
| H | 0.34970400 | 2.03269100 | 2.50903800 |
| H | 0.08544700 | 4.14770000 | 1.24935900 |
| H | 0.08547600 | 4.14771600 | -1.24935400 |
| H | 0.34972200 | 2.03270000 | -2.50904700 |
| C | 3.57963000 | 0.36807300 | 0.00000000 |
| H | 3.20069500 | 0.88339000 | -0.88718500 |
| H | 3.20071000 | 0.88334800 | 0.88728100 |
| H | 4.67336700 | 0.44252600 | 0.00000000 |
| Co | -1.00618500 | -0.34279100 | 0.00000000 |
| C | -2.42303700 | -1.69107600 | -0.71228100 |
| H | -2.18408700 | -2.53164000 | -1.35266400 |
| C | -2.78236500 | -0.36486900 | -1.15293200 |
| H | -2.85107200 | -0.03719200 | -2.18384700 |
| C | -2.78236000 | -0.36477600 | 1.15293000 |
| H | -2.85104200 | -0.03702300 | 2.18382300 |
| C | -3.03806000 | 0.43347900 | 0.00000000 |
| H | -3.29400600 | 1.48680700 | 0.00000000 |
| C | -2.42303300 | -1.69101900 | 0.71238000 |
| H | -2.18405500 | -2.53154700 | 1.35279900 |

**2Co-6**($C_1$) / M06-L

| | | | |
|---|---|---|---|
| C | 0.50383500 | 0.76392600 | 0.73317400 |
| C | 0.49686100 | 0.77851900 | -0.71740500 |
| C | 0.56181400 | -0.53473000 | -1.30676400 |
| C | 1.45316600 | -1.60017000 | -0.76684300 |
| C | 1.46063700 | -1.61496600 | 0.72393300 |
| C | 0.57389600 | -0.56142100 | 1.29468500 |
| C | 0.29378200 | 1.99223100 | 1.43792200 |
| C | 0.11880100 | 3.16541300 | 0.74879900 |
| C | 0.10799000 | 3.17924400 | -0.67965800 |
| C | 0.27493300 | 2.02028100 | -1.39431300 |
| P | 3.16824000 | -1.36337700 | -0.02749400 |
| H | 0.35271600 | -0.58487200 | -2.37546600 |
| H | 1.35837100 | -2.55826300 | -1.27363400 |
| H | 1.37099300 | -2.58327200 | 1.21193800 |
| H | 0.37764000 | -0.63383700 | 2.36441300 |
| H | 0.30424600 | 1.98155900 | 2.52503800 |
| H | -0.01805000 | 4.09728200 | 1.28922900 |
| H | -0.03785000 | 4.12122400 | -1.19982400 |
| H | 0.27010500 | 2.03140200 | -2.48154100 |
| C | 3.45590800 | 0.46037900 | -0.01111600 |
| H | 3.04402000 | 0.96323700 | -0.88893900 |
| H | 3.05197400 | 0.94607200 | 0.87996700 |
| H | 4.53796100 | 0.61171100 | -0.01459300 |
| Co | -0.99439800 | -0.36385300 | 0.00270000 |
| C | -2.45448500 | -1.28686400 | -1.07891400 |
| H | -2.28754500 | -1.74506100 | -2.04465000 |
| C | -2.84070300 | 0.07456900 | -0.85957900 |
| H | -3.01248200 | 0.81676300 | -1.62756100 |
| C | -2.54847700 | -0.93087200 | 1.19335900 |
| H | -2.46813000 | -1.07739200 | 2.26251500 |
| C | -2.90871100 | 0.28829500 | 0.54649500 |
| H | -3.12755500 | 1.22671300 | 1.03897000 |
| C | -2.28095200 | -1.92449500 | 0.18843600 |
| H | -2.00103500 | -2.95461000 | 0.36039700 |

**2Co-7**($C_1$) / BP86

| | | | |
|---|---|---|---|
| C | -0.73224200 | 0.30116700 | -0.75130600 |
| C | -0.73224200 | 0.37171600 | 0.72479200 |
| C | -1.77732300 | -0.14169400 | 1.45174300 |
| C | -2.99048200 | -0.67924300 | 0.79883600 |
| C | -2.98918200 | -0.75381800 | -0.72699900 |
| C | -1.77552300 | -0.28112100 | -1.42687500 |
| C | 0.51702700 | 0.76107800 | -1.37322400 |
| C | 1.29833300 | 1.83722500 | -0.80415300 |
| C | 1.29996400 | 1.90392800 | 0.63213300 |
| C | 0.51827400 | 0.88658700 | 1.30015000 |
| P | -4.23903900 | 0.52052000 | -0.02619400 |
| C | -5.77581400 | -0.56136900 | 0.02110400 |
| H | -1.73026800 | -0.16171300 | 2.54816000 |
| H | -3.49994800 | -1.49153800 | 1.33510300 |
| H | -3.49835700 | -1.61465300 | -1.18190800 |
| H | -1.72693300 | -0.40534300 | -2.51633500 |
| H | 0.64152500 | 0.56316300 | -2.44681400 |
| H | 1.92725900 | 2.49422300 | -1.41549700 |
| H | 1.93114100 | 2.61334600 | 1.17911400 |
| H | 0.64374600 | 0.78917400 | 2.38736000 |
| H | -6.37958000 | -0.38797200 | -0.88779100 |
| H | -5.54670200 | -1.64013600 | 0.08200200 |
| H | -6.39424900 | -0.29010400 | 0.89548300 |
| Co | 1.98390100 | 0.15718400 | -0.00660500 |
| C | 2.97508700 | -1.15723200 | 1.22791100 |
| H | 2.75170100 | -1.29646300 | 2.28835900 |
| C | 3.94408100 | -0.22812300 | 0.68498600 |
| H | 4.57161800 | 0.45291000 | 1.26444800 |
| C | 2.90781500 | -1.33343700 | -1.08571500 |
| H | 2.62380200 | -1.62733400 | -2.09897800 |
| C | 3.90084200 | -0.33477700 | -0.74449500 |
| H | 4.48977900 | 0.24970300 | -1.45506200 |
| C | 2.35029000 | -1.86756500 | 0.13423200 |
| H | 1.58229300 | -2.63894900 | 0.21489500 |

**2Co-7**($C_1$) / B3LYP

| | | | |
|---|---|---|---|
| C | -0.74575100 | 0.31036300 | -0.74264600 |
| C | -0.74600300 | 0.34147200 | 0.73160000 |
| C | -1.78141600 | -0.17969700 | 1.44036400 |
| C | -2.99529100 | -0.70133000 | 0.77639300 |
| C | -2.99459400 | -0.73374000 | -0.74548200 |
| C | -1.78024400 | -0.24058500 | -1.42973200 |
| C | 0.50391900 | 0.79683200 | -1.34650300 |
| C | 1.25251900 | 1.86446600 | -0.75185600 |
| C | 1.25303700 | 1.89391600 | 0.67618400 |
| C | 0.50407000 | 0.85199500 | 1.31477500 |
| P | -4.23930900 | 0.50118900 | -0.01122400 |
| C | -5.77024500 | -0.57611700 | 0.00965100 |
| H | -1.73711700 | -0.22374400 | 2.52745100 |
| H | -3.48629300 | -1.52992700 | 1.28626600 |
| H | -3.48540300 | -1.58325100 | -1.21998300 |
| H | -1.73481900 | -0.33017500 | -2.51397000 |
| H | 0.62976600 | 0.63342000 | -2.41638400 |
| H | 1.87948500 | 2.53293000 | -1.33605800 |
| H | 1.87999900 | 2.58600500 | 1.23218700 |
| H | 0.62970000 | 0.73290300 | 2.39053200 |
| H | -6.37524900 | -0.37357900 | -0.88228400 |
| H | -5.54363100 | -1.64811800 | 0.03329000 |
| H | -6.37852800 | -0.33506900 | 0.88968400 |
| Co | 1.97502100 | 0.16927900 | -0.00243800 |
| C | 3.03395300 | -1.16673200 | 1.19555600 |
| H | 2.82988900 | -1.31803200 | 2.24936000 |
| C | 3.97984800 | -0.23399100 | 0.65264000 |
| H | 4.60478700 | 0.44204300 | 1.22449200 |
| C | 2.93240100 | -1.32016100 | -1.10069100 |
| H | 2.63834100 | -1.60525700 | -2.10421600 |
| C | 3.91325800 | -0.32368900 | -0.76740200 |
| H | 4.48132700 | 0.26863400 | -1.47525700 |
| C | 2.40432200 | -1.86622200 | 0.11251100 |
| H | 1.64913200 | -2.63783100 | 0.19689700 |

**2Co-7**($C_1$) / M06-L

| | | | |
|---|---|---|---|
| C | -0.71317800 | 0.35826200 | -0.73590400 |
| C | -0.71346000 | 0.37775100 | 0.72798500 |
| C | -1.74218500 | -0.16537800 | 1.42944600 |
| C | -2.94488900 | -0.67722700 | 0.76522300 |
| C | -2.94440100 | -0.69716800 | -0.74717400 |
| C | -1.74147200 | -0.20279500 | -1.42365800 |
| C | 0.53287000 | 0.82393100 | -1.33276100 |
| C | 1.31583300 | 1.86617500 | -0.73597800 |
| C | 1.31609100 | 1.88497600 | 0.68806900 |
| C | 0.53258200 | 0.85922800 | 1.31257300 |
| P | -4.18278800 | 0.51286600 | -0.00717100 |
| C | -5.66742600 | -0.59783000 | 0.00646000 |
| H | -1.68940800 | -0.22850400 | 2.51354900 |
| H | -3.44372400 | -1.50771200 | 1.26178300 |
| H | -3.44317600 | -1.54034600 | -1.22211400 |
| H | -1.68794000 | -0.29361900 | -2.50575100 |
| H | 0.65815500 | 0.65884500 | -2.40197300 |
| H | 1.95672500 | 2.51959000 | -1.31890900 |
| H | 1.95701000 | 2.55378600 | 1.25341200 |
| H | 0.65721800 | 0.72261900 | 2.38585000 |
| H | -6.28520200 | -0.41326800 | -0.87656400 |
| H | -5.39991600 | -1.65854700 | 0.01651200 |
| H | -6.28270200 | -0.39575500 | 0.88732500 |
| Co | 1.95832700 | 0.15675100 | -0.00101000 |
| C | 2.89908900 | -1.20199700 | 1.18244700 |
| H | 2.67158200 | -1.34474800 | 2.23065200 |
| C | 3.88317000 | -0.30358000 | 0.65807900 |
| H | 4.52856300 | 0.33876000 | 1.24141600 |
| C | 2.80597000 | -1.32274800 | -1.11036000 |
| H | 2.49566200 | -1.56923900 | -2.11718000 |
| C | 3.82251500 | -0.37412300 | -0.76065000 |
| H | 4.41534700 | 0.20359500 | -1.45672200 |
| C | 2.24369000 | -1.85784700 | 0.09000800 |
| H | 1.45001000 | -2.58851300 | 0.16070500 |

**2Co-8**($C_1$) / BP86

| | | | |
|---|---|---|---|
| C | 1.96586800 | -1.81539300 | -0.93994700 |
| C | 1.46985400 | 0.06766700 | 1.12961600 |
| C | 0.21086400 | -0.33479500 | 1.71555100 |
| C | -0.78374300 | -1.02477600 | 0.92064300 |
| C | -0.55992300 | -1.30144500 | -0.52212600 |
| C | 0.63106000 | -1.82508400 | -1.22853200 |
| C | -1.78885800 | -1.53098900 | -1.27948500 |
| C | -3.04416700 | -1.64231800 | -0.71076100 |
| C | -3.19494000 | -1.55966800 | 0.71621000 |
| C | -2.09786600 | -1.25397600 | 1.49543700 |
| H | 2.63946600 | -2.32331800 | -1.64447000 |
| H | 1.97886900 | 0.84826500 | 1.72138000 |
| H | -0.08872200 | -0.00978300 | 2.72205700 |
| H | 0.35999900 | -2.31942800 | -2.17491600 |
| H | -1.68218300 | -1.69648700 | -2.36031300 |
| H | -3.91511700 | -1.85224200 | -1.34319600 |
| H | -4.17458400 | -1.73293500 | 1.17777300 |
| H | -2.19606500 | -1.16586400 | 2.58519100 |
| P | 2.74395300 | -1.10031400 | 0.51426200 |
| C | 3.97734000 | 0.05022700 | -0.29462100 |
| H | 3.49004600 | 0.75432200 | -0.99024400 |
| H | 4.51566300 | 0.61738400 | 0.48489300 |
| H | 4.72283400 | -0.54733200 | -0.84773300 |
| Co | -0.17828000 | 0.74894600 | 0.12214200 |
| C | -1.83038600 | 1.92001100 | -0.47050300 |
| H | -2.86715400 | 1.57726200 | -0.47340100 |
| C | -0.88634900 | 1.76237100 | -1.56096900 |
| H | -1.10075700 | 1.28616800 | -2.52022800 |
| C | 0.23065000 | 2.74869500 | 0.21875400 |
| H | 1.01864200 | 3.18531000 | 0.83709500 |
| C | 0.38276900 | 2.29003600 | -1.15111100 |
| H | 1.29593800 | 2.32031800 | -1.74793100 |
| C | -1.14461900 | 2.54280900 | 0.62213700 |
| H | -1.56792900 | 2.78129700 | 1.60052800 |

**2Co-8**($C_1$) / B3LYP

| | | | |
|---|---|---|---|
| C | 1.92425100 | -1.82566000 | -0.95221100 |
| C | 1.45595000 | 0.00659700 | 1.15335800 |
| C | 0.19433700 | -0.38611900 | 1.70911000 |
| C | -0.80148600 | -1.05034000 | 0.90818000 |
| C | -0.59153100 | -1.31992500 | -0.52025500 |
| C | 0.60177200 | -1.82807000 | -1.23720300 |
| C | -1.81176600 | -1.53580800 | -1.27925600 |
| C | -3.06361100 | -1.61804800 | -0.72079100 |
| C | -3.21362500 | -1.52093000 | 0.69878900 |
| C | -2.11893200 | -1.24149000 | 1.47444700 |
| H | 2.58587200 | -2.31574600 | -1.66758200 |
| H | 1.96183500 | 0.75839200 | 1.76739100 |
| H | -0.11194600 | -0.06255400 | 2.70334500 |
| H | 0.33026200 | -2.30350000 | -2.18187100 |
| H | -1.70481500 | -1.70321400 | -2.35029900 |
| H | -3.93026100 | -1.81248100 | -1.34887700 |
| H | -4.19068800 | -1.66421900 | 1.15585900 |
| H | -2.22000900 | -1.14553600 | 2.55419400 |
| P | 2.72555800 | -1.14587900 | 0.50618800 |
| C | 3.92256300 | 0.03125200 | -0.30404100 |
| H | 3.42137400 | 0.72965400 | -0.98252100 |
| H | 4.45518100 | 0.59768500 | 0.46868100 |
| H | 4.66846000 | -0.54151900 | -0.86687500 |
| Co | -0.15377300 | 0.74087300 | 0.13146600 |
| C | -1.76123500 | 1.95816700 | -0.56868400 |
| H | -2.78368400 | 1.61471100 | -0.67049800 |
| C | -0.73178400 | 1.83525400 | -1.57155400 |
| H | -0.85748900 | 1.39228900 | -2.55254000 |
| C | 0.20329800 | 2.77657700 | 0.31337600 |
| H | 0.92490200 | 3.19869300 | 1.00336100 |
| C | 0.47827200 | 2.35725800 | -1.03945700 |
| H | 1.43591200 | 2.40420900 | -1.54255600 |
| C | -1.18982600 | 2.57132300 | 0.57853900 |
| H | -1.69630600 | 2.77753500 | 1.51428100 |

**2Co-8**($C_1$) / M06-L

| | | | |
|---|---|---|---|
| C | 1.93655000 | -1.79433500 | -0.93333600 |
| C | 1.44932900 | 0.02874800 | 1.14259700 |
| C | 0.19378000 | -0.35817300 | 1.71522800 |
| C | -0.79630100 | -1.02629000 | 0.91728100 |
| C | -0.57073700 | -1.29969400 | -0.50973100 |
| C | 0.61465700 | -1.80453600 | -1.21415200 |
| C | -1.78550500 | -1.48700600 | -1.27489200 |
| C | -3.04042800 | -1.53901500 | -0.73208100 |
| C | -3.20556400 | -1.44524200 | 0.68015900 |
| C | -2.11734900 | -1.19608800 | 1.46643600 |
| H | 2.59964400 | -2.27609700 | -1.64993400 |
| H | 1.95233600 | 0.79874700 | 1.73714100 |
| H | -0.11617100 | -0.02863700 | 2.70674100 |
| H | 0.34379500 | -2.27085100 | -2.16359900 |
| H | -1.66663700 | -1.65488600 | -2.34417400 |
| H | -3.90098600 | -1.71016500 | -1.37126100 |
| H | -4.18863200 | -1.56637800 | 1.12427300 |
| H | -2.22412000 | -1.09958800 | 2.54404900 |
| P | 2.71770700 | -1.11082500 | 0.51612700 |
| C | 3.88389700 | 0.07505500 | -0.28466500 |
| H | 3.36020300 | 0.77152900 | -0.94639700 |
| H | 4.41732600 | 0.64335600 | 0.48149900 |
| H | 4.62934900 | -0.47239400 | -0.86631000 |
| Co | -0.15829100 | 0.72543100 | 0.12870500 |
| C | -1.77893200 | 1.89724300 | -0.42522000 |
| H | -2.81031900 | 1.57186000 | -0.38731500 |
| C | -0.88143000 | 1.70112000 | -1.52932400 |
| H | -1.12895000 | 1.19617200 | -2.45424100 |
| C | 0.29888500 | 2.69359500 | 0.17351000 |
| H | 1.11115200 | 3.10734500 | 0.75722000 |
| C | 0.39887100 | 2.20662900 | -1.17635200 |
| H | 1.28638900 | 2.19727300 | -1.79311900 |
| C | -1.05342300 | 2.52814900 | 0.61954000 |
| H | -1.43392800 | 2.78747200 | 1.59848700 |

**2Co-9**($C_1$) / BP86

| | | | |
|---|---|---|---|
| C | -2.26541800 | -1.09658700 | 1.31811500 |
| C | -1.49495800 | 0.62520400 | -0.83856000 |
| C | -0.55890500 | -0.21228100 | -1.55367400 |
| C | 0.31357600 | -1.13855400 | -0.86469600 |
| C | 0.23222700 | -1.29309100 | 0.60690200 |
| C | -0.98116500 | -1.53601100 | 1.43153600 |
| C | 1.43531500 | -1.85507700 | 1.21720400 |
| C | 2.51052600 | -2.34440500 | 0.49766200 |
| C | 2.46975300 | -2.34989400 | -0.93964000 |
| C | 1.40636500 | -1.75856700 | -1.59226400 |
| H | -2.98533200 | -1.47730200 | 2.05761700 |
| H | -1.77736900 | 1.51570800 | -1.42712300 |
| H | -0.34002700 | -0.02095000 | -2.61506500 |
| H | -0.78014900 | -2.21497500 | 2.27663700 |
| H | 1.43561500 | -1.95967000 | 2.31100000 |
| H | 3.36683400 | -2.78491300 | 1.02244000 |
| H | 3.28213500 | -2.81553900 | -1.51060300 |
| H | 1.36780900 | -1.73474600 | -2.68922100 |
| P | -2.88585300 | 0.25546300 | 0.29471800 |
| C | -4.06473400 | -0.66568700 | -0.84547000 |
| H | -4.91443500 | -1.05384000 | -0.25591100 |
| H | -4.46776400 | 0.04151700 | -1.59158700 |
| H | -3.57065100 | -1.50389300 | -1.36519200 |
| Co | 0.39882700 | 0.74755500 | -0.10871100 |
| C | 2.37770200 | 1.35934800 | 0.28363500 |
| H | 3.25019000 | 0.70355500 | 0.24690200 |
| C | 1.52495800 | 1.56260100 | 1.44411800 |
| H | 1.65703900 | 1.08780800 | 2.41879200 |
| C | 0.64263800 | 2.77042100 | -0.33023200 |
| H | -0.01982700 | 3.40298200 | -0.92614400 |
| C | 0.45949000 | 2.44460600 | 1.07725000 |
| H | -0.35603100 | 2.78508700 | 1.71737100 |
| C | 1.84681800 | 2.12745700 | -0.80163500 |
| H | 2.24631900 | 2.17634800 | -1.81699300 |

**2Co-9**($C_1$) / B3LYP

| | | | |
|---|---|---|---|
| C | -2.28354300 | -0.95410900 | 1.36002500 |
| C | -1.47582700 | 0.65934000 | -0.85042900 |
| C | -0.57638300 | -0.22036200 | -1.53814200 |
| C | 0.24825100 | -1.17312300 | -0.84480300 |
| C | 0.17841500 | -1.31644900 | 0.61229500 |
| C | -1.03374100 | -1.45441600 | 1.46285700 |
| C | 1.34514400 | -1.93386900 | 1.21920500 |
| C | 2.39310400 | -2.46102400 | 0.50481000 |
| C | 2.34916500 | -2.45610800 | -0.92621000 |
| C | 1.31442300 | -1.82861300 | -1.57013000 |
| H | -2.99563600 | -1.26774100 | 2.12522100 |
| H | -1.72090200 | 1.53755600 | -1.45595800 |
| H | -0.34069500 | -0.04933600 | -2.58901600 |
| H | -0.85629200 | -2.10983600 | 2.31905800 |
| H | 1.34373600 | -2.03476700 | 2.30408500 |
| H | 3.22498400 | -2.93408800 | 1.02214900 |
| H | 3.13653000 | -2.94452200 | -1.49688300 |
| H | 1.27766700 | -1.80063200 | -2.65798100 |
| P | -2.88603900 | 0.35383700 | 0.27052500 |
| C | -4.03903900 | -0.62269200 | -0.83532500 |
| H | -4.89492800 | -0.97731600 | -0.24863000 |
| H | -4.42373000 | 0.03661300 | -1.62207500 |
| H | -3.54060800 | -1.48172600 | -1.29652000 |
| Co | 0.41642600 | 0.73770800 | -0.11151000 |
| C | 2.42660900 | 1.29745700 | 0.33393800 |
| H | 3.25930700 | 0.60483100 | 0.35917200 |
| C | 1.54560500 | 1.59011200 | 1.44063100 |
| H | 1.61173800 | 1.15660700 | 2.43153500 |
| C | 0.81446800 | 2.76092600 | -0.40530700 |
| H | 0.21947500 | 3.39901100 | -1.04849800 |
| C | 0.55609100 | 2.50473400 | 0.99299900 |
| H | -0.26292600 | 2.90812300 | 1.57531300 |
| C | 1.99908000 | 2.05685100 | -0.78799700 |
| H | 2.43844500 | 2.03960500 | -1.77856400 |

**2Co-9**($C_1$) / M06-L

| | | | |
|---|---|---|---|
| C | -2.25736200 | -1.03920000 | 1.32828600 |
| C | -1.48322700 | 0.64390200 | -0.81174500 |
| C | -0.57505100 | -0.19962700 | -1.53515700 |
| C | 0.28104800 | -1.13276900 | -0.86065600 |
| C | 0.20840900 | -1.28742600 | 0.59710700 |
| C | -0.99198200 | -1.49337700 | 1.42790700 |
| C | 1.40018500 | -1.84753400 | 1.19876600 |
| C | 2.47287000 | -2.31203800 | 0.48729900 |
| C | 2.43667600 | -2.30069300 | -0.93806500 |
| C | 1.37615000 | -1.72847100 | -1.58176500 |
| H | -2.95964200 | -1.39750700 | 2.07995000 |
| H | -1.74475800 | 1.53396100 | -1.39301200 |
| H | -0.35177100 | -0.00619500 | -2.58529300 |
| H | -0.79122500 | -2.15716600 | 2.27250500 |
| H | 1.39480200 | -1.95777900 | 2.28206700 |
| H | 3.32308900 | -2.74426600 | 1.00579500 |
| H | 3.25011900 | -2.74084700 | -1.50667000 |
| H | 1.34048400 | -1.69191000 | -2.66796800 |
| P | -2.87782200 | 0.28123500 | 0.28992000 |
| C | -3.98948400 | -0.67091100 | -0.84974600 |
| H | -4.83736400 | -1.07560700 | -0.29050400 |
| H | -4.38770700 | 0.00149900 | -1.61373100 |
| H | -3.46278900 | -1.49430200 | -1.33976900 |
| Co | 0.39779400 | 0.73654100 | -0.10415100 |
| C | 2.36225800 | 1.28330700 | 0.27083400 |
| H | 3.20589500 | 0.60694300 | 0.22594400 |
| C | 1.53184900 | 1.50808500 | 1.42576100 |
| H | 1.64762700 | 1.02209000 | 2.38564100 |
| C | 0.68169100 | 2.73120900 | -0.32496800 |
| H | 0.03120900 | 3.36360200 | -0.91461600 |
| C | 0.49737800 | 2.40915800 | 1.06887300 |
| H | -0.30528900 | 2.75688700 | 1.70387800 |
| C | 1.85429600 | 2.06589400 | -0.79819100 |
| H | 2.23999900 | 2.09840000 | -1.80818400 |

**2Co-10**($C_1$) / BP86

| | | | |
|---|---|---|---|
| C | 3.17152900 | -1.35910700 | -0.49086700 |
| C | 3.17146800 | 1.36283200 | -0.48166500 |
| C | 1.82159900 | 1.57745000 | -0.38705800 |
| C | 0.82221300 | 0.69896900 | 0.20123500 |
| C | 0.82228000 | -0.70072400 | 0.19770900 |
| C | 1.82181500 | -1.57509300 | -0.39678800 |
| C | -0.45277800 | -1.29929500 | 0.67883000 |
| C | -1.14228700 | -0.72119400 | 1.82221900 |
| C | -1.14254200 | 0.71140800 | 1.82477000 |
| C | -0.45290000 | 1.29469400 | 0.68486900 |
| H | 3.78293900 | -2.05751500 | -1.08177500 |
| H | 3.78293400 | 2.06586300 | -1.06698300 |
| H | 1.42158800 | 2.51004800 | -0.81743300 |
| H | 1.42187900 | -2.50471000 | -0.83363400 |
| H | -0.57836400 | -2.37875100 | 0.51527500 |
| H | -1.69542100 | -1.31698100 | 2.55662500 |
| H | -1.69853100 | 1.30366000 | 2.55990200 |
| H | -0.57961600 | 2.37469100 | 0.52569200 |
| P | 4.00542400 | -0.00111200 | 0.41667200 |
| C | 5.66336700 | 0.00249000 | -0.44630900 |
| H | 5.58329200 | 0.00688800 | -1.54754300 |
| H | 6.23558500 | 0.89050400 | -0.12600900 |
| H | 6.23620400 | -0.88761800 | -0.13305800 |
| Co | -1.96864900 | -0.00275800 | 0.17179100 |
| C | -2.98408800 | 1.13033000 | -1.21664800 |
| H | -2.70014400 | 2.14593400 | -1.50318700 |
| C | -3.92921300 | 0.78612900 | -0.16932600 |
| H | -4.46068600 | 1.49662100 | 0.46792400 |
| C | -3.09288400 | -1.17732900 | -1.08746900 |
| H | -2.90442400 | -2.23979500 | -1.26148200 |
| C | -4.00069800 | -0.63747100 | -0.09483400 |
| H | -4.59430300 | -1.22139300 | 0.61210200 |
| C | -2.49525700 | -0.08328100 | -1.82245500 |
| H | -1.79051200 | -0.16113600 | -2.65214400 |

**2Co-10**($C_1$) / B3LYP

| | | | |
|---|---|---|---|
| C | 3.15315700 | -1.36920900 | -0.46192600 |
| C | 3.15370300 | 1.37115200 | -0.45662100 |
| C | 1.81585000 | 1.57400800 | -0.35959800 |
| C | 0.81845100 | 0.69271100 | 0.23314900 |
| C | 0.81837200 | -0.69256700 | 0.23154600 |
| C | 1.81531500 | -1.57200000 | -0.36519300 |
| C | -0.43508400 | -1.30167300 | 0.73590000 |
| C | -1.12910500 | -0.71249200 | 1.85010000 |
| C | -1.12945000 | 0.70906100 | 1.85055500 |
| C | -0.43531800 | 1.30022500 | 0.73845600 |
| H | 3.75169000 | -2.08925400 | -1.02274100 |
| H | 3.75267100 | 2.09326900 | -1.01425400 |
| H | 1.41243800 | 2.49893800 | -0.77984500 |
| H | 1.41122200 | -2.49494900 | -0.78911900 |
| H | -0.54892400 | -2.37533900 | 0.59108600 |
| H | -1.70040500 | -1.29569900 | 2.56703700 |
| H | -1.70423200 | 1.29078800 | 2.56592100 |
| H | -0.55077400 | 2.37383200 | 0.59429800 |
| P | 4.01692800 | -0.00080600 | 0.38973300 |
| C | 5.62603400 | 0.00074800 | -0.54618100 |
| H | 5.49243900 | 0.00344100 | -1.63382100 |
| H | 6.20985300 | 0.88251600 | -0.25901800 |
| H | 6.20913000 | -0.88288200 | -0.26330100 |
| Co | -1.95036500 | -0.00251100 | 0.17929200 |
| C | -2.95974500 | 1.10205000 | -1.27977200 |
| H | -2.65076500 | 2.09243800 | -1.59417900 |
| C | -3.91903900 | 0.81576200 | -0.24341300 |
| H | -4.43839500 | 1.55285800 | 0.35809000 |
| C | -3.13082100 | -1.18120500 | -1.08117300 |
| H | -2.97159000 | -2.24430600 | -1.22344200 |
| C | -4.03500100 | -0.59358600 | -0.13336100 |
| H | -4.65066500 | -1.13496200 | 0.57549000 |
| C | -2.49905700 | -0.13239000 | -1.83240500 |
| H | -1.78734400 | -0.25436000 | -2.63946000 |

**2Co-10**($C_1$) / M06-L

| | | | |
|---|---|---|---|
| C | 3.13360800 | -1.34614200 | -0.49339000 |
| C | 3.13398300 | 1.35387600 | -0.47258600 |
| C | 1.79826300 | 1.56352800 | -0.38735700 |
| C | 0.81050300 | 0.69089700 | 0.20417600 |
| C | 0.81053400 | -0.69347700 | 0.19509200 |
| C | 1.79798000 | -1.55722300 | -0.41030800 |
| C | -0.45111100 | -1.28797800 | 0.67356400 |
| C | -1.13161100 | -0.72119000 | 1.81112100 |
| C | -1.13170800 | 0.69770200 | 1.81946600 |
| C | -0.45137400 | 1.27865900 | 0.68982200 |
| H | 3.74240200 | -2.03492600 | -1.07962400 |
| H | 3.74314700 | 2.05204500 | -1.04723200 |
| H | 1.39590200 | 2.48216100 | -0.81980800 |
| H | 1.39516100 | -2.46883300 | -0.85699700 |
| H | -0.57487900 | -2.35780300 | 0.50759600 |
| H | -1.68581900 | -1.31348100 | 2.53189500 |
| H | -1.68880400 | 1.28076600 | 2.54552100 |
| H | -0.57616700 | 2.35031200 | 0.53680200 |
| P | 3.95192300 | -0.00306500 | 0.41252900 |
| C | 5.58691300 | 0.00374600 | -0.44046200 |
| H | 5.50019400 | 0.01259600 | -1.53083100 |
| H | 6.15961500 | 0.88041900 | -0.13000800 |
| H | 6.15988100 | -0.87761700 | -0.14417900 |
| Co | -1.94676000 | -0.00319400 | 0.17342700 |
| C | -2.92878600 | 1.11561600 | -1.22196500 |
| H | -2.62457300 | 2.11498600 | -1.50459300 |
| C | -3.86473300 | 0.79614000 | -0.18111000 |
| H | -4.38183600 | 1.51172600 | 0.44375600 |
| C | -3.06105500 | -1.16718400 | -1.06959800 |
| H | -2.87414000 | -2.22240500 | -1.22163000 |
| C | -3.95230800 | -0.61459300 | -0.09427200 |
| H | -4.54518500 | -1.17929800 | 0.61222700 |
| C | -2.45155300 | -0.09700300 | -1.80468100 |
| H | -1.74651000 | -0.19067100 | -2.61844400 |

**2Co-11**($C_s$) / BP86

| | | | |
|---|---|---|---|
| C | 2.41054600 | 2.30022200 | 1.37917300 |
| C | 2.41054600 | 2.30022200 | -1.37917300 |
| C | 1.47365600 | 1.31283900 | -1.58342900 |
| C | 0.44361900 | 0.81242000 | -0.70154800 |
| C | 0.44361900 | 0.81242000 | 0.70154800 |
| C | 1.47365600 | 1.31283900 | 1.58342900 |
| C | -0.67538800 | 0.03081900 | 1.29595400 |
| C | -2.00740800 | 0.11389800 | 0.71636400 |
| C | -2.00740800 | 0.11389800 | -0.71636400 |
| C | -0.67538800 | 0.03081900 | -1.29595400 |
| H | 3.19222100 | 2.40364300 | 2.14604100 |
| H | 3.19222100 | 2.40364300 | -2.14604100 |
| H | 1.51002400 | 0.79914400 | -2.56011100 |
| H | 1.51002400 | 0.79914400 | 2.56011100 |
| H | -0.61379900 | -0.16631600 | 2.37528500 |
| H | -2.92692200 | 0.07725400 | 1.31083400 |
| H | -2.92692200 | 0.07725400 | -1.31083400 |
| H | -0.61379900 | -0.16631600 | -2.37528500 |
| P | 2.50528900 | 3.51202900 | 0.00000000 |
| C | 0.77496100 | 4.22648800 | 0.00000000 |
| H | 0.66556200 | 4.86599000 | 0.89380300 |
| H | 0.66556200 | 4.86599000 | -0.89380300 |
| H | -0.02233800 | 3.46606300 | 0.00000000 |
| Co | -1.11623200 | -1.50389300 | 0.00000000 |
| C | -0.63725000 | -3.13606700 | -1.15691500 |
| H | -0.31245500 | -3.07303000 | -2.19849500 |
| C | -2.00740800 | -3.31188700 | -0.71382100 |
| H | -2.88292300 | -3.38874700 | -1.36245800 |
| C | -0.63725000 | -3.13606700 | 1.15691500 |
| H | -0.31245500 | -3.07303000 | 2.19849500 |
| C | -2.00740800 | -3.31188700 | 0.71382100 |
| H | -2.88292300 | -3.38874700 | 1.36245800 |
| C | 0.22530800 | -3.07236100 | 0.00000000 |
| H | 1.31174200 | -2.96885700 | 0.00000000 |

**2Co-11**($C_s$) / B3LYP

| | | | |
|---|---|---|---|
| C | 3.17675800 | -1.38122800 | -0.91557600 |
| C | 3.17613400 | 1.39696800 | -0.89264200 |
| C | 1.86428100 | 1.58571600 | -0.57694100 |
| C | 0.91962900 | 0.69343800 | 0.06045000 |
| C | 0.91990000 | -0.69512600 | 0.04941500 |
| C | 1.86507100 | -1.57615600 | -0.60301100 |
| C | -0.29717900 | -1.30468300 | 0.63833800 |
| C | -0.90081200 | -0.72609700 | 1.81005200 |
| C | -0.90092100 | 0.69530600 | 1.82096600 |
| C | -0.29768000 | 1.29262000 | 0.65919500 |
| H | 3.65343700 | -2.15788400 | -1.51546600 |
| H | 3.65231800 | 2.18379900 | -1.47949900 |
| H | 1.43393000 | 2.55410100 | -0.85111400 |
| H | 1.43527300 | -2.54009400 | -0.89322300 |
| H | -0.42420900 | -2.37669100 | 0.49282000 |
| H | -1.41257600 | -1.31566400 | 2.56571700 |
| H | -1.41450900 | 1.27249500 | 2.58491600 |
| H | -0.42622900 | 2.36657200 | 0.53008400 |
| P | 4.27491100 | 0.00429700 | -0.43255700 |
| C | 4.11085200 | -0.01097200 | 1.42524100 |
| H | 4.62197200 | -0.90115500 | 1.81019800 |
| H | 4.62213500 | 0.87271900 | 1.82467300 |
| H | 3.07565400 | -0.01372700 | 1.77700400 |
| Co | -1.84796700 | -0.00406400 | 0.21284700 |
| C | -2.97155700 | 1.11667900 | -1.14426100 |
| H | -2.69434000 | 2.11441400 | -1.46501100 |
| C | -3.84450600 | 0.80602000 | -0.04138500 |
| H | -4.31963600 | 1.52867800 | 0.61186000 |
| C | -3.11194700 | -1.17103700 | -0.97327400 |
| H | -2.95698700 | -2.23033300 | -1.14524100 |
| C | -3.94124000 | -0.60630900 | 0.05373800 |
| H | -4.49595100 | -1.16446000 | 0.79893300 |
| C | -2.54656700 | -0.10511100 | -1.75203500 |
| H | -1.90014600 | -0.20767500 | -2.61479000 |

**2Co-11**($C_s$) / M06-L

| | | | |
|---|---|---|---|
| C | -3.18449900 | 1.37349100 | -0.89471100 |
| C | -3.18636200 | -1.35721900 | -0.91692800 |
| C | -1.86955400 | -1.56171700 | -0.63818500 |
| C | -0.92090400 | -0.69524300 | 0.00088400 |
| C | -0.92044100 | 0.69223800 | 0.01240800 |
| C | -1.86744200 | 1.57072900 | -0.61235700 |
| C | 0.30638300 | 1.27505900 | 0.58554900 |
| C | 0.89218400 | 0.69288900 | 1.76843100 |
| C | 0.89238500 | -0.72644900 | 1.75634100 |
| C | 0.30589700 | -1.28852700 | 0.56389900 |
| H | -3.67326400 | 2.13438000 | -1.50178600 |
| H | -3.67645800 | -2.10678200 | -1.53693600 |
| H | -1.44600800 | -2.52062500 | -0.95154000 |
| H | -1.44194400 | 2.53400500 | -0.90947700 |
| H | 0.44381100 | 2.34670500 | 0.44367200 |
| H | 1.38597600 | 1.27408400 | 2.54017800 |
| H | 1.38523400 | -1.32095100 | 2.51854400 |
| H | 0.44241900 | -2.35777100 | 0.40423800 |
| P | -4.24238700 | 0.00423500 | -0.32948300 |
| C | -3.88144800 | -0.01008700 | 1.48230300 |
| H | -4.34346100 | 0.87000600 | 1.93680200 |
| H | -4.34482300 | -0.89623400 | 1.92343700 |
| H | -2.81685800 | -0.01271500 | 1.72784400 |
| Co | 1.83587600 | -0.00389000 | 0.19415300 |
| C | 3.02535100 | -1.15116800 | -0.99280200 |
| H | 2.82728200 | -2.19415100 | -1.20280600 |
| C | 3.83538600 | -0.66027700 | 0.08266500 |
| H | 4.34702100 | -1.26741000 | 0.81695400 |
| C | 2.96091700 | 1.13872200 | -1.06089600 |
| H | 2.70548300 | 2.15567900 | -1.32831200 |
| C | 3.79148000 | 0.75507300 | 0.04441400 |
| H | 4.26467000 | 1.43160600 | 0.74292200 |
| C | 2.50871200 | -0.03872600 | -1.73315300 |
| H | 1.87981900 | -0.08103300 | -2.61078600 |

**Table S50**. The total energies (E, in hartree), relative energies (ΔE, in kcal/mol), and the number of imaginary vibrational frequencies (Nimg) for the 1-methyl-1*H*-phosphanorcaradiene and 1-methyl-1*H*-phosphepine structures.

| | **1-1** ($C_s$, $^1A'$) | **1-2** ($C_s$, $^1A'$) | **1-3** ($C_s$, $^1A'$) | **1-4** ($C_s$, $^1A'$) |
|---|---|---|---|---|
| **B3LYP** | | | | |
| -E | 613.50318 | 613.50102 | 613.49776 | 613.49594 |
| ZPE | 87.2 | 87.0 | 86.3 | 86.7 |
| ΔE | 0.0 | 1.4 | 3.4 | 4.5 |
| Nimg | 0 | 0 | 0 | 0 |
| **BP86** | | | | |
| -E | 613.51715 | 613.51385 | 613.50666 | 613.50486 |
| ZPE | 84.6 | 84.4 | 83.6 | 84.1 |
| ΔE | 0.0 | 2.1 | 6.6 | 7.7 |
| Nimg | 0 | 0 | 0 | 0 |
| **M06-L** | | | | |
| -E | 613.45304 | 613.44776 | 613.43551 | 613.43416 |
| ZPE | 87.7 | 87.6 | 86.5 | 87.0 |
| ΔE | 0.0 | 3.3 | 11.0 | 11.8 |
| Nimg | 0 | 0 | 0 | 0 |

**Table S51.** The total energies (E, in hartree), relative energies (ΔE, in kcal/mol), and the number of imaginary vibrational frequencies (Nimg) for the $(C_6H_6PCH_3)Fe(CO)_3$ structures.

| | **1Fe-1** ($C_s$, $^1A'$) | **1Fe-2** ($C_1$, $^1A$) | **1Fe-3** ($C_1$, $^1A$) | **1Fe-4** ($C_s$, $^1A'$) | **1Fe-5** ($C_1$, $^1A$) | **1Fe-6** ($C_1$, $^1A$) | **1Fe-7** ($C_s$, $^1A'$) | **1Fe-8** ($C_s$, $^1A'$) |
|---|---|---|---|---|---|---|---|---|
| **B3LYP** | | | | | | | | |
| -E-2217 | 0.37868 | 0.37615 | 0.37624 | 0.37272 | 0.37426 | 0.37199 | 0.34968 | 0.34820 |
| ZPE | 104.5 | 103.9 | 104.2 | 104.8 | 103.4 | 104.1 | 103.4 | 103.5 |
| ΔE | 0.0 | 1.6 | 1.5 | 3.7 | 2.8 | 4.2 | 18.2 | 19.1 |
| Nimg | 0 | 0 | 0 | 0 | 0 | 0 | 1(17i) | 1(13i) |
| **BP86** | | | | | | | | |
| -E-2217 | 0.64735 | 0.64332 | 0.64122 | 0.64152 | 0.63925 | 0.63536 | 0.61565 | 0.61362 |
| ZPE | 101.6 | 101.0 | 101.2 | 101.9 | 100.6 | 101.1 | 100.6 | 100.7 |
| ΔE | 0.0 | 2.5 | 2.8 | 3.7 | 5.1 | 7.5 | 19.9 | 21.2 |
| Nimg | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| **M06-L** | | | | | | | | |
| -E-2217 | 0.26356 | 0.25359 | 0.25376 | 0.25953 | 0.24727 | 0.24711 | 0.22711 | 0.22463 |
| ZPE | 104.7 | 103.8 | 104.0 | 105.2 | 103.3 | 104.1 | 103.1 | 103.4 |
| ΔE | 0.0 | 6.3 | 6.1 | 2.5 | 10.2 | 10.3 | 22.9 | 24.4 |
| Nimg | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |

**Table S52**. The total energies (E, in hartree), relative energies (ΔE, in kcal/mol), and the number of imaginary vibrational frequencies (Nimg) for the $(C_6H_6PCH_3)Co(C_5H_5)$ structures.

| | **1Co-1** ($C_1$, $^1A$) | **1Co-2** ($C_s$, $^1A'$) | **1Co-3** ($C_s$, $^1A'$) | **1Co-4** ($C_1$, $^1A$) | **1Co-5** ($C_1$, $^1A$) | **1Co-6** ($C_s$, $^1A$) | **1Co-7** ($C_1$, $^1A$) | **1Co-8** ($C_s$, $^1A'$) |
|---|---|---|---|---|---|---|---|---|
| **B3LYP** | | | | | | | | |
| -(E+2189) | 0.89626 | 0.89414 | 0.88948 | 0.89234 | 0.88861 | 0.88849 | 0.88389 | 0.88263 |
| ZPE | 140.4 | 140.7 | 141.0 | 140.5 | 140.1 | 139.5 | 139.8 | 140.1 |
| ΔE | 0.0 | 1.3 | 4.3 | 2.5 | 4.8 | 4.9 | 7.8 | 8.6 |
| Nimg | 0 | 0 | 1(13i) | 0 | 0 | 0 | 0 | 0 |
| **BP86** | | | | | | | | |
| -(E+2190) | 0.14678 | 0.14787 | 0.14329 | 0.14143 | 0.14118 | 0.13698 | 0.13500 | 0.13377 |
| ZPE | 136.3 | 136.6 | 136.8 | 136.3 | 135.9 | 135.5 | 135.6 | 135.9 |
| ΔE | 0.0 | -0.7 | 2.2 | 3.4 | 3.5 | 6.1 | 7.4 | 8.2 |
| Nimg | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| **M06-L** | | | | | | | | |
| -(E+2189) | 0.77428 | 0.77857 | 0.77594 | 0.76739 | 0.76595 | 0.75912 | 0.76116 | 0.75955 |
| ZPE | 140.9 | 141.0 | 141.4 | 140.8 | 140.2 | 139.7 | 140.1 | 140.3 |
| ΔE | 0.0 | -2.7 | -1.0 | 4.3 | 5.2 | 9.5 | 8.2 | 9.2 |
| Nimg | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |

**Table S53**. The total energies (E, in hartree), relative energies (ΔE, in kcal/mol), and the number of imaginary vibrational frequencies (Nimg) for the 3-methyl-3H-benzo[*d*]phosphepine and 1-methyl-1H-naphtho[2,3-*b*]phosphirene structures.

| | **2-1** ($C_s$, $^1A'$) | **2-2** ($C_s$, $^1A'$) | **2-3** ($C_s$, $^1A'$) | **2-4** ($C_s$, $^1A'$) |
|---|---|---|---|---|
| **B3LYP** | | | | |
| -E | 767.16691 | 767.16360 | 767.14636 | 767.14259 |
| ZPE | 116.1 | 116.3 | 116.4 | 116.1 |
| ΔE | 0.0 | 2.1 | 12.9 | 15.3 |
| Nimg | 0 | 0 | 0 | 0 |
| **BP86** | | | | |
| -E | 767.17341 | 767.16977 | 767.16077 | 767.15591 |
| ZPE | 112.6 | 112.8 | 113.0 | 112.6 |
| ΔE | 0.0 | 2.3 | 7.9 | 11.0 |
| Nimg | 0 | 0 | 0 | 0 |

| | | | | |
|---|---|---|---|---|
| **M06-L** | | | | |
| -E | 767.08912 | 767.08618 | 767.08166 | 767.07450 |
| ZPE | 116.2 | 116.6 | 117.2 | 116.4 |
| ΔE | 0.0 | 1.8 | 4.7 | 9.2 |
| Nimg | 0 | 0 | 0 | 0 |

**Table S54.** The total energies (E, in hartree), relative energies (ΔE, in kcal/mol), and the number of imaginary vibrational frequencies (Nimg) for the $(C_{10}H_8PCH_3)Fe(CO)_3$ structures.

| | **2Fe-1** ($C_1$, $^1$A) | **2Fe-2** ($C_s$, $^1$A') | **2Fe-3** ($C_s$, $^1$A') | **2Fe-4** ($C_s$, $^1$A') | **2Fe-5** ($C_1$, $^1$A) | **2Fe-6** ($C_1$, $^1$A) | **2Fe-7** ($C_1$, $^1$A) |
|---|---|---|---|---|---|---|---|
| **B3LYP** | | | | | | | |
| -(E+2371) | 0.03919 | 0.02607 | 0.02630 | 0.02632 | 0.01856 | 0.01602 | 0.01488 |
| ZPE | 133.4 | 133.6 | 133.1 | 133.4 | 133.8 | 133.6 | 133.4 |
| ΔE | 0.0 | 8.2 | 8.1 | 8.1 | 12.9 | 14.5 | 15.3 |
| Nimg | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| **BP86** | | | | | | | |
| -(E+2371) | 0.30338 | 0.29343 | 0.29055 | 0.29001 | 0.28622 | 0.28491 | 0.28300 |
| ZPE | 129.6 | 129.9 | 129.5 | 129.7 | 130.0 | 129.8 | 129.6 |
| ΔE | 0.0 | 6.2 | 8.1 | 8.4 | 10.8 | 11.6 | 12.8 |
| Nimg | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| **M06-L** | | | | | | | |
| -(E+2370) | 0.90171 | 0.89765 | 0.88845 | 0.88829 | 0.89331 | 0.88868 | 0.88403 |
| ZPE | 133.3 | 133.9 | 132.9 | 133.2 | 134.4 | 133.7 | 133.9 |
| ΔE | 0.0 | 2.5 | 8.3 | 8.4 | 5.3 | 8.2 | 11.1 |
| Nimg | 0 | 0 | 0 | 0 | 0 | 0 | 0 |

| | **2Fe-8** ($C_1$, $^1$A) | **2Fe-9** ($C_1$, $^1$A) | **2Fe-10** ($C_1$, $^1$A) | **2Fe-11** ($C_1$, $^1$A) | **2Fe-12** ($C_s$, $^1$A') | **2Fe-13** ($C_s$, $^1$A') |
|---|---|---|---|---|---|---|
| **B3LYP** | | | | | | |
| -(E+2371) | 0.01423 | 0.00962 | 0.00599 | 0.00355 | -0.00349 | 0.00188 |
| ZPE | 133.0 | 132.9 | 133.2 | 132.4 | 133.3 | 132.8 |
| ΔE | 15.7 | 18.6 | 20.8 | 22.4 | 26.8 | 23.4 |
| Nimg | 0 | 0 | 0 | 0 | 0 | 0 |
| **BP86** | | | | | | |
| -(E+2371) | 0.27753 | 0.27149 | 0.27440 | 0.26604 | 0.26553 | 0.26428 |
| ZPE | 129.1 | 129.1 | 129.4 | 128.5 | 129.5 | 129.0 |
| ΔE | 16.2 | 20.0 | 18.2 | 23.4 | 24.3 | 24.5 |
| Nimg | 0 | 0 | 0 | 0 | 0 | 0 |

| **M06-L** | | | | | | |
|---|---|---|---|---|---|---|
| -(E+2370) | 0.87904 | 0.87158 | 0.87698 | 0.86314 | 0.87097 | 0.86229 |
| ZPE | 133.1 | 132.9 | 133.5 | 132.4 | 134.0 | 132.8 |
| ΔE | 14.2 | 18.9 | 15.5 | 24.2 | 19.3 | 24.7 |
| Nimg | 0 | 0 | 0 | 0 | 0 | 0 |

**Table S55.** The total energies (E, in hartree), relative energies (ΔE, in kcal/mol), and the number of imaginary vibrational frequencies (Nimg) for the $(C_{10}H_8PCH_3)Co(C_5H_5)$ structures.

| | **2Co-1** ($C_1$, $^1A$) | **2Co-2** ($C_1$, $^1A$) | **2Co-3** ($C_1$, $^1A$) | **2Co-4** ($C_s$, $^1A'$) | **2Co-5** ($C_1$, $^1A$) | **2Co-6** ($C_1$, $^1A$) | **2Co-7** ($C_1$, $^1A$) |
|---|---|---|---|---|---|---|---|
| **B3LYP** | | | | | | | |
| -(E+2343) | 0.56024 | 0.56027 | 0.55130 | 0.54088 | 0.53536 | 0.53496 | 0.53363 |
| ZPE | 169.6 | 169.9 | 169.7 | 169.9 | 169.9 | 170.1 | 169.8 |
| ΔE | 0.0 | 0.0 | 5.6 | 12.1 | 15.6 | 15.9 | 16.7 |
| Nimg | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| **BP86** | | | | | | | |
| -(E+2343) | 0.80980 | 0.80967 | 0.80009 | 0.79329 | 0.79001 | 0.78784 | 0.78750 |
| ZPE | 164.7 | 164.9 | 164.7 | 164.8 | 164.8 | 164.9 | 164.7 |
| ΔE | 0.0 | 0.1 | 6.1 | 10.4 | 12.4 | 13.8 | 14.0 |
| Nimg | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| M06-L | | | | | | | |
| -(E+2343) | 0.42201 | 0.42271 | 0.41351 | 0.41138 | 0.40787 | 0.40831 | 0.40280 |
| ZPE | 169.8 | 170.4 | 170.2 | 170.5 | 170.6 | 170.7 | 170.3 |
| ΔE | 0.0 | -0.4 | 5.3 | 6.7 | 8.9 | 8.6 | 12.1 |
| Nimg | 0 | 0 | 0 | 0 | 0 | 0 | 0 |

| | **2Co-8** ($C_1$, $^1A$) | **2Co-9** ($C_1$, $^1A$) | **2Co-10** ($C_1$, $^1A$) | **2Co-11** ($C_s$, $^1A'$) |
|---|---|---|---|---|
| **B3LYP** | | | | |
| -(E+2343) | 0.53620 | 0.53234 | 0.52340 | 0.52256 |
| ZPE | 169.4 | 169.4 | 168.7 | 169.2 |
| ΔE | 15.1 | 17.5 | 23.1 | 23.6 |
| Nimg | 0 | 0 | 0 | 0 |
| **BP86** | | | | |
| -(E+2343) | 0.78464 | 0.77934 | 0.77081 | 0.77017 |
| ZPE | 164.2 | 164.3 | 164.1 | 164.1 |
| ΔE | 16.2 | 19.1 | 24.5 | 24.9 |
| Nimg | 0 | 0 | 0 | 0 |
| **BP86** | | | | |
| -(E+2343) | 0.40009 | 0.39360 | 0.38218 | 0.38258 |
| ZPE | 169.7 | 169.6 | 168.9 | 169.5 |
| ΔE | 13.8 | 17.8 | 25.0 | 24.7 |
| Nimg | 0 | 0 | 0 | 0 |

**Table S56.** Harmonic ν(CO) vibrational frequencies (in $cm^{-1}$) predicted for the isomers of $(C_6H_6PCH_3)Fe(CO)_3$ by BP86 method. Infrared intensities (in km/mol) are in parentheses.

| | BP86 |
|---|---|
| **1Fe-1** | 1959(707), 1966(826), 2018(827) |
| **1Fe-2** | 1943(715), 1958(793), 2007(838) |
| **1Fe-3** | 1962(649), 1971(766), 2021(763) |
| **1Fe-4** | 1959(702), 1966(814), 2018(854) |
| **1Fe-5** | 1944(922), 1955(562), 2010(706) |
| **1Fe-6** | 1963(638), 1979(806), 2027(744) |
| **1Fe-7** | 1950(610), 1970(758), 2013(750) |
| **1Fe-8** | 1961(592), 1976(768), 2020(802) |

**Table S57.** Harmonic ν(CO) vibrational frequencies (in $cm^{-1}$) predicted for the isomers of $(C_{10}H_8PCH_3)Fe(CO)_3$ by BP86 method. Infrared intensities (in km/mol) are in parentheses.

| | BP86 |
|---|---|
| **2Fe-1** | 1940(697), 1955(788), 2003(825) |
| **2Fe-2** | 1961(656), 1963(719), 2017(906) |
| **2Fe-3** | 1950(603), 1971(756), 2013(849) |
| **2Fe-4** | 1961(585), 1978(754), 2020(918) |
| **2Fe-5** | 1961(648), 1964(710), 2016(937) |
| **2Fe-6** | 1961(674), 1974(789), 2021(990) |
| **2Fe-7** | 1959(673), 1972(792), 2019(1016) |
| **2Fe-8** | 1957(572), 1964(656), 2013(833) |
| **2Fe-9** | 1958(537), 1971(707), 2017(842) |
| **2Fe-10** | 1954(696), 1966(812), 2020(861) |
| **2Fe-11** | 1960(697), 1973(844), 2021(851) |
| **2Fe-12** | 1955(689), 1965(800), 2019(914) |
| **2Fe-13** | 1963(690), 1977(829), 2025(832) |

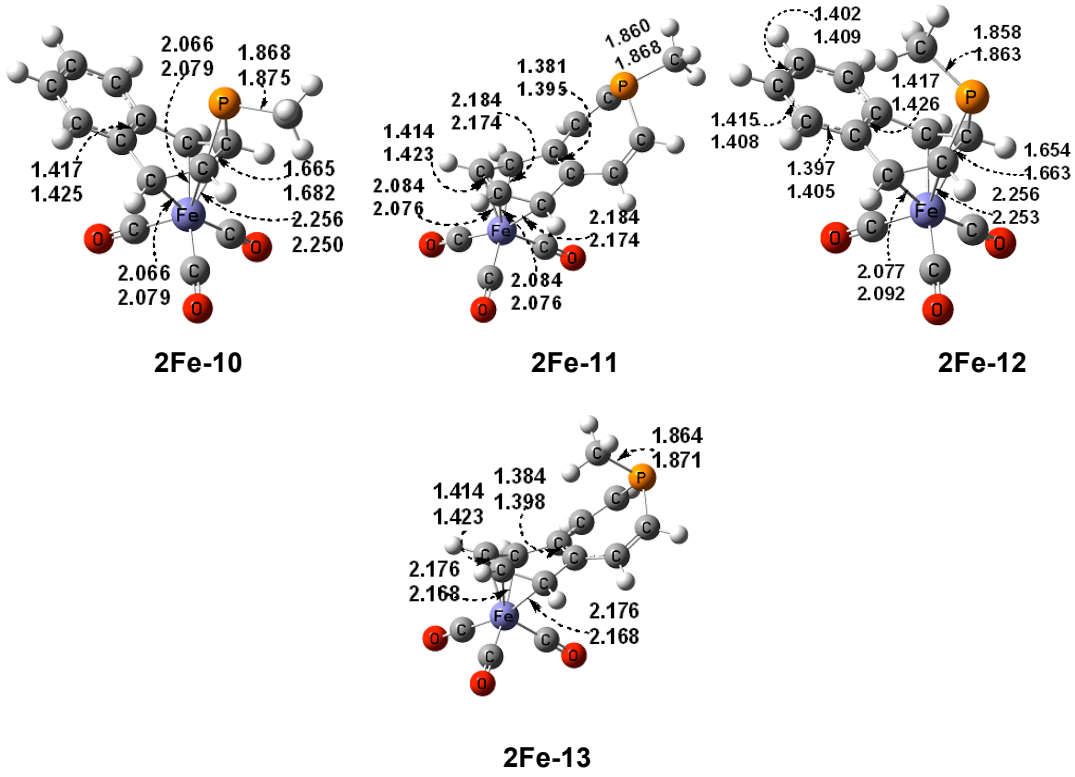


**Figure S1.** The four higher-lying $(C_{10}H_8PCH_3)Fe(CO)_3$ structures. Distances (in Å) are predicted by B3LYP (upper) and BP86 (lower).

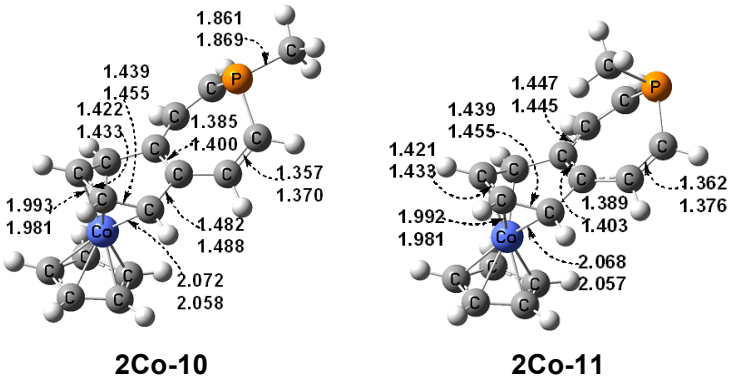


**Figure S2.** The two higher-lying $(C_{10}H_8PCH_3)Co(C_5H_5)$ structures. Distances (in Å) are predicted by B3LYP (upper) and BP86 (lower).

**Complete reference 41.**

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