Major Differences Between Trifluorophosphine and Carbonyl Ligands in Binuclear Cyclopentadienyliron Complexes

Shida Gong,[a] Qiong Luo,*[,a] Qian-shu Li,[a] Yaoming Xie,[b] R. Bruce King,*[,a,b] and Henry F. Schaefer III[b]

[a] MOE Key Laboratory of Theoretical Chemistry of Environment, Center for Computational Quantum Chemistry, South China Normal University, Guangzhou 510631, P. R. China
[b]Department of Chemistry and Center for Computational Chemistry, University of Georgia, Athens, Georgia 30602, USA

Supplementary Material

Figure S1-S4. The optimized geometries (distances in Å) and the relative energies (kcal/mol) of the $Cp_2Fe_2(PF_3)_n$ (n = 5, 4, 3, 2) structures by the B3LYP, the BP86, and the B3LYP* method.

Figure S5. The optimized geometries (distances in Å) and the relative energies (kcal/mol) of the $CpFe(PF_3)_n$ (n=2, 1) structures by the B3LYP, the BP86, and the B3LYP* method.

Tables S1-S2. Atomic population, NBO analysis, and Fe-Fe bonding for the singlet $Cp_2Fe_2(PF_3)_n$ (n = 5, 4, 3, 2) structures.

Table S3. Reaction energies (kcal/mol) for some reactions of $Cp_2Fe_2(PF_3)_n$ (n = 5, 4, 3, 2) derivatives by three methods.

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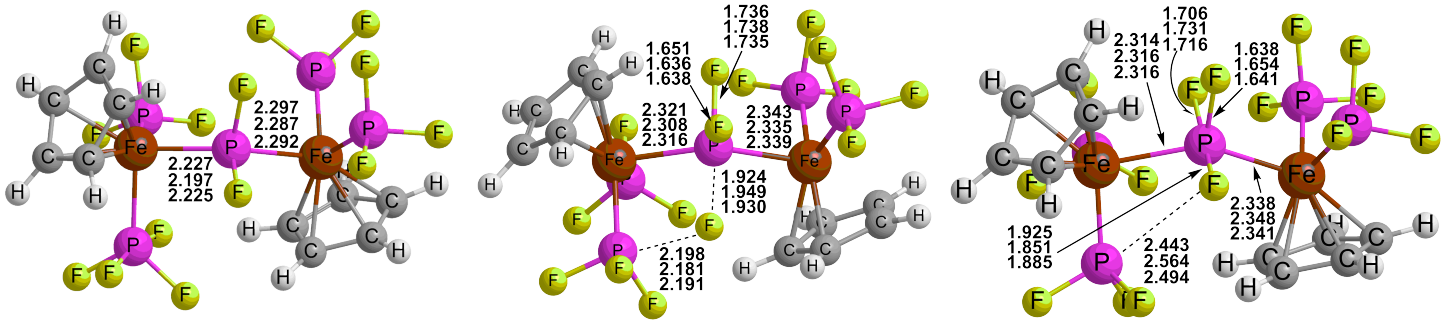
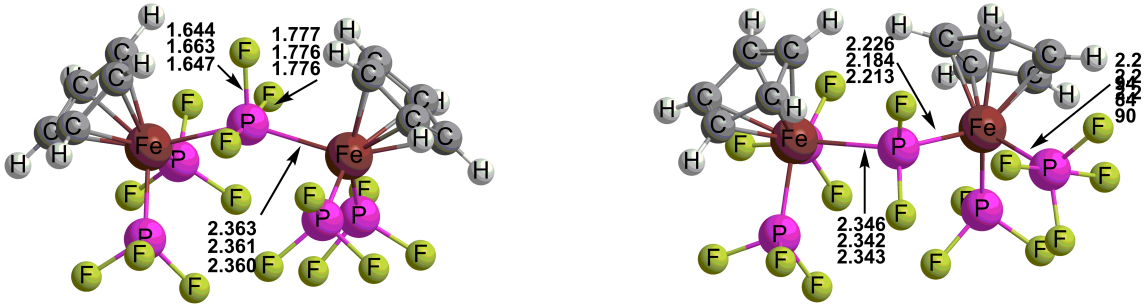
Table S17-S36. Cartesian coordinates and energies for the $Cp_2Fe_2(PF_3)_n$ (n = 5, 4, 3, 2) structures.

Table S37-S41. Cartesian coordinates and energies for the $CpFe(PF_3)_n$ (n = 2, 1) structures.

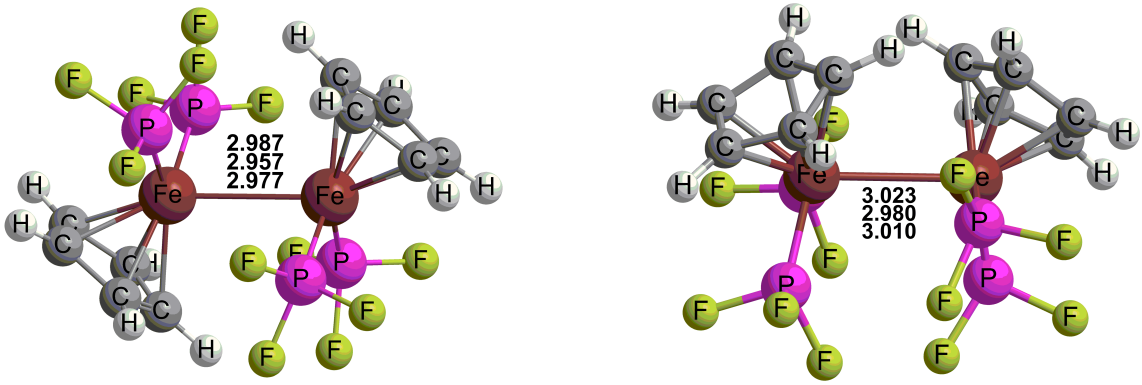


25-1S(C_1, 0.0, 0.0, 0.0) **TS_{mig}(C_1, 8.4, 5.1, 7.5)** **25-2S(C_1, 8.3, 4.7, 7.5)**



25-3S(C_2, 10.6, 7.4, 9.7) **25-4S(C_1, 12.9, 9.4, 12.1)**

Figure S1. The optimized geometries (distances in Å) and the relative energies (kcal/mol) of the $Cp_2Fe_2(PF_3)_5$ structures as well as the migration transition state structure between **25-1S** and **25-2S** by the B3LYP (top, former), the BP86 (middle, middle), and the B3LYP* (bottom, later) method.



24-1S(C_2, 0.0, 0.0, 0.0) **24-2S(C_2, 4.9, 5.0, 5.1)**

Figure S2. The optimized geometries (distances in Å) and the relative energies (kcal/mol) of the $Cp_2Fe_2(PF_3)_4$ structures by the B3LYP (top, former), the BP86 (middle, middle), and the B3LYP* (bottom, later) method.

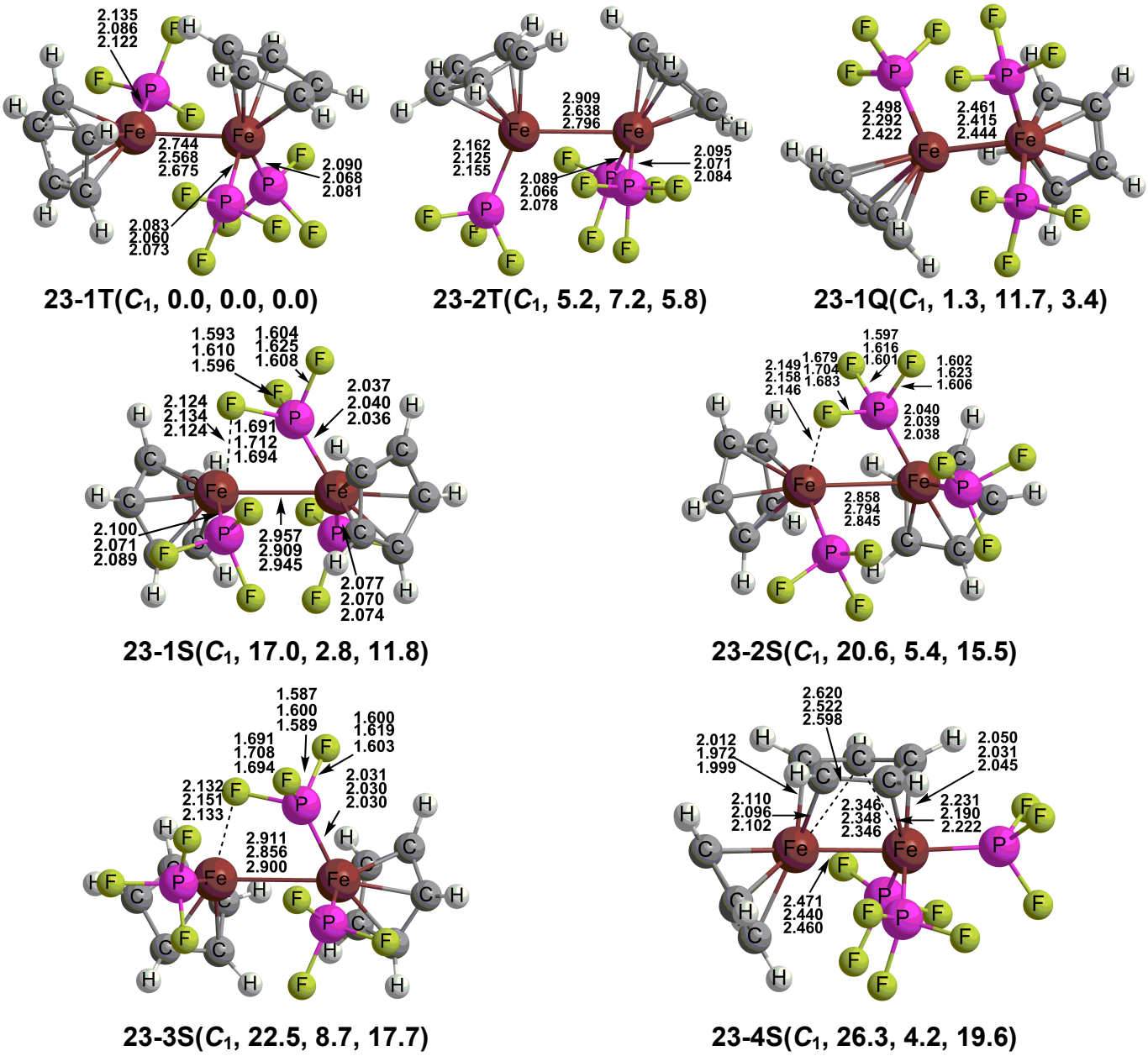


Figure S3. The optimized geometries (distances in Å) and the relative energies (kcal/mol) of the $Cp_2Fe_2(PF_3)_3$ structures by the B3LYP (top, former), the BP86 (middle, middle), and the B3LYP* (bottom, later) method.

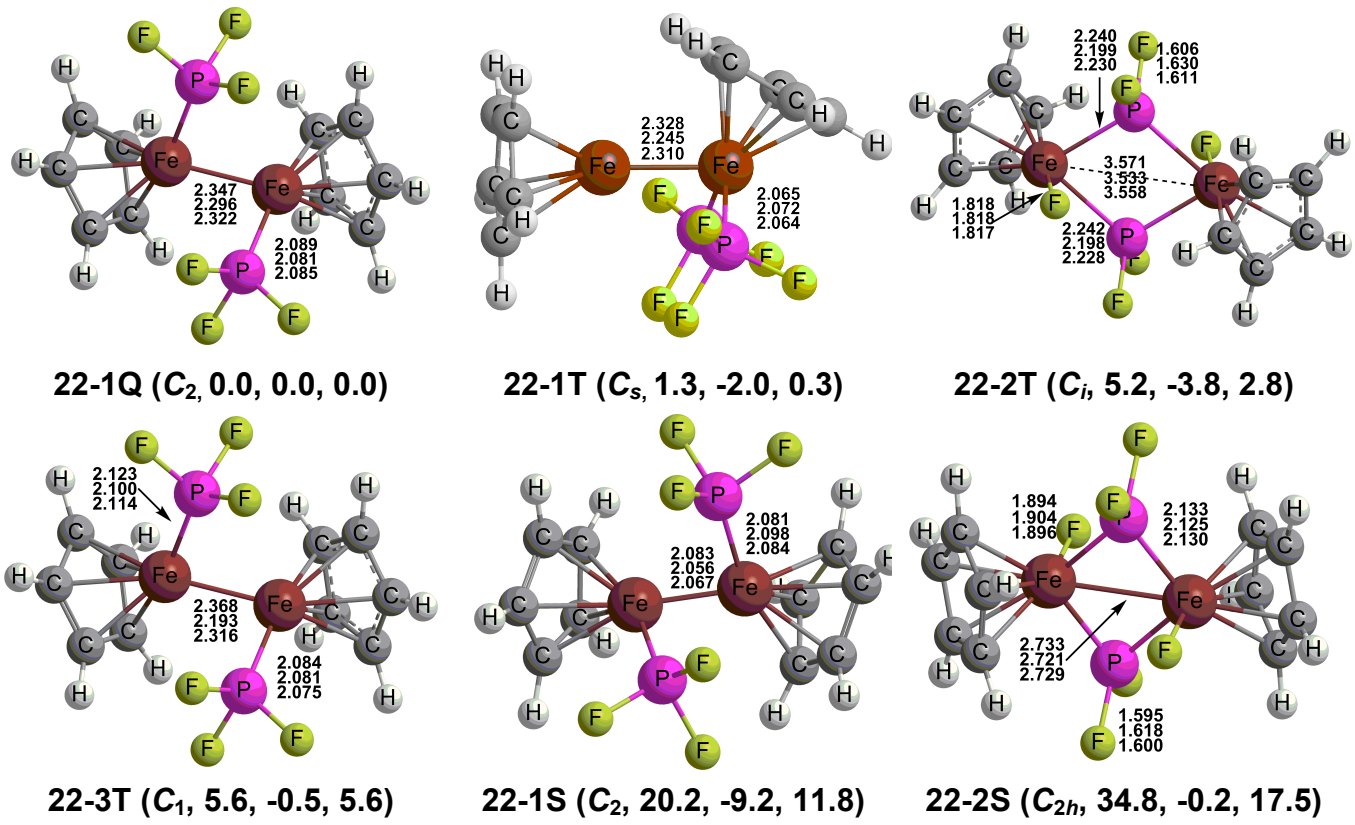


Figure S4. The optimized geometries (distances in Å) and the relative energies (kcal/mol) of the $Cp_2Fe_2(PF_3)_2$ structures by the B3LYP (top, former), the BP86 (middle, middle), and the B3LYP* (bottom, later) method.

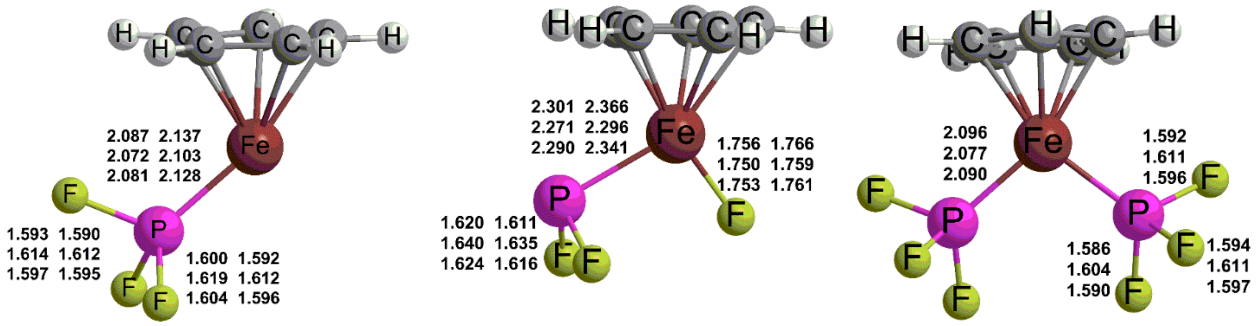


Figure S5. The optimized geometries (distances in Å) and the relative energies (kcal/mol) of the $CpFe(PF_3)_n$ (n = 2, 1) structures by the B3LYP (top, former), the BP86 (middle, middle), and the B3LYP* (bottom, later) method. For the bond distances in the same line, the left are for the doublet structures and the right are for quartet structures.

Table S1. Atomic population, NBO analysis, and iron–iron bonding for the singlet $Cp_2Fe_2(PF_3)_n$ (n =5, 4, 3, 2) structures by the B3LYP method.

Structures	Natural charge on Fe/Fe	Wiberg bond index	Fe-Fe distance (Å)	Formal Fe-Fe bond order
25-1S	-0.60/-0.52	0.03	4.240	0
25-2S	-0.57/-0.54	0.03	4.417	0
25-3S	-0.56/-0.56	0.03	4.560	0
25-4S	-0.60/-0.55	0.03	4.186	0
24-1S	-0.50/-0.50	0.37	2.987	1
24-2S	-0.50/-0.50	0.37	3.023	1
23-1T	0.46/-0.53	0.27	2.744	1
23-2T	0.46/-0.46	0.21	2.909	1
23-1Q	0.91/-0.79	0.31	2.461	1
23-1S	0.05/-0.56	0.32	2.957	1
23-2S	0.06/-0.58	0.32	2.858	1
23-3S	0.07/-0.57	0.34	2.911	1
23-4S	0.26/-0.83	0.37	2.471	2
22-1Q	0.24/0.24	0.49	2.347	2
22-1T	0.66/-0.71	0.46	2.310	2
22-2T	0.28/0.28	0.06	3.558	0
22-3T	0.39/-0.06	0.50	2.316	2
22-1S	-0.16/-0.16	1.01	2.083	3
22-2S	-0.02/-0.02	0.25	2.733	1

Table S2. Atomic population, NBO analysis, and iron–iron bonding for the singlet $Cp_2Fe_2(PF_3)_n$ (n=5, 4, 3, 2) structures by the BP86 method.

Structures	Natural charge on Fe/Fe	Wiberg bond index	Fe-Fe distance (Å)	Formal Fe-Fe bond order
25-1S	-0.74/-0.69	0.04	4.119	0
25-2S	-0.70/-0.69	0.03	4.414	0
25-3S	-0.69/-0.69	0.03	4.548	0
25-4S	-0.73/-0.70	0.04	4.134	0
24-1S	-0.59/-0.59	0.34	2.957	1
24-2S	-0.58/-0.58	0.35	2.980	1
23-1T	0.26/-0.69	0.39	2.568	1
23-2T	0.22/-0.66	0.38	2.638	1
23-1Q	0.62/-0.75	0.37	2.415	1
23-1S	-0.12/-0.60	0.32	2.909	1
23-2S	-0.11/-0.63	0.32	2.794	1
23-3S	-0.11/-0.60	0.34	2.856	1
23-4S	0.13/-0.86	0.40	2.440	2
22-1Q	0.12/0.12	0.53	2.296	2
22-1T	0.66/-0.71	0.46	2.310	2
22-2T	0.28/0.28	0.06	3.558	0
22-3T	0.39/-0.06	0.50	2.316	2
22-1S	-0.24/-0.24	1.04	2.056	3
22-2S	-0.13/-0.13	0.26	2.721	1

Table S3. SCF reaction energies (ΔE, 0K, kcal/mol) and reaction Gibbs free energies (ΔG,298.15K, kcal/mol) for some reactions of $Cp_2Fe_2(PF_3)_n$ (n = 5, 4, 3, 2) derivatives by three methods. These energies of each compound are based on their singlet or doublet global minima.

Reaction	B3LYP		BP86		B3LYP*	
	ΔE	ΔG	ΔE	ΔG	ΔE	ΔG
$Cp_2Fe_2(PF_3)_5 \rightarrow Cp_2Fe_2(PF_3)_4 + PF_3$	24.1	12.6	19.9	7.1	23.1	11.1
$Cp_2Fe_2(PF3)_4 \rightarrow Cp_2Fe_2(PF_3)_3 + PF_3$	27.5	10.4	35.6	19.3	30.3	13.4
$Cp_2Fe_2(PF3)_3 \rightarrow Cp_2Fe_2(PF_3)_2 + PF_3$	22.7	6.9	16.1	0.4	21.6	5.9
$Cp_2Fe_2(PF_3)_4 \rightarrow 2CpFe(PF_3)_2$	0.8	-21.8	18.9	-3.3	7.3	-15.3
$Cp_2Fe_2(PF_3)_3 \rightarrow CpFe(PF_3) + CpFe(PF_3)_2$	17.2	-3.3	34.5	13.8	23.5	3.2
$Cp_2Fe_2(PF_3)_2 \rightarrow 2CpFe(PF_3)$	38.4	18.6	69.4	49.8	48.4	29.2
$2Cp_2Fe_2(PF_3)_4 \rightarrow Cp_2Fe_2(PF_3)_5 + Cp_2Fe_2(PF_3)_3$	3.4	-2.2	15.7	12.2	7.3	2.3
$2Cp_2Fe_2(PF_3)_3 \rightarrow Cp_2Fe_2(PF_3)_4 + Cp_2Fe_2(PF_3)_2$	-4.9	-3.5	-19.4	-18.9	-8.7	-7.5
$2CpFe(PF_3)_2H \rightarrow Cp_2Fe_2(PF_3)_4 + H_2$	21.8	31.7	18.0	29.2	19.8	26.5
$2CpFe(CO)_2H \rightarrow Cp_2Fe_2(CO)_4 + H_2$	2.6	6.0	-7.2	-3.6	0.0	3.4
$Fe(PF_3)_3 + C_5H_6 \rightarrow C_5H_6Fe(PF_3)_3 + 2PF_3$	0.6	-11.7	0.9	-11.1	1.2	-10.8
$C_5H_6Fe(PF_3)_3 \rightarrow CpFe(PF_3)_2H + PF_3$	6.3	-9.4	15.2	-1.4	8.8	-5.5

Table S4. Harmonic vibrational frequencies (cm^{-1}) and corresponding infrared intensities (km/mol, in parentheses) predicted for the $Cp_2Fe_2(PF_3)_5$ structures by the B3LYP method.

Structures	Frequencies
25-1S	22(0), 27(1), 36(0), 43(0), 47(0), 55(0), 63(0), 66(1), 72(0), 79(0), 82(0), 86(0), 95(0), 113(3), 114(1), 124(1), 128(0), 141(1), 149(0), 165(0), 177(4), 181(1), 191(1), 201(4), 206(3), 209(1), 212(4), 217(2), 225(4), 230(4), 240(1), 257(0), 277(2), 281(0), 294(1), 305(2), 351(4), 354(8), 356(1), 365(4), 368(4), 374(9), 375(9), 386(2), 394(1), 418(20), 419(12), 427(5), 437(4), 445(5), 448(115), 462(97), 474(54), 500(4), 503(83), 505(160), 512(108), 521(64), 590(1), 594(1), 596(2), 598(0), 690(190), 722(71), 756(95), 799(250), 826(95), 839(84), 842(83), 842(11), 844(101), 845(99), 848(186), 849(72), 852(75), 853(138), 861(5), 869(311), 870(304), 872(346), 879(127), 884(1), 892(56), 895(192), 911(277), 921(1), 944(0), 970(2), 974(2), 986(2), 1017(15), 1021(12), 1031(6), 1034(8), 1072(1), 1074(0), 1083(0), 1099(2), 1143(1), 1144(1), 1277(0), 1282(0), 1405(1), 1405(1), 1408(1), 1410(1), 1459(8), 1461(4), 1466(10), 1466(7), 3240(0), 3242(0), 3252(1), 3260(0), 3264(1), 3265(7), 3272(36), 3274(1), 3281(27), 3291(3)
25-2S	23(0), 30(4), 34(0), 37(0), 43(0), 51(0), 61(0), 65(0), 68(0), 80(1), 82(1), 91(0), 94(0), 98(1), 112(2), 118(0), 129(4), 137(6), 143(1), 155(1), 162(25), 183(1), 197(0), 200(0), 204(8), 210(2), 212(14), 219(7), 228(6), 232(25), 250(6), 251(1), 275(4), 280(3), 294(2), 302(5), 304(16), 339(6), 355(1), 357(4), 367(23), 369(5), 373(5), 380(3), 384(8), 393(5), 406(8), 408(9), 417(13), 423(4), 436(12), 438(23), 447(3), 472(221), 501(28), 504(187), 510(117), 518(83), 593(20), 594(4), 596(5), 598(10), 603(89), 754(79), 811(233), 822(107), 834(296), 838(80), 838(98), 840(38), 843(2), 845(63), 847(136), 852(67), 856(94), 859(251), 863(71), 864(38), 867(279), 875(85), 878(329), 884(43), 888(31), 895(222), 898(44), 916(403), 944(4), 949(2), 962(1), 968(2), 1014(14), 1018(12), 1031(8), 1035(8), 1072(0), 1074(0), 1079(1), 1088(1), 1140(1), 1142(1), 1275(0), 1281(0), 1404(1), 1405(1), 1405(1), 1407(1), 1454(4), 1460(5), 1467(7), 1467(7), 3242(0), 3243(0), 3246(0), 3246(0), 3265(1), 3268(1), 3272(2), 3277(1), 3285(3), 3288(2)
TS_{mig}	132*i*, 28(1), 36(0), 42(0), 49(1), 54(0), 60(0), 64(0), 68(0), 72(0), 81(0), 88(1), 99(2), 103(0), 119(1), 126(1), 133(2), 138(4), 147(1), 158(1), 182(10), 185(1), 194(0), 199(1), 203(1), 212(1), 218(19), 220(1), 225(5), 239(2), 258(7), 266(4), 279(2), 281(1), 292(2), 304(3), 328(6), 343(2), 357(7), 360(2), 364(11), 367(1), 372(12), 377(7), 393(3), 403(10), 408(2), 414(2), 429(25), 434(21), 438(13), 443(7), 450(31), 468(185), 502(61), 505(181), 510(64), 517(92), 562(138), 594(1), 595(2), 600(1), 601(1), 757(80), 785(190), 830(67), 837(174), 838(417), 842(71), 843(76), 844(3), 845(52), 848(35), 851(98), 861(118), 863(266), 866(26), 871(168), 872(125), 874(364), 879(188), 882(76), 887(18), 897(62), 900(24), 912(375), 952(0), 963(5), 966(1), 967(1), 1014(14), 1019(15), 1033(6), 1033(8), 1074(0), 1075(0), 1078(0), 1084(1), 1141(1), 1143(1), 1275(0), 1276(0), 1404(1), 1406(2), 1408(1), 1408(1), 1454(4), 1456(5), 1467(9), 1470(6), 3241(0), 3241(0), 3251(0), 3253(0), 3267(1), 3269(2), 3273(1), 3286(3), 3288(2), 3316(3)
25-3S	28(0), 32(1), 39(0), 44(0), 53(0), 55(0), 57(0), 65(0), 65(1), 69(0), 79(0), 85(0), 86(0), 97(1), 115(1), 115(1), 125(0), 134(0), 145(0), 166(1), 166(0), 187(0), 199(2), 202(0), 206(17), 214(0), 215(4), 217(2), 227(30), 238(1), 246(0), 250(0), 280(1), 281(1), 301(1), 303(5), 348(2), 351(1), 352(1), 358(28), 367(5), 371(11), 373(0), 375(7), 379(7), 399(7), 406(1), 417(1), 424(9), 429(2), 434(94), 438(10), 449(0), 455(172), 501(3), 505(145), 515(11), 520(165), 547(232), 594(3), 594(0), 599(1), 599(1), 740(123), 829(2), 831(183), 840(407), 841(3), 843(11), 843(4), 847(238), 847(3), 852(112), 858(31), 862(155), 864(24), 865(369), 868(138), 870(12), 875(375), 876(10), 889(55), 893(26), 894(39), 897(203), 918(526), 950(7), 951(0), 962(4), 962(1), 1017(17), 1018(10), 1031(1), 1031(16), 1073(0), 1073(0), 1079(2), 1082(0), 1142(2), 1142(0), 1276(0), 1276(0), 1404(1), 1405(0),

	1407(1), 1407(2), 1455(6), 1455(2), 1468(12), 1468(2), 3241(0), 3241(0), 3248(0), 3248(0), 3264(1), 3264(1), 3275(1), 3275(2), 3292(3), 3292(3)
25-4S	14(0), 27(0), 39(0), 52(0), 53(0), 57(0), 67(0), 69(0), 72(0), 78(0), 83(0), 90(0), 94(1), 100(0), 113(1), 121(1), 130(0), 147(1), 154(0), 167(2), 173(2), 177(0), 194(10), 197(2), 201(1), 208(1), 215(2), 219(2), 225(0), 243(1), 252(1), 261(2), 270(1), 282(0), 297(2), 304(3), 348(7), 354(0), 360(8), 362(9), 371(0), 372(3), 378(7), 380(2), 398(7), 408(2), 429(29), 435(250), 439(15), 441(15), 450(14), 455(0), 493(75), 505(108), 511(22), 513(35), 519(161), 552(29), 592(2), 595(0), 596(1), 598(2), 723(118), 774(168), 782(50), 805(485), 833(7), 840(118), 840(10), 843(23), 845(10), 845(184), 847(91), 849(7), 855(125), 857(141), 862(196), 871(88), 879(92), 880(184), 881(93), 885(43), 890(31), 896(493), 904(15), 923(436), 946(9), 960(4), 969(1), 976(2), 1018(21), 1021(5), 1030(7), 1035(8), 1075(0), 1078(0), 1080(0), 1081(2), 1142(1), 1142(1), 1275(0), 1279(0), 1404(0), 1406(1), 1408(2), 1408(2), 1455(6), 1456(1), 1465(8), 1471(7), 3242(0), 3244(0), 3252(4), 3257(0), 3265(0), 3267(3), 3273(2), 3277(2), 3283(3), 3284(2)

Table S5. Harmonic vibrational frequencies (cm^{-1}) and corresponding infrared intensities (km/mol, in parentheses) predicted for the $Cp_2Fe_2(PF_3)_5$ structures by the BP86 method.

Structures	Frequencies
25-1S	20(1), 27(0), 35(0), 41(0), 47(0), 63(1), 66(0), 71(1), 78(0), 87(0), 98(0), 100(1), 103(0), 111(0), 123(0), 131(1), 140(1), 145(0), 158(0), 167(2), 172(1), 180(3), 197(1), 199(3), 207(2), 214(1), 222(3), 227(5), 233(2), 243(4), 246(0), 259(1), 283(2), 286(0), 305(4), 309(4), 343(1), 348(8), 353(2), 357(2), 361(1), 365(9), 367(5), 383(5), 399(2), 414(4), 427(8), 433(111), 439(23), 443(13), 448(125), 462(95), 475(44), 488(2), 504(122), 507(64), 511(67), 521(41), 569(3), 572(1), 572(0), 576(2), 688(66), 700(128), 743(35), 763(367), 774(83), 799(167), 802(107), 808(93), 810(12), 812(214), 813(105), 816(45), 821(177), 823(146), 825(62), 831(373), 833(66), 842(145), 849(144), 852(24), 855(29), 860(178), 868(187), 881(2), 904(0), 919(0), 933(1), 941(1), 982(14), 987(10), 1001(8), 1009(10), 1040(0), 1047(0), 1047(1), 1054(1), 1109(1), 1110(0), 1224(0), 1230(0), 1365(1), 1365(1), 1367(1), 1370(0), 1399(7), 1403(6), 1414(8), 1421(11), 3170(0), 3175(0), 3178(2), 3186(3), 3186(0), 3195(2), 3196(3), 3197(1), 3207(1), 3217(3)
25-2S	23(0), 29(0), 38(0), 41(0), 54(0), 57(0), 60(0), 67(0), 69(0), 75(0), 81(0), 89(0), 95(0), 99(0), 108(0), 120(0), 131(0), 141(1), 148(1), 158(3), 177(3), 183(9), 201(1), 205(2), 207(2), 212(14), 216(2), 219(2), 226(2), 231(18), 250(0), 253(3), 281(2), 284(4), 302(5), 307(7), 325(6), 340(9), 345(2), 349(3), 356(14), 357(14), 359(3), 366(4), 370(6), 394(1), 410(6), 413(1), 416(69), 422(11), 434(24), 442(61), 447(48), 459(124), 496(28), 499(135), 505(99), 511(63), 564(20), 569(7), 570(9), 573(29), 576(66), 716(76), 782(128), 784(92), 795(366), 795(185), 799(172), 805(54), 810(27), 812(136), 813(18), 814(43), 817(27), 818(49), 824(161), 827(97), 832(110), 835(121), 840(388), 844(94), 853(62), 857(3), 863(123), 876(407), 903(4), 904(1), 925(0), 932(2), 984(13), 987(10), 999(8), 1001(7), 1040(0), 1041(0), 1047(1), 1054(2), 1108(1), 1110(2), 1224(0), 1229(0), 1364(1), 1366(1), 1366(1), 1367(1), 1400(6), 1406(6), 1412(10), 1416(8), 3169(0), 3170(0), 3172(0), 3173(0), 3192(1), 3195(1), 3197(2), 3203(1), 3210(3), 3213(5)
TS_{mig}	138*i*, 30(1), 39(0), 45(0), 49(1), 54(1), 61(1), 64(0), 68(1), 73(0), 82(0), 88(0), 100(1), 108(0), 119(1), 127(1), 134(1), 138(2), 149(2), 160(0), 184(4), 187(3), 196(0), 204(2), 208(1), 211(2), 215(10), 223(3), 227(6), 240(2), 260(2), 269(3), 284(4), 284(3), 295(3), 310(6), 326(8), 337(2), 348(4), 351(5), 355(10), 355(5), 361(11), 366(4), 384(3), 398(1), 406(2), 413(16), 425(31), 431(67), 438(3), 443(120), 449(48), 460(48), 493(69), 500(119), 505(57), 511(78), 562(102), 569(16), 569(1), 575(1), 576(3), 721(69), 746(169), 787(79), 795(176), 798(493), 804(47), 805(72), 811(15), 812(27), 814(9), 816(61), 824(375), 829(118), 831(44), 835(63), 836(225), 838(130), 840(174), 846(129), 852(8), 861(28), 869(89), 876(285), 916(0), 921(4), 925(1), 929(0), 983(13), 988(13), 1000(1), 1000(14), 1043(1), 1043(0), 1046(0), 1049(1), 1109(2), 1111(1), 1223(0), 1224(0), 1365(1), 1367(2), 1368(0), 1369(0), 1401(5), 1402(6), 1415(11), 1417(8), 3167(0), 3168(0), 3178(0), 3181(0), 3194(1), 3196(2), 3199(1), 3211(2), 3211(2), 3232(6)
25-3S	22(0), 31(0), 40(1), 46(0), 54(0), 57(0), 62(0), 65(0), 66(0), 71(0), 75(0), 83(0), 84(0), 99(0), 116(1), 118(1), 123(1), 137(0), 148(0), 165(0), 169(1), 195(0), 202(3), 205(0), 209(10), 212(4), 213(0), 221(4), 226(15), 235(1), 247(1), 253(1), 285(3), 286(4), 307(2), 309(10), 337(1), 339(1), 345(2), 350(30), 356(2), 358(9), 360(0), 366(7), 368(5), 396(5), 411(1), 411(22), 418(123), 431(4), 432(113), 436(3), 444(80), 450(0), 498(1), 500(124), 508(9), 512(127), 556(164), 570(7), 570(0), 573(1), 573(1), 697(117), 788(5), 789(178), 801(608), 803(10), 810(68), 812(18), 813(8), 814(34), 814(97), 822(207), 824(330), 827(74), 831(12), 833(8), 834(14), 836(39), 839(142), 853(87), 855(192), 860(8), 863(57), 882(557), 907(7), 908(0), 929(2), 929(0), 988(15), 988(9), 998(2), 998(16), 1042(1), 1042(0), 1046(2), 1049(0), 1110(3), 1110(0), 1224(0), 1224(0), 1365(0), 1366(1), 1369(1), 1369(1), 1402(9), 1402(2), 1414(13), 1414(3), 3168(0), 3168(0), 3173(0), 3173(0), 3193(1), 3193(1), 3201(1), 3202(2), 3214(2), 3215(2)
25-4S	17(0), 25(0), 37(0), 47(0), 52(0), 57(0), 66(0), 70(0), 76(0), 83(0), 89(0), 92(0), 95(0), 102(0), 113(0), 124(1), 131(0), 152(0), 158(0), 168(2), 171(3), 181(1), 196(7), 200(0), 205(1), 212(3), 216(1), 220(3), 228(2), 244(0), 255(1), 261(1),

	270(1), 285(1), 304(5), 310(4), 339(2), 344(2), 351(14), 354(7), 358(1), 363(5), 368(3), 378(5), 395(6), 408(3), 429(222), 430(66), 437(13), 445(69), 449(23), 452(12), 474(55), 494(3), 500(105), 507(30), 513(121), 541(25), 566(3), 567(1), 571(1), 572(2), 699(29), 733(161), 743(87), 761(462), 788(5), 801(39), 801(400), 809(16), 811(103), 811(3), 812(2), 820(237), 821(6), 824(51), 831(33), 836(65), 842(234), 845(58), 846(13), 848(88), 856(16), 857(395), 870(3), 887(469), 902(20), 918(4), 936(0), 937(1), 988(18), 992(5), 998(7), 1000(7), 1043(0), 1046(1), 1047(0), 1052(2), 1109(2), 1110(1), 1223(0), 1229(0), 1364(0), 1366(0), 1368(2), 1370(1), 1401(8), 1403(2), 1414(11), 1416(7), 3168(0), 3170(0), 3175(5), 3185(0), 3191(0), 3195(3), 3199(2), 3202(4), 3208(1), 3210(2)

Table S6. Harmonic vibrational frequencies (cm^{-1}) and corresponding infrared intensities (km/mol, in parentheses) predicted for the $Cp_2Fe_2(PF_3)_5$ structures by the B3LYP* method.

Structures	Frequencies
25-1S	12(0), 27(1), 38(0), 47(0), 52(0), 54(0), 59(0), 69(0), 74(1), 79(0), 85(1), 91(0), 104(0), 114(2), 123(1), 129(2), 143(0), 150(1), 157(0), 165(0), 180(5), 184(1), 193(2), 203(4), 210(3), 213(2), 217(3), 222(2), 230(0), 232(6), 244(1), 262(0), 280(2), 287(0), 300(0), 301(4), 351(3), 353(1), 358(3), 363(13), 367(4), 373(6), 374(6), 386(1), 391(15), 419(5), 423(20), 430(3), 434(10), 442(1), 451(132), 460(60), 471(68), 496(7), 501(124), 505(120), 513(113), 518(60), 589(2), 590(3), 592(1), 594(1), 685(191), 721(78), 754(77), 790(265), 818(107), 828(203), 832(74), 835(64), 836(105), 838(7), 839(8), 841(54), 844(27), 849(217), 860(93), 861(566), 863(16), 867(257), 874(206), 879(0), 889(298), 891(149), 902(51), 928(12), 941(0), 962(1), 966(3), 986(1), 1010(15), 1015(10), 1024(8), 1029(6), 1065(0), 1069(1), 1076(0), 1094(5), 1136(2), 1137(1), 1263(0), 1274(0), 1395(1), 1395(1), 1400(1), 1402(0), 1448(11), 1449(7), 1453(6), 1455(9), 3223(0), 3223(0), 3236(1), 3242(0), 3246(28), 3246(1), 3251(19), 3255(1), 3265(15), 3274(3)
25-2S	24(0), 31(0), 35(0), 43(0), 47(1), 53(0), 61(0), 66(1), 69(0), 79(1), 81(1), 90(0), 94(0), 99(1), 112(1), 119(0), 130(1), 140(2), 144(2), 156(3), 171(17), 182(2), 200(0), 203(1), 204(6), 213(13), 213(2), 220(5), 227(3), 232(27), 251(3), 252(2), 277(2), 282(2), 298(3), 304(6), 316(11), 342(7), 352(1), 355(4), 364(21), 366(6), 369(5), 376(3), 380(7), 396(4), 408(7), 410(10), 419(14), 424(8), 436(17), 440(29), 448(7), 468(219), 499(32), 503(174), 509(114), 517(79), 584(67), 588(11), 589(7), 591(25), 594(25), 745(80), 808(202), 814(88), 825(364), 829(62), 829(141), 832(47), 837(1), 837(56), 839(100), 844(67), 846(101), 849(120), 851(128), 855(57), 859(255), 866(108), 870(377), 876(45), 881(18), 886(91), 889(144), 906(405), 934(4), 939(1), 953(1), 959(3), 1007(14), 1010(12), 1022(8), 1026(8), 1064(0), 1065(0), 1071(1), 1080(2), 1132(1), 1134(1), 1263(0), 1268(0), 1394(1), 1395(1), 1395(1), 1397(1), 1440(5), 1447(5), 1453(8), 1454(7), 3222(0), 3224(0), 3226(0), 3227(0), 3245(2), 3248(2), 3252(2), 3259(2), 3265(3), 3269(4)
TS_{mig}	135*i*, 28(1), 37(0), 43(0), 49(0), 54(1), 60(0), 64(0), 68(0), 72(0), 82(0), 89(1), 100(2), 105(0), 119(1), 126(1), 133(2), 138(3), 148(1), 158(0), 183(9), 186(0), 196(0), 201(2), 205(1), 212(1), 218(16), 222(2), 226(6), 240(2), 259(5), 268(4), 281(3), 283(1), 293(2), 306(3), 327(6), 342(2), 355(8), 357(1), 362(12), 364(1), 369(12), 374(5), 391(3), 404(7), 408(1), 413(4), 430(35), 433(18), 438(11), 445(15), 451(54), 466(161), 499(66), 504(168), 509(60), 516(90), 564(132), 588(3), 588(1), 594(1), 595(1), 750(77), 776(185), 820(79), 827(172), 829(469), 834(60), 835(76), 837(6), 837(4), 840(30), 843(96), 853(175), 855(250), 858(18), 863(180), 864(65), 866(332), 870(204), 873(96), 880(8), 889(53), 894(32), 904(360), 944(0), 954(5), 956(1), 958(1), 1006(14), 1011(14), 1024(6), 1024(9), 1066(0), 1066(0), 1070(0), 1075(1), 1134(1), 1135(1), 1263(0), 1263(0), 1394(1), 1396(2), 1398(1), 1399(1), 1441(4), 1442(6), 1454(9), 1457(7), 3221(0), 3221(0), 3231(0), 3234(0), 3247(1), 3249(2), 3253(1), 3266(3), 3267(2), 3295(4)
25-3S	27(0), 33(1), 39(0), 45(0), 53(0), 56(0), 57(0), 65(0), 66(1), 69(0), 78(0), 85(0), 86(0), 98(1), 115(1), 116(1), 125(1), 135(0), 145(0), 166(0), 167(1), 189(0), 201(2), 204(0), 207(16), 214(0), 215(3), 219(3), 228(26), 237(1), 247(0), 252(1), 282(2), 283(1), 304(1), 305(6), 347(1), 348(1), 350(1), 356(28), 365(4), 368(10), 371(0), 373(7), 376(6), 399(3), 408(1), 417(1), 425(23), 430(3), 434(114), 437(8), 450(0), 452(159), 500(2), 504(141), 514(11), 518(156), 550(217), 588(4), 588(0), 593(1), 593(1), 731(122), 820(2), 821(181), 832(497), 833(6), 836(7), 836(5), 839(1), 839(158), 843(124), 850(34), 854(165), 855(403), 857(14), 860(80), 862(12), 867(320), 867(14), 881(69), 884(63), 886(28), 889(169), 910(532), 940(7), 941(0), 954(4), 954(1), 1010(17), 1010(10), 1023(1), 1023(16), 1065(0), 1065(0), 1071(2), 1074(0), 1134(2), 1134(0), 1264(0), 1264(0), 1394(0), 1395(0), 1397(1), 1397(2),

	1442(7), 1442(2), 1454(13), 1454(2), 3222(0), 3222(0), 3228(0), 3228(0), 3244(2), 3244(1), 3255(1), 3255(2), 3271(3), 3271(3)
25-4S	13(0), 28(0), 40(0), 52(0), 54(0), 57(0), 68(0), 70(0), 74(0), 79(0), 83(0), 91(0), 95(1), 101(0), 113(0), 122(1), 131(0), 148(0), 156(0), 168(2), 174(2), 177(0), 194(10), 198(2), 202(1), 211(2), 216(1), 220(2), 226(0), 244(1), 254(0), 262(1), 271(1), 283(0), 300(2), 306(3), 346(6), 350(0), 358(10), 360(8), 369(0), 370(4), 376(6), 379(1), 398(6), 408(1), 429(42), 436(278), 440(2), 443(14), 450(10), 452(2), 489(74), 503(100), 508(22), 512(39), 518(152), 550(28), 587(3), 589(0), 590(1), 592(1), 719(93), 765(179), 773(47), 796(480), 824(6), 830(174), 833(41), 836(104), 837(69), 837(13), 839(8), 844(65), 847(132), 849(155), 854(164), 863(84), 871(68), 872(244), 873(39), 877(21), 882(23), 887(487), 895(10), 915(448), 936(12), 950(4), 961(0), 967(2), 1011(20), 1013(5), 1022(7), 1026(8), 1066(0), 1069(0), 1072(0), 1074(2), 1134(1), 1134(1), 1262(0), 1267(0), 1395(0), 1396(0), 1398(3), 1398(1), 1441(7), 1443(1), 1452(8), 1457(7), 3222(0), 3224(0), 3232(4), 3238(0), 3246(0), 3247(3), 3253(2), 3258(2), 3263(3), 3263(2)

Table S7. Harmonic vibrational frequencies (cm^{-1}) and corresponding infrared intensities (km/mol, in parentheses) predicted for the $Cp_2Fe_2(PF_3)_4$ structures by the B3LYP method.

Structures	Frequencies
24-1S	12*i*, 27(0), 46(0), 52(0), 72(0), 73(0), 76(0), 79(0), 82(0), 93(0), 96(0), 103(0), 108(0), 126(0), 137(0), 145(0), 151(2), 166(0), 196(1), 209(1), 218(2), 222(2), 223(2), 227(0), 250(13), 252(0), 268(9), 273(0), 306(0), 307(5), 352(1), 355(3), 357(1), 361(1), 372(9), 372(3), 378(19), 380(3), 406(141), 407(3), 421(1), 424(36), 432(18), 435(0), 505(133), 511(61), 513(211), 523(22), 590(0), 591(1), 596(0), 596(1), 799(28), 808(106), 809(175), 816(0), 817(445), 819(451), 823(20), 825(160), 836(472), 839(169), 842(30), 845(15), 846(91), 849(300), 857(135), 864(87), 878(37), 880(17), 882(10), 884(76), 890(3), 891(20), 946(11), 949(0), 954(4), 955(0), 1018(25), 1018(2), 1035(15), 1035(1), 1077(0), 1077(0), 1085(0), 1085(1), 1141(4), 1142(0), 1279(0), 1279(0), 1403(1), 1404(2), 1412(0), 1412(3), 1452(0), 1452(9), 1471(14), 1471(0), 3247(0), 3247(0), 3257(0), 3257(0), 3268(1), 3268(1), 3272(0), 3272(0), 3301(3), 3301(0)
24-2S	34(0), 44(0), 48(0), 60(0), 61(0), 65(0), 69(0), 74(0), 77(0), 79(0), 85(0), 95(0), 100(0), 122(0), 128(1), 133(0), 137(2), 155(0), 201(0), 208(1), 213(4), 216(0), 223(2), 224(1), 244(6), 252(1), 263(8), 269(1), 301(6), 303(0), 345(0), 352(15), 355(0), 356(0), 374(0), 375(11), 379(4), 380(9), 401(194), 408(0), 419(1), 424(2), 431(2), 432(4), 501(68), 511(97), 516(196), 525(68), 585(1), 588(0), 591(0), 591(0), 793(0), 794(343), 813(293), 814(134), 820(494), 824(115), 828(65), 829(247), 836(2), 841(1), 841(8), 844(0), 848(37), 848(6), 856(4), 859(14), 861(81), 863(265), 868(77), 880(108), 880(44), 913(207), 916(505), 929(5), 947(0), 948(3), 1013(19), 1016(3), 1033(2), 1038(16), 1071(1), 1077(0), 1078(0), 1089(2), 1140(3), 1142(3), 1277(0), 1279(0), 1402(3), 1404(0), 1411(3), 1411(0), 1452(5), 1452(1), 1471(12), 1472(0), 3244(0), 3244(0), 3248(0), 3249(0), 3264(0), 3264(1), 3276(3), 3277(0), 3298(2), 3300(1)

Table S8. Harmonic vibrational frequencies (cm^{-1}) and corresponding infrared intensities (km/mol, in parentheses) predicted for the $Cp_2Fe_2(PF_3)_4$ structures by the BP86 method.

Structures	Frequencies
24-1S	27*i*, 28(0), 45(0), 48(0), 64(0), 73(0), 74(0), 78(1), 82(0), 94(0), 100(0), 103(0), 109(0), 129(0), 140(1), 149(1), 152(1), 166(0), 194(2), 208(0), 219(2), 223(3), 226(5), 228(0), 247(9), 250(0), 272(7), 274(0), 309(0), 312(10), 338(1), 345(1), 347(13), 349(2), 360(10), 361(2), 369(3), 369(8), 411(86), 411(0), 422(0), 423(16), 435(50), 437(0), 499(75), 504(121), 507(52), 513(44), 564(0), 564(2), 568(0), 569(1), 761(7), 771(121), 771(105), 775(1), 778(149), 782(550), 783(21), 794(82), 798(539), 800(246), 808(36), 812(10), 812(7), 817(183), 819(309), 827(93), 846(15), 848(142), 853(0), 854(0), 866(7), 867(4), 902(14), 906(0), 912(1), 912(0), 983(24), 983(1), 1002(1), 1002(17), 1044(1), 1044(0), 1049(0), 1049(2), 1109(5), 1109(0), 1225(0), 1225(0), 1363(2), 1364(1), 1371(0), 1372(0), 1396(0), 1396(12), 1417(16), 1417(0), 3171(0), 3171(0), 3184(0), 3184(0), 3194(1), 3194(1), 3196(0), 3196(0), 3214(3), 3214(0)
24-2S	32(0), 43(0), 47(0), 57(0), 65(0), 66(0), 68(0), 74(0), 76(0), 79(0), 86(0), 94(0), 100(0), 125(0), 129(1), 134(0), 138(1), 160(0), 199(0), 204(0), 214(5), 215(0), 226(4), 226(1), 243(7), 250(0), 267(2), 274(5), 304(9), 304(1), 331(0), 341(9), 346(24), 348(0), 362(0), 362(8), 369(1), 371(6), 407(139), 413(0), 416(2), 424(0), 430(2), 431(17), 496(42), 503(85), 509(134), 514(37), 555(2), 562(0), 562(1), 563(1), 757(0), 760(195), 776(142), 781(412), 784(554), 789(35), 790(31), 794(136), 799(2), 806(1), 808(14), 809(0), 812(0), 815(31), 822(3), 823(78), 829(226), 830(62), 835(98), 848(9), 848(27), 870(13), 880(700), 887(4), 914(0), 915(0), 980(16), 984(3), 1000(2), 1006(19), 1037(2), 1044(0), 1045(1), 1056(2), 1107(3), 1110(4), 1225(0), 1227(0), 1362(2), 1364(0), 1369(1), 1370(0), 1398(8), 1399(2), 1417(12), 1418(0), 3168(0), 3168(0), 3171(0), 3171(0), 3189(1), 3189(0), 3199(3), 3200(0), 3216(1), 3217(2)

Table S9. Harmonic vibrational frequencies (cm^{-1}) and corresponding infrared intensities (km/mol, in parentheses) predicted for the $Cp_2Fe_2(PF_3)_4$ structures by the B3LYP* method.

Structures	Frequencies
24-1S	12*i*, 28(0), 47(0), 52(0), 73(0), 73(0), 77(0), 79(0), 82(0), 94(0), 97(0), 104(0), 108(0), 128(0), 138(0), 146(0), 152(2), 166(0), 196(1), 209(0), 219(2), 223(2), 224(3), 228(0), 250(12), 252(0), 269(7), 274(0), 307(0), 309(6), 349(1), 353(4), 355(1), 358(2), 369(9), 370(3), 376(16), 377(3), 408(128), 408(2), 422(0), 424(31), 433(24), 436(0), 504(107), 510(68), 511(190), 521(28), 585(0), 585(1), 589(0), 590(1), 790(12), 800(108), 800(156), 807(0), 808(262), 812(597), 814(31), 818(127), 827(495), 831(207), 834(32), 837(14), 838(60), 842(295), 848(146), 855(93), 871(44), 873(18), 875(4), 877(71), 885(3), 886(15), 936(11), 939(0), 944(4), 945(0), 1009(25), 1009(2), 1026(16), 1026(1), 1069(0), 1069(0), 1076(0), 1076(1), 1134(4), 1134(0), 1267(0), 1267(0), 1393(1), 1394(2), 1402(0), 1402(1), 1438(0), 1438(10), 1458(14), 1458(0), 3227(0), 3227(0), 3237(0), 3237(0), 3248(1), 3248(2), 3251(0), 3251(0), 3279(3), 3279(0)
24-2S	33(0), 44(0), 48(0), 60(0), 62(0), 66(0), 69(0), 73(0), 77(0), 78(0), 85(0), 96(0), 101(0), 123(0), 128(1), 133(0), 138(1), 157(0), 200(0), 207(0), 214(5), 216(0), 224(3), 225(1), 244(6), 252(0), 264(6), 271(2), 303(7), 304(0), 342(0), 350(18), 352(2), 354(0), 371(0), 372(10), 376(2), 378(8), 403(179), 409(0), 419(0), 424(1), 431(2), 432(6), 500(60), 509(93), 515(181), 522(63), 578(1), 583(0), 584(0), 585(0), 785(0), 787(286), 805(139), 806(341), 812(433), 815(170), 819(55), 820(214), 828(0), 834(1), 834(10), 836(0), 840(4), 841(39), 847(2), 851(11), 853(102), 855(250), 860(85), 872(86), 872(37), 903(58), 908(656), 919(4), 937(0), 938(3), 1005(19), 1007(3), 1025(2), 1030(17), 1062(1), 1068(0), 1069(0), 1081(2), 1132(3), 1135(3), 1265(0), 1267(0), 1392(3), 1394(0), 1400(2), 1401(0), 1438(6), 1439(1), 1458(12), 1459(0), 3224(0), 3224(0), 3228(0), 3228(0), 3243(0), 3244(1), 3256(3), 3256(0), 3277(2), 3279(1)

Table S10. Harmonic vibrational frequencies (cm^{-1}) and corresponding infrared intensities (km/mol, in parentheses) predicted for the $Cp_2Fe_2(PF_3)_3$ structures by the B3LYP method.

Structures	Frequencies
23-1T	18(0), 31(0), 31(0), 45(0), 51(0), 57(0), 63(0), 70(0), 74(0), 80(1), 88(0), 93(1), 110(0), 121(1), 125(0), 187(0), 197(1), 209(9), 214(2), 221(1), 245(0), 245(2), 269(1), 291(1), 300(1), 304(4), 346(0), 348(10), 353(8), 358(4), 363(5), 369(6), 375(8), 402(68), 421(0), 437(7), 494(106), 511(144), 518(80), 587(0), 589(3), 595(1), 602(0), 792(4), 806(202), 811(17), 816(88), 817(388), 825(130), 827(54), 833(272), 836(16), 838(41), 840(13), 841(146), 842(107), 845(29), 847(14), 851(190), 861(112), 869(97), 876(531), 903(24), 913(1), 920(3), 927(1), 1007(12), 1014(12), 1029(12), 1030(17), 1069(3), 1071(2), 1072(1), 1073(1), 1134(1), 1135(1), 1273(0), 1275(0), 1381(15), 1390(1), 1395(1), 1401(2), 1442(4), 1452(14), 1465(0), 1469(3), 3232(1), 3240(0), 3243(0), 3247(0), 3252(1), 3257(1), 3260(0), 3261(0), 3272(0), 3272(1)
23-2T	17(0), 24(0), 34(0), 39(0), 43(0), 50(0), 56(0), 63(1), 70(1), 77(1), 94(0), 96(0), 107(0), 128(0), 134(0), 182(0), 190(0), 201(9), 215(2), 220(2), 238(0), 243(2), 263(2), 280(6), 290(1), 303(2), 339(1), 347(16), 351(2), 357(2), 361(10), 364(2), 368(8), 398(57), 417(0), 432(3), 489(94), 509(138), 517(98), 585(0), 591(5), 597(0), 603(1), 776(11), 790(105), 805(93), 813(181), 817(161), 819(146), 823(318), 828(37), 835(50), 838(47), 840(65), 840(1), 842(23), 845(20), 847(35), 855(144), 860(177), 863(43), 876(6), 894(777), 909(9), 917(10), 920(1), 1006(20), 1012(8), 1031(4), 1033(16), 1072(2), 1072(2), 1076(7), 1078(2), 1135(1), 1137(2), 1273(0), 1281(0), 1380(15), 1389(3), 1394(2), 1407(5), 1447(2), 1455(15), 1466(0), 1479(3), 3235(1), 3240(0), 3244(0), 3245(0), 3252(1), 3255(1), 3257(0), 3267(2), 3269(0), 3287(1)
23-1S	14(1), 37(0), 48(0), 61(0), 72(0), 77(0), 84(0), 87(0), 105(1), 106(0), 124(1), 126(0), 144(1), 154(0), 162(0), 211(1), 222(4), 226(1), 231(4), 247(5), 258(2), 274(6), 279(3), 322(9), 331(8), 346(3), 356(2), 362(6), 374(22), 379(10), 380(7), 393(5), 413(41), 417(58), 429(15), 445(5), 504(143), 519(57), 524(55), 583(3), 589(3), 591(0), 596(0), 623(116), 798(125), 803(317), 808(207), 815(527), 823(70), 826(173), 830(179), 839(34), 841(23), 842(16), 845(158), 846(30), 848(12), 856(45), 863(1), 875(167), 883(3), 889(5), 927(2), 932(1), 935(3), 950(1), 1011(13), 1015(14), 1033(10), 1034(9), 1075(1), 1076(0), 1082(0), 1083(1), 1138(4), 1139(6), 1277(0), 1280(0), 1398(1), 1399(1), 1402(3), 1408(3), 1447(4), 1458(3), 1465(5), 1473(4), 3239(0), 3242(0), 3242(0), 3251(0), 3265(0), 3266(0), 3271(0), 3279(1), 3291(3), 3293(1)
23-2S	23(0), 37(0), 50(0), 57(0), 64(0), 77(0), 83(0), 94(0), 100(1), 104(0), 118(1), 126(0), 143(0), 146(0), 156(1), 197(1), 221(2), 224(3), 226(3), 238(1), 268(8), 274(3), 277(3), 305(5), 325(8), 347(14), 352(0), 361(21), 374(10), 378(1), 382(19), 394(6), 412(95), 417(1), 429(12), 444(3), 502(58), 516(159), 523(44), 588(3), 588(3), 590(0), 594(1), 646(107), 800(65), 804(425), 814(128), 816(135), 822(183), 833(122), 835(31), 838(43), 841(7), 842(22), 843(46), 847(6), 848(38), 854(180), 864(124), 866(4), 873(60), 886(648), 923(0), 924(2), 925(1), 933(1), 1010(10), 1015(15), 1029(11), 1035(4), 1072(0), 1074(1), 1077(2), 1080(2), 1137(5), 1140(5), 1275(0), 1279(0), 1396(1), 1401(1), 1403(3), 1405(2), 1447(3), 1455(2), 1465(3), 1471(3), 3238(0), 3243(0), 3246(0), 3251(0), 3260(0), 3263(0), 3264(0), 3267(0), 3273(1), 3280(2)
23-3S	26(0), 43(0), 48(0), 56(0), 68(0), 78(0), 84(0), 88(0), 100(0), 106(0), 114(1), 123(0), 128(0), 144(0), 159(0), 208(0), 216(2), 223(2), 227(5), 243(3), 258(1), 263(5), 277(7), 320(10), 338(2),

	345(4), 357(1), 361(3), 366(21), 370(1), 375(7), 382(9), 411(15), 419(65), 431(19), 445(2), 495(84), 521(105), 524(67), 581(3), 588(2), 591(3), 594(1), 619(118), 804(68), 807(225), 815(234), 815(374), 824(51), 827(62), 832(11), 835(9), 840(4), 841(11), 844(0), 846(44), 849(27), 852(27), 853(96), 865(23), 872(215), 898(755), 916(1), 920(7), 926(4), 928(1), 1010(14), 1012(13), 1030(7), 1036(5), 1073(0), 1074(3), 1075(1), 1087(2), 1136(4), 1140(7), 1274(0), 1281(0), 1397(1), 1400(1), 1402(6), 1406(3), 1445(3), 1457(2), 1470(5), 1472(2), 3237(0), 3240(0), 3243(0), 3243(0), 3255(0), 3266(1), 3267(0), 3273(3), 3274(0), 3292(1)
23-4S	38(0), 46(0), 51(0), 54(0), 59(0), 61(0), 76(0), 87(0), 93(0), 104(0), 120(1), 140(1), 144(0), 156(1), 188(0), 200(0), 207(1), 215(6), 222(4), 226(2), 231(1), 247(1), 290(2), 333(5), 338(2), 343(1), 347(5), 357(6), 366(7), 370(3), 374(2), 385(4), 397(39), 409(3), 420(19), 451(0), 500(144), 513(110), 520(93), 583(1), 586(0), 620(2), 644(14), 785(20), 796(37), 804(7), 805(4), 810(47), 814(330), 818(115), 821(332), 835(10), 838(177), 840(67), 841(260), 844(60), 847(42), 851(10), 859(41), 869(197), 879(27), 886(605), 894(19), 917(4), 939(4), 949(17), 976(4), 1017(1), 1021(16), 1032(9), 1041(2), 1056(1), 1073(0), 1082(1), 1103(3), 1144(5), 1261(0), 1279(0), 1352(4), 1367(12), 1398(5), 1403(1), 1407(1), 1453(3), 1456(2), 1471(2), 3218(0), 3220(0), 3231(3), 3234(0), 3236(2), 3245(0), 3246(2), 3256(0), 3262(0), 3281(1)
23-1Q	19(0), 23(0), 33(0), 37(0), 42(0), 51(0), 55(0), 64(1), 71(0), 79(1), 85(1), 97(0), 103(0), 111(0), 125(1), 137(0), 142(1), 183(3), 206(1), 209(3), 216(7), 223(2), 232(3), 257(1), 272(2), 306(23), 315(4), 337(4), 347(5), 348(2), 356(0), 371(7), 376(9), 424(117), 428(1), 453(6), 471(68), 525(117), 531(70), 589(0), 595(1), 601(0), 607(0), 783(73), 786(34), 796(118), 801(257), 808(207), 814(264), 826(112), 827(97), 831(19), 841(47), 843(162), 843(8), 845(39), 849(70), 850(136), 855(117), 866(140), 871(17), 882(457), 895(21), 902(5), 917(3), 922(0), 1007(8), 1017(22), 1022(23), 1032(9), 1065(0), 1068(1), 1071(1), 1077(0), 1131(1), 1135(1), 1271(0), 1277(0), 1376(1), 1386(0), 1396(0), 1402(0), 1438(4), 1454(2), 1460(1), 1468(3), 3221(3), 3224(0), 3233(0), 3244(0), 3246(0), 3247(0), 3252(0), 3260(0), 3261(1), 3268(0)

Table S11. Harmonic vibrational frequencies (cm^{-1}) and corresponding infrared intensities (km/mol, in parentheses) predicted for the $Cp_2Fe_2(PF_3)_3$ structures by the BP86 method.

Structures	Frequencies
23-1T	14(0), 32(0), 49(0), 58(0), 60(0), 64(0), 74(0), 77(0), 81(0), 86(0), 93(0), 105(0), 124(1), 136(3), 147(0), 197(0), 199(1), 219(3), 221(5), 227(3), 247(2), 258(2), 265(1), 277(3), 308(5), 334(9), 340(1), 346(4), 348(4), 356(5), 360(4), 367(3), 368(5), 421(79), 427(5), 442(17), 490(78), 509(66), 511(59), 555(0), 564(0), 566(1), 571(1), 762(95), 773(140), 778(193), 779(208), 780(14), 785(259), 789(125), 797(57), 798(48), 803(4), 806(24), 808(108), 810(1), 815(62), 820(295), 828(66), 832(31), 836(33), 843(464), 872(1), 873(8), 885(1), 909(2), 974(12), 981(11), 998(6), 1003(13), 1038(1), 1039(1), 1041(0), 1043(0), 1100(3), 1107(1), 1221(0), 1228(0), 1349(7), 1353(2), 1355(0), 1360(0), 1385(5), 1402(7), 1413(4), 1421(2), 3159(0), 3165(1), 3170(0), 3171(0), 3179(0), 3181(1), 3186(0), 3188(0), 3193(0), 3203(1)
23-2T	23(0), 27(0), 41(0), 47(0), 55(0), 63(0), 78(0), 79(0), 83(0), 103(0), 104(0), 120(0), 124(1), 142(1), 149(0), 189(0), 197(0), 210(5), 221(3), 231(4), 245(4), 253(1), 270(6), 302(3), 309(6), 319(2), 337(5), 344(4), 347(0), 350(2), 353(11), 356(6), 368(4), 412(48), 420(28), 433(12), 481(70), 506(81), 509(61), 555(0), 562(1), 564(0), 566(1), 746(40), 756(44), 760(276), 768(24), 773(323), 780(225), 790(67), 795(40), 802(32), 804(23), 805(36), 807(2), 809(15), 811(15), 814(32), 818(112), 823(121), 837(5), 846(2), 862(735), 878(7), 882(8), 891(0), 977(14), 980(11), 1002(6), 1006(12), 1040(2), 1041(3), 1046(1), 1050(3), 1106(3), 1109(3), 1222(0), 1230(0), 1340(0), 1358(1), 1360(4), 1370(1), 1396(4), 1404(13), 1419(1), 1425(3), 3165(0), 3166(0), 3172(1), 3172(0), 3181(0), 3185(0), 3186(0), 3195(0), 3197(3), 3201(3)
23-1S	31(0), 35(0), 61(0), 71(0), 75(0), 76(0), 83(0), 89(1), 107(0), 110(0), 130(0), 132(1), 148(1), 158(1), 168(0), 208(2), 217(3), 228(2), 232(3), 243(3), 258(5), 276(4), 286(6), 313(10), 324(10), 338(11), 346(7), 361(16), 363(2), 368(7), 385(7), 407(5), 418(69), 422(21), 430(4), 446(17), 499(83), 506(24), 509(55), 553(4), 560(0), 566(1), 574(0), 606(123), 758(172), 760(108), 761(228), 776(341), 784(167), 788(267), 793(153), 800(47), 806(65), 808(25), 811(5), 813(45), 815(81), 828(26), 835(1), 843(153), 854(1), 872(2), 888(2), 891(2), 899(2), 910(2), 979(12), 985(12), 992(11), 1003(9), 1040(0), 1044(0), 1047(3), 1048(1), 1105(8), 1106(3), 1224(0), 1226(0), 1357(1), 1358(1), 1362(1), 1369(2), 1395(3), 1395(7), 1410(6), 1423(5), 3161(0), 3164(1), 3167(0), 3179(0), 3189(0), 3189(0), 3195(0), 3199(1), 3213(2), 3215(1)
23-2S	22(0), 45(0), 54(0), 59(0), 64(0), 80(0), 88(0), 92(0), 102(0), 110(0), 122(0), 131(0), 141(1), 152(0), 167(0), 194(2), 218(2), 222(3), 226(5), 238(1), 264(2), 277(5), 285(6), 298(11), 312(6), 338(33), 342(10), 358(10), 366(5), 375(8), 386(12), 407(7), 411(65), 421(13), 433(5), 440(16), 496(35), 504(103), 509(33), 554(3), 560(3), 565(1), 568(0), 621(114), 749(215), 757(105), 770(176), 780(159), 784(52), 789(119), 794(132), 800(13), 803(1), 807(20), 809(10), 812(8), 815(10), 818(297), 825(17), 836(41), 844(221), 850(426), 864(1), 884(1), 885(0), 897(2), 979(12), 983(10), 991(12), 1004(4), 1037(1), 1041(2), 1044(1), 1050(2), 1104(5), 1106(6), 1221(0), 1228(0), 1356(1), 1361(1), 1361(2), 1365(1), 1393(5), 1396(4), 1411(3), 1420(3), 3161(0), 3163(0), 3171(0), 3177(2), 3179(0), 3188(0), 3189(1), 3190(0), 3197(1), 3206(2)
23-3S	28(0), 35(0), 54(0), 60(0), 70(0), 80(0), 81(0), 89(0), 101(0), 107(0), 116(0), 128(0), 131(0), 149(0), 166(0), 206(0), 216(3), 222(1), 225(5), 238(2), 259(6), 269(6), 280(2), 317(12), 327(2),

	332(4), 346(8), 352(1), 358(11), 362(7), 376(13), 394(4), 415(55), 423(29), 433(1), 442(17), 486(60), 508(43), 510(70), 546(2), 559(2), 563(1), 565(1), 609(117), 764(267), 766(107), 771(173), 775(33), 779(67), 783(173), 789(53), 799(61), 805(43), 806(7), 810(36), 811(20), 814(4), 819(78), 825(126), 828(93), 836(2), 865(660), 873(1), 879(21), 880(8), 891(3), 977(11), 978(16), 998(6), 1000(5), 1037(2), 1041(1), 1045(1), 1052(2), 1103(7), 1105(6), 1220(0), 1227(0), 1356(3), 1357(1), 1358(2), 1366(2), 1391(6), 1394(2), 1419(6), 1421(3), 3160(0), 3163(0), 3165(0), 3166(0), 3181(1), 3183(2), 3191(1), 3194(0), 3195(1), 3207(2)
23-4S	38(0), 46(0), 51(0), 56(0), 60(0), 70(0), 83(0), 89(0), 92(0), 100(0), 121(1), 144(1), 154(0), 156(1), 188(0), 203(2), 204(1), 215(9), 221(2), 224(4), 227(1), 241(1), 296(2), 328(8), 330(6), 331(2), 337(7), 351(4), 355(0), 359(0), 367(12), 386(32), 403(3), 409(16), 417(5), 453(7), 489(114), 498(59), 509(76), 552(0), 555(0), 609(2), 638(12), 752(11), 765(4), 766(13), 773(67), 777(114), 778(213), 782(3), 783(279), 799(4), 799(222), 802(87), 807(354), 810(2), 813(27), 819(18), 828(35), 835(162), 850(178), 853(392), 862(27), 867(13), 900(4), 907(12), 943(5), 983(2), 986(11), 1000(8), 1010(1), 1019(2), 1039(0), 1052(1), 1065(1), 1110(6), 1206(0), 1227(0), 1300(3), 1317(6), 1338(6), 1358(1), 1370(1), 1388(2), 1397(4), 1426(2), 3125(4), 3135(0), 3143(4), 3155(1), 3155(2), 3164(1), 3166(2), 3177(1), 3185(0), 3200(1)
23-1Q	10(0), 27(0), 37(0), 47(0), 52(0), 56(0), 59(0), 64(0), 77(0), 79(1), 93(0), 96(0), 109(0), 123(1), 146(0), 160(3), 162(0), 183(3), 200(0), 202(0), 217(2), 226(4), 230(4), 251(1), 275(4), 310(5), 320(8), 326(3), 330(4), 337(1), 345(1), 357(4), 365(7), 414(97), 415(22), 444(25), 457(56), 509(81), 519(54), 563(1), 566(1), 572(2), 585(0), 745(117), 756(10), 762(116), 772(39), 780(76), 783(328), 788(477), 793(35), 796(23), 797(112), 802(97), 808(26), 808(12), 810(3), 811(93), 813(84), 823(106), 838(37), 839(298), 852(141), 859(25), 873(2), 892(1), 976(7), 985(18), 995(18), 1002(9), 1035(1), 1039(1), 1040(0), 1045(1), 1100(2), 1103(0), 1224(0), 1226(0), 1334(1), 1349(0), 1352(0), 1362(1), 1384(6), 1405(4), 1411(2), 1419(3), 3148(2), 3155(1), 3161(0), 3172(0), 3172(0), 3177(0), 3179(0), 3188(0), 3188(1), 3197(1)

Table S12. Harmonic vibrational frequencies (cm^{-1}) and corresponding infrared intensities (km/mol, in parentheses) predicted for the $Cp_2Fe_2(PF_3)_3$ structures by the B3LYP* method.

Structures	Frequencies
23-1T	17(0), 29(0), 34(0), 49(0), 54(0), 60(0), 66(0), 74(0), 77(0), 85(0), 90(0), 100(1), 115(0), 126(1), 131(0), 189(0), 200(1), 212(9), 216(2), 225(2), 247(1), 248(1), 272(2), 296(1), 305(1), 309(5), 346(7), 349(2), 352(11), 357(4), 364(4), 368(5), 374(7), 410(80), 424(0), 440(11), 492(105), 512(123), 517(75), 579(2), 582(0), 588(1), 592(0), 786(10), 796(112), 801(101), 807(397), 808(147), 814(72), 820(29), 824(396), 829(97), 830(18), 831(1), 833(48), 835(22), 838(17), 841(13), 844(210), 852(93), 862(100), 869(527), 894(27), 908(1), 912(3), 917(1), 1000(11), 1007(12), 1020(5), 1024(23), 1061(2), 1063(1), 1064(1), 1065(2), 1126(2), 1130(1), 1260(0), 1264(0), 1372(11), 1383(1), 1385(1), 1391(2), 1429(4), 1440(17), 1454(2), 1455(2), 3214(1), 3222(0), 3223(0), 3227(0), 3234(0), 3236(1), 3240(0), 3244(0), 3252(1), 3255(0)
23-2T	16(0), 27(0), 36(0), 41(0), 46(0), 57(0), 62(0), 68(0), 77(0), 88(1), 102(0), 103(0), 116(0), 133(0), 142(0), 183(0), 195(0), 203(10), 218(3), 225(3), 241(1), 246(2), 265(4), 289(5), 297(2), 307(3), 344(3), 346(12), 348(1), 356(2), 360(10), 363(3), 368(6), 404(75), 419(0), 434(3), 485(92), 511(125), 515(89), 580(0), 580(4), 590(0), 593(1), 769(17), 782(103), 790(45), 802(217), 805(171), 808(259), 812(296), 819(28), 826(39), 831(1), 832(35), 833(32), 834(6), 836(15), 839(22), 848(100), 853(156), 856(72), 870(8), 887(768), 903(6), 904(17), 911(1), 1000(20), 1005(6), 1024(4), 1029(15), 1064(3), 1066(1), 1069(7), 1071(2), 1129(2), 1131(2), 1262(0), 1270(0), 1371(11), 1383(2), 1387(2), 1399(5), 1434(3), 1443(21), 1457(1), 1466(3), 3218(1), 3223(0), 3224(0), 3225(0), 3236(0), 3238(0), 3239(0), 3250(1), 3251(1), 3268(2)
23-1S	19(0), 36(0), 55(0), 62(0), 73(0), 77(0), 83(0), 88(0), 106(0), 107(0), 126(1), 128(0), 145(1), 155(0), 164(0), 210(1), 221(4), 227(1), 232(4), 247(4), 259(3), 276(6), 282(3), 323(7), 327(10), 345(6), 353(2), 363(5), 371(21), 376(10), 382(6), 397(6), 415(71), 419(25), 429(14), 445(7), 504(127), 517(48), 521(56), 576(3), 583(1), 585(1), 592(0), 622(118), 790(118), 794(299), 795(176), 807(502), 815(56), 817(214), 822(205), 830(50), 833(2), 835(35), 836(98), 839(55), 841(27), 849(35), 856(2), 868(161), 877(2), 887(4), 919(2), 922(1), 928(3), 941(1), 1002(13), 1007(14), 1022(10), 1025(9), 1066(1), 1067(0), 1072(0), 1075(1), 1130(4), 1131(6), 1264(0), 1267(0), 1388(1), 1389(1), 1392(2), 1399(3), 1433(4), 1443(4), 1450(6), 1461(4), 3219(0), 3221(0), 3222(0), 3232(0), 3245(0), 3245(1), 3250(0), 3259(1), 3271(3), 3273(1)
23-2S	25(0), 38(0), 51(0), 58(0), 64(0), 78(0), 84(0), 96(0), 101(1), 105(0), 119(0), 128(0), 144(0), 148(0), 158(0), 197(1), 221(2), 224(3), 227(4), 239(1), 269(7), 277(3), 280(4), 304(6), 321(8), 346(22), 349(0), 361(17), 372(7), 380(15), 382(5), 397(6), 412(91), 420(3), 429(10), 443(5), 502(53), 514(146), 520(40), 580(4), 581(2), 584(0), 587(1), 641(108), 791(111), 793(309), 806(162), 807(95), 813(227), 823(98), 826(46), 830(60), 833(16), 834(6), 835(18), 839(1), 842(26), 846(218), 857(91), 860(31), 867(56), 878(636), 914(1), 915(1), 917(0), 923(1), 1001(11), 1007(14), 1020(11), 1028(4), 1063(0), 1066(1), 1069(2), 1072(2), 1129(5), 1132(5), 1262(0), 1267(0), 1386(1), 1390(1), 1393(3), 1395(2), 1434(4), 1440(2), 1452(3), 1459(3), 3217(0), 3222(0), 3227(0), 3232(0), 3239(0), 3242(0), 3245(0), 3246(0), 3253(1), 3260(2)
23-3S	26(0), 41(0), 50(0), 57(0), 68(0), 78(0), 84(0), 88(0), 101(0), 107(0), 116(1), 123(0), 129(0), 146(0), 161(0), 208(0), 217(2), 224(2), 227(5), 242(2), 259(2), 267(6), 278(5), 320(11), 336(3),

	342(4), 355(2), 359(2), 366(21), 371(4), 372(6), 385(8), 415(39), 419(36), 430(22), 444(4), 494(78), 519(92), 521(66), 573(3), 581(1), 584(2), 587(1), 618(118), 796(107), 800(235), 804(225), 807(233), 815(109), 818(64), 823(14), 827(16), 833(8), 833(14), 837(4), 838(42), 841(39), 845(36), 846(65), 857(99), 862(126), 890(748), 907(1), 911(9), 917(3), 917(2), 1002(14), 1004(13), 1022(7), 1027(5), 1064(1), 1065(1), 1066(1), 1079(2), 1128(4), 1132(7), 1261(0), 1268(0), 1387(1), 1389(1), 1391(6), 1396(2), 1432(4), 1442(2), 1457(5), 1459(2), 3217(0), 3220(0), 3223(0), 3223(0), 3235(0), 3246(1), 3248(0), 3252(2), 3253(0), 3271(1)
23-4S	38(0), 46(0), 51(0), 55(0), 59(0), 62(0), 76(0), 87(0), 92(0), 103(0), 120(1), 141(1), 146(0), 157(1), 188(0), 201(1), 207(1), 216(7), 223(4), 225(2), 230(1), 246(1), 293(2), 333(6), 336(3), 341(1), 345(6), 355(5), 365(2), 368(7), 371(2), 391(20), 397(22), 408(3), 418(19), 454(2), 497(137), 510(96), 518(89), 576(0), 579(0), 618(2), 642(12), 778(17), 790(22), 795(10), 799(6), 802(45), 806(302), 809(131), 811(305), 827(11), 828(188), 831(61), 833(306), 836(37), 839(38), 843(12), 853(38), 862(180), 873(11), 878(613), 886(26), 905(5), 930(4), 939(16), 968(4), 1008(1), 1012(15), 1024(9), 1033(1), 1047(1), 1064(0), 1074(1), 1093(3), 1136(5), 1247(0), 1266(0), 1339(4), 1355(9), 1384(5), 1392(1), 1398(2), 1436(3), 1441(3), 1460(3), 3195(1), 3197(0), 3207(3), 3213(0), 3214(1), 3223(1), 3225(1), 3235(0), 3242(0), 3261(2)
23-1Q	16(0), 23(0), 32(0), 42(0), 43(0), 52(0), 58(0), 64(1), 72(0), 81(1), 90(0), 101(0), 104(0), 114(0), 129(0), 143(1), 150(1), 186(3), 205(0), 209(1), 218(8), 222(3), 231(4), 256(1), 272(3), 309(16), 313(4), 334(4), 344(4), 346(3), 353(0), 367(6), 373(8), 421(122), 424(0), 451(9), 468(69), 521(108), 528(67), 582(0), 589(1), 593(0), 602(0), 778(64), 780(45), 787(130), 795(199), 801(115), 806(311), 817(175), 818(32), 824(26), 831(257), 834(101), 835(9), 836(35), 839(62), 841(27), 847(133), 855(135), 859(13), 873(434), 885(50), 893(6), 901(6), 912(1), 998(8), 1009(21), 1015(21), 1023(10), 1057(1), 1060(1), 1061(0), 1068(0), 1124(1), 1127(1), 1260(0), 1263(0), 1365(1), 1376(0), 1384(0), 1392(0), 1424(5), 1442(3), 1448(1), 1456(3), 3201(2), 3205(0), 3213(0), 3224(0), 3226(0), 3228(0), 3233(0), 3238(0), 3242(1), 3246(0)

Table S13. Harmonic vibrational frequencies (cm^{-1}) and corresponding infrared intensities (km/mol, in parentheses) predicted for the $Cp_2Fe_2(PF_3)_2$ structures by the B3LYP method.

Structures	Frequencies
22-1Q	19*i*, 34(0), 34(0), 37(0), 43(0), 54(2), 58(0), 73(0), 78(0), 89(1), 94(0), 154(0), 194(4), 210(12), 219(0), 222(0), 257(4), 258(1), 285(3), 288(1), 311(7), 335(0), 352(9), 352(50), 363(25), 370(6), 386(10), 389(3), 502(188), 518(46), 584(1), 587(0), 598(1), 600(0), 791(69), 796(11), 800(331), 805(544), 807(3), 808(75), 823(50), 826(92), 831(50), 836(34), 838(66), 840(7), 840(17), 843(7), 843(95), 853(368), 899(0), 899(0), 904(0), 907(1), 1008(17), 1010(8), 1026(22), 1027(14), 1065(4), 1067(0), 1068(2), 1070(1), 1132(2), 1133(0), 1272(0), 1272(0), 1381(2), 1381(0), 1392(15), 1392(6), 1445(9), 1445(1), 1468(2), 1468(1), 3234(0), 3234(0), 3240(0), 3240(0), 3250(0), 3250(0), 3253(2), 3253(0), 3264(0), 3264(1)
22-1T	62*i*, 24(0), 27(0), 43(0), 44(0), 47(0), 48(0), 82(0), 91(0), 103(1), 112(0), 159(0), 196(0), 220(2), 229(4), 253(0), 264(0), 273(1), 278(2), 311(7), 338(3), 348(9), 359(7), 372(7), 380(7), 426(0), 439(46), 459(62), 495(1), 525(118), 532(60), 576(1), 594(0), 596(1), 783(1), 789(32), 797(259), 801(14), 807(122), 810(407), 818(16), 822(139), 825(33), 835(34), 838(47), 838(26), 842(5), 847(103), 872(2), 874(441), 885(1), 905(1), 920(0), 929(2), 998(12), 1007(14), 1021(9), 1031(20), 1058(1), 1061(10), 1067(1), 1068(0), 1130(1), 1134(2), 1269(0), 1274(0), 1353(0), 1392(33), 1394(0), 1398(6), 1435(0), 1439(12), 1459(3), 1474(2), 3230(0), 3233(1), 3240(0), 3240(0), 3243(0), 3249(0), 3251(0), 3259(0), 3260(0), 3267(0)
22-2T	18*i*, 28(0), 32(0), 76(4), 93(2), 95(0), 97(0), 130(0), 131(2), 135(0), 159(7), 166(0), 186(9), 187(0), 203(0), 207(0), 221(0), 232(0), 251(2), 269(7), 329(0), 333(3), 335(45), 366(0), 381(40), 388(26), 391(0), 401(0), 414(0), 532(157), 588(2), 588(0), 589(0), 589(1), 622(0), 624(59), 810(412), 816(0), 825(321), 828(0), 832(75), 838(0), 838(8), 842(0), 842(3), 844(0), 864(0), 866(23), 866(0), 866(1), 932(1), 933(0), 934(0), 934(1), 1024(0), 1024(25), 1026(0), 1026(18), 1073(0), 1074(0), 1077(1), 1077(0), 1138(2), 1139(0), 1278(0), 1278(0), 1392(0), 1393(0), 1399(2), 1400(0), 1459(12), 1459(0), 1465(0), 1465(14), 3245(0), 3245(0), 3248(0), 3248(0), 3259(0), 3259(1), 3259(2), 3259(0), 3270(0), 3270(0)
22-3T	19(0), 31(0), 39(0), 40(0), 46(0), 55(0), 68(0), 76(1), 86(1), 91(0), 114(1), 150(1), 192(6), 198(3), 218(1), 222(1), 245(1), 273(2), 280(1), 297(3), 313(2), 341(10), 347(6), 355(14), 366(12), 370(8), 387(4), 395(14), 502(150), 512(63), 585(0), 594(1), 595(1), 605(0), 786(15), 796(275), 804(65), 809(79), 809(64), 816(410), 819(60), 826(21), 829(164), 834(92), 838(12), 843(19), 844(22), 846(2), 849(302), 856(75), 891(2), 900(1), 907(0), 917(1), 1008(12), 1016(14), 1022(21), 1027(17), 1065(1), 1068(2), 1070(0), 1071(1), 1132(2), 1133(0), 1272(0), 1273(0), 1379(8), 1388(2), 1389(0), 1393(2), 1446(3), 1452(4), 1461(1), 1465(1), 3234(0), 3236(0), 3237(0), 3241(0), 3248(0), 3252(0), 3253(0), 3255(0), 3262(1), 3266(0)
22-1S	30(0), 33(0), 34(0), 40(0), 49(0), 60(0), 79(0), 98(0), 113(2), 121(0), 130(0), 189(0), 213(2), 231(8), 232(0), 236(0), 288(5), 291(3), 334(0), 347(0), 360(41), 364(0), 365(6), 380(12), 394(7), 414(4), 420(6), 459(0), 511(163), 525(64), 581(1), 585(1), 591(1), 592(1), 797(358), 799(25), 805(396), 820(236), 821(2), 824(22), 826(5), 832(1), 833(9), 839(4), 841(7), 842(6), 845(7), 853(69), 857(16), 861(431), 904(1), 905(2), 921(1), 922(6), 1010(29), 1011(0), 1024(3), 1024(19), 1068(0), 1069(0), 1070(0), 1071(1), 1135(11), 1135(0), 1271(0), 1272(0), 1392(1), 1396(0), 1397(3), 1398(0), 1444(7), 1445(0), 1465(1), 1465(3), 3241(0), 3241(0), 3245(0), 3245(0), 3254(0), 3254(0), 3260(0), 3260(0), 3269(0), 3269(0)
22-2S	35(1), 36(0), 36(3), 104(7), 105(3), 123(0), 127(0), 132(0), 135(0), 141(0), 159(1), 172(0), 183(0), 191(12), 216(0), 241(0), 257(0), 270(5), 282(0), 307(10), 345(43), 347(0), 373(37), 375(0), 390(0), 417(0), 419(0), 444(0), 461(39), 545(350), 555(105), 557(0), 593(2), 594(0), 594(0), 594(1), 831(0), 834(240), 837(103),

	841(0), 844(0), 845(417), 846(51), 849(0), 851(60), 867(0), 872(0), 875(16), 876(0), 877(40), 933(4), 934(0), 947(0), 949(0), 1007(23), 1007(0), 1032(16), 1033(0), 1076(1), 1077(0), 1079(1), 1079(0), 1136(3), 1136(0), 1278(0), 1278(0), 1391(0), 1392(0), 1406(3), 1407(0), 1449(0), 1449(11), 1478(10), 1478(0), 3253(0), 3253(0), 3254(0), 3255(0), 3264(0), 3264(2), 3269(0), 3269(3), 3277(1), 3277(0)

Table S14. Harmonic vibrational frequencies (cm^{-1}) and corresponding infrared intensities (km/mol, in parentheses) predicted for the $Cp_2Fe_2(PF_3)_2$ structures by the BP86 method.

Structures	Frequencies
22-1Q	30(0), 30(0), 49(0), 53(0), 55(0), 69(0), 75(0), 83(1), 87(0), 95(0), 99(0), 169(0), 199(12), 207(3), 221(0), 233(0), 261(3), 269(7), 303(3), 308(4), 317(0), 318(2), 334(46), 347(3), 354(8), 361(8), 386(19), 399(7), 497(101), 503(23), 559(1), 564(1), 571(1), 571(0), 752(27), 752(355), 758(46), 767(44), 774(287), 780(35), 785(263), 788(34), 790(82), 802(71), 806(23), 808(50), 809(19), 810(2), 811(10), 817(215), 860(1), 862(1), 867(3), 867(0), 981(19), 983(5), 992(15), 993(22), 1033(1), 1036(0), 1037(0), 1041(1), 1103(3), 1103(1), 1220(0), 1221(0), 1343(4), 1344(1), 1351(2), 1353(0), 1396(0), 1396(9), 1411(1), 1412(1), 3165(0), 3165(0), 3169(0), 3169(1), 3180(0), 3180(1), 3181(0), 3182(0), 3192(0), 3192(1)
22-1T	27(0), 31(0), 43(0), 44(0), 55(0), 57(0), 80(0), 94(0), 97(1), 101(1), 104(0), 170(0), 188(0), 214(3), 225(5), 243(1), 271(3), 293(2), 301(1), 305(3), 313(10), 335(14), 360(5), 361(1), 368(5), 417(2), 428(7), 459(84), 476(2), 510(78), 520(36), 550(0), 567(0), 571(1), 743(41), 752(12), 758(339), 760(20), 769(20), 775(29), 777(488), 788(32), 794(0), 798(35), 806(28), 806(75), 809(5), 811(3), 836(390), 840(2), 844(3), 863(5), 882(0), 889(1), 966(10), 973(12), 993(9), 998(19), 1029(5), 1029(1), 1035(0), 1036(1), 1099(2), 1101(5), 1218(0), 1223(0), 1311(0), 1350(0), 1351(17), 1360(5), 1383(5), 1391(8), 1415(3), 1419(2), 3155(0), 3161(1), 3165(0), 3166(0), 3171(0), 3173(0), 3177(0), 3186(0), 3187(0), 3193(0)
22-2T	19*i*, 33(0), 38(0), 78(5), 93(1), 95(0), 115(0), 124(0), 134(0), 136(0), 166(0), 171(7), 186(0), 195(5), 207(0), 208(0), 229(0), 237(0), 256(2), 274(4), 321(5), 323(0), 323(17), 366(0), 376(28), 390(0), 394(0), 394(35), 395(0), 529(198), 560(0), 561(2), 565(1), 566(0), 612(0), 619(39), 756(402), 762(0), 773(253), 779(0), 796(82), 798(0), 804(8), 808(0), 810(0), 811(3), 831(20), 832(0), 834(0), 834(1), 888(1), 890(0), 892(0), 892(1), 993(0), 993(22), 994(16), 994(0), 1042(0), 1042(0), 1046(1), 1046(0), 1108(4), 1108(0), 1227(0), 1227(0), 1351(0), 1352(0), 1362(2), 1363(0), 1408(13), 1408(0), 1411(0), 1412(14), 3171(0), 3171(0), 3175(0), 3175(0), 3185(1), 3185(0), 3186(0), 3186(0), 3195(0), 3195(0)
22-3T	31(0), 39(0), 53(0), 57(0), 62(0), 72(0), 80(1), 94(0), 104(0), 108(0), 125(0), 170(1), 193(7), 213(2), 220(2), 222(1), 264(5), 281(7), 290(0), 303(3), 328(6), 332(26), 351(5), 364(6), 368(7), 389(13), 399(4), 427(7), 493(122), 501(29), 548(0), 553(0), 560(1), 574(2), 737(198), 754(147), 769(422), 772(111), 777(100), 778(5), 784(57), 794(90), 796(60), 802(53), 803(24), 809(5), 810(8), 813(7), 818(155), 822(11), 860(1), 865(2), 870(1), 879(4), 984(7), 986(14), 989(13), 990(18), 1033(0), 1034(2), 1038(0), 1041(1), 1102(6), 1103(3), 1219(0), 1222(0), 1334(1), 1349(2), 1355(0), 1360(0), 1396(4), 1404(3), 1405(2), 1409(1), 3164(0), 3165(0), 3168(0), 3174(0), 3180(0), 3182(1), 3184(0), 3188(0), 3194(0), 3196(0)
22-1S	38(0), 38(0), 46(0), 51(0), 54(0), 69(0), 89(0), 108(0), 121(1), 130(0), 143(1), 196(0), 209(6), 228(2), 234(1), 239(0), 284(4), 286(7), 326(0), 326(7), 350(45), 356(4), 359(0), 380(10), 392(0), 418(5), 422(10), 480(3), 498(100), 513(37), 554(1), 557(1), 563(1), 565(1), 744(30), 744(297), 767(402), 780(174), 781(0), 785(22), 793(23), 801(0), 803(14), 808(11), 809(9), 810(10), 811(0), 820(309), 828(98), 830(6), 860(0), 862(1), 883(2), 884(7), 977(24), 978(0), 994(21), 994(2), 1035(0), 1036(0), 1041(0), 1042(0), 1102(13), 1103(0), 1221(0), 1221(0), 1353(0), 1355(0), 1356(1), 1358(0), 1390(11), 1390(0), 1415(1), 1416(3), 3169(0), 3169(0), 3174(0), 3174(0), 3182(0), 3183(0), 3187(0), 3187(0), 3197(0), 3197(0)
22-2S	41(3), 42(1), 42(0), 102(4), 104(2), 124(0), 129(0), 130(0), 137(0), 138(0), 165(2), 169(0), 182(0), 190(8), 214(0), 239(0), 258(0), 271(6), 281(0), 306(11), 362(40), 366(0), 375(0), 377(14), 391(0), 411(0), 426(0), 444(0), 456(29), 533(152), 534(211), 541(0), 563(3), 565(0), 569(0), 570(1), 777(0), 783(249), 798(408), 805(0), 806(102), 808(0), 815(2), 815(0), 816(52), 827(0), 834(0), 839(18), 850(12), 850(0), 886(0),

	886(3), 901(1), 904(0), 978(25), 978(0), 999(16), 999(0), 1043(0), 1045(0), 1046(1), 1046(0), 1102(5), 1102(0), 1226(0), 1226(0), 1352(0), 1352(1), 1362(2), 1363(0), 1399(8), 1399(0), 1416(0), 1416(13), 3177(0), 3177(0), 3179(0), 3179(0), 3189(2), 3189(0), 3193(0), 3193(2), 3200(1), 3201(0)

Table S15. Harmonic vibrational frequencies (cm^{-1}) and corresponding infrared intensities (km/mol, in parentheses) predicted for the $Cp_2Fe_2(PF_3)_2$ structures by the B3LYP* method.

Structures	Frequencies
22-1Q	11*i*, 6(0), 39(0), 41(1), 47(0), 60(0), 62(2), 73(0), 78(0), 88(1), 92(0), 161(0), 197(5), 209(9), 219(0), 223(0), 259(1), 260(4), 286(3), 291(1), 311(6), 333(0), 349(44), 350(8), 360(24), 368(6), 386(11), 391(4), 501(162), 515(38), 577(1), 581(0), 593(1), 593(0), 779(37), 788(20), 790(367), 795(42), 799(502), 801(30), 813(66), 816(61), 820(37), 826(62), 827(71), 832(17), 833(24), 836(49), 836(3), 845(352), 885(1), 890(0), 893(0), 895(1), 1001(18), 1002(7), 1015(21), 1015(16), 1055(3), 1059(0), 1059(2), 1060(2), 1125(2), 1125(0), 1258(0), 1258(0), 1370(2), 1371(0), 1381(5), 1381(10), 1431(1), 1432(9), 1453(2), 1454(1), 3216(0), 3216(0), 3221(0), 3221(0), 3232(0), 3232(0), 3234(1), 3234(0), 3245(0), 3245(1)
22-1T	17(0), 27(0), 38(0), 43(0), 47(0), 48(0), 73(0), 82(0), 91(0), 103(1), 111(0), 162(0), 196(0), 220(2), 229(4), 252(0), 275(2), 276(1), 281(1), 310(6), 334(3), 351(0), 357(12), 369(7), 377(7), 424(0), 438(37), 459(69), 490(2), 523(108), 530(53), 571(1), 588(0), 590(1), 775(1), 780(25), 790(275), 791(14), 798(116), 804(488), 808(10), 816(33), 820(54), 827(31), 831(29), 832(52), 834(5), 838(73), 865(2), 867(437), 875(1), 896(1), 910(0), 920(2), 990(13), 998(12), 1014(9), 1023(20), 1051(1), 1053(9), 1059(1), 1059(0), 1123(1), 1127(3), 1257(0), 1262(0), 1342(0), 1383(32), 1383(0), 1388(4), 1424(2), 1428(10), 1448(3), 1461(2), 3210(0), 3213(1), 3220(0), 3220(0), 3223(0), 3229(0), 3232(0), 3239(0), 3240(0), 3248(0)
22-2T	19*i*, 30(0), 34(0), 77(4), 93(2), 95(0), 101(0), 128(2), 130(0), 134(0), 162(7), 167(0), 187(0), 188(8), 204(0), 206(0), 223(0), 233(0), 252(2), 271(6), 327(0), 330(2), 332(37), 367(0), 384(32), 385(33), 391(0), 398(0), 410(0), 532(173), 582(0), 583(1), 583(1), 584(0), 622(0), 625(54), 799(409), 805(0), 814(308), 818(0), 823(75), 828(0), 830(6), 835(0), 835(0), 835(3), 857(0), 858(13), 858(8), 859(0), 922(1), 923(0), 924(0), 924(1), 1016(0), 1016(24), 1018(18), 1018(0), 1065(0), 1065(0), 1068(1), 1069(0), 1131(2), 1131(0), 1266(0), 1266(0), 1382(0), 1382(0), 1390(2), 1391(0), 1446(12), 1446(0), 1452(0), 1452(14), 3225(0), 3225(0), 3228(0), 3228(0), 3239(2), 3239(0), 3239(1), 3239(0), 3249(0), 3249(0)
22-3T	29(0), 35(0), 41(0), 42(0), 52(0), 59(0), 70(0), 80(1), 83(0), 91(0), 111(1), 151(0), 198(6), 204(1), 217(2), 220(1), 253(2), 278(3), 283(1), 295(6), 318(2), 339(5), 347(22), 356(3), 362(11), 376(9), 384(7), 400(13), 499(160), 510(50), 576(0), 586(1), 587(0), 600(0), 782(14), 789(275), 796(143), 800(32), 801(86), 806(428), 811(97), 819(72), 824(14), 827(85), 830(24), 832(2), 837(46), 838(11), 842(260), 848(53), 888(0), 895(1), 900(0), 902(1), 1002(12), 1007(11), 1012(20), 1014(18), 1055(1), 1058(1), 1059(1), 1061(1), 1125(3), 1126(0), 1256(0), 1258(0), 1368(4), 1379(2), 1382(0), 1385(1), 1431(3), 1439(5), 1448(1), 1450(2), 3215(0), 3217(0), 3219(0), 3220(0), 3231(0), 3231(1), 3233(0), 3237(0), 3244(0), 3245(0)
22-1S	35(0), 35(0), 37(0), 45(0), 48(0), 62(0), 83(0), 101(0), 116(1), 128(0), 135(0), 195(0), 214(3), 231(6), 235(0), 236(0), 288(5), 290(3), 332(0), 343(0), 357(43), 363(5), 363(0), 379(13), 394(4), 416(5), 422(7), 467(1), 509(144), 522(56), 575(1), 579(1), 584(1), 586(1), 784(324), 786(25), 796(414), 811(224), 811(0), 816(24), 816(7), 823(1), 826(7), 831(3), 833(6), 835(5), 836(7), 846(82), 852(13), 853(395), 893(1), 894(1), 910(1), 912(6), 1001(28), 1002(0), 1017(20), 1017(2), 1060(0), 1060(0), 1062(0), 1063(1), 1127(11), 1128(0), 1259(0), 1260(0), 1382(1), 1386(0), 1386(2), 1388(0), 1431(8), 1431(0), 1452(1), 1453(3), 3222(0), 3222(0), 3226(0), 3227(0), 3235(0), 3235(0), 3241(0), 3241(0), 3250(0), 3250(0)
22-2S	36(1), 36(0), 37(3), 103(6), 105(3), 124(0), 129(0), 131(0), 134(0), 139(0), 161(1), 172(0), 183(0), 191(12), 216(0), 241(0), 257(0), 271(6), 281(0), 306(10), 350(44), 352(0), 373(27), 375(0), 390(0), 417(0), 419(0), 443(0), 460(38), 543(341), 552(94), 555(0), 586(2), 587(0), 589(0), 589(1), 820(0), 823(261), 829(166),

	833(0), 835(0), 836(351), 839(23), 841(0), 842(56), 858(0), 863(0), 868(33), 869(0), 870(13), 922(4), 922(0), 937(0), 939(0), 1000(24), 1000(0), 1024(16), 1024(0), 1068(1), 1069(0), 1070(1), 1070(0), 1128(3), 1128(0), 1266(0), 1266(0), 1381(0), 1382(0), 1395(3), 1396(0), 1437(0), 1437(10), 1463(11), 1463(0), 3233(0), 3233(0), 3235(0), 3235(0), 3244(3), 3244(0), 3248(0), 3249(4), 3256(1), 3256(0)

Table S16. Harmonic vibrational frequencies (cm^{-1}) and corresponding infrared intensities (km/mol, in parentheses) predicted for the isolated PF_3 structures by the B3LYP, BP86, and B3LYP* method. The stretching vibrational frequencies of the P-F bonds ν(PF) are in **bold**.

B3LYP	BP86	B3LYP*
331(5), 331(5), 465(28), **845(194), 845(194), 878(142)**	313(4), 313(4), 439(22), **813(178), 813(178), 841(124)**	327(5), 327(5), 459(27), **838(190), 838(190), 870(138)**

Table S17. Cartesian coordinates (Å) and energies (in hartree) for the optimized structure **25-1S**.

	B3LYP (-6120.03920)			BP86 (-6120.56623)			B3LYP* (-6118.37022)		
	X	Y	Z	X	Y	Z	X	Y	Z
Fe	-1.955184	-0.180855	-0.556544	1.985294	-0.059340	0.622049	-1.948053	-0.271768	-0.547355
Fe	2.094587	0.053524	0.675443	-1.914507	0.121077	-0.691517	2.061063	0.043374	0.705114
P	2.041267	1.724912	-0.650492	-1.813603	1.686578	0.687040	1.916240	1.742719	-0.557248
P	2.505987	-1.493791	-0.928696	-2.965626	-1.303548	0.701713	2.576559	-1.390320	-0.968980
P	-3.165626	-1.144258	0.897903	3.177841	-1.288403	-0.596246	-3.255015	-0.875646	1.005982
P	-2.325369	1.812402	0.064690	2.251161	1.665918	-0.524853	-2.133664	1.807519	-0.180535
F	0.907838	2.017771	-1.725390	-1.424252	1.577832	2.244356	0.729913	2.033121	-1.584768
F	3.292249	2.073155	-1.552654	-3.082216	2.649932	0.852236	3.120820	2.163551	-1.497006
F	1.963651	3.139442	0.079300	-0.760298	2.879151	0.364739	1.821669	3.137313	0.217324
F	1.457859	-2.453473	-1.693981	-2.314271	-2.015848	2.004396	1.627395	-2.451780	-1.736263
F	3.942860	-1.710229	-1.594811	-4.531368	-1.720514	0.591805	4.002594	-1.399102	-1.697639
F	2.209472	-0.380264	-2.241361	-3.512016	-0.066028	1.767478	2.083220	-0.280109	-2.227205
F	-3.137826	-0.798895	2.430950	3.362535	-1.007762	-2.153825	-3.499557	-0.018431	2.308300
F	-3.100360	-2.717141	1.007130	2.915828	-2.860483	-0.657784	-3.070158	-2.288206	1.693177
F	-4.732030	-1.024373	0.677503	4.740190	-1.375707	-0.232028	-4.777040	-1.062836	0.584627
F	-3.138160	2.111260	1.385582	3.677189	1.899277	-1.225967	-3.461825	2.329631	0.518485
F	-3.174343	2.715999	-0.922046	2.172774	3.085719	0.209488	-2.163384	2.804632	-1.412092
F	-1.144376	2.833920	0.306727	1.361159	2.024568	-1.808581	-1.109334	2.609698	0.722594
P	-0.093553	-0.349917	0.778779	0.071579	-0.774573	-0.405542	-0.092678	-0.510029	0.776795
F	-0.254362	-1.824898	1.462054	0.013955	-2.295871	0.194417	-0.153560	-2.075260	1.234277
F	-0.620740	0.487194	2.096928	0.607132	-1.247231	-1.903137	-0.675815	0.082791	2.200406
F	2.831502	-2.787423	0.069649	-2.628318	-2.693923	-0.179597	3.105234	-2.670786	-0.036828
C	2.945171	-1.083095	2.285985	-3.447308	-0.491228	-2.046497	3.982260	-0.332804	1.535284
H	2.811005	-2.151383	2.392595	-4.200155	-1.257271	-1.848431	4.820640	-0.731339	0.971874
C	3.983839	-0.437147	1.535742	-3.577634	0.909344	-1.755839	3.657779	1.046348	1.695508
H	4.784802	-0.933437	0.999463	-4.439774	1.393223	-1.291231	4.225494	1.882577	1.294645
C	3.777620	0.968894	1.619089	-2.354865	1.559061	-2.186464	2.462768	1.137589	2.496008
H	4.412485	1.729019	1.175034	-2.141155	2.630053	-2.129832	1.953876	2.050514	2.789663
C	2.112459	-0.068026	2.834190	-2.152541	-0.721264	-2.618701	3.003331	-1.104408	2.250363
H	1.230983	-0.233225	3.442055	-1.750953	-1.689080	-2.923475	2.960433	-2.186296	2.298693
C	2.598556	1.203079	2.411978	-1.477890	0.558275	-2.714508	2.087529	-0.193821	2.850033
H	2.172678	2.168400	2.658939	-0.480315	0.730850	-3.121789	1.225294	-0.465982	3.450173
C	-0.851228	-0.524899	-2.369987	0.889828	-0.360795	2.422843	-0.935238	-0.675972	-2.390849
H	0.213716	-0.382243	-2.503416	-0.175233	-0.595688	2.499508	0.082077	-0.375153	-2.621604
C	-1.858572	0.451968	-2.596536	1.470453	0.952274	2.410682	-2.124646	0.065149	-2.661638
H	-1.684596	1.467983	-2.934501	0.925421	1.894653	2.473241	-2.161745	1.042535	-3.134914
C	-3.140882	-0.144222	-2.330938	2.911560	0.807125	2.335370	-3.252202	-0.677810	-2.190436

H	-4.108846	0.333686	-2.430725	3.641684	1.620315	2.334835	-4.296024	-0.385477	-2.257887
C	-1.490709	-1.731182	-1.939818	1.954737	-1.320388	2.320806	-1.324985	-1.906531	-1.761903
H	-0.990693	-2.659520	-1.690893	1.833653	-2.405622	2.288941	-0.653160	-2.695763	-1.440936
C	-2.904105	-1.497996	-1.948404	3.206652	-0.589878	2.289711	-2.746917	-1.910646	-1.645636
H	-3.668605	-2.231557	-1.710708	4.205911	-1.029323	2.236353	-3.346415	-2.721595	-1.238584

Table S18. Cartesian coordinates (Å) and energies (in hartree) for the optimized structure **25-2S**.

	B3LYP (-6120.02593)			BP86 (-6120.55877)			B3LYP* (-6118.35832)		
	X	Y	Z	X	Y	Z	X	Y	Z
Fe	2.299915	-0.193582	-0.534413	2.301569	-0.182585	-0.538052	2.301643	-0.188806	-0.531794
Fe	-1.977375	-0.233017	0.568713	-1.969927	-0.202291	0.575828	-1.974315	-0.220123	0.569537
P	-3.117562	-1.126401	-0.974469	-3.098026	-1.153546	-0.907249	-3.102886	-1.138269	-0.955983
P	-2.327858	1.815687	-0.036057	-2.411769	1.769388	-0.048942	-2.357265	1.801451	-0.040758
P	2.197485	1.782548	0.286610	2.238835	1.755584	0.269797	2.207329	1.775994	0.276356
P	2.554821	-1.217004	1.273168	2.559724	-1.182717	1.260857	2.549122	-1.198905	1.276584
F	-4.602295	-1.537951	-0.576578	-4.592842	-1.575626	-0.476992	-4.588173	-1.557635	-0.550792
F	-2.708450	-2.514170	-1.605128	-2.682414	-2.578603	-1.498285	-2.685529	-2.535331	-1.570122
F	-3.464695	-0.367375	-2.314304	-3.481880	-0.449110	-2.287000	-3.460040	-0.400119	-2.308860
F	-2.426943	2.341254	-1.513208	-2.541954	2.261586	-1.554530	-2.481168	2.307693	-1.526666
F	-1.584725	3.021212	0.658617	-1.648355	3.021650	0.583562	-1.587820	3.018279	0.613680
F	-3.798786	2.274443	0.400896	-3.889990	2.237053	0.409236	-3.817434	2.275209	0.422097
F	1.220755	2.209790	1.449969	1.222306	2.226991	1.409299	1.203190	2.214945	1.417880
F	2.110071	3.054935	-0.636886	2.173225	3.038616	-0.676596	2.124779	3.044448	-0.660481
F	3.546990	2.212827	1.025181	3.584215	2.193243	1.045309	3.543747	2.220117	1.034949
F	4.039871	-1.567258	1.715101	4.068765	-1.531984	1.697643	4.037737	-1.551604	1.720588
F	1.964655	-2.672315	1.505638	1.981980	-2.661219	1.525501	1.956982	-2.655410	1.526850
F	2.073609	-0.593799	2.657226	2.099236	-0.547591	2.669121	2.073839	-0.563069	2.662096
P	-0.024507	-0.409071	-0.660987	-0.035023	-0.360475	-0.686494	-0.026078	-0.389450	-0.671329
F	-0.432859	-0.414493	-2.246852	-0.462646	-0.494492	-2.279128	-0.437336	-0.466072	-2.258488
F	0.015059	-2.114626	-0.676456	0.029650	-2.088628	-0.603035	0.024968	-2.103926	-0.632262
C	-3.346258	-0.606766	2.177529	-3.300122	-0.571160	2.201894	-3.329853	-0.590652	2.185162
H	-4.422431	-0.494804	2.118500	-4.387422	-0.482713	2.158347	-4.408813	-0.483851	2.131586
C	-2.593084	-1.799518	1.886314	-2.521628	-1.755721	1.908702	-2.572007	-1.781557	1.893586
H	-3.004885	-2.756306	1.581897	-2.920895	-2.735339	1.631477	-2.982178	-2.743901	1.597361
C	-1.214976	-1.522029	2.093275	-1.133469	-1.440546	2.076874	-1.190999	-1.495905	2.088240
H	-0.409888	-2.229356	1.937909	-0.311185	-2.137467	1.909506	-0.382594	-2.200828	1.926920
C	-2.413755	0.393084	2.573785	-2.375121	0.468906	2.547719	-2.397530	0.418670	2.566201
H	-2.661228	1.407698	2.869689	-2.641664	1.489377	2.837262	-2.648259	1.435121	2.860428
C	-1.093387	-0.153777	2.506339	-1.033253	-0.054334	2.463680	-1.072888	-0.123635	2.493258
H	-0.179416	0.368884	2.756969	-0.119534	0.500049	2.681616	-0.158048	0.406442	2.733690
C	2.353717	-1.249568	-2.390705	2.304644	-1.253767	-2.369838	2.344121	-1.261170	-2.374346
H	1.535296	-1.865139	-2.741639	1.473390	-1.869006	-2.716696	1.522547	-1.879090	-2.719834
C	3.428477	-1.685623	-1.569074	3.392642	-1.699714	-1.550772	3.421947	-1.693240	-1.550337
H	3.593592	-2.703770	-1.231699	3.546828	-2.724416	-1.201528	3.584660	-2.710495	-1.202745
C	4.275747	-0.549959	-1.294550	4.262688	-0.568509	-1.292140	4.273848	-0.557036	-1.286995
H	5.181390	-0.552533	-0.698754	5.176471	-0.577088	-0.693888	5.180997	-0.556928	-0.689876

C	2.504442	0.155899	-2.617479	2.471389	0.157460	-2.608737	2.498329	0.143676	-2.613479
H	1.831995	0.786380	-3.186937	1.794995	0.799657	-3.176165	1.824342	0.772996	-3.186246
C	3.708831	0.571955	-1.958716	3.693464	0.567800	-1.952037	3.706045	0.563409	-1.957703
H	4.112749	1.579619	-1.956265	4.114543	1.577216	-1.962694	4.113335	1.571845	-1.965260
F	-0.047529	1.505561	-0.854967	-0.050601	1.463728	-0.999774	-0.051737	1.477272	-0.935126

Table S19. Cartesian coordinates (Å) and energies (in hartree) for the optimized structure $\mathbf{TS_{mig}}$.

	B3LYP (-6120.02582)			BP86 (-6120.55811)			B3LYP* (-6118.35829)		
	X	Y	Z	X	Y	Z	X	Y	Z
Fe	-2.214593	0.059131	0.592798	-2.198622	0.046638	0.606247	-2.207826	0.056706	0.594859
Fe	2.030894	-0.126365	-0.583237	2.008207	-0.124560	-0.590637	2.022298	-0.126219	-0.583868
P	2.233671	1.826233	0.247214	2.239046	1.794958	0.237044	2.227335	1.816650	0.244499
P	3.116223	-1.174605	0.903958	3.110869	-1.154183	0.858236	3.112060	-1.167067	0.892246
P	-2.652437	-1.500935	-0.876442	-2.637884	-1.449796	-0.880020	-2.644901	-1.487208	-0.876529
P	-2.089865	1.660240	-0.748520	-2.090605	1.650870	-0.699852	-2.080267	1.655778	-0.737028
F	2.835458	2.093072	1.680404	2.880579	2.046062	1.676258	2.839258	2.081371	1.677913
F	3.210075	2.792313	-0.557045	3.219626	2.779386	-0.579260	3.199451	2.790024	-0.564018
F	1.013448	2.831552	0.314332	1.023357	2.830648	0.345481	1.005320	2.825240	0.324425
F	3.068320	-2.753749	0.891300	3.096697	-2.753823	0.834965	3.071476	-2.750574	0.880579
F	2.957471	-0.938855	2.449474	2.969066	-0.937610	2.426488	2.957860	-0.932625	2.442169
F	0.489799	0.562962	1.856823	0.492661	0.542417	1.883024	0.489538	0.553293	1.866170
F	-2.205777	-1.496670	-2.398664	-2.175621	-1.431308	-2.418997	-2.194126	-1.479231	-2.401969
F	-2.694340	-3.044337	-0.548880	-2.743441	-3.017539	-0.584284	-2.703991	-3.036101	-0.557263
F	-4.223982	-1.428517	-1.226468	-4.218479	-1.328632	-1.265378	-4.218135	-1.402051	-1.234879
F	-3.386110	2.018648	-1.596915	-3.416893	2.016795	-1.535313	-3.379533	2.019706	-1.586076
F	-1.842010	3.119493	-0.182730	-1.849804	3.126331	-0.116472	-1.831588	3.118288	-0.168124
F	-1.060418	1.724667	-1.960260	-1.076356	1.753077	-1.947102	-1.051078	1.725452	-1.954544
P	0.033351	-0.517782	0.577508	0.036187	-0.527941	0.592078	0.034073	-0.522571	0.583515
F	0.255514	-1.766958	1.609759	0.275932	-1.803332	1.613481	0.260053	-1.778236	1.611381
F	-0.503289	-1.901468	-0.647394	-0.523338	-1.928782	-0.642269	-0.507972	-1.909527	-0.644964
F	4.698943	-1.033325	0.837082	4.709696	-0.984682	0.781200	4.698111	-1.021100	0.821879
C	3.291196	0.248770	-2.275337	3.254259	0.260036	-2.274195	3.275997	0.252472	-2.275291
H	4.175552	0.875299	-2.267092	4.147358	0.888473	-2.268690	4.161373	0.881015	-2.268308
C	1.944130	0.675840	-2.557582	1.897592	0.695467	-2.541018	1.926178	0.679476	-2.552302
H	1.633036	1.682163	-2.816199	1.585366	1.712026	-2.792758	1.612974	1.687789	-2.808987
C	1.092979	-0.460429	-2.470145	1.034374	-0.444925	-2.444292	1.073970	-0.458618	-2.461683
H	0.023612	-0.470870	-2.621697	-0.044566	-0.450029	-2.589707	0.002256	-0.469185	-2.610892
C	3.249281	-1.150878	-2.023935	3.208034	-1.148470	-2.015876	3.235257	-1.148854	-2.021511
H	4.106901	-1.775327	-1.792619	4.072460	-1.782304	-1.796910	4.095536	-1.774336	-1.793552
C	1.887669	-1.592282	-2.114781	1.833698	-1.588663	-2.100267	1.871379	-1.591630	-2.109451
H	1.517000	-2.594880	-1.944936	1.458615	-2.597805	-1.926208	1.500695	-2.595943	-1.937048
C	-2.391127	1.114349	2.430300	-2.354419	1.068313	2.449516	-2.376345	1.100990	2.434671
H	-1.753265	1.942181	2.715187	-1.707629	1.894742	2.749375	-1.731423	1.924187	2.724637
C	-3.642362	1.198078	1.723202	-3.607828	1.168524	1.728055	-3.626159	1.197004	1.722706
H	-4.127475	2.111224	1.392040	-4.094895	2.096007	1.413215	-4.105664	2.117104	1.396202
C	-4.138633	-0.117398	1.529545	-4.113365	-0.152113	1.510054	-4.131743	-0.116132	1.520049

H	-5.047731	-0.385005	1.003852	-5.028476	-0.409630	0.972887	-5.042295	-0.375508	0.988678
C	-2.144925	-0.263524	2.702461	-2.108054	-0.324649	2.693067	-2.138238	-0.282041	2.697663
H	-1.274335	-0.660381	3.208915	-1.235493	-0.736920	3.201969	-1.269983	-0.688613	3.204872
C	-3.201165	-1.031108	2.132985	-3.173627	-1.084301	2.104160	-3.200182	-1.040303	2.120763
H	-3.291442	-2.111546	2.170566	-3.263276	-2.173622	2.117072	-3.296718	-2.122479	2.150278

Table S20. Cartesian coordinates (Å) and energies (in hartree) for the optimized structure **25-3S**.

	B3LYP (-6120.02234)			BP86 (-6120.55438)			B3LYP* (-6118.35478)		
	X	Y	Z	X	Y	Z	X	Y	Z
Fe	0.299571	-2.260447	0.441944	0.318670	-2.251402	0.449300	0.303918	-2.254601	0.442053
Fe	-0.299571	2.260447	0.441944	-0.318670	2.251402	0.449300	-0.303918	2.254601	0.442053
P	-1.428974	1.932713	-1.307876	-1.448708	1.914879	-1.272258	-1.430712	1.921894	-1.299665
P	1.621674	2.419111	-0.450032	1.545779	2.446719	-0.478629	1.603084	2.417466	-0.454744
P	-1.621674	-2.419111	-0.450032	-1.545779	-2.446719	-0.478629	-1.603084	-2.417466	-0.454744
P	1.428974	-1.932713	-1.307876	1.448708	-1.914879	-1.272258	1.430712	-1.921894	-1.299665
F	-1.751777	3.226269	-2.176338	-1.838703	3.230342	-2.116824	-1.766630	3.218645	-2.165946
F	-2.920249	1.420082	-1.204589	-2.939946	1.344368	-1.168972	-2.922820	1.398793	-1.196476
F	-0.944892	1.010460	-2.493681	-0.945376	1.037411	-2.505708	-0.942958	1.006195	-2.493625
F	2.244039	1.348971	-1.424525	2.175468	1.400513	-1.502072	2.230242	1.346656	-1.431349
F	2.883779	2.696911	0.457166	2.848824	2.729539	0.405707	2.871704	2.702146	0.448928
F	1.812017	3.681438	-1.402991	1.698421	3.745416	-1.421122	1.787881	3.681597	-1.412594
F	-2.244039	-1.348971	-1.424525	-2.175468	-1.400513	-1.502072	-2.230242	-1.346656	-1.431349
F	-2.883779	-2.696911	0.457166	-2.848824	-2.729539	0.405707	-2.871704	-2.702146	0.448928
F	-1.812017	-3.681438	-1.402991	-1.698421	-3.745416	-1.421122	-1.787881	-3.681597	-1.412594
F	1.751777	-3.226269	-2.176338	1.838703	-3.230342	-2.116824	1.766630	-3.218645	-2.165946
F	2.920249	-1.420082	-1.204589	2.939946	-1.344368	-1.168972	2.922820	-1.398793	-1.196476
F	0.944892	-1.010460	-2.493681	0.945376	-1.037411	-2.505708	0.942958	-1.006195	-2.493625
P	0.000000	0.000000	1.063637	0.000000	0.000000	1.084816	0.000000	0.000000	1.071429
F	0.000000	0.000000	2.707201	0.000000	0.000000	2.748066	0.000000	0.000000	2.718862
F	1.756824	0.246397	1.162993	1.754802	0.253133	1.183587	1.755687	0.247329	1.172428
C	-1.013010	4.256410	0.809773	-1.018559	4.241119	0.802605	-1.018360	4.247773	0.803169
H	-1.177668	5.009258	0.047214	-1.177646	4.994333	0.027785	-1.184186	4.998653	0.036127
C	-1.976267	3.297484	1.289611	-1.988899	3.278708	1.281332	-1.980426	3.286860	1.285105
H	-3.004862	3.202412	0.957340	-3.026226	3.188977	0.947167	-3.010992	3.189550	0.952925
C	-1.355103	2.500860	2.287828	-1.365634	2.466591	2.283546	-1.356317	2.490229	2.285113
H	-1.812005	1.668004	2.805729	-1.832438	1.631655	2.806837	-1.813091	1.656485	2.805914
C	0.192896	4.042095	1.534897	0.199997	4.010034	1.522499	0.191461	4.033408	1.525768
H	1.109733	4.612258	1.420997	1.125623	4.581805	1.409554	1.109221	4.605470	1.409987
C	0.000000	2.941352	2.431677	0.000000	2.904002	2.429157	0.000000	2.932893	2.427074
H	0.740686	2.522924	3.102090	0.746423	2.477734	3.101561	0.743718	2.514759	3.097565
C	1.355103	-2.500860	2.287828	1.365634	-2.466591	2.283546	1.356317	-2.490229	2.285113
H	1.812005	-1.668004	2.805729	1.832438	-1.631655	2.806837	1.813091	-1.656485	2.805914
C	1.976267	-3.297484	1.289611	1.988899	-3.278708	1.281332	1.980426	-3.286860	1.285105
H	3.004862	-3.202412	0.957340	3.026226	-3.188977	0.947167	3.010992	-3.189550	0.952925
C	1.013010	-4.256410	0.809773	1.018559	-4.241119	0.802605	1.018360	-4.247773	0.803169
H	1.177668	-5.009258	0.047214	1.177646	-4.994333	0.027785	1.184186	-4.998653	0.036127

C	0.000000	-2.941352	2.431677	0.000000	-2.904002	2.429157	0.000000	-2.932893	2.427074
H	-0.740686	-2.522924	3.102090	-0.746423	-2.477734	3.101561	-0.743718	-2.514759	3.097565
C	-0.192896	-4.042095	1.534897	-0.199997	-4.010034	1.522499	-0.191461	-4.033408	1.525768
H	-1.109733	-4.612258	1.420997	-1.125623	-4.581805	1.409554	-1.109221	-4.605470	1.409987
F	-1.756824	-0.246397	1.162993	-1.754802	-0.253133	1.183587	-1.755687	-0.247329	1.172428

Table S21. Cartesian coordinates (Å) and energies (in hartree) for the optimized structure **25-4S**.

	B3LYP (-6120.01871)			BP86 (-6120.55119)			B3LYP* (-6118.35098)		
	X	Y	Z	X	Y	Z	X	Y	Z
Fe	2.295262	-0.287839	-0.499288	2.258508	-0.314907	-0.498648	2.285410	-0.293291	-0.497498
Fe	-1.837582	0.375083	-0.522285	-1.823224	0.339916	-0.554610	-1.826528	0.369807	-0.526538
P	-1.792567	1.219924	1.415501	-1.734252	1.329241	1.285266	-1.777171	1.228959	1.396195
P	-3.275247	-1.296857	0.111349	-3.260289	-1.250280	0.234951	-3.268824	-1.284600	0.125737
P	2.104704	1.761802	-0.059516	2.119219	1.726725	-0.100952	2.097200	1.752104	-0.072683
P	2.668705	-0.948778	1.486418	2.649956	-0.902871	1.478485	2.658771	-0.932822	1.485539
F	-3.050402	1.262834	2.364125	-3.020453	1.611182	2.186588	-3.035249	1.279788	2.350966
F	-1.460688	2.776037	1.499918	-1.231821	2.863263	1.251930	-1.449079	2.790765	1.466837
F	-0.752170	0.716997	2.502126	-0.779059	0.820053	2.466084	-0.732578	0.738905	2.489905
F	-3.460273	-1.906760	1.577977	-3.380238	-1.753084	1.764198	-3.451192	-1.875071	1.603559
F	-4.351539	-1.943689	-0.896702	-4.404771	-1.962314	-0.682474	-4.351966	-1.941048	-0.874682
F	-4.484729	-0.185184	0.509155	-4.445685	-0.090340	0.600898	-4.474826	-0.162891	0.511650
F	1.362455	2.297741	1.221477	1.656629	2.312067	1.306456	1.359702	2.303155	1.208990
F	1.450280	2.737471	-1.129047	1.268036	2.706943	-1.049110	1.441412	2.726493	-1.149820
F	3.453734	2.576306	0.113105	3.493135	2.551991	-0.223546	3.450832	2.569431	0.089511
F	4.128978	-0.644315	2.027063	4.125643	-0.553910	2.008538	4.122574	-0.621448	2.024465
F	2.665135	-2.494065	1.787220	2.684584	-2.457089	1.833571	2.659696	-2.479061	1.803052
F	1.866460	-0.437709	2.732827	1.850089	-0.370378	2.738435	1.857218	-0.412047	2.732706
P	0.019959	-0.841466	-0.358645	-0.012371	-0.856883	-0.317239	0.013777	-0.846357	-0.350999
F	0.010247	-1.810767	0.941854	-0.014558	-1.763878	1.046849	0.004968	-1.806937	0.959701
F	-0.050483	-1.992962	-1.500714	-0.083683	-2.097970	-1.395176	-0.056257	-2.013457	-1.483624
F	-2.304784	-2.605081	-0.244778	-2.322464	-2.604678	-0.081686	-2.304130	-2.602545	-0.217694
C	-3.337016	0.746033	-2.028538	-3.344818	0.526475	-2.047613	-3.327991	0.718448	-2.028583
H	-4.311943	0.274596	-2.042850	-4.311610	0.019926	-2.036268	-4.304602	0.245798	-2.039608
C	-3.017911	1.960661	-1.367145	-3.070622	1.810155	-1.478887	-3.009827	1.942876	-1.380067
H	-3.714895	2.579524	-0.813336	-3.794980	2.440454	-0.957902	-3.708297	2.566260	-0.829368
C	-1.616935	2.225889	-1.580185	-1.672467	2.110476	-1.713077	-1.607666	2.207348	-1.595652
H	-1.067472	3.087469	-1.221290	-1.147752	3.016649	-1.406212	-1.057101	3.073134	-1.242603
C	-2.145380	0.224440	-2.625658	-2.127821	0.006643	-2.618245	-2.134537	0.191821	-2.622231
H	-2.064283	-0.700348	-3.185227	-2.016105	-0.960136	-3.113616	-2.052603	-0.741000	-3.172100
C	-1.092748	1.163713	-2.365058	-1.100135	1.005974	-2.422491	-1.080804	1.135731	-2.370084
H	-0.065731	1.079634	-2.701976	-0.062228	0.941756	-2.757951	-0.052097	1.050485	-2.707903
C	2.772663	-1.953234	-1.732877	2.703074	-2.026861	-1.648240	2.758300	-1.968887	-1.710796
H	2.306540	-2.927334	-1.649944	2.241414	-3.005564	-1.507246	2.292273	-2.944192	-1.616039
C	3.963223	-1.522110	-1.068057	3.914524	-1.554463	-1.022917	3.951621	-1.528466	-1.051146
H	4.563912	-2.123651	-0.392680	4.540055	-2.126894	-0.331725	4.555861	-2.123599	-0.370072
C	4.229692	-0.171387	-1.435696	4.170594	-0.216596	-1.466921	4.217525	-0.180773	-1.435941

H	5.055661	0.437982	-1.086710	5.001690	0.420084	-1.155898	5.043510	0.435216	-1.092433
C	2.319630	-0.868854	-2.552559	2.221628	-0.975815	-2.509534	2.301297	-0.892116	-2.540884
H	1.453058	-0.892350	-3.201370	1.337840	-1.036441	-3.146070	1.432111	-0.923729	-3.189142
C	3.210797	0.225981	-2.369693	3.116962	0.140129	-2.392239	3.193377	0.207328	-2.370360
H	3.146079	1.188269	-2.867967	3.036368	1.087556	-2.933069	3.125792	1.166856	-2.877881

Table S22. Cartesian coordinates (Å) and energies (in hartree) for the optimized structure **24-1S**.

	B3LYP (-5478.94162)			BP86 (-5479.46227)			B3LYP* (-5477.49550)		
	X	Y	Z	X	Y	Z	X	Y	Z
C	-0.666238	3.430457	-0.553798	-0.644073	3.406302	-0.544316	-0.647186	3.424549	-0.553608
H	-0.049814	4.176710	-1.041037	-0.027545	4.165190	-1.030424	-0.027866	4.170551	-1.041996
C	-0.827314	3.259420	0.845857	-0.803328	3.220825	0.864661	-0.807625	3.252223	0.848073
H	-0.353829	3.860034	1.615254	-0.334996	3.826967	1.644674	-0.332324	3.852814	1.619192
C	-1.722008	2.155657	1.066857	-1.707838	2.108161	1.078214	-1.708401	2.149996	1.068776
H	-2.054470	1.790709	2.030817	-2.040043	1.733103	2.047759	-2.041524	1.784126	2.034452
C	-1.477784	2.437201	-1.211564	-1.460335	2.409395	-1.211802	-1.463069	2.432503	-1.212020
H	-1.592961	2.314632	-2.282362	-1.570680	2.288812	-2.291657	-1.577505	2.308850	-2.284796
C	-2.141245	1.673589	-0.208109	-2.126174	1.629046	-0.207972	-2.129843	1.669060	-0.207644
H	-2.861012	0.884945	-0.375463	-2.848418	0.831928	-0.383104	-2.853468	0.881161	-0.375601
Fe	0.000688	1.493417	-0.007698	0.006380	1.478702	-0.004624	0.009292	1.488307	-0.007035
P	1.379672	1.337112	-1.577851	1.373774	1.348749	-1.564036	1.382854	1.331224	-1.573589
P	1.362907	1.423883	1.580835	1.366116	1.435743	1.562746	1.367928	1.416934	1.576222
F	0.865191	1.091841	3.053875	0.866837	1.153618	3.066323	0.870297	1.088350	3.054415
F	2.713683	0.583112	1.629003	2.728541	0.578505	1.642219	2.720099	0.570615	1.626993
F	2.045241	2.818408	1.966551	2.082065	2.845680	1.906664	2.058265	2.812101	1.960764
F	1.462453	2.599941	-2.550680	1.417617	2.606821	-2.576817	1.463069	2.591352	-2.556383
F	1.379672	0.263412	-2.760157	1.417617	0.245548	-2.746468	1.385998	0.249339	-2.754621
F	2.945809	1.234853	-1.274957	2.962082	1.309301	-1.260854	2.953669	1.233765	-1.272202
C	0.666238	-3.430457	-0.553798	0.644073	-3.406302	-0.544316	0.647186	-3.424549	-0.553608
H	0.049814	-4.176710	-1.041037	0.027545	-4.165190	-1.030424	0.027866	-4.170551	-1.041996
C	0.827314	-3.259420	0.845857	0.803328	-3.220825	0.864661	0.807625	-3.252223	0.848073
H	0.353829	-3.860034	1.615254	0.334996	-3.826967	1.644674	0.332324	-3.852814	1.619192
C	1.722008	-2.155657	1.066857	1.707838	-2.108161	1.078214	1.708401	-2.149996	1.068776
H	2.054470	-1.790709	2.030817	2.040043	-1.733103	2.047759	2.041524	-1.784126	2.034452
C	1.477784	-2.437201	-1.211564	1.460335	-2.409395	-1.211802	1.463069	-2.432503	-1.212020
H	1.592961	-2.314632	-2.282362	1.570680	-2.288812	-2.291657	1.577505	-2.308850	-2.284796
C	2.141245	-1.673589	-0.208109	2.126174	-1.629046	-0.207972	2.129843	-1.669060	-0.207644
H	2.861012	-0.884945	-0.375463	2.848418	-0.831928	-0.383104	2.853468	-0.881161	-0.375601
Fe	-0.000688	-1.493417	-0.007698	-0.006380	-1.478702	-0.004624	-0.009292	-1.488307	-0.007035
P	-1.379672	-1.337112	-1.577851	-1.373774	-1.348749	-1.564036	-1.382854	-1.331224	-1.573589
P	-1.362907	-1.423883	1.580835	-1.366116	-1.435743	1.562746	-1.367928	-1.416934	1.576222
F	-0.865191	-1.091841	3.053875	-0.866837	-1.153618	3.066323	-0.870297	-1.088350	3.054415
F	-2.713683	-0.583112	1.629003	-2.728541	-0.578505	1.642219	-2.720099	-0.570615	1.626993
F	-2.045241	-2.818408	1.966551	-2.082065	-2.845680	1.906664	-2.058265	-2.812101	1.960764
F	-1.462453	-2.599941	-2.550680	-1.417617	-2.606821	-2.576817	-1.463069	-2.591352	-2.556383
F	-1.379672	-0.263412	-2.760157	-1.417617	-0.245548	-2.746468	-1.385998	-0.249339	-2.754621
F	-2.945809	-1.234853	-1.274957	-2.962082	-1.309301	-1.260854	-2.953669	-1.233765	-1.272202

Table S23. Cartesian coordinates (Å) and energies (in hartree) for the optimized structure **24-2S**.

	B3LYP (-5478.93384)			BP86 (-5479.45431)			B3LYP* (-5477.48739)		
	X	Y	Z	X	Y	Z	X	Y	Z
C	0.793576	3.366318	-1.171080	0.870923	3.318441	-1.134307	0.787195	3.359135	-1.160649
H	1.088025	4.184668	-0.522339	1.187618	4.133918	-0.478425	1.079655	4.179162	-0.509791
C	-0.489827	3.189655	-1.750893	-0.424412	3.176994	-1.725499	-0.496485	3.180517	-1.744750
H	-1.350437	3.832181	-1.602868	-1.275688	3.844830	-1.575283	-1.360522	3.821920	-1.597255
C	-0.443516	1.999753	-2.558292	-0.398305	1.989915	-2.553591	-0.444881	1.990979	-2.555568
H	-1.261857	1.619524	-3.159507	-1.230838	1.632205	-3.164706	-1.263076	1.608945	-3.159533
C	1.642779	2.287169	-1.610295	1.704859	2.218646	-1.589210	1.641507	2.281533	-1.601978
H	2.681491	2.144415	-1.340584	2.746615	2.047560	-1.313856	2.681594	2.139709	-1.328950
C	0.876973	1.463072	-2.479633	0.917571	1.414562	-2.472969	0.878537	1.455939	-2.475068
H	1.241043	0.580132	-2.985359	1.268043	0.523884	-2.993295	1.246976	0.573737	-2.983294
Fe	-0.027155	1.511175	-0.531686	0.010254	1.489839	-0.541652	-0.029005	1.504678	-0.532316
P	0.653991	2.027035	1.392441	0.656080	2.012037	1.372737	0.644910	2.021683	1.387110
P	-2.000848	1.083638	-0.020819	-1.960434	1.118217	-0.025416	-1.998474	1.079217	-0.022614
F	-3.000082	0.315432	-1.004393	-3.013658	0.409722	-1.030421	-3.002959	0.314744	-1.011017
F	-2.467079	0.415810	1.345154	-2.458579	0.434071	1.341747	-2.469045	0.405361	1.343046
F	-2.952434	2.367462	0.111900	-2.870267	2.448746	0.150908	-2.950236	2.366530	0.115742
F	0.066036	3.400034	1.957069	0.010254	3.378801	1.943288	0.036694	3.387378	1.958924
F	2.183745	2.430890	1.554110	2.188396	2.471826	1.553579	2.172578	2.449331	1.548122
F	0.489827	1.214117	2.734084	0.508562	1.196758	2.735583	0.496485	1.203814	2.731813
C	-0.793576	-3.366318	-1.171080	-0.870923	-3.318441	-1.134307	-0.787195	-3.359135	-1.160649
H	-1.088025	-4.184668	-0.522339	-1.187618	-4.133918	-0.478425	-1.079655	-4.179162	-0.509791
C	0.489827	-3.189655	-1.750893	0.424412	-3.176994	-1.725499	0.496485	-3.180517	-1.744750
H	1.350437	-3.832181	-1.602868	1.275688	-3.844830	-1.575283	1.360522	-3.821920	-1.597255
C	0.443516	-1.999753	-2.558292	0.398305	-1.989915	-2.553591	0.444881	-1.990979	-2.555568
H	1.261857	-1.619524	-3.159507	1.230838	-1.632205	-3.164706	1.263076	-1.608945	-3.159533
C	-1.642779	-2.287169	-1.610295	-1.704859	-2.218646	-1.589210	-1.641507	-2.281533	-1.601978
H	-2.681491	-2.144415	-1.340584	-2.746615	-2.047560	-1.313856	-2.681594	-2.139709	-1.328950
C	-0.876973	-1.463072	-2.479633	-0.917571	-1.414562	-2.472969	-0.878537	-1.455939	-2.475068
H	-1.241043	-0.580132	-2.985359	-1.268043	-0.523884	-2.993295	-1.246976	-0.573737	-2.983294
Fe	0.027155	-1.511175	-0.531686	-0.010254	-1.489839	-0.541652	0.029005	-1.504678	-0.532316
P	-0.653991	-2.027035	1.392441	-0.656080	-2.012037	1.372737	-0.644910	-2.021683	1.387110
P	2.000848	-1.083638	-0.020819	1.960434	-1.118217	-0.025416	1.998474	-1.079217	-0.022614
F	3.000082	-0.315432	-1.004393	3.013658	-0.409722	-1.030421	3.002959	-0.314744	-1.011017
F	2.467079	-0.415810	1.345154	2.458579	-0.434071	1.341747	2.469045	-0.405361	1.343046
F	2.952434	-2.367462	0.111900	2.870267	-2.448746	0.150908	2.950236	-2.366530	0.115742
F	-0.066036	-3.400034	1.957069	-0.010254	-3.378801	1.943288	-0.036694	-3.387378	1.958924
F	-2.183745	-2.430890	1.554110	-2.188396	-2.471826	1.553579	-2.172578	-2.449331	1.548122
F	-0.489827	-1.214117	2.734084	-0.508562	-1.196758	2.735583	-0.496485	-1.203814	2.731813

Table S24. Cartesian coordinates (Å) and energies (in hartree) for the optimized structure **23-1T**.

	B3LYP (-4837.86565)			BP86 (-4838.33784)			B3LYP* (-4836.62819)		
	X	Y	Z	X	Y	Z	X	Y	Z
C	2.488013	-0.441952	2.187731	2.321135	-0.648346	2.201954	2.430574	-0.471949	2.193843
H	3.521898	-0.115292	2.159605	3.392038	-0.429233	2.210389	3.475628	-0.175662	2.167278
C	2.010408	-1.735111	1.860210	1.718605	-1.900223	1.863127	1.916280	-1.757516	1.879071
H	2.614394	-2.579649	1.545982	2.244226	-2.810365	1.563764	2.497624	-2.624801	1.577605
C	0.577666	-1.739720	2.031750	0.282477	-1.757423	2.004642	0.482748	-1.718518	2.044152
H	-0.075626	-2.591258	1.883441	-0.456046	-2.543059	1.830024	-0.196137	-2.552835	1.898618
C	1.351786	0.368893	2.560224	1.257479	0.279410	2.552970	1.315981	0.376252	2.553146
H	1.388532	1.405439	2.877222	1.394623	1.322108	2.849074	1.381640	1.417498	2.856572
C	0.183729	-0.447282	2.493442	0.001998	-0.413011	2.442945	0.121729	-0.405816	2.484639
H	-0.822108	-0.145288	2.762806	-0.980501	-0.016825	2.712929	-0.877507	-0.073482	2.751158
Fe	1.102070	-0.297117	0.557727	1.003374	-0.386154	0.579102	1.063277	-0.311440	0.568681
P	1.128134	-1.523813	-1.134746	0.873838	-1.544591	-1.128982	1.066162	-1.543145	-1.109252
F	0.236748	-1.276597	-2.430060	-0.020482	-1.173542	-2.420791	0.185058	-1.286752	-2.415916
F	0.825688	-3.073411	-0.950402	0.432429	-3.086044	-0.997587	0.731656	-3.089992	-0.918376
F	2.502779	-1.707025	-1.922112	2.220785	-1.824083	-1.975999	2.441160	-1.761431	-1.896755
C	-1.164785	2.837341	0.516520	-0.530360	2.929144	-0.048576	-1.047546	2.846592	0.503851
H	-0.365029	3.208688	1.146550	0.465902	3.322323	0.159904	-0.236181	3.198699	1.133122
C	-2.473832	2.466339	0.939416	-1.594857	2.806952	0.907440	-2.365114	2.507605	0.928227
H	-2.841295	2.452697	1.960876	-1.521267	3.016413	1.978696	-2.733693	2.502497	1.951412
C	-3.219996	2.094669	-0.218618	-2.747760	2.310257	0.224813	-3.115740	2.136967	-0.229227
H	-4.245911	1.740348	-0.225799	-3.728905	2.115256	0.665592	-4.149794	1.800809	-0.235776
C	-1.112537	2.712656	-0.921623	-1.041918	2.553192	-1.344617	-0.996803	2.714650	-0.936279
H	-0.278920	2.988087	-1.557250	-0.467282	2.541824	-2.274129	-0.153774	2.966167	-1.572446
C	-2.389466	2.262651	-1.367172	-2.406223	2.159701	-1.183212	-2.281240	2.286741	-1.381232
H	-2.679676	2.068744	-2.394815	-3.088046	1.828277	-1.970431	-2.574830	2.088990	-2.409172
Fe	-1.368837	0.734934	-0.041794	-1.189448	0.812480	-0.014113	-1.310523	0.756804	-0.047383
P	-2.418832	-1.121683	0.039238	-2.494607	-0.813527	0.053444	-2.418522	-1.051832	0.028734
F	-2.067416	-2.378821	-0.867505	-2.334302	-2.169230	-0.796129	-2.101906	-2.334866	-0.859417
F	-3.977573	-1.097990	-0.279497	-4.030676	-0.536756	-0.359785	-3.974932	-0.976343	-0.316966
F	-2.534748	-1.911410	1.423860	-2.834733	-1.523529	1.469998	-2.589425	-1.823743	1.422411
P	2.049703	1.329616	-0.332752	2.204751	1.044868	-0.287386	2.068757	1.258405	-0.336935
F	3.645463	1.321528	-0.347649	3.757867	0.676003	-0.533709	3.668572	1.196401	-0.343647
F	1.864440	1.726865	-1.863821	1.976118	1.695275	-1.746914	1.910243	1.639648	-1.880082
F	1.930030	2.802585	0.277158	2.528547	2.425200	0.505296	2.005605	2.751655	0.247472

Table S25. Cartesian coordinates (Å) and energies (in hartree) for the optimized structure **23-2T**.

	B3LYP (-4837.85741)			BP86 (-4838.32640)			B3LYP* (-4836.61889)		
	X	Y	Z	X	Y	Z	X	Y	Z
C	-2.266589	2.550030	0.951116	2.215894	2.092970	-1.519275	-2.194547	2.555678	0.927719
H	-2.482610	2.560431	2.014568	2.602926	1.751397	-2.482633	-2.414221	2.572386	1.992233
C	-3.174344	2.180111	-0.080771	2.931129	2.059001	-0.265731	-3.091049	2.149721	-0.103111
H	-4.198924	1.853196	0.064611	3.956763	1.704588	-0.130243	-4.112151	1.807309	0.044280
C	-2.505753	2.292218	-1.336962	2.090505	2.602141	0.758549	-2.420806	2.257736	-1.361948
H	-2.939623	2.081164	-2.309221	2.344964	2.679769	1.818964	-2.848055	2.019754	-2.332978
C	-1.016150	2.870467	0.344227	0.905503	2.603138	-1.256055	-0.946061	2.880698	0.320306
H	-0.140659	3.241619	0.863646	0.125479	2.771825	-2.001962	-0.074203	3.265968	0.838959
C	-1.167129	2.711595	-1.085981	0.823813	2.907043	0.169231	-1.089180	2.697448	-1.111203
H	-0.425704	2.935938	-1.844697	-0.020674	3.359960	0.691270	-0.344347	2.913878	-1.871137
Fe	-1.304834	0.776480	-0.129980	1.095457	0.802251	-0.147953	-1.223562	0.788922	-0.126411
P	-2.431652	-1.054969	0.092404	2.323004	-0.921049	0.044112	-2.383909	-1.013351	0.095659
F	-2.093034	-2.199067	1.137884	1.967728	-2.445332	-0.302992	-2.075076	-2.184600	1.123360
F	-2.695381	-1.979461	-1.170527	3.014491	-1.185273	1.471387	-2.688275	-1.910213	-1.181790
F	-3.956168	-0.873213	0.511791	3.689858	-0.877774	-0.814676	-3.904098	-0.793712	0.532224
C	2.156430	2.279669	-0.554763	-2.216791	2.200450	-0.418776	2.147829	2.252293	-0.554818
H	1.487316	3.111881	-0.726512	-1.665841	3.092392	-0.717376	1.508324	3.106546	-0.740634
C	2.632211	1.373198	-1.544288	-2.538547	1.807288	0.923214	2.617434	1.330248	-1.535870
H	2.412305	1.412546	-2.606090	-2.258401	2.334149	1.839725	2.407237	1.366315	-2.601799
C	3.537039	0.444992	-0.900065	-3.370421	0.616092	0.853993	3.494060	0.384699	-0.876210
H	4.072193	-0.360959	-1.389256	-3.783548	0.075388	1.708152	4.016129	-0.438358	-1.354960
C	2.692073	1.883287	0.703081	-2.791431	1.237333	-1.310521	2.664254	1.852621	0.712205
H	2.529518	2.377095	1.655281	-2.731741	1.252364	-2.401838	2.499420	2.353627	1.662539
C	3.572547	0.756650	0.476566	-3.524908	0.262402	-0.517127	3.521749	0.704443	0.501714
H	4.143393	0.237197	1.237621	-4.084600	-0.590351	-0.907084	4.072386	0.174960	1.273354
Fe	1.556772	0.257545	-0.079793	-1.475407	0.229366	0.003145	1.518852	0.244889	-0.076425
P	0.968324	-1.254434	-1.395905	-0.744653	-0.623523	1.736595	0.926888	-1.256564	-1.385570
F	0.217078	-2.578116	-0.944564	0.049217	-2.018425	1.811134	0.176453	-2.586549	-0.935895
F	2.120434	-1.970582	-2.237233	-1.825480	-0.991391	2.889195	2.079199	-1.976560	-2.235322
F	0.050594	-0.930920	-2.664625	0.216211	0.198234	2.759028	0.008193	-0.938787	-2.662408
P	1.071856	-0.593094	1.772001	-1.009330	-1.220625	-1.399832	1.016254	-0.591759	1.764387
F	0.756560	-2.135383	1.951733	-0.753558	-2.755944	-1.018918	0.678602	-2.132599	1.950912
F	2.183955	-0.483726	2.911047	-2.145367	-1.497298	-2.521592	2.126888	-0.493742	2.914402
F	-0.128209	-0.055156	2.686015	0.199076	-1.104878	-2.480355	-0.179515	-0.037671	2.687186

Table S26. Cartesian coordinates (Å) and energies (in hartree) for the optimized structure **23-1S**.

	B3LYP (-4837.83855)			BP86 (-4838.33334)			B3LYP* (-4836.60917)		
	X	Y	Z	X	Y	Z	X	Y	Z
C	-2.422245	2.195829	0.833961	-2.436586	2.049295	0.983131	-2.445681	2.138914	0.877182
H	-2.800190	2.220881	1.850152	-2.830468	1.970656	1.999041	-2.835255	2.126400	1.891282
C	-3.099210	1.670577	-0.294430	-3.086568	1.607467	-0.207564	-3.102748	1.638527	-0.276268
H	-4.092491	1.237276	-0.305107	-4.072339	1.142380	-0.273962	-4.090579	1.189466	-0.312260
C	-2.220152	1.807670	-1.434655	-2.192953	1.881084	-1.326520	-2.212209	1.825113	-1.403619
H	-2.455116	1.523812	-2.455516	-2.405835	1.677554	-2.379816	-2.431424	1.567368	-2.436983
C	-1.124700	2.651167	0.408934	-1.143453	2.594397	0.613720	-1.149363	2.629534	0.479227
H	-0.380232	3.121677	1.039781	-0.413197	3.029413	1.299349	-0.416495	3.092258	1.132809
C	-1.018292	2.435091	-1.001195	-1.012479	2.511916	-0.817402	-1.024687	2.459796	-0.937207
H	-0.192113	2.713922	-1.640801	-0.183580	2.885343	-1.418592	-0.195340	2.775196	-1.558866
Fe	-1.319462	0.575036	0.033135	-1.277983	0.569300	0.050702	-1.310865	0.566646	0.039237
P	-1.982269	-1.143929	-0.925682	-1.950104	-1.089357	-0.989589	-1.959710	-1.135669	-0.952045
F	-1.828554	-2.627091	-0.361609	-1.805839	-2.616259	-0.492935	-1.801430	-2.630319	-0.409513
F	-1.551653	-1.483138	-2.434246	-1.523279	-1.360907	-2.533145	-1.519250	-1.450281	-2.467214
F	-3.550232	-1.238574	-1.227103	-3.536022	-1.172148	-1.298436	-3.528800	-1.235117	-1.264814
C	2.353335	-2.348079	0.780440	2.328323	-2.337193	0.752016	2.356405	-2.332859	0.778430
H	2.500514	-2.566256	1.833997	2.461863	-2.593161	1.807620	2.497444	-2.560428	1.832954
C	3.246367	-1.605797	-0.037956	3.239704	-1.558435	-0.032095	3.253170	-1.576747	-0.027474
H	4.220605	-1.225410	0.246035	4.216442	-1.182587	0.279761	4.224621	-1.191944	0.267394
C	2.614825	-1.459660	-1.330187	2.609398	-1.351592	-1.323795	2.625436	-1.416267	-1.320782
H	3.043082	-0.969631	-2.198884	3.046877	-0.822368	-2.175461	3.056311	-0.912916	-2.183064
C	1.176363	-2.653076	0.032731	1.152761	-2.625020	-0.026152	1.184237	-2.638721	0.019112
H	0.318484	-3.204586	0.393481	0.289568	-3.200501	0.308454	0.325967	-3.199814	0.369997
C	1.346021	-2.104426	-1.283113	1.322078	-2.005115	-1.317871	1.355421	-2.069432	-1.288992
H	0.644483	-2.166642	-2.105267	0.632776	-2.045330	-2.162651	0.659208	-2.127130	-2.118581
Fe	1.416998	-0.540736	0.139616	1.411971	-0.534496	0.143529	1.419078	-0.531844	0.144320
P	2.151692	1.329122	-0.473329	2.078958	1.323926	-0.481978	2.120276	1.336463	-0.474916
F	1.908416	2.707317	0.287935	1.860703	2.721625	0.300627	1.870749	2.720610	0.284765
F	1.913963	1.862024	-1.958747	1.791708	1.874571	-1.977852	1.867073	1.867096	-1.964542
F	3.743662	1.459207	-0.543279	3.687606	1.483923	-0.616622	3.714890	1.486922	-0.561580
P	-0.637125	-0.191650	1.792553	-0.585178	-0.285205	1.768748	-0.628412	-0.223855	1.787304
F	-0.766428	-1.686575	2.326535	-0.728858	-1.806628	2.274211	-0.749007	-1.727917	2.307141
F	1.006269	-0.066899	2.168902	1.062099	-0.121386	2.207246	1.012994	-0.078777	2.179007
F	-1.035586	0.516421	3.174977	-1.037260	0.374142	3.183984	-1.048352	0.462833	3.178978

Table S27. Cartesian coordinates (Å) and energies (in hartree) for the optimized structure **23-2S**.

	B3LYP (-4837.83280)			BP86 (-4838.32926)			B3LYP* (-4836.60349)		
	X	Y	Z	X	Y	Z	X	Y	Z
C	-1.860864	-2.234468	1.592635	-1.829240	-1.934529	1.860047	-1.842402	-2.189199	1.643088
H	-2.171174	-3.176313	1.153318	-2.199320	-2.913809	1.546870	-2.152398	-3.143793	1.226828
C	-2.686347	-1.100202	1.806900	-2.598475	-0.731527	1.952667	-2.670174	-1.049643	1.830800
H	-3.742841	-1.023962	1.576271	-3.665147	-0.633433	1.735864	-3.728716	-0.980170	1.597809
C	-1.871466	-0.066204	2.409629	-1.718911	0.335642	2.418341	-1.855574	0.001475	2.409625
H	-2.209782	0.920893	2.705605	-2.002848	1.377577	2.582320	-2.196053	0.997008	2.680914
C	-0.535534	-1.906398	2.030770	-0.473495	-1.618278	2.248195	-0.515825	-1.848192	2.075547
H	0.316447	-2.574056	1.996403	0.357407	-2.325939	2.272622	0.339592	-2.515414	2.055268
C	-0.552459	-0.570566	2.556157	-0.416824	-0.218280	2.605673	-0.534473	-0.498233	2.568997
H	0.283046	-0.026140	2.977310	0.458256	0.339563	2.941074	0.301585	0.059252	2.976906
Fe	-1.096944	-0.571418	0.504078	-1.016529	-0.463013	0.591158	-1.080355	-0.553389	0.520696
P	-2.247785	0.883634	-0.463237	-2.272690	0.704013	-0.592725	-2.249139	0.851810	-0.490987
F	-2.026464	1.331609	-1.968945	-2.008289	1.062962	-2.131976	-2.017465	1.276946	-2.005001
F	-2.480186	2.325316	0.174592	-2.783841	2.144676	-0.088075	-2.529396	2.300839	0.118340
F	-3.804098	0.550287	-0.606752	-3.757489	0.107500	-0.825102	-3.797900	0.475828	-0.653092
C	2.684504	-1.889760	0.341745	2.746841	-1.797830	0.405797	2.688022	-1.868233	0.362354
H	2.278384	-2.892957	0.296912	2.394293	-2.829265	0.461516	2.287087	-2.876449	0.342724
C	2.644717	-0.997952	1.461186	2.671894	-0.804907	1.443159	2.644320	-0.947593	1.459669
H	2.207178	-1.201625	2.430986	2.283564	-0.947236	2.453756	2.215269	-1.130467	2.439630
C	3.296676	0.213503	1.089429	3.265903	0.412505	0.939835	3.290172	0.261248	1.053224
H	3.449801	1.075726	1.730092	3.394895	1.339981	1.504797	3.441812	1.141202	1.673218
C	3.372783	-1.216595	-0.714625	3.366758	-1.177298	-0.737980	3.364401	-1.213803	-0.716365
H	3.504794	-1.600407	-1.721878	3.482110	-1.642918	-1.721710	3.489890	-1.620602	-1.717643
C	3.751383	0.081038	-0.274324	3.703390	0.180261	-0.423111	3.741005	0.098066	-0.309377
H	4.281529	0.831540	-0.848883	4.184447	0.906042	-1.082017	4.263025	0.839284	-0.906679
Fe	1.639950	-0.101201	-0.173448	1.634190	-0.101161	-0.213620	1.638856	-0.098368	-0.182090
P	1.115563	1.919847	0.033646	1.016745	1.880269	-0.085248	1.094741	1.909928	0.015126
F	0.154258	2.734125	-0.931847	-0.032006	2.650613	-1.033525	0.110099	2.718566	-0.939798
F	2.335624	2.956206	-0.041823	2.210248	2.964994	-0.303211	2.307419	2.960550	-0.086526
F	0.566607	2.468818	1.425344	0.552327	2.524862	1.325150	0.565068	2.470898	1.416038
P	-0.385161	-1.438550	-1.199163	-0.307442	-1.559777	-0.974795	-0.368866	-1.463802	-1.157669
F	-1.268159	-1.647275	-2.519997	-1.287103	-1.966735	-2.203700	-1.268987	-1.713636	-2.464133
F	0.795560	-0.629867	-2.077404	0.780945	-0.823802	-2.059078	0.793332	-0.660521	-2.073052
F	0.280727	-2.888435	-1.259634	0.369312	-3.025533	-0.902180	0.305607	-2.914868	-1.194460

Table S28. Cartesian coordinates (Å) and energies (in hartree) for the optimized structure **23-3S**.

	B3LYP (-4837.82980)			BP86 (-4838.32393)			B3LYP* (-4836.60003)		
	X	Y	Z	X	Y	Z	X	Y	Z
C	1.915059	-2.869473	-0.350218	1.794352	-2.851835	-0.544215	1.898495	-2.863444	-0.381849
H	2.016098	-3.542939	0.495792	1.916698	-3.595540	0.249484	2.002190	-3.550471	0.455523
C	2.911509	-1.969695	-0.805117	2.802054	-1.945751	-0.987976	2.897767	-1.961509	-0.831682
H	3.922759	-1.881765	-0.426211	3.839244	-1.909429	-0.649385	3.913208	-1.881726	-0.456659
C	2.330729	-1.192558	-1.879959	2.183506	-1.053063	-1.958805	2.310169	-1.160924	-1.887492
H	2.835358	-0.431230	-2.465862	2.683141	-0.250127	-2.508241	2.814213	-0.389987	-2.465028
C	0.721191	-2.660620	-1.102289	0.560910	-2.557866	-1.227030	0.698010	-2.639417	-1.124401
H	-0.199362	-3.214897	-0.984119	-0.368940	-3.112649	-1.104442	-0.224596	-3.194450	-1.007350
C	0.985803	-1.619048	-2.057944	0.801399	-1.431977	-2.107287	0.958241	-1.579696	-2.064040
H	0.292510	-1.206593	-2.780070	0.088094	-0.952847	-2.779824	0.262444	-1.154264	-2.779010
Fe	1.223086	-0.848757	-0.122968	1.170687	-0.858112	-0.175620	1.217406	-0.850535	-0.131169
P	2.374067	0.916922	0.192897	2.391411	0.804585	0.242243	2.368970	0.898353	0.201425
F	2.324970	1.817956	1.491796	2.419870	1.609827	1.630305	2.334712	1.781445	1.519301
F	2.382166	2.068454	-0.898763	2.470232	2.065319	-0.756814	2.379687	2.074447	-0.871642
F	3.955371	0.692913	0.184027	3.985108	0.511084	0.189162	3.955125	0.672122	0.176768
C	-2.315661	-1.600523	-1.466606	-2.426621	-1.484666	-1.482196	-2.324152	-1.580643	-1.477257
H	-1.740701	-2.118617	-2.223418	-1.914321	-2.030061	-2.277479	-1.756396	-2.101197	-2.240954
C	-2.979951	-0.352163	-1.642089	-3.008888	-0.178526	-1.607137	-2.976167	-0.321934	-1.642307
H	-2.993267	0.238125	-2.552714	-3.008816	0.439811	-2.509297	-2.985768	0.275977	-2.550423
C	-3.683501	-0.034162	-0.421127	-3.650538	0.163653	-0.346345	-3.673602	-0.003382	-0.415400
H	-4.280158	0.852786	-0.242367	-4.184796	1.090945	-0.129387	-4.260991	0.890550	-0.229035
C	-2.565046	-2.043179	-0.132286	-2.664274	-1.943100	-0.142471	-2.574461	-2.029467	-0.143621
H	-2.214759	-2.963911	0.321498	-2.359838	-2.902954	0.283446	-2.231448	-2.958217	0.304297
C	-3.429529	-1.079629	0.501681	-3.436737	-0.925485	0.551030	-3.426794	-1.058473	0.501234
H	-3.797089	-1.134733	1.520365	-3.776767	-0.980455	1.587833	-3.792439	-1.116630	1.522542
Fe	-1.604509	-0.159313	-0.044977	-1.589219	-0.134513	-0.054412	-1.597688	-0.157861	-0.049125
P	-1.099302	1.759970	-0.645337	-1.002073	1.772724	-0.595531	-1.083643	1.762108	-0.632214
F	-0.173554	2.750846	0.184465	-0.082568	2.733853	0.299945	-0.164987	2.748311	0.215695
F	-2.305862	2.787783	-0.870382	-2.189419	2.846947	-0.840459	-2.291221	2.793537	-0.860657
F	-0.442772	2.019739	-2.079850	-0.289249	2.053967	-2.018425	-0.414175	2.033696	-2.062170
P	-0.706646	-0.257686	1.774170	-0.679610	-0.335005	1.749542	-0.704054	-0.275533	1.769279
F	-0.160022	0.948627	2.647697	-0.114684	0.829678	2.690672	-0.154490	0.922513	2.656812
F	-1.393554	-1.070047	2.968759	-1.416930	-1.176904	2.919996	-1.401452	-1.094508	2.958055
F	0.725500	-1.143848	1.929299	0.727777	-1.292805	1.884386	0.723780	-1.173995	1.918649

Table S29. Cartesian coordinates (Å) and energies (in hartree) for the optimized structure **23-4S**.

	B3LYP (-4837.82377)			BP86 (-4838.33112)			B3LYP* (-4836.59698)		
	X	Y	Z	X	Y	Z	X	Y	Z
C	-0.759245	-0.799533	-2.264729	-0.736796	-0.746396	-2.265567	-0.755488	-0.788444	-2.264150
H	-1.749995	-0.807713	-2.707019	-1.705021	-0.715197	-2.774512	-1.742027	-0.789482	-2.721067
C	0.255161	0.192457	-2.489070	0.354140	0.194626	-2.459504	0.274797	0.192967	-2.483652
H	0.085192	1.145762	-2.980338	0.242532	1.173021	-2.937140	0.115815	1.152724	-2.970647
C	1.567961	-0.461156	-2.396416	1.632348	-0.533548	-2.358368	1.581628	-0.473639	-2.386988
H	2.439179	-0.153126	-2.965790	2.516224	-0.306638	-2.964514	2.454671	-0.183432	-2.967410
C	-0.104507	-1.880183	-1.590720	-0.149376	-1.864713	-1.565961	-0.113367	-1.876489	-1.584825
H	-0.571626	-2.828037	-1.339121	-0.673926	-2.798415	-1.337848	-0.592674	-2.821184	-1.335294
C	1.351216	-1.709444	-1.756985	1.326913	-1.755728	-1.662257	1.346922	-1.718224	-1.735309
H	2.053343	-2.535079	-1.691977	1.987792	-2.622637	-1.559210	2.040025	-2.553969	-1.665850
C	3.026365	1.386644	0.525094	2.976391	1.416062	0.566820	3.011885	1.390970	0.535340
H	2.716887	2.417641	0.652941	2.669305	2.452434	0.724504	2.701999	2.423187	0.669316
C	3.705766	0.854778	-0.619427	3.645985	0.905445	-0.609220	3.690821	0.864268	-0.615464
H	4.006981	1.417961	-1.496462	3.937533	1.495941	-1.482623	3.990633	1.434198	-1.491235
C	3.920034	-0.537731	-0.393010	3.875009	-0.500043	-0.417215	3.906696	-0.530832	-0.398143
H	4.388435	-1.232177	-1.083216	4.356788	-1.180000	-1.125789	4.377588	-1.222007	-1.093039
C	2.794298	0.327863	1.438957	2.745778	0.331298	1.455992	2.778165	0.326419	1.442537
H	2.286374	0.411056	2.391656	2.228374	0.389933	2.415660	2.266359	0.403797	2.396056
C	3.323258	-0.877879	0.857416	3.264100	-0.874709	0.833794	3.303356	-0.879413	0.850596
H	3.282810	-1.868679	1.296892	3.225930	-1.882544	1.255495	3.260810	-1.874760	1.284706
Fe	1.836439	-0.144554	-0.427943	1.825428	-0.129830	-0.437366	1.831598	-0.142521	-0.431137
Fe	-0.632849	-0.111117	-0.338415	-0.612496	-0.108537	-0.341634	-0.626756	-0.110391	-0.338722
P	-2.747295	-0.109379	-0.373126	-2.713037	-0.066813	-0.395782	-2.737026	-0.099819	-0.378939
P	-0.333438	-1.184372	1.411438	-0.350989	-1.236576	1.377521	-0.338167	-1.193709	1.404690
P	-0.386837	1.852499	0.346579	-0.363493	1.839213	0.377266	-0.379796	1.848123	0.352504
F	-3.536643	0.818311	-1.403356	-3.479061	0.930379	-1.405746	-3.521477	0.842626	-1.405076
F	-3.508173	-1.460163	-0.747263	-3.505298	-1.399990	-0.843704	-3.504772	-1.446838	-0.769484
F	-3.599854	0.259677	0.911059	-3.590383	0.263506	0.903658	-3.595517	0.260694	0.908065
F	0.328291	2.239475	1.714793	0.316045	2.213858	1.788957	0.328853	2.231734	1.729979
F	-1.683317	2.751696	0.603287	-1.679277	2.747810	0.617786	-1.679856	2.749022	0.606960
F	0.351350	2.922437	-0.578661	0.403387	2.946111	-0.517685	0.365624	2.926908	-0.564580
F	0.113040	-0.519676	2.789424	0.076720	-0.613654	2.800896	0.107849	-0.537278	2.791255
F	-1.602367	-1.951300	2.019891	-1.647092	-2.023034	1.942540	-1.613556	-1.960609	2.007040
F	0.615538	-2.468930	1.491682	0.603190	-2.540484	1.440388	0.609879	-2.483791	1.482211

Table S30. Cartesian coordinates (Å) and energies (in hartree) for the optimized structure **23-1Q**.

	B3LYP (-4837.86362)			BP86 (-4838.31918)			B3LYP* (-4836.62273)		
	X	Y	Z	X	Y	Z	X	Y	Z
C	2.560318	-1.004680	2.070799	2.573194	-0.625179	2.143086	2.567818	-0.843145	2.110891
H	3.634136	-0.855759	2.042775	3.635516	-0.372072	2.102524	3.636535	-0.649155	2.084761
C	1.864501	-2.168103	1.655957	1.993195	-1.887676	1.824106	1.925011	-2.051947	1.738175
H	2.310349	-3.070555	1.252115	2.530370	-2.782529	1.499726	2.412464	-2.951320	1.372010
C	0.457075	-1.938727	1.846384	0.557612	-1.776204	1.996494	0.505211	-1.874188	1.910297
H	-0.331015	-2.654691	1.642736	-0.167758	-2.573917	1.826008	-0.253366	-2.629961	1.727361
C	1.586505	-0.042780	2.521125	1.498275	0.278794	2.516450	1.548596	0.094862	2.517377
H	1.805836	0.945534	2.910899	1.619450	1.323322	2.814716	1.723167	1.109594	2.864855
C	0.284281	-0.626781	2.401117	0.251132	-0.439430	2.446375	0.271890	-0.549043	2.413870
H	-0.641103	-0.198246	2.775365	-0.726770	-0.070753	2.772736	-0.676358	-0.146376	2.765052
Fe	1.208015	-0.495659	0.496314	1.178099	-0.383153	0.546333	1.205065	-0.454346	0.512060
P	0.816209	-1.451727	-1.286071	0.919327	-1.515576	-1.158817	0.860068	-1.490208	-1.235803
F	0.769119	-0.702019	-2.688762	0.410954	-0.908978	-2.560851	0.805070	-0.789983	-2.666955
F	-0.546668	-2.288683	-1.476733	-0.050414	-2.804471	-1.121553	-0.469053	-2.384069	-1.412974
F	1.754157	-2.658063	-1.761787	2.187070	-2.300904	-1.781101	1.853625	-2.676170	-1.656680
C	-0.830455	2.851451	-0.808332	-0.987002	2.667929	-0.856078	-0.891637	2.780143	-0.834482
H	0.045163	3.128346	-1.385353	-0.122505	2.953676	-1.460118	-0.018664	3.057653	-1.418687
C	-0.987388	2.991043	0.612681	-1.117282	2.818021	0.581339	-1.042881	2.928285	0.590152
H	-0.245927	3.394626	1.294600	-0.355374	3.225721	1.251228	-0.297221	3.337510	1.267282
C	-2.307814	2.563596	0.948618	-2.458997	2.444946	0.935312	-2.369085	2.518379	0.930704
H	-2.746099	2.565509	1.942315	-2.882011	2.454663	1.944483	-2.804053	2.526276	1.927971
C	-2.053360	2.338051	-1.335474	-2.252112	2.211380	-1.362246	-2.125021	2.280673	-1.354818
H	-2.255369	2.127776	-2.381454	-2.478718	2.002675	-2.412087	-2.332667	2.066838	-2.401024
C	-2.970146	2.187194	-0.256935	-3.166462	2.118557	-0.267440	-3.042026	2.149242	-0.272520
H	-3.999786	1.850997	-0.337971	-4.211203	1.800928	-0.327618	-4.075535	1.817404	-0.347329
Fe	-0.850513	0.799340	0.122047	-0.932572	0.699628	0.094862	-0.879120	0.756486	0.109297
P	-2.743357	-0.830327	0.151565	-2.596973	-0.876198	0.101842	-2.697828	-0.842614	0.133824
F	-3.516850	-1.113287	-1.197802	-3.104782	-1.501996	-1.286955	-3.436338	-1.202146	-1.222239
F	-4.002923	-0.491692	1.059076	-4.054885	-0.600244	0.731359	-3.995251	-0.530471	1.004291
F	-2.558356	-2.330774	0.636944	-2.332066	-2.266463	0.872647	-2.464831	-2.322182	0.672316
P	2.294686	1.086052	-0.267340	2.162676	1.178575	-0.372171	2.249577	1.124210	-0.312085
F	3.891829	0.976714	-0.282004	3.777782	1.121451	-0.437891	3.850805	1.040047	-0.357290
F	2.149876	1.651385	-1.747315	1.953521	1.611800	-1.906895	2.068891	1.654096	-1.804728
F	2.281438	2.501889	0.487119	2.118432	2.665484	0.270143	2.225596	2.559269	0.412655

Table S31. Cartesian coordinates (Å) and energies (in hartree) for the optimized structure **22-1Q**.

	B3LYP (-4196.77547)			BP86 (-4197.22066)			B3LYP* (-4195.75551)		
	X	Y	Z	X	Y	Z	X	Y	Z
C	-0.262095	2.119130	1.799675	-1.830461	1.048724	1.842556	-1.815866	1.122619	1.799882
H	0.699701	2.069189	2.298053	-1.212616	1.774882	2.376561	-1.176222	1.838365	2.308630
C	-0.562401	2.911511	0.636320	-2.654682	1.335426	0.686285	-2.615017	1.395420	0.631797
H	0.143173	3.532026	0.094142	-2.767183	2.311507	0.207899	-2.658447	2.342553	0.100748
C	-1.937043	2.721185	0.323393	-3.296090	0.111012	0.294620	-3.321476	0.202915	0.299795
H	-2.479953	3.169378	-0.502174	-3.974360	-0.026721	-0.551538	-4.003998	0.065815	-0.534942
C	-1.476088	1.496010	2.235254	-1.996238	-0.337751	2.180525	-2.082985	-0.222515	2.215410
H	-1.582253	0.829977	3.085409	-1.495493	-0.869147	2.993759	-1.630265	-0.732764	3.061837
C	-2.497941	1.838416	1.314589	-2.876351	-0.923039	1.212990	-2.982808	-0.798973	1.279301
H	-3.530048	1.504379	1.351558	-3.186513	-1.971113	1.177084	-3.361842	-1.817979	1.299693
C	2.497941	-1.838416	1.314589	2.876351	0.923039	1.212990	2.982808	0.798973	1.279301
H	3.530048	-1.504379	1.351558	3.186513	1.971113	1.177084	3.361842	1.817979	1.299693
C	1.937043	-2.721185	0.323393	3.296090	-0.111012	0.294620	3.321476	-0.202915	0.299795
H	2.479953	-3.169378	-0.502174	3.974360	0.026721	-0.551538	4.003998	-0.065815	-0.534942
C	0.562401	-2.911511	0.636320	2.654682	-1.335426	0.686285	2.615017	-1.395420	0.631797
H	-0.143173	-3.532026	0.094142	2.767183	-2.311507	0.207899	2.658447	-2.342553	0.100748
C	1.476088	-1.496010	2.235254	1.996238	0.337751	2.180525	2.082985	0.222515	2.215410
H	1.582253	-0.829977	3.085409	1.495493	0.869147	2.993759	1.630265	0.732764	3.061837
C	0.262095	-2.119130	1.799675	1.830461	-1.048724	1.842556	1.815866	-1.122619	1.799882
H	-0.699701	-2.069189	2.298053	1.212616	-1.774882	2.376561	1.176222	-1.838365	2.308630
Fe	-0.844733	0.814421	0.162510	-1.145343	-0.076747	0.124402	-1.154405	-0.124571	0.151956
Fe	0.844733	-0.814421	0.162510	1.145343	0.076747	0.124402	1.154405	0.124571	0.151956
P	1.886829	0.654871	-0.895842	0.530788	1.803238	-0.860593	0.645360	1.863679	-0.879560
F	3.252516	0.251254	-1.626298	1.689332	2.628073	-1.647104	1.815866	2.672303	-1.623005
F	1.281692	1.454583	-2.139271	-0.530788	1.883318	-2.081750	-0.377060	1.921310	-2.111601
F	2.497941	1.907957	-0.119987	0.004070	3.085103	-0.030164	0.079579	3.130166	-0.082119
P	-1.886829	-0.654871	-0.895842	-0.530788	-1.803238	-0.860593	-0.645360	-1.863679	-0.879560
F	-3.252516	-0.251254	-1.626298	-1.689332	-2.628073	-1.647104	-1.815866	-2.672303	-1.623005
F	-2.497941	-1.907957	-0.119987	-0.004070	-3.085103	-0.030164	-0.079579	-3.130166	-0.082119
F	-1.281692	-1.454583	-2.139271	0.530788	-1.883318	-2.081750	0.377060	-1.921310	-2.111601

Table S32. Cartesian coordinates (Å) and energies (in hartree) for the optimized structure **22-1T**.

	B3LYP (-4196.77335)			BP86 (-4197.22382)			B3LYP* (-4195.75512)		
	X	Y	Z	X	Y	Z	X	Y	Z
C	-2.467143	-0.834630	0.712576	-2.397445	-1.184266	0.714031	-2.458280	-0.891593	0.712694
H	-2.892105	-0.074436	1.358399	-2.925661	-0.483719	1.365012	-2.900893	-0.139871	1.359856
C	-1.831631	-2.051585	1.150668	-1.558502	-2.286440	1.156399	-1.786194	-2.091903	1.151682
H	-1.693140	-2.351792	2.184298	-1.365849	-2.556868	2.198414	-1.638081	-2.387721	2.187379
C	-1.461134	-2.815098	0.000000	-1.065005	-2.988230	0.000000	-1.395037	-2.847224	0.000000
H	-0.969839	-3.781178	0.000000	-0.416856	-3.867023	0.000000	-0.875872	-3.800832	0.000000
C	-2.467143	-0.834630	-0.712576	-2.397445	-1.184266	-0.714031	-2.458280	-0.891593	-0.712694
H	-2.892105	-0.074436	-1.358399	-2.925661	-0.483719	-1.365012	-2.900893	-0.139871	-1.359856
C	-1.831631	-2.051585	-1.150668	-1.558502	-2.286440	-1.156399	-1.786194	-2.091903	-1.151682
H	-1.693140	-2.351792	-2.184298	-1.365849	-2.556868	-2.198414	-1.638081	-2.387721	-2.187379
Fe	-0.461541	-0.944548	0.000000	-0.401210	-0.981086	0.000000	-0.451598	-0.950512	0.000000
P	0.876478	-0.761785	-1.561790	0.884475	-0.561866	-1.569537	0.879533	-0.725791	-1.561304
F	0.391579	-0.155564	-2.962514	0.312438	-0.017094	-2.983373	0.380947	-0.122724	-2.962772
F	1.445813	-2.111510	-2.216347	1.612064	-1.849902	-2.244582	1.475607	-2.064375	-2.224445
F	2.283286	-0.024511	-1.477629	2.225076	0.327113	-1.496827	2.276444	0.037267	-1.475048
C	-1.230713	3.248456	-0.709125	-1.480100	2.962317	-0.715263	-1.274426	3.195742	-0.710202
H	-2.098838	3.282789	-1.359487	-2.349744	2.892853	-1.374710	-2.143835	3.215984	-1.362707
C	0.145812	3.201606	-1.145290	-0.094267	3.064710	-1.152689	0.105475	3.169420	-1.146169
H	0.479080	3.162541	-2.177947	0.245697	3.052124	-2.192242	0.440206	3.131958	-2.180506
C	0.985330	3.238809	0.000000	0.737944	3.213631	0.000000	0.945122	3.225092	0.000000
H	2.068697	3.179254	0.000000	1.830295	3.255468	0.000000	2.031089	3.178088	0.000000
C	-1.230713	3.248456	0.709125	-1.480100	2.962317	0.715263	-1.274426	3.195742	0.710202
H	-2.098838	3.282789	1.359487	-2.349744	2.892853	1.374710	-2.143835	3.215984	1.362707
C	0.145812	3.201606	1.145290	-0.094267	3.064710	1.152689	0.105475	3.169420	1.146169
H	0.479080	3.162541	2.177947	0.245697	3.052124	2.192242	0.440206	3.131958	2.180506
Fe	-0.372939	1.381370	0.000000	-0.426591	1.263716	0.000000	-0.386455	1.358416	0.000000
P	0.876478	-0.761785	1.561790	0.884475	-0.561866	1.569537	0.879533	-0.725791	1.561304
F	0.391579	-0.155564	2.962514	0.312438	-0.017094	2.983373	0.380947	-0.122724	2.962772
F	2.283286	-0.024511	1.477629	2.225076	0.327113	1.496827	2.276444	0.037267	1.475048
F	1.445813	-2.111510	2.216347	1.612064	-1.849902	2.244582	1.475607	-2.064375	2.224445

Table S33. Cartesian coordinates (Å) and energies (in hartree) for the optimized structure **22-2T**.

	B3LYP (-4196.76723)			BP86 (-4197.22676)			B3LYP* (-4195.75101)		
	X	Y	Z	X	Y	Z	X	Y	Z
C	0.229619	3.775572	1.048381	0.230310	3.738992	1.055620	0.228588	3.764554	1.049959
C	0.713776	3.845269	-0.291055	0.726041	3.815106	-0.286080	0.716274	3.836590	-0.289253
C	-0.258925	3.253008	-1.146820	-0.224758	3.179567	-1.152795	-0.248933	3.231944	-1.148089
C	-1.351239	2.795200	-0.333392	-1.327019	2.704269	-0.343468	-1.342891	2.767467	-0.336544
C	-1.045074	3.139732	1.028347	-1.031638	3.056065	1.029665	-1.041421	3.115106	1.027652
H	0.771703	4.086639	1.935319	0.763524	4.063567	1.953249	0.767416	4.079989	1.939802
H	1.685932	4.219082	-0.595070	1.701777	4.207385	-0.584988	1.688905	4.216634	-0.591185
H	-0.181063	3.137671	-2.222614	-0.133687	3.062536	-2.235479	-0.166993	3.116042	-2.225494
H	-2.257310	2.315547	-0.686541	-2.228303	2.203905	-0.705320	-2.246950	2.281627	-0.692513
H	-1.667652	2.924715	1.890262	-1.659589	2.827570	1.894388	-1.665557	2.895329	1.889720
Fe	0.371105	1.730644	0.235967	0.406776	1.702352	0.240368	0.382623	1.721268	0.237003
F	2.023581	1.253446	0.824683	2.089873	1.340386	0.825602	2.042559	1.273291	0.823357
P	0.475421	0.069418	-1.265975	0.445909	0.066042	-1.227748	0.466521	0.068315	-1.256946
F	-0.263144	0.355179	-2.664023	-0.304478	0.389801	-2.637651	-0.275817	0.368671	-2.654854
F	1.958750	-0.107009	-1.857015	1.931030	-0.146154	-1.863381	1.948016	-0.122969	-1.859540
C	1.045074	-3.139732	-1.028347	1.031638	-3.056065	-1.029665	1.041421	-3.115106	-1.027652
C	1.351239	-2.795200	0.333392	1.327019	-2.704269	0.343468	1.342891	-2.767467	0.336544
C	0.258925	-3.253008	1.146820	0.224758	-3.179567	1.152795	0.248933	-3.231944	1.148089
C	-0.713776	-3.845269	0.291055	-0.726041	-3.815106	0.286080	-0.716274	-3.836590	0.289253
C	-0.229619	-3.775572	-1.048381	-0.230310	-3.738992	-1.055620	-0.228588	-3.764554	-1.049959
H	1.667652	-2.924715	-1.890262	1.659589	-2.827570	-1.894388	1.665557	-2.895329	-1.889720
H	2.257310	-2.315547	0.686541	2.228303	-2.203905	0.705320	2.246950	-2.281627	0.692513
H	0.181063	-3.137671	2.222614	0.133687	-3.062536	2.235479	0.166993	-3.116042	2.225494
H	-1.685932	-4.219082	0.595070	-1.701777	-4.207385	0.584988	-1.688905	-4.216634	0.591185
H	-0.771703	-4.086639	-1.935319	-0.763524	-4.063567	-1.953249	-0.767416	-4.079989	-1.939802
Fe	-0.371105	-1.730644	-0.235967	-0.406776	-1.702352	-0.240368	-0.382623	-1.721268	-0.237003
F	-2.023581	-1.253446	-0.824683	-2.089873	-1.340386	-0.825602	-2.042559	-1.273291	-0.823357
P	-0.475421	-0.069418	1.265975	-0.445909	-0.066042	1.227748	-0.466521	-0.068315	1.256946
F	-1.958750	0.107009	1.857015	-1.931030	0.146154	1.863381	-1.948016	0.122969	1.859540
F	0.263144	-0.355179	2.664023	0.304478	-0.389801	2.637651	0.275817	-0.368671	2.654854

Table S34. Cartesian coordinates (Å) and energies (in hartree) for the optimized structure **22-3T**.

	B3LYP (-4196.76658)			BP86 (-4197.22149)			B3LYP* (-4195.74664)		
	X	Y	Z	X	Y	Z	X	Y	Z
C	1.201325	2.155004	1.487110	1.202238	1.985427	1.644642	0.973813	1.938459	1.739148
H	0.416743	2.893970	1.605783	0.369731	2.493511	2.135281	0.059021	2.366038	2.139682
C	2.301966	2.240049	0.577317	1.779570	2.345894	0.369377	1.729067	2.462092	0.633980
H	2.466691	3.029542	-0.149177	1.457986	3.171917	-0.269696	1.462014	3.332923	0.040272
C	3.102338	1.078212	0.743855	2.832486	1.418923	0.068450	2.855782	1.618282	0.421316
H	4.007485	0.839654	0.195751	3.442819	1.408181	-0.837316	3.617399	1.735648	-0.344304
C	1.343339	0.945234	2.252214	1.890031	0.809520	2.119020	1.649672	0.773156	2.227918
H	0.690108	0.616295	3.052794	1.684562	0.266131	3.045251	1.339371	0.151021	3.062459
C	2.510988	0.275229	1.788739	2.906144	0.468643	1.151789	2.800507	0.564489	1.405337
H	2.900832	-0.665586	2.162824	3.597064	-0.375508	1.221932	3.526070	-0.237562	1.518131
Fe	1.104359	0.463117	0.168533	0.966357	0.389500	0.315901	1.044888	0.477718	0.187163
P	1.550869	-1.291108	-0.864212	1.337555	-1.368344	-0.733869	1.606555	-1.252957	-0.809289
F	1.755746	-2.648199	-0.045995	1.518836	-2.775296	0.044489	1.783537	-2.624660	-0.000124
F	2.933036	-1.398959	-1.660772	2.787109	-1.429876	-1.463057	3.063711	-1.299879	-1.476619
F	0.638729	-1.900106	-2.027207	0.529976	-1.956567	-2.010994	0.823089	-1.871295	-2.062845
C	-1.732048	-1.537567	2.016498	-1.386590	-1.570699	1.866687	-1.435681	-1.791994	1.850645
H	-1.158036	-1.544289	2.937394	-0.638064	-1.691490	2.653184	-0.700285	-1.945131	2.635789
C	-1.536011	-2.422901	0.899145	-1.585071	-2.462740	0.739262	-1.518745	-2.539909	0.620235
H	-0.787761	-3.205584	0.832889	-1.002358	-3.361051	0.523280	-0.850246	-3.341789	0.318608
C	-2.529650	-2.116603	-0.079981	-2.706328	-1.972367	-0.010907	-2.649646	-2.057605	-0.106424
H	-2.642424	-2.597266	-1.046628	-3.089759	-2.399331	-0.942047	-2.978694	-2.402135	-1.083834
C	-2.840818	-0.688500	1.715830	-2.391897	-0.538337	1.796581	-2.528608	-0.866587	1.878102
H	-3.249613	0.087866	2.354790	-2.519922	0.291877	2.495755	-2.747580	-0.152774	2.668560
C	-3.321809	-1.041356	0.415670	-3.197638	-0.789174	0.630327	-3.264264	-1.021602	0.665388
H	-4.146500	-0.567647	-0.106949	-4.025009	-0.167380	0.278895	-4.138121	-0.445427	0.371118
Fe	-1.116703	-0.350279	0.286933	-1.038893	-0.470573	0.094736	-1.078964	-0.446378	0.189550
P	-1.318814	1.423200	-0.863010	-1.197608	1.441653	-0.758522	-1.391231	1.381479	-0.825840
F	-1.488350	2.822915	-0.123172	-1.335377	2.772646	0.148760	-1.542193	2.743004	-0.004161
F	-2.658984	1.525002	-1.727683	-2.637453	1.654204	-1.493887	-2.790650	1.511221	-1.598859
F	-0.364081	1.919023	-2.045353	-0.368427	2.090542	-1.986044	-0.515738	1.955371	-2.036052

Table S35. Cartesian coordinates (Å) and energies (in hartree) for the optimized structure **22-1S**.

	B3LYP (-4196.74325)			BP86 (-4197.23540)			B3LYP* (-4195.73674)		
	X	Y	Z	X	Y	Z	X	Y	Z
C	0.000000	3.092912	1.156340	0.000000	3.068248	1.166192	0.000000	3.086416	1.158347
C	0.774759	3.394280	0.000000	0.777620	3.375835	0.000000	0.774956	3.389712	0.000000
C	0.000000	3.092912	-1.156340	0.000000	3.068248	-1.166192	0.000000	3.086416	-1.158347
C	-1.294139	2.618598	-0.705403	-1.285055	2.550232	-0.714225	-1.290907	2.600145	-0.707293
C	-1.294139	2.618598	0.705403	-1.285055	2.550232	0.714225	-1.290907	2.600145	0.707293
H	0.313613	3.222072	2.186268	0.319282	3.199727	2.202953	0.314895	3.216120	2.189938
H	1.819139	3.685295	0.000000	1.826704	3.680724	0.000000	1.820349	3.684653	0.000000
H	0.313613	3.222072	-2.186268	0.319282	3.199727	-2.202953	0.314895	3.216120	-2.189938
H	-2.109315	2.286139	-1.337889	-2.104341	2.207586	-1.349896	-2.106371	2.263745	-1.340678
H	-2.109315	2.286139	1.337889	-2.104341	2.207586	1.349896	-2.106371	2.263745	1.340678
Fe	0.265499	1.340237	0.000000	0.267917	1.334078	0.000000	0.266984	1.338018	0.000000
F	2.094751	0.847824	0.000000	2.120799	0.894428	0.000000	2.100706	0.857990	0.000000
P	0.000000	0.000000	-1.638496	0.000000	0.000000	-1.632547	0.000000	0.000000	-1.636212
F	-1.157165	0.269368	-2.702527	-1.162762	0.273184	-2.724233	-1.157274	0.274233	-2.706045
F	1.157165	-0.269368	-2.702527	1.162762	-0.273184	-2.724233	1.157274	-0.274233	-2.706045
C	1.294139	-2.618598	-0.705403	1.285055	-2.550232	-0.714225	1.290907	-2.600145	-0.707293
C	1.294139	-2.618598	0.705403	1.285055	-2.550232	0.714225	1.290907	-2.600145	0.707293
C	0.000000	-3.092912	1.156340	0.000000	-3.068248	1.166192	0.000000	-3.086416	1.158347
C	-0.774759	-3.394280	0.000000	-0.777620	-3.375835	0.000000	-0.774956	-3.389712	0.000000
C	0.000000	-3.092912	-1.156340	0.000000	-3.068248	-1.166192	0.000000	-3.086416	-1.158347
H	2.109315	-2.286139	-1.337889	2.104341	-2.207586	-1.349896	2.106371	-2.263745	-1.340678
H	2.109315	-2.286139	1.337889	2.104341	-2.207586	1.349896	2.106371	-2.263745	1.340678
H	-0.313613	-3.222072	2.186268	-0.319282	-3.199727	2.202953	-0.314895	-3.216120	2.189938
H	-1.819139	-3.685295	0.000000	-1.826704	-3.680724	0.000000	-1.820349	-3.684653	0.000000
H	-0.313613	-3.222072	-2.186268	-0.319282	-3.199727	-2.202953	-0.314895	-3.216120	-2.189938
Fe	-0.265499	-1.340237	0.000000	-0.267917	-1.334078	0.000000	-0.266984	-1.338018	0.000000
F	-2.094751	-0.847824	0.000000	-2.120799	-0.894428	0.000000	-2.100706	-0.857990	0.000000
P	0.000000	0.000000	1.638496	0.000000	0.000000	1.632547	0.000000	0.000000	1.636212
F	-1.157165	0.269368	2.702527	-1.162762	0.273184	2.724233	-1.157274	0.274233	2.706045
F	1.157165	-0.269368	2.702527	1.162762	-0.273184	2.724233	1.157274	-0.274233	2.706045

Table S36. Cartesian coordinates (Å) and energies (in hartree) for the optimized structure **22-2S**.

	B3LYP (-4196.73587)			BP86 (-4197.22104)			B3LYP* (-4195.72756)		
	X	Y	Z	X	Y	Z	X	Y	Z
C	-1.288965	1.961809	1.658464	-1.330226	2.068016	1.588539	-1.294608	2.002330	1.629828
H	-2.125336	1.442007	2.111326	-2.195925	1.583331	2.046030	-2.145876	1.498916	2.078426
C	-1.315521	2.663383	0.398647	-1.310160	2.691927	0.276231	-1.294608	2.680990	0.354581
H	-2.169753	2.737128	-0.265855	-2.158627	2.763581	-0.408614	-2.142368	2.759190	-0.320717
C	-0.033335	3.223207	0.169932	0.005748	3.189057	0.039940	0.002077	3.213163	0.131579
H	0.271735	3.786369	-0.704695	0.354639	3.679432	-0.871338	0.330024	3.752723	-0.752014
C	0.033335	2.073411	2.188380	-0.005748	2.151504	2.143280	0.024612	2.095685	2.174789
H	0.393575	1.640588	3.115410	0.321752	1.768236	3.112753	0.365851	1.675517	3.116920
C	0.815873	2.833387	1.259290	0.825764	2.828726	1.172202	0.832510	2.824444	1.237546
H	1.864989	3.085740	1.370523	1.893615	3.035347	1.280532	1.888055	3.055405	1.353546
Fe	0.073893	1.038996	0.375283	0.022968	1.027721	0.408482	0.065099	1.031585	0.385295
P	1.695279	0.651271	-0.870717	1.654848	0.521809	-0.809758	1.687882	0.603889	-0.850458
F	3.047684	-0.007395	-0.328089	3.025611	-0.140311	-0.253869	3.033963	-0.087149	-0.318323
F	2.416662	1.961059	-1.447981	2.416031	1.833398	-1.402275	2.440866	1.909288	-1.411393
F	1.643041	-0.115802	-2.265218	1.605156	-0.242969	-2.227710	1.622066	-0.141908	-2.259940
C	1.288965	-1.961809	1.658464	1.330226	-2.068016	1.588539	1.294608	-2.002330	1.629828
H	2.125336	-1.442007	2.111326	2.195925	-1.583331	2.046030	2.145876	-1.498916	2.078426
C	1.315521	-2.663383	0.398647	1.310160	-2.691927	0.276231	1.294608	-2.680990	0.354581
H	2.169753	-2.737128	-0.265855	2.158627	-2.763581	-0.408614	2.142368	-2.759190	-0.320717
C	0.033335	-3.223207	0.169932	-0.005748	-3.189057	0.039940	-0.002077	-3.213163	0.131579
H	-0.271735	-3.786369	-0.704695	-0.354639	-3.679432	-0.871338	-0.330024	-3.752723	-0.752014
C	-0.033335	-2.073411	2.188380	0.005748	-2.151504	2.143280	-0.024612	-2.095685	2.174789
H	-0.393575	-1.640588	3.115410	-0.321752	-1.768236	3.112753	-0.365851	-1.675517	3.116920
C	-0.815873	-2.833387	1.259290	-0.825764	-2.828726	1.172202	-0.832510	-2.824444	1.237546
H	-1.864989	-3.085740	1.370523	-1.893615	-3.035347	1.280532	-1.888055	-3.055405	1.353546
Fe	-0.073893	-1.038996	0.375283	-0.022968	-1.027721	0.408482	-0.065099	-1.031585	0.385295
P	-1.695279	-0.651271	-0.870717	-1.654848	-0.521809	-0.809758	-1.687882	-0.603889	-0.850458
F	-3.047684	0.007395	-0.328089	-3.025611	0.140311	-0.253869	-3.033963	0.087149	-0.318323
F	-2.416662	-1.961059	-1.447981	-2.416031	-1.833398	-1.402275	-2.440866	-1.909288	-1.411393
F	-1.643041	0.115802	-2.265218	-1.605156	0.242969	-2.227710	-1.622066	0.141908	-2.259940

Table S37. Cartesian coordinates (Å) and energies (in hartree) for the optimized structure **11-1D**.

	B3LYP (-2098.34100)			BP86 (-2098.56238)			B3LYP* (-2097.82977)		
	X	Y	Z	X	Y	Z	X	Y	Z
C	0.944066	2.548045	0.000000	0.961230	2.551457	0.000000	0.941180	2.544092	0.000000
H	1.906540	3.052164	0.000000	1.938406	3.045117	0.000000	1.905789	3.048725	0.000000
C	0.186672	2.185409	1.168236	0.204599	2.172628	1.174376	0.186958	2.174654	1.170879
H	0.483324	2.346507	2.199801	0.509773	2.323858	2.213819	0.483503	2.337507	2.204231
C	-0.994305	1.530976	0.728913	-0.993410	1.521009	0.731986	-0.991207	1.511020	0.730600
H	-1.779450	1.127923	1.359350	-1.781823	1.111278	1.368201	-1.774179	1.099716	1.361773
C	0.186672	2.185409	-1.168236	0.204599	2.172628	-1.174376	0.186958	2.174654	-1.170879
H	0.483324	2.346507	-2.199801	0.509773	2.323858	-2.213819	0.483503	2.337507	-2.204231
C	-0.994305	1.530976	-0.728913	-0.993410	1.521009	-0.731986	-0.991207	1.511020	-0.730600
H	-1.779450	1.127923	-1.359350	-1.781823	1.111278	-1.368201	-1.774179	1.099716	-1.361773
Fe	0.691943	0.459021	0.000000	0.666553	0.467449	0.000000	0.690932	0.463671	0.000000
P	-0.098363	-1.472199	0.000000	-0.094587	-1.459443	0.000000	-0.097209	-1.461771	0.000000
F	0.186672	-2.512616	-1.181241	0.204599	-2.505587	-1.198231	0.186958	-2.505671	-1.183930
F	-1.684696	-1.612265	0.000000	-1.698926	-1.634360	0.000000	-1.687983	-1.604735	0.000000
F	0.186672	-2.512616	1.181241	0.204599	-2.505587	1.198231	0.186958	-2.505671	1.183930

Table S38. Cartesian coordinates (Å) and energies (in hartree) for the optimized structure **11-1Q**.

	B3LYP (-2098.37634)			BP86 (-2098.57454)			B3LYP* (-2097.85974)		
	X	Y	Z	X	Y	Z	X	Y	Z
C	-0.152175	2.105432	1.155715	-0.150125	2.052379	1.162007	-0.153643	2.090394	1.156903
H	-0.491241	2.064257	2.186216	-0.490294	1.989464	2.199717	-0.492936	2.043314	2.189120
C	-0.978052	1.989822	0.000000	-0.981097	1.931956	0.000000	-0.980103	1.971644	0.000000
H	-2.049252	1.814704	0.000000	-2.055759	1.730801	0.000000	-2.051614	1.786895	0.000000
C	-0.152175	2.105432	-1.155715	-0.150125	2.052379	-1.162007	-0.153643	2.090394	-1.156903
H	-0.491241	2.064257	-2.186216	-0.490294	1.989464	-2.199717	-0.492936	2.043314	-2.189120
C	1.200788	2.297375	0.719574	1.211413	2.259136	0.724094	1.200301	2.288975	0.720433
H	2.061083	2.475179	1.357772	2.078699	2.432508	1.368022	2.061846	2.467775	1.359969
C	1.200788	2.297375	-0.719574	1.211413	2.259136	-0.724094	1.200301	2.288975	-0.720433
H	2.061083	2.475179	-1.357772	2.078699	2.432508	-1.368022	2.061846	2.467775	-1.359969
Fe	0.671588	0.323054	0.000000	0.667012	0.333679	0.000000	0.673449	0.324762	0.000000
P	-0.342399	-1.558218	0.000000	-0.337623	-1.514303	0.000000	-0.339941	-1.546625	0.000000
F	-0.152175	-2.592855	1.195084	-0.150125	-2.562996	1.210265	-0.153643	-2.585097	1.197826
F	-0.152175	-2.592855	-1.195084	-0.150125	-2.562996	-1.210265	-0.153643	-2.585097	-1.197826
F	-1.932401	-1.557881	0.000000	-1.949516	-1.525760	0.000000	-1.934497	-1.544896	0.000000

Table S39. Cartesian coordinates (Å) and energies (in hartree) for the optimized structure **11-2D**.

	B3LYP (-2098.33631)			BP86 (-2098.55537)			B3LYP* (-2097.82499)		
	X	Y	Z	X	Y	Z	X	Y	Z
C	1.852745	0.939185	1.151621	1.778966	0.897234	1.157657	1.834292	0.929211	1.151738
C	1.852745	-0.426545	0.716370	1.778966	-0.485381	0.719132	1.834292	-0.441060	0.716355
C	1.852745	-0.426545	-0.716370	1.778966	-0.485381	-0.719132	1.834292	-0.441060	-0.716355
C	1.852745	0.939185	-1.151621	1.778966	0.897234	-1.157657	1.834292	0.929211	-1.151738
C	1.879092	1.775742	0.000000	1.855012	1.740763	0.000000	1.874437	1.767269	0.000000
H	1.803232	1.275377	2.182655	1.719255	1.234856	2.196686	1.780012	1.265711	2.184619
H	1.859732	-1.300461	1.359234	1.764083	-1.363170	1.370679	1.836282	-1.315392	1.361941
H	1.859732	-1.300461	-1.359234	1.764083	-1.363170	-1.370679	1.836282	-1.315392	-1.361941
H	1.803232	1.275377	-2.182655	1.719255	1.234856	-2.196686	1.780012	1.265711	-2.184619
H	1.810671	2.858785	0.000000	1.787609	2.832361	0.000000	1.805906	2.852292	0.000000
Fe	0.056527	0.450080	0.000000	0.076305	0.478791	0.000000	0.063064	0.453237	0.000000
F	-1.337379	1.517512	0.000000	-1.313120	1.543411	0.000000	-1.331248	1.515729	0.000000
P	-1.098103	-1.539924	0.000000	-1.032918	-1.502379	0.000000	-1.084393	-1.528001	0.000000
F	-2.102152	-1.215310	1.229080	-2.069535	-1.209229	1.237146	-2.094481	-1.206670	1.230644
F	-2.102152	-1.215310	-1.229080	-2.069535	-1.209229	-1.237146	-2.094481	-1.206670	-1.230644

Table S40. Cartesian coordinates (Å) and energies (in hartree) for the optimized structure **11-2Q**.

	B3LYP (-2098.36591)			BP86 (-2098.56446)			B3LYP* (-2097.84936)		
	X	Y	Z	X	Y	Z	X	Y	Z
C	1.906869	1.077344	1.157081	1.845225	1.068594	1.164454	1.889674	1.075268	1.158518
C	1.906869	-0.279398	0.723978	1.845225	-0.299469	0.728936	1.889674	-0.283410	0.725074
C	1.906869	-0.279398	-0.723978	1.845225	-0.299469	-0.728936	1.889674	-0.283410	-0.725074
C	1.906869	1.077344	-1.157081	1.845225	1.068594	-1.164454	1.889674	1.075268	-1.158518
C	1.888921	1.910839	0.000000	1.829333	1.906198	0.000000	1.871123	1.909364	0.000000
H	1.879503	1.418087	2.187544	1.805633	1.412803	2.201985	1.858708	1.416900	2.190651
H	1.956134	-1.157724	1.359316	1.897843	-1.184765	1.368210	1.939285	-1.163512	1.361205
H	1.956134	-1.157724	-1.359316	1.897843	-1.184765	-1.368210	1.939285	-1.163512	-1.361205
H	1.879503	1.418087	-2.187544	1.805633	1.412803	-2.201985	1.858708	1.416900	-2.190651
H	1.827690	2.994861	0.000000	1.751258	2.997477	0.000000	1.804837	2.995090	0.000000
Fe	-0.025216	0.531406	0.000000	-0.024768	0.519486	0.000000	-0.027531	0.525340	0.000000
F	-1.589347	1.350569	0.000000	-1.571536	1.357603	0.000000	-1.585699	1.346713	0.000000
P	-0.998695	-1.624629	0.000000	-0.923666	-1.593232	0.000000	-0.975937	-1.614702	0.000000
F	-2.036510	-1.453234	1.219684	-1.987601	-1.441490	1.232024	-2.019643	-1.445504	1.222210
F	-2.036510	-1.453234	-1.219684	-1.987601	-1.441490	-1.232024	-2.019643	-1.445504	-1.222210

Table S41. Cartesian coordinates (Å) and energies (in hartree) for the optimized structure **12-1D**.

	B3LYP (-2739.47020)			BP86 (-2739.71604)			B3LYP* (-2738.74196)		
	X	Y	Z	X	Y	Z	X	Y	Z
C	-2.110856	-1.086923	0.706459	-2.040945	-1.105086	0.712818	-2.091171	-1.091607	0.707500
H	-1.974665	-1.947353	1.352222	-1.876087	-1.968295	1.361735	-1.946671	-1.952218	1.354405
C	-2.110856	-1.086923	-0.706459	-2.040945	-1.105086	-0.712818	-2.091171	-1.091607	-0.707500
H	-1.974665	-1.947353	-1.352222	-1.876087	-1.968295	-1.361735	-1.946671	-1.952218	-1.354405
C	-2.318052	0.277779	-1.152215	-2.304548	0.259762	-1.160664	-2.312093	0.273102	-1.153782
H	-2.394108	0.600965	-2.185001	-2.380546	0.584695	-2.201396	-2.388399	0.596547	-2.188517
C	-2.318052	0.277779	1.152215	-2.304548	0.259762	1.160664	-2.312093	0.273102	1.153782
H	-2.394108	0.600965	2.185001	-2.380546	0.584695	2.201396	-2.388399	0.596547	2.188517
C	-2.493962	1.097440	0.000000	-2.502852	1.080125	0.000000	-2.494180	1.092480	0.000000
H	-2.657118	2.170581	0.000000	-2.691938	2.157384	0.000000	-2.664200	2.166559	0.000000
Fe	-0.522406	0.206062	0.000000	-0.547527	0.224492	0.000000	-0.525978	0.211885	0.000000
P	0.805074	0.022547	1.611205	0.784467	0.027687	1.581979	0.799722	0.023915	1.604625
P	0.805074	0.022547	-1.611205	0.784467	0.027687	-1.581979	0.799722	0.023915	-1.604625
F	1.335077	1.319885	-2.369845	1.533573	1.318757	-2.189272	1.353872	1.321939	-2.352601
F	2.209428	-0.705513	-1.494747	2.082415	-0.911399	-1.502263	2.195863	-0.727277	-1.489533
F	0.285255	-0.746968	-2.903888	0.221230	-0.540384	-2.980330	0.273728	-0.728801	-2.909639
F	0.285255	-0.746968	2.903888	0.221230	-0.540384	2.980330	0.273728	-0.728801	2.909639
F	1.335077	1.319885	2.369845	1.533573	1.318757	2.189272	1.353872	1.321939	2.352601
F	2.209428	-0.705513	1.494747	2.082415	-0.911399	1.502263	2.195863	-0.727277	1.489533