Structures of Dimetallocenes $M_2(C_5H_5)_2$ (M = Zn, Cu, Ni, Co, Fe) and Their Perfluorinated Derivatives

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Supporting Information

Table S1: Total energies and relative energies for optimized low-energy structures of the $M_2(C_5X_5)_2$ (M=Zn, Cu, Ni, Co, Fe; X=H, F) complexes at the OPBE/cc-pVTZ level.

Table S2: Vibrational frequencies and infrared intensities for optimized low-energy structures of the $M_2(C_5X_5)_2$ (M=Zn, Cu, Ni, Co, Fe; X=H, F) complexes at the OPBE/cc-pVTZ level.

Table S3: Cartesian coordinates for optimized low-energy structures of the $M_2(C_5X_5)_2$ (M=Zn, Cu, Ni, Co, Fe; X=H, F) complexes at the OPBE/cc-pVTZ level.

Table S4: The M-C distances for optimized low-energy structures of the $M_2(C_5X_5)_2$ (M=Zn, Cu, Ni, Co, Fe; X=H, F) complexes at the OPBE/cc-pVTZ level.

Complete Gaussian 09 reference.

Table S1. Total energies (E_{tot}, in hartree) and relative energies (ΔE, in kcal/mol) for various optimized low-energy structures of the $M_2(C_5X_5)_2$ (M=Zn, Cu, Ni, Co, Fe; X=H, F) complexes at the OPBE/cc-pVTZ level.

Complex	Structure	Multiplicity	OPBE/cc-pVTZ	
			E_{tot}	ΔE
$Zn_2(C_5H_5)_2$	**Zn-H-1S**	1	-3946.91267	0.00
$Zn_2(C_5F_5)_2$	**Zn-F-1S**	1	-4939.00761	0.00
$Cu_2(C_5H_5)_2$	**Cu-H-1S**	1	-3669.09969	0.00
$Cu_2(C_5F_5)_2$	**Cu-F-1S**	1	-4661.20800	0.00
$Ni_2(C_5H_5)_2$	**Ni-H-1T**	3	-3404.60485	0.00
	Ni-H-2S	1	-3404.60391	0.59
	Ni-H-3S	1	-3404.60102	2.41
$Ni_2(C_5F_5)_2$	**Ni-F-1S**	1	-4396.73450	0.00
	Ni-F-2S	1	-4396.72769	4.27
	Ni-F-3S	1	-4396.72504	5.93
	Ni-F-4T	3	-4396.71584	11.71
$Co_2(C_5H_5)_2$	**Co-H-1T**	3	-3153.35576	0.00
	Co-H-2T	3	-3153.35025	3.46
	Co-H-3Q	5	-3153.34806	4.83
	Co-H-4T	3	-3153.34592	6.18
$Co_2(C_5F_5)_2$	**Co-F-1S**	1	-4145.50589	0.00
	Co-F-2T	3	-4145.50372	1.36
	Co-F-3S	1	-4145.50262	2.05
	Co-F-4T	3	-4145.48800	11.22
$Fe_2(C_5H_5)_2$	**Fe-H-1E**	7	-2915.10325	0.00
	Fe-H-2Q	5	-2915.10116	1.31
	Fe-H-3T	3	-2915.09716	3.82
	Fe-H-4Q	5	-2915.09174	7.22
$Fe_2(C_5F_5)_2$	**Fe-F-1Q**	5	-3907.25599	0.00
	Fe-F-2T	3	-3907.25298	1.89
	Fe-F-3T	3	-3907.24998	3.77

Table S2. Vibrational frequencies (in cm^{-1}) and infrared intensities (in km/mol, given in parentheses) for optimized low-energy structures of the $M_2(C_5X_5)_2$ (M=Zn, Cu, Ni, Co, Fe; X=H, F) complexes at the OPBE/cc-pVTZ level.

Structure	OPBE/cc-pVTZ
Zn-H-1S	15(0), 30(0), 30(0), 73(0), 73(0), 150(0), 196(2), 196(2), 197(0), 197(0), 286(105), 364(0), 609(0), 609(0), 609(0), 609(0), 753(1), 753(1), 755(0), 755(0), 781(436), 786(0), 828(0), 828(0), 828(0), 828(0), 860(0), 860(0), 861(0), 861(0), 1010(33), 1010(33), 1011(0), 1011(0), 1056(0), 1056(0), 1057(0), 1057(0), 1133(17), 1134(0), 1234(0), 1234(0), 1374(0), 1374(0), 1375(0), 1375(0), 1431(3), 1431(3), 1432(0), 1432(0), 3187(0), 3187(0), 3187(0), 3187(0), 3204(0), 3204(0), 3205(6), 3205(6), 3218(6), 3218(0)
Zn-F-1S	7i(0), 7i(0), 2(0), 2(0), 6(0), 87(0), 95(0), 95(0), 105(1), 105(1), 175(15), 178(0), 178(0), 178(0), 178(0), 234(0), 234(0), 235(0), 235(0), 235(0), 235(0), 259(0), 261(0), 261(0), 299(0), 299(0), 304(0), 304(0), 353(142), 397(0), 519(0), 519(0), 519(0), 519(0), 529(0), 529(0), 530(0), 530(0), 603(0), 604(0), 759(0), 759(0), 984(0), 984(0), 985(312), 985(312), 1176(0), 1176(0), 1178(0), 1178(0), 1469(0), 1469(0), 1470(0), 1470(0), 1551(446), 1561(451), 1561(451), 1561(0), 1561(0), 1566(0)
Cu-H-1S	40*i*(1), 52(0), 67(1), 103(0), 118(3), 129(0), 129(5), 193(0), 285(1), 325(0), 345(0), 366(3), 606(0), 607(4), 634(2), 638(0), 708(0), 719(44), 725(153), 726(0), 749(39), 756(0), 788(22), 792(0), 808(6), 808(0), 835(5), 843(0), 857(0), 858(22), 985(27), 985(0), 991(0), 992(31), 1041(2), 1043(0), 1058(3), 1059(0), 1101(1), 1105(0), 1224(0), 1224(0), 1339(1), 1340(0), 1364(0), 1368(4), 1411(0), 1412(1), 1443(4), 1445(0), 3127(1), 3127(0), 3150(1), 3150(0), 3173(5), 3173(0), 3176(5), 3176(0), 3196(0), 3196(16)
Cu-F-1S	21(0), 31(1), 65(0), 72(0), 86(0), 92(2), 106(0), 128(2), 148(0), 158(8), 159(0), 168(0), 174(0), 190(0), 200(4), 204(0), 218(2), 232(0), 234(3), 242(0), 271(0), 288(3), 292(0), 294(0), 310(1), 316(0), 396(0), 397(21), 450(7), 463(0), 504(5), 505(0), 517(8), 521(0), 603(41), 604(0), 624(0), 628(59), 662(67), 676(0), 747(1), 747(0), 944(0), 950(323), 968(0), 969(300), 1124(45), 1127(0), 1147(51), 1148(0), 1294(211), 1299(0), 1379(144), 1379(0), 1445(0), 1448(363), 1522(308), 1526(0), 1589(458), 1592(0)
Ni-H-1T	67(0), 95(0), 127(0), 140(0), 165(1), 178(0), 254(0), 280(0), 300(0), 318(1), 339(1), 409(0), 594(0), 600(0), 622(3), 622(0), 704(0), 706(36), 712(16), 716(0), 748(55), 757(0), 764(2), 775(0), 780(0), 796(0), 827(3), 830(0), 844(1), 850(0), 972(0), 974(33), 989(30), 991(0), 1028(1), 1032(0), 1036(0), 1039(0), 1086(10), 1090(0), 1220(0), 1220(0), 1337(3), 1339(0), 1341(0), 1350(1), 1386(0), 1390(0), 1408(0), 1409(1), 3138(0), 3138(0), 3148(6), 3149(0), 3154(3), 3155(0), 3189(0), 3189(11), 3194(6), 3194(0)
Ni-H-2S	31(0), 97(0), 144(0), 148(4), 164(0), 247(0), 312(1), 322(0), 331(0), 336(3), 359(9), 444(0), 565(6), 598(0), 620(0), 632(14), 680(54), 694(0), 700(49), 732(0), 737(26), 752(0), 758(10), 776(0), 777(3), 790(0), 843(0), 847(0), 866(5), 868(0), 945(25), 948(0), 995(36), 1000(0), 1016(7), 1025(0), 1028(0), 1030(0), 1085(9), 1088(0), 1214(0), 1214(0), 1316(2), 1316(0), 1342(44), 1355(0), 1359(0), 1362(11), 1417(4), 1418(0), 3140(1), 3141(0), 3152(3), 3153(0), 3162(0), 3163(0), 3168(15), 3168(0), 3181(14), 3181(0)
Ni-H-3S	101(0), 102(0), 143(0), 157(2), 184(1), 288(1), 306(1), 316(0), 338(2), 347(2), 395(0), 422(0), 578(0), 604(0), 613(0), 618(13), 658(0), 697(21), 725(0), 733(31), 749(14), 756(7), 761(0), 780(1), 781(1), 800(5), 838(1), 850(2), 868(5), 870(0), 934(1), 937(16), 992(0), 997(32), 1009(2), 1009(2), 1030(0), 1032(0), 1082(14), 1084(1), 1212(0), 1212(0), 1302(1), 1308(2), 1335(34), 1340(2), 1366(0), 1368(9), 1418(2), 1421(1), 3122(2), 3123(2), 3154(3), 3154(1), 3165(0), 3165(0), 3174(1), 3175(21), 3187(10), 3187(1)
Ni-F-1S	39(0), 53(0), 92(0), 102(1), 119(4), 144(1), 155(0), 158(1), 163(0), 163(0), 199(8), 207(3), 217(1), 220(0), 227(0), 228(0), 239(0), 241(0), 266(1), 284(0), 307(3), 313(8), 324(3), 372(1), 396(1), 408(2), 432(2), 444(11), 456(0), 478(21), 489(4), 502(7), 504(0), 526(4), 588(1), 592(43), 618(21), 649(82), 660(6), 708(14), 726(0), 730(1), 907(219), 934(227), 934(122), 946(95), 1077(96), 1091(5), 1104(71), 1133(39), 1274(50), 1280(159), 1343(79), 1346(105), 1435(217), 1438(256), 1454(180), 1481(234), 1520(183), 1555(307)
Ni-F-2S	31(0), 46(0), 74(0), 115(2), 117(2), 142(11), 149(0), 155(2), 161(1), 161(0), 183(4), 202(0), 207(1), 209(10), 221(0), 232(1), 232(2), 243(3), 253(0), 269(0), 281(2), 289(5), 301(1), 319(0), 344(43), 376(2), 408(18), 435(25), 454(7), 480(12), 482(3), 498(25), 506(16), 512(2), 577(67), 596(10), 599(10), 625(0), 633(65), 649(4), 733(2), 733(1), 935(296), 936(0), 940(17), 945(276), 1091(34), 1096(9), 1103(144), 1127(28), 1302(35), 1303(134), 1364(39), 1385(0), 1434(7), 1441(353), 1442(448), 1450(57), 1511(615), 1526(5)
Ni-F-3S	15(0), 20(0), 39(0), 73(1), 113(0), 141(0), 156(2), 164(1), 171(0), 174(0), 190(1), 195(1), 199(1), 209(6), 233(0), 236(0), 239(0), 246(0), 260(3), 275(13), 294(0), 303(4), 328(11), 330(5), 369(7), 395(3), 397(1), 443(9), 460(0), 493(12), 500(0), 501(18), 509(14), 516(5), 542(4), 544(1), 596(47), 638(28), 661(38), 678(1), 725(1), 749(0), 922(156), 929(120), 966(198), 978(170), 1051(8), 1103(191), 1152(12), 1158(0), 1258(118), 1339(73), 1385(169), 1400(284), 1431(18), 1442(2), 1512(489), 1514(309), 1526(93), 1575(260)
Ni-F-4T	40(0), 45(0), 62(0), 101(1), 113(0), 134(0), 143(0), 146(3), 154(2), 162(0), 168(0), 184(5), 186(9), 202(0), 205(10), 218(0), 223(0), 225(3), 245(0), 250(0), 272(6), 286(0), 295(0), 311(0), 315(0), 329(5), 341(0), 342(21), 415(38), 433(0), 482(7), 482(0), 494(14), 513(0), 550(36), 562(0), 598(107), 606(0), 608(9), 621(0), 735(0), 736(1), 939(0), 942(292), 945(0), 955(326), 1096(0), 1110(55), 1114(20), 1120(0), 1348(0), 1355(154), 1369(31), 1374(0), 1423(433), 1434(0), 1468(0), 1475(363), 1509(615), 1525(0)

Co-H-1T	69(0), 103(0), 105(0), 165(3), 175(0), 313(6), 325(1), 330(2), 349(1), 362(3), 364(1), 455(0), 588(2), 599(0), 623(0), 631(7), 692(30), 697(9), 729(23), 745(3), 747(8), 760(21), 772(1), 776(1), 783(5), 784(1), 838(0), 838(0), 859(2), 862(0), 947(1), 948(25), 990(32), 994(0), 1016(0), 1025(0), 1027(0), 1031(0), 1083(19), 1086(0), 1214(0), 1214(0), 1322(6), 1328(0), 1338(16), 1351(0), 1364(0), 1372(6), 1407(3), 1409(0), 3134(12), 3135(0), 3136(0), 3136(0), 3151(2), 3152(0), 3168(3), 3168(19), 3175(10), 3176(2)
Co-H-2T	44(0), 73(0), 93(0), 159(2), 190(0), 271(1), 313(5), 368(2), 393(23), 403(5), 419(11), 470(5), 564(0), 580(3), 580(3), 633(9), 714(18), 723(16), 728(7), 755(24), 758(3), 785(2), 786(8), 797(4), 803(4), 818(1), 851(3), 855(2), 855(3), 870(1), 917(4), 955(4), 988(3), 995(4), 1001(14), 1021(0), 1029(5), 1047(0), 1073(13), 1109(8), 1205(0), 1216(0), 1293(0), 1315(8), 1336(1), 1345(1), 1359(2), 1388(1), 1398(0), 1419(1), 2969(29), 3112(1), 3128(13), 3139(8), 3160(20), 3167(16), 3182(0), 3188(3), 3197(8), 3208(7)
Co-H-3Q	33(0), 37(0), 53(0), 72(6), 121(0), 230(0), 317(0), 322(1), 352(1), 365(3), 367(0), 389(0), 574(0), 580(0), 582(1), 587(0), 711(0), 722(21), 742(0), 753(1), 769(90), 779(0), 783(0), 789(30), 794(0), 796(0), 843(2), 846(0), 846(0), 847(1), 962(0), 966(23), 983(0), 983(40), 1032(12), 1034(0), 1041(1), 1042(0), 1098(12), 1101(0), 1214(0), 1214(0), 1323(0), 1326(0), 1358(3), 1361(0), 1392(0), 1392(2), 1404(0), 1405(0), 3080(6), 3081(0), 3176(0), 3177(0), 3185(3), 3185(0), 3194(10), 3194(0), 3203(0), 3203(7)
Co-H-4T	12(0), 32(0), 94(1), 95(2), 170(2), 258(2), 323(1), 351(1), 369(11), 384(8), 386(7), 453(3), 554(1), 585(1), 587(0), 599(1), 709(13), 730(6), 733(19), 763(8), 778(5), 780(7), 792(2), 793(19), 798(2), 805(0), 837(0), 861(4), 863(0), 864(2), 943(13), 982(9), 990(10), 1006(11), 1019(0), 1020(1), 1042(0), 1049(1), 1072(14), 1123(10), 1211(0), 1229(0), 1310(0), 1321(17), 1344(1), 1359(0), 1377(2), 1394(2), 1404(2), 1432(2), 3141(2), 3146(0), 3160(8), 3161(13), 3173(8), 3179(0), 3180(0), 3194(9), 3198(6), 3209(6)
Co-F-1S	16(0), 53(0), 60(0), 98(1), 128(0), 154(0), 161(0), 171(1), 172(0), 175(0), 187(3), 204(1), 209(5), 227(4), 231(0), 236(0), 239(0), 251(0), 252(1), 288(2), 298(0), 311(1), 362(14), 390(20), 433(6), 437(6), 450(6), 461(2), 482(7), 494(3), 499(1), 507(2), 527(7), 549(1), 559(0), 562(74), 595(18), 632(18), 701(2), 723(58), 729(0), 747(0), 900(156), 933(147), 963(178), 977(182), 1073(3), 1087(29), 1154(2), 1173(0), 1277(143), 1321(107), 1352(235), 1438(176), 1440(9), 1462(7), 1505(317), 1518(102), 1538(275), 1560(288)
Co-F-2T	41(0), 49(16), 77(0), 110(0), 116(4), 154(0), 156(0), 160(0), 163(0), 173(0), 175(0), 208(4), 218(0), 226(0), 227(0), 239(0), 240(0), 243(1), 262(4), 294(0), 296(1), 311(2), 350(16), 391(1), 414(19), 423(16), 467(0), 474(1), 479(7), 502(0), 510(1), 513(6), 533(16), 538(8), 589(71), 595(1), 601(24), 613(0), 712(69), 722(0), 727(0), 761(3), 865(189), 876(376), 938(23), 949(168), 1058(55), 1080(78), 1134(34), 1148(51), 1252(129), 1287(24), 1328(64), 1353(187), 1435(131), 1460(108), 1493(87), 1503(359), 1541(185), 1568(320)
Co-F-3S	11(0), 50(0), 58(0), 81(1), 118(0), 141(1), 161(0), 169(0), 175(0), 178(1), 202(1), 203(1), 206(5), 215(2), 230(0), 238(0), 238(0), 254(2), 257(0), 279(2), 308(0), 323(2), 372(3), 373(9), 422(20), 426(18), 457(4), 464(4), 483(6), 500(4), 500(4), 516(15), 530(4), 557(0), 559(3), 591(56), 623(29), 646(30), 673(67), 699(0), 710(1), 746(0), 910(133), 928(139), 967(184), 972(221), 1072(5), 1084(34), 1154(7), 1169(0), 1307(102), 1316(13), 1393(231), 1413(193), 1444(5), 1458(1), 1466(464), 1511(244), 1539(262), 1553(268)
Co-F-4T	26(0), 40(0), 66(0), 121(0), 122(3), 140(0), 149(2), 151(0), 159(3), 167(0), 173(6), 206(1), 206(5), 223(1), 228(0), 231(0), 235(0), 241(0), 249(0), 292(1), 298(0), 312(6), 317(7), 334(0), 379(5), 391(3), 417(13), 430(14), 483(2), 493(32), 494(0), 504(1), 507(6), 510(2), 580(55), 584(3), 594(26), 607(4), 721(0), 722(52), 730(29), 735(0), 899(24), 900(375), 938(19), 944(239), 1061(150), 1072(0), 1123(4), 1130(76), 1262(144), 1272(14), 1325(32), 1332(141), 1424(143), 1445(4), 1485(12), 1491(428), 1539(677), 1553(0)
Fe-H-1E	46(0), 70(0), 118(0), 129(0), 150(0), 154(0), 183(1), 263(0), 284(1), 350(0), 365(1), 409(0), 598(1), 606(0), 622(0), 623(6), 685(0), 694(24), 708(0), 715(21), 725(55), 747(0), 771(17), 780(0), 787(0), 788(1), 827(2), 836(0), 837(0), 840(0), 962(31), 963(0), 983(30), 985(0), 1031(4), 1031(0), 1041(2), 1044(0), 1082(18), 1086(0), 1218(0), 1219(0), 1320(0), 1322(2), 1351(0), 1354(0), 1385(0), 1387(0), 1395(1), 1398(0), 3112(5), 3113(0), 3165(0), 3165(0), 3176(2), 3177(0), 3185(9), 3185(0), 3195(5), 3195(0)
Fe-H-2Q	86(0), 96(0), 130(2), 159(3), 170(2), 303(0), 307(0), 329(5), 359(5), 391(0), 429(0), 443(0), 602(1), 610(0), 629(0), 642(6), 664(1), 695(36), 703(16), 725(0), 736(7), 738(28), 750(1), 764(0), 779(0), 781(3), 832(0), 842(1), 849(1), 858(0), 935(31), 939(0), 988(1), 994(37), 1009(0), 1014(0), 1021(0), 1024(0), 1074(27), 1076(0), 1210(0), 1210(0), 1316(0), 1319(20), 1319(0), 1326(0), 1356(5), 1356(0), 1398(2), 1400(1), 3147(1), 3148(0), 3155(0), 3155(0), 3168(1), 3169(0), 3177(0), 3177(18), 3185(6), 3185(0)
Fe-H-3T	30(1), 86(0), 123(3), 143(0), 160(4), 278(3), 355(3), 370(0), 435(21), 446(18), 457(20), 519(11), 577(1), 582(0), 626(1), 635(7), 726(10), 751(4), 769(12), 776(8), 785(14), 793(0), 803(6), 807(13), 814(11), 817(0), 849(6), 856(0), 865(1), 867(1), 928(9), 957(7), 995(8), 996(10), 997(2), 1028(0), 1041(1), 1048(0), 1065(11), 1121(13), 1202(0), 1226(0), 1284(1), 1297(1), 1361(1), 1369(1), 1375(2), 1385(0), 1411(2), 1414(1), 3086(10), 3100(31), 3155(5), 3166(1), 3170(18), 3175(0), 3178(16), 3187(5), 3190(14), 3205(11)

Fe-H-4Q	51(1), 101(2), 126(1), 171(6), 199(1), 276(3), 311(2), 339(0), 407(7), 432(12), 449(26), 540(23), 569(2), 587(12), 600(5), 602(34), 722(2), 758(12), 763(15), 782(39), 790(0), 803(2), 805(3), 815(21), 820(3), 831(8), 861(3), 862(0), 876(3), 887(0), 919(2), 956(1), 972(6), 999(3), 1013(1), 1032(1), 1037(3), 1051(0), 1073(10), 1114(15), 1171(5), 1220(0), 1225(2), 1312(1), 1343(3), 1346(1), 1379(0), 1395(1), 1404(2), 1419(2), 3025(45), 3074(16), 3144(6), 3146(4), 3169(12), 3180(1), 3185(0), 3185(21), 3195(9), 3208(7)
Fe-F-1Q	31(0), 60(1), 80(0), 105(3), 131(0), 144(1), 158(1), 169(0), 170(1), 174(0), 181(0), 187(7), 211(7), 220(0), 233(0), 235(0), 240(0), 248(1), 250(0), 280(1), 293(0), 317(1), 392(23), 398(9), 440(2), 447(26), 463(2), 474(5), 487(5), 491(1), 495(1), 510(0), 521(2), 562(1), 568(23), 589(38), 596(49), 626(66), 628(0), 700(0), 741(20), 741(0), 903(59), 942(138), 961(177), 968(175), 1065(106), 1075(67), 1138(9), 1177(7), 1226(205), 1265(125), 1393(79), 1416(102), 1438(212), 1450(4), 1495(107), 1531(280), 1536(154), 1566(355)
Fe-F-2T	32(0), 39(5), 78(0), 103(0), 116(6), 141(0), 150(3), 163(3), 164(0), 171(0), 178(0), 188(2), 202(0), 208(0), 238(0), 239(0), 244(0), 250(1), 255(0), 292(0), 301(4), 323(1), 399(28), 422(3), 423(42), 429(0), 459(38), 487(1), 489(1), 492(0), 499(0), 507(0), 529(13), 557(88), 565(6), 567(0), 573(1), 592(26), 674(303), 705(112), 718(0), 718(0), 773(18), 801(309), 886(0), 948(275), 1056(15), 1077(78), 1119(0), 1163(32), 1282(133), 1319(83), 1357(0), 1383(198), 1454(60), 1475(84), 1505(0), 1515(428), 1535(206), 1563(302)
Fe-F-3T	12(1), 36(0), 81(1), 83(1), 119(2), 156(0), 163(0), 172(0), 173(3), 176(1), 188(1), 200(4), 202(4), 229(1), 231(0), 236(0), 240(0), 248(1), 254(0), 287(3), 295(0), 311(1), 391(13), 418(10), 442(9), 448(4), 459(21), 467(16), 473(1), 481(5), 491(0), 501(4), 521(2), 560(15), 560(0), 573(100), 592(24), 607(3), 664(89), 690(5), 714(1), 744(0), 896(127), 928(122), 961(202), 964(248), 1084(2), 1084(19), 1152(0), 1172(1), 1296(131), 1319(83), 1358(289), 1437(161), 1454(20), 1454(4), 1495(356), 1505(38), 1520(293), 1555(328)

Table S3. Cartesian coordinates (in Å) for optimized low-energy structures of the $M_2(C_5X_5)_2$ (M=Zn, Cu, Ni, Co, Fe; X=H, F) complexes at the OPBE/cc-pVTZ level.

$Zn_2(C_5H_5)_2$ (**Zn-H-1S**) OPBE/cc-pVTZ	$Zn_2(C_5F_5)_2$ (**Zn-F-1S**) OPBE/cc-pVTZ
0 1	0 1
C,0,-0.7112726968,-0.9789828766,3.0947300646	Zn,0,0.,0.,0.008931761
C,0,-1.1508633951,0.373938187,3.0947300646	C,0,1.2124469255,0.,1.9678133438
C,0,0.0000000022,1.2100893859,3.0947300646	C,0,0.3746667048,1.1531055491,1.9678133438
C,0,1.1508633964,0.3739381829,3.0947300646	C,0,-0.9808901675,0.712658422,1.9678133438
C,0,0.7112726932,-0.9789828792,3.0947300646	C,0,-0.9808901675,-0.712658422,1.9678133438
C,0,-0.0000000022,-1.2100893859,-3.0947300646	C,0,0.3746667047,-1.1531055491,1.9678133438
C,0,1.1508633951,-0.373938187,-3.0947300646	Zn,0,0.,0.,-2.323931761
C,0,0.7112726968,0.9789828766,-3.0947300646	C,0,0.9808901675,-0.712658422,-4.2828133438
C,0,-0.7112726932,0.9789828792,-3.0947300646	C,0,-0.3746667048,-1.1531055491,-4.2828133438
C,0,-1.1508633964,-0.3739381829,-3.0947300646	C,0,-1.2124469255,0.,-4.2828133438
Zn,0,0.,0.,1.1720401437	C,0,-0.3746667047,1.1531055491,-4.2828133438
Zn,0,0.,0.,-1.1720401437	C,0,0.9808901675,0.712658422,-4.2828133438
H,0,-1.349160554,-1.8569601872,3.1005595054	F,0,2.5383874222,0.,2.0441871112
H,0,-2.1829876259,0.7092956807,3.1005595054	F,0,0.7844048518,2.4141498988,2.0441871112
H,0,0.0000000042,2.295329026,3.1005595054	F,0,-2.0535985629,1.4920266914,2.0441871112
H,0,2.1829876285,0.7092956727,3.1005595054	F,0,-2.0535985629,-1.4920266914,2.0441871112
H,0,1.3491605472,-1.8569601921,3.1005595054	F,0,0.7844048518,-2.4141498988,2.0441871112
H,0,-0.0000000042,-2.295329026,-3.1005595054	F,0,2.0535985629,-1.4920266914,-4.3591871112
H,0,2.1829876259,-0.7092956807,-3.1005595054	F,0,-0.7844048518,-2.4141498988,-4.3591871112
H,0,1.349160554,1.8569601872,-3.1005595054	F,0,-2.5383874222,0.,-4.3591871112
H,0,-1.3491605472,1.8569601921,-3.1005595054	F,0,-0.7844048518,2.4141498988,-4.3591871112
H,0,-2.1829876285,-0.7092956727,-3.1005595054	F,0,2.0535985629,1.4920266914,-4.3591871112
$Cu_2(C_5H_5)_2$ (**Cu-H-1S**) OPBE/cc-pVTZ	$Cu_2(C_5F_5)_2$ (**Cu-F-1S**) OPBE/cc-pVTZ
0 1	0 1
C,0,1.9527627415,1.5511020694,-0.1852811883	C,0,2.0271403916,0.50502214,0.1762321777
C,0,1.7229248803,0.6839245366,0.9324707275	C,0,2.3584403684,-0.4141809046,1.2451551302
C,0,1.9737269464,-0.6741206945,0.4892709944	C,0,2.2015910502,-1.7211550995,0.8184876719
C,0,2.3475664785,-0.5941939445,-0.8951792769	C,0,1.8913492533,-1.7368946589,-0.5834259364
C,0,2.3179061443,0.7419627803,-1.2994737917	C,0,1.8104994892,-0.3930763237,-1.004992089
C,0,-1.9737269464,0.6741206945,-0.4892709944	C,0,-2.2015910502,1.7211550995,-0.8184876719
C,0,-1.7229248803,-0.6839245366,-0.9324707275	C,0,-2.3584403684,0.4141809046,-1.2451551302
C,0,-1.9527627415,-1.5511020694,0.1852811883	C,0,-2.0271403916,-0.50502214,-0.1762321777
C,0,-2.3179061443,-0.7419627803,1.2994737917	C,0,-1.8104994892,0.3930763237,1.004992089
C,0,-2.3475664785,0.5941939445,0.8951792769	C,0,-1.8913492533,1.7368946589,0.5834259364
Cu,0,-0.1027110578,1.2122262274,0.0317248863	Cu,0,0.1366532871,0.9993081157,0.6795721118
Cu,0,0.1027110578,-1.2122262274,-0.0317248863	Cu,0,-0.1366532871,-0.9993081157,-0.6795721118
H,0,2.0335552474,2.6361048894,-0.1363700829	F,0,2.8089128417,1.6016381083,-0.0746838278
H,0,1.6611844236,0.986905587,1.9752567807	F,0,2.5627598349,-0.0620813369,2.5108731366
H,0,2.2418659112,-1.4852667767,1.1688268047	F,0,2.1135177706,-2.7847343803,1.6065835538
H,0,2.6476663434,-1.4363714178,-1.5136252163	F,0,1.9901019578,-2.8150591242,-1.3695038832
H,0,2.5246295999,1.108610701,-2.300840704	F,0,2.1162036235,0.0406546827,-2.2275571087
H,0,-2.2418659112,1.4852667767,-1.1688268047	F,0,-2.1135177706,2.7847343803,-1.6065835538
H,0,-1.6611844236,-0.986905587,-1.9752567807	F,0,-2.5627598349,0.0620813369,-2.5108731366
H,0,-2.0335552474,-2.6361048894,0.1363700829	F,0,-2.8089128417,-1.6016381083,0.0746838278
H,0,-2.5246295999,-1.108610701,2.300840704	F,0,-2.1162036235,-0.0406546827,2.2275571087
H,0,-2.6476663434,1.4363714178,1.5136252163	F,0,-1.9901019578,2.8150591242,1.3695038832

$Ni_2(C_5H_5)_2$ (**Ni-H-1T**) OPBE/cc-pVTZ	$Ni_2(C_5F_5)_2$ (**Ni-F-1S**) OPBE/cc-pVTZ
0 3	0 1
C,0,1.3101246668,0.,2.111496559	Ni,0,1.5626711866,0.574886485,0.
C,0,0.4863604047,1.1509706782,1.9193016107	C,0,0.4718263172,2.0131496494,0.716217764
C,0,-0.8798572727,0.7175277705,1.7603311122	C,0,0.4718263172,2.0131496494,-0.716217764
C,0,-0.8798572727,-0.7175277705,1.7603311122	C,0,-0.8341298448,1.4060468466,-1.1275913439
C,0,0.4863604047,-1.1509706782,1.9193016107	C,0,-1.7227670047,1.3263834902,0.
C,0,0.8798572727,-0.7175277705,-1.7603311122	C,0,-0.8341298448,1.4060468466,1.1275913439
C,0,-0.4863604047,-1.1509706782,-1.9193016107	Ni,0,-0.5019163064,-0.2376403597,0.
C,0,-1.3101246668,0.,-2.111496559	C,0,0.550616112,-1.6233343189,1.1208920056
C,0,-0.4863604047,1.1509706782,-1.9193016107	C,0,-0.730853422,-2.1247055189,0.7147845517
C,0,0.8798572727,0.7175277705,-1.7603311122	C,0,-0.730853422,-2.1247055189,-0.7147845517
Ni,0,1.1235736979,0.,0.1406189687	C,0,0.550616112,-1.6233343189,-1.1208920056
Ni,0,-1.1235736979,0.,-0.1406189687	C,0,1.4942190132,-1.4276098768,0.
H,0,2.358080902,0.,2.4071141958	F,0,0.9908869671,3.0090966086,1.4653688212
H,0,0.8021088874,2.1846056004,2.0257785477	F,0,0.9908869671,3.0090966086,-1.4653688212
H,0,-1.7453377392,1.3614422939,1.9129194913	F,0,-1.2292804736,1.377598798,-2.3938412182
H,0,-1.7453377392,-1.3614422939,1.9129194913	F,0,-3.039492755,1.1590798621,0.
H,0,0.8021088874,-2.1846056004,2.0257785477	F,0,-1.2292804736,1.377598798,2.3938412182
H,0,1.7453377392,-1.3614422939,-1.9129194913	F,0,0.9226381876,-1.5882863941,2.3943432949
H,0,-0.8021088874,-2.1846056004,-2.0257785477	F,0,-1.7074584925,-2.5511530121,1.4987679789
H,0,-2.358080902,0.,-2.4071141958	F,0,-1.7074584925,-2.5511530121,-1.4987679789
H,0,-0.8021088874,2.1846056004,-2.0257785477	F,0,0.9226381876,-1.5882863941,-2.3943432949
H,0,1.7453377392,1.3614422939,-1.9129194913	F,0,2.6618881632,-2.1893739294,0.
$Ni_2(C_5H_5)_2$ (**Ni-H-2S**) OPBE/cc-pVTZ	$Ni_2(C_5F_5)_2$ (**Ni-F-2S** OPBE/cc-pVTZ
0 1	0 1
C,0,-0.0888721124,0.1115142557,-0.0684929817	C,0,1.8386621769,1.7571008727,0.0811359933
C,0,-0.0881370291,-0.1437292945,1.3423408299	C,0,1.4593991,0.8407150508,1.1209019005
C,0,1.2840608074,-0.2826465323,1.8189287416	C,0,1.6390009759,-0.5791707002,0.6686670648
C,0,2.1176441117,-0.3247083719,0.6688429406	C,0,1.8577825059,-0.4734775339,-0.7503675714
C,0,1.2421031481,-0.210851979,-0.4929770462	C,0,1.8746364608,0.9384238327,-1.1039017247
C,0,0.6744605589,-3.7218116047,-0.2529363756	C,0,-1.8577825059,0.4734775339,-0.7503675714
C,0,2.0466583954,-3.8607288425,0.2236515361	C,0,-1.8746364608,-0.9384238327,-1.1039017247
C,0,2.0473934787,-4.1159723927,1.6344853477	C,0,-1.8386621769,-1.7571008727,0.0811359933
C,0,0.7164182182,-3.7936061581,2.0589694122	C,0,-1.4593991,-0.8407150508,1.1209019005
C,0,-0.1591227454,-3.6797497651,0.8971494254	C,0,-1.6390009759,0.5791707002,0.6686670648
Ni,0,0.0604361714,-1.800209919,0.1096428827	Ni,0,0.0317015288,1.1558723011,-0.2237054232
Ni,0,1.8980851949,-2.204248218,1.4563494832	Ni,0,-0.0317015288,-1.1558723011,-0.2237054232
H,0,-0.9143859164,0.4669217472,-0.6798244292	F,0,2.1351176258,3.0505985861,0.1827371227
H,0,-0.9477210804,-0.03703376,2.0005541731	F,0,1.4051663075,1.147656148,2.4091958476
H,0,1.5977536555,-0.0697542921,2.8401739078	F,0,2.3441750787,-1.4271697232,1.4502435638
H,0,3.1925322651,-0.1502253403,0.6398752392	F,0,2.5464242684,-1.380696219,-1.4658175675
H,0,1.6027832469,-0.1657298406,-1.5183488531	F,0,2.1462168191,1.3768582466,-2.3260892022
H,0,0.3607677108,-3.9347038449,-1.2741815418	F,0,-2.5464242684,1.380696219,-1.4658175675
H,0,2.9062424467,-3.967424377,-0.4345618071	F,0,-2.1462168191,-1.3768582466,-2.3260892022
H,0,2.8729072827,-4.4713798842,2.2458167952	F,0,-2.1351176258,-3.0505985861,0.1827371227
H,0,0.3557381194,-3.8387282964,3.0843412191	F,0,-1.4051663075,-1.147656148,2.4091958476
H,0,-1.2340108988,-3.8542327967,0.9261171268	F,0,-2.3441750787,1.4271697232,1.4502435638

$Ni_2(C_5H_5)_2$ (**Ni-H-3S**) OPBE/cc-pVTZ 0 1 Ni,0,0.0580329883,-1.3407040686,0. C,0,-0.901318755,-0.7325482049,1.7291969948 C,0,0.4957184987,-0.9449814893,1.8648733764 C,0,1.1187249021,0.386566528,1.77767913 C,0,0.1140573548,1.3975122471,1.8989877736 C,0,-1.1189967734,0.7185334959,1.6516916748 Ni,0,0.093254584,0.9199287454,0. C,0,-0.901318755,-0.7325482049,-1.7291969948 C,0,-1.1189967734,0.7185334959,-1.6516916748 C,0,0.1140573548,1.3975122471,-1.8989877736 C,0,1.1187249021,0.386566528,-1.77767913 C,0,0.4957184987,-0.9449814893,-1.8648733764 H,0,-1.6945757415,-1.4381105271,1.9702564764 H,0,0.9840055881,-1.8226217965,2.2919520955 H,0,2.1889775796,0.5578100047,1.8619123602 H,0,0.2568685861,2.4572764334,2.0911911128 H,0,-2.1024834057,1.1824362852,1.6598572014 H,0,-1.6945757415,-1.4381105271,-1.9702564764 H,0,-2.1024834057,1.1824362852,-1.6598572014 H,0,0.2568685861,2.4572764334,-2.0911911128 H,0,2.1889775796,0.5578100047,-1.8619123602 H,0,0.9840055881,-1.8226217965,-2.2919520955	$Ni_2(C_5F_5)_2$ (**Ni-F-3S**) OPBE/cc-pVTZ 0 1 Ni,0,1.0988689685,-1.2750472973,0. C,0,-1.1733217678,-0.9429976305,-0.7275681684 C,0,-0.2769078739,-2.0667187311,-1.1173994487 C,0,0.0819866156,-2.9047357575,0. C,0,-0.2769078739,-2.0667187311,1.1173994487 C,0,-1.1733217678,-0.9429976305,0.7275681684 Ni,0,-0.2353643866,0.6130900526,0. C,0,0.6720327556,2.0329192826,-1.1470810172 C,0,-0.5955163321,2.5544375528,-0.7078851587 C,0,-0.5955163321,2.5544375528,0.7078851587 C,0,0.6720327556,2.0329192826,1.1470810172 C,0,1.4729441683,1.7152120845,0. F,0,-2.3206796742,-0.7768792044,-1.4361557413 F,0,-0.0625191065,-2.3912166482,-2.3856716538 F,0,0.5608398567,-4.1479150993,0. F,0,-0.0625191065,-2.3912166482,2.3856716538 F,0,-2.3206796742,-0.7768792044,1.4361557413 F,0,1.076715591,1.9898783629,-2.4087572666 F,0,-1.560504424,2.9927426584,-1.5001614551 F,0,-1.560504424,2.9927426584,1.5001614551 F,0,1.076715591,1.9898783629,2.4087572666 F,0,2.8034738167,1.5385852479,0.
	$Ni_2(C_5F_5)_2$ (**Ni-F-4T**) OPBE/cc-pVTZ 0 3 C,0,1.3123085796,0.,2.166300696 C,0,0.5095750857,1.1534588515,1.8862406029 C,0,-0.8707237676,0.7260486494,1.6619784481 C,0,-0.8707237676,-0.7260486494,1.6619784481 C,0,0.5095750857,-1.1534588515,1.8862406029 C,0,0.8707237676,-0.7260486494,-1.6619784481 C,0,-0.5095750857,-1.1534588515,-1.8862406029 C,0,-1.3123085796,0.,-2.166300696 C,0,-0.5095750857,1.1534588515,-1.8862406029 C,0,0.8707237676,0.7260486494,-1.6619784481 Ni,0,1.1100403182,0.,0.1795180753 Ni,0,-1.1100403182,0.,-0.1795180753 F,0,2.5767394529,0.,2.587970961 F,0,0.8566451944,2.4135988762,2.1246071867 F,0,-1.9040753441,1.4656304285,2.1085036699 F,0,-1.9040753441,-1.4656304285,2.1085036699 F,0,0.8566451944,-2.4135988762,2.1246071867 F,0,1.9040753441,-1.4656304285,-2.1085036699 F,0,-0.8566451944,-2.4135988762,-2.1246071867 F,0,-2.5767394529,0.,-2.587970961 F,0,-0.8566451944,2.4135988762,-2.1246071867 F,0,1.9040753441,1.4656304285,-2.1085036699

$Co_2(C_5H_5)_2$ (**Co-H-1T**) OPBE/cc-pVTZ 0 3 C,0,1.9915542162,1.460845415,-0.063398149 C,0,1.718477631,0.7011274636,1.1195204688 C,0,1.7266083087,-0.7220262595,0.7866060359 C,0,1.8435159813,-0.8245032446,-0.6327194032 C,0,1.8588940419,0.5359185634,-1.1474603211 C,0,-1.8435159813,0.8245032446,-0.6327194032 C,0,-1.8588940419,-0.5359185634,-1.1474603211 C,0,-1.9915542162,-1.460845415,-0.063398149 C,0,-1.718477631,-0.7011274636,1.1195204688 C,0,-1.7266083087,0.7220262595,0.7866060359 Co,0,0.0837213995,1.0827639189,-0.1085567424 Co,0,-0.0837213995,-1.0827639189,-0.1085567424 H,0,2.2297703666,2.5221319496,-0.1240082274 H,0,1.7500530795,1.0858196653,2.1365427643 H,0,1.9453108175,-1.5067256999,1.509616363 H,0,2.1701040818,-1.6980666486,-1.1962966515 H,0,1.96095977,0.7822367873,-2.2018461393 H,0,-2.1701040818,1.6980666486,-1.1962966515 H,0,-1.96095977,-0.7822367873,-2.2018461393 H,0,-2.2297703666,-2.5221319496,-0.1240082274 H,0,-1.7500530795,-1.0858196653,2.1365427643 H,0,-1.9453108175,1.5067256999,1.509616363	$Co_2(C_5F_5)_2$ (**Co-F-1S**) OPBE/cc-pVTZ 0 1 Co,0,0.2951702048,1.4673909768,0. C,0,-1.3680697358,1.6036139525,0.7381921165 C,0,-1.3680697358,1.6036139525,-0.7381921165 C,0,-1.807699165,0.2358876889,-1.1334131928 C,0,-2.3560468886,-0.4601616987,0. C,0,-1.807699165,0.2358876889,1.1334131928 Co,0,-0.4401419316,-0.7168812981,0. C,0,0.963141049,-1.5880853615,1.1625611551 C,0,0.0109101899,-2.5599353634,0.7163220824 C,0,0.0109101899,-2.5599353634,-0.7163220824 C,0,0.963141049,-1.5880853615,-1.1625611551 C,0,1.5336335899,-0.9717000202,0. F,0,-1.7542156837,2.6580488172,1.508983745 F,0,-1.7542156837,2.6580488172,-1.508983745 F,0,-2.0955888672,-0.0759673097,-2.3969720566 F,0,-3.2298341601,-1.4641933293,0. F,0,-2.0955888672,-0.0759673097,2.3969720566 F,0,1.3213799563,-1.3625413046,2.4175658685 F,0,-0.6706479391,-3.3837326497,1.4947755112 F,0,-0.6706479391,-3.3837326497,-1.4947755112 F,0,1.3213799563,-1.3625413046,-2.4175658685 F,0,2.5671177755,-0.1106674335,0.
$Co_2(C_5H_5)_2$ (**Co-H-2T**) OPBE/cc-pVTZ 0 3 Co,0,0.3137228342,1.1498311799,0. C,0,-1.4384450937,1.6323354938,0.7145944216 C,0,-1.4384450937,1.6323354938,-0.7145944216 C,0,-1.8913545684,0.2843844305,-1.1296308004 C,0,-2.4601207,-0.4034397857,0. C,0,-1.8913545684,0.2843844305,1.1296308004 Co,0,-0.603571919,-0.8729806678,0. C,0,0.9134773796,-1.5513173971,1.1527143746 C,0,0.1497319017,-2.6802201448,0.708612292 C,0,0.1497319017,-2.6802201448,-0.708612292 C,0,0.9134773796,-1.5513173971,-1.1527143746 C,0,1.4232049325,-0.8501520502,0. H,0,-1.479510939,2.5086178926,1.3633879563 H,0,-1.479510939,2.5086178926,-1.3633879563 H,0,-2.081697005,0.0231451095,-2.1685965285 H,0,-3.1946769739,-1.206398794,0. H,0,-2.081697005,0.0231451095,2.1685965285 H,0,1.0995605306,-1.2807366998,2.1872541381 H,0,-0.3348483619,-3.4051542139,1.3545086099 H,0,-0.3348483619,-3.4051542139,-1.3545086099 H,0,1.0995605306,-1.2807366998,-2.1872541381 H,0,2.215932344,-0.080604739,0.	$Co_2(C_5F_5)_2$ (**Co-F-2T**) OPBE/cc-pVTZ 0 3 Co,0,1.8904414588,-0.7277547471,0. C,0,-1.7074896591,-1.0380173108,-0.7151356394 C,0,-0.4133502848,-1.4960789511,-1.1170287709 C,0,0.408655113,-2.0289132053,0. C,0,-0.4133502848,-1.4960789511,1.1170287709 C,0,-1.7074896591,-1.0380173108,0.7151356394 Co,0,-0.2680904745,0.1699437488,0. C,0,0.7587555633,1.5041950914,-1.1248771938 C,0,-0.4974172473,2.0477222254,-0.7144583906 C,0,-0.4974172473,2.0477222254,0.7144583906 C,0,0.7587555633,1.5041950914,1.1248771938 C,0,1.6846997191,1.2694240012,0. F,0,-2.7293020909,-0.7195567684,-1.4929023597 F,0,-0.087457625,-1.6696632698,-2.3968378088 F,0,0.6730047298,-3.4125973196,0. F,0,-0.087457625,-1.6696632698,2.3968378088 F,0,-2.7293020909,-0.7195567684,1.4929023597 F,0,1.1274993313,1.4245565215,-2.4004796576 F,0,-1.4595940273,2.5126938211,-1.4943882042 F,0,-1.4595940273,2.5126938211,1.4943882042 F,0,1.1274993313,1.4245565215,2.4004796576 F,0,2.9293488944,1.9217153545,0.

$Co_2(C_5H_5)_2$ (**Co-H-3Q**) OPBE/cc-pVTZ	$Co_2(C_5F_5)_2$ (**Co-F-3S**) OPBE/cc-pVTZ
0 5	0 1
Co,0,-0.6551570663,-0.9294108122,0.	Co,0,1.2039910852,-1.3244199316,0.
C,0,1.3567630257,-1.341952541,0.	C,0,-1.2265990662,-0.8413465101,-0.7287666602
C,0,0.7184323532,-1.9255385895,1.1630674009	C,0,-0.2535399708,-1.8894386843,-1.1290615045
C,0,-0.2959920732,-2.8197534204,0.7175937595	C,0,0.0418446843,-2.7510415323,0.
C,0,-0.2959920732,-2.8197534204,-0.7175937595	C,0,-0.2535399708,-1.8894386843,1.1290615045
C,0,0.7184323532,-1.9255385895,-1.1630674009	C,0,-1.2265990662,-0.8413465101,0.7287666602
Co,0,0.6551570663,0.9294108122,0.	Co,0,-0.0662009908,0.5143860625,0.
C,0,0.2959920732,2.8197534204,0.7175937595	C,0,0.6966556368,1.9762251152,-1.1700739159
C,0,0.2959920732,2.8197534204,-0.7175937595	C,0,-0.6189120864,2.3083072472,-0.7185592717
C,0,-0.7184323532,1.9255385895,-1.1630674009	C,0,-0.6189120864,2.3083072472,0.7185592717
C,0,-1.3567630257,1.341952541,0.	C,0,0.6966556368,1.9762251152,1.1700739159
C,0,-0.7184323532,1.9255385895,1.1630674009	C,0,1.4946390894,1.7541022718,0.
H,0,0.9835866425,-1.7233765814,2.1961496059	F,0,-2.337179193,-0.6283290868,-1.462155302
H,0,-0.9436687229,-3.412653492,1.3561401409	F,0,-0.0968542682,-2.2395170134,-2.4097545142
H,0,-0.9436687229,-3.412653492,-1.3561401409	F,0,0.5168504694,-4.001292647,0.
H,0,0.9835866425,-1.7233765814,-2.1961496059	F,0,-0.0968542682,-2.2395170134,2.4097545142
H,0,2.334976097,-0.8498236069,0.	F,0,-2.337179193,-0.6283290868,1.462155302
H,0,-2.334976097,0.8498236069,0.	F,0,1.1309914831,1.9965228218,-2.4250911911
H,0,-0.9835866425,1.7233765814,-2.1961496059	F,0,-1.6416855709,2.6457751597,-1.4860187501
H,0,0.9436687229,3.412653492,1.3561401409	F,0,-1.6416855709,2.6457751597,1.4860187501
H,0,0.9436687229,3.412653492,-1.3561401409	F,0,1.1309914831,1.9965228218,2.4250911911
H,0,-0.9835866425,1.7233765814,2.1961496059	F,0,2.8044690938,1.475388168,0.
$Co_2(C_5H_5)_2$ (**Co-H-4T**) OPBE/cc-pVTZ	$Co_2(C_5F_5)_2$ (**Co-F-4T**) OPBE/cc-pVTZ
0 3	0 3
Co,0,-1.231238552,-0.9970997796,0.	Co,0,-0.8272830744,-0.7981766308,0.2800122725
C,0,-0.8741009075,1.3730383537,-0.7182882636	C,0,0.2617628096,-1.5864888796,-1.1436303057
C,0,-1.9840673606,0.5140884402,-1.1373259467	C,0,1.3631531869,-1.001164858,-0.3135137924
C,0,-2.7911690021,0.1658651378,0.	C,0,0.9878592987,-1.5591826185,0.9974628477
C,0,-1.9840673606,0.5140884402,1.1373259467	C,0,-0.0293892621,-2.5563213637,0.9138182371
C,0,-0.8741009075,1.3730383537,0.7182882636	C,0,-0.4527603557,-2.6148468256,-0.4492048087
Co,0,0.5912050401,0.1533011677,0.	Co,0,0.8272830744,0.7981766308,0.2800122725
C,0,2.4661202213,0.7967360586,-0.7059822618	C,0,-0.2617628096,1.5864888796,-1.1436303057
C,0,2.4661202213,0.7967360586,0.7059822618	C,0,-1.3631531869,1.001164858,-0.3135137924
C,0,2.1081903652,-0.5168403568,1.1519238203	C,0,-0.9878592987,1.5591826185,0.9974628477
C,0,1.9187898592,-1.3510800954,0.	C,0,0.0293892621,2.5563213637,0.9138182371
C,0,2.1081903652,-0.5168403568,-1.1519238203	C,0,0.4527603557,2.6148468256,-0.4492048087
H,0,-2.2651472174,0.3592024314,-2.177602669	F,0,0.2039079064,-1.4361852853,-2.4593659211
H,0,-3.7726975911,-0.3048256479,0.	F,0,2.6738047296,-1.1560926549,-0.7515196843
H,0,-2.2651472174,0.3592024314,2.177602669	F,0,1.720233925,-1.3718827305,2.1050857404
H,0,-0.438700204,2.1347277006,1.3613408771	F,0,-0.47323473,-3.3139589505,1.9092132856
H,0,-0.438700204,2.1347277006,-1.3613408771	F,0,-1.3591009209,-3.4432185769,-0.9509789332
H,0,1.7425840306,-2.421333987,0.	F,0,-0.2039079064,1.4361852853,-2.4593659211
H,0,2.0218459506,-0.830405031,2.1876943419	F,0,-2.6738047296,1.1560926549,-0.7515196843
H,0,2.6661992356,1.6493008791,-1.3472776457	F,0,-1.720233925,1.3718827305,2.1050857404
H,0,2.6661992356,1.6493008791,1.3472776457	F,0,0.47323473,3.3139589505,1.9092132856
H,0,2.0218459506,-0.830405031,-2.1876943419	F,0,1.3591009209,3.4432185769,-0.9509789332

$Fe_2(C_5H_5)_2$ (**Fe-H-1E**) OPBE/cc-pVTZ	$Fe_2(C_5F_5)_2$ (**Fe-F-1Q**) OPBE/cc-pVTZ
0 7	0 5
C,0,-0.7249601608,2.2230024061,-0.8370362217	Fe,0,1.8519950476,-1.0821630376,0.
C,0,-0.6865793313,2.3770327672,0.5874649936	C,0,-1.4965007697,-0.9373001271,-0.7133554008
C,0,0.5972914421,1.9613837036,1.0379910063	C,0,-0.2187571788,-1.4928658712,-1.1042174482
C,0,1.4254542803,1.6335708204,-0.0985478465	C,0,0.384912898,-2.324482061,0.
C,0,0.5390628405,1.6839985639,-1.2441809108	C,0,-0.2187571788,-1.4928658712,1.1042174482
C,0,-1.4254542803,-1.6335708204,0.0985478465	C,0,-1.4965007697,-0.9373001271,0.7133554008
C,0,-0.5972914421,-1.9613837036,-1.0379910063	Fe,0,-0.0668086714,0.2453791339,0.
C,0,0.6865793313,-2.3770327672,-0.5874649936	C,0,0.6714866561,1.7143549456,-1.1588243737
C,0,0.7249601608,-2.2230024061,0.8370362217	C,0,-0.6307155544,2.0908352915,-0.7135505602
C,0,-0.5390628405,-1.6839985639,1.2441809108	C,0,-0.6307155544,2.0908352915,0.7135505602
Fe,0,-0.9976239368,0.3437114671,0.0136876867	C,0,0.6714866561,1.7143549456,1.1588243737
Fe,0,0.9976239368,-0.3437114671,-0.0136876867	C,0,1.4907071222,1.4549267474,0.
H,0,-1.5171009545,2.5463715621,-1.5072961594	F,0,-2.5091394174,-0.6160636223,-1.5078444586
H,0,-1.460542348,2.8148958999,1.2120030862	F,0,0.0377262931,-1.7366656637,-2.4017236479
H,0,0.9412292528,2.0233828148,2.0666016322	F,0,0.1887725494,-3.6840133915,0.
H,0,2.5142244257,1.7112569203,-0.133250957	F,0,0.0377262931,-1.7366656637,2.4017236479
H,0,0.8473286322,1.5705225743,-2.2800158276	F,0,-2.5091394174,-0.6160636223,1.5078444586
H,0,-2.5142244257,-1.7112569203,0.133250957	F,0,1.0863928505,1.7022403031,-2.4193795016
H,0,-0.9412292528,-2.0233828148,-2.0666016322	F,0,-1.643173935,2.4347858585,-1.4922366915
H,0,1.460542348,-2.8148958999,-1.2120030862	F,0,-1.643173935,2.4347858585,1.4922366915
H,0,1.5171009545,-2.5463715621,1.5072961594	F,0,1.0863928505,1.7022403031,2.4193795016
H,0,-0.8473286322,-1.5705225743,2.2800158276	F,0,2.8571305266,1.3952308774,0.
$Fe_2(C_5H_5)_2$ (**Fe-H-2Q** OPBE/cc-pVTZ	$Fe_2(C_5F_5)_2$ (**Fe-F-2T**) OPBE/cc-pVTZ
0 5	0 3
C,0,-0.71362421,-1.91960581,-0.97808504	Fe,0,0.,0.,-2.04163403
C,0,0.71362421,-1.91960581,-0.97808504	C,0,-0.715669,-1.62332499,1.27950411
C,0,1.13853002,-1.76820801,0.41461667	C,0,-1.138578,-1.61301011,-0.08240489
C,0,0.,-1.93440007,1.27331084	C,0,0.,-1.65130319,-1.00199088
C,0,-1.13853002,-1.76820801,0.41461667	C,0,1.138578,-1.61301011,-0.08240489
C,0,-0.71362421,1.91960581,-0.97808504	C,0,0.715669,-1.62332499,1.27950411
C,0,-1.13853002,1.76820801,0.41461667	Fe,0,0.,0.,0.31823297
C,0,0.,1.93440007,1.27331084	C,0,-1.138578,1.61301011,-0.08240489
C,0,1.13853002,1.76820801,0.41461667	C,0,-0.715669,1.62332499,1.27950411
C,0,0.71362421,1.91960581,-0.97808504	C,0,0.715669,1.62332499,1.27950411
Fe,0,0.,0.,-1.06872996	C,0,1.138578,1.61301011,-0.08240489
Fe,0,0.,0.,0.98480904	C,0,0.,1.65130319,-1.00199088
H,0,-1.36160135,-2.22827771,-1.79533697	F,0,-1.493926,-1.7333729,2.34669412
H,0,1.36160135,-2.22827771,-1.79533697	F,0,-2.413171,-1.64884615,-0.47887488
H,0,2.17584207,-1.83618707,0.7323425	F,0,0.,-2.5033873,-2.17505881
H,0,0.,-2.16140418,2.33784582	F,0,2.413171,-1.64884615,-0.47887488
H,0,-2.17584207,-1.83618707,0.7323425	F,0,1.493926,-1.7333729,2.34669412
H,0,-1.36160135,2.22827771,-1.79533697	F,0,-2.413171,1.64884615,-0.47887488
H,0,-2.17584207,1.83618707,0.7323425	F,0,-1.493926,1.7333729,2.34669412
H,0,0.,2.16140418,2.33784582	F,0,1.493926,1.7333729,2.34669412
H,0,2.17584207,1.83618707,0.7323425	F,0,2.413171,1.64884615,-0.47887488
H,0,1.36160135,2.22827771,-1.79533697	F,0,0.,2.5033873,-2.17505881

$Fe_2(C_5H_5)_2$ (**Fe-H-3T**) OPBE/cc-pVTZ 0 3 Fe,0,-1.2475000337,-1.3902181167,0. C,0,-0.7021093469,1.6603160961,0. C,0,-1.1788500014,0.9319584292,-1.1411166646 C,0,-2.285159907,0.0518217885,-0.7294276866 C,0,-2.285159907,0.0518217885,0.7294276866 C,0,-1.1788500014,0.9319584292,1.1411166646 Fe,0,0.3425051164,0.0165390733,0. C,0,2.020483725,0.0251207631,-1.1534983605 C,0,2.2467552724,0.8289781572,0. C,0,2.020483725,0.0251207631,1.1534983605 C,0,1.7008317489,-1.3024908135,0.7186467356 C,0,1.7008317489,-1.3024908135,-0.7186467356 H,0,-0.1680405175,2.6065577701,0. H,0,-1.0121821672,1.2225804168,-2.1752297553 H,0,-3.1262774962,-0.1931895624,-1.3831248673 H,0,-3.1262774962,-0.1931895624,1.3831248673 H,0,-1.0121821672,1.2225804168,2.1752297553 H,0,2.0882583825,0.355999053,-2.1852834691 H,0,2.4938036847,1.8853511551,0. H,0,2.0882583825,0.355999053,2.1852834691 H,0,1.5537013112,-2.1624938801,1.3658149104 H,0,1.5537013112,-2.1624938801,-1.3658149104	$Fe_2(C_5F_5)_2$ (**Fe-F-3T**) OPBE/cc-pVTZ 0 3 Fe,0,-1.2669289306,-1.517929207,0. C,0,-0.6983409167,1.669934837,0. C,0,-1.1210081771,0.8985245483,-1.1388458038 C,0,-2.1932016794,-0.0450356546,-0.7359559702 C,0,-2.1932016794,-0.0450356546,0.7359559702 C,0,-1.1210081771,0.8985245483,1.1388458038 Fe,0,0.3324534598,0.0090825621,0. C,0,1.9893471233,0.028840485,-1.1559316697 C,0,2.2135030359,0.8369056059,0. C,0,1.9893471233,0.028840485,1.1559316697 C,0,1.6554505795,-1.2942803049,0.7185574873 C,0,1.6554505795,-1.2942803049,-0.7185574873 F,0,-0.1962590479,2.904305099,0. F,0,-1.0075422453,1.3073574873,-2.4059591587 F,0,-3.3001118832,-0.1916896862,-1.5043412792 F,0,-3.3001118832,-0.1916896862,1.5043412792 F,0,-1.0075422453,1.3073574873,2.4059591587 F,0,2.1726516111,0.4024663863,-2.4146960332 F,0,2.6172205694,2.0973705603,0. F,0,2.1726516111,0.4024663863,2.4146960332 F,0,1.5471032391,-2.3729497212,1.5055407018 F,0,1.5471032391,-2.3729497212,-1.5055407018
$Fe_2(C_5H_5)_2$ (**Fe-H-4Q** OPBE/cc-pVTZ 0 5 Fe,0,0.2355749826,-1.7552907251,-0.1768850031 C,0,1.5596305787,1.1458319862,0.725539095 C,0,1.5687812618,-0.2674538242,1.0203215832 C,0,2.0113338811,-1.0550965043,-0.1760213373 C,0,1.5429898374,-0.0801595596,-1.2176245097 C,0,1.5508512776,1.2650346983,-0.6936386331 Fe,0,-0.1340991535,0.4581920044,-0.0428281724 C,0,-1.8032543797,0.270588981,1.0961945318 C,0,-1.6204221079,1.6511499921,0.7816003074 C,0,-1.6139064749,1.7888933604,-0.6297389347 C,0,-1.7855324391,0.4941517987,-1.2073794202 C,0,-1.9324967743,-0.4658749245,-0.1389800496 H,0,1.5962056813,1.9495750333,1.4553507395 H,0,1.6453477143,-0.6313086379,2.0437133456 H,0,2.9623516532,-1.6007614687,-0.2280923128 H,0,1.5814283086,-0.2720155246,-2.2885766969 H,0,1.5749635967,2.1796924818,-1.2792860502 H,0,-1.8603840418,-0.1484900468,2.0962552127 H,0,-1.4784962142,2.4470485271,1.5051643422 H,0,-1.466433981,2.710149854,-1.1834420808 H,0,-1.8265092332,0.2729726588,-2.2693618544 H,0,-2.3122119736,-1.4874461603,-0.2422841022	

Table S4: All the M-C distances for optimized low-energy structures of the $M_2(C_5X_5)_2$ (M=Zn, Cu, Ni, Co, Fe; X=H, F) complexes at the OPBE/cc-pVTZ level.

Structure	M-C	distance	M-C	distance
Zn-H-1S	Zn1-C1	2.272	Zn2-C1	4.435
	Zn1-C2	2.272	Zn2-C2	4.435
	Zn1-C3	2.272	Zn2-C3	4.435
	Zn1-C4	2.272	Zn2-C4	4.435
	Zn1-C5	2.272	Zn2-C5	4.435
	Zn1-C6	4.435	Zn2-C6	2.272
	Zn1-C7	4.435	Zn2-C7	2.272
	Zn1-C8	4.435	Zn2-C8	2.272
	Zn1-C9	4.435	Zn2-C9	2.272
	Zn1-C10	4.435	Zn2-C10	2.272
Zn-F-1S	Zn1-C1	2.304	Zn2-C1	4.460
	Zn1-C2	2.304	Zn2-C2	4.460
	Zn1-C3	2.304	Zn2-C3	4.460
	Zn1-C4	2.304	Zn2-C4	4.460
	Zn1-C5	2.304	Zn2-C5	4.460
	Zn1-C6	4.460	Zn2-C6	2.304
	Zn1-C7	4.460	Zn2-C7	2.304
	Zn1-C8	4.460	Zn2-C8	2.304
	Zn1-C9	4.460	Zn2-C9	2.304
	Zn1-C10	4.460	Zn2-C10	2.304
Cu-H-1S	Cu1-C1	2.103	Cu2-C1	2.674
	Cu1-C2	2.842	Cu2-C2	2.015
	Cu1-C3	3.182	Cu2-C3	2.483
	Cu1-C4	2.802	Cu2-C4	3.215
	Cu1-C5	2.094	Cu2-C5	3.329
	Cu1-C6	2.483	Cu2-C6	3.182
	Cu1-C7	3.214	Cu2-C7	2.802
	Cu1-C8	3.329	Cu2-C8	2.094
	Cu1-C9	2.674	Cu2-C9	2.103
	Cu1-C10	2.015	Cu2-C10	2.842
Cu-F-1S	Cu1-C1	2.065	Cu2-C1	2.753
	Cu1-C2	2.771	Cu2-C2	2.018
	Cu1-C3	3.205	Cu2-C3	2.693
	Cu1-C4	2.869	Cu2-C4	3.418
	Cu1-C5	2.160	Cu2-C5	3.487
	Cu1-C6	2.693	Cu2-C6	3.205
	Cu1-C7	3.418	Cu2-C7	2.869
	Cu1-C8	3.487	Cu2-C8	2.160
	Cu1-C9	2.753	Cu2-C9	2.065
	Cu1-C10	2.018	Cu2-C10	2.771
Ni-H-1T	Ni1-C1	2.046	Ni2-C1	2.674
	Ni1-C2	2.857	Ni2-C2	2.212
	Ni1-C3	3.316	Ni2-C3	1.980
	Ni1-C4	2.857	Ni2-C4	2.212
	Ni1-C5	2.046	Ni2-C5	2.674
	Ni1-C6	1.980	Ni2-C6	3.316
	Ni1-C7	2.212	Ni2-C7	2.857
	Ni1-C8	2.674	Ni2-C8	2.046
	Ni1-C9	2.674	Ni2-C9	2.046
	Ni1-C10	2.212	Ni2-C10	2.857

Ni-H-2S	Ni1-C1	2.050	Ni2-C1	2.593
	Ni1-C2	2.864	Ni2-C2	2.070
	Ni1-C3	3.411	Ni2-C3	1.926
	Ni1-C4	2.864	Ni2-C4	2.070
	Ni1-C5	2.050	Ni2-C5	2.593
	Ni1-C6	1.926	Ni2-C6	3.411
	Ni1-C7	2.070	Ni2-C7	2.864
	Ni1-C8	2.593	Ni2-C8	2.050
	Ni1-C9	2.593	Ni2-C9	2.050
	Ni1-C10	2.070	Ni2-C10	2.864
Ni-H-3S	Ni1-C1	1.958	Ni2-C1	3.333
	Ni1-C2	2.120	Ni2-C2	2.697
	Ni1-C3	2.668	Ni2-C3	1.956
	Ni1-C4	2.590	Ni2-C4	2.069
	Ni1-C5	2.059	Ni2-C5	2.890
	Ni1-C6	1.958	Ni2-C6	3.333
	Ni1-C7	2.120	Ni2-C7	2.696
	Ni1-C8	2.668	Ni2-C8	1.956
	Ni1-C9	2.590	Ni2-C9	2.069
	Ni1-C10	2.059	Ni2-C10	2.890
Ni-F-1S	Ni1-C1	1.984	Ni2-C1	3.370
	Ni1-C2	2.021	Ni2-C2	2.776
	Ni1-C3	2.555	Ni2-C3	1.942
	Ni1-C4	2.555	Ni2-C4	1.942
	Ni1-C5	2.021	Ni2-C5	2.776
	Ni1-C6	2.031	Ni2-C6	3.614
	Ni1-C7	2.070	Ni2-C7	2.667
	Ni1-C8	2.324	Ni2-C8	2.004
	Ni1-C9	2.070	Ni2-C9	2.667
	Ni1-C10	2.031	Ni2-C10	3.614
Ni-F-2S	Ni1-C1	1.980	Ni2-C1	2.528
	Ni1-C2	2.832	Ni2-C2	1.986
	Ni1-C3	3.475	Ni2-C3	1.929
	Ni1-C4	2.966	Ni2-C4	2.054
	Ni1-C5	2.077	Ni2-C5	2.503
	Ni1-C6	1.929	Ni2-C6	3.475
	Ni1-C7	1.986	Ni2-C7	2.832
	Ni1-C8	2.528	Ni2-C8	1.980
	Ni1-C9	2.503	Ni2-C9	2.077
	Ni1-C10	2.054	Ni2-C10	2.966
Ni-F-3S	Ni1-C1	1.957	Ni2-C1	2.409
	Ni1-C2	1.957	Ni2-C2	2.409
	Ni1-C3	2.904	Ni2-C3	1.941
	Ni1-C4	3.532	Ni2-C4	1.921
	Ni1-C5	2.904	Ni2-C5	1.941
	Ni1-C6	2.098	Ni2-C6	4.247
	Ni1-C7	2.098	Ni2-C7	4.247
	Ni1-C8	2.038	Ni2-C8	3.527
	Ni1-C9	2.033	Ni2-C9	3.014
	Ni1-C10	2.038	Ni2-C10	3.527

Ni-F-4T	Ni1-C1	1.994	Ni2-C1	2.578
	Ni1-C2	2.867	Ni2-C2	2.146
	Ni1-C3	3.372	Ni2-C3	1.997
	Ni1-C4	2.867	Ni2-C4	2.146
	Ni1-C5	1.994	Ni2-C5	2.578
	Ni1-C6	1.997	Ni2-C6	3.372
	Ni1-C7	2.146	Ni2-C7	2.867
	Ni1-C8	2.578	Ni2-C8	1.994
	Ni1-C9	2.578	Ni2-C9	1.994
	Ni1-C10	2.146	Ni2-C10	2.867
Co-H-1T	Co1-C1	2.014	Co2-C1	2.648
	Co1-C2	2.734	Co2-C2	2.128
	Co1-C3	3.283	Co2-C3	1.945
	Co1-C4	2.818	Co2-C4	2.080
	Co1-C5	2.052	Co2-C5	2.600
	Co1-C6	1.945	Co2-C6	3.283
	Co1-C7	2.128	Co2-C7	2.734
	Co1-C8	2.648	Co2-C8	2.014
	Co1-C9	2.600	Co2-C9	2.052
	Co1-C10	2.080	Co2-C10	2.818
Co-H-2T	Co1-C1	1.915	Co2-C1	3.179
	Co1-C2	2.067	Co2-C2	2.624
	Co1-C3	2.736	Co2-C3	1.953
	Co1-C4	2.736	Co2-C4	1.953
	Co1-C5	2.067	Co2-C5	2.624
	Co1-C6	2.082	Co2-C6	3.899
	Co1-C7	2.022	Co2-C7	2.997
	Co1-C8	2.027	Co2-C8	2.287
	Co1-C9	2.022	Co2-C9	2.997
	Co1-C10	2.082	Co2-C10	3.899
Co-H-3Q	Co1-C1	2.377	Co2-C1	2.054
	Co1-C2	3.083	Co2-C2	2.057
	Co1-C3	3.934	Co2-C3	2.054
	Co1-C4	3.934	Co2-C4	2.054
	Co1-C5	3.083	Co2-C5	2.057
	Co1-C6	2.054	Co2-C6	3.934
	Co1-C7	2.057	Co2-C7	3.083
	Co1-C8	2.054	Co2-C8	2.377
	Co1-C9	2.057	Co2-C9	3.083
	Co1-C10	2.054	Co2-C10	3.934
Co-H-4T	Co1-C1	2.038	Co2-C1	2.502
	Co1-C2	2.838	Co2-C2	2.036
	Co1-C3	3.382	Co2-C3	1.946
	Co1-C4	2.838	Co2-C4	2.036
	Co1-C5	2.038	Co2-C5	2.502
	Co1-C6	2.104	Co2-C6	4.170
	Co1-C7	2.019	Co2-C7	3.565
	Co1-C8	2.006	Co2-C8	3.170
	Co1-C9	2.019	Co2-C9	3.565
	Co1-C10	2.104	Co2-C10	4.170

Co-F-1S	Co1-C1	1.933	Co2-C1	3.278
	Co1-C2	2.016	Co2-C2	2.688
	Co1-C3	2.606	Co2-C3	1.825
	Co1-C4	2.606	Co2-C4	1.825
	Co1-C5	2.016	Co2-C5	2.688
	Co1-C6	2.028	Co2-C6	4.100
	Co1-C7	2.020	Co2-C7	3.337
	Co1-C8	1.990	Co2-C8	2.736
	Co1-C9	2.020	Co2-C9	3.337
	Co1-C10	2.028	Co2-C10	4.100
Co-F-2T	Co1-C1	2.011	Co2-C1	3.681
	Co1-C2	2.011	Co2-C2	2.673
	Co1-C3	2.301	Co2-C3	1.972
	Co1-C4	2.011	Co2-C4	2.673
	Co1-C5	2.011	Co2-C5	3.681
	Co1-C6	2.022	Co2-C6	3.730
	Co1-C7	2.025	Co2-C7	2.744
	Co1-C8	2.241	Co2-C8	2.008
	Co1-C9	2.025	Co2-C9	2.744
	Co1-C10	2.022	Co2-C10	3.730
Co-F-3S	Co1-C1	1.928	Co2-C1	2.583
	Co1-C2	2.662	Co2-C2	1.928
	Co1-C3	3.267	Co2-C3	1.840
	Co1-C4	2.662	Co2-C4	1.928
	Co1-C5	1.928	Co2-C5	2.583
	Co1-C6	2.010	Co2-C6	4.127
	Co1-C7	2.022	Co2-C7	3.538
	Co1-C8	1.993	Co2-C8	3.092
	Co1-C9	2.022	Co2-C9	3.538
	Co1-C10	2.010	Co2-C10	4.127
Co-F-4T	Co1-C1	1.969	Co2-C1	2.278
	Co1-C2	2.469	Co2-C2	2.095
	Co1-C3	3.520	Co2-C3	2.032
	Co1-C4	3.717	Co2-C4	1.993
	Co1-C5	2.834	Co2-C5	1.958
	Co1-C6	1.993	Co2-C6	3.717
	Co1-C7	2.032	Co2-C7	3.520
	Co1-C8	2.095	Co2-C8	2.469
	Co1-C9	2.278	Co2-C9	1.969
	Co1-C10	1.958	Co2-C10	2.834
Fe-H-1E	Fe1-C1	2.025	Fe2-C1	2.747
	Fe1-C2	2.565	Fe2-C2	2.492
	Fe1-C3	3.256	Fe2-C3	2.136
	Fe1-C4	3.199	Fe2-C4	2.081
	Fe1-C5	2.416	Fe2-C5	2.396
	Fe1-C6	2.081	Fe2-C6	3.199
	Fe1-C7	2.396	Fe2-C7	2.416
	Fe1-C8	2.747	Fe2-C8	2.025
	Fe1-C9	2.492	Fe2-C9	2.565
	Fe1-C10	2.136	Fe2-C10	3.256

Fe-H-2Q	Fe1-C1	1.956	Fe2-C1	3.038
	Fe1-C2	2.179	Fe2-C2	2.574
	Fe1-C3	2.837	Fe2-C3	2.050
	Fe1-C4	2.837	Fe2-C4	2.050
	Fe1-C5	2.179	Fe2-C5	2.574
	Fe1-C6	1.956	Fe2-C6	3.038
	Fe1-C7	2.179	Fe2-C7	2.574
	Fe1-C8	2.837	Fe2-C8	2.050
	Fe1-C9	2.837	Fe2-C9	2.050
	Fe1-C10	2.179	Fe2-C10	2.574
Fe-H-3T	Fe1-C1	1.948	Fe2-C1	3.099
	Fe1-C2	2.111	Fe2-C2	2.588
	Fe1-C3	2.727	Fe2-C3	1.920
	Fe1-C4	2.727	Fe2-C4	1.920
	Fe1-C5	2.111	Fe2-C5	2.588
	Fe1-C6	2.070	Fe2-C6	4.139
	Fe1-C7	2.036	Fe2-C7	3.743
	Fe1-C8	2.025	Fe2-C8	3.036
	Fe1-C9	2.025	Fe2-C9	3.036
	Fe1-C10	2.036	Fe2-C10	3.743
Fe-H-4Q	Fe1-C1	1.978	Fe2-C1	3.335
	Fe1-C2	2.117	Fe2-C2	2.366
	Fe1-C3	2.629	Fe2-C3	1.909
	Fe1-C4	2.135	Fe2-C4	2.329
	Fe1-C5	1.983	Fe2-C5	3.314
	Fe1-C6	2.075	Fe2-C6	4.023
	Fe1-C7	2.021	Fe2-C7	3.195
	Fe1-C8	2.024	Fe2-C8	2.523
	Fe1-C9	2.029	Fe2-C9	3.144
	Fe1-C10	2.077	Fe2-C10	3.996
Fe-F-1Q	Fe1-C1	1.988	Fe2-C1	3.427
	Fe1-C2	2.065	Fe2-C2	2.382
	Fe1-C3	2.609	Fe2-C3	1.922
	Fe1-C4	2.065	Fe2-C4	2.382
	Fe1-C5	1.988	Fe2-C5	3.427
	Fe1-C6	2.057	Fe2-C6	4.092
	Fe1-C7	2.011	Fe2-C7	3.249
	Fe1-C8	1.972	Fe2-C8	2.563
	Fe1-C9	2.011	Fe2-C9	3.249
	Fe1-C10	2.057	Fe2-C10	4.092
Fe-F-2T	Fe1-C1	2.018	Fe2-C1	3.765
	Fe1-C2	2.015	Fe2-C2	2.782
	Fe1-C3	2.114	Fe2-C3	1.951
	Fe1-C4	2.015	Fe2-C4	2.782
	Fe1-C5	2.018	Fe2-C5	3.765
	Fe1-C6	2.018	Fe2-C6	3.765
	Fe1-C7	2.015	Fe2-C7	2.782
	Fe1-C8	2.114	Fe2-C8	1.951
	Fe1-C9	2.015	Fe2-C9	2.782
	Fe1-C10	2.018	Fe2-C10	3.765

Fe-F-3T	Fe1-C1	1.955	Fe2-C1	3.238
	Fe1-C2	2.050	Fe2-C2	2.675
	Fe1-C3	2.631	Fe2-C3	1.889
	Fe1-C4	2.631	Fe2-C4	1.889
	Fe1-C5	2.050	Fe2-C5	2.675
	Fe1-C6	2.055	Fe2-C6	4.202
	Fe1-C7	2.020	Fe2-C7	3.786
	Fe1-C8	1.991	Fe2-C8	3.018
	Fe1-C9	1.991	Fe2-C9	3.018
	Fe1-C10	2.020	Fe2-C10	3.786

Complete Gaussian 09 reference

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