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Perfluoroolefin Complexes Versus Perfluorometallacycles and Perfluorocarbene Complexes in Cyclopentadienylcobalt Chemistry

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Supporting Information

Table S1: Total energies and relative energies for optimized low-lying structures of the $CpCo(L)(C_3F_6)$ and $CpCo(L)(C_4F_8)$ (L = CO, PMe_3) complexes at the M06-L/cc-pVTZ level.

Table S2. Total energies and relative energies for optimized low-lying structures of the $CpCo(L)(C_3F_6)$ and $CpCo(L)(C_4F_8)$ (L = CO, PMe_3) complexes at the DLPNO-CCSD(T)/cc-pVTZ//M06-L/cc-pVTZ and DLPNO-CCSD(T)/aug-cc-pVTZ// M06-L/cc-pVTZ levels of theory.

Table S3: Vibrational frequencies and infrared intensities for optimized low-lying structures of the $CpCo(L)(C_3F_6)$ and $CpCo(L)(C_4F_8)$ (L = CO, PMe_3) complexes at the M06-L/cc-pVTZ level.

Table S4: Cartesian coordinates for optimized low-lying structures of the $CpCo(L)(C_3F_6)$ and $CpCo(L)(C_4F_8)$ (L = CO, PMe_3) complexes at the M06-L/cc-pVTZ level.

Table S5: Topological data at the bond critical points for the interactions between the cobalt atom and the C=C double bond in optimized lowest-energy structures of the $CpCo(L)(C_3F_6)$ and $CpCo(L)(C_4F_8)$ (L = CO, PMe_3) complexes at the M06-L/cc-pVTZ level of theory.

Figure S1: Bond paths for optimized lowest-energy structures of the $CpCo(L)(C_3F_6)$ and $CpCo(L)(C_4F_8)$ (L = CO, PMe_3) complexes at the M06-L/cc-pVTZ level of theory.

Complete Gaussian 09 reference.

Table S1. Total energies (E_{tot}, in hartree) and relative energies (ΔE, in kcal/mol) for optimized low-lying structures of the $CpCo(L)(C_3F_6)$ and $CpCo(L)(C_4F_8)$ (L = CO, PMe_3) complexes at the M06-L/cc-pVTZ level.

Complex	Structure	Multiplicity	M06-L/cc-pVTZ	
			E_{tot}	ΔE
$CpCo(CO)(C_3F_6)$	**CO-C_3F_6-1**	1	-2403.261010	0.0
	CO-C_3F_6-2	1	-2403.247699	8.4
	CO-C_3F_6-3	1	-2403.244144	10.6
	CO-C_3F_6-4	1	-2403.240817	12.7
$CpCo(PMe_3)(C_3F_6)$	**PMe_3-C_3F_6-1**	1	-2751.054204	0.0
	PMe_3-C_3F_6-2	1	-2751.038555	9.8
	PMe_3-C_3F_6-3	1	-2751.036844	10.9
	PMe_3-C_3F_6-4	1	-2751.028633	16.0
$CpCo(CO)(C_4F_8)$	**CO-C_4F_8-1**	1	-2641.121687	0.0
	CO-C_4F_8-2	1	-2641.113333	5.2
	CO-C_4F_8-3	1	-2641.098501	14.5
	CO-C_4F_8-4	1	-2641.094891	16.8
	CO-C_4F_8-5	1	-2641.090590	19.5
	CO-C_4F_8-6	1	-2641.088601	20.8
	CO-C_4F_8-7	1	-2641.085581	22.7
	CO-C_4F_8-8	1	-2641.083824	23.8
	CO-C_4F_8-9	1	-2641.076052	28.6
$CpCo(PMe_3)(C_4F_8)$	**PMe_3-C_4F_8-1**	1	-2988.908196	0.0
	PMe_3-C_4F_8-2	1	-2988.905757	1.5
	PMe_3-C_4F_8-3	1	-2988.891878	10.2
	PMe_3-C_4F_8-4	1	-2988.890418	11.2
	PMe_3-C_4F_8-5	1	-2988.889101	12.0
	PMe_3-C_4F_8-6	1	-2988.884054	15.1
	PMe_3-C_4F_8-7	1	-2988.875219	20.7
	PMe_3-C_4F_8-8	1	-2988.870048	23.9
	PMe_3-C_4F_8-9	1	-2988.865239	27.0

Table S2. Total energies (E_{tot}, in hartree) and relative energies (ΔE, in kcal/mol) for optimized low-lying structures of the CpCo(L)(C_3F_6) and CpCo(L)(C_4F_8) (L = CO, PMe_3) complexes at the DLPNO-CCSD(T)/cc-pVTZ//M06-L/cc-pVTZ and DLPNO-CCSD(T)/*aug*-cc-pVTZ//M06-L/cc-pVTZ levels of theory.

Complex	Structure	DLPNO-CCSD(T)/cc-pVTZ //M06-L/cc-pVTZ		DLPNO-CCSD(T)/aug-cc-pVTZ //M06-L/cc-pVTZ	
		E_{tot}	ΔE	E_{tot}	ΔE
CpCo(CO)(C_3F_6)	**CO-C_3F_6-1**	-2400.930776	0.0	-2401.041919	0.0
	CO-C_3F_6-2	-2400.926205	2.9	-2401.036235	3.6
	CO-C_3F_6-3	-2400.911462	12.1	-2401.024433	11.0
	CO-C_3F_6-4	-2400.918098	8.0	-2401.028177	8.6
CpCo(PMe_3)(C_3F_6)	**PMe_3-C_3F_6-1**	-2748.216418	0.0	-2748.337196	0.0
	PMe_3-C_3F_6-2	-2748.201111	9.6	-2748.323345	8.7
	PMe_3-C_3F_6-3	-2748.207007	5.9	-2748.325366	7.4
	PMe_3-C_3F_6-4	-2748.199918	10.4	-2748.318701	11.6
CpCo(CO)(C_4F_8)	**CO-C_4F_8-1**	-2638.463821	0.0	-2638.595083	0.0
	CO-C_4F_8-2	-2638.455259	5.4	-2638.586617	5.3
	CO-C_4F_8-3	-2638.436666	17.0	-2638.568431	16.7
	CO-C_4F_8-4	-2638.434021	18.7	-2638.567051	17.6
	CO-C_4F_8-5	-2638.430020	21.2	-2638.564315	19.3
	CO-C_4F_8-6	-2638.426150	23.6	-2638.558888	22.7
	CO-C_4F_8-7	-2638.433364	19.1	-2638.563382	19.9
	CO-C_4F_8-8	-2638.431210	20.5	-2638.561857	20.8
	CO-C_4F_8-9	-2638.421190	26.8	-2638.551955	27.1
CpCo(PMe_3)(C_4F_8)	**PMe_3-C_4F_8-1**	-2985.741304	0.0	-2985.882486	0.0
	PMe_3-C_4F_8-2	-2985.738626	1.7	-2985.879781	1.7
	PMe_3-C_4F_8-3	-2985.723022	11.5	-2985.863908	11.7
	PMe_3-C_4F_8-4	-2985.723656	11.1	-2985.867241	9.6
	PMe_3-C_4F_8-5	-2985.721814	12.2	-2985.864474	11.3
	PMe_3-C_4F_8-6	-2985.715216	16.4	-2985.857244	15.8
	PMe_3-C_4F_8-7	-2985.715682	16.1	-2985.854910	17.3
	PMe_3-C_4F_8-8	-2985.707890	21.0	-2985.847485	22.0
	PMe_3-C_4F_8-9	-2985.704184	23.3	-2985.843908	24.2

Table S3. Vibrational frequencies (in cm^{-1}) and infrared intensities (in km/mol, given in parentheses) for optimized low-lying structures of the $CpCo(L)(C_3F_6)$ and $CpCo(L)(C_4F_8)$ (L = CO, PMe_3) complexes at the M06-L/cc-pVTZ level.

Structure	ν
CO-C_3F_6-1	42(0), 46(0), 60(0), 98(0), 115(0), 128(0), 140(1), 166(1), 213(0), 228(3), 258(0), 273(1), 281(2), 342(1), 364(1), 371(0), 387(4), 410(4), 489(1), 513(16), 521(9), 523(26), 567(12), 591(1), 606(2), 611(8), 615(5), 683(184), 753(27), 782(50), 828(4), 832(27), 836(3), 842(35), 868(4), 920(1), 924(1), 995(198), 1018(6), 1048(6), 1082(6), 1082(6), 1103(138), 1135(163), 1149(2), 1158(105), 1196(305), 1282(0), 1307(345), 1397(1), 1403(6), 1447(124), 1452(21), 1486(2), 2096(687), 3221(0), 3226(0), 3238(1), 3241(1), 3250(1)
CO-C_3F_6-2	26(0), 39(0), 66(0), 91(0), 111(0), 133(0), 156(1), 175(0), 187(2), 200(0), 265(8), 300(0), 310(1), 347(0), 373(3), 398(3), 402(7), 461(7), 492(25), 514(11), 533(1), 541(3), 552(0), 567(15), 603(1), 612(0), 690(42), 709(12), 742(27), 833(3), 835(7), 842(5), 850(34), 878(2), 928(55), 934(43), 942(8), 990(109), 1031(3), 1049(4), 1069(7), 1086(5), 1091(18), 1101(19), 1121(444), 1153(4), 1190(19), 1235(842), 1261(266), 1288(0), 1403(1), 1408(0), 1460(4), 1475(2), 2093(695), 3219(1), 3231(1), 3240(0), 3246(0), 3258(1)
CO-C_3F_6-3	58(0), 69(0), 70(0), 109(0), 115(1), 141(0), 191(1), 199(0), 207(2), 223(0), 260(2), 265(5), 286(0), 294(1), 344(0), 372(1), 378(6), 392(0), 402(3), 510(19), 527(17), 531(15), 570(18), 576(13), 590(24), 608(3), 616(4), 644(3), 804(21), 834(17), 840(0), 848(40), 852(3), 867(14), 897(320), 932(1), 935(1), 990(290), 1024(4), 1047(12), 1074(6), 1083(6), 1096(2), 1103(86), 1137(266), 1151(8), 1162(73), 1257(173), 1284(0), 1330(254), 1398(0), 1405(1), 1458(2), 1482(3), 2108(653), 3222(0), 3225(0), 3238(1), 3242(1), 3252(1)
CO-C_3F_6-4	28(0), 44(0), 51(0), 67(0), 93(0), 121(1), 136(2), 148(0), 190(1), 218(1), 273(2), 277(2), 308(1), 354(0), 374(1), 384(3), 393(4), 417(8), 439(3), 488(3), 529(35), 534(8), 570(25), 581(5), 606(8), 607(5), 614(0), 683(2), 742(42), 824(2), 831(19), 839(4), 841(29), 865(6), 882(78), 924(1), 927(10), 1029(2), 1042(4), 1063(118), 1084(2), 1085(2), 1143(270), 1151(5), 1157(17), 1185(368), 1207(91), 1224(290), 1283(0), 1304(253), 1401(1), 1404(0), 1457(3), 1473(1), 2087(795), 3218(1), 3230(1), 3239(1), 3244(1), 3255(1)
PMe_3-C_3F_6-1	50(0), 61(0), 70(1), 90(0), 109(0), 123(0), 135(3), 152(1), 171(0), 181(1), 182(2), 199(1), 206(1), 214(3), 228(1), 243(1), 261(1), 266(2), 275(2), 278(1), 296(1), 309(2), 333(4), 350(8), 369(2), 386(5), 419(3), 447(11), 487(1), 528(4), 588(2), 597(3), 606(1), 609(4), 676(51), 691(100), 731(10), 734(12), 765(26), 786(54), 794(0), 801(3), 821(67), 836(24), 838(2), 857(5), 862(6), 869(9), 913(9), 924(3), 958(19), 960(10), 973(106), 983(271), 1018(10), 1047(7), 1059(134), 1076(37), 1081(3), 1089(52), 1132(197), 1150(13), 1167(318), 1281(0), 1291(338), 1314(9), 1318(8), 1336(6), 1397(72), 1401(6), 1406(37), 1446(0), 1453(3), 1458(1), 1460(1), 1463(6), 1470(7), 1479(2), 1481(3), 3040(18), 3044(13), 3051(17), 3141(5), 3142(15), 3156(4), 3158(3), 3159(4), 3188(0), 3202(6), 3223(2), 3231(4), 3238(3), 3254(1)
PMe_3-C_3F_6-2	3(0), 63(0), 65(0), 110(0), 120(4), 131(1), 146(1), 178(3), 191(1), 202(0), 203(0), 215(1), 218(2), 219(1), 245(0), 246(3), 259(4), 259(1), 272(4), 277(1), 291(0), 292(0), 307(0), 335(4), 352(7), 383(2), 391(1), 403(0), 448(9), 542(0), 563(7), 575(19), 605(2), 614(5), 625(2), 680(13), 736(10), 738(12), 801(0), 822(35), 822(11), 832(2), 838(2), 842(44), 845(2), 859(0), 869(2), 898(281), 923(3), 927(1), 952(151), 961(25), 975(153), 978(139), 1022(9), 1026(6), 1044(9), 1055(347), 1082(12), 1089(1), 1100(54), 1139(143), 1151(5), 1222(98), 1281(0), 1292(205), 1315(8), 1317(8), 1337(7), 1398(1), 1408(0), 1449(0), 1458(0), 1459(2), 1461(0), 1466(5), 1467(11), 1480(7), 1481(1), 3043(22), 3043(5), 3054(17), 3143(0), 3144(17), 3160(3), 3161(0), 3161(3), 3192(0), 3217(1), 3223(1), 3235(5), 3238(3), 3248(3)
PMe_3-C_3F_6-3	44(0), 47(0), 76(0), 94(1), 105(0), 115(0), 134(2), 142(1), 151(0), 167(2), 176(0), 181(2), 191(0), 217(1), 219(2), 229(3), 249(0), 274(6), 279(1), 301(3), 306(1), 315(0), 345(5), 350(4), 380(11), 408(2), 421(8), 500(4), 532(2), 542(0), 551(0), 595(1), 605(1), 676(5), 680(38), 697(16), 724(13), 734(17), 736(14), 799(0), 818(6), 825(24), 833(3), 840(30), 857(8), 859(2), 870(4), 910(25), 918(89), 924(16), 959(20), 963(21), 971(165), 980(76), 1027(7), 1042(8), 1044(7), 1062(54), 1085(0), 1088(4), 1100(404), 1151(16), 1173(10), 1217(956), 1255(296), 1283(0), 1316(7), 1321(8), 1340(3), 1402(1), 1408(1), 1449(0), 1458(1), 1460(4), 1461(1), 1465(4), 1471(3), 1473(9), 1481(3), 3042(20), 3044(14), 3051(16), 3138(6), 3140(12), 3147(7), 3160(5), 3174(1), 3200(0), 3208(5), 3226(3), 3233(3), 3241(2), 3253(2)
PMe_3-C_3F_6-4	9(0), 35(0), 59(0), 67(0), 83(0), 90(0), 132(2), 139(1), 151(1), 167(0), 176(1), 181(0), 187(1), 213(1), 222(3), 231(0), 248(0), 259(1), 268(4), 275(3), 294(0), 311(6), 347(10), 356(4), 384(6), 397(1), 416(6), 429(6), 480(28), 534(2), 562(1), 596(1), 607(1), 631(5), 662(25), 678(20), 729(74), 731(7), 732(12), 795(0), 809(2), 823(34), 833(11), 838(11), 840(33), 861(15), 863(50), 864(4), 908(5), 915(8), 956(5), 959(17), 973(155), 1025(37), 1031(236), 1036(38), 1072(128), 1080(3), 1083(10), 1112(79), 1148(14), 1170(277), 1202(164), 1211(264), 1280(0), 1312(11), 1316(11), 1328(149), 1334(8), 1398(1), 1405(1), 1449(0), 1456(2), 1460(1), 1461(0), 1464(7), 1469(0), 1471(10), 1480(2), 3041(23), 3042(17), 3043(16), 3139(6), 3141(3), 3141(22), 3154(5), 3173(1), 3175(1), 3213(1), 3220(3), 3234(6), 3235(6), 3248(3)

CO-C_4F_8-1	39(0), 49(0), 60(0), 84(0), 105(0), 127(0), 136(0), 152(1), 162(2), 175(1), 194(1), 208(0), 246(1), 263(1), 310(0), 316(0), 344(0), 349(1), 363(3), 378(1), 403(2), 409(4), 494(16), 508(18), 517(10), 542(2), 547(7), 555(12), 567(8), 607(3), 612(2), 626(8), 686(195), 712(37), 761(25), 795(3), 821(4), 833(27), 838(15), 842(18), 886(4), 933(2), 942(7), 974(116), 1002(215), 1021(8), 1052(7), 1083(1), 1085(1), 1095(3), 1105(7), 1151(2), 1158(394), 1172(75), 1199(95), 1258(516), 1285(0), 1295(361), 1399(21), 1403(149), 1412(144), 1451(6), 1486(2), 2098(661), 3217(1), 3230(0), 3241(1), 3248(0), 3260(1)
CO-C_4F_8-2	39(0), 44(1), 57(0), 68(0), 94(0), 106(0), 118(0), 139(0), 153(0), 186(0), 208(1), 240(2), 246(1), 273(2), 277(0), 291(4), 310(1), 335(2), 366(1), 386(1), 406(3), 429(0), 501(6), 508(10), 516(22), 520(8), 536(11), 556(22), 576(10), 605(1), 610(0), 617(0), 694(60), 703(125), 768(1), 778(38), 828(5), 833(12), 839(2), 846(48), 888(2), 913(90), 928(2), 949(6), 1018(5), 1056(5), 1076(28), 1082(12), 1085(58), 1095(24), 1137(41), 1150(1), 1156(152), 1173(226), 1190(443), 1270(401), 1286(0), 1303(296), 1401(1), 1404(0), 1440(51), 1453(3), 1486(2), 2102(657), 3220(0), 3227(1), 3239(0), 3243(1), 3261(1)
CO-C_4F_8-3	42(0), 50(0), 62(0), 71(0), 96(0), 115(0), 133(0), 140(1), 162(1), 178(0), 210(0), 225(1), 235(3), 262(0), 280(2), 289(3), 320(1), 349(0), 368(1), 369(0), 380(4), 410(3), 444(1), 510(9), 517(15), 523(17), 536(16), 555(7), 585(15), 607(7), 609(7), 616(1), 635(5), 694(169), 756(39), 768(40), 831(7), 835(11), 837(2), 844(48), 878(8), 917(195), 926(12), 935(1), 1017(5), 1049(6), 1076(12), 1082(2), 1085(22), 1096(98), 1140(52), 1149(1), 1167(97), 1194(395), 1209(376), 1268(147), 1283(0), 1331(146), 1397(1), 1403(6), 1440(105), 1451(6), 1486(2), 2096(660), 3219(0), 3224(1), 3238(1), 3238(1), 3250(1)
CO-C_4F_8-4	54(0), 61(0), 67(0), 80(1), 103(1), 112(0), 132(0), 145(1), 194(0), 202(0), 209(1), 225(0), 254(1), 257(1), 265(4), 282(1), 308(0), 327(0), 346(1), 377(1), 385(4), 403(3), 447(1), 497(6), 518(28), 525(10), 544(8), 552(12), 581(35), 596(1), 609(4), 615(4), 626(13), 717(43), 813(14), 834(14), 841(0), 848(38), 857(21), 872(48), 880(87), 903(252), 935(1), 941(0), 1025(4), 1047(2), 1058(31), 1084(5), 1086(27), 1092(24), 1118(175), 1130(74), 1151(1), 1155(62), 1182(368), 1229(192), 1285(0), 1313(320), 1320(141), 1399(0), 1404(2), 1458(3), 1481(4), 2115(609), 3222(0), 3229(0), 3240(0), 3243(0), 3255(1)
CO-C_4F_8-5	47(0), 53(0), 83(0), 106(0), 114(0), 138(1), 145(0), 172(0), 193(1), 221(3), 231(0), 236(0), 254(3), 270(3), 272(2), 277(3), 299(3), 329(1), 349(1), 371(2), 375(3), 382(0), 399(2), 447(3), 512(19), 520(25), 533(11), 554(26), 584(9), 595(12), 607(4), 616(3), 620(2), 659(13), 827(12), 833(16), 839(1), 851(43), 857(10), 865(6), 911(312), 939(5), 940(1), 982(310), 1024(8), 1032(16), 1044(9), 1060(18), 1067(131), 1088(10), 1093(3), 1117(144), 1152(3), 1167(236), 1173(116), 1233(108), 1263(143), 1284(0), 1347(116), 1395(0), 1410(1), 1459(3), 1485(4), 2124(588), 3222(0), 3229(0), 3239(0), 3246(0), 3255(1)
CO-C_4F_8-6	49(0), 56(0), 61(0), 73(0), 106(1), 111(0), 133(0), 137(0), 190(1), 200(1), 210(1), 222(0), 244(1), 254(6), 271(1), 271(1), 311(0), 336(0), 367(5), 375(0), 375(7), 394(0), 401(3), 507(14), 523(28), 530(11), 537(6), 554(13), 584(7), 604(0), 608(3), 618(4), 642(10), 687(148), 799(7), 812(106), 835(4), 841(0), 848(39), 854(5), 867(11), 933(1), 936(1), 992(233), 1025(4), 1047(11), 1068(9), 1076(30), 1083(15), 1094(3), 1100(158), 1151(26), 1153(25), 1161(30), 1208(393), 1238(440), 1270(176), 1284(0), 1302(214), 1399(0), 1406(1), 1459(2), 1481(3), 2110(637), 3222(0), 3226(0), 3238(0), 3242(0), 3253(1)
CO-C_4F_8-7	29(0), 42(0), 55(0), 72(0), 80(0), 89(0), 117(2), 129(0), 147(0), 159(0), 188(0), 212(1), 253(0), 289(1), 302(1), 310(1), 324(0), 346(0), 374(1), 387(2), 394(4), 424(9), 434(3), 511(8), 525(16), 536(4), 540(28), 553(4), 583(6), 604(9), 612(13), 615(0), 641(8), 730(26), 745(48), 824(2), 828(25), 836(56), 839(0), 843(19), 873(18), 924(1), 926(10), 979(94), 1030(2), 1045(13), 1085(2), 1088(0), 1090(224), 1140(21), 1151(8), 1157(46), 1168(46), 1184(0), 1227(162), 1240(461), 1251(255), 1285(0), 1285(546), 1402(1), 1405(0), 1458(3), 1475(1), 2086(798), 3218(1), 3231(1), 3240(2), 3246(1), 3258(1)
CO-C_4F_8-8	17(0), 38(0), 50(0), 71(0), 82(0), 105(0), 132(0), 137(0), 155(1), 178(0), 201(2), 215(1), 226(4), 272(2), 298(0), 304(1), 331(0), 367(2), 374(1), 397(4), 403(5), 452(2), 458(7), 490(26), 519(5), 526(7), 547(2), 565(25), 588(0), 598(4), 607(4), 610(0), 688(35), 713(18), 749(41), 832(5), 834(3), 842(3), 849(50), 873(51), 879(34), 934(2), 936(2), 960(69), 1033(4), 1041(2), 1048(30), 1075(58), 1087(0), 1090(16), 1098(251), 1152(24), 1156(58), 1188(34), 1198(539), 1225(219), 1239(355), 1285(0), 1295(269), 1403(1), 1408(0), 1462(4), 1471(2), 2096(640), 3219(1), 3231(0), 3240(0), 3245(0), 3256(1)
CO-C_4F_8-9	29(0), 30(0), 42(0), 56(0), 79(0), 111(1), 124(0), 130(0), 135(0), 170(0), 186(1), 217(2), 254(0), 264(6), 295(1), 311(3), 321(2), 347(1), 374(0), 380(3), 391(4), 405(10), 447(3), 460(6), 494(5), 520(27), 530(10), 571(17), 589(2), 590(33), 607(0), 612(0), 656(8), 683(3), 749(33), 823(5), 830(23), 839(23), 841(18), 863(73), 872(15), 924(2), 925(0), 1005(172), 1030(4), 1041(10), 1080(74), 1085(0), 1099(97), 1118(62), 1150(4), 1151(27), 1182(39), 1197(338), 1212(510), 1230(171), 1248(119), 1284(0), 1351(61), 1401(0), 1402(0), 1456(3), 1473(1), 2082(676), 3219(1), 3221(0), 3234(2), 3241(2), 3249(1)

PMe_3-C_4F_8-1	51(0), 61(0), 82(0), 96(0), 101(1), 117(2), 141(0), 146(1), 167(1), 176(0), 177(1), 188(1), 193(0), 199(1), 208(0), 216(1), 223(0), 249(3), 266(0), 273(2), 277(0), 284(1), 304(1), 320(0), 328(1), 337(3), 347(1), 356(5), 369(5), 394(4), 417(3), 434(6), 519(3), 539(4), 541(2), 567(0), 600(1), 604(7), 621(2), 677(30), 697(116), 708(34), 728(19), 737(12), 765(41), 778(8), 787(5), 800(0), 818(64), 832(2), 842(2), 862(3), 870(12), 891(11), 931(16), 943(5), 955(131), 964(21), 966(4), 975(179), 989(196), 1025(6), 1051(9), 1057(9), 1073(19), 1085(1), 1096(10), 1121(243), 1134(151), 1154(9), 1183(73), 1244(543), 1280(371), 1287(2), 1316(8), 1320(20), 1338(52), 1346(277), 1401(4), 1411(5), 1449(0), 1453(5), 1459(0), 1461(2), 1467(10), 1469(4), 1482(1), 1483(4), 3043(16), 3046(13), 3059(19), 3142(8), 3143(8), 3161(5), 3165(3), 3166(2), 3203(0), 3209(6), 3228(2), 3234(4), 3245(2), 3261(1)
PMe_3-C_4F_8-2	28(0), 53(0), 67(1), 69(0), 95(0), 100(0), 115(0), 130(1), 142(0), 169(2), 169(1), 173(1), 185(2), 205(1), 216(3), 224(1), 235(0), 240(1), 264(1), 269(1), 273(1), 285(0), 290(1), 295(0), 305(0), 328(6), 336(3), 350(8), 377(5), 407(3), 425(2), 456(7), 465(1), 532(1), 538(14), 574(3), 598(2), 604(0), 609(1), 677(25), 707(75), 708(58), 732(13), 736(12), 770(0), 782(46), 797(1), 810(6), 824(34), 833(0), 842(45), 860(5), 868(3), 872(3), 914(7), 927(108), 929(3), 958(21), 965(28), 978(125), 1006(164), 1015(8), 1045(24), 1055(8), 1080(3), 1091(3), 1125(92), 1138(231), 1151(33), 1153(233), 1186(386), 1246(268), 1282(108), 1284(71), 1312(9), 1319(6), 1337(10), 1387(133), 1403(1), 1406(3), 1446(0), 1456(4), 1458(2), 1462(6), 1463(2), 1471(7), 1481(5), 1485(1), 3042(18), 3045(12), 3050(18), 3141(2), 3141(16), 3153(5), 3160(5), 3165(0), 3191(0), 3207(4), 3222(3), 3232(3), 3238(3), 3277(1)
PMe_3-C_4F_8-3	39(0), 47(0), 60(0), 68(0), 84(0), 91(0), 129(1), 133(4), 152(1), 168(0), 171(0), 182(0), 191(1), 196(0), 217(1), 226(4), 236(1), 239(0), 250(2), 260(1), 273(1), 276(1), 284(1), 286(1), 309(4), 328(4), 347(5), 350(5), 372(2), 378(2), 408(1), 435(5), 449(10), 526(1), 531(11), 576(9), 599(1), 607(5), 610(1), 650(17), 674(113), 686(82), 731(14), 736(10), 757(34), 766(0), 803(0), 813(5), 823(39), 833(6), 838(29), 854(2), 863(6), 868(3), 908(1), 914(10), 925(94), 964(21), 965(19), 978(172), 1014(14), 1022(113), 1049(9), 1075(159), 1079(10), 1082(47), 1107(82), 1137(164), 1150(3), 1192(262), 1213(336), 1257(77), 1280(0), 1309(164), 1317(11), 1318(13), 1337(4), 1397(87), 1401(0), 1406(27), 1448(0), 1455(3), 1459(2), 1460(3), 1464(6), 1472(9), 1479(3), 1483(2), 3042(15), 3043(16), 3049(16), 3139(4), 3140(16), 3151(6), 3155(5), 3175(0), 3186(0), 3209(3), 3222(4), 3234(3), 3238(5), 3259(1)
PMe_3-C_4F_8-4	44(0), 70(0), 80(0), 96(0), 126(1), 133(5), 151(0), 160(0), 177(1), 178(1), 184(1), 192(1), 200(1), 206(0), 220(3), 229(1), 238(1), 242(2), 252(2), 259(2), 268(0), 271(1), 279(1), 294(3), 300(3), 302(1), 329(1), 344(7), 352(1), 374(1), 380(2), 405(6), 430(3), 461(4), 521(11), 579(7), 590(11), 607(1), 608(2), 615(2), 654(13), 678(10), 735(10), 741(11), 805(0), 808(9), 821(43), 832(3), 837(1), 841(23), 861(3), 865(15), 870(2), 906(273), 924(18), 933(3), 952(161), 963(20), 974(115), 978(156), 1001(37), 1011(208), 1034(15), 1036(20), 1040(6), 1083(3), 1092(24), 1095(100), 1146(189), 1155(11), 1160(162), 1217(93), 1255(115), 1283(0), 1315(11), 1320(8), 1338(90), 1338(30), 1402(1), 1408(0), 1446(0), 1458(0), 1460(0), 1464(6), 1466(9), 1470(2), 1473(5), 1479(3), 3045(14), 3046(10), 3058(17), 3145(7), 3146(6), 3161(2), 3163(2), 3168(1), 3203(0), 3207(5), 3229(2), 3235(3), 3245(0), 3259(1)
PMe_3-C_4F_8-5	30(0), 51(0), 68(0), 96(0), 114(0), 126(0), 138(2), 143(3), 156(0), 170(0), 175(3), 193(0), 200(2), 217(2), 221(1), 229(1), 243(2), 248(3), 263(0), 267(0), 275(1), 276(4), 289(1), 298(2), 313(0), 328(1), 329(1), 339(2), 355(5), 381(3), 392(2), 437(7), 447(1), 518(3), 532(4), 579(8), 594(5), 595(7), 607(4), 612(3), 679(13), 711(44), 732(10), 741(11), 804(8), 805(11), 825(11), 834(8), 838(26), 843(8), 859(1), 870(51), 871(10), 875(89), 905(219), 921(9), 963(19), 964(13), 967(11), 980(138), 997(56), 1028(11), 1043(58), 1046(210), 1070(53), 1081(5), 1090(18), 1103(34), 1154(133), 1155(26), 1171(275), 1208(87), 1278(229), 1283(2), 1288(252), 1317(7), 1319(9), 1338(6), 1404(1), 1408(1), 1450(0), 1459(0), 1462(1), 1462(3), 1468(10), 1469(5), 1478(2), 1487(5), 3041(12), 3050(12), 3055(17), 3142(8), 3149(6), 3156(3), 3163(1), 3171(2), 3200(0), 3213(3), 3227(2), 3236(5), 3246(0), 3267(2)
PMe_3-C_4F_8-6	39(0), 56(0), 60(0), 70(0), 106(0), 114(1), 128(5), 148(1), 163(1), 188(1), 189(0), 192(1), 206(1), 216(2), 221(0), 230(3), 233(0), 243(1), 250(2), 252(1), 259(3), 271(1), 285(0), 291(2), 296(0), 315(0), 335(7), 351(7), 371(0), 383(3), 386(3), 396(0), 449(8), 515(4), 536(2), 579(3), 600(1), 602(2), 612(5), 635(9), 677(73), 685(73), 727(15), 737(9), 796(0), 808(2), 808(89), 815(17), 824(3), 839(25), 842(5), 853(30), 863(3), 870(13), 914(1), 925(1), 960(0), 963(22), 975(153), 978(249), 1019(7), 1023(7), 1046(6), 1056(231), 1069(40), 1080(12), 1088(0), 1116(52), 1142(35), 1152(5), 1201(355), 1225(360), 1253(92), 1280(0), 1300(265), 1316(8), 1317(6), 1337(6), 1402(1), 1404(0), 1444(0), 1457(1), 1458(3), 1460(4), 1461(2), 1470(8), 1479(6), 1480(5), 3048(23), 3049(17), 3049(5), 3144(7), 3149(2), 3149(13), 3165(5), 3184(0), 3184(0), 3219(0), 3223(2), 3235(4), 3240(4), 3252(1)

PMe_3-C_4F_8-7	28(0), 34(0), 58(0), 64(0), 64(0), 75(0), 95(1), 117(2), 132(1), 161(0), 163(0), 170(1), 173(0), 190(0), 206(0), 213(1), 219(2), 246(0), 252(0), 258(1), 267(3), 281(3), 291(0), 304(1), 314(3), 327(0), 346(2), 350(11), 385(7), 391(1), 411(4), 456(21), 519(10), 532(7), 536(3), 541(9), 575(3), 604(2), 609(2), 636(6), 678(21), 726(32), 729(14), 734(10), 742(47), 798(0), 804(2), 820(39), 825(41), 834(4), 839(11), 854(30), 862(2), 865(5), 908(0), 914(14), 955(6), 960(20), 973(98), 976(154), 1009(237), 1024(15), 1040(11), 1080(1), 1081(1), 1124(50), 1144(42), 1150(9), 1159(68), 1176(1), 1223(166), 1227(465), 1257(222), 1280(1), 1284(452), 1313(10), 1318(10), 1336(3), 1399(1), 1406(0), 1449(0), 1455(2), 1462(0), 1463(2), 1465(6), 1471(0), 1473(10), 1482(2), 3041(20), 3042(18), 3043(17), 3138(4), 3139(7), 3141(20), 3153(6), 3173(1), 3177(1), 3214(1), 3222(5), 3235(7), 3237(4), 3255(2)
PMe_3-C_4F_8-8	40(0), 43(0), 48(0), 72(0), 98(0), 103(1), 116(1), 122(0), 140(1), 146(1), 163(2), 176(1), 179(1), 188(1), 215(2), 226(1), 229(3), 243(3), 251(0), 275(2), 282(1), 285(1), 295(1), 305(4), 322(2), 345(0), 354(8), 376(0), 380(11), 405(1), 416(7), 448(1), 508(9), 528(5), 547(2), 583(1), 594(1), 602(6), 604(1), 677(13), 680(36), 706(12), 725(14), 735(12), 745(37), 799(0), 821(3), 826(28), 831(1), 841(35), 853(56), 859(6), 865(30), 875(4), 909(3), 932(5), 957(5), 963(66), 964(58), 976(141), 1026(6), 1028(22), 1042(4), 1050(38), 1075(228), 1082(54), 1090(15), 1149(305), 1152(116), 1162(159), 1189(192), 1203(167), 1241(314), 1267(333), 1282(0), 1315(8), 1322(6), 1340(5), 1403(1), 1408(1), 1449(0), 1459(2), 1460(1), 1462(5), 1466(3), 1471(1), 1475(10), 1481(3), 3044(21), 3044(13), 3052(16), 3139(6), 3141(13), 3147(7), 3161(6), 3178(1), 3199(0), 3208(5), 3225(3), 3233(3), 3241(1), 3253(2)
PMe_3-C_4F_8-9	24(0), 30(0), 32(0), 60(0), 64(0), 81(0), 111(1), 123(0), 136(0), 157(0), 172(1), 176(1), 183(1), 198(2), 214(1), 216(1), 232(1), 234(0), 245(1), 253(0), 270(3), 279(3), 285(3), 289(2), 321(2), 339(1), 352(11), 364(2), 375(1), 390(7), 408(2), 432(8), 479(19), 512(19), 529(13), 550(9), 593(5), 601(5), 609(1), 617(3), 678(22), 694(2), 730(15), 732(19), 739(89), 799(0), 804(16), 813(45), 825(29), 837(17), 842(14), 862(7), 863(12), 866(7), 917(3), 927(11), 959(9), 961(18), 975(157), 989(115), 1026(10), 1044(8), 1058(192), 1081(1), 1090(1), 1107(167), 1136(39), 1150(10), 1165(45), 1176(120), 1210(295), 1226(366), 1249(31), 1285(0), 1316(10), 1316(11), 1335(161), 1336(62), 1402(1), 1406(1), 1450(0), 1457(2), 1461(0), 1462(2), 1466(6), 1472(0), 1472(9), 1482(3), 3041(16), 3043(27), 3044(12), 3138(8), 3140(7), 3142(16), 3153(5), 3176(1), 3179(1), 3215(1), 3222(5), 3236(7), 3239(4), 3261(2)

Table S4. Cartesian coordinates (in Å) for optimized low-lying structures of the $CpCo(L)(C_3F_6)$ and $CpCo(L)(C_4F_8)$ (L = CO, PMe_3) complexes at the M06-L/cc-pVTZ level.

$CpCo(CO)(C_3F_6)$ (**CO-C_3F_6-1**) M06-L/cc-pVTZ Co,0,1.1609893606,0.193450392,-0.0320269963 C,0,1.1946679168,1.9464026447,-0.17284228 O,0,1.3097167167,3.0815193667,-0.2692159426 C,0,-1.7924858456,0.8728844481,-0.4306226654 C,0,-0.7716209991,-0.0523035683,0.1725572974 C,0,-0.1032453708,0.182713711,1.4271694056 F,0,-1.8840807348,0.6873305751,-1.7541980955 F,0,-0.3419182926,1.3112811853,2.1137915238 F,0,-0.0454435063,-0.8365579,2.298430255 F,0,-1.5082264011,2.1593506683,-0.2147601256 F,0,-3.0100751776,0.639471043,0.0819087685 C,0,2.5225507457,-0.3043825358,-1.5528096088 C,0,1.6017045626,-1.3454643993,-1.3718816049 C,0,1.6923881737,-1.7763402691,-0.0124721253 C,0,2.7107736421,-1.0230612179,0.633148549 C,0,3.2025998154,-0.0937433518,-0.3038104203 H,0,2.6759769781,0.2639070774,-2.4545888568 H,0,0.9013499084,-1.7155044783,-2.101628242 H,0,1.0831971636,-2.5368943159,0.4454370888 H,0,3.0070485902,-1.1109305021,1.6644184097 H,0,3.9545513691,0.6556362276,-0.1199588038 F,0,-1.202322415,-1.3362519007,-0.0271867305	$CpCo(CO)(C_3F_6)$ (**CO-C_3F_6-2**) M06-L/cc-pVTZ Co,0,1.294888379,-0.4273747815,-0.010546883 C,0,0.7037001739,-2.08494677,-0.1525309448 O,0,0.4941402067,-3.2095693715,-0.1944403945 C,0,-0.4314483399,1.9029280145,0.0376563417 C,0,-0.2855999067,0.4065923708,-0.1537016898 C,0,-1.6159734022,-0.1838196789,-0.5442599461 F,0,-0.1000610601,2.5628427668,-1.0946451952 F,0,0.3689494567,2.3914632722,1.005411378 F,0,-1.6695190128,2.2979227091,0.3654450709 F,0,-1.5397925379,-1.4274606723,-1.0374709757 F,0,-2.2206545079,0.5522613246,-1.4977876286 C,0,3.0221669961,0.0615163103,-1.02026291 C,0,2.6183879196,1.1317499875,-0.1721799604 C,0,2.6234181476,0.6626625429,1.1674537212 C,0,3.0063843042,-0.6966012233,1.1545068931 C,0,3.26255238,-1.0631399809,-0.1976763333 H,0,3.1058914975,0.0949147414,-2.0929637116 H,0,2.3460529803,2.1220562271,-0.4933214396 H,0,2.3309227045,1.2307074986,2.0331560882 H,0,3.076582946,-1.3475920445,2.0092822901 H,0,3.5415355949,-2.0460235385,-0.5401322399 F,0,-2.4572909194,-0.2465374041,0.5050535691
$CpCo(CO)(C_3F_6)$ (**CO-C_3F_6-3**) M06-L/cc-pVTZ Co,0,0.7274068676,0.1837767703,0. C,0,0.3202083299,1.8975073683,0. O,0,0.1285582273,3.0242099313,0. C,0,-0.8232630636,-0.2784712628,-1.1435134982 C,0,-1.8275165033,-0.103409691,0. C,0,-0.8232630636,-0.2784712628,1.1435134982 F,0,-2.8791049864,-0.9449859684,0. F,0,-1.0865689571,0.4751112774,2.2289223212 F,0,-2.309388416,1.1590955235,0. F,0,-0.8145385376,-1.5723958805,1.5586555616 C,0,2.106112398,-0.8694167979,1.1518397756 C,0,2.7056661547,0.3260324742,0.7162176327 C,0,2.7056661547,0.3260324742,-0.7162176327 C,0,2.106112398,-0.8694167979,-1.1518397756 C,0,1.7070063462,-1.606652101,0. H,0,1.9178048787,-1.1516145996,2.1741538209 H,0,3.077925427,1.1160795725,1.346495384 H,0,3.077925427,1.1160795725,-1.346495384 H,0,1.9178048787,-1.1516145996,-2.1741538209 H,0,1.1863563665,-2.5485161511,0. F,0,-0.8145385376,-1.5723958805,-1.5586555616 F,0,-1.0865689571,0.4751112774,-2.2289223212	$CpCo(CO)(C_3F_6)$ (**CO-C_3F_6-4**) M06-L/cc-pVTZ Co,0,-1.6890879448,0.2118512926,0.0095147716 C,0,-2.1825628661,1.7571588824,-0.6420267693 O,0,-2.5398952177,2.7604306039,-1.0676255688 C,0,1.9588093267,-0.8148194633,-1.019134935 C,0,0.0182247817,0.6358313684,-0.1452191759 C,0,1.2715260227,-0.1619191243,0.2058500529 F,0,2.2886043906,0.0989211145,-1.9237658003 F,0,1.1350663106,-1.699527328,-1.5887370009 F,0,3.0608411564,-1.456532326,-0.6412501736 F,0,0.4878518821,1.7851015945,-0.6629473487 F,0,0.995663323,-1.1672883016,1.065779978 C,0,-3.5970903993,-0.5964960589,0.1351604059 C,0,-2.7559350393,-1.4605657696,-0.6104768052 C,0,-1.6835631937,-1.8390917424,0.2364932976 C,0,-1.8752937788,-1.2206733284,1.5045077988 C,0,-3.057290348,-0.449592868,1.4432363089 H,0,-4.4794088436,-0.1027275011,-0.2376581103 H,0,-2.8964382572,-1.7583559569,-1.6352373905 H,0,-0.8613321812,-2.479257254,-0.0320028133 H,0,-1.2154715887,-1.3057012256,2.3503097553 H,0,-3.4678429227,0.1546910691,2.2338267184 F,0,2.1921323873,0.6342253226,0.7949230044
$CpCo(PMe_3)(C_3F_6)$ (**PMe_3-C_3F_6-1**) M06-L/cc-pVTZ Co,0,-0.5742563,-0.8060624551,-0.0071016064 C,0,2.3765142878,-0.0878604661,-0.0329025771 C,0,0.9718930245,0.3305106994,0.2987590663 C,0,0.2958274907,-0.0809727604,1.510371904 F,0,2.6300034601,0.0560892521,-1.3460603208 F,0,0.9300510836,-0.9120062912,2.3740816448 F,0,-0.2664057312,0.9046497188,2.268042912 F,0,2.6405981781,-1.3615054921,0.2840559725 F,0,3.2783227033,0.6704543992,0.613652403 C,0,-3.112742258,0.7897572923,-1.6164795709 H,0,-2.4806358876,1.0276741673,-2.469041514 H,0,-3.5690467297,-0.1802973721,-1.7944202657 H,0,-3.9009650418,1.5384416056,-1.5465167984	$CpCo(PMe_3)(C_3F_6)$ (**PMe_3-C_3F_6-2**) M06-L/cc-pVTZ Co,0,-0.2619921816,0.7048564901,0. C,0,1.0100886765,-0.2156851785,-1.1631862201 C,0,1.802346967,-0.8488202038,0. C,0,1.0100886765,-0.2156851785,1.1631862201 F,0,3.1053247135,-0.5031921666,0. F,0,0.548541434,-1.1634244441,-2.045524211 F,0,0.548541434,-1.1634244441,2.045524211 F,0,1.7375910271,-2.2023820465,0. F,0,1.8246695755,0.5841792752,1.9104298865 C,0,-0.275682541,2.4444007412,1.149726055 C,0,-1.5882017158,2.1968305198,0.7161892573 C,0,-1.5882017158,2.1968305198,-0.7161892573 C,0,-0.275682541,2.4444007412,-1.149726055

C,0,-3.3622364628,0.5518209002,1.2143554599 C,0,-1.7335220466,2.5571617232,0.0654606186 H,0,-2.8843148067,0.6529461647,2.1856576615 H,0,-4.1590522102,1.2900320444,1.1292964376 H,0,-3.793558985,-0.4447093106,1.1522196661 H,0,-2.6699456394,3.1143495576,0.065920069 H,0,-1.1898691067,2.7530325991,0.9832866884 H,0,-1.1199608745,2.8848705134,-0.7679896149 P,0,-2.1011208721,0.7768252707,-0.090424077 C,0,0.1145072507,-2.7357189733,0.0941967539 C,0,-1.2526407644,-2.7125520837,0.4746926099 C,0,-1.9789424847,-2.2005979773,-0.6215104464 C,0,-1.0741085188,-1.9461267287,-1.7043998906 C,0,0.2143568877,-2.2787605308,-1.2537609912 H,0,0.9367905611,-3.0374474724,0.7184668848 H,0,-1.6563291745,-3.0033268226,1.4298190964 H,0,-3.0468227194,-2.0485367752,-0.6461802233 H,0,-1.3371940582,-1.5676087298,-2.6776884942 H,0,1.1305170854,-2.1675129404,-1.8096062178 F,0,0.9040448392,1.6793945636,0.0002204602	C,0,0.5570973977,2.5712572882,0. H,0,0.062849491,2.4628582438,2.1717404565 H,0,-2.4439572637,2.0430292157,1.3521100677 H,0,-2.4439572637,2.0430292157,-1.3521100677 H,0,0.062849491,2.4628582438,-2.1717404565 H,0,1.6203272899,2.7423868446,0. P,0,-1.6905330667,-0.9768847663,0. C,0,-1.1525127746,-2.7187142433,0. H,0,-0.5550295335,-2.9293592594,0.8805963968 H,0,-0.5550295335,-2.9293592594,-0.8805963968 H,0,-2.036567454,-3.3552296255,0. C,0,-2.8289110376,-0.9603014754,-1.4284650892 H,0,-3.4222653829,-0.0496164177,-1.4306682303 H,0,-3.5012911326,-1.8169073589,-1.3990836202 H,0,-2.2488827219,-0.9956129168,-2.3477145084 C,0,-2.8289110376,-0.9603014754,1.4284650892 H,0,-3.4222653829,-0.0496164177,1.4306682303 H,0,-3.5012911326,-1.8169073589,1.3990836202 H,0,-2.2488827219,-0.9956129168,2.3477145084 F,0,1.8246695755,0.5841792752,-1.9104298865
CpCo(PMe$_3$)(C$_3$F$_6$) (**PMe$_3$-C$_3$F$_6$-3**) M06-L/cc-pVTZ Co,0,0.7185815779,-0.7679053626,0.0368881616 C,0,-0.6649795928,1.8655616572,0.2193661131 C,0,-0.6107332499,0.4251867573,-0.1831532403 C,0,-1.9723249814,0.0115707446,-0.6789743172 F,0,-0.5454977637,2.7244571916,-0.8218665467 F,0,0.3163642662,2.2138457134,1.0886222217 F,0,-1.8118061471,2.1925609218,0.8467829234 F,0,-1.938737223,-1.0316139235,-1.5321659662 F,0,-2.6147095611,0.9925465991,-1.3460774063 C,0,0.3321803437,-2.6190773513,-0.8586717348 C,0,1.7119781063,-2.5058997774,-0.5840843142 C,0,1.8621901127,-2.3039258133,0.81895791 C,0,0.5775588968,-2.2729568179,1.4057328861 C,0,-0.3744391451,-2.4639321777,0.3588113578 H,0,-0.1120992195,-2.7452968036,-1.8307483487 H,0,2.510470094,-2.5692731429,-1.3041457025 H,0,2.7936236268,-2.1738799492,1.3465614044 H,0,0.3569536142,-2.1210679125,2.4487153711 H,0,-1.4442281762,-2.4724651097,0.4751563831 P,0,2.4623799192,0.6051406541,0.0625694399 C,0,3.0999353431,1.1518834978,1.688028264 H,0,3.3214664712,0.2806112832,2.3010371791 H,0,2.3549210769,1.7490537491,2.2030717835 H,0,4.0114504995,1.7371377226,1.5702681536 C,0,2.5032794415,2.1372394025,-0.9336554138 H,0,2.1700891406,1.9203711173,-1.9457294632 H,0,3.5221973277,2.5207062578,-0.9696199683 H,0,1.8524391801,2.8977143222,-0.5204580224 C,0,3.9574862429,-0.2084951646,-0.6248940305 H,0,4.1959852624,-1.1223453881,-0.0871998566 H,0,4.8123407716,0.4640679126,-0.5629486872 H,0,3.7915787115,-0.4612843754,-1.6697093318 F,0,-2.7999760571,-0.3665176345,0.3272896184	CpCo(PMe$_3$)(C$_3$F$_6$) (**PMe$_3$-C$_3$F$_6$-4**) M06-L/cc-pVTZ Co,0,-1.2359379615,0.5775474938,-0.1271476321 C,0,2.763546555,-0.8390177967,-0.6169600075 C,0,0.2690476119,-0.3149923233,-0.0384630752 C,0,1.6756735551,0.209746428,-0.2792973309 F,0,3.056036556,-1.6047841982,0.4289760575 F,0,0.4354591463,-1.6357020295,0.3289439815 F,0,1.6842998967,1.0926941831,-1.309898761 F,0,3.8840020446,-0.2205783759,-0.9948471686 F,0,2.3627820114,-1.6172157543,-1.6246585655 C,0,-2.7811794378,1.9536200786,0.1066809862 C,0,-1.6238482957,2.3930655332,0.7871776114 C,0,-0.5835464855,2.5124149052,-0.1775333485 C,0,-1.1135521257,2.1599856395,-1.449216959 C,0,-2.4713181675,1.8055038611,-1.276447252 H,0,-3.73615441,1.7480522723,0.5613910934 H,0,-1.5428529752,2.5948395269,1.8417526094 H,0,0.4303828213,2.8144258419,0.0209121162 H,0,-0.5623036547,2.1331514898,-2.3737004691 H,0,-3.1523120541,1.4906237771,-2.0498132242 P,0,-2.4012943436,-1.2140188954,0.2536153018 C,0,-2.1896406756,-2.0450766956,1.8678190357 H,0,-1.1524086417,-2.3385011666,1.9943574719 H,0,-2.8254529534,-2.9270612966,1.9409298006 H,0,-2.4487344575,-1.3550970179,2.6674589795 C,0,-2.1746957095,-2.5862474878,-0.9324162254 H,0,-1.1302491239,-2.880310158,-0.9590556593 H,0,-2.7852567693,-3.4463580796,-0.6588569837 H,0,-2.4601648619,-2.2519802923,-1.9271877528 C,0,-4.2208489544,-1.0126464537,0.2037655976 H,0,-4.7162488194,-1.9783532186,0.2975262667 H,0,-4.5520586932,-0.3748299123,1.0197962102 H,0,-4.5251170912,-0.5525641389,-0.7337169118 F,0,2.1332112241,0.8901804108,0.8129365871
CpCo(CO)(C$_4$F$_8$) (**CO-C$_4$F$_8$-1**) M06-L/cc-pVTZ Co,0,1.1130644902,0.1192097475,-0.0445033802 C,0,1.2080336844,1.8748798809,-0.1670058531 O,0,1.4089791381,2.9973797084,-0.2607816447 C,0,-1.6729612446,1.1109447015,-0.4714934514 C,0,-1.5759919359,-1.3494997495,-0.102766966 C,0,-0.8825217412,-0.025910001,0.1433085239 C,0,-0.1736305317,0.1370399904,1.3960757037 F,0,-1.9636792268,-1.4564330958,-1.382798417	CpCo(CO)(C$_4$F$_8$) (**CO-C$_4$F$_8$-2**) M06-L/cc-pVTZ Co,0,0.3561429823,1.3242422855,0.7139865623 C,0,2.0326668551,1.3963985972,1.2572868361 O,0,3.0945154025,1.5313271067,1.6596514982 C,0,-1.0281423367,-1.2773808711,1.5112062279 C,0,0.2320257669,-0.603292733,1.0199194042 C,0,0.4665124559,-0.2973388785,-0.3671207366 C,0,1.706322605,-0.7246627717,-1.1164550754 F,0,-0.9908518956,-2.591137216,1.2550307125

F,0,-1.443038101,1.2154539658,-1.7914314224 F,0,-2.6742765018,-1.4783806682,0.6569737721 F,0,-0.8203171369,-2.4256538673,0.1617990506 F,0,-0.3178239725,1.2433509445,2.135065524 F,0,-0.161209228,-0.9056455242,2.2465311194 F,0,-1.3845018525,2.3009138139,0.0666198367 F,0,-2.9961022547,0.9370019394,-0.32932282 C,0,2.3263238144,-0.4991179289,-1.6539864081 C,0,1.5818939826,-1.5858222038,-1.1745493837 C,0,1.8974642854,-1.7752838637,0.207044221 C,0,2.8580230164,-0.8094486094,0.5838904687 C,0,3.0985367817,0.0001100078,-0.5550718509 H,0,2.3004758793,-0.0890068108,-2.6486406232 H,0,0.8604061167,-2.1574946812,-1.733659318 H,0,1.4659164631,-2.5196550857,0.8520229398 H,0,3.299906081,-0.6886058923,1.5577227673 H,0,3.7564219943,0.8535252818,-0.5914733887	F,0,-1.1469312656,-1.1336690284,2.8370015039 F,0,-2.1431870469,-0.794269799,0.9538230316 F,0,-0.5886175164,-0.4881330135,-1.2211624199 F,0,1.8276457724,-0.0220244363,-2.2496026264 F,0,1.6262525028,-2.0186268741,-1.4581785608 F,0,2.8279293807,-0.5643743425,-0.4140486611 F,0,1.2695786442,-1.1778201743,1.7051439893 C,0,0.1925795686,3.3772946116,0.4790309766 C,0,-0.5515629003,2.7300382628,-0.5237787665 C,0,-1.5191016476,1.9148862953,0.1285217166 C,0,-1.4006688209,2.1024328759,1.5359658401 C,0,-0.3360644904,2.9905579545,1.7600811482 H,0,1.0311400627,4.0356971592,0.3226790534 H,0,-0.3887504215,2.7940896698,-1.5861867447 H,0,-2.2185739693,1.2607233864,-0.3610068528 H,0,-1.9901426097,1.6071404965,2.2890822376 H,0,0.0351295919,3.3163873571,2.7170207058
CpCo(CO)(C_4F_8) (**CO-C_4F_8-3**) M06-L/cc-pVTZ Co,0,-0.9903315981,0.4584784066,0.1451592423 C,0,-1.694115905,-0.1128716447,1.6530462524 O,0,-2.2059245621,-0.4213762255,2.6294154784 C,0,2.0096678252,-0.1979377535,2.139114102 C,0,1.2503479668,-1.265649249,1.3117358135 C,0,0.5615133648,-0.7347618447,0.0812103843 C,0,-0.6200553106,-1.3144777822,-0.5154890418 F,0,0.3712708202,-1.8506926985,2.1507324469 F,0,2.6836701434,-0.7817700083,3.1239312537 F,0,2.1656152758,-2.2002557794,0.9569561433 F,0,-0.6015813414,-1.4957553898,-1.8454959572 F,0,1.5214054855,-0.3597489177,-0.8226167352 F,0,-1.217962792,-2.3772578876,0.0429357037 F,0,1.1515523463,0.6718409887,2.6802564857 F,0,2.8675853308,0.4806764969,1.3815301113 C,0,-0.0790858569,2.2509859558,-0.4106227424 C,0,-1.154608269,2.5319559664,0.4422262537 C,0,-2.3463760445,2.0021329345,-0.1629915242 C,0,-1.999441745,1.4204868993,-1.3988599523 C,0,-0.5903095127,1.5382234348,-1.5397443081 H,0,0.9598842514,2.4675254015,-0.223894149 H,0,-1.0993965202,3.0206154849,1.4004962784 H,0,-3.3345861904,2.0408054318,0.2646384503 H,0,-2.6670070024,0.9275229457,-2.0846191291 H,0,-0.0014673398,1.1472245239,-2.3520171509	CpCo(CO)(C_4F_8) (**CO-C_4F_8-4**) M06-L/cc-pVTZ Co,0,1.0511547545,0.0174950188,-0.1131831817 C,0,1.5078573764,1.4043986557,-1.1070511059 O,0,1.8925324144,2.2799251093,-1.7307803034 C,0,-0.8580319425,-0.024702398,-0.6970538028 C,0,-1.1804733055,1.2444645791,0.0848682888 C,0,-0.0301064566,1.1636350534,1.0875153791 F,0,-2.4178877306,1.2898939503,0.6138262875 F,0,0.4665220727,2.3576823459,1.4659908339 F,0,-1.0292363267,2.3422991875,-0.6961983542 F,0,-0.4319168049,0.530111601,2.2169791881 C,0,2.1847825762,-0.8310760433,1.4024077605 C,0,3.0061713967,-0.6266996733,0.2756019319 C,0,2.4657302672,-1.3812165148,-0.8158073509 C,0,1.3114347945,-2.037092817,-0.3545893356 C,0,1.1157619429,-1.685206807,1.0125978291 H,0,2.3049403564,-0.3723668081,2.3695156329 H,0,3.8778335022,0.0050156918,0.2339868168 H,0,2.859062642,-1.4142700983,-1.817789604 H,0,0.6435608817,-2.640258419,-0.9463185897 H,0,0.293655939,-1.9971492203,1.6328648665 C,0,-1.2194066001,-0.0723212275,-2.1686193617 F,0,-0.9323348005,-1.2813595129,-2.6761718577 F,0,-2.5274821452,0.1397315044,-2.3632744647 F,0,-0.5527716252,0.8336201412,-2.8894175854 F,0,-1.533718599,-1.0763572286,-0.1098606776
CpCo(CO)(C_4F_8) (**CO-C_4F_8-5**) M06-L/cc-pVTZ Co,0,0.9891140889,0.1361454693,0.1418523645 C,0,0.7292762725,0.7363341258,1.7867729373 O,0,0.6235023339,1.1310153553,2.8510352866 C,0,-1.7024534527,-0.9297083289,-0.2160010078 C,0,-1.8496422325,0.5835000179,-0.0522074095 C,0,-0.3494124293,-1.3414686895,0.3984724714 C,0,-0.5392709667,1.2155880258,-0.5391346228 F,0,0.0052244034,-2.5308162323,-0.1644494132 F,0,-0.5543055803,-1.6147884708,1.7179962063 F,0,-2.740437787,-1.5835449612,0.3310023285 F,0,-1.6783313631,-1.2132615008,-1.5368451632 F,0,-2.0055429002,0.8575136088,1.2644338843 F,0,-2.9270376658,1.0498294348,-0.7029720063 F,0,-0.6011130148,1.2595265453,-1.9007397062 F,0,-0.4815650456,2.5111339226,-0.1313057377 C,0,3.0513155723,-0.2528339037,0.3588772254 C,0,2.4651674047,-1.2033260925,-0.4900165081 C,0,1.8663290231,-0.5117880877,-1.585693279 C,0,2.1552932832,0.8741854763,-1.4265918371	CpCo(CO)(C_4F_8) (**CO-C_4F_8-6**) M06-L/cc-pVTZ Co,0,1.2782361299,0.1074363664,0. C,0,1.2070644419,1.8714220523,0. O,0,1.2572927258,3.0127724956,0. C,0,-0.3298045348,-0.0524957101,-1.1353927812 C,0,-2.7178457119,-0.2708768272,0. C,0,-1.2986475698,0.313618262,0. C,0,-0.3298045348,-0.0524957101,1.1353927812 F,0,-3.379620742,0.1478793099,-1.0824756523 F,0,-1.4586364623,1.6737256289,0. F,0,-3.379620742,0.1478793099,1.0824756523 F,0,-2.7271367839,-1.6000873505,0. F,0,-0.4569630104,0.7476258258,2.2115907418 F,0,-0.556821788,-1.322454327,1.5711757565 F,0,-0.556821788,-1.322454327,-1.5711757565 F,0,-0.4569630104,0.7476258258,-2.2115907418 C,0,2.4422134857,-1.1785870623,1.1512565477 C,0,3.2531031661,-0.1148184048,0.7157521005 C,0,3.2531031661,-0.1148184048,-0.7157521005 C,0,2.4422134857,-1.1785870623,-1.1512565477

C,0,2.8553457954,1.0443337857,-0.2212761796 H,0,3.5401272914,-0.4572811545,1.2968789787 H,0,2.4019761945,-2.2615663279,-0.306958047 H,0,1.3161802533,-0.9586155818,-2.3967120643 H,0,1.8120604427,1.663183258,-2.0735383749 H,0,3.1752679387,1.9822362161,0.2004870337	C,0,1.9146812638,-1.8314136106,0. H,0,2.2053435813,-1.4205134544,2.1738147286 H,0,3.7642282848,0.5929401107,1.3465370191 H,0,3.7642282848,0.5929401107,-1.3465370191 H,0,2.2053435813,-1.4205134544,-2.1738147286 H,0,1.2325152716,-2.6638865402,0.
CpCo(CO)(C_4F_8) (**CO-C_4F_8-7**) M06-L/cc-pVTZ Co,0,1.8660206785,-0.0981401694,-0.2840225137 C,0,2.2282864121,-0.9170884133,-1.7854593542 O,0,2.502728843,-1.446116568,-2.7654170956 C,0,-1.9933873888,-1.2609511809,0.657961904 C,0,-1.8103254496,1.1742243173,-0.1235395594 C,0,0.1394761852,-0.4152518984,-0.4722868677 C,0,-1.0418192911,-0.0539908299,0.426131163 F,0,-2.1586384593,1.0101469442,-1.3936829331 F,0,-2.8057943172,-1.457634164,-0.375746966 F,0,-1.0301360479,2.2544348113,-0.0386261045 F,0,-2.9119610693,1.4125170422,0.5885724571 F,0,-0.4138852149,-1.057823082,-1.5234956478 F,0,-0.6048139554,0.3134700705,1.670340014 F,0,-2.7393465406,-1.0607692665,1.74131408 F,0,-1.2797125715,-2.3703086049,0.8564358371 C,0,3.8086533758,0.5297130716,0.0838847377 C,0,2.931567708,1.6436265034,0.1135606325 C,0,1.9774138034,1.4011363166,1.1328556905 C,0,2.2783289148,0.1475821859,1.738631059 C,0,3.4105543391,-0.3934178767,1.0910191777 H,0,4.6219515321,0.3887370579,-0.6089550525 H,0,2.9730435949,2.5041604736,-0.5316474494 H,0,1.1603892596,2.047159563,1.4016956318 H,0,1.7198174948,-0.3155699205,2.5334233841 H,0,3.8776437539,-1.3395994629,1.3038198456	CpCo(CO)(C_4F_8) (**CO-C_4F_8-8**) M06-L/cc-pVTZ Co,0,0.9781758563,-0.6442215924,0.4303675248 C,0,0.7642587884,-2.17632448,-0.4248765736 O,0,0.721969956,-3.2395750762,-0.8450466991 C,0,-0.3775224833,1.8202524661,-0.3128911647 C,0,-0.0935379752,0.3621028728,-0.6084740392 C,0,-0.7001924991,-0.0648179711,-1.9230980611 C,0,-2.1044357667,-0.7267165032,-1.818574587 F,0,0.5775466004,2.6018546745,-0.86456937 F,0,-0.381959744,2.1065272524,1.0038690635 F,0,-1.5552713063,2.2666129971,-0.7693417802 F,0,-2.0157839313,-1.8846352281,-1.1580361777 F,0,-2.5808337607,-0.9781062978,-3.0336620179 F,0,-2.970736876,0.0505988419,-1.1785345762 F,0,0.0692615411,-0.9913104229,-2.5579688493 F,0,-0.8187304168,0.967472927,-2.7982018722 C,0,2.9112637472,-0.2368826842,1.0124650495 C,0,2.0232710869,0.7585390381,1.5069587404 C,0,1.0819832783,0.1276155767,2.3617735791 C,0,1.3688528608,-1.2557465802,2.3878051947 C,0,2.5060977985,-1.4767779469,1.5618766185 H,0,3.727835257,-0.0806756892,0.3286782906 H,0,2.0515094382,1.8063037062,1.2630547738 H,0,0.261578657,0.612810192,2.8605368935 H,0,0.8186831163,-2.0115298862,2.9219020511 H,0,2.950894717,-2.4347937664,1.3481324687
CpCo(CO)(C_4F_8) (**CO-C_4F_8-9**) M06-L/cc-pVTZ Co,0,1.7912506934,0.2315911688,-0.0677640195 C,0,2.5860181823,1.7998189158,-0.0612645377 O,0,3.2251574642,2.7514046131,-0.0185753243 C,0,0.1353502402,0.8182173227,-0.2080174333 C,0,1.5082664831,-1.6033783908,0.8124155114 C,0,1.5601395692,-1.7344246432,-0.6048997583 C,0,2.8284702779,-1.2842320514,-1.0479425961 C,0,3.5490906313,-0.85995329,0.0985612313 C,0,2.7400454915,-1.0653545324,1.251253869 H,0,0.6551861582,-1.8259753311,1.4318536018 H,0,0.7550786821,-2.0810548975,-1.2307316938 H,0,3.1741123751,-1.2474158343,-2.0664967295 H,0,4.5349509972,-0.4250225778,0.0950831908 H,0,3.0092471963,-0.8297803513,2.2665092815 C,0,-0.50659835,2.1928318435,-0.26807065 C,0,-1.3074532172,2.6015948888,1.0052158365 F,0,-0.909089218,-0.0415695737,-0.1959484107 F,0,-2.4272329337,1.8670097435,1.0859748978 F,0,-1.3922942573,2.246951899,-1.2941656381 F,0,0.4126473597,3.1523097311,-0.4774364916 C,0,-0.5474856776,2.4419528828,2.3424310187 F,0,-0.388031792,1.1510810281,2.6366080525 F,0,-1.2433894734,3.0093002944,3.3209324981 F,0,0.6500595779,3.0179932554,2.2807014621 F,0,-1.6538740705,3.8942397563,0.8836191111	
CpCo(PMe_3)(C_4F_8) (**PMe_3-C_4F_8-1**) M06-L/cc-pVTZ Co,0,0.81434468,-0.3247316244,-0.3364029641 C,0,-2.0076681977,0.6142158683,-0.9258771898 C,0,-1.7311732557,-0.3919222486,1.3313952125	CpCo(PMe_3)(C_4F_8) (**PMe_3-C_4F_8-2**) M06-L/cc-pVTZ Co,0,-0.3758550415,-0.8671048774,-0.2426363645 C,0,2.4239011581,-0.7607540198,0.9439701884 C,0,1.1137491703,-0.054841536,0.6789550314

C,0,-1.0261280492,0.2976528575,0.1801636584	C,0,0.7483186977,0.6713506541,-0.526489231
C,0,0.0667969091,1.2491067389,0.3951335887	F,0,3.4271431008,0.1187575938,1.1082141356
F,0,-1.3297031312,-1.6795491465,1.5034196114	F,0,2.3383928165,-1.470549415,2.0796715484
F,0,-2.6298073929,-0.4962525568,-1.3711686758	F,0,2.8049675627,-1.6081496053,-0.0168613054
F,0,-3.0573369637,-0.4633373109,1.1624014123	F,0,0.8892067504,0.6659353321,1.8378146042
F,0,-1.5399036679,0.2141958989,2.5134918775	C,0,0.044266406,-2.9105227327,-0.1912109082
F,0,0.0552665269,2.3896981256,-0.334996573	C,0,-1.3366596806,-2.7067533378,-0.0493328788
F,0,0.3784168101,1.6430346621,1.6596990718	C,0,-1.7972333757,-2.0145160347,-1.2242787363
F,0,-1.4590390483,1.1899292853,-2.0039808696	C,0,-0.7010874143,-1.8081474855,-2.0800877224
F,0,-2.9702182222,1.4623193897,-0.5158934549	C,0,0.4476390561,-2.3378465659,-1.4318382215
C,0,1.9349152567,-2.8693684601,1.6453712401	H,0,0.6977191962,-3.3769310808,0.5272394936
H,0,0.9673105142,-3.3666355312,1.6326273963	H,0,-1.9458645465,-3.0150803965,0.7836777601
H,0,2.501159496,-3.2131706374,0.7848301368	H,0,-2.8154056536,-1.7201815315,-1.4242171466
H,0,2.4647883105,-3.1567456203,2.5526448817	H,0,-0.7173877252,-1.3066823719,-3.0334883237
C,0,3.3370352992,-0.3584774774,1.8362662198	H,0,1.4467865026,-2.333630784,-1.8242282424
C,0,1.0089383483,-0.820374572,3.2913310694	C,0,-1.7544978206,1.5181972458,2.0249949623
H,0,3.2408506559,0.7178815444,1.9658331508	H,0,-1.3958197816,0.9877127362,2.9022135154
H,0,3.8166899555,-0.7773292572,2.7200704363	H,0,-1.0172239691,2.2659329559,1.7563178455
H,0,3.9702790287,-0.5366151243,0.9718293429	H,0,-2.7041537035,1.9993178846,2.2575031859
H,0,1.7537495955,-1.1996311871,3.9901928729	C,0,-2.8060486131,1.3920688051,-0.615988033
H,0,0.8260871037,0.2286030183,3.4945086793	C,0,-3.417932088,-0.6110566471,1.306167976
H,0,0.0836676376,-1.3676452979,3.4312674799	H,0,-3.1972196015,0.7678338234,-1.4163934114
P,0,1.6621809918,-1.060080156,1.599689079	H,0,-3.622791533,1.9731512707,-0.1889640327
C,0,1.1795563007,0.3117683244,-2.2684147465	H,0,-2.0671446154,2.065568712,-1.0411614557
C,0,2.4068540025,0.0738112481,-1.6106119121	H,0,-4.214587083,0.0627755046,1.6188885667
C,0,2.4041559449,-1.2918380715,-1.2223800554	H,0,-3.8156882563,-1.2948701137,0.5611176012
C,0,1.2024287057,-1.9145887222,-1.6704484971	H,0,-3.0993992359,-1.1931875729,2.168023081
C,0,0.4445038167,-0.9104392786,-2.3014031686	P,0,-2.0027700714,0.3469645236,0.6490780279
H,0,0.8406471222,1.2576474626,-2.6513749681	C,0,1.5846321421,0.9026827762,-1.7587026984
H,0,3.1924372693,0.787775853,-1.4292585539	F,0,2.2707779366,-0.171461274,-2.1574986465
H,0,3.2060148463,-1.7883590707,-0.6993478198	F,0,0.7997956151,1.2785884837,-2.7853862664
H,0,0.9278607642,-2.9473646838,-1.5401571207	F,0,2.4744765572,1.8901463307,-1.5745755191
H,0,-0.5439747137,-1.0302879421,-2.7113451486	F,0,0.2129011115,1.9299495096,-0.2558197993
CpCo(PMe_3)(C_4F_8) (**PMe_3-C_4F_8-3**) M06-L/cc-pVTZ	CpCo(PMe_3)(C_4F_8) (**PMe_3-C_4F_8-4**) M06-L/cc-pVTZ
Co,0,-0.8541414745,-0.9813834794,-0.0269369117	Co,0,-1.1741163627,-0.0235145558,0.122006418
C,0,0.9969383899,-1.0977449274,0.5535900438	C,0,1.6239806878,0.2275654453,-0.2956582237
C,0,0.0359516957,-1.4022974715,1.5942582748	C,0,1.5187548897,-1.1156292319,0.4295108958
F,0,-0.058613475,-2.6787622445,2.0456135262	C,0,0.4543716018,1.1016957084,0.1688572174
F,0,0.0424944074,-0.6033755477,2.6885529859	C,0,0.0479813759,-1.5849791968,0.3224822559
C,0,-0.9886074235,-2.1226014688,-1.7741209848	F,0,0.4211066687,2.2134992766,-0.6323752193
C,0,-1.8693951255,-1.0318048647,-1.8617971948	F,0,0.8008409466,1.6070502803,1.4095813144
C,0,-2.7950598147,-1.1248120576,-0.7649732377	F,0,2.8307241129,0.7943189728,-0.1084623589
C,0,-2.4837899736,-2.2740773671,-0.0195845347	F,0,1.481890717,-0.0037403844,-1.626796519
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P,0,-0.8526991035,1.2162512074,0.1232430933	C,0,-1.6276879198,0.6708486499,-1.7887562854
C,0,0.2645984968,1.9982710463,-1.0938238715	C,0,-1.900545599,-0.7086982175,-1.7176567355
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H,0,-0.4909920591,3.1500035897,1.5313365164	H,0,-1.4132844418,2.4965733893,2.5578210544
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C,0,1.9918484107,-2.0626772933,-0.0229489416	H,0,-3.0436291401,-0.9206698042,3.922512705

C,0,3.298768757,-2.2242106563,0.8043844962 F,0,2.3793485745,-1.660252203,-1.264055622 F,0,1.4677675126,-3.3000131629,-0.1455558313 F,0,3.9830940499,-3.2834316388,0.3718579354 F,0,4.0837918313,-1.1579416129,0.6994196109 F,0,3.0035059395,-2.4123120116,2.0909752504	H,0,-2.5157033194,-2.0623481995,2.6753554258 H,0,-3.7767199768,-0.8854768028,2.312501715 C,0,-0.2758059964,-0.1900532464,3.5738724218 H,0,0.1027259728,-1.2031193555,3.4924994239 H,0,0.551157817,0.500961064,3.4595638064 H,0,-0.7340578852,-0.0509664521,4.5525555823
CpCo(PMe_3)(C_4F_8) (**PMe_3-C_4F_8-5**) M06-L/cc-pVTZ Co,0,-0.41614641,0.6812890135,0.1595604718 C,0,2.4111084077,0.1825785475,-0.9037089341 C,0,1.0675926148,-0.4355867337,-0.5677396443 C,0,1.0968210244,-1.334263021,0.6829901372 C,0,0.0467921284,-0.611901185,1.5405751967 F,0,2.3062185798,-1.4034032145,1.2910813544 F,0,3.3424431907,-0.7464487121,-1.1609842148 F,0,0.7675439463,-1.1848900635,-1.7097724892 F,0,-0.9235094873,-1.4780493501,1.9915563493 F,0,0.7321738778,-2.602706023,0.3856164457 F,0,0.6087315249,-0.1025258375,2.6710422091 F,0,2.8795119471,0.9529162443,0.0896256119 F,0,2.3316629605,0.9492726061,-2.0072203838 C,0,-1.0603025344,2.1959929538,1.42459114 C,0,-1.7660496647,2.2887111959,0.2068340742 C,0,-0.8345740816,2.5031752897,-0.8515479772 C,0,0.4470057117,2.5511924881,-0.2712334155 C,0,0.324761508,2.3429334631,1.1262448844 H,0,-1.4857580291,2.0125288796,2.3971926803 H,0,-2.835297033,2.2126569703,0.0932512513 H,0,-1.065816491,2.6232991291,-1.8963940827 H,0,1.3711175731,2.6838595497,-0.8040849796 H,0,1.1359293177,2.2964365603,1.8317335647 P,0,-2.0158420681,-0.6280730686,-0.6479883466 C,0,-1.8453760901,-2.4274038309,-0.8805432743 H,0,-1.6797985935,-2.9082280728,0.0780924951 H,0,-1.0102758319,-2.6580097027,-1.5316202336 H,0,-2.7695973649,-2.8033644177,-1.3180702886 C,0,-2.5783789134,-0.0890230156,-2.2981189849 H,0,-2.9253075679,0.9408985284,-2.2623544557 H,0,-3.3873016672,-0.7216720119,-2.6612286618 H,0,-1.7433582496,-0.145287387,-2.9930759763 C,0,-3.5407162638,-0.5839768741,0.3590138005 H,0,-3.9444979267,0.4217551442,0.4276991556 H,0,-4.2990945925,-1.2359520303,-0.0724219774 H,0,-3.3072404521,-0.9301660117,1.3627514985	CpCo(PMe_3)(C_4F_8) (**PMe_3-C_4F_8-6**) M06-L/cc-pVTZ Co,0,-0.9176720046,-0.6313243458,0. C,0,0.6431012436,-0.2617763852,1.132519967 C,0,2.9997162781,0.2185074919,0. C,0,1.4728426668,0.3609317412,0. C,0,0.6431012436,-0.2617763852,-1.132519967 F,0,3.5139193287,0.8166114303,1.0820933883 F,0,1.2465973564,1.7232513769,0. F,0,3.5139193287,0.8166114303,-1.0820933883 F,0,3.4055278679,-1.0459863062,0. F,0,0.569078688,0.5555254287,-2.2198717671 F,0,1.2639933837,-1.397383506,-1.5874372294 F,0,1.2639933837,-1.397383506,1.5874372294 F,0,0.569078688,0.5555254287,2.2198717671 C,0,-1.5513531093,-2.2476329604,-1.1495817364 C,0,-2.6858895348,-1.5403947297,-0.7165531995 C,0,-2.6858895348,-1.5403947297,0.7165531995 C,0,-1.5513531093,-2.2476329604,1.1495817364 C,0,-0.8268777312,-2.6714672751,0. H,0,-1.2435613455,-2.3906781875,-2.1719615003 H,0,-3.4284443029,-1.0895473346,-1.353070426 H,0,-3.4284443029,-1.0895473346,1.353070426 H,0,-1.2435613455,-2.3906781875,2.1719615003 H,0,0.1079935781,-3.2038792729,0. P,0,-1.7115965069,1.4556429343,0. C,0,-1.363457743,2.5440148038,1.4241286744 H,0,-1.6543771273,2.0479852632,2.3465824985 H,0,-0.3040819578,2.7670576949,1.4825664863 H,0,-1.9286411514,3.469606749,1.3208816934 C,0,-3.5445287521,1.524670944,0. H,0,-3.9510535834,1.0370870227,0.8818264063 H,0,-3.8704017073,2.5640039577,0. H,0,-3.9510535834,1.0370870227,-0.8818264063 C,0,-1.363457743,2.5440148038,-1.4241286744 H,0,-1.9286411514,3.469606749,-1.3208816934 H,0,-0.3040819578,2.7670576949,-1.4825664863 H,0,-1.6543771273,2.0479852632,-2.3465824985
CpCo(PMe_3)(C_4F_8) (**PMe_3-C_4F_8-7**) M06-L/cc-pVTZ Co,0,-1.7541792034,0.7586396871,-0.2029425088 C,0,2.2053282004,1.9236876815,-0.2833500043 C,0,1.744357274,-0.2155233213,-1.6019567695 C,0,-0.1960989755,1.2445403079,-0.8399465126 C,0,1.2104864518,0.7521268867,-0.5196300855 F,0,1.6357518743,0.3015552598,-2.8223903591 F,0,2.6696064455,2.4275035782,-1.4255583628 F,0,1.0452745258,-1.3524689904,-1.5684891532 F,0,3.0277543269,-0.5266103801,-1.3956170719 F,0,0.0350413345,2.2446485587,-1.773198644 F,0,1.2134511815,0.0320913723,0.6480742489 F,0,3.2481695429,1.5132723191,0.4367378958 F,0,1.6104410892,2.9069544281,0.3984253982 C,0,-3.4974439891,-0.2006788886,0.40731051 C,0,-2.6005487827,-1.1347858298,-0.1561914798 C,0,-1.4039202346,-1.088600028,0.6119664064 C,0,-1.5769459069,-0.1356719543,1.6524943432 C,0,-2.8696215704,0.4232497766,1.5246647958 H,0,-4.4875912988,0.0164003465,0.0424385983	CpCo(PMe_3)(C_4F_8) (**PMe_3-C_4F_8-8**) M06-L/cc-pVTZ Co,0,1.1079385448,-0.3515840665,0.167883085 C,0,-1.3799817645,-1.7768746506,-0.6307843986 C,0,-0.6377455614,-0.7933776599,0.217673619 C,0,-1.6302633181,-0.0570183526,1.084730454 C,0,-2.3870965901,1.1502309362,0.3917525493 F,0,-1.6606078525,-2.9400278089,0.0004763046 F,0,-0.7138313265,-2.127519891,-1.7576400949 F,0,-2.564836502,-1.2945786731,-1.068584274 F,0,-3.6635309488,0.8698856646,0.1760259493 F,0,-1.8271260246,1.4649269388,-0.7824556918 F,0,-2.335085379,2.2474203636,1.1567304904 F,0,-1.0391799774,0.4538371768,2.1963819268 F,0,-2.5999044632,-0.8933151481,1.5579569403 C,0,1.7260810102,0.9472818331,1.6956013211 C,0,2.8524254612,0.3337646944,1.1086502384 C,0,2.8544043537,0.6607099671,-0.2794789701 C,0,1.7198812427,1.4572985806,-0.5514642705 C,0,1.0181573467,1.631787668,0.6785742662 H,0,1.4252369175,0.8682577659,2.7259137337

H,0,-2.7872918978,-1.7630908768,-1.0104735316 H,0,-0.5188632968,-1.6734643485,0.4361584396 H,0,-0.8371346808,0.1332719843,2.3871344456 H,0,-3.307128195,1.174843883,2.1609710788 P,0,-2.7279251863,2.4444302736,-1.1714420971 C,0,-2.729762758,2.5193944137,-2.9979451507 H,0,-1.709634213,2.5177432481,-3.3676335294 H,0,-3.2406413148,3.4147931076,-3.3512263351 H,0,-3.2380923696,1.6435427685,-3.3944761559 C,0,-2.0958779362,4.0925797518,-0.6953449727 H,0,-1.0321705414,4.1561922261,-0.9017992545 H,0,-2.6170268228,4.8842125605,-1.2331084087 H,0,-2.2438956566,4.2347751941,0.3729021825 C,0,-4.513777382,2.6536860364,-0.8223138896 H,0,-4.8797308447,3.5845857213,-1.2540257219 H,0,-5.0814923465,1.8299660355,-1.2485305677 H,0,-4.6916938233,2.6723926906,0.2506165131	H,0,3.5857848303,-0.2670988766,1.6194509538 H,0,3.5835577485,0.3407814814,-1.0066937942 H,0,1.4284216467,1.8498520317,-1.5112554167 H,0,0.1129996693,2.1978339421,0.8118904974 P,0,1.9500240077,-2.2253983865,-0.6778767593 C,0,2.2304521673,-2.2853551545,-2.4850583715 H,0,2.8508480413,-1.4429240531,-2.7837932537 H,0,1.2863976628,-2.2163518165,-3.0148965833 H,0,2.7353163388,-3.2084805953,-2.7682413811 C,0,1.239056486,-3.8710981853,-0.3202550069 H,0,1.0474406388,-3.961283882,0.7461894441 H,0,1.9458963416,-4.643336219,-0.6209763716 H,0,0.3040252269,-4.0228820907,-0.8449799548 C,0,3.6552033747,-2.5273321123,-0.0686472778 H,0,4.3124723747,-1.6919430955,-0.2946642588 H,0,4.0635160519,-3.4246936956,-0.5322204922 H,0,3.642945124,-2.6701882605,1.0095096484
$CpCo(PMe_3)(C_4F_8)$ (**PMe_3-C_4F_8-9**) M06-L/cc-pVTZ Co,0,1.6189312387,-0.1413174967,0.5427728311 C,0,-3.6928269765,-0.2804719613,0.9533293965 C,0,-2.2510892049,0.1162141401,0.545521109 C,0,-1.1540766088,-0.1063290399,1.6221118497 C,0,0.1741637841,0.5459458434,1.2687960124 F,0,-2.2859163603,1.414417163,0.1963255731 F,0,-4.4783830279,-0.2281657948,-0.1231332368 F,0,-1.9334529947,-0.6081111334,-0.5467435763 F,0,-1.6436268756,0.3773641347,2.7957861651 F,0,-1.0175506821,-1.4441123282,1.7769416368 F,0,-0.0148728821,1.8609610699,1.6383452247 F,0,-4.180606506,0.5531017881,1.8632687316 F,0,-3.7283771016,-1.5183331854,1.4379950159 C,0,1.7850452786,-2.1530811171,0.9684027591 C,0,0.9892967883,-1.9486377234,-0.1912571009 C,0,1.7876968575,-1.2982851657,-1.1717952523 C,0,3.0674337136,-1.0986947537,-0.6070288296 C,0,3.0726010616,-1.6216139046,0.7176782833 H,0,1.4510721627,-2.605037372,1.8869265437 H,0,-0.0406294115,-2.2350195195,-0.3057667492 H,0,1.4748946695,-1.0103169942,-2.1611550785 H,0,3.8978598708,-0.6139092989,-1.0925974247 H,0,3.9084415642,-1.6207119086,1.3977103426 P,0,2.6768279597,1.7494828112,0.7359370952 C,0,2.0232157128,3.185609792,-0.186284564 H,0,2.6271182576,4.0744634942,-0.0054349576 H,0,0.998499055,3.3787434396,0.1144129196 H,0,2.0305507666,2.9642860511,-1.2509979741 C,0,4.4248946639,1.7573019486,0.1889183172 H,0,4.4858182113,1.5966156179,-0.884840039 H,0,4.9813178928,0.9651520267,0.6853121671 H,0,4.8928876229,2.7130785262,0.4219452875 C,0,2.854977167,2.4054900663,2.4329230496 H,0,3.4085661754,1.6905038035,3.03735499 H,0,3.3896582829,3.3549459128,2.4300300869 H,0,1.8762833048,2.5449063384,2.8800609354	

Table S5: Topological data at the bond critical points for the interactions between the cobalt atom and the C=C double bond in optimized lowest-energy structures of the CpCo(L)(C_3F_6) and CpCo(L)(C_4F_8) (L = CO, PMe_3) complexes at the M06-L/cc-pVTZ level of theory. All values are in a.u.

Structures	Bonds	ρ_r	$\nabla^2\rho_r$	G_r	V_r	H_r
CO-C_3F_6-1	Co–C^1	0.124	0.228	0.109	-0.162	-0.052
	Co–C^2	0.115	0.243	0.107	-0.153	-0.046
PMe_3-C_3F_6-1	Co–C^1	0.132	0.267	0.125	-0.183	-0.058
	Co–C^2	0.117	0.280	0.117	-0.164	-0.047
CO-C_4F_8-1	Co–C^1	0.123	0.212	0.105	-0.157	-0.052
	Co–C^2	0.101	0.261	0.102	-0.138	-0.036
PMe_3-C_4F_8-1	Co–C^1	0.133	0.248	0.121	-0.180	-0.059
	Co–C^2	0.100	0.304	0.111	-0.146	-0.035

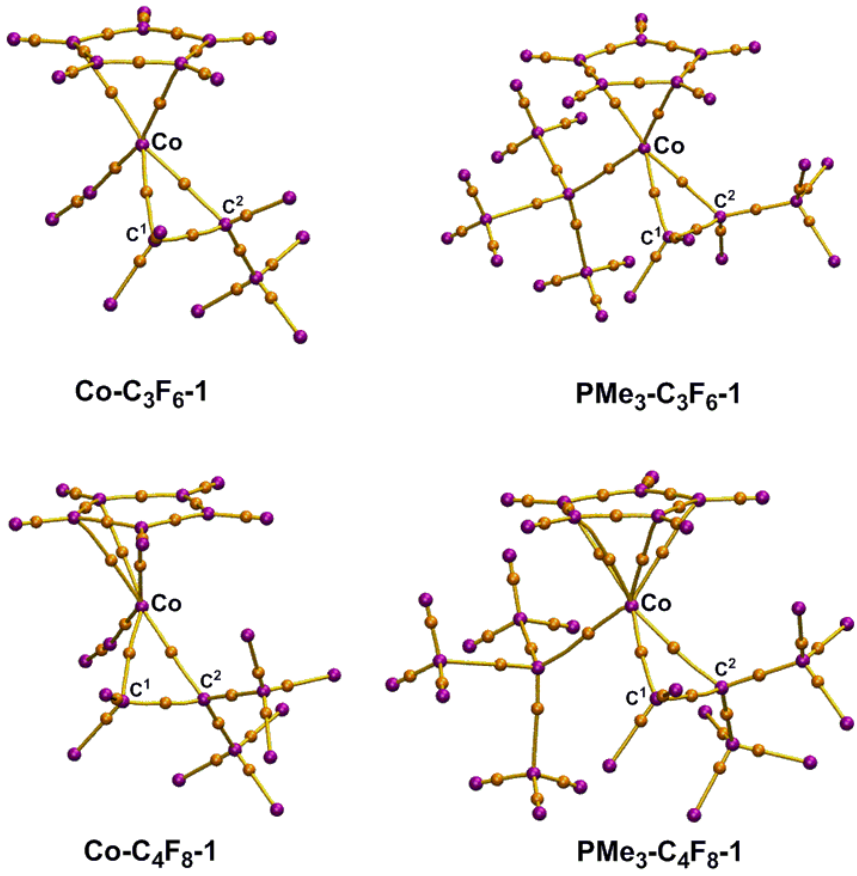

Figure S1: Bond paths for optimized lowest-energy structures of the CpCo(L)(C_3F_6) and CpCo(L)(C_4F_8) (L = CO, PMe_3) complexes at the M06-L/cc-pVTZ level of theory. Orange dots are bond critical points.

Complete Gaussian 09 reference

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