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Supporting Information

Cyclopentadienone-like Behavior of Fluorenone and 4,5-Diazafluoren-9-one

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Table 1. Crystal data and structure refinement for compound 4.

Identification code	schepp24
Measurement device	Nonius KappaCCD
Empirical formula	C23 H23 Co O
Formula weight	374.34
Temperature	100(2) K
Wavelength	0.71073 A
Crystal system, space group	Triclinic P 21/c
Unit cell dimensions	a = 6.9000(4) A alpha = 90 deg. b = 15.5450(14) A beta = 94.207(6) deg. c = 15.9470(14) A gamma = 90 deg.
Volume	1705.9(2) A^3
Z, Calculated density	4, 1.458 Mg/m^3
Absorption coefficient	1.013 mm^-1
F(000)	784
Crystal size, colour and habit	0.3 x 0.2 x 0.09 mm^3, black needle
Theta range for data collection	3.24 to 30.00 deg.
Index ranges	-9<=h<=9, -21<=k<=21, -22<=l<=22
Reflections collected / unique	40774 / 4977 [R(int) = 0.0379]
Completeness to theta = 30.00	99.8%
Absorption correction	multi-scan (Sadabs)
Max. and min. transmission	1.000000 and 0.653717
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4977 / 0 / 236
Goodness-of-fit on F^2	1.041
Final R indices [I>2sigma(I)]	R1 = 0.0298, wR2 = 0.0653 [4105]
R indices (all data)	R1 = 0.0434, wR2 = 0.0718
Largest diff. peak and hole	0.405 and -0.316 e.A^-3
remarks	Disorder of Co(1):Co(1A) (97:3). The resulting small changes of the C- and O-coordinates cannot be determined because of the small percentage of the disorder. Thus the bond lengths and angles at Co(1A) are unreliable.

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for compound 4.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Co(1)	1026(1)	2293(1)	1452(1)	13(1)
Co(1A)	-3660(3)	2300(12)	1458(11)	94(7)
O(1)	3724(2)	2906(1)	3044(1)	30(1)
C(1)	3608(2)	2686(1)	2290(1)	21(1)
C(2)	3714(2)	1815(1)	1935(1)	21(1)
C(3)	4035(2)	1006(1)	2344(1)	29(1)
C(4)	4146(2)	287(1)	1867(1)	34(1)
C(5)	3940(2)	320(1)	973(1)	31(1)
C(6)	3657(2)	1077(1)	552(1)	24(1)
C(7)	3548(2)	1845(1)	1030(1)	19(1)
C(8)	3248(2)	2732(1)	785(1)	16(1)
C(9)	3042(2)	3140(1)	-17(1)	19(1)
C(10)	2792(2)	4010(1)	-40(1)	22(1)
C(11)	2725(2)	4507(1)	709(1)	24(1)
C(12)	2906(2)	4135(1)	1483(1)	22(1)
C(13)	3205(2)	3231(1)	1543(1)	18(1)
C(14)	-1041(2)	1817(1)	2181(1)	17(1)
C(15)	-1167(2)	1397(1)	1370(1)	16(1)
C(16)	-1548(2)	2033(1)	742(1)	17(1)
C(17)	-1606(2)	2847(1)	1157(1)	18(1)
C(18)	-1320(2)	2708(1)	2051(1)	17(1)
C(19)	-675(2)	1387(1)	3013(1)	23(1)
C(20)	-950(2)	451(1)	1236(1)	21(1)
C(21)	-1794(2)	1902(1)	-187(1)	23(1)
C(22)	-1964(2)	3692(1)	733(1)	25(1)
C(23)	-1258(2)	3381(1)	2719(1)	25(1)

Table 3. Bond lengths [A] and angles [deg] for compound 4.

Co(1)-C(17)	2.0326(14)
Co(1)-C(7)	2.0335(14)
Co(1)-C(18)	2.0427(14)
Co(1)-C(14)	2.0442(14)
Co(1)-C(8)	2.0468(14)
Co(1)-C(15)	2.0555(14)
Co(1)-C(16)	2.0744(14)
Co(1)-C(2)	2.0916(14)
Co(1)-C(13)	2.0918(14)
Co(1)-C(1)	2.2326(14)
Co(1A)-C(17)	1.751(19)
Co(1A)-C(18)	1.918(19)
Co(1A)-C(16)	1.960(19)
Co(1A)-C(7)#1	2.118(19)
Co(1A)-C(2)#1	2.153(19)
Co(1A)-C(14)	2.202(19)
Co(1A)-C(15)	2.231(19)
Co(1A)-C(8)#1	2.413(19)
Co(1A)-C(1)#1	2.457(19)
O(1)-C(1)	1.2466(18)
C(1)-C(2)	1.471(2)
C(1)-C(13)	1.4723(19)
C(1)-Co(1A)#2	2.457(19)
C(2)-C(3)	1.427(2)
C(2)-C(7)	1.440(2)
C(2)-Co(1A)#2	2.153(19)
C(3)-C(4)	1.356(3)
C(4)-C(5)	1.424(3)
C(5)-C(6)	1.361(2)
C(6)-C(7)	1.422(2)
C(7)-C(8)	1.4434(19)
C(7)-Co(1A)#2	2.118(19)
C(8)-C(9)	1.4268(19)
C(8)-C(13)	1.4372(19)
C(8)-Co(1A)#2	2.413(19)
C(9)-C(10)	1.363(2)
C(10)-C(11)	1.424(2)
C(11)-C(12)	1.361(2)
C(12)-C(13)	1.423(2)
C(14)-C(18)	1.4121(19)
C(14)-C(15)	1.4444(19)
C(14)-C(19)	1.4925(19)
C(15)-C(16)	1.4198(19)
C(15)-C(20)	1.4942(19)
C(16)-C(17)	1.427(2)
C(16)-C(21)	1.4936(19)
C(17)-C(18)	1.4416(19)
C(17)-C(22)	1.4911(19)
C(18)-C(23)	1.4897(19)
C(17)-Co(1)-C(7)	147.07(6)
C(17)-Co(1)-C(18)	41.43(5)
C(7)-Co(1)-C(18)	171.46(6)
C(17)-Co(1)-C(14)	68.69(6)
C(7)-Co(1)-C(14)	135.54(6)
C(18)-Co(1)-C(14)	40.43(5)
C(17)-Co(1)-C(8)	115.40(6)
C(7)-Co(1)-C(8)	41.43(5)
C(18)-Co(1)-C(8)	141.94(5)
C(14)-Co(1)-C(8)	175.75(5)
C(17)-Co(1)-C(15)	68.35(5)
C(7)-Co(1)-C(15)	113.03(6)

C(18)-Co(1)-C(15)	68.79(6)
C(14)-Co(1)-C(15)	41.26(5)
C(8)-Co(1)-C(15)	140.36(5)
C(17)-Co(1)-C(16)	40.65(6)
C(7)-Co(1)-C(16)	118.18(6)
C(18)-Co(1)-C(16)	68.92(6)
C(14)-Co(1)-C(16)	68.55(5)
C(8)-Co(1)-C(16)	115.19(5)
C(15)-Co(1)-C(16)	40.21(5)
C(17)-Co(1)-C(2)	171.25(6)
C(7)-Co(1)-C(2)	40.82(6)
C(18)-Co(1)-C(2)	130.65(6)
C(14)-Co(1)-C(2)	107.37(6)
C(8)-Co(1)-C(2)	68.42(6)
C(15)-Co(1)-C(2)	114.27(6)
C(16)-Co(1)-C(2)	146.31(6)
C(17)-Co(1)-C(13)	110.29(6)
C(7)-Co(1)-C(13)	68.45(6)
C(18)-Co(1)-C(13)	109.78(6)
C(14)-Co(1)-C(13)	137.89(5)
C(8)-Co(1)-C(13)	40.62(5)
C(15)-Co(1)-C(13)	178.49(6)
C(16)-Co(1)-C(13)	139.09(5)
C(2)-Co(1)-C(13)	66.97(6)
C(17)-Co(1)-C(1)	133.11(6)
C(7)-Co(1)-C(1)	68.08(6)
C(18)-Co(1)-C(1)	105.01(6)
C(14)-Co(1)-C(1)	108.58(5)
C(8)-Co(1)-C(1)	67.93(5)
C(15)-Co(1)-C(1)	140.82(5)
C(16)-Co(1)-C(1)	173.51(6)
C(2)-Co(1)-C(1)	39.62(6)
C(13)-Co(1)-C(1)	39.64(5)
C(17)-Co(1A)-C(18)	46.0(5)
C(17)-Co(1A)-C(16)	44.8(5)
C(18)-Co(1A)-C(16)	73.9(7)
C(17)-Co(1A)-C(7)#1	144.0(10)
C(18)-Co(1A)-C(7)#1	169.2(10)
C(16)-Co(1A)-C(7)#1	116.1(9)
C(17)-Co(1A)-C(2)#1	170.8(11)
C(18)-Co(1A)-C(2)#1	130.0(9)
C(16)-Co(1A)-C(2)#1	144.4(10)
C(7)#1-Co(1A)-C(2)#1	39.4(3)
C(17)-Co(1A)-C(14)	70.1(7)
C(18)-Co(1A)-C(14)	39.3(4)
C(16)-Co(1A)-C(14)	67.5(6)
C(7)#1-Co(1A)-C(14)	138.3(9)
C(2)#1-Co(1A)-C(14)	112.1(8)
C(17)-Co(1A)-C(15)	69.2(6)
C(18)-Co(1A)-C(15)	67.3(6)
C(16)-Co(1A)-C(15)	38.9(4)
C(7)#1-Co(1A)-C(15)	117.2(8)
C(2)#1-Co(1A)-C(15)	118.3(8)
C(14)-Co(1A)-C(15)	38.0(3)
C(17)-Co(1A)-C(8)#1	116.7(9)
C(18)-Co(1A)-C(8)#1	144.3(10)
C(16)-Co(1A)-C(8)#1	118.0(8)
C(7)#1-Co(1A)-C(8)#1	36.4(3)
C(2)#1-Co(1A)-C(8)#1	61.0(5)
C(14)-Co(1A)-C(8)#1	173.0(9)
C(15)-Co(1A)-C(8)#1	143.8(9)
C(17)-Co(1A)-C(1)#1	134.3(10)
C(18)-Co(1A)-C(1)#1	107.7(8)
C(16)-Co(1A)-C(1)#1	176.7(10)
C(7)#1-Co(1A)-C(1)#1	62.6(5)
C(2)#1-Co(1A)-C(1)#1	36.5(3)

C(14)-Co(1A)-C(1)#1	115.7(8)
C(15)-Co(1A)-C(1)#1	144.3(9)
C(8)#1-Co(1A)-C(1)#1	58.9(4)
O(1)-C(1)-C(2)	128.37(14)
O(1)-C(1)-C(13)	128.26(14)
C(2)-C(1)-C(13)	103.27(12)
O(1)-C(1)-Co(1)	130.10(11)
C(2)-C(1)-Co(1)	65.02(8)
C(13)-C(1)-Co(1)	65.01(7)
O(1)-C(1)-Co(1A)#2	126.1(5)
C(2)-C(1)-Co(1A)#2	60.4(4)
C(13)-C(1)-Co(1A)#2	79.1(4)
Co(1)-C(1)-Co(1A)#2	102.7(4)
C(3)-C(2)-C(7)	119.10(14)
C(3)-C(2)-C(1)	130.19(15)
C(7)-C(2)-C(1)	110.63(12)
C(3)-C(2)-Co(1)	125.83(11)
C(7)-C(2)-Co(1)	67.42(8)
C(1)-C(2)-Co(1)	75.36(8)
C(3)-C(2)-Co(1A)#2	111.4(5)
C(7)-C(2)-Co(1A)#2	69.0(5)
C(1)-C(2)-Co(1A)#2	83.1(5)
Co(1)-C(2)-Co(1A)#2	119.5(5)
C(4)-C(3)-C(2)	118.86(16)
C(3)-C(4)-C(5)	121.70(15)
C(6)-C(5)-C(4)	121.76(16)
C(5)-C(6)-C(7)	118.18(16)
C(6)-C(7)-C(2)	120.38(13)
C(6)-C(7)-C(8)	131.97(14)
C(2)-C(7)-C(8)	107.64(12)
C(6)-C(7)-Co(1)	122.97(10)
C(2)-C(7)-Co(1)	71.76(8)
C(8)-C(7)-Co(1)	69.78(8)
C(6)-C(7)-Co(1A)#2	111.8(5)
C(2)-C(7)-Co(1A)#2	71.6(5)
C(8)-C(7)-Co(1A)#2	83.0(5)
Co(1)-C(7)-Co(1A)#2	124.0(5)
C(9)-C(8)-C(13)	120.48(12)
C(9)-C(8)-C(7)	132.17(13)
C(13)-C(8)-C(7)	107.34(12)
C(9)-C(8)-Co(1)	125.86(10)
C(13)-C(8)-Co(1)	71.37(8)
C(7)-C(8)-Co(1)	68.79(8)
C(9)-C(8)-Co(1A)#2	123.4(5)
C(13)-C(8)-Co(1A)#2	81.3(4)
C(7)-C(8)-Co(1A)#2	60.6(4)
Co(1)-C(8)-Co(1A)#2	110.3(4)
C(10)-C(9)-C(8)	117.99(13)
C(9)-C(10)-C(11)	121.82(14)
C(12)-C(11)-C(10)	121.55(14)
C(11)-C(12)-C(13)	118.97(13)
C(12)-C(13)-C(8)	119.18(12)
C(12)-C(13)-C(1)	129.86(13)
C(8)-C(13)-C(1)	110.86(12)
C(12)-C(13)-Co(1)	125.75(11)
C(8)-C(13)-Co(1)	68.01(8)
C(1)-C(13)-Co(1)	75.34(8)
C(18)-C(14)-C(15)	108.28(12)
C(18)-C(14)-C(19)	125.68(13)
C(15)-C(14)-C(19)	126.04(13)
C(18)-C(14)-Co(1)	69.73(8)
C(15)-C(14)-Co(1)	69.79(8)
C(19)-C(14)-Co(1)	126.09(10)
C(18)-C(14)-Co(1A)	59.4(5)
C(15)-C(14)-Co(1A)	72.1(5)
C(19)-C(14)-Co(1A)	134.2(5)

Co(1)-C(14)-Co(1A)	99.1(5)
C(16)-C(15)-C(14)	108.15(12)
C(16)-C(15)-C(20)	126.91(13)
C(14)-C(15)-C(20)	124.93(12)
C(16)-C(15)-Co(1)	70.61(8)
C(14)-C(15)-Co(1)	68.95(8)
C(20)-C(15)-Co(1)	126.55(10)
C(16)-C(15)-Co(1A)	60.1(5)
C(14)-C(15)-Co(1A)	69.9(5)
C(20)-C(15)-Co(1A)	135.5(5)
Co(1)-C(15)-Co(1A)	97.8(5)
C(15)-C(16)-C(17)	107.53(12)
C(15)-C(16)-C(21)	127.39(13)
C(17)-C(16)-C(21)	125.06(13)
C(15)-C(16)-Co(1A)	80.9(5)
C(17)-C(16)-Co(1A)	59.8(6)
C(21)-C(16)-Co(1A)	124.9(6)
C(15)-C(16)-Co(1)	69.18(8)
C(17)-C(16)-Co(1)	68.10(8)
C(21)-C(16)-Co(1)	126.76(10)
Co(1A)-C(16)-Co(1)	106.5(5)
C(16)-C(17)-C(18)	108.60(12)
C(16)-C(17)-C(22)	125.44(13)
C(18)-C(17)-C(22)	125.94(13)
C(16)-C(17)-Co(1A)	75.4(6)
C(18)-C(17)-Co(1A)	73.1(6)
C(22)-C(17)-Co(1A)	116.3(6)
C(16)-C(17)-Co(1)	71.25(8)
C(18)-C(17)-Co(1)	69.66(8)
C(22)-C(17)-Co(1)	126.38(11)
Co(1A)-C(17)-Co(1)	117.3(6)
C(14)-C(18)-C(17)	107.40(12)
C(14)-C(18)-C(23)	125.90(13)
C(17)-C(18)-C(23)	126.66(13)
C(14)-C(18)-Co(1A)	81.2(6)
C(17)-C(18)-Co(1A)	60.9(6)
C(23)-C(18)-Co(1A)	124.3(6)
C(14)-C(18)-Co(1)	69.85(8)
C(17)-C(18)-Co(1)	68.91(8)
C(23)-C(18)-Co(1)	124.93(11)
Co(1A)-C(18)-Co(1)	109.4(6)

Symmetry transformations used to generate equivalent atoms:
#1 x-1,y,z #2 x+1,y,z

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Table 4. Anisotropic displacement parameters (A^2 x 10^3) for compound 4.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Co(1)	15(1)	12(1)	12(1)	2(1)	1(1)	1(1)
O(1)	34(1)	40(1)	16(1)	2(1)	-4(1)	-6(1)
C(1)	20(1)	25(1)	18(1)	5(1)	-3(1)	-4(1)
C(2)	15(1)	21(1)	26(1)	7(1)	-1(1)	-1(1)
C(3)	18(1)	29(1)	39(1)	17(1)	-3(1)	-1(1)
C(4)	17(1)	21(1)	61(1)	16(1)	0(1)	2(1)
C(5)	19(1)	17(1)	57(1)	-1(1)	5(1)	2(1)
C(6)	18(1)	19(1)	38(1)	-4(1)	7(1)	1(1)
C(7)	16(1)	15(1)	25(1)	2(1)	3(1)	0(1)
C(8)	17(1)	14(1)	16(1)	-1(1)	2(1)	-1(1)
C(9)	21(1)	21(1)	15(1)	0(1)	2(1)	-3(1)
C(10)	26(1)	22(1)	19(1)	5(1)	-1(1)	-2(1)
C(11)	29(1)	14(1)	28(1)	2(1)	0(1)	0(1)
C(12)	26(1)	18(1)	21(1)	-4(1)	0(1)	-2(1)
C(13)	20(1)	18(1)	15(1)	0(1)	-1(1)	-2(1)
C(14)	18(1)	17(1)	14(1)	2(1)	1(1)	-1(1)
C(15)	17(1)	16(1)	16(1)	1(1)	1(1)	0(1)
C(16)	16(1)	19(1)	14(1)	2(1)	0(1)	0(1)
C(17)	18(1)	17(1)	17(1)	4(1)	2(1)	2(1)
C(18)	20(1)	16(1)	16(1)	-1(1)	3(1)	1(1)
C(19)	29(1)	25(1)	16(1)	6(1)	1(1)	-2(1)
C(20)	22(1)	16(1)	24(1)	-1(1)	2(1)	-1(1)
C(21)	26(1)	30(1)	14(1)	1(1)	0(1)	-3(1)
C(22)	26(1)	20(1)	28(1)	8(1)	2(1)	5(1)
C(23)	34(1)	21(1)	22(1)	-7(1)	7(1)	0(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for compound 4.

	x	y	z	U(eq)
H(3)	4170	972	2940	35
H(4)	4366	-252	2137	40
H(5)	4003	-199	662	37
H(6)	3534	1090	-45	29
H(9)	3078	2815	-521	23
H(10)	2659	4292	-569	27
H(11)	2550	5112	666	28
H(12)	2834	4474	1976	26
H(19A)	229	1735	3374	35
H(19B)	-109	817	2933	35
H(19C)	-1903	1326	3279	35
H(20A)	-2071	150	1439	31
H(20B)	243	248	1545	31
H(20C)	-879	335	635	31
H(21A)	-1242	1345	-331	35
H(21B)	-1122	2362	-469	35
H(21C)	-3180	1914	-372	35
H(22A)	-1352	3695	197	37
H(22B)	-1408	4153	1094	37
H(22C)	-3366	3784	628	37
H(23A)	-2432	3342	3027	38
H(23B)	-1193	3951	2461	38
H(23C)	-109	3292	3108	38

Table 6. Crystal data and structure refinement for compound 5.

Identification code	schepp11
Measurement device	Nonius KappaCCD
Empirical formula	C21 H21 Co N2 O x 6H2O
Formula weight	484.42
Temperature	100(2) K
Wavelength	0.71073 A
Crystal system, space group	Orthorhombic P m n 21
Unit cell dimensions	a = 18.76700(10) A alpha = 90 deg. b = 9.11100(10) A beta = 90 deg. c = 6.7660(2) A gamma = 90 deg.
Volume	1156.89(4) A^3
Z, Calculated density	2, 1.391 Mg/m^3
Absorption coefficient	0.785 mm^-1
F(000)	512
Crystal size, colour and habit	0.30 x 0.22 x 0.10 mm^3, dark-brown needles
Theta range for data collection	3.20 to 29.98 deg.
Index ranges	-26<=h<=26, -12<=k<=12, -9<=l<=9
Reflections collected / unique	17475 / 3229 [R(int) = 0.033]
Completeness to theta = 29.98	98.9%
Absorption correction	Multi-Scan
Max. and min. transmission	0.9257 and 0.7987
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3229 / 1 / 183
Goodness-of-fit on F^2	1.048
Final R indices [I>2sigma(I)]	R1 = 0.0258, wR2 = 0.0654 [3097]
R indices (all data)	R1 = 0.0274, wR2 = 0.0663
Absolute structure parameter	0.530(12)
Largest diff. peak and hole	0.335 and -0.323 e.A^-3
remarks	disorder Co(1): Co(1a) 95:5 H(12A)-H(12C) disorder caused by symmetry (50:50).

Table 7. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for compound 5.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Co(1)	0	1404(1)	3581(1)	14(1)
Co(1A)	0	1406(5)	-1216(17)	18(2)
O(1)	0	4365(1)	1191(3)	25(1)
N(1)	850(1)	-688(1)	988(2)	17(1)
C(1)	384(1)	478(1)	1064(2)	14(1)
C(2)	616(1)	1988(1)	1153(2)	16(1)
C(3)	1359(1)	2289(1)	1171(2)	20(1)
C(4)	1813(1)	1118(2)	1082(3)	22(1)
C(5)	1531(1)	-347(1)	1003(3)	21(1)
C(6)	0	2966(2)	1160(3)	17(1)
C(7)	377(1)	2425(2)	6083(3)	26(1)
C(8)	610(1)	915(2)	6011(3)	27(1)
C(9)	0	-3(2)	6004(4)	26(1)
C(10)	843(1)	3754(2)	6133(4)	49(1)
C(11)	1367(1)	392(3)	5951(3)	50(1)
C(12)	0	-1660(3)	5975(5)	51(1)
O(2)	3937(1)	3707(1)	-3752(2)	24(1)
O(3)	2821(1)	3769(1)	-6483(4)	35(1)
O(4)	2940(1)	3675(2)	-594(2)	35(1)

Table 8. Bond lengths [A] and angles [deg] for compound 5.

Co(1)-C(1)#1	2.0319(15)
Co(1)-C(1)	2.0319(15)
Co(1)-C(8)	2.0526(17)
Co(1)-C(8)#1	2.0526(17)
Co(1)-C(7)	2.0574(16)
Co(1)-C(7)#1	2.0574(16)
Co(1)-C(2)#1	2.0783(15)
Co(1)-C(2)	2.0783(15)
Co(1)-C(9)	2.081(2)
Co(1)-C(6)	2.170(2)
Co(1A)-C(1)#1	1.901(10)
Co(1A)-C(1)	1.901(10)
Co(1A)-C(2)	2.047(9)
Co(1A)-C(2)#1	2.047(9)
Co(1A)-C(6)	2.146(10)
Co(1A)-C(7)#2	2.169(10)
Co(1A)-C(7)#3	2.169(10)
Co(1A)-C(8)#2	2.243(10)
Co(1A)-C(8)#3	2.243(10)
Co(1A)-C(9)#3	2.277(11)
O(1)-C(6)	1.275(2)
N(1)-C(5)	1.3142(17)
N(1)-C(1)	1.3776(15)
C(1)-C(1)#1	1.441(2)
C(1)-C(2)	1.4441(16)
C(2)-C(3)	1.4203(17)
C(2)-C(6)	1.4602(17)
C(3)-C(4)	1.3667(18)
C(3)-H(3)	0.9500
C(4)-C(5)	1.4368(17)
C(4)-H(4)	0.9500
C(5)-H(5)	0.9500
C(6)-C(2)#1	1.4602(17)
C(7)-C(7)#1	1.416(3)
C(7)-C(8)	1.444(2)
C(7)-C(10)	1.494(2)
C(7)-Co(1A)#4	2.169(10)
C(8)-C(9)	1.418(2)
C(8)-C(11)	1.498(2)
C(8)-Co(1A)#4	2.243(10)
C(9)-C(8)#1	1.418(2)
C(9)-C(12)	1.511(3)
C(9)-Co(1A)#4	2.277(11)
C(10)-H(10A)	0.9800
C(10)-H(10B)	0.9800
C(10)-H(10C)	0.9800
C(11)-H(11A)	0.9800
C(11)-H(11B)	0.9800
C(11)-H(11C)	0.9800
C(12)-H(12A)	0.9800
C(12)-H(12B)	0.9800
C(12)-H(12C)	0.9800
O(2)-H(2A)	0.84(2)
O(2)-H(2B)	0.78(2)
O(3)-H(3A)	0.82(6)
O(3)-H(3B)	0.78(3)
O(4)-H(4A)	0.88(2)
O(4)-H(4B)	0.85(4)
C(1)#1-Co(1)-C(1)	41.53(7)
C(1)#1-Co(1)-C(8)	141.17(6)
C(1)-Co(1)-C(8)	112.54(6)

C(1)#1-Co(1)-C(8)#1	112.54(6)
C(1)-Co(1)-C(8)#1	141.17(6)
C(8)-Co(1)-C(8)#1	67.82(10)
C(1)#1-Co(1)-C(7)	177.62(6)
C(1)-Co(1)-C(7)	139.03(6)
C(8)-Co(1)-C(7)	41.15(6)
C(8)#1-Co(1)-C(7)	68.35(7)
C(1)#1-Co(1)-C(7)#1	139.03(6)
C(1)-Co(1)-C(7)#1	177.62(6)
C(8)-Co(1)-C(7)#1	68.35(7)
C(8)#1-Co(1)-C(7)#1	41.15(6)
C(7)-Co(1)-C(7)#1	40.26(10)
C(1)#1-Co(1)-C(2)#1	41.12(5)
C(1)-Co(1)-C(2)#1	68.98(6)
C(8)-Co(1)-C(2)#1	177.68(7)
C(8)#1-Co(1)-C(2)#1	112.21(6)
C(7)-Co(1)-C(2)#1	136.56(6)
C(7)#1-Co(1)-C(2)#1	110.06(5)
C(1)#1-Co(1)-C(2)	68.98(6)
C(1)-Co(1)-C(2)	41.12(5)
C(8)-Co(1)-C(2)	112.21(6)
C(8)#1-Co(1)-C(2)	177.68(7)
C(7)-Co(1)-C(2)	110.06(5)
C(7)#1-Co(1)-C(2)	136.56(6)
C(2)#1-Co(1)-C(2)	67.65(8)
C(1)#1-Co(1)-C(9)	113.88(7)
C(1)-Co(1)-C(9)	113.88(7)
C(8)-Co(1)-C(9)	40.11(6)
C(8)#1-Co(1)-C(9)	40.11(6)
C(7)-Co(1)-C(9)	68.29(7)
C(7)#1-Co(1)-C(9)	68.29(7)
C(2)#1-Co(1)-C(9)	141.30(5)
C(2)-Co(1)-C(9)	141.30(5)
C(1)#1-Co(1)-C(6)	68.87(6)
C(1)-Co(1)-C(6)	68.87(6)
C(8)-Co(1)-C(6)	138.33(6)
C(8)#1-Co(1)-C(6)	138.33(6)
C(7)-Co(1)-C(6)	108.94(7)
C(7)#1-Co(1)-C(6)	108.94(7)
C(2)#1-Co(1)-C(6)	40.13(5)
C(2)-Co(1)-C(6)	40.13(5)
C(9)-Co(1)-C(6)	177.02(9)
C(1)#1-Co(1A)-C(1)	44.5(2)
C(1)#1-Co(1A)-C(2)	72.2(4)
C(1)-Co(1A)-C(2)	42.7(2)
C(1)#1-Co(1A)-C(2)#1	42.7(2)
C(1)-Co(1A)-C(2)#1	72.2(4)
C(2)-Co(1A)-C(2)#1	68.8(4)
C(1)#1-Co(1A)-C(6)	71.7(4)
C(1)-Co(1A)-C(6)	71.7(4)
C(2)-Co(1A)-C(6)	40.68(19)
C(2)#1-Co(1A)-C(6)	40.68(19)
C(1)#1-Co(1A)-C(7)#2	138.64(7)
C(1)-Co(1A)-C(7)#2	176.4(3)
C(2)-Co(1A)-C(7)#2	137.2(2)
C(2)#1-Co(1A)-C(7)#2	111.38(14)
C(6)-Co(1A)-C(7)#2	110.4(2)
C(1)#1-Co(1A)-C(7)#3	176.4(3)
C(1)-Co(1A)-C(7)#3	138.64(7)
C(2)-Co(1A)-C(7)#3	111.38(14)
C(2)#1-Co(1A)-C(7)#3	137.2(2)
C(6)-Co(1A)-C(7)#3	110.4(2)
C(7)#2-Co(1A)-C(7)#3	38.1(2)
C(1)#1-Co(1A)-C(8)#2	113.38(14)
C(1)-Co(1A)-C(8)#2	141.6(3)
C(2)-Co(1A)-C(8)#2	174.4(4)

C(2)#1-Co(1A)-C(8)#2	114.72(7)
C(6)-Co(1A)-C(8)#2	139.35(18)
C(7)#2-Co(1A)-C(8)#2	38.17(18)
C(7)#3-Co(1A)-C(8)#2	63.1(3)
C(1)#1-Co(1A)-C(8)#3	141.6(3)
C(1)-Co(1A)-C(8)#3	113.38(14)
C(2)-Co(1A)-C(8)#3	114.72(7)
C(2)#1-Co(1A)-C(8)#3	174.4(4)
C(6)-Co(1A)-C(8)#3	139.35(18)
C(7)#2-Co(1A)-C(8)#3	63.1(3)
C(7)#3-Co(1A)-C(8)#3	38.17(18)
C(8)#2-Co(1A)-C(8)#3	61.4(3)
C(1)#1-Co(1A)-C(9)#3	114.8(2)
C(1)-Co(1A)-C(9)#3	114.8(2)
C(2)-Co(1A)-C(9)#3	142.47(13)
C(2)#1-Co(1A)-C(9)#3	142.47(13)
C(6)-Co(1A)-C(9)#3	172.8(4)
C(7)#2-Co(1A)-C(9)#3	62.9(3)
C(7)#3-Co(1A)-C(9)#3	62.9(3)
C(8)#2-Co(1A)-C(9)#3	36.55(18)
C(8)#3-Co(1A)-C(9)#3	36.55(18)
C(5)-N(1)-C(1)	115.79(11)
N(1)-C(1)-C(1)#1	129.44(7)
N(1)-C(1)-C(2)	122.96(12)
C(1)#1-C(1)-C(2)	107.59(7)
N(1)-C(1)-Co(1A)	123.6(2)
C(1)#1-C(1)-Co(1A)	67.73(12)
C(2)-C(1)-Co(1A)	74.04(18)
N(1)-C(1)-Co(1)	125.22(11)
C(1)#1-C(1)-Co(1)	69.24(4)
C(2)-C(1)-Co(1)	71.16(8)
Co(1A)-C(1)-Co(1)	111.2(2)
C(3)-C(2)-C(1)	118.76(12)
C(3)-C(2)-C(6)	131.24(11)
C(1)-C(2)-C(6)	109.98(11)
C(3)-C(2)-Co(1A)	127.7(2)
C(1)-C(2)-Co(1A)	63.24(18)
C(6)-C(2)-Co(1A)	73.31(16)
C(3)-C(2)-Co(1)	126.08(12)
C(1)-C(2)-Co(1)	67.72(7)
C(6)-C(2)-Co(1)	73.31(10)
Co(1A)-C(2)-Co(1)	103.8(2)
C(4)-C(3)-C(2)	117.36(11)
C(4)-C(3)-H(3)	121.3
C(2)-C(3)-H(3)	121.3
C(3)-C(4)-C(5)	119.88(12)
C(3)-C(4)-H(4)	120.1
C(5)-C(4)-H(4)	120.1
N(1)-C(5)-C(4)	125.25(12)
N(1)-C(5)-H(5)	117.4
C(4)-C(5)-H(5)	117.4
O(1)-C(6)-C(2)#1	127.60(7)
O(1)-C(6)-C(2)	127.60(7)
C(2)#1-C(6)-C(2)	104.80(15)
O(1)-C(6)-Co(1A)	132.4(3)
C(2)#1-C(6)-Co(1A)	66.01(14)
C(2)-C(6)-Co(1A)	66.01(14)
O(1)-C(6)-Co(1)	130.03(17)
C(2)#1-C(6)-Co(1)	66.56(9)
C(2)-C(6)-Co(1)	66.56(9)
Co(1A)-C(6)-Co(1)	97.5(2)
C(7)#1-C(7)-C(8)	107.62(9)
C(7)#1-C(7)-C(10)	125.80(13)
C(8)-C(7)-C(10)	126.58(18)
C(7)#1-C(7)-Co(1)	69.87(5)
C(8)-C(7)-Co(1)	69.25(9)

C(10)-C(7)-Co(1)	125.92(14)
C(7)#1-C(7)-Co(1A)#4	70.94(10)
C(8)-C(7)-Co(1A)#4	73.71(17)
C(10)-C(7)-Co(1A)#4	121.3(2)
Co(1)-C(7)-Co(1A)#4	112.8(2)
C(9)-C(8)-C(7)	108.49(13)
C(9)-C(8)-C(11)	125.32(18)
C(7)-C(8)-C(11)	126.19(18)
C(9)-C(8)-Co(1)	71.02(11)
C(7)-C(8)-Co(1)	69.60(9)
C(11)-C(8)-Co(1)	125.19(14)
C(9)-C(8)-Co(1A)#4	73.02(17)
C(7)-C(8)-Co(1A)#4	68.12(17)
C(11)-C(8)-Co(1A)#4	124.7(2)
Co(1)-C(8)-Co(1A)#4	109.99(18)
C(8)-C(9)-C(8)#1	107.75(19)
C(8)-C(9)-C(12)	126.12(9)
C(8)#1-C(9)-C(12)	126.12(9)
C(8)-C(9)-Co(1)	68.87(11)
C(8)#1-C(9)-Co(1)	68.87(11)
C(12)-C(9)-Co(1)	127.27(19)
C(8)-C(9)-Co(1A)#4	70.43(14)
C(8)#1-C(9)-Co(1A)#4	70.43(14)
C(12)-C(9)-Co(1A)#4	125.0(3)
Co(1)-C(9)-Co(1A)#4	107.7(2)
C(7)-C(10)-H(10A)	109.5
C(7)-C(10)-H(10B)	109.5
H(10A)-C(10)-H(10B)	109.5
C(7)-C(10)-H(10C)	109.5
H(10A)-C(10)-H(10C)	109.5
H(10B)-C(10)-H(10C)	109.5
C(8)-C(11)-H(11A)	109.5
C(8)-C(11)-H(11B)	109.5
H(11A)-C(11)-H(11B)	109.5
C(8)-C(11)-H(11C)	109.5
H(11A)-C(11)-H(11C)	109.5
H(11B)-C(11)-H(11C)	109.5
C(9)-C(12)-H(12A)	109.5
C(9)-C(12)-H(12B)	109.5
H(12A)-C(12)-H(12B)	109.5
C(9)-C(12)-H(12C)	109.5
H(12A)-C(12)-H(12C)	109.5
H(12B)-C(12)-H(12C)	109.5
H(2A)-O(2)-H(2B)	107(2)
H(3A)-O(3)-H(3B)	92(5)
H(4A)-O(4)-H(4B)	95(2)

Symmetry transformations used to generate equivalent atoms:
#1 -x,y,z #2 -x,y,z-1 #3 x,y,z-1
#4 x,y,z+1

Table 9. Anisotropic displacement parameters (A^2 x 10^3) for compound 5.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Co(1)	11(1)	12(1)	20(1)	-1(1)	0	0
Co(1A)	11(2)	8(2)	35(5)	3(3)	0	0
O(1)	17(1)	9(1)	47(1)	1(1)	0	0
N(1)	14(1)	13(1)	25(1)	0(1)	1(1)	2(1)
C(1)	11(1)	10(1)	21(1)	0(1)	0(1)	0(1)
C(2)	14(1)	10(1)	24(1)	1(1)	2(1)	-1(1)
C(3)	14(1)	14(1)	30(1)	0(1)	1(1)	-2(1)
C(4)	12(1)	18(1)	35(1)	1(1)	3(1)	-2(1)
C(5)	15(1)	15(1)	32(1)	0(1)	3(1)	2(1)
C(6)	13(1)	11(1)	29(1)	1(1)	0	0
C(7)	29(1)	26(1)	21(1)	-4(1)	-3(1)	-10(1)
C(8)	20(1)	39(1)	23(1)	-2(1)	-3(1)	7(1)
C(9)	39(1)	19(1)	21(1)	2(1)	0	0
C(10)	64(2)	47(1)	36(1)	-5(1)	-4(1)	-34(1)
C(11)	30(1)	87(2)	34(1)	-2(1)	-5(1)	26(1)
C(12)	100(3)	20(1)	33(1)	4(1)	0	0
O(2)	16(1)	12(1)	44(1)	-1(1)	0(1)	0(1)
O(3)	24(1)	43(1)	39(1)	2(1)	-6(1)	-1(1)
O(4)	29(1)	35(1)	42(1)	4(1)	7(1)	-4(1)

Table 10. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for compound 5.

	x	y	z	U(eq)
H(3)	1533	3267	1242	23
H(4)	2313	1272	1072	26
H(5)	1863	-1133	958	25
H(10A)	823	4198	7451	73
H(10B)	676	4465	5149	73
H(10C)	1335	3472	5832	73
H(11A)	1531	192	7299	75
H(11B)	1668	1151	5353	75
H(11C)	1396	-508	5163	75
H(12A)	-475	-2016	5612	77
H(12B)	126	-2032	7289	77
H(12C)	349	-2010	5006	77
H(2A)	4262(12)	4340(2)	-3880(4)	28(5)
H(2B)	4117(11)	2930(3)	-3810(4)	30(5)
H(3A)	3210(3)	3680(5)	-5930(11)	130(2)
H(3B)	2999(13)	3740(2)	-7530(4)	18(5)
H(4A)	2673(13)	4390(3)	-1050(4)	46(7)
H(4B)	3233(13)	3690(2)	-1540(6)	35(6)

Table 11. Atomic distances (Å) for **4** as determined by single-crystal X-ray diffraction at 100 K in comparison to the calculated values as well as the respective calculated values for fluorenone (**1**), cyclopentadienone (CpO) and the cyclopentadienone complex [CpCo(CpO)]. The crystallographers' atom numbering scheme was used (Figure 1). Computational method: B3LYP/ECP-31g(d) (ECP = Stevens, Basch, and Krauss),[11] full optimization in C_1 symmetry.

Parameter	**4** (exp)	**4** (calcd)	**1** (calcd)	CpO (calcd)	[CpCo(CpO)] (calcd)
C(1)-C(2)	1.471	1.501	1.546	1.529	1.497
C(1)-C(13)	1.472	1.499	1.546	1.529	1.496
C(2)-C(3)	1.427	1.439	1.405		
C(2)-C(7)	1.440	1.451	1.425	1.364	1.436
C(3)-C(4)	1.356	1.393	1.417		
C(4)-C(5)	1.424	1.450	1.410		
C(5)-C(6)	1.361	1.392	1.414		
C(6)-C(7)	1.422	1.439	1.406		
C(7)-C(8)	1.443	1.464	1.501	1.519	1.447
C(8)-C(9)	1.427	1.443	1.406		
C(8)-C(13)	1.437	1.455	1.425	1.364	1.436
C(9)-C(10)	1.363	1.391	1.414		
C(10)-C(11)	1.424	1.451	1.410		
C(11)-C(12)	1.361	1.392	1.417		
C(12)-(C(13)	1.423	1.440	1.405		
C(1)-O(1)	1.247	1.247	1.257	1.529	1.497

Table 12. Calculated geometric parameters (Cartesian coordinates in Å).

a) 4

C	6.0	-0.4586430340	2.5340901401	-0.7851148051
C	6.0	0.9562268348	2.4175547392	-0.6532069896
C	6.0	1.2531585406	2.1792361638	0.7495404247
C	6.0	0.0225422319	2.2030348027	1.4861770156
C	6.0	-1.0403368355	2.3572134019	0.5305028756
Co	27.0	0.0358637917	0.6653590472	0.0137475831
C	6.0	0.6597006190	-1.1886845362	0.6096442967
C	6.0	-0.8038509168	-1.1474187620	0.6164766510
C	6.0	-1.2369967366	-0.8898667352	-0.7443611373
C	6.0	-0.0693203887	-0.9011993569	-1.6877975169
C	6.0	1.1043226497	-0.9715562922	-0.7581248153
O	8.0	-0.0754419982	-0.7816273790	-2.9286043426
H	1.0	-0.0998992661	2.0306507918	2.5653430801
H	1.0	-2.1179318282	2.3364799637	0.7521035897
C	6.0	2.5126018955	-0.9352154182	-1.0585849436
H	1.0	2.2545047817	1.9991510516	1.1677504040
C	6.0	-2.6415835498	-0.7786224116	-1.0359513936
H	1.0	-1.0156387565	2.6642061334	-1.7245112599
C	6.0	1.6294105678	-1.3935786545	1.6581225059
H	1.0	1.6875379994	2.4366696330	-1.4740048469
C	6.0	-1.7690035188	-1.3049209720	1.6726158078
C	6.0	3.4286534694	-1.1178277170	-0.0268210574
C	6.0	2.9818389973	-1.3526275415	1.3340042768
H	1.0	2.8329578481	-0.7852474009	-2.1055862982
H	1.0	4.5143957500	-1.1021948331	-0.2388496538
H	1.0	3.7371269792	-1.5096762407	2.1275690220

b) 1

O	8.0	0.0000000000	0.0000000000	-2.8783866996
C	6.0	0.0000000000	0.0000000000	-1.6215268592
C	6.0	-1.2173404647	0.0000000000	-0.6683496375
C	6.0	1.2173404647	0.0000000000	-0.6683496375
C	6.0	-0.7505410512	0.0000000000	0.6775630226
C	6.0	0.7505410512	0.0000000000	0.6775630226
C	6.0	-2.5932057595	0.0000000000	-0.9510725129
C	6.0	2.5932057595	0.0000000000	-0.9510725129
C	6.0	-1.6599831285	0.0000000000	1.7503829667
C	6.0	1.6599831285	0.0000000000	1.7503829667
C	6.0	-3.5082002204	0.0000000000	0.1309551389
C	6.0	3.5082002204	0.0000000000	0.1309551389
C	6.0	-3.0448859241	0.0000000000	1.4629126601
C	6.0	3.0448859241	0.0000000000	1.4629126601
H	1.0	-2.9539097911	0.0000000000	-1.9898165144
H	1.0	2.9539097911	0.0000000000	-1.9898165144
H	1.0	-4.5886481786	0.0000000000	-0.0679456804
H	1.0	4.5886481786	0.0000000000	-0.0679456804
H	1.0	-3.7701325043	0.0000000000	2.2886069317
H	1.0	3.7701325043	0.0000000000	2.2886069317
H	1.0	-1.3083805888	0.0000000000	2.7912109930
H	1.0	1.3083805888	0.0000000000	2.7912109930

c) [CpCo(CpO)]

C	6.0	-1.0640288140	1.4047659768	-0.9147622818
C	6.0	-1.5330335693	0.0559950398	-1.0631928800
C	6.0	-2.0158494763	-0.4713652445	0.2519430887
C	6.0	-1.4132574298	0.5066435840	1.2108907719
C	6.0	-0.9858744154	1.6808876477	0.5039014705
O	8.0	-2.6090601600	-1.5387142165	0.4931165602
Co	27.0	0.2254128881	0.1510691570	0.0017061489
C	6.0	1.3926303230	-1.4870564298	0.5102850109
C	6.0	1.8384732260	-0.3072518954	1.2146437743
C	6.0	2.2616411112	0.6703339112	0.2446552414
C	6.0	2.0405965421	0.1141607397	-1.0595072220
C	6.0	1.5030330395	-1.2174843193	-0.8948743015
H	1.0	2.6330817399	1.6821344571	0.4649573268
H	1.0	2.2209698013	0.6173589045	-2.0213093970
H	1.0	-1.4384725215	0.3913568273	2.3049714748
H	1.0	1.8412794095	-0.1724255841	2.3061958965
H	1.0	-1.6740306384	-0.4692578205	-2.0209556738
H	1.0	1.2005041226	-1.8928472579	-1.7084161146
H	1.0	-0.6238720209	2.6200934464	0.9503793827
H	1.0	0.9942292940	-2.4050494541	0.9659614033
H	1.0	-0.7665324539	2.0914243251	-1.7221830892

d) CpO

O	8.0	0.0000000000	0.0000000000	-2.0099876960
C	6.0	0.0000000000	0.0000000000	-0.7817486348
C	6.0	-1.2222095492	0.0000000000	0.1367357480
C	6.0	1.2222095492	0.0000000000	0.1367357480
C	6.0	-0.7594150152	0.0000000000	1.4195674985
C	6.0	0.7594150152	0.0000000000	1.4195674985
H	1.0	-2.2623256563	0.0000000000	-0.2298584823
H	1.0	2.2623256563	0.0000000000	-0.2298584823
H	1.0	-1.3692871854	0.0000000000	2.3417055124
H	1.0	1.3692871854	0.0000000000	2.3417055124