[6 + 4] and [4 + 2] Cycloaddition Reactions of Cobaloxime 1,3-Dienyl Complexes and Tropones.

Ramakrishna R. Pidaparthi, Mark E. Welker,* and Cynthia S. Day
Department of Chemistry, Wake Forest University, P.O. Box 7486, Winston-Salem, NC 27109 (USA), email: welker@wfu.edu, FAX: (336)-758-4321

Supporting Information

Table 1. Crystal data and structure refinement for Compound (5B)

Empirical formula	C25 H32 Co N5 O5
Formula weight	541.49
Temperature	193(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	P2(1)/n
Unit cell dimensions	a = 8.173(3) Å
	b = 22.819(8) Å, β = 99.147(5)°
	c = 13.929(5) Å
Volume	2564.9(15) $Å^3$
Z	4
Density (calculated)	1.402 g/cm^3
Absorption coefficient	0.714 mm^{-1}
F(000)	1136
Crystal size	0.46 x 0.26 x 0.10 mm^3
Theta range for data collection	3.99 to 24.15°
Index ranges	$-9 \leq h \leq 9$, $-26 \leq k \leq 26$, $-16 \leq l \leq 16$
Reflections collected	16838
Independent reflections	4067 [R(int) = 0.1118]
Completeness to theta = 24.15°	99.1 %
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4067 / 32 / 335
Goodness-of-fit on F^2	0.901
Final R indices [I>2sigma(I)]	R1 = 0.0682, wR2 = 0.1463
R indices (all data)	R1 = 0.1236, wR2 = 0.1586
Largest diff. peak and hole	0.831 and -0.448 $e^-/Å^3$

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for Compound(5B). U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Co(1)	-725(1)	-528(1)	-2565(1)	30(1)
O(1)	-97(5)	-660(2)	-4496(3)	47(1)
O(2)	1358(5)	-854(2)	-813(3)	54(1)
O(3)	-1365(5)	-408(2)	-639(3)	48(1)
O(4)	-2796(5)	-189(2)	-4327(3)	45(1)
O(5)	1290(7)	-2381(2)	-2862(6)	114(3)
N(1)	487(6)	-744(2)	-3555(3)	32(1)
N(2)	1163(6)	-835(2)	-1790(4)	37(1)
N(3)	-1931(6)	-320(2)	-1578(3)	33(1)
N(4)	-2592(5)	-221(2)	-3342(3)	32(1)
N(5)	316(5)	291(2)	-2485(3)	34(1)
C(1)	1912(7)	-985(3)	-3282(5)	41(2)
C(2)	2319(7)	-1040(3)	-2235(5)	45(2)
C(3)	-3348(7)	-54(2)	-1854(4)	35(1)
C(4)	-3743(7)	4(3)	-2897(4)	33(1)
C(5)	3007(8)	-1180(3)	-3989(5)	63(2)
C(6)	3852(8)	-1328(3)	-1725(5)	63(2)
C(7)	-4401(7)	174(3)	-1153(4)	53(2)
C(8)	-5277(7)	301(3)	-3416(4)	47(2)
C(9)	324(7)	617(3)	-3279(4)	42(2)
C(10)	960(8)	1179(3)	-3235(6)	52(2)
C(11)	1634(8)	1411(3)	-2364(6)	61(2)
C(12)	1653(8)	1075(3)	-1536(5)	54(2)
C(13)	1009(7)	515(3)	-1626(5)	42(2)
C(14)	-1747(7)	-1315(2)	-2638(4)	34(1)
C(15)	-1807(8)	-1637(3)	-1831(6)	56(2)
C(16)	-2417(11)	-2242(4)	-1835(8)	98(3)
C(17)	-1122(13)	-2671(4)	-2202(11)	147(5)
C(18)	-198(11)	-2373(3)	-2922(8)	82(3)
C(19)	-1174(11)	-2082(4)	-3851(8)	103(4)
C(20)	-2346(8)	-1582(3)	-3588(5)	54(2)

C(21)	-1914(19)	-3256(5)	-2570(19)	210(11)
C(22)	-2453(13)	-3368(8)	-3556(19)	320(20)
C(23)	-2551(13)	-3071(8)	-4200(19)	294(17)
C(24)	-2041(15)	-2492(5)	-4519(11)	162(6)
C(25)	-2793(14)	-2442(5)	-797(9)	146(5)

Table 3. Bond lengths [Å] and angles [°] for Compound(5B)

Co(1)-N(4)	1.862(4)
Co(1)-N(2)	1.872(5)
Co(1)-N(3)	1.875(4)
Co(1)-N(1)	1.886(4)
Co(1)-C(14)	1.976(6)
Co(1)-N(5)	2.050(5)
O(1)-N(1)	1.336(5)
O(2)-N(2)	1.345(6)
O(3)-N(3)	1.332(5)
O(4)-N(4)	1.357(6)
O(5)-C(18)	1.206(9)
N(1)-C(1)	1.290(7)
N(2)-C(2)	1.298(7)
N(3)-C(3)	1.311(7)
N(4)-C(4)	1.311(6)
N(5)-C(9)	1.333(7)
N(5)-C(13)	1.341(7)
C(1)-C(2)	1.449(9)
C(1)-C(5)	1.500(8)
C(2)-C(6)	1.490(8)
C(3)-C(4)	1.443(8)
C(3)-C(7)	1.494(7)
C(4)-C(8)	1.505(7)
C(9)-C(10)	1.382(8)
C(10)-C(11)	1.358(9)
C(11)-C(12)	1.383(9)
C(12)-C(13)	1.380(8)
C(14)-C(15)	1.350(8)
C(14)-C(20)	1.469(8)
C(15)-C(16)	1.467(10)

C(16)-C(17)	1.584(12)
C(16)-C(25)	1.592(13)
C(17)-C(18)	1.509(14)
C(17)-C(21)	1.535(18)
C(18)-C(19)	1.557(13)
C(19)-C(24)	1.426(13)
C(19)-C(20)	1.569(10)
C(21)-C(22)	1.40(3)
C(22)-C(23)	1.1161
C(23)-C(24)	1.47(2)

N(4)-Co(1)-N(2)	179.6(2)
N(4)-Co(1)-N(3)	81.6(2)
N(2)-Co(1)-N(3)	98.8(2)
N(4)-Co(1)-N(1)	98.6(2)
N(2)-Co(1)-N(1)	81.0(2)
N(3)-Co(1)-N(1)	179.5(2)
N(4)-Co(1)-C(14)	90.7(2)
N(2)-Co(1)-C(14)	89.6(2)
N(3)-Co(1)-C(14)	90.0(2)
N(1)-Co(1)-C(14)	89.6(2)
N(4)-Co(1)-N(5)	89.00(19)
N(2)-Co(1)-N(5)	90.73(19)
N(3)-Co(1)-N(5)	89.52(18)
N(1)-Co(1)-N(5)	90.90(18)
C(14)-Co(1)-N(5)	179.5(2)
C(1)-N(1)-O(1)	121.0(5)
C(1)-N(1)-Co(1)	116.8(4)
O(1)-N(1)-Co(1)	122.2(4)
C(2)-N(2)-O(2)	119.5(5)
C(2)-N(2)-Co(1)	117.1(4)
O(2)-N(2)-Co(1)	123.4(4)
C(3)-N(3)-O(3)	120.7(5)
C(3)-N(3)-Co(1)	116.4(4)
O(3)-N(3)-Co(1)	122.8(4)
C(4)-N(4)-O(4)	118.4(4)

C(4)-N(4)-Co(1)	117.1(4)
O(4)-N(4)-Co(1)	124.4(3)
C(9)-N(5)-C(13)	118.1(5)
C(9)-N(5)-Co(1)	121.3(4)
C(13)-N(5)-Co(1)	120.6(4)
N(1)-C(1)-C(2)	112.7(5)
N(1)-C(1)-C(5)	122.5(6)
C(2)-C(1)-C(5)	124.8(6)
N(2)-C(2)-C(1)	112.4(5)
N(2)-C(2)-C(6)	123.6(6)
C(1)-C(2)-C(6)	123.9(6)
N(3)-C(3)-C(4)	112.6(5)
N(3)-C(3)-C(7)	122.9(5)
C(4)-C(3)-C(7)	124.5(5)
N(4)-C(4)-C(3)	112.2(5)
N(4)-C(4)-C(8)	123.7(5)
C(3)-C(4)-C(8)	124.1(5)
N(5)-C(9)-C(10)	122.1(6)
C(11)-C(10)-C(9)	120.0(7)
C(10)-C(11)-C(12)	118.5(7)
C(13)-C(12)-C(11)	119.0(6)
N(5)-C(13)-C(12)	122.3(6)
C(15)-C(14)-C(20)	118.2(6)
C(15)-C(14)-Co(1)	121.6(5)
C(20)-C(14)-Co(1)	120.1(4)
C(14)-C(15)-C(16)	124.6(7)
C(15)-C(16)-C(17)	109.7(7)
C(15)-C(16)-C(25)	112.4(8)
C(17)-C(16)-C(25)	110.6(8)
C(18)-C(17)-C(21)	113.4(12)
C(18)-C(17)-C(16)	111.6(7)
C(21)-C(17)-C(16)	112.1(9)
O(5)-C(18)-C(17)	123.6(10)
O(5)-C(18)-C(19)	116.2(9)
C(17)-C(18)-C(19)	120.0(8)
C(24)-C(19)-C(18)	113.4(10)

C(24)-C(19)-C(20)	111.8(8)
C(18)-C(19)-C(20)	111.5(7)
C(14)-C(20)-C(19)	112.6(6)
C(22)-C(21)-C(17)	122.5(17)
C(23)-C(22)-C(21)	130.5(12)
C(22)-C(23)-C(24)	142.9(10)
C(19)-C(24)-C(23)	121.8(14)

Table 4. Anisotropic displacement parameters ($Å^2 x 10^3$) for Compound(5B). The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Co(1)	23(1)	39(1)	29(1)	0(1)	7(1)	1(1)
O(1)	51(3)	65(3)	29(3)	-6(2)	17(2)	6(2)
O(2)	44(3)	78(4)	37(3)	9(2)	-1(2)	14(2)
O(3)	43(3)	76(3)	25(2)	8(2)	9(2)	3(2)
O(4)	37(3)	72(4)	27(3)	0(2)	3(2)	9(2)
O(5)	40(4)	56(4)	250(8)	0(4)	37(4)	9(3)
N(1)	29(3)	38(3)	34(3)	-4(2)	16(2)	2(2)
N(2)	25(3)	50(3)	34(3)	5(2)	1(2)	-1(2)
N(3)	29(3)	46(3)	25(3)	0(2)	10(2)	-5(2)
N(4)	30(3)	42(3)	21(3)	1(2)	-1(2)	3(2)
N(5)	28(3)	48(3)	27(3)	0(2)	11(2)	6(2)
C(1)	28(4)	40(4)	57(5)	-8(3)	19(3)	-2(3)
C(2)	29(4)	32(4)	73(5)	0(3)	8(3)	5(3)
C(3)	24(3)	44(4)	39(4)	-6(3)	15(3)	-2(3)
C(4)	22(3)	43(4)	34(4)	-9(3)	4(3)	1(3)
C(5)	44(4)	65(5)	89(6)	-14(4)	38(4)	7(4)
C(6)	34(4)	63(5)	90(6)	8(4)	2(4)	14(4)
C(7)	40(4)	80(5)	47(4)	-8(4)	30(3)	6(4)
C(8)	30(4)	60(4)	48(4)	-2(3)	0(3)	12(3)
C(9)	39(4)	48(4)	41(4)	5(3)	17(3)	6(3)
C(10)	40(4)	47(5)	77(6)	12(4)	30(4)	0(3)
C(11)	52(5)	46(5)	89(6)	-17(5)	22(4)	-14(4)
C(12)	43(4)	58(5)	60(5)	-16(4)	7(4)	-9(4)
C(13)	33(3)	49(4)	45(4)	-9(3)	10(3)	-3(3)
C(14)	27(3)	30(3)	47(4)	1(3)	12(3)	6(3)
C(15)	37(4)	53(5)	80(5)	10(4)	15(4)	-6(3)
C(16)	79(7)	78(7)	144(9)	33(6)	36(6)	20(5)
C(17)	70(7)	65(7)	313(17)	33(9)	51(9)	23(6)
C(18)	44(5)	36(5)	173(10)	3(5)	36(6)	1(4)
C(19)	63(6)	96(8)	163(10)	-45(7)	56(7)	-14(6)
C(20)	32(4)	48(4)	85(5)	-14(4)	16(4)	-2(3)

C(21)	87(10)	40(7)	530(40)	35(13)	132(16)	11(7)
C(22)	150(20)	161(19)	710(70)	-160(30)	200(30)	-2(14)
C(23)	89(12)	190(20)	610(40)	-280(20)	73(17)	-28(11)
C(24)	146(11)	103(9)	255(15)	-126(10)	89(11)	-59(8)
C(25)	129(10)	106(9)	209(13)	92(8)	45(9)	6(7)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for Compound(5B).

	x	y	z	U(eq)
H(2O)	690(90)	-690(30)	-630(50)	64
H(4O)	-2260(90)	-400(30)	-4370(50)	55
H(5A)	2506	-1066	-4649	95
H(5B)	3135	-1607	-3956	95
H(5C)	4096	-994	-3824	95
H(6A)	3974	-1245	-1027	95
H(6B)	4816	-1175	-1983	95
H(6C)	3773	-1752	-1831	95
H(7A)	-3748	187	-499	80
H(7B)	-5357	-86	-1152	80
H(7C)	-4788	569	-1347	80
H(8A)	-6255	137	-3187	70
H(8B)	-5363	236	-4118	70
H(8C)	-5211	722	-3281	70
H(9)	-122	457	-3896	50
H(10)	925	1403	-3813	63
H(11)	2083	1796	-2324	73
H(12)	2103	1227	-915	65
H(13)	1059	280	-1059	50
H(15)	-1428	-1460	-1219	67
H(16)	-3475	-2265	-2305	118
H(17)	-279	-2766	-1621	176
H(19)	-332	-1890	-4195	124
H(20A)	-2438	-1276	-4096	65
H(20B)	-3466	-1746	-3583	65
H(21)	-2042	-3553	-2110	252
H(22)	-2790	-3760	-3702	390
H(23)	-3199	-3260	-4738	353
H(24)	-2297	-2390	-5187	194
H(25A)	-3384	-2128	-515	219

H(25B)	-1748	-2524	-368	219
H(25C)	-3479	-2796	-869	219

Table 7. Hydrogen bonds for Compound(5B) [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(2)-H(2O)...O(3)	0.74(7)	1.79(7)	2.494(6)	157(8)
O(4)-H(4O)...O(1)	0.66(6)	1.90(7)	2.498(5)	151(9)

Table 1. Crystal data and structure refinement for $Co(C_4H_7N_2O_2)_2(C_7H_{10}N_2)(C_{19}H_{23}O_6)$ (15a).

Empirical formula	C34 H47 Co N6 O10
Formula weight	758.71
Temperature	193(2) K
Wavelength	0.71073 Å
Crystal system	Orthorhombic
Space group	Pna2(1) – C_{2v}^{9} (No.33)
Unit cell dimensions	a = 9.199(1) Å
	b = 29.552(4) Å
	c = 14.318(2) Å
Volume	3892.5(9) $Å^3$
Z	4
Density (calculated)	1.295 g/cm^3
Absorption coefficient	0.501 mm^{-1}
F(000)	1600
Crystal size	0.22 x 0.19 x 0.04 mm^3
Theta range for data collection	3.81 to 24.15°
Index ranges	$-10 \leq h \leq 10$, $-34 \leq k \leq 33$, $-16 \leq l \leq 16$
Reflections collected	24196
Independent reflections	6189 [R(int) = 0.0820]
Completeness to theta = 24.15°	99.2 %
Absorption correction	Multi-scan (SADABS)
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	6189 / 1 / 461
Goodness-of-fit on F^2	1.204
Final R indices [$I>2\sigma(I)$]	R1 = 0.0794, wR2 = 0.1736
R indices (all data)	R1 = 0.0949, wR2 = 0.1805
Absolute structure parameter	0.03(3)
Largest diff. peak and hole	0.685 and -0.539 $e^-/Å^3$

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for $Co(C_4H_7N_2O_2)_2(C_7H_{10}N_2)(C_{19}H_{23}O_6)$. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Co(1)	3542(1)	-473(1)	5166(1)	32(1)
O(1)	733(6)	-367(2)	5972(4)	55(2)
O(2)	4392(5)	-285(2)	3290(3)	39(1)
O(3)	6271(5)	-645(2)	4299(3)	40(1)
O(4)	2713(6)	-620(2)	7043(3)	48(1)
O(5)	5215(6)	1654(2)	6951(4)	57(2)
O(6)	5342(8)	1832(2)	5445(4)	80(2)
O(7)	1545(12)	1494(4)	3589(9)	146(4)
O(8)	-171(10)	1150(3)	4303(6)	105(3)
O(9)	58(6)	1689(2)	5894(5)	70(2)
O(10)	592(6)	1503(2)	7598(4)	58(2)
N(1)	1552(6)	-316(2)	5218(6)	43(1)
N(2)	3296(6)	-280(2)	3932(4)	32(1)
N(3)	5497(5)	-646(2)	5113(5)	35(1)
N(4)	3801(6)	-634(2)	6414(4)	37(1)
C(1)	963(8)	-162(2)	4448(5)	38(2)
C(2)	2019(8)	-147(2)	3663(5)	37(2)
C(3)	6054(7)	-794(3)	5869(5)	38(2)
C(4)	5064(9)	-783(3)	6655(5)	43(2)
C(5)	-580(8)	-31(3)	4352(8)	68(3)
C(6)	1640(9)	22(3)	2708(6)	57(2)
C(7)	7584(8)	-993(3)	5925(6)	52(2)
C(8)	5397(10)	-911(3)	7628(6)	64(2)
N(5)	2972(5)	-1127(2)	4834(4)	34(1)
N(6)	1764(8)	-2454(2)	4162(5)	63(2)
C(9)	3260(8)	-1322(2)	4018(5)	44(2)
C(10)	2894(8)	-1739(3)	3729(6)	49(2)
C(11)	2163(8)	-2033(3)	4393(6)	50(2)
C(12)	1920(7)	-1841(2)	5252(6)	49(2)
C(13)	2297(8)	-1405(2)	5434(4)	41(2)

C(14)	1050(12)	-2734(4)	4813(8)	92(4)
C(15)	1913(14)	-2611(4)	3146(8)	98(4)
C(16)	4097(7)	154(2)	5515(4)	33(2)
C(17)	5233(6)	364(2)	5152(6)	36(1)
C(18)	5722(7)	838(2)	5361(5)	39(2)
C(19)	4410(7)	1114(2)	5793(5)	38(2)
C(20)	3781(7)	840(2)	6595(5)	33(2)
C(21)	3131(7)	391(2)	6228(5)	35(2)
C(22)	3304(8)	1193(2)	5025(5)	40(2)
C(23)	1919(7)	1307(2)	5124(6)	43(2)
C(24)	1126(8)	1446(2)	6017(5)	39(2)
C(25)	1564(7)	1315(2)	6950(4)	30(1)
C(26)	2681(7)	1059(2)	7215(5)	37(2)
C(27)	7095(8)	852(3)	5942(6)	51(2)
C(28)	5004(8)	1558(2)	6154(6)	44(2)
C(29)	6028(16)	2267(5)	5669(12)	137(5)
C(30)	7090(20)	2404(7)	5076(16)	195(8)
C(31)	995(13)	1311(5)	4216(10)	106(5)
C(32)	-1044(16)	1148(5)	3436(10)	129(6)
C(33)	-1767(13)	1553(5)	3320(8)	103(4)
C(34)	757(12)	1365(4)	8534(7)	90(3)

Table 3. Bond lengths [Å] and angles [°] for $Co(C_4H_7N_2O_2)_2(C_7H_{10}N_2)(C_{19}H_{23}O_6)$

Co(1)-N(4)	1.864(6)
Co(1)-N(2)	1.869(5)
Co(1)-N(3)	1.872(5)
Co(1)-N(1)	1.890(5)
Co(1)-C(16)	1.987(6)
Co(1)-N(5)	2.058(6)
O(1)-N(1)	1.325(9)
O(2)-N(2)	1.365(7)
O(3)-N(3)	1.365(7)
O(4)-N(4)	1.347(7)
O(5)-C(28)	1.192(9)
O(6)-C(28)	1.335(9)
O(6)-C(29)	1.468(16)
O(7)-C(31)	1.164(14)
O(8)-C(31)	1.180(12)
O(8)-C(32)	1.479(12)
O(9)-C(24)	1.228(9)
O(10)-C(25)	1.403(8)
O(10)-C(34)	1.409(11)
N(1)-C(1)	1.310(10)
N(2)-C(2)	1.297(9)
N(3)-C(3)	1.275(9)
N(4)-C(4)	1.290(9)
C(1)-C(5)	1.478(10)
C(1)-C(2)	1.486(10)
C(2)-C(6)	1.497(10)
C(3)-C(4)	1.449(10)
C(3)-C(7)	1.528(10)
C(4)-C(8)	1.476(10)
N(5)-C(9)	1.330(9)
N(5)-C(13)	1.341(8)
N(6)-C(11)	1.339(9)
N(6)-C(14)	1.410(12)
N(6)-C(15)	1.533(12)

C(9)-C(10)	1.342(10)
C(10)-C(11)	1.453(11)
C(11)-C(12)	1.373(11)
C(12)-C(13)	1.359(10)
C(16)-C(17)	1.321(9)
C(16)-C(21)	1.523(9)
C(17)-C(18)	1.502(9)
C(18)-C(27)	1.514(10)
C(18)-C(19)	1.583(9)
C(19)-C(22)	1.515(10)
C(19)-C(28)	1.513(9)
C(19)-C(20)	1.521(10)
C(20)-C(26)	1.495(9)
C(20)-C(21)	1.547(9)
C(22)-C(23)	1.325(9)
C(23)-C(24)	1.529(11)
C(23)-C(31)	1.553(16)
C(24)-C(25)	1.448(10)
C(25)-C(26)	1.331(9)
C(29)-C(30)	1.35(2)
C(32)-C(33)	1.377(15)

N(4)-Co(1)-N(2)	177.0(3)
N(4)-Co(1)-N(3)	81.2(3)
N(2)-Co(1)-N(3)	99.3(3)
N(4)-Co(1)-N(1)	98.5(3)
N(2)-Co(1)-N(1)	81.1(3)
N(3)-Co(1)-N(1)	178.3(2)
N(4)-Co(1)-C(16)	87.9(2)
N(2)-Co(1)-C(16)	89.1(2)
N(3)-Co(1)-C(16)	91.0(2)
N(1)-Co(1)-C(16)	90.6(2)
N(4)-Co(1)-N(5)	90.8(2)
N(2)-Co(1)-N(5)	92.2(2)
N(3)-Co(1)-N(5)	88.8(2)
N(1)-Co(1)-N(5)	89.6(2)

C(16)-Co(1)-N(5)	178.7(2)
C(28)-O(6)-C(29)	117.6(9)
C(31)-O(8)-C(32)	114.0(12)
C(25)-O(10)-C(34)	116.5(6)
C(1)-N(1)-O(1)	119.4(6)
C(1)-N(1)-Co(1)	116.9(6)
O(1)-N(1)-Co(1)	123.7(6)
C(2)-N(2)-O(2)	118.2(5)
C(2)-N(2)-Co(1)	118.8(5)
O(2)-N(2)-Co(1)	123.0(4)
C(3)-N(3)-O(3)	121.0(5)
C(3)-N(3)-Co(1)	116.5(5)
O(3)-N(3)-Co(1)	122.4(4)
C(4)-N(4)-O(4)	120.0(6)
C(4)-N(4)-Co(1)	117.3(5)
O(4)-N(4)-Co(1)	122.6(5)
N(1)-C(1)-C(5)	124.5(8)
N(1)-C(1)-C(2)	112.1(6)
C(5)-C(1)-C(2)	123.4(8)
N(2)-C(2)-C(1)	111.0(6)
N(2)-C(2)-C(6)	125.7(7)
C(1)-C(2)-C(6)	123.2(7)
N(3)-C(3)-C(4)	113.5(6)
N(3)-C(3)-C(7)	123.2(7)
C(4)-C(3)-C(7)	123.2(7)
N(4)-C(4)-C(3)	111.5(6)
N(4)-C(4)-C(8)	121.8(7)
C(3)-C(4)-C(8)	126.7(7)
C(9)-N(5)-C(13)	112.9(6)
C(9)-N(5)-Co(1)	124.0(5)
C(13)-N(5)-Co(1)	123.1(4)
C(11)-N(6)-C(14)	120.7(8)
C(11)-N(6)-C(15)	119.5(8)
C(14)-N(6)-C(15)	119.4(8)
N(5)-C(9)-C(10)	128.2(7)
C(9)-C(10)-C(11)	117.6(7)

N(6)-C(11)-C(12)	124.1(8)
N(6)-C(11)-C(10)	121.3(8)
C(12)-C(11)-C(10)	114.5(7)
C(13)-C(12)-C(11)	121.4(8)
N(5)-C(13)-C(12)	125.2(7)
C(17)-C(16)-C(21)	120.6(6)
C(17)-C(16)-Co(1)	122.8(5)
C(21)-C(16)-Co(1)	116.5(4)
C(16)-C(17)-C(18)	126.6(6)
C(17)-C(18)-C(27)	112.6(6)
C(17)-C(18)-C(19)	109.3(5)
C(27)-C(18)-C(19)	114.0(6)
C(22)-C(19)-C(28)	111.0(5)
C(22)-C(19)-C(20)	112.0(6)
C(28)-C(19)-C(20)	110.0(6)
C(22)-C(19)-C(18)	107.9(6)
C(28)-C(19)-C(18)	107.8(6)
C(20)-C(19)-C(18)	108.1(5)
C(26)-C(20)-C(19)	118.3(5)
C(26)-C(20)-C(21)	108.2(5)
C(19)-C(20)-C(21)	110.4(5)
C(16)-C(21)-C(20)	113.3(5)
C(23)-C(22)-C(19)	127.4(7)
C(22)-C(23)-C(24)	128.0(8)
C(22)-C(23)-C(31)	116.1(8)
C(24)-C(23)-C(31)	115.9(7)
O(9)-C(24)-C(25)	120.7(7)
O(9)-C(24)-C(23)	114.8(7)
C(25)-C(24)-C(23)	124.5(6)
C(26)-C(25)-O(10)	121.8(6)
C(26)-C(25)-C(24)	129.0(6)
O(10)-C(25)-C(24)	109.1(6)
C(25)-C(26)-C(20)	126.9(6)
O(5)-C(28)-O(6)	123.2(7)
O(5)-C(28)-C(19)	126.3(7)
O(6)-C(28)-C(19)	110.5(7)

C(30)-C(29)-O(6)	115.7(16)
O(7)-C(31)-O(8)	131.6(15)
O(7)-C(31)-C(23)	114.3(13)
O(8)-C(31)-C(23)	113.9(10)
C(33)-C(32)-O(8)	111.1(10)

Table 4. Anisotropic displacement parameters ($Å^2 x 10^3$) for $Co(C_4H_7N_2O_2)_2(C_7H_{10}N_2)(C_{19}H_{23}O_6)$. The anisotropic displacement factor exponent takes the form: $-2\Pi^2[h^2 a^{*2} U_{11} + ... + 2 h k a^* b^* U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Co(1)	36(1)	32(1)	28(1)	-5(1)	5(1)	-2(1)
O(1)	49(3)	48(3)	68(4)	-7(3)	35(3)	-7(2)
O(2)	49(3)	41(3)	26(3)	3(2)	6(2)	5(2)
O(3)	37(3)	43(3)	39(3)	-9(2)	18(2)	1(2)
O(4)	64(4)	45(3)	35(3)	-6(2)	21(3)	-8(3)
O(5)	64(4)	56(3)	51(4)	-26(3)	-8(3)	-12(3)
O(6)	134(6)	31(3)	76(5)	-3(3)	5(4)	-29(3)
O(8)	112(7)	117(6)	86(6)	24(4)	-67(5)	-23(5)
O(9)	55(3)	76(4)	78(4)	18(3)	-1(3)	32(3)
O(10)	55(3)	68(4)	52(4)	-11(3)	3(3)	28(3)
N(1)	43(3)	39(3)	49(4)	-13(4)	11(4)	-5(2)
N(2)	34(3)	27(3)	34(3)	4(2)	2(3)	-1(2)
N(3)	44(3)	30(3)	31(3)	-1(3)	-9(3)	-2(2)
N(4)	47(4)	40(3)	25(3)	2(3)	6(3)	-15(3)
C(1)	39(4)	23(4)	51(5)	-11(3)	-6(4)	-1(3)
C(2)	42(4)	32(4)	39(4)	-14(3)	6(3)	-9(3)
C(3)	32(4)	47(4)	34(4)	-4(3)	-4(3)	-11(3)
C(4)	58(5)	44(4)	26(4)	-2(3)	-21(4)	-10(4)
C(5)	45(5)	49(5)	110(8)	-25(5)	-1(5)	4(4)
C(6)	69(6)	44(4)	57(6)	7(4)	-9(4)	13(4)
C(7)	50(5)	45(4)	61(5)	7(4)	-18(4)	-2(3)
C(8)	94(7)	58(5)	39(5)	9(4)	-15(5)	-2(5)
N(5)	27(3)	37(3)	37(3)	1(2)	-1(2)	-4(2)
N(6)	75(5)	34(4)	80(5)	-18(4)	3(4)	-15(3)
C(9)	50(4)	35(4)	46(5)	-2(3)	22(4)	-3(3)
C(10)	49(4)	47(5)	51(5)	-6(4)	9(4)	5(4)
C(11)	57(5)	39(4)	53(5)	-14(4)	-11(4)	-2(4)
C(12)	49(4)	48(4)	50(5)	-4(4)	-10(4)	-10(3)
C(13)	62(5)	41(4)	21(4)	-5(3)	-10(3)	0(4)
C(14)	92(7)	59(6)	124(11)	-6(6)	6(6)	-31(5)

C(15)	133(10)	74(7)	88(9)	-25(6)	-17(7)	-17(7)
C(16)	39(4)	34(4)	27(3)	-3(3)	-7(3)	-1(3)
C(17)	43(3)	34(3)	31(3)	-14(4)	8(4)	-2(3)
C(18)	45(4)	38(4)	35(5)	-1(3)	13(3)	-8(3)
C(19)	43(4)	28(4)	42(4)	-10(3)	-1(3)	8(3)
C(20)	33(4)	33(4)	33(4)	-5(3)	-1(3)	5(3)
C(21)	35(4)	36(4)	36(4)	-2(3)	8(3)	-7(3)
C(22)	65(5)	31(3)	25(4)	-2(3)	-16(4)	-2(3)
C(23)	54(4)	37(4)	39(4)	-3(4)	3(5)	-3(3)
C(24)	30(4)	45(4)	41(5)	3(4)	-5(3)	-8(3)
C(25)	35(4)	33(4)	23(3)	-2(3)	4(3)	5(3)
C(26)	47(4)	38(4)	27(4)	-10(3)	-2(3)	3(3)
C(27)	44(4)	60(5)	48(5)	-11(4)	8(4)	-2(4)
C(28)	41(4)	36(4)	55(5)	-9(4)	-7(4)	-5(3)
C(31)	50(6)	133(11)	136(12)	98(10)	3(7)	20(7)
C(32)	140(12)	109(10)	139(12)	-42(9)	-96(10)	29(9)
C(33)	98(9)	121(10)	92(9)	-19(7)	-14(7)	32(7)
C(34)	88(7)	110(9)	72(8)	2(6)	31(6)	35(7)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for $Co(C_4H_7N_2O_2)_2(C_7H_{10}N_2)(C_{19}H_{23}O_6)$

	x	y	z	U(eq)
H(2O)	5060(80)	-470(20)	3670(50)	39(19)
H(4O)	1590(80)	-580(20)	6750(50)	42(19)
H(5A)	-1059	-51	4962	102
H(5B)	-1063	-235	3911	102
H(5C)	-641	281	4121	102
H(6A)	2508	16	2312	85
H(6B)	1276	333	2753	85
H(6C)	888	-172	2436	85
H(7A)	7757	-1188	5382	78
H(7B)	7678	-1172	6499	78
H(7C)	8299	-748	5931	78
H(8A)	5285	-646	8034	96
H(8B)	6399	-1021	7666	96
H(8C)	4728	-1149	7831	96
H(9)	3792	-1144	3585	52
H(10)	3106	-1838	3113	59
H(12)	1478	-2017	5730	59
H(13)	2064	-1288	6034	49
H(14A)	1713	-2805	5329	138
H(14B)	751	-3016	4506	138
H(14C)	191	-2578	5056	138
H(15A)	2926	-2578	2944	147
H(15B)	1285	-2426	2745	147
H(15C)	1623	-2929	3098	147
H(17)	5797	198	4714	43
H(18)	5959	983	4748	47
H(20)	4619	755	7004	39
H(21A)	2967	184	6762	43
H(21B)	2175	454	5938	43
H(22)	3642	1156	4403	49

H(26)	2790	1011	7868	45
H(27A)	7880	697	5608	76
H(27B)	6922	701	6541	76
H(27C)	7373	1168	6054	76
H(29A)	5262	2502	5684	165
H(29B)	6446	2246	6305	165
H(30A)	7938	2501	5435	293
H(30B)	6730	2658	4700	293
H(30C)	7356	2153	4664	293
H(32A)	-398	1096	2894	155
H(32B)	-1758	898	3461	155
H(33A)	-2450	1527	2797	155
H(33B)	-1063	1793	3188	155
H(33C)	-2302	1626	3892	155
H(34A)	-10	1502	8915	135
H(34B)	1709	1462	8766	135
H(34C)	686	1035	8571	135

Table 6. Torsion angles [°] for $Co(C_4H_7N_2O_2)_2(C_7H_{10}N_2)(C_{19}H_{23}O_6)$

N(4)-Co(1)-N(1)-C(1)	177.3(5)
N(2)-Co(1)-N(1)-C(1)	0.3(5)
N(3)-Co(1)-N(1)-C(1)	-103(12)
C(16)-Co(1)-N(1)-C(1)	89.3(5)
N(5)-Co(1)-N(1)-C(1)	-92.0(5)
N(4)-Co(1)-N(1)-O(1)	-4.8(5)
N(2)-Co(1)-N(1)-O(1)	178.2(5)
N(3)-Co(1)-N(1)-O(1)	75(12)
C(16)-Co(1)-N(1)-O(1)	-92.7(5)
N(5)-Co(1)-N(1)-O(1)	86.0(5)
N(4)-Co(1)-N(2)-C(2)	-85(5)
N(3)-Co(1)-N(2)-C(2)	177.0(5)
N(1)-Co(1)-N(2)-C(2)	-1.4(5)
C(16)-Co(1)-N(2)-C(2)	-92.1(5)
N(5)-Co(1)-N(2)-C(2)	87.9(5)
N(4)-Co(1)-N(2)-O(2)	97(5)
N(3)-Co(1)-N(2)-O(2)	-1.0(5)
N(1)-Co(1)-N(2)-O(2)	-179.4(5)
C(16)-Co(1)-N(2)-O(2)	89.9(5)
N(5)-Co(1)-N(2)-O(2)	-90.1(5)
N(4)-Co(1)-N(3)-C(3)	2.0(5)
N(2)-Co(1)-N(3)-C(3)	178.9(5)
N(1)-Co(1)-N(3)-C(3)	-78(12)
C(16)-Co(1)-N(3)-C(3)	89.7(5)
N(5)-Co(1)-N(3)-C(3)	-89.1(5)
N(4)-Co(1)-N(3)-O(3)	177.7(4)
N(2)-Co(1)-N(3)-O(3)	-5.3(4)
N(1)-Co(1)-N(3)-O(3)	98(12)
C(16)-Co(1)-N(3)-O(3)	-94.6(4)
N(5)-Co(1)-N(3)-O(3)	86.7(4)
N(2)-Co(1)-N(4)-C(4)	-99(5)
N(3)-Co(1)-N(4)-C(4)	-1.0(5)
N(1)-Co(1)-N(4)-C(4)	177.3(5)
C(16)-Co(1)-N(4)-C(4)	-92.4(5)

N(5)-Co(1)-N(4)-C(4)	87.6(5)
N(2)-Co(1)-N(4)-O(4)	84(5)
N(3)-Co(1)-N(4)-O(4)	-177.6(5)
N(1)-Co(1)-N(4)-O(4)	0.7(5)
C(16)-Co(1)-N(4)-O(4)	91.0(5)
N(5)-Co(1)-N(4)-O(4)	-89.0(5)
O(1)-N(1)-C(1)-C(5)	0.9(10)
Co(1)-N(1)-C(1)-C(5)	178.9(5)
O(1)-N(1)-C(1)-C(2)	-177.4(5)
Co(1)-N(1)-C(1)-C(2)	0.6(7)
O(2)-N(2)-C(2)-C(1)	-179.9(5)
Co(1)-N(2)-C(2)-C(1)	2.0(7)
O(2)-N(2)-C(2)-C(6)	-2.6(9)
Co(1)-N(2)-C(2)-C(6)	179.3(5)
N(1)-C(1)-C(2)-N(2)	-1.6(8)
C(5)-C(1)-C(2)-N(2)	-179.9(6)
N(1)-C(1)-C(2)-C(6)	-179.0(6)
C(5)-C(1)-C(2)-C(6)	2.7(10)
O(3)-N(3)-C(3)-C(4)	-178.3(5)
Co(1)-N(3)-C(3)-C(4)	-2.5(8)
O(3)-N(3)-C(3)-C(7)	-2.1(10)
Co(1)-N(3)-C(3)-C(7)	173.7(5)
O(4)-N(4)-C(4)-C(3)	176.7(6)
Co(1)-N(4)-C(4)-C(3)	0.0(8)
O(4)-N(4)-C(4)-C(8)	-4.6(10)
Co(1)-N(4)-C(4)-C(8)	178.7(6)
N(3)-C(3)-C(4)-N(4)	1.6(9)
C(7)-C(3)-C(4)-N(4)	-174.6(6)
N(3)-C(3)-C(4)-C(8)	-177.1(7)
C(7)-C(3)-C(4)-C(8)	6.8(12)
N(4)-Co(1)-N(5)-C(9)	-147.4(6)
N(2)-Co(1)-N(5)-C(9)	32.9(6)
N(3)-Co(1)-N(5)-C(9)	-66.3(6)
N(1)-Co(1)-N(5)-C(9)	114.0(6)
C(16)-Co(1)-N(5)-C(9)	-147(11)
N(4)-Co(1)-N(5)-C(13)	31.0(5)

N(2)-Co(1)-N(5)-C(13)	-148.7(5)
N(3)-Co(1)-N(5)-C(13)	112.1(5)
N(1)-Co(1)-N(5)-C(13)	-67.6(6)
C(16)-Co(1)-N(5)-C(13)	31(11)
C(13)-N(5)-C(9)-C(10)	3.8(11)
Co(1)-N(5)-C(9)-C(10)	-177.7(6)
N(5)-C(9)-C(10)-C(11)	-3.9(12)
C(14)-N(6)-C(11)-C(12)	-0.3(13)
C(15)-N(6)-C(11)-C(12)	172.0(9)
C(14)-N(6)-C(11)-C(10)	-179.7(9)
C(15)-N(6)-C(11)-C(10)	-7.4(12)
C(9)-C(10)-C(11)-N(6)	-179.9(7)
C(9)-C(10)-C(11)-C(12)	0.6(11)
N(6)-C(11)-C(12)-C(13)	-177.3(7)
C(10)-C(11)-C(12)-C(13)	2.2(11)
C(9)-N(5)-C(13)-C(12)	-0.4(10)
Co(1)-N(5)-C(13)-C(12)	-179.0(5)
C(11)-C(12)-C(13)-N(5)	-2.5(11)
N(4)-Co(1)-C(16)-C(17)	119.7(6)
N(2)-Co(1)-C(16)-C(17)	-60.7(6)
N(3)-Co(1)-C(16)-C(17)	38.6(6)
N(1)-Co(1)-C(16)-C(17)	-141.8(6)
N(5)-Co(1)-C(16)-C(17)	119(11)
N(4)-Co(1)-C(16)-C(21)	-60.9(5)
N(2)-Co(1)-C(16)-C(21)	118.7(5)
N(3)-Co(1)-C(16)-C(21)	-142.1(5)
N(1)-Co(1)-C(16)-C(21)	37.6(5)
N(5)-Co(1)-C(16)-C(21)	-61(11)
C(21)-C(16)-C(17)-C(18)	-0.4(11)
Co(1)-C(16)-C(17)-C(18)	179.0(5)
C(16)-C(17)-C(18)-C(27)	107.8(8)
C(16)-C(17)-C(18)-C(19)	-20.0(10)
C(17)-C(18)-C(19)-C(22)	-70.2(7)
C(27)-C(18)-C(19)-C(22)	162.7(6)
C(17)-C(18)-C(19)-C(28)	169.9(6)
C(27)-C(18)-C(19)-C(28)	42.9(8)

C(17)-C(18)-C(19)-C(20)	51.0(7)
C(27)-C(18)-C(19)-C(20)	-76.0(7)
C(22)-C(19)-C(20)-C(26)	-70.9(7)
C(28)-C(19)-C(20)-C(26)	53.0(8)
C(18)-C(19)-C(20)-C(26)	170.4(6)
C(22)-C(19)-C(20)-C(21)	54.5(7)
C(28)-C(19)-C(20)-C(21)	178.4(5)
C(18)-C(19)-C(20)-C(21)	-64.2(7)
C(17)-C(16)-C(21)-C(20)	-11.0(9)
Co(1)-C(16)-C(21)-C(20)	169.6(4)
C(26)-C(20)-C(21)-C(16)	174.8(6)
C(19)-C(20)-C(21)-C(16)	43.9(8)
C(28)-C(19)-C(22)-C(23)	-80.2(9)
C(20)-C(19)-C(22)-C(23)	43.2(9)
C(18)-C(19)-C(22)-C(23)	162.0(6)
C(19)-C(22)-C(23)-C(24)	8.5(11)
C(19)-C(22)-C(23)-C(31)	-173.3(8)
C(22)-C(23)-C(24)-O(9)	154.1(7)
C(31)-C(23)-C(24)-O(9)	-24.1(10)
C(22)-C(23)-C(24)-C(25)	-25.4(11)
C(31)-C(23)-C(24)-C(25)	156.4(8)
C(34)-O(10)-C(25)-C(26)	-7.1(11)
C(34)-O(10)-C(25)-C(24)	172.7(8)
O(9)-C(24)-C(25)-C(26)	-179.7(7)
C(23)-C(24)-C(25)-C(26)	-0.2(11)
O(9)-C(24)-C(25)-O(10)	0.6(9)
C(23)-C(24)-C(25)-O(10)	-179.9(6)
O(10)-C(25)-C(26)-C(20)	179.7(6)
C(24)-C(25)-C(26)-C(20)	0.0(12)
C(19)-C(20)-C(26)-C(25)	43.6(10)
C(21)-C(20)-C(26)-C(25)	-82.7(8)
C(29)-O(6)-C(28)-O(5)	1.0(13)
C(29)-O(6)-C(28)-C(19)	-176.0(9)
C(22)-C(19)-C(28)-O(5)	137.7(8)
C(20)-C(19)-C(28)-O(5)	13.2(10)
C(18)-C(19)-C(28)-O(5)	-104.5(9)

C(22)-C(19)-C(28)-O(6)	-45.5(8)
C(20)-C(19)-C(28)-O(6)	-170.0(6)
C(18)-C(19)-C(28)-O(6)	72.4(7)
C(28)-O(6)-C(29)-C(30)	141.5(15)
C(32)-O(8)-C(31)-O(7)	6(2)
C(32)-O(8)-C(31)-C(23)	-179.2(9)
C(22)-C(23)-C(31)-O(7)	-46.6(15)
C(24)-C(23)-C(31)-O(7)	131.9(12)
C(22)-C(23)-C(31)-O(8)	137.4(11)
C(24)-C(23)-C(31)-O(8)	-44.2(14)
C(31)-O(8)-C(32)-C(33)	-85.3(17)

Table 7. Hydrogen bonds for $Co(C_4H_7N_2O_2)_2(C_7H_{10}N_2)(C_{19}H_{23}O_6)$ [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(2)-H(2O)...O(3)	0.98(7)	1.53(8)	2.491(7)	167(6)
O(4)-H(4O)...O(1)	1.12(7)	1.49(8)	2.495(8)	145(6)

Least-squares planes (x,y,z in crystal coordinates) and deviations from them

(* indicates atom used to define plane)

2.4011 (0.0155) x + 27.6265 (0.0177) y + 3.4470 (0.0266) z = 1.3329 (0.0144)

* -0.0357 (0.0027) N1

* 0.0400 (0.0029) N2

* -0.0359 (0.0026) N3

* 0.0403 (0.0028) N4

* -0.0087 (0.0023) Co1

-2.0669 (0.0059) N5

1.9782 (0.0066) C16

Rms deviation of fitted atoms = 0.0342