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Aminoguanidinium Hydrolysis Effected by a Hydroxo-Bridged Dicobalt(II) Complex as a Functional Model for Arginase and Catalyzed by Mononuclear Cobalt(II) Complexes

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the 40% probability thermal ellipsoids, with hydrogen atoms omitted for clarity.

Figure S3. ORTEP diagram of $[Co_2(XDK)(NO_3)_2(CH_3OH)_3(H_2O)_2]$ (**1**) (the other molecule in the asymmetric unit) showing the 40% probability thermal ellipsoids, with hydrogen atoms omitted for clarity.

Figure S4. ORTEP diagram of $[Co_2(\mu\text{-}OH)(XDK)(bpy)_2(EtOH)](NO_3)\cdot 2EtOH$ (**2**) showing the 40% probability thermal ellipsoids, with hydrogen atoms omitted for clarity.

Figure S5. ORTEP diagram of $[Co_2(\mu\text{-}Cl)(XDK)(bpy)_2(EtOH)_2]\cdot(NO_3)\cdot 3EtOH$ (**3**) showing the 40% probability thermal ellipsoids, with hydrogen atoms omitted for clarity.

Figure S6. ORTEP diagram of $[Co_2(XDK)(py)_3(NO_3)_2]\cdot MeOH\cdot 0.5Et_2O$ (**4**) showing the 40% probability thermal ellipsoids, with hydrogen atoms omitted for clarity.

Figure S7. ORTEP diagram of $[Co(XDK)(bpy)(H_2O)]\cdot 3H_2O\cdot 0.5EtOH$ (**5**) showing the 40% probability thermal ellipsoids, with hydrogen atoms omitted for clarity.

Figure S8. ORTEP diagram of $[Zn(XDK)(bpy)(H_2O)]\cdot 1.25H_2O$ (**6**) showing the 40% probability thermal ellipsoids, with hydrogen atoms omitted for clarity..

Figure S9. Hydrolysis of 0.05 M aminoguanidinium nitrate catalyzed by 0.0025 M $[Co(XDK)(bpy)(H_2O)]$ (**5**) in 37 °C incubator and 1:1 $MeOH/H_2O$ solution (0.10 M CHES buffer, pH 9.5, CHES: 2-(cyclohexylamino)-ethanesulfonic acid). Product urea was detected for 12 turnovers.

Figure S10. UV-vis studies of 0.05 M aminoguanidine nitrate hydrolysis by 0.0025 M **5** in 1:1 $MeOH/H_2O$ solution (0.10 M CHES buffer, pH 9.5) at 37 °C. Spectra a, b and c were taken at 0, 3, 30 minutes after 500 μL of 0.1 M aminoguanidine nitrate solution was injected into 500 μL of 0.005 M **5** in methanol to initiate reaction.

Figure S11. Standard calibration curve for urea determination.

Table S1. Crystal data and structure refinement for [Co2(XDK)(NO3)2(CH3OH)3-(H2O)1.625] 2.5MeOH 0.5Et2O.

Identification code	[Co2(XDK)(NO3)2(CH3OH)3(H2O)1.625] 2.5MeOH 0.5Et2O
Empirical formula	C38.25 H65.75 Co2 N4 O20.38
Formula weight	1025.56
Temperature	293(2) K
Wavelength	0.71073 A
Crystal system	Triclinic
Space group	P-1
Unit cell dimensions	a = 11.6456(2) A alpha = 70.3790(10) deg. b = 18.8160(2) A beta = 89.5860(10) deg. c = 23.1313(5) A gamma = 85.6410(10) deg.
Volume, Z	4759.59(14) A^3, 4
Density (calculated)	1.431 Mg/m^3
Absorption coefficient	0.777 mm^-1
F(000)	2161
Crystal size	0.20 x 0.20 x 0.10 mm
Theta range for data collection	1.15 to 23.00 deg.
Limiting indices	-15<=h<=14, -25<=k<=24, -15<=l<=30
Reflections collected	20697
Independent reflections	12927 [R(int) = 0.0331]
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	12236 / 0 / 1124
Goodness-of-fit on F^2	1.043
Observed reflections [I>2sigma(I)]	9044
Final R indices [I>2sigma(I)]	R1 = 0.0597, wR2 = 0.1456
R indices (all data)	R1 = 0.0960, wR2 = 0.1664
Largest diff. peak and hole	0.901 and -0.579 e.A^-3

Table S2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for [Co2(XDK)(NO3)2(CH3OH)3-(H2O)1.625] 2.5MeOH 0.5Et2O. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Co(1)	6880(1)	2832(1)	6391(1)	32(1)
Co(2)	8562(1)	2506(1)	4797(1)	27(1)
O(101)	6191(3)	2993(2)	5549(2)	30(1)
O(102)	7013(3)	3058(2)	4655(2)	29(1)
O(103)	3825(3)	2136(2)	5954(2)	29(1)
O(104)	5427(3)	1924(2)	4227(2)	26(1)
O(201)	7936(3)	1898(2)	6562(2)	31(1)
O(202)	8686(3)	1893(2)	5677(2)	32(1)
O(203)	6850(3)	288(2)	7234(2)	34(1)
O(204)	8436(3)	286(2)	5440(2)	26(1)
N(101)	4546(4)	2017(2)	5081(2)	21(1)
N(201)	7656(3)	279(2)	6344(2)	18(1)
C(101)	6221(5)	3229(3)	4972(3)	23(1)
C(102)	3903(4)	2421(3)	5401(3)	23(1)
C(103)	4760(5)	2293(3)	4444(3)	22(1)
C(104)	5780(5)	4573(3)	4457(3)	31(2)
C(105)	2246(5)	3341(4)	5360(3)	40(2)
C(106)	3867(6)	3027(4)	3430(3)	38(2)
C(107)	5255(5)	3803(3)	4609(3)	24(1)
C(108)	4158(5)	3814(3)	4986(3)	26(1)
C(109)	3327(5)	3189(3)	5032(3)	26(1)
C(110)	3047(5)	3194(3)	4388(3)	31(2)
C(111)	4139(5)	3046(3)	4067(3)	24(1)
C(112)	4944(5)	3685(3)	4007(3)	26(1)
C(201)	8703(5)	1698(3)	6246(3)	23(1)
C(202)	8610(5)	201(3)	5977(3)	21(1)
C(203)	7726(5)	195(3)	6971(3)	22(1)
C(204)	10571(5)	1803(4)	6645(3)	34(2)
C(205)	10517(5)	-446(4)	5956(3)	33(2)
C(206)	8755(5)	-486(3)	7962(3)	31(2)
C(207)	9759(4)	1214(3)	6598(2)	22(1)
C(208)	10360(5)	730(3)	6242(3)	25(1)
C(209)	9783(4)	-4(3)	6289(3)	23(1)
C(210)	9637(5)	-470(3)	6965(3)	25(1)
C(211)	8898(5)	-22(3)	7289(2)	23(1)
C(212)	9484(5)	700(3)	7246(2)	23(1)
C(301)	6088(4)	1143(3)	5716(2)	20(1)
C(302)	5021(4)	1253(3)	5433(2)	17(1)
C(303)	4359(4)	653(3)	5478(2)	20(1)
C(304)	4831(4)	-74(3)	5807(2)	20(1)
C(305)	5901(5)	-209(3)	6100(2)	21(1)
C(306)	6519(5)	418(3)	6047(2)	19(1)
C(307)	3162(5)	773(3)	5196(3)	28(1)
C(308)	6381(5)	-1003(3)	6464(3)	29(1)
N(1)	7685(5)	4212(4)	5992(3)	51(2)
N(2)	10141(5)	2464(4)	4025(3)	50(2)
O(1A)	6673(5)	4083(3)	6201(3)	44(2)
O(1B)	7073(17)	4490(12)	6388(10)	58(5)
O(2)	8144(6)	4791(3)	5755(3)	81(2)
O(3A)	8257(6)	3576(4)	5984(3)	36(2)
O(3B)	7756(19)	3662(12)	5981(9)	33(5)
O(4)	9233(4)	2904(3)	3869(2)	49(1)
O(5)	10871(5)	2401(4)	3653(3)	79(2)
O(6)	10251(4)	2077(3)	4589(2)	51(1)
O(7A)	5416(5)	2362(4)	6750(3)	43(2)

C(3A)	4592(10)	2739(7)	7061(5)	66(3)
O(7B)	5325(14)	3576(10)	6498(8)	39(4)
C(3B)	4290(23)	3326(16)	6811(13)	42(7)
O(7C)	5555(12)	1908(9)	6769(7)	20(3)
O(8)	7288(4)	2827(3)	7277(2)	46(1)
C(1)	7306(8)	2180(4)	7818(3)	67(2)
O(9)	9293(4)	3404(2)	4997(2)	45(1)
C(2)	9381(7)	4136(4)	4537(4)	62(2)
O(10)	7848(3)	1640(2)	4540(2)	31(1)
Co(3)	5885(1)	2592(1)	-256(1)	28(1)
Co(4)	7434(1)	2828(1)	1396(1)	28(1)
O(401)	5658(4)	1891(2)	572(2)	45(1)
O(402)	6522(3)	1968(2)	1400(2)	39(1)
O(403)	6496(3)	292(2)	421(2)	31(1)
O(404)	8084(3)	495(2)	2130(2)	25(1)
O(501)	7373(3)	3054(2)	-345(2)	37(1)
O(502)	8045(3)	3164(2)	520(2)	38(1)
O(503)	9140(3)	1979(2)	-810(2)	32(1)
O(504)	10664(3)	2237(2)	898(2)	31(1)
N(401)	7293(4)	341(2)	1293(2)	19(1)
N(501)	9973(4)	2093(2)	34(2)	23(1)
C(401)	5774(5)	1733(3)	1141(3)	28(1)
C(402)	6361(5)	218(3)	957(3)	26(1)
C(403)	7254(5)	322(3)	1906(3)	23(1)
C(404)	3887(5)	1809(4)	1588(3)	38(2)
C(405)	4687(5)	-532(4)	1016(3)	42(2)
C(406)	6459(5)	-338(4)	2933(3)	32(2)
C(407)	4878(5)	1233(3)	1545(3)	25(1)
C(408)	4437(5)	687(3)	1241(3)	30(2)
C(409)	5265(5)	-22(3)	1304(3)	28(1)
C(410)	5570(5)	-439(3)	1978(3)	27(1)
C(411)	6156(5)	78(3)	2258(3)	24(1)
C(412)	5356(5)	789(3)	2194(3)	25(1)
C(501)	8029(5)	3313(3)	-46(3)	27(1)
C(502)	10532(5)	2507(3)	346(3)	25(1)
C(503)	9697(5)	2363(3)	-598(3)	26(1)
C(504)	8159(5)	4659(3)	-582(3)	37(2)
C(505)	12003(5)	3411(4)	269(3)	41(2)
C(506)	10379(7)	3082(4)	-1631(3)	50(2)
C(507)	8868(5)	3890(3)	-429(3)	27(1)
C(508)	9968(5)	3895(3)	-72(3)	29(1)
C(509)	10931(5)	3268(3)	-38(3)	28(1)
C(510)	11195(5)	3257(3)	-677(3)	33(2)
C(511)	10121(5)	3115(3)	-988(3)	30(2)
C(512)	9175(5)	3757(3)	-1031(3)	32(2)
C(601)	8632(4)	1212(3)	658(2)	19(1)
C(602)	8390(4)	479(3)	989(2)	20(1)
C(603)	9175(5)	-139(3)	1046(3)	21(1)
C(604)	10234(5)	4(3)	768(2)	24(1)
C(605)	10527(4)	733(3)	439(2)	21(1)
C(606)	9697(5)	1331(3)	385(2)	21(1)
C(607)	8900(5)	-935(3)	1410(3)	31(2)
C(608)	11717(5)	865(3)	176(3)	32(2)
N(3)	5079(6)	3783(3)	1350(3)	52(2)
N(4)	4402(6)	2732(5)	-1121(3)	63(2)
O(11)	5916(4)	3589(3)	1059(2)	48(1)
O(12)	5209(6)	3691(4)	1899(3)	104(3)
O(13)	4166(5)	4043(3)	1081(3)	74(2)
O(14)	4252(4)	2313(3)	-584(3)	57(1)
O(15)	3751(5)	2797(5)	-1552(3)	112(3)
O(16)	5298(5)	3102(3)	-1196(2)	56(1)
O(17)	6900(5)	2614(3)	2306(2)	69(2)
C(4)	7402(8)	2246(6)	2869(4)	85(3)
O(18)	8414(5)	3631(3)	1542(3)	71(2)
C(5)	8164(10)	4413(5)	1314(5)	102(4)
O(19)	5008(4)	3483(2)	-22(2)	43(1)

C(6)	4742(7)	4228(4)	-431(4)	59(2)
O(20)	6762(3)	1693(2)	-514(2)	35(1)
O(21)	8860(3)	2011(2)	1732(2)	29(1)
C(1S)	6390(11)	4613(8)	7629(6)	126(4)
O(1SA)	6679(13)	3849(8)	7793(6)	92(4)
O(1SB)	5959(13)	3900(8)	7656(7)	93(4)
C(3SA)	11374(11)	2986(7)	2123(6)	55(3)
C(3SB)	10349(17)	3741(12)	1834(10)	61(5)
O(3S)	10348(10)	3213(6)	2316(5)	174(4)
C(4S)	9398(17)	6098(11)	3328(9)	85(6)
C(5S)	8156(17)	5996(11)	3117(9)	87(6)
O(4S)	8274(10)	5286(7)	2996(6)	82(4)
C(6S)	7198(17)	5130(11)	2731(9)	84(6)
C(7S)	7368(17)	4327(12)	2829(9)	87(6)
O(2S)	10217(19)	4766(12)	2585(10)	169(8)
C(2S)	11003(24)	4542(15)	2960(13)	125(9)

Table S3. Bond lengths [A] and angles [deg] for [Co2(XDK)(NO3)2-(CH3OH)3(H2O)1.625] 2.5MeOH 0.5Et2O.

Co(1)-O(3B)	1.90(2)
Co(1)-O(201)	1.992(4)
Co(1)-O(7A)	2.024(6)
Co(1)-O(101)	2.030(4)
Co(1)-O(8)	2.105(4)
Co(1)-O(3A)	2.202(7)
Co(1)-O(1A)	2.238(6)
Co(1)-O(7B)	2.27(2)
Co(1)-O(7C)	2.35(2)
Co(1)-Co(2)	4.3634(11)
Co(2)-O(202)	1.975(4)
Co(2)-O(102)	1.984(4)
Co(2)-O(9)	2.133(4)
Co(2)-O(10)	2.136(4)
Co(2)-O(6)	2.181(4)
Co(2)-O(4)	2.182(4)
O(101)-C(101)	1.258(7)
O(102)-C(101)	1.264(7)
O(103)-C(102)	1.216(7)
O(104)-C(103)	1.218(6)
O(201)-C(201)	1.263(7)
O(202)-C(201)	1.241(7)
O(203)-C(203)	1.216(6)
O(204)-C(202)	1.215(6)
N(101)-C(102)	1.405(7)
N(101)-C(103)	1.414(7)
N(101)-C(302)	1.460(7)
N(201)-C(203)	1.407(7)
N(201)-C(202)	1.422(7)
N(201)-C(306)	1.460(7)
C(101)-C(107)	1.534(8)
C(102)-C(109)	1.516(8)
C(103)-C(111)	1.522(8)
C(104)-C(107)	1.545(8)
C(105)-C(109)	1.522(8)
C(106)-C(111)	1.523(8)
C(107)-C(112)	1.532(8)
C(107)-C(108)	1.544(8)
C(108)-C(109)	1.555(8)
C(109)-C(110)	1.524(8)
C(110)-C(111)	1.522(8)
C(111)-C(112)	1.550(8)
C(201)-C(207)	1.534(8)
C(202)-C(209)	1.510(8)
C(203)-C(211)	1.517(8)
C(204)-C(207)	1.542(8)
C(205)-C(209)	1.526(7)
C(206)-C(211)	1.523(8)
C(207)-C(212)	1.533(7)
C(207)-C(208)	1.546(7)
C(208)-C(209)	1.553(8)
C(209)-C(210)	1.529(8)
C(210)-C(211)	1.523(8)
C(211)-C(212)	1.541(7)
C(301)-C(302)	1.378(7)
C(301)-C(306)	1.379(7)
C(302)-C(303)	1.389(7)
C(303)-C(304)	1.396(8)
C(303)-C(307)	1.512(7)
C(304)-C(305)	1.388(7)
C(305)-C(306)	1.398(7)

C(305)-C(308)	1.513(8)
N(1)-O(3B)	1.04(2)
N(1)-O(2)	1.207(8)
N(1)-O(1A)	1.281(8)
N(1)-O(3A)	1.331(9)
N(1)-O(1B)	1.37(2)
N(2)-O(5)	1.233(7)
N(2)-O(6)	1.263(7)
N(2)-O(4)	1.268(7)
O(7A)-C(3A)	1.472(12)
O(7B)-C(3B)	1.43(3)
O(8)-C(1)	1.421(8)
O(9)-C(2)	1.441(8)
Co(3)-O(401)	1.957(4)
Co(3)-O(501)	1.977(4)
Co(3)-O(19)	2.120(4)
Co(3)-O(16)	2.153(5)
Co(3)-O(20)	2.160(4)
Co(3)-O(14)	2.214(5)
Co(3)-Co(4)	4.4062(11)
Co(4)-O(402)	2.000(4)
Co(4)-O(502)	2.048(4)
Co(4)-O(18)	2.076(5)
Co(4)-O(17)	2.105(5)
Co(4)-O(21)	2.135(4)
Co(4)-O(11)	2.160(4)
O(401)-C(401)	1.255(7)
O(402)-C(401)	1.246(7)
O(403)-C(402)	1.211(6)
O(404)-C(403)	1.216(6)
O(501)-C(501)	1.259(7)
O(502)-C(501)	1.244(7)
O(503)-C(503)	1.224(7)
O(504)-C(502)	1.212(7)
N(401)-C(403)	1.406(7)
N(401)-C(402)	1.417(7)
N(401)-C(602)	1.453(7)
N(501)-C(503)	1.407(7)
N(501)-C(502)	1.418(7)
N(501)-C(606)	1.449(7)
C(401)-C(407)	1.547(8)
C(402)-C(409)	1.519(8)
C(403)-C(411)	1.527(8)
C(404)-C(407)	1.549(8)
C(405)-C(409)	1.534(8)
C(406)-C(411)	1.523(8)
C(407)-C(412)	1.536(8)
C(407)-C(408)	1.543(8)
C(408)-C(409)	1.551(8)
C(409)-C(410)	1.522(8)
C(410)-C(411)	1.536(8)
C(411)-C(412)	1.535(8)
C(501)-C(507)	1.556(8)
C(502)-C(509)	1.515(8)
C(503)-C(511)	1.518(8)
C(504)-C(507)	1.543(8)
C(505)-C(509)	1.525(8)
C(506)-C(511)	1.535(8)
C(507)-C(508)	1.531(8)
C(507)-C(512)	1.531(8)
C(508)-C(509)	1.548(8)
C(509)-C(510)	1.514(8)
C(510)-C(511)	1.531(9)
C(511)-C(512)	1.550(8)
C(601)-C(602)	1.383(7)
C(601)-C(606)	1.388(7)

C(602)-C(603)	1.394(7)
C(603)-C(604)	1.389(8)
C(603)-C(607)	1.508(8)
C(604)-C(605)	1.394(8)
C(605)-C(606)	1.399(7)
C(605)-C(608)	1.514(7)
N(3)-O(13)	1.217(8)
N(3)-O(12)	1.231(8)
N(3)-O(11)	1.280(7)
N(4)-O(15)	1.224(8)
N(4)-O(14)	1.247(8)
N(4)-O(16)	1.277(8)
O(17)-C(4)	1.364(9)
O(18)-C(5)	1.394(10)
O(19)-C(6)	1.416(8)
C(1S)-O(1SA)	1.37(2)
C(1S)-O(1SB)	1.45(2)
C(3SA)-O(3S)	1.36(2)
C(3SB)-O(3S)	1.22(2)
C(4S)-C(5S)	1.58(3)
C(5S)-O(4S)	1.45(2)
O(4S)-C(6S)	1.49(2)
C(6S)-C(7S)	1.45(3)
O(2S)-C(2S)	1.21(3)

O(3B)-Co(1)-O(201)	106.8(7)
O(201)-Co(1)-O(7A)	99.6(2)
O(3B)-Co(1)-O(101)	85.5(6)
O(201)-Co(1)-O(101)	104.1(2)
O(7A)-Co(1)-O(101)	87.5(2)
O(3B)-Co(1)-O(8)	94.7(6)
O(201)-Co(1)-O(8)	87.9(2)
O(7A)-Co(1)-O(8)	86.8(2)
O(101)-Co(1)-O(8)	167.5(2)
O(201)-Co(1)-O(3A)	92.7(2)
O(7A)-Co(1)-O(3A)	167.5(3)
O(101)-Co(1)-O(3A)	91.3(2)
O(8)-Co(1)-O(3A)	91.8(2)
O(201)-Co(1)-O(1A)	148.1(2)
O(7A)-Co(1)-O(1A)	109.8(2)
O(101)-Co(1)-O(1A)	89.6(2)
O(8)-Co(1)-O(1A)	81.9(2)
O(3A)-Co(1)-O(1A)	57.8(2)
O(3B)-Co(1)-O(7B)	94.1(8)
O(201)-Co(1)-O(7B)	157.7(4)
O(101)-Co(1)-O(7B)	84.9(4)
O(8)-Co(1)-O(7B)	82.5(4)
O(3B)-Co(1)-O(7C)	170.2(7)
O(201)-Co(1)-O(7C)	80.1(4)
O(101)-Co(1)-O(7C)	86.1(4)
O(8)-Co(1)-O(7C)	92.4(4)
O(7B)-Co(1)-O(7C)	80.2(6)
O(202)-Co(2)-O(102)	107.1(2)
O(202)-Co(2)-O(9)	89.3(2)
O(102)-Co(2)-O(9)	91.7(2)
O(202)-Co(2)-O(10)	94.0(2)
O(102)-Co(2)-O(10)	88.1(2)
O(9)-Co(2)-O(10)	176.6(2)
O(202)-Co(2)-O(6)	93.8(2)
O(102)-Co(2)-O(6)	159.0(2)
O(9)-Co(2)-O(6)	91.3(2)
O(10)-Co(2)-O(6)	87.6(2)
O(202)-Co(2)-O(4)	152.7(2)
O(102)-Co(2)-O(4)	100.3(2)
O(9)-Co(2)-O(4)	90.3(2)
O(10)-Co(2)-O(4)	86.4(2)

O(6)-Co(2)-O(4)	58.9(2)
C(101)-O(101)-Co(1)	152.3(4)
C(101)-O(102)-Co(2)	137.7(4)
C(201)-O(201)-Co(1)	132.3(4)
C(201)-O(202)-Co(2)	162.7(4)
C(102)-N(101)-C(103)	124.8(5)
C(102)-N(101)-C(302)	117.3(4)
C(103)-N(101)-C(302)	117.9(4)
C(203)-N(201)-C(202)	124.9(4)
C(203)-N(201)-C(306)	118.4(4)
C(202)-N(201)-C(306)	116.6(4)
O(101)-C(101)-O(102)	125.6(5)
O(101)-C(101)-C(107)	118.6(5)
O(102)-C(101)-C(107)	115.8(5)
O(103)-C(102)-N(101)	118.7(5)
O(103)-C(102)-C(109)	123.6(5)
N(101)-C(102)-C(109)	117.7(5)
O(104)-C(103)-N(101)	119.0(5)
O(104)-C(103)-C(111)	123.5(5)
N(101)-C(103)-C(111)	117.5(5)
C(112)-C(107)-C(101)	112.4(4)
C(112)-C(107)-C(108)	109.7(5)
C(101)-C(107)-C(108)	113.2(5)
C(112)-C(107)-C(104)	108.8(5)
C(101)-C(107)-C(104)	103.7(4)
C(108)-C(107)-C(104)	108.8(4)
C(107)-C(108)-C(109)	116.4(4)
C(102)-C(109)-C(105)	108.9(5)
C(102)-C(109)-C(110)	109.0(5)
C(105)-C(109)-C(110)	111.6(5)
C(102)-C(109)-C(108)	109.6(5)
C(105)-C(109)-C(108)	108.7(5)
C(110)-C(109)-C(108)	109.1(5)
C(111)-C(110)-C(109)	110.7(5)
C(103)-C(111)-C(106)	108.9(5)
C(103)-C(111)-C(110)	109.9(5)
C(106)-C(111)-C(110)	111.3(5)
C(103)-C(111)-C(112)	108.7(4)
C(106)-C(111)-C(112)	109.1(5)
C(110)-C(111)-C(112)	108.9(5)
C(107)-C(112)-C(111)	115.6(5)
O(202)-C(201)-O(201)	125.0(5)
O(202)-C(201)-C(207)	118.2(5)
O(201)-C(201)-C(207)	116.7(5)
O(204)-C(202)-N(201)	118.6(5)
O(204)-C(202)-C(209)	124.1(5)
N(201)-C(202)-C(209)	117.3(5)
O(203)-C(203)-N(201)	119.0(5)
O(203)-C(203)-C(211)	123.0(5)
N(201)-C(203)-C(211)	118.0(4)
C(201)-C(207)-C(212)	113.2(4)
C(201)-C(207)-C(204)	103.6(4)
C(212)-C(207)-C(204)	109.1(4)
C(201)-C(207)-C(208)	112.0(5)
C(212)-C(207)-C(208)	109.4(5)
C(204)-C(207)-C(208)	109.3(4)
C(207)-C(208)-C(209)	115.2(4)
C(202)-C(209)-C(205)	108.1(5)
C(202)-C(209)-C(210)	109.0(4)
C(205)-C(209)-C(210)	111.7(5)
C(202)-C(209)-C(208)	109.5(4)
C(205)-C(209)-C(208)	109.0(4)
C(210)-C(209)-C(208)	109.6(5)
C(211)-C(210)-C(209)	111.0(5)
C(203)-C(211)-C(206)	109.6(4)
C(203)-C(211)-C(210)	108.8(4)

C(206)-C(211)-C(210)	111.1(5)
C(203)-C(211)-C(212)	109.4(4)
C(206)-C(211)-C(212)	109.2(4)
C(210)-C(211)-C(212)	108.8(4)
C(207)-C(212)-C(211)	116.1(4)
C(302)-C(301)-C(306)	119.2(5)
C(301)-C(302)-C(303)	121.8(5)
C(301)-C(302)-N(101)	120.1(5)
C(303)-C(302)-N(101)	118.0(5)
C(302)-C(303)-C(304)	117.4(5)
C(302)-C(303)-C(307)	122.1(5)
C(304)-C(303)-C(307)	120.5(5)
C(305)-C(304)-C(303)	122.5(5)
C(304)-C(305)-C(306)	117.4(5)
C(304)-C(305)-C(308)	121.3(5)
C(306)-C(305)-C(308)	121.2(5)
C(301)-C(306)-C(305)	121.6(5)
C(301)-C(306)-N(201)	120.7(5)
C(305)-C(306)-N(201)	117.7(5)
O(3B)-N(1)-O(2)	137.3(13)
O(3B)-N(1)-O(1A)	87.1(13)
O(2)-N(1)-O(1A)	132.3(7)
O(2)-N(1)-O(3A)	116.7(6)
O(1A)-N(1)-O(3A)	110.5(7)
O(3B)-N(1)-O(1B)	128(2)
O(2)-N(1)-O(1B)	93.7(10)
O(5)-N(2)-O(6)	121.4(7)
O(5)-N(2)-O(4)	122.6(7)
O(6)-N(2)-O(4)	115.9(5)
O(1B)-O(1A)-N(1)	69.0(11)
N(1)-O(1A)-Co(1)	95.7(4)
N(1)-O(3A)-Co(1)	95.9(5)
N(1)-O(3B)-Co(1)	130(2)
N(2)-O(4)-Co(2)	92.4(4)
N(2)-O(6)-Co(2)	92.6(4)
C(3A)-O(7A)-Co(1)	121.3(6)
C(3B)-O(7B)-Co(1)	126(2)
C(1)-O(8)-Co(1)	124.7(4)
C(2)-O(9)-Co(2)	122.0(4)
O(401)-Co(3)-O(501)	113.1(2)
O(401)-Co(3)-O(19)	90.1(2)
O(501)-Co(3)-O(19)	93.0(2)
O(401)-Co(3)-O(16)	149.4(2)
O(501)-Co(3)-O(16)	97.5(2)
O(19)-Co(3)-O(16)	90.9(2)
O(401)-Co(3)-O(20)	90.8(2)
O(501)-Co(3)-O(20)	87.3(2)
O(19)-Co(3)-O(20)	178.8(2)
O(16)-Co(3)-O(20)	87.9(2)
O(401)-Co(3)-O(14)	91.1(2)
O(501)-Co(3)-O(14)	155.5(2)
O(19)-Co(3)-O(14)	90.9(2)
O(16)-Co(3)-O(14)	58.3(2)
O(20)-Co(3)-O(14)	88.3(2)
O(402)-Co(4)-O(502)	101.5(2)
O(402)-Co(4)-O(18)	170.8(2)
O(502)-Co(4)-O(18)	86.6(2)
O(402)-Co(4)-O(17)	86.2(2)
O(502)-Co(4)-O(17)	172.2(2)
O(18)-Co(4)-O(17)	85.7(2)
O(402)-Co(4)-O(21)	87.1(2)
O(502)-Co(4)-O(21)	92.3(2)
O(18)-Co(4)-O(21)	88.4(2)
O(17)-Co(4)-O(21)	89.0(2)
O(402)-Co(4)-O(11)	88.9(2)
O(502)-Co(4)-O(11)	88.7(2)

O(18)-Co(4)-O(11)	95.6(2)
O(17)-Co(4)-O(11)	90.5(2)
O(21)-Co(4)-O(11)	175.9(2)
C(401)-O(401)-Co(3)	148.6(4)
C(401)-O(402)-Co(4)	147.6(4)
C(501)-O(501)-Co(3)	139.6(4)
C(501)-O(502)-Co(4)	157.6(4)
C(403)-N(401)-C(402)	125.3(5)
C(403)-N(401)-C(602)	116.9(4)
C(402)-N(401)-C(602)	117.7(4)
C(503)-N(501)-C(502)	124.4(5)
C(503)-N(501)-C(606)	117.6(5)
C(502)-N(501)-C(606)	117.9(5)
O(402)-C(401)-O(401)	125.3(6)
O(402)-C(401)-C(407)	118.2(6)
O(401)-C(401)-C(407)	116.4(6)
O(403)-C(402)-N(401)	118.3(5)
O(403)-C(402)-C(409)	124.4(5)
N(401)-C(402)-C(409)	117.2(5)
O(404)-C(403)-N(401)	119.2(5)
O(404)-C(403)-C(411)	123.3(5)
N(401)-C(403)-C(411)	117.5(5)
C(412)-C(407)-C(408)	110.3(5)
C(412)-C(407)-C(401)	112.0(5)
C(408)-C(407)-C(401)	111.3(5)
C(412)-C(407)-C(404)	109.0(5)
C(408)-C(407)-C(404)	110.2(5)
C(401)-C(407)-C(404)	103.8(5)
C(407)-C(408)-C(409)	114.9(5)
C(402)-C(409)-C(410)	109.0(5)
C(402)-C(409)-C(405)	107.9(5)
C(410)-C(409)-C(405)	111.3(5)
C(402)-C(409)-C(408)	109.7(5)
C(410)-C(409)-C(408)	109.7(5)
C(405)-C(409)-C(408)	109.2(5)
C(409)-C(410)-C(411)	110.6(5)
C(406)-C(411)-C(403)	109.5(5)
C(406)-C(411)-C(412)	109.6(5)
C(403)-C(411)-C(412)	108.5(4)
C(406)-C(411)-C(410)	110.6(5)
C(403)-C(411)-C(410)	108.5(4)
C(412)-C(411)-C(410)	110.0(5)
C(411)-C(412)-C(407)	116.0(5)
O(502)-C(501)-O(501)	126.1(5)
O(502)-C(501)-C(507)	117.5(5)
O(501)-C(501)-C(507)	116.3(5)
O(504)-C(502)-N(501)	118.8(5)
O(504)-C(502)-C(509)	123.8(5)
N(501)-C(502)-C(509)	117.5(5)
O(503)-C(503)-N(501)	118.8(5)
O(503)-C(503)-C(511)	122.8(5)
N(501)-C(503)-C(511)	118.3(5)
C(508)-C(507)-C(512)	110.1(5)
C(508)-C(507)-C(504)	109.9(5)
C(512)-C(507)-C(504)	108.5(5)
C(508)-C(507)-C(501)	113.1(5)
C(512)-C(507)-C(501)	111.6(5)
C(504)-C(507)-C(501)	103.5(4)
C(507)-C(508)-C(509)	116.5(5)
C(510)-C(509)-C(502)	109.0(5)
C(510)-C(509)-C(505)	110.7(5)
C(502)-C(509)-C(505)	108.6(5)
C(510)-C(509)-C(508)	109.8(5)
C(502)-C(509)-C(508)	109.3(4)
C(505)-C(509)-C(508)	109.3(5)
C(509)-C(510)-C(511)	111.0(5)

C(503)-C(511)-C(510)	108.7(5)
C(503)-C(511)-C(506)	108.4(5)
C(510)-C(511)-C(506)	111.8(5)
C(503)-C(511)-C(512)	109.2(5)
C(510)-C(511)-C(512)	108.6(5)
C(506)-C(511)-C(512)	110.0(5)
C(507)-C(512)-C(511)	116.3(5)
C(602)-C(601)-C(606)	118.6(5)
C(601)-C(602)-C(603)	122.0(5)
C(601)-C(602)-N(401)	119.6(5)
C(603)-C(602)-N(401)	118.3(5)
C(604)-C(603)-C(602)	117.6(5)
C(604)-C(603)-C(607)	121.0(5)
C(602)-C(603)-C(607)	121.4(5)
C(603)-C(604)-C(605)	122.5(5)
C(604)-C(605)-C(606)	117.4(5)
C(604)-C(605)-C(608)	120.6(5)
C(606)-C(605)-C(608)	121.9(5)
C(601)-C(606)-C(605)	121.7(5)
C(601)-C(606)-N(501)	119.8(5)
C(605)-C(606)-N(501)	118.4(5)
O(13)-N(3)-O(12)	121.4(7)
O(13)-N(3)-O(11)	119.3(7)
O(12)-N(3)-O(11)	119.3(7)
O(15)-N(4)-O(14)	123.8(8)
O(15)-N(4)-O(16)	121.2(8)
O(14)-N(4)-O(16)	115.0(6)
N(3)-O(11)-Co(4)	130.3(4)
N(4)-O(14)-Co(3)	92.3(4)
N(4)-O(16)-Co(3)	94.3(4)
C(4)-O(17)-Co(4)	134.5(5)
C(5)-O(18)-Co(4)	126.0(6)
C(6)-O(19)-Co(3)	125.3(4)
O(4S)-C(5S)-C(4S)	105(2)
C(5S)-O(4S)-C(6S)	112.3(14)
C(7S)-C(6S)-O(4S)	103(2)

Symmetry transformations used to generate equivalent atoms:

Table S4. Anisotropic displacement parameters (A^2 x 10^3) for [Co2(XDK)-(NO3)2(CH3OH)3(H2O)1.625] 2.5MeOH 0.5Et2O. 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)	46(1)	25(1)	23(1)	-9(1)	-5(1)	6(1)
Co(2)	23(1)	31(1)	23(1)	-4(1)	2(1)	-2(1)
O(101)	30(2)	35(3)	24(3)	-8(2)	-5(2)	0(2)
O(102)	21(2)	34(3)	31(2)	-11(2)	2(2)	2(2)
O(103)	30(2)	30(2)	25(3)	-6(2)	6(2)	-3(2)
O(104)	32(2)	24(2)	22(2)	-7(2)	-2(2)	-2(2)
O(201)	29(2)	36(3)	28(2)	-12(2)	3(2)	6(2)
O(202)	35(2)	33(3)	22(3)	-3(2)	-2(2)	3(2)
O(203)	22(2)	55(3)	25(2)	-15(2)	3(2)	-4(2)
O(204)	29(2)	33(2)	17(2)	-11(2)	0(2)	0(2)
N(101)	21(3)	20(3)	23(3)	-8(2)	-3(2)	-2(2)
N(201)	15(2)	20(3)	17(3)	-5(2)	-1(2)	-1(2)
C(101)	28(3)	18(3)	25(4)	-8(3)	-4(3)	-7(3)
C(102)	17(3)	20(3)	30(4)	-6(3)	-1(3)	-5(2)
C(103)	22(3)	22(3)	23(3)	-8(3)	-4(3)	-9(3)
C(104)	33(4)	24(3)	35(4)	-7(3)	1(3)	-4(3)
C(105)	27(4)	34(4)	56(5)	-9(3)	4(3)	2(3)
C(106)	48(4)	26(4)	36(4)	-4(3)	-14(3)	-1(3)
C(107)	26(3)	19(3)	25(3)	-7(3)	1(3)	-3(3)
C(108)	30(3)	19(3)	29(4)	-6(3)	-1(3)	-2(3)
C(109)	23(3)	22(3)	33(4)	-8(3)	3(3)	-1(3)
C(110)	29(3)	20(3)	37(4)	-3(3)	-9(3)	-1(3)
C(111)	24(3)	23(3)	22(3)	-5(3)	-10(3)	0(3)
C(112)	32(3)	19(3)	24(3)	-2(3)	-4(3)	1(3)
C(201)	28(3)	20(3)	23(4)	-6(3)	-3(3)	-10(3)
C(202)	24(3)	13(3)	28(4)	-9(3)	6(3)	-4(2)
C(203)	19(3)	22(3)	27(4)	-11(3)	4(3)	-4(2)
C(204)	25(3)	44(4)	33(4)	-13(3)	-1(3)	-10(3)
C(205)	23(3)	46(4)	33(4)	-19(3)	-2(3)	8(3)
C(206)	29(3)	37(4)	24(4)	-5(3)	1(3)	-9(3)
C(207)	14(3)	27(3)	22(3)	-7(3)	2(2)	-2(2)
C(208)	17(3)	27(3)	28(3)	-4(3)	4(3)	-3(3)
C(209)	16(3)	26(3)	27(3)	-10(3)	1(3)	3(2)
C(210)	23(3)	18(3)	29(4)	-5(3)	-4(3)	3(3)
C(211)	20(3)	25(3)	21(3)	-5(3)	-3(2)	-2(3)
C(212)	17(3)	28(3)	24(3)	-11(3)	-5(2)	2(2)
C(301)	21(3)	17(3)	22(3)	-7(3)	7(2)	-6(2)
C(302)	19(3)	15(3)	18(3)	-5(2)	0(2)	-1(2)
C(303)	18(3)	25(3)	19(3)	-10(3)	4(2)	-6(3)
C(304)	21(3)	20(3)	21(3)	-8(3)	5(2)	-11(2)
C(305)	26(3)	20(3)	17(3)	-7(3)	-2(2)	0(3)
C(306)	24(3)	22(3)	13(3)	-9(3)	3(2)	-2(3)
C(307)	26(3)	34(4)	28(4)	-13(3)	-2(3)	-5(3)
C(308)	33(4)	23(3)	31(4)	-8(3)	-4(3)	-2(3)
N(1)	50(4)	42(4)	51(4)	-5(3)	-1(3)	0(3)
N(2)	34(4)	78(5)	49(4)	-32(4)	14(3)	-23(4)
O(2)	113(5)	27(3)	96(5)	-8(3)	-11(4)	-21(3)
O(4)	43(3)	60(3)	39(3)	-8(2)	7(2)	-8(3)
O(5)	56(4)	128(6)	68(4)	-48(4)	43(3)	-24(3)
O(6)	32(3)	76(4)	43(3)	-20(3)	2(2)	2(2)
O(8)	66(3)	47(3)	25(3)	-13(2)	-10(2)	3(2)
C(1)	100(7)	59(6)	29(5)	-6(4)	-4(4)	21(5)
O(9)	42(3)	32(3)	57(3)	-7(2)	-7(2)	-13(2)
C(2)	65(5)	39(5)	77(6)	-10(4)	4(4)	-21(4)
O(10)	35(2)	35(3)	28(2)	-16(2)	2(2)	-3(2)
Co(3)	25(1)	31(1)	24(1)	-5(1)	-1(1)	-5(1)

Co(4)	33(1)	27(1)	26(1)	-9(1)	0(1)	-1(1)
O(401)	61(3)	40(3)	30(3)	-5(2)	11(2)	-10(2)
O(402)	26(2)	37(3)	46(3)	-1(2)	0(2)	-13(2)
O(403)	33(2)	36(3)	27(3)	-15(2)	1(2)	-9(2)
O(404)	19(2)	35(2)	22(2)	-8(2)	-3(2)	-5(2)
O(501)	28(2)	46(3)	46(3)	-24(2)	6(2)	-14(2)
O(502)	30(2)	43(3)	34(3)	-5(2)	6(2)	-9(2)
O(503)	39(3)	33(3)	24(2)	-9(2)	4(2)	-4(2)
O(504)	29(2)	29(2)	31(3)	-6(2)	-5(2)	-4(2)
N(401)	20(2)	21(3)	19(3)	-8(2)	2(2)	-6(2)
N(501)	24(3)	20(3)	22(3)	-4(2)	5(2)	-4(2)
C(401)	21(3)	20(3)	33(4)	0(3)	7(3)	8(3)
C(402)	31(3)	21(3)	27(4)	-11(3)	0(3)	-2(3)
C(403)	28(3)	15(3)	23(3)	-3(3)	1(3)	1(3)
C(404)	21(3)	39(4)	46(4)	-4(3)	1(3)	4(3)
C(405)	36(4)	46(4)	50(5)	-21(4)	3(3)	-20(3)
C(406)	31(3)	40(4)	23(3)	-9(3)	6(3)	-4(3)
C(407)	20(3)	28(3)	24(3)	-4(3)	-1(3)	-3(3)
C(408)	16(3)	40(4)	32(4)	-10(3)	1(3)	-9(3)
C(409)	25(3)	29(4)	32(4)	-13(3)	1(3)	-13(3)
C(410)	24(3)	26(3)	32(4)	-10(3)	6(3)	-6(3)
C(411)	22(3)	28(3)	20(3)	-5(3)	3(2)	-2(3)
C(412)	22(3)	28(3)	27(3)	-11(3)	9(3)	-5(3)
C(501)	23(3)	19(3)	35(4)	-4(3)	8(3)	3(3)
C(502)	15(3)	27(4)	36(4)	-13(3)	1(3)	2(3)
C(503)	26(3)	32(4)	23(4)	-12(3)	7(3)	1(3)
C(504)	32(4)	26(4)	45(4)	-2(3)	-1(3)	3(3)
C(505)	31(4)	29(4)	56(5)	-4(3)	-4(3)	-10(3)
C(506)	79(5)	40(4)	27(4)	-5(3)	23(4)	-11(4)
C(507)	25(3)	22(3)	30(4)	-5(3)	4(3)	-3(3)
C(508)	28(3)	18(3)	40(4)	-8(3)	4(3)	-7(3)
C(509)	20(3)	24(3)	37(4)	-6(3)	4(3)	-4(3)
C(510)	30(4)	23(4)	42(4)	-5(3)	15(3)	-3(3)
C(511)	37(4)	25(4)	23(3)	-1(3)	13(3)	-3(3)
C(512)	37(4)	23(4)	29(4)	2(3)	5(3)	-8(3)
C(601)	17(3)	22(3)	20(3)	-9(3)	-2(2)	0(2)
C(602)	20(3)	25(3)	16(3)	-8(3)	0(2)	-5(3)
C(603)	25(3)	23(3)	20(3)	-13(3)	2(3)	-4(3)
C(604)	30(3)	26(4)	20(3)	-11(3)	-2(3)	4(3)
C(605)	19(3)	23(3)	21(3)	-11(3)	-3(2)	1(3)
C(606)	22(3)	19(3)	21(3)	-7(3)	0(3)	-5(3)
C(607)	39(4)	21(3)	35(4)	-13(3)	6(3)	-3(3)
C(608)	26(3)	34(4)	38(4)	-15(3)	5(3)	-2(3)
N(3)	60(5)	46(4)	49(4)	-18(3)	6(4)	10(3)
N(4)	43(4)	105(6)	45(5)	-37(4)	-13(4)	21(4)
O(11)	55(3)	44(3)	40(3)	-13(2)	1(2)	19(2)
O(12)	102(5)	148(7)	58(4)	-46(4)	-4(4)	64(5)
O(13)	53(4)	72(4)	79(4)	-8(3)	-3(3)	21(3)
O(14)	39(3)	85(4)	55(4)	-33(3)	-4(3)	-10(3)
O(15)	65(4)	215(9)	73(5)	-78(5)	-39(4)	25(5)
O(16)	50(3)	70(4)	37(3)	-6(3)	-7(2)	6(3)
O(17)	81(4)	93(4)	27(3)	-20(3)	-2(3)	29(3)
C(4)	86(7)	118(9)	39(5)	-15(5)	-1(5)	12(6)
O(18)	104(5)	37(3)	76(4)	-23(3)	-18(3)	-20(3)
C(5)	156(11)	53(6)	108(9)	-34(6)	30(8)	-40(7)
O(19)	41(3)	33(3)	51(3)	-11(2)	3(2)	6(2)
C(6)	61(5)	41(5)	67(6)	-11(4)	0(4)	4(4)
O(20)	39(3)	38(3)	31(3)	-16(2)	-4(2)	-4(2)
O(21)	27(2)	31(2)	28(2)	-8(2)	-5(2)	-1(2)

Table S5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for [Co2(XDK)(NO3)2(CH3OH)3-(H2O)1.625] 2.5MeOH 0.5Et2O.

	x	y	z	U(eq)
H(10A)	5979(5)	4654(3)	4832(3)	47
H(10B)	5229(5)	4971(3)	4226(3)	47
H(10C)	6460(5)	4574(3)	4219(3)	47
H(10D)	1875(5)	3826(4)	5129(3)	61
H(10E)	2453(5)	3337(4)	5762(3)	61
H(10F)	1730(5)	2955(4)	5395(3)	61
H(10G)	3475(6)	3500(4)	3188(3)	58
H(10H)	3384(6)	2623(4)	3465(3)	58
H(10I)	4571(6)	2944(4)	3235(3)	58
H(10J)	3733(5)	4303(3)	4807(3)	31
H(10K)	4392(5)	3770(3)	5399(3)	31
H(11A)	2524(5)	2807(3)	4414(3)	37
H(11B)	2666(5)	3680(3)	4151(3)	37
H(11C)	5651(5)	3575(3)	3819(3)	32
H(11D)	4578(5)	4156(3)	3732(3)	32
H(20A)	11266(5)	1547(4)	6861(3)	51
H(20B)	10198(5)	2107(4)	6863(3)	51
H(20C)	10756(5)	2122(4)	6240(3)	51
H(20D)	11268(5)	-582(4)	6148(3)	50
H(20E)	10589(5)	-137(4)	5535(3)	50
H(20F)	10157(5)	-896(4)	5977(3)	50
H(20G)	9497(5)	-623(3)	8163(3)	46
H(20H)	8387(5)	-936(3)	7991(3)	46
H(20I)	8289(5)	-191(3)	8156(3)	46
H(20J)	11149(5)	592(3)	6394(3)	30
H(20K)	10386(5)	1039(3)	5813(3)	30
H(21A)	9279(5)	-930(3)	6993(3)	30
H(21B)	10388(5)	-614(3)	7167(3)	30
H(21C)	8989(5)	994(3)	7436(2)	27
H(21D)	10197(5)	552(3)	7485(2)	27
H(30A)	6511(4)	1554(3)	5685(2)	24
H(30B)	4412(4)	-485(3)	5831(2)	23
H(30C)	2849(5)	293(3)	5277(3)	42
H(30D)	3199(5)	1024(3)	4761(3)	42
H(30E)	2678(5)	1080(3)	5372(3)	42
H(30F)	7125(5)	-985(3)	6632(3)	44
H(30G)	6453(5)	-1301(3)	6199(3)	44
H(30H)	5871(5)	-1227(3)	6791(3)	44
H(1A)	7516(8)	2318(4)	8165(3)	100
H(1B)	7858(8)	1796(4)	7776(3)	100
H(1C)	6556(8)	1991(4)	7878(3)	100
H(2A)	9732(7)	4461(4)	4716(4)	93
H(2B)	8626(7)	4353(4)	4381(4)	93
H(2C)	9845(7)	4081(4)	4208(4)	93
H(40A)	3584(5)	2089(4)	1184(3)	57
H(40B)	4175(5)	2152(4)	1770(3)	57
H(40C)	3288(5)	1544(4)	1837(3)	57
H(40D)	3990(5)	-691(4)	1228(3)	62
H(40E)	5200(5)	-968(4)	1048(3)	62
H(40F)	4509(5)	-256(4)	591(3)	62
H(40G)	5768(5)	-491(4)	3154(3)	47
H(40H)	6828(5)	-8(4)	3099(3)	47
H(40I)	6970(5)	-777(4)	2971(3)	47
H(40J)	4294(5)	964(3)	808(3)	35
H(40K)	3708(5)	521(3)	1421(3)	35
H(41A)	6084(5)	-883(3)	2016(3)	32

H(41B)	4876(5)	-604(3)	2200(3)	32
H(41C)	5774(5)	1127(3)	2337(3)	30
H(41D)	4711(5)	640(3)	2464(3)	30
H(50A)	7471(5)	4653(3)	-806(3)	56
H(50B)	8610(5)	5055(3)	-828(3)	56
H(50C)	7956(5)	4750(3)	-209(3)	56
H(50D)	11819(5)	3416(4)	673(3)	62
H(50E)	12268(5)	3891(4)	29(3)	62
H(50F)	12597(5)	3017(4)	298(3)	62
H(50G)	10648(7)	3554(4)	-1884(3)	75
H(50H)	9689(7)	2990(4)	-1811(3)	75
H(50I)	10959(7)	2679(4)	-1599(3)	75
H(50J)	9758(5)	3855(3)	344(3)	34
H(50K)	10281(5)	4382(3)	-258(3)	34
H(51A)	11798(5)	2863(3)	-653(3)	40
H(51B)	11472(5)	3738(3)	-922(3)	40
H(51C)	9422(5)	4224(3)	-1318(3)	39
H(51D)	8481(5)	3645(3)	-1202(3)	39
H(60A)	8091(4)	1616(3)	619(2)	23
H(60B)	10768(5)	-403(3)	803(2)	29
H(60C)	8136(5)	-926(3)	1567(3)	46
H(60D)	9443(5)	-1147(3)	1745(3)	46
H(60E)	8945(5)	-1238(3)	1148(3)	46
H(60F)	11768(5)	1396(3)	-35(3)	48
H(60G)	11853(5)	594(3)	-107(3)	48
H(60H)	12283(5)	688(3)	502(3)	48
H(4A)	6872(8)	2270(6)	3183(4)	127
H(4B)	8084(8)	2484(6)	2909(4)	127
H(4C)	7604(8)	1727(6)	2911(4)	127
H(5A)	8753(10)	4656(5)	1448(5)	153
H(5B)	7433(10)	4539(5)	1465(5)	153
H(5C)	8133(10)	4583(5)	874(5)	153
H(6A)	4343(7)	4526(4)	-216(4)	88
H(6B)	4262(7)	4213(4)	-762(4)	88
H(6C)	5442(7)	4450(4)	-593(4)	88

Table S6. Crystal data and structure refinement for [Co2(OH)(XDK)(bpy)2-(EtOH)](NO3).2EtOH

Identification code	[Co2(OH)(XDK)(bpy)2(EtOH)](NO3).2EtOH
Empirical formula	C58 H73 Co2 N7 O15
Formula weight	1226.09
Temperature	293(2) K
Wavelength	0.71073 A
Crystal system	Monoclinic
Space group	P2(1)/c
Unit cell dimensions	a = 12.3880(4) A alpha = 90 deg. b = 16.7363(6) A beta = 94.1760(10) deg. c = 27.9451(10) A gamma = 90 deg.
Volume, Z	5778.5(3) A^3, 4
Density (calculated)	1.409 Mg/m^3
Absorption coefficient	0.648 mm^-1
F(000)	2576
Crystal size	0.25 x 0.25 x 0.15 mm
Theta range for data collection	1.42 to 22.50 deg.
Limiting indices	-16<=h<=12, -18<=k<=22, -29<=l<=37
Reflections collected	22848
Independent reflections	7492 [R(int) = 0.0795]
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	7109 / 0 / 733
Goodness-of-fit on F^2	1.039
Observed reflections [I>2sigma(I)]	4870
Final R indices [I>2sigma(I)]	R1 = 0.0647, wR2 = 0.1328
R indices (all data)	R1 = 0.1164, wR2 = 0.1543
Largest diff. peak and hole	0.676 and -0.316 e.A^-3

Table S7. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for [Co2(OH)(XDK)(bpy)2(EtOH)]-(NO3).2EtOH. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Co(1)	6539(1)	6913(1)	1402(1)	27(1)
Co(2)	8746(1)	6296(1)	948(1)	27(1)
O(101)	6776(3)	7282(2)	690(1)	29(1)
O(102)	7924(3)	6531(3)	308(1)	33(1)
O(103)	6051(3)	9191(3)	405(2)	37(1)
O(104)	8776(3)	8132(2)	-388(1)	33(1)
O(201)	7873(3)	7573(2)	1702(1)	28(1)
O(202)	9390(3)	7010(2)	1475(1)	31(1)
O(203)	8029(3)	9589(3)	1820(2)	35(1)
O(204)	11091(3)	8542(3)	1292(2)	36(1)
N(101)	7412(4)	8644(3)	14(2)	24(1)
N(201)	9530(4)	9021(3)	1557(2)	23(1)
C(101)	7032(5)	6912(4)	328(2)	30(2)
C(102)	6295(5)	8746(4)	89(2)	29(2)
C(103)	7803(5)	8194(3)	-359(2)	24(2)
C(104)	5770(5)	5993(4)	-82(2)	38(2)
C(105)	4409(5)	8775(4)	-262(3)	44(2)
C(106)	7464(5)	7836(4)	-1218(2)	39(2)
C(107)	6221(4)	6846(4)	-108(2)	26(2)
C(108)	5277(5)	7447(4)	-82(2)	30(2)
C(109)	5484(5)	8315(4)	-249(2)	30(2)
C(110)	5926(5)	8298(4)	-746(2)	32(2)
C(111)	6985(5)	7829(4)	-728(2)	27(2)
C(112)	6748(5)	6956(4)	-585(2)	28(2)
C(201)	8852(5)	7362(4)	1775(2)	25(2)
C(202)	10571(5)	8676(4)	1633(2)	30(2)
C(203)	8861(5)	9246(4)	1925(2)	28(2)
C(204)	9189(5)	6693(4)	2534(2)	43(2)
C(205)	12205(5)	8544(5)	2203(2)	47(2)
C(206)	8751(5)	9617(4)	2779(2)	43(2)
C(207)	9400(5)	7487(4)	2279(2)	28(2)
C(208)	10623(5)	7623(4)	2272(2)	31(2)
C(209)	10968(5)	8482(4)	2149(2)	31(2)
C(210)	10475(5)	9072(4)	2486(2)	34(2)
C(211)	9242(5)	9024(4)	2437(2)	28(2)
C(212)	8885(5)	8174(4)	2553(2)	33(2)
C(301)	8518(4)	8821(4)	774(2)	22(2)
C(302)	8166(4)	9105(3)	325(2)	22(1)
C(303)	8488(5)	9853(4)	169(2)	27(2)
C(304)	9182(5)	10300(4)	474(2)	32(2)
C(305)	9537(5)	10033(4)	928(2)	30(2)
C(306)	9189(5)	9288(4)	1077(2)	24(2)
C(307)	8070(5)	10181(4)	-316(2)	37(2)
C(308)	10268(6)	10545(4)	1261(2)	46(2)
N(1)	4906(4)	6430(3)	1232(2)	35(1)
N(2)	5544(4)	7939(3)	1401(2)	31(1)
N(3)	10211(4)	6528(3)	570(2)	29(1)
N(4)	9523(4)	5195(3)	917(2)	27(1)
C(1)	4633(5)	5669(4)	1200(2)	41(2)
C(2)	3582(6)	5398(5)	1232(2)	47(2)
C(3)	2786(6)	5937(5)	1301(2)	45(2)
C(4)	3044(5)	6742(5)	1310(2)	44(2)
C(5)	4118(5)	6973(4)	1277(2)	32(2)
C(6)	4460(5)	7813(4)	1294(2)	29(2)
C(7)	3768(5)	8470(4)	1207(2)	37(2)

C(8)	4177(6)	9226(4)	1242(2)	40(2)
C(9)	5252(5)	9344(4)	1355(2)	35(2)
C(10)	5906(5)	8686(4)	1426(2)	31(2)
C(11)	10544(5)	7236(4)	429(2)	38(2)
C(12)	11427(5)	7344(4)	159(3)	44(2)
C(13)	11985(5)	6674(5)	32(2)	41(2)
C(14)	11652(5)	5929(4)	175(2)	37(2)
C(15)	10763(5)	5877(4)	446(2)	30(2)
C(16)	10355(5)	5121(4)	631(2)	30(2)
C(17)	10768(5)	4370(4)	529(2)	38(2)
C(18)	10343(5)	3698(4)	726(2)	38(2)
C(19)	9519(5)	3772(4)	1034(2)	39(2)
C(20)	9143(5)	4524(4)	1117(2)	37(2)
O(1)	7468(3)	5947(2)	1313(1)	32(1)
O(2)	6265(3)	6625(3)	2142(2)	43(1)
C(21)	6041(7)	5836(5)	2285(3)	67(2)
C(22)	6220(8)	5689(6)	2806(3)	88(3)
N(5)	6631(5)	3873(5)	1130(3)	60(2)
O(3)	6637(4)	4410(4)	826(3)	79(2)
O(4)	6912(7)	3987(6)	1557(3)	147(4)
O(5)	6492(6)	3173(4)	1013(2)	103(2)
O(1SA)	5087(28)	7530(21)	2691(13)	90(14)
O(1SB)	5411(19)	7622(14)	2726(8)	49(7)
O(1SC)	4841(14)	7632(10)	2526(6)	35(5)
C(1S)	5034(9)	8463(7)	2613(4)	106(4)
C(2SA)	5727(15)	8803(12)	3013(8)	79(6)
C(2SB)	5988(17)	8812(13)	2714(8)	91(7)
O(2SA)	6302(20)	2295(14)	1767(9)	75(7)
O(2SB)	6808(14)	2263(10)	1927(6)	55(5)
O(2SC)	6077(13)	1997(11)	1657(6)	44(5)
C(3S)	6962(8)	1535(7)	1747(4)	93(3)
C(4SA)	7816(11)	1514(8)	1405(5)	84(4)
C(4SB)	6929(24)	1232(19)	2252(12)	83(11)

Table S8. Bond lengths [A] and angles [deg] for [Co2(OH)(XDK)-(bpy)2(EtOH)](NO3).2EtOH.

Co(1)-O(1)	2.011(4)
Co(1)-O(201)	2.108(4)
Co(1)-N(2)	2.113(5)
Co(1)-O(101)	2.125(4)
Co(1)-O(2)	2.173(4)
Co(1)-N(1)	2.198(5)
Co(1)-Co(2)	3.2651(11)
Co(2)-O(202)	2.015(4)
Co(2)-O(102)	2.030(4)
Co(2)-O(1)	2.031(4)
Co(2)-N(4)	2.083(5)
Co(2)-N(3)	2.198(5)
O(101)-C(101)	1.245(7)
O(102)-C(101)	1.281(7)
O(103)-C(102)	1.211(7)
O(104)-C(103)	1.219(6)
O(201)-C(201)	1.266(7)
O(202)-C(201)	1.255(7)
O(203)-C(203)	1.197(7)
O(204)-C(202)	1.211(7)
N(101)-C(103)	1.400(7)
N(101)-C(102)	1.424(7)
N(101)-C(302)	1.451(7)
N(201)-C(202)	1.414(7)
N(201)-C(203)	1.417(7)
N(201)-C(306)	1.448(7)
C(101)-C(107)	1.526(8)
C(102)-C(109)	1.511(8)
C(103)-C(111)	1.521(8)
C(104)-C(107)	1.536(8)
C(105)-C(109)	1.536(8)
C(106)-C(111)	1.533(8)
C(107)-C(112)	1.537(8)
C(107)-C(108)	1.549(8)
C(108)-C(109)	1.553(8)
C(109)-C(110)	1.529(8)
C(110)-C(111)	1.526(8)
C(111)-C(112)	1.548(8)
C(201)-C(207)	1.533(8)
C(202)-C(209)	1.524(8)
C(203)-C(211)	1.521(8)
C(204)-C(207)	1.541(8)
C(205)-C(209)	1.532(8)
C(206)-C(211)	1.533(8)
C(207)-C(208)	1.533(8)
C(207)-C(212)	1.544(8)
C(208)-C(209)	1.545(9)
C(209)-C(210)	1.521(8)
C(210)-C(211)	1.526(8)
C(211)-C(212)	1.531(8)
C(301)-C(302)	1.382(8)
C(301)-C(306)	1.385(8)
C(302)-C(303)	1.394(8)
C(303)-C(304)	1.385(8)
C(303)-C(307)	1.518(8)
C(304)-C(305)	1.387(8)
C(305)-C(306)	1.393(8)
C(305)-C(308)	1.515(8)
N(1)-C(1)	1.320(8)
N(1)-C(5)	1.346(8)
N(2)-C(10)	1.327(8)

N(2)-C(6)	1.371(7)
N(3)-C(11)	1.324(8)
N(3)-C(15)	1.346(8)
N(4)-C(20)	1.354(8)
N(4)-C(16)	1.355(7)
C(1)-C(2)	1.387(9)
C(2)-C(3)	1.360(10)
C(3)-C(4)	1.385(10)
C(4)-C(5)	1.394(9)
C(5)-C(6)	1.468(9)
C(6)-C(7)	1.404(8)
C(7)-C(8)	1.364(9)
C(8)-C(9)	1.360(9)
C(9)-C(10)	1.373(8)
C(11)-C(12)	1.386(9)
C(12)-C(13)	1.378(9)
C(13)-C(14)	1.381(9)
C(14)-C(15)	1.385(8)
C(15)-C(16)	1.471(9)
C(16)-C(17)	1.393(9)
C(17)-C(18)	1.374(9)
C(18)-C(19)	1.388(9)
C(19)-C(20)	1.368(9)
O(2)-C(21)	1.413(8)
C(21)-C(22)	1.479(10)
N(5)-O(5)	1.225(8)
N(5)-O(4)	1.233(8)
N(5)-O(3)	1.238(8)
O(1SA)-C(1S)	1.58(4)
O(1SB)-C(1S)	1.51(3)
O(1SC)-C(1S)	1.43(2)
C(1S)-C(2SB)	1.33(2)
C(1S)-C(2SA)	1.47(2)
O(2SA)-C(3S)	1.51(2)
O(2SB)-C(3S)	1.34(2)
O(2SC)-C(3S)	1.35(2)
C(3S)-C(4SA)	1.48(2)
C(3S)-C(4SB)	1.50(3)

O(1)-Co(1)-O(201)	91.8(2)
O(1)-Co(1)-N(2)	172.8(2)
O(201)-Co(1)-N(2)	90.9(2)
O(1)-Co(1)-O(101)	89.9(2)
O(201)-Co(1)-O(101)	93.6(2)
N(2)-Co(1)-O(101)	83.3(2)
O(1)-Co(1)-O(2)	94.0(2)
O(201)-Co(1)-O(2)	84.9(2)
N(2)-Co(1)-O(2)	92.9(2)
O(101)-Co(1)-O(2)	175.9(2)
O(1)-Co(1)-N(1)	101.7(2)
O(201)-Co(1)-N(1)	163.8(2)
N(2)-Co(1)-N(1)	76.8(2)
O(101)-Co(1)-N(1)	95.2(2)
O(2)-Co(1)-N(1)	85.4(2)
O(202)-Co(2)-O(102)	132.5(2)
O(202)-Co(2)-O(1)	94.9(2)
O(102)-Co(2)-O(1)	98.0(2)
O(202)-Co(2)-N(4)	113.2(2)
O(102)-Co(2)-N(4)	109.8(2)
O(1)-Co(2)-N(4)	98.3(2)
O(202)-Co(2)-N(3)	87.1(2)
O(102)-Co(2)-N(3)	85.5(2)
O(1)-Co(2)-N(3)	173.0(2)
N(4)-Co(2)-N(3)	74.7(2)
C(101)-O(101)-Co(1)	132.6(4)
C(101)-O(102)-Co(2)	115.9(4)

C(201)-O(201)-Co(1)	129.2(4)
C(201)-O(202)-Co(2)	124.4(4)
C(103)-N(101)-C(102)	124.5(5)
C(103)-N(101)-C(302)	119.3(5)
C(102)-N(101)-C(302)	116.0(5)
C(202)-N(201)-C(203)	125.1(5)
C(202)-N(201)-C(306)	117.8(5)
C(203)-N(201)-C(306)	116.3(5)
O(101)-C(101)-O(102)	123.7(6)
O(101)-C(101)-C(107)	119.5(6)
O(102)-C(101)-C(107)	116.7(5)
O(103)-C(102)-N(101)	118.5(5)
O(103)-C(102)-C(109)	124.0(6)
N(101)-C(102)-C(109)	117.4(5)
O(104)-C(103)-N(101)	119.5(5)
O(104)-C(103)-C(111)	122.3(5)
N(101)-C(103)-C(111)	118.1(5)
C(101)-C(107)-C(112)	112.8(5)
C(101)-C(107)-C(104)	104.5(5)
C(112)-C(107)-C(104)	109.4(5)
C(101)-C(107)-C(108)	111.7(5)
C(112)-C(107)-C(108)	109.5(5)
C(104)-C(107)-C(108)	108.8(5)
C(107)-C(108)-C(109)	116.8(5)
C(102)-C(109)-C(110)	108.1(5)
C(102)-C(109)-C(105)	108.2(5)
C(110)-C(109)-C(105)	110.8(5)
C(102)-C(109)-C(108)	112.0(5)
C(110)-C(109)-C(108)	109.5(5)
C(105)-C(109)-C(108)	108.3(5)
C(111)-C(110)-C(109)	110.1(5)
C(103)-C(111)-C(110)	110.1(5)
C(103)-C(111)-C(106)	108.7(5)
C(110)-C(111)-C(106)	110.8(5)
C(103)-C(111)-C(112)	109.5(5)
C(110)-C(111)-C(112)	108.4(5)
C(106)-C(111)-C(112)	109.4(5)
C(107)-C(112)-C(111)	115.9(5)
O(202)-C(201)-O(201)	124.9(6)
O(202)-C(201)-C(207)	117.2(5)
O(201)-C(201)-C(207)	117.7(5)
O(204)-C(202)-N(201)	119.3(6)
O(204)-C(202)-C(209)	123.5(6)
N(201)-C(202)-C(209)	117.2(5)
O(203)-C(203)-N(201)	119.3(6)
O(203)-C(203)-C(211)	123.3(6)
N(201)-C(203)-C(211)	117.4(5)
C(201)-C(207)-C(208)	112.3(5)
C(201)-C(207)-C(204)	103.2(5)
C(208)-C(207)-C(204)	109.6(5)
C(201)-C(207)-C(212)	112.7(5)
C(208)-C(207)-C(212)	109.9(5)
C(204)-C(207)-C(212)	108.8(5)
C(207)-C(208)-C(209)	115.5(5)
C(210)-C(209)-C(202)	109.3(5)
C(210)-C(209)-C(205)	109.8(5)
C(202)-C(209)-C(205)	109.3(5)
C(210)-C(209)-C(208)	109.7(5)
C(202)-C(209)-C(208)	109.4(5)
C(205)-C(209)-C(208)	109.4(5)
C(209)-C(210)-C(211)	110.8(5)
C(203)-C(211)-C(210)	108.1(5)
C(203)-C(211)-C(212)	110.6(5)

C(212)-C(211)-C(206)	109.7(5)
C(211)-C(212)-C(207)	116.8(5)
C(302)-C(301)-C(306)	119.8(6)
C(301)-C(302)-C(303)	121.0(5)
C(301)-C(302)-N(101)	120.6(5)
C(303)-C(302)-N(101)	118.4(5)
C(304)-C(303)-C(302)	118.1(6)
C(304)-C(303)-C(307)	120.6(6)
C(302)-C(303)-C(307)	121.2(6)
C(303)-C(304)-C(305)	122.1(6)
C(304)-C(305)-C(306)	118.5(6)
C(304)-C(305)-C(308)	121.1(6)
C(306)-C(305)-C(308)	120.4(6)
C(301)-C(306)-C(305)	120.5(6)
C(301)-C(306)-N(201)	121.0(5)
C(305)-C(306)-N(201)	118.6(5)
C(1)-N(1)-C(5)	118.3(6)
C(1)-N(1)-Co(1)	126.6(5)
C(5)-N(1)-Co(1)	113.2(4)
C(10)-N(2)-C(6)	118.6(5)
C(10)-N(2)-Co(1)	124.8(4)
C(6)-N(2)-Co(1)	115.9(4)
C(11)-N(3)-C(15)	118.2(6)
C(11)-N(3)-Co(2)	125.9(4)
C(15)-N(3)-Co(2)	115.7(4)
C(20)-N(4)-C(16)	118.0(5)
C(20)-N(4)-Co(2)	122.8(4)
C(16)-N(4)-Co(2)	118.6(4)
N(1)-C(1)-C(2)	123.2(7)
C(3)-C(2)-C(1)	119.1(7)
C(2)-C(3)-C(4)	118.6(7)
C(3)-C(4)-C(5)	119.3(7)
N(1)-C(5)-C(4)	121.4(6)
N(1)-C(5)-C(6)	116.1(5)
C(4)-C(5)-C(6)	122.5(6)
N(2)-C(6)-C(7)	119.5(6)
N(2)-C(6)-C(5)	115.5(5)
C(7)-C(6)-C(5)	124.9(6)
C(8)-C(7)-C(6)	119.7(6)
C(9)-C(8)-C(7)	120.3(6)
C(8)-C(9)-C(10)	118.3(6)
N(2)-C(10)-C(9)	123.7(6)
N(3)-C(11)-C(12)	123.6(7)
C(13)-C(12)-C(11)	117.7(7)
C(12)-C(13)-C(14)	119.6(6)
C(13)-C(14)-C(15)	118.8(6)
N(3)-C(15)-C(14)	122.0(6)
N(3)-C(15)-C(16)	114.3(5)
C(14)-C(15)-C(16)	123.7(6)
N(4)-C(16)-C(17)	120.6(6)
N(4)-C(16)-C(15)	115.1(5)
C(17)-C(16)-C(15)	124.3(6)
C(18)-C(17)-C(16)	120.0(6)
C(17)-C(18)-C(19)	119.6(6)
C(20)-C(19)-C(18)	117.6(7)
N(4)-C(20)-C(19)	124.1(6)
Co(1)-O(1)-Co(2)	107.8(2)
C(21)-O(2)-Co(1)	121.6(4)
O(2)-C(21)-C(22)	114.5(7)
O(5)-N(5)-O(4)	115.5(9)
O(5)-N(5)-O(3)	121.2(8)
O(4)-N(5)-O(3)	122.5(8)
C(2SB)-C(1S)-O(1SC)	126.8(14)
O(1SC)-C(1S)-C(2SA)	125.8(13)
C(2SB)-C(1S)-O(1SB)	96.3(14)
C(2SA)-C(1S)-O(1SB)	92.7(13)

C(2SB)-C(1S)-O(1SA)	112(2)
C(2SA)-C(1S)-O(1SA)	105(2)
O(2SB)-C(3S)-C(4SA)	113.2(12)
O(2SC)-C(3S)-C(4SA)	120.3(12)
O(2SB)-C(3S)-C(4SB)	87(2)
O(2SC)-C(3S)-C(4SB)	107(2)
C(4SA)-C(3S)-O(2SA)	117.3(12)
C(4SB)-C(3S)-O(2SA)	101(2)

Symmetry transformations used to generate equivalent atoms:

Table S9. Anisotropic displacement parameters (A^2 x 10^3) for [Co2(OH)-(XDK)(bpy)2(EtOH)](NO3).2EtOH. 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)	26(1)	24(1)	32(1)	3(1)	5(1)	2(1)
Co(2)	27(1)	25(1)	29(1)	-1(1)	4(1)	4(1)
O(101)	37(3)	24(3)	25(3)	-2(2)	-2(2)	3(2)
O(102)	29(3)	41(3)	28(3)	0(2)	1(2)	6(2)
O(103)	39(3)	36(3)	37(3)	-9(2)	7(2)	6(2)
O(104)	36(3)	29(3)	34(3)	-4(2)	7(2)	2(2)
O(201)	27(3)	25(3)	31(3)	1(2)	2(2)	3(2)
O(202)	29(2)	36(3)	28(3)	-9(2)	4(2)	1(2)
O(203)	33(3)	35(3)	37(3)	-3(2)	7(2)	8(2)
O(204)	31(3)	47(3)	31(3)	1(2)	7(2)	2(2)
N(101)	30(3)	21(3)	22(3)	0(2)	1(2)	1(2)
N(201)	19(3)	31(3)	20(3)	-1(2)	0(2)	-1(2)
C(101)	35(4)	27(4)	28(4)	0(3)	2(3)	-3(3)
C(102)	26(4)	29(4)	30(4)	3(3)	-2(3)	2(3)
C(103)	37(4)	19(4)	18(4)	1(3)	2(3)	-1(3)
C(104)	35(4)	35(4)	42(4)	-6(3)	-4(3)	-6(3)
C(105)	40(4)	38(5)	53(5)	-4(4)	-7(4)	15(3)
C(106)	47(4)	40(4)	28(4)	-3(3)	-6(3)	-3(3)
C(107)	24(3)	22(4)	32(4)	-4(3)	0(3)	-1(3)
C(108)	26(4)	31(4)	34(4)	-2(3)	-1(3)	-4(3)
C(109)	21(3)	30(4)	37(4)	-5(3)	-4(3)	6(3)
C(110)	36(4)	27(4)	33(4)	0(3)	-9(3)	-3(3)
C(111)	31(4)	25(4)	25(4)	0(3)	-2(3)	-2(3)
C(112)	28(4)	30(4)	25(4)	-8(3)	-3(3)	-3(3)
C(201)	32(4)	21(4)	24(4)	4(3)	3(3)	-4(3)
C(202)	26(4)	32(4)	32(4)	-4(3)	0(3)	-7(3)
C(203)	32(4)	21(4)	32(4)	-4(3)	5(3)	-1(3)
C(204)	48(4)	40(5)	40(4)	12(4)	5(4)	7(4)
C(205)	34(4)	67(6)	39(4)	-5(4)	-6(3)	-1(4)
C(206)	57(5)	44(5)	29(4)	-9(3)	8(4)	0(4)
C(207)	31(4)	27(4)	27(4)	6(3)	4(3)	1(3)
C(208)	31(4)	38(4)	24(4)	3(3)	-5(3)	7(3)
C(209)	24(4)	42(5)	26(4)	2(3)	0(3)	-4(3)
C(210)	38(4)	34(4)	29(4)	-1(3)	0(3)	0(3)
C(211)	33(4)	28(4)	23(4)	-6(3)	5(3)	-4(3)
C(212)	33(4)	42(4)	23(4)	-7(3)	2(3)	-1(3)
C(301)	24(4)	16(4)	28(4)	3(3)	5(3)	0(3)
C(302)	22(3)	21(4)	24(4)	-2(3)	-1(3)	1(3)
C(303)	37(4)	23(4)	22(4)	2(3)	6(3)	3(3)
C(304)	48(4)	17(4)	30(4)	-2(3)	3(3)	-4(3)
C(305)	32(4)	29(4)	28(4)	-6(3)	1(3)	-4(3)
C(306)	24(4)	25(4)	23(4)	0(3)	5(3)	-2(3)
C(307)	48(4)	26(4)	36(4)	4(3)	4(3)	1(3)
C(308)	62(5)	36(5)	39(5)	-2(4)	5(4)	-20(4)
N(1)	36(3)	30(4)	39(4)	-1(3)	3(3)	1(3)
N(2)	28(3)	34(4)	32(3)	-2(3)	6(3)	-2(3)
N(3)	30(3)	31(4)	25(3)	1(3)	-1(2)	3(3)
N(4)	30(3)	25(3)	26(3)	-1(3)	0(3)	6(3)
C(1)	42(5)	38(5)	43(5)	-5(4)	7(4)	0(4)
C(2)	49(5)	46(5)	45(5)	-4(4)	-3(4)	-14(4)
C(3)	39(5)	60(6)	36(5)	2(4)	-5(4)	-25(4)
C(4)	31(4)	73(6)	28(4)	-1(4)	-3(3)	0(4)
C(5)	31(4)	35(4)	30(4)	-7(3)	-2(3)	-2(4)
C(6)	24(4)	43(5)	22(4)	-2(3)	8(3)	6(3)
C(7)	25(4)	55(5)	31(4)	-2(4)	2(3)	10(4)
C(8)	46(5)	40(5)	35(4)	3(4)	10(4)	18(4)

C(9)	32(4)	29(4)	43(4)	-1(3)	7(3)	7(3)
C(10)	32(4)	31(4)	31(4)	1(3)	2(3)	3(3)
C(11)	38(4)	40(5)	37(4)	-3(4)	3(4)	-2(4)
C(12)	40(4)	40(5)	54(5)	4(4)	10(4)	-4(4)
C(13)	32(4)	58(6)	36(4)	6(4)	8(3)	-4(4)
C(14)	27(4)	55(5)	31(4)	-2(4)	9(3)	8(4)
C(15)	27(4)	33(4)	28(4)	-6(3)	-1(3)	0(3)
C(16)	26(4)	36(5)	26(4)	-9(3)	-6(3)	11(3)
C(17)	33(4)	41(5)	38(4)	-8(4)	1(3)	5(4)
C(18)	42(4)	28(4)	42(4)	-10(4)	-11(4)	10(4)
C(19)	42(4)	31(5)	43(4)	0(3)	-9(4)	4(4)
C(20)	32(4)	36(5)	41(4)	3(4)	-3(3)	8(3)
O(1)	17(2)	38(3)	43(3)	-10(2)	12(2)	8(2)
O(2)	49(3)	41(3)	39(3)	16(2)	5(2)	-6(2)
C(21)	96(7)	56(6)	50(5)	12(4)	14(5)	-13(5)
C(22)	124(8)	83(8)	58(6)	30(5)	10(6)	-6(6)
N(5)	61(5)	63(6)	54(5)	-16(5)	0(4)	-13(4)
O(3)	62(4)	62(4)	110(5)	12(4)	-7(4)	5(3)
O(4)	177(8)	206(10)	62(5)	-34(5)	38(5)	-115(7)
O(5)	175(7)	54(5)	75(5)	-5(4)	-22(4)	-19(5)

Table S10. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for [Co2(OH)(XDK)-(bpy)2(EtOH)](NO3).2EtOH.

	x	y	z	U(eq)
H(10A)	5248(5)	5905(4)	-348(2)	57
H(10B)	5429(5)	5927(4)	213(2)	57
H(10C)	6350(5)	5616(4)	-95(2)	57
H(10D)	3882(5)	8510(4)	-476(3)	66
H(10E)	4518(5)	9309(4)	-374(3)	66
H(10F)	4157(5)	8793(4)	54(3)	66
H(10G)	6954(5)	7607(4)	-1455(2)	58
H(10H)	8121(5)	7530(4)	-1201(2)	58
H(10I)	7617(5)	8377(4)	-1306(2)	58
H(10J)	5081(5)	7468(4)	248(2)	36
H(10K)	4656(5)	7239(4)	-274(2)	36
H(11A)	5400(5)	8051(4)	-974(2)	39
H(11B)	6051(5)	8840(4)	-852(2)	39
H(11C)	6278(5)	6717(4)	-839(2)	34
H(11D)	7424(5)	6661(4)	-567(2)	34
H(20A)	9507(5)	6714(4)	2858(2)	64
H(20B)	9506(5)	6262(4)	2366(2)	64
H(20C)	8423(5)	6608(4)	2538(2)	64
H(20D)	12512(5)	8171(5)	1990(2)	71
H(20E)	12457(5)	8423(5)	2528(2)	71
H(20F)	12421(5)	9076(5)	2125(2)	71
H(20G)	8985(5)	9484(4)	3104(2)	64
H(20H)	7976(5)	9590(4)	2738(2)	64
H(20I)	8986(5)	10148(4)	2709(2)	64
H(20J)	10901(5)	7261(4)	2039(2)	37
H(20K)	10962(5)	7483(4)	2584(2)	37
H(21A)	10702(5)	9609(4)	2411(2)	41
H(21B)	10734(5)	8954(4)	2814(2)	41
H(21C)	8106(5)	8142(4)	2490(2)	39
H(21D)	9043(5)	8084(4)	2894(2)	39
H(30A)	8305(4)	8318(4)	872(2)	27
H(30B)	9416(5)	10795(4)	371(2)	38
H(30C)	7603(5)	9795(4)	-479(2)	55
H(30D)	8670(5)	10291(4)	-505(2)	55
H(30E)	7674(5)	10665(4)	-272(2)	55
H(30F)	10431(6)	10265(4)	1558(2)	69
H(30G)	9908(6)	11038(4)	1323(2)	69
H(30H)	10927(6)	10655(4)	1113(2)	69
H(1A)	5172(5)	5295(4)	1154(2)	49
H(2A)	3424(6)	4856(5)	1206(2)	57
H(3A)	2083(6)	5768(5)	1341(2)	54
H(4A)	2508(5)	7125(5)	1337(2)	53
H(7A)	3035(5)	8389(4)	1126(2)	44
H(8A)	3719(6)	9662(4)	1189(2)	48
H(9A)	5537(5)	9857(4)	1382(2)	42
H(10L)	6643(5)	8767(4)	1496(2)	37
H(11E)	10164(5)	7686(4)	517(2)	46
H(12A)	11636(5)	7851(4)	67(3)	53
H(13A)	12583(5)	6722(5)	-149(2)	50
H(14A)	12019(5)	5471(4)	91(2)	45
H(17A)	11331(5)	4325(4)	329(2)	45
H(18A)	10606(5)	3195(4)	652(2)	46
H(19A)	9233(5)	3327(4)	1179(2)	47
H(20L)	8591(5)	4578(4)	1323(2)	44
H(21E)	6492(7)	5471(5)	2118(3)	80
H(21F)	5293(7)	5714(5)	2185(3)	80

H(22A)	6051(8)	5143(6)	2874(3)	132
H(22B)	5763(8)	6037(6)	2975(3)	132
H(22C)	6964(8)	5793(6)	2908(3)	132

Table S11. Crystal data and structure refinement for [Co2Cl(XDK)(bpy)2-(EtOH)2](NO3).3EtOH.

Identification code	[Co2Cl(XDK)(bpy)2(EtOH)2](NO3).3EtOH
Empirical formula	C62 H84 Cl Co2 N7 O16
Formula weight	1336.67
Temperature	293(2) K
Wavelength	0.71073 A
Crystal system	orthorhombic
Space group	Pnma
Unit cell dimensions	a = 25.5097(5) A alpha = 90 deg. b = 17.9514(4) A beta = 90 deg. c = 14.1510(3) A gamma = 90 deg.
Volume, Z	6480.2(2) A^3, 4
Density (calculated)	1.370 Mg/m^3
Absorption coefficient	0.625 mm^-1
F(000)	2816
Crystal size	0.50 x 0.30 x 0.10 mm
Theta range for data collection	1.60 to 28.23 deg.
Limiting indices	-29<=h<=32, -23<=k<=12, -18<=l<=16
Reflections collected	37716
Independent reflections	7793 [R(int) = 0.0365]
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	7790 / 0 / 417
Goodness-of-fit on F^2	1.031
Observed reflections [I>2sigma(I)]	6075
Final R indices [I>2sigma(I)]	R1 = 0.0518, wR2 = 0.1349
R indices (all data)	R1 = 0.0722, wR2 = 0.1474
Largest diff. peak and hole	0.746 and -0.890 e.A^-3

Table S12. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for [Co2Cl(XDK)(bpy)2-(EtOH)2](NO3).3EtOH. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Co(1)	1232(1)	1458(1)	2620(1)	25(1)
N(1)	1652(1)	517(1)	2128(1)	28(1)
N(2)	1323(1)	778(1)	3867(1)	34(1)
C(1)	1793(1)	407(1)	1232(2)	34(1)
C(2)	2143(1)	-140(2)	965(2)	46(1)
C(3)	2364(1)	-578(2)	1656(3)	56(1)
C(4)	2225(1)	-467(2)	2585(2)	51(1)
C(5)	1859(1)	72(1)	2805(2)	34(1)
C(6)	1653(1)	197(2)	3772(2)	36(1)
C(7)	1770(1)	-270(2)	4532(2)	50(1)
C(8)	1546(1)	-131(2)	5398(2)	60(1)
C(9)	1209(1)	460(2)	5492(2)	55(1)
C(10)	1103(1)	909(2)	4713(2)	43(1)
O(1)	514(1)	869(1)	2407(2)	56(1)
C(11)	-19(1)	1071(2)	2543(3)	61(1)
C(12)	-279(2)	676(3)	3281(4)	103(2)
O(101)	1948(1)	1877(1)	3015(1)	27(1)
O(103)	3104(1)	1239(1)	2125(2)	52(1)
O(201)	1162(1)	1878(1)	1278(1)	32(1)
O(203)	1957(1)	1242(1)	-706(1)	37(1)
C(102)	3147(1)	1803(2)	2587(2)	36(1)
C(105)	3601(2)	1087(3)	3849(3)	74(1)
C(108)	2795(1)	1795(2)	4257(2)	33(1)
C(109)	3293(1)	1804(2)	3634(2)	42(1)
C(203)	1706(1)	1805(1)	-853(2)	31(1)
C(206)	1121(1)	1095(2)	-1911(2)	50(1)
C(211)	1170(1)	1801(2)	-1313(2)	34(1)
C(212)	734(1)	1794(1)	-548(2)	31(1)
N(101)	3084(1)	2500	2153(2)	30(1)
N(201)	1920(1)	2500	-609(2)	29(1)
C(101)	2091(1)	2500	3327(2)	23(1)
C(104)	2076(1)	2500	5053(2)	34(1)
C(107)	2458(1)	2500	4201(2)	26(1)
C(110)	3609(2)	2500	3847(3)	52(1)
C(201)	1040(1)	2500	936(2)	26(1)
C(204)	127(1)	2500	499(3)	37(1)
C(207)	680(1)	2500	57(2)	27(1)
C(210)	1110(2)	2500	-1918(3)	39(1)
C(301)	2504(1)	2500	762(2)	30(1)
C(302)	3007(1)	2500	1132(2)	31(1)
C(303)	3450(2)	2500	555(3)	37(1)
C(304)	3369(2)	2500	-417(3)	38(1)
C(305)	2877(2)	2500	-825(3)	34(1)
C(306)	2446(1)	2500	-213(2)	29(1)
C(307)	3996(2)	2500	969(3)	54(1)
C(308)	2811(2)	2500	-1887(3)	45(1)
Cl(1)	767(1)	2500	3385(1)	36(1)
C(1SA)	-88(4)	1519(6)	6207(7)	81(3)
C(2SA)	-554(5)	1008(6)	6349(9)	85(3)
O(1SA)	-553(2)	684(4)	7371(4)	77(2)
C(1SB)	-358(6)	1243(9)	6043(11)	116(4)
C(2SB)	-674(4)	1093(6)	6940(8)	84(3)
O(1SB)	-380(5)	1244(7)	7806(8)	160(4)
O(2S)	-428(4)	155(5)	8951(6)	128(3)
C(3S)	-253(2)	214(3)	9903(4)	86(1)

N(5)	-1054(3)	2143(5)	8554(5)	73(2)
O(3S)	-1186(4)	1575(7)	8620(9)	148(4)
O(4S)	-1321(4)	2500	8763(7)	171(3)
O(5SA)	-570(7)	2500	8151(13)	147(6)
O(5SB)	-577(9)	2093(12)	8371(14)	123(6)

Table S13. Bond lengths [A] and angles [deg] for [Co2Cl(XDK)-(bpy)2(EtOH)2](NO3).3EtOH.

Co(1)-O(201)	2.052(2)
Co(1)-O(101)	2.054(2)
Co(1)-N(1)	2.120(2)
Co(1)-O(1)	2.135(2)
Co(1)-N(2)	2.158(2)
Co(1)-Cl(1)	2.4651(6)
Co(1)-Co(1)#1	3.7400(7)
N(1)-C(1)	1.332(3)
N(1)-C(5)	1.354(3)
N(2)-C(10)	1.343(3)
N(2)-C(6)	1.347(4)
C(1)-C(2)	1.378(4)
C(2)-C(3)	1.377(5)
C(3)-C(4)	1.376(5)
C(4)-C(5)	1.380(4)
C(5)-C(6)	1.483(4)
C(6)-C(7)	1.397(4)
C(7)-C(8)	1.375(5)
C(8)-C(9)	1.373(5)
C(9)-C(10)	1.392(4)
O(1)-C(11)	1.420(4)
C(11)-C(12)	1.427(5)
O(101)-C(101)	1.257(2)
O(103)-C(102)	1.210(4)
O(201)-C(201)	1.255(2)
O(203)-C(203)	1.215(3)
C(102)-N(101)	1.404(3)
C(102)-C(109)	1.528(4)
C(105)-C(109)	1.538(4)
C(108)-C(107)	1.533(3)
C(108)-C(109)	1.545(4)
C(109)-C(110)	1.518(4)
C(203)-N(201)	1.405(3)
C(203)-C(211)	1.515(4)
C(206)-C(211)	1.530(4)
C(211)-C(210)	1.526(3)
C(211)-C(212)	1.551(4)
C(212)-C(207)	1.536(3)
N(101)-C(102)#1	1.404(3)
N(101)-C(302)	1.457(4)
N(201)-C(203)#1	1.405(3)
N(201)-C(306)	1.455(5)
C(101)-O(101)#1	1.257(2)
C(101)-C(107)	1.550(4)
C(104)-C(107)	1.549(5)
C(107)-C(108)#1	1.533(3)
C(110)-C(109)#1	1.518(4)
C(201)-O(201)#1	1.255(2)
C(201)-C(207)	1.547(4)
C(204)-C(207)	1.543(5)
C(207)-C(212)#1	1.536(3)
C(210)-C(211)#1	1.526(3)
C(301)-C(302)	1.386(5)
C(301)-C(306)	1.388(5)
C(302)-C(303)	1.395(5)
C(303)-C(304)	1.390(6)
C(303)-C(307)	1.510(6)
C(304)-C(305)	1.382(6)
C(305)-C(306)	1.399(5)
C(305)-C(308)	1.511(5)
Cl(1)-Co(1)#1	2.4651(6)

C(1SA)-C(2SA)	1.52(2)
C(2SA)-O(1SA)	1.559(14)
C(1SB)-C(2SB)	1.53(2)
C(2SB)-O(1SB)	1.46(2)
O(2S)-C(3S)	1.423(10)
C(3S)-C(3S)#2	1.526(9)
N(5)-O(4S)	0.980(8)
N(5)-O(3S)	1.076(12)
N(5)-O(5SB)	1.25(2)
N(5)-O(5SA)	1.50(2)

O(201)-Co(1)-O(101)	101.24(7)
O(201)-Co(1)-N(1)	91.87(7)
O(101)-Co(1)-N(1)	86.04(7)
O(201)-Co(1)-O(1)	88.67(9)
O(101)-Co(1)-O(1)	169.27(9)
N(1)-Co(1)-O(1)	89.56(8)
O(201)-Co(1)-N(2)	166.95(8)
O(101)-Co(1)-N(2)	83.62(7)
N(1)-Co(1)-N(2)	76.28(8)
O(1)-Co(1)-N(2)	85.83(9)
O(201)-Co(1)-Cl(1)	94.93(5)
O(101)-Co(1)-Cl(1)	91.78(5)
N(1)-Co(1)-Cl(1)	173.14(6)
O(1)-Co(1)-Cl(1)	91.45(7)
N(2)-Co(1)-Cl(1)	97.02(7)
C(1)-N(1)-C(5)	118.7(2)
C(1)-N(1)-Co(1)	124.6(2)
C(5)-N(1)-Co(1)	115.8(2)
C(10)-N(2)-C(6)	119.0(2)
C(10)-N(2)-Co(1)	125.8(2)
C(6)-N(2)-Co(1)	115.1(2)
N(1)-C(1)-C(2)	122.8(3)
C(3)-C(2)-C(1)	118.5(3)
C(4)-C(3)-C(2)	119.3(3)
C(3)-C(4)-C(5)	119.5(3)
N(1)-C(5)-C(4)	121.1(3)
N(1)-C(5)-C(6)	115.2(2)
C(4)-C(5)-C(6)	123.7(3)
N(2)-C(6)-C(7)	121.5(3)
N(2)-C(6)-C(5)	115.5(2)
C(7)-C(6)-C(5)	122.9(3)
C(8)-C(7)-C(6)	119.3(3)
C(9)-C(8)-C(7)	119.1(3)
C(8)-C(9)-C(10)	119.5(3)
N(2)-C(10)-C(9)	121.6(3)
C(11)-O(1)-Co(1)	132.4(2)
O(1)-C(11)-C(12)	114.7(3)
C(101)-O(101)-Co(1)	132.9(2)
C(201)-O(201)-Co(1)	134.8(2)
O(103)-C(102)-N(101)	119.9(2)
O(103)-C(102)-C(109)	123.2(3)
N(101)-C(102)-C(109)	116.9(3)
C(107)-C(108)-C(109)	115.1(2)
C(110)-C(109)-C(102)	108.8(3)
C(110)-C(109)-C(105)	112.2(3)
C(102)-C(109)-C(105)	108.3(3)
C(110)-C(109)-C(108)	109.4(3)
C(102)-C(109)-C(108)	110.7(2)
C(105)-C(109)-C(108)	107.4(3)
O(203)-C(203)-N(201)	119.5(2)
O(203)-C(203)-C(211)	123.1(2)
N(201)-C(203)-C(211)	117.4(2)
C(203)-C(211)-C(210)	109.1(2)
C(203)-C(211)-C(206)	108.3(2)
C(210)-C(211)-C(206)	111.2(2)

C(203)-C(211)-C(212)	110.4(2)
C(210)-C(211)-C(212)	109.1(2)
C(206)-C(211)-C(212)	108.7(2)
C(207)-C(212)-C(211)	116.5(2)
C(102)-N(101)-C(102)#1	126.2(3)
C(102)-N(101)-C(302)	116.7(2)
C(102)#1-N(101)-C(302)	116.7(2)
C(203)-N(201)-C(203)#1	125.3(3)
C(203)-N(201)-C(306)	116.9(2)
C(203)#1-N(201)-C(306)	116.9(2)
O(101)-C(101)-O(101)#1	125.7(3)
O(101)-C(101)-C(107)	117.1(2)
O(101)#1-C(101)-C(107)	117.1(2)
C(108)#1-C(107)-C(108)	111.3(3)
C(108)#1-C(107)-C(104)	108.2(2)
C(108)-C(107)-C(104)	108.2(2)
C(108)#1-C(107)-C(101)	112.3(2)
C(108)-C(107)-C(101)	112.3(2)
C(104)-C(107)-C(101)	104.0(3)
C(109)#1-C(110)-C(109)	110.9(3)
O(201)#1-C(201)-O(201)	125.5(3)
O(201)#1-C(201)-C(207)	117.2(2)
O(201)-C(201)-C(207)	117.2(2)
C(212)-C(207)-C(212)#1	111.2(3)
C(212)-C(207)-C(204)	108.0(2)
C(212)#1-C(207)-C(204)	108.0(2)
C(212)-C(207)-C(201)	113.2(2)
C(212)#1-C(207)-C(201)	113.2(2)
C(204)-C(207)-C(201)	102.6(3)
C(211)-C(210)-C(211)#1	110.5(3)
C(302)-C(301)-C(306)	118.3(3)
C(301)-C(302)-C(303)	121.9(3)
C(301)-C(302)-N(101)	119.9(3)
C(303)-C(302)-N(101)	118.2(3)
C(304)-C(303)-C(302)	117.3(4)
C(304)-C(303)-C(307)	121.4(3)
C(302)-C(303)-C(307)	121.3(4)
C(305)-C(304)-C(303)	123.3(3)
C(304)-C(305)-C(306)	117.0(3)
C(304)-C(305)-C(308)	121.2(3)
C(306)-C(305)-C(308)	121.9(4)
C(301)-C(306)-C(305)	122.2(3)
C(301)-C(306)-N(201)	118.7(3)
C(305)-C(306)-N(201)	119.1(3)
Co(1)#1-Cl(1)-Co(1)	98.68(3)
C(1SB)-C(1SA)-C(2SA)	23.0(12)
C(1SB)-C(1SA)-C(2SB)	47.7(12)
C(2SA)-C(1SA)-C(2SB)	26.0(5)
C(1SB)-C(2SA)-C(2SB)	129(2)
C(1SB)-C(2SA)-C(1SA)	25.9(14)
C(2SB)-C(2SA)-C(1SA)	106.6(13)
C(1SB)-C(2SA)-O(1SA)	135(2)
C(2SB)-C(2SA)-O(1SA)	37.4(9)
C(1SA)-C(2SA)-O(1SA)	110.2(8)
C(2SB)-O(1SA)-O(1SB)	79.7(9)
C(2SB)-O(1SA)-C(2SA)	33.1(7)
O(1SB)-O(1SA)-C(2SA)	99.0(8)
C(2SA)-C(1SB)-C(1SA)	131(3)
C(2SA)-C(1SB)-C(2SB)	27.2(13)
C(1SA)-C(1SB)-C(2SB)	107(2)
C(2SA)-C(2SB)-O(1SA)	109(2)
C(2SA)-C(2SB)-O(1SB)	129.2(14)
O(1SA)-C(2SB)-O(1SB)	57.8(8)
C(2SA)-C(2SB)-C(1SB)	23.4(11)
O(1SA)-C(2SB)-C(1SB)	118.0(11)
O(1SB)-C(2SB)-C(1SB)	113.0(10)

C(2SA)-C(2SB)-C(1SA)	47.4(10)
O(1SA)-C(2SB)-C(1SA)	111.6(9)
O(1SB)-C(2SB)-C(1SA)	88.8(8)
C(1SB)-C(2SB)-C(1SA)	25.2(6)
O(1SA)-O(1SB)-C(2SB)	42.5(6)
O(1SA)-O(1SB)-O(5SB)	143.0(12)
C(2SB)-O(1SB)-O(5SB)	112.8(11)
O(2S)-C(3S)-C(3S)#2	113.5(6)
O(4S)-N(5)-O(3S)	112.1(10)
O(4S)-N(5)-O(5SB)	142(2)
O(3S)-N(5)-O(5SB)	104.7(14)
O(4S)-N(5)-O(5SA)	113.9(10)
O(3S)-N(5)-O(5SA)	133.8(10)
N(5)-O(3S)-O(4S)	32.1(6)
N(5)-O(4S)-O(3S)	35.7(5)

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

Table S14. Anisotropic displacement parameters (A^2 x 10^3) for [Co2Cl(XDK)(bpy)2(EtOH)2](NO3).3EtOH. 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)	25(1)	29(1)	21(1)	1(1)	-1(1)	-3(1)
N(1)	34(1)	23(1)	28(1)	2(1)	-1(1)	-4(1)
N(2)	43(1)	35(1)	23(1)	4(1)	0(1)	-12(1)
C(1)	43(1)	29(1)	30(1)	-1(1)	1(1)	-2(1)
C(2)	55(2)	40(2)	42(2)	-7(1)	6(1)	6(1)
C(3)	67(2)	41(2)	61(2)	-6(2)	2(2)	22(2)
C(4)	63(2)	36(2)	53(2)	6(1)	-10(2)	12(2)
C(5)	40(1)	27(1)	37(1)	5(1)	-6(1)	-6(1)
C(6)	44(1)	32(1)	31(1)	6(1)	-8(1)	-10(1)
C(7)	59(2)	50(2)	42(2)	18(1)	-11(1)	-9(2)
C(8)	70(2)	70(2)	38(2)	24(2)	-13(2)	-19(2)
C(9)	70(2)	70(2)	25(1)	8(1)	1(1)	-30(2)
C(10)	51(2)	49(2)	28(1)	0(1)	4(1)	-17(1)
O(1)	34(1)	71(2)	63(1)	-18(1)	4(1)	-19(1)
C(11)	34(2)	76(3)	71(2)	14(2)	-5(1)	-17(2)
C(12)	80(3)	99(4)	130(4)	51(3)	54(3)	17(3)
O(101)	26(1)	24(1)	31(1)	-2(1)	-3(1)	0(1)
O(103)	78(2)	43(1)	36(1)	0(1)	9(1)	20(1)
O(201)	43(1)	32(1)	23(1)	1(1)	-4(1)	8(1)
O(203)	45(1)	30(1)	35(1)	-2(1)	3(1)	5(1)
C(102)	34(1)	46(2)	30(1)	3(1)	6(1)	14(1)
C(105)	67(2)	105(3)	48(2)	18(2)	9(2)	58(2)
C(108)	32(1)	44(2)	24(1)	5(1)	-4(1)	10(1)
C(109)	33(1)	63(2)	31(1)	4(1)	-1(1)	19(1)
C(203)	42(1)	32(1)	18(1)	-2(1)	4(1)	1(1)
C(206)	62(2)	45(2)	41(2)	-19(1)	-6(1)	-3(2)
C(211)	45(2)	33(1)	23(1)	-6(1)	-5(1)	0(1)
C(212)	36(1)	30(1)	26(1)	-3(1)	-6(1)	-4(1)
N(101)	26(1)	42(2)	24(1)	0	2(1)	0
N(201)	38(2)	28(2)	20(1)	0	-1(1)	0
C(101)	22(2)	26(2)	20(1)	0	2(1)	0
C(104)	31(2)	45(2)	26(2)	0	2(1)	0
C(107)	25(2)	29(2)	23(2)	0	-2(1)	0
C(110)	24(2)	99(4)	33(2)	0	-3(2)	0
C(201)	27(2)	32(2)	18(1)	0	0(1)	0
C(204)	33(2)	41(2)	38(2)	0	-4(2)	0
C(207)	31(2)	26(2)	24(2)	0	-5(1)	0
C(210)	51(2)	46(2)	20(2)	0	-7(2)	0
C(301)	31(2)	34(2)	25(2)	0	6(1)	0
C(302)	32(2)	36(2)	25(2)	0	3(1)	0
C(303)	33(2)	42(2)	36(2)	0	9(2)	0
C(304)	37(2)	40(2)	37(2)	0	17(2)	0
C(305)	47(2)	29(2)	27(2)	0	9(2)	0
C(306)	35(2)	29(2)	24(2)	0	2(1)	0
C(307)	31(2)	84(4)	48(3)	0	6(2)	0
C(308)	67(3)	42(2)	28(2)	0	13(2)	0
Cl(1)	32(1)	40(1)	35(1)	0	8(1)	0

Table S15. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for [Co2Cl(XDK)(bpy)2-(EtOH)2](NO3).3EtOH.

	x	y	z	U(eq)
H(1A)	1650(1)	711(1)	768(2)	40
H(2A)	2226(1)	-211(2)	331(2)	55
H(3A)	2606(1)	-946(2)	1497(3)	68
H(4A)	2377(1)	-752(2)	3060(2)	61
H(7A)	1998(1)	-670(2)	4454(2)	60
H(8A)	1622(1)	-435(2)	5913(2)	72
H(9A)	1052(1)	560(2)	6071(2)	66
H(10A)	876(1)	1310(2)	4780(2)	51
H(11A)	-207(1)	988(2)	1956(3)	73
H(11B)	-35(1)	1600(2)	2681(3)	73
H(12A)	-635(2)	844(3)	3326(4)	154
H(12B)	-102(2)	766(3)	3869(4)	154
H(12C)	-274(2)	152(3)	3143(4)	154
H(10B)	3388(2)	662(3)	3705(3)	110
H(10C)	3695(2)	1078(3)	4505(3)	110
H(10D)	3913(2)	1075(3)	3469(3)	110
H(10E)	2582(1)	1372(2)	4075(2)	40
H(10F)	2900(1)	1721(2)	4909(2)	40
H(20A)	783(1)	1083(2)	-2209(2)	74
H(20B)	1161(1)	665(2)	-1514(2)	74
H(20C)	1390(1)	1094(2)	-2387(2)	74
H(21A)	401(1)	1704(1)	-860(2)	37
H(21B)	798(1)	1376(1)	-129(2)	37
H(10G)	2273(1)	2500	5631(2)	51
H(10I)	1860(1)	2063	5027(2)	51
H(11C)	3710(2)	2500	4508(3)	63
H(11D)	3926(2)	2500	3468(3)	63
H(20D)	-131(1)	2500	5(3)	56
H(20E)	83(1)	2063	883(3)	56
H(21C)	768(2)	2500	-2217(3)	46
H(21D)	1374(2)	2500	-2410(3)	46
H(30A)	2213(1)	2500	1157(2)	36
H(30B)	3660(2)	2500	-811(3)	46
H(30C)	4249(2)	2500	467(3)	81
H(30E)	4043(2)	2063	1352(3)	81
H(30F)	3149(2)	2500	-2185(3)	68
H(30G)	2620(2)	2063	-2075(3)	68

Table S16. Crystal data and structure refinement for [Co2(XDK)(py)3-(NO3)2].MeOH.0.5Et2O.

Identification code	[Co2(XDK)(py)3(NO3)2].MeOH.0.5Et2O
Empirical formula	C50 H62 Co2 N7 O15.50
Formula weight	1126.93
Temperature	293(2) K
Wavelength	0.71073 A
Crystal system	monoclinic
Space group	P2(1)/n
Unit cell dimensions	a = 18.0846(4) A alpha = 90 deg. b = 12.3862(3) A beta = 102.7790(10) deg. c = 25.9939(5) A gamma = 90 deg.
Volume, Z	5678.4(2) A^3, 4
Density (calculated)	1.318 Mg/m^3
Absorption coefficient	0.653 mm^-1
F(000)	2356
Crystal size	0.25 x 0.10 x 0.10 mm
Theta range for data collection	1.25 to 22.50 deg.
Limiting indices	-17<=h<=24, -16<=k<=16, -33<=l<=32
Reflections collected	23083
Independent reflections	7407 [R(int) = 0.0271]
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	7252 / 4 / 685
Goodness-of-fit on F^2	1.095
Observed reflections [I>2sigma(I)]	6195
Final R indices [I>2sigma(I)]	R1 = 0.0462, wR2 = 0.1381
R indices (all data)	R1 = 0.0599, wR2 = 0.1517
Largest diff. peak and hole	0.747 and -0.638 e.A^-3