Electronic Supporting Information (ESI)

Solvent-induced structural diversities from discrete cup-shaped Co_8 cluster to Co_8 cluster-based chains accompanied by in situ ligand conversion

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Experimental Section

Materials and methods.

All chemicals were of reagent grade and used as purchased without further purification.

Elemental analyses (C, H, and N) were performed on a Perkin-Elmer 240C analyzer (Perkin-Elmer, USA). Thermogravimetric (TG) analyses were carried out on a Rigaku standard TG-DTA analyzer with a heating rate of 10°C min^{-1} from ambient temperature to 700 °C under nitrogen gas. Powder X-ray diffraction (PXRD) spectra were recorded on a Bruker D8 FOCUS diffractometer with a Cu-target tube and a graphite monochromator. Simulation of the XRPD spectra were carried out by the single-crystal data and diffraction-crystal module of the Mercury (Hg) program available free of charge *via* the Internet at http://www.iucr.org. The magnetic measurements were performed by using an MPMS XL-5 SQUID magnetometer. Diamagnetic corrections were estimated by using Pascal constants and background corrections by experimental measurement on sample holders.

Synthesis of 1-3

The ligand Hbms·HCl was prepared according to the method described in the literature.[1] A mixture of Hbms·HCl, HBTA and $Co(NO_3)_2 \cdot 6H_2O$ in the molar ratio of 1:1:2 in 10 ml MeOH/EtOH/n-PrOH/n-BuOH was sealed in a Teflon-lined autoclave, and heated to 90°C for 2 days then slowly cooled to 30°C in 36 h. Yield: ca. 12%, 30%, 15% and 10% with respect to HBTA for MeOH/EtOH/n-PrOH/n-BuOH system, respectively.

X-ray Crystallography.

The crystallographic data of **1-3** were collected on a Rigaku Saturn 724 diffractometer at 113 K with Mo-Kα radiation (λ = 0.71073 Å). The program *CrystalClear* was used for integration of the diffraction profiles. The crystal data was solved by direct methods and refined by a

full-matrix least-square method on F^2 using the *SHELXL-97* crystallographic software package.[2] In spite of the low temperature data set obtained at about 113 K for these three compounds, highly disordered solvents still exist within the lattice interstices. The diffraction data were treated by the "SQUEEZE" method as implemented in PLATON[3] and the results were appended to the bottom of the CIF file. All non-hydrogen atoms were refined anisotropically, and hydrogen atoms of the organic ligands were generated theoretically onto the specific atoms and refined isotropically with fixed thermal factors. Hydrogen atoms on coordinated water molecules and hydroxyl of coordinated alcohol/n-butanol can't be generated and were included in the molecular formula directly. In addition, the relatively high R_1 and wR_2 factors of compounds **1-3** might be due to the weak high-angle diffractions and the disorder of solvents atoms. Full crystallographic data for **1**, **2** and **3** have been deposited with the CCDC (940365-940367). These data can be obtained free of charge from The Cambridge Crystallographic Data Centre *via* www.ccdc.cam.ac.uk/data_request/cif.

The detail of structure refinements

(1) Solvent assignment for **1**:

The PLATON SQUEEZE procedure was used to treat regions of diffuse solvent which could not be modeled properly in terms of atomic sites. Their contribution to the diffraction pattern was removed and modified F^2 was written to a new HKL file. The number of located electrons, 748 in two voids per unit cell, is included in the formula, formula weight, calculated density, μ and $F(000)$. The main framework of **1** is dianionic. Considering the sources of cation and the acidic reaction environment in the formation of **1**, the negative charge may be balanced by two protonated water molecules. Similar cases are common in literature.[4] In the refinement of **1**, highly disordered BTA^- ligands are generated. However, these units cannot be modeled properly.

There are four formula units in one unit cell. On base of charge balance considerations, volume/count_electrons analysis, TG analyses and elemental analyses, this residual electron density was assigned to two and half molecules of 1*H*-Benzotriazole (HBTA), two molecules of protonated water and one water molecule. So SQUEEZE removed these disordered units per unit cell. The TENTATIVE formula for **1** is $[Co_8(BTA)_6(BIC)_3Cl_6]\cdot(HBTA)_{2.5}(H_3O)_2(H_2O)$.[5]

Crystal data for **1**: $C_{75}H_{56.5}Cl_6Co_8N_{31.5}O_9$, Mr = 2227.14; Monoclinic, $P2_1/c$; a = 18.867(4) Å, b = 17.119(3) Å, c = 28.504(5) Å, α = γ = 90°, β= 112.252(11)°; V = 8521(3) Å^3; Z = 4; D_{calc} = 1.736 g/cm^3; T = 113 K.; Reflections collected/unique = 79926 / 20307, R_{int} = 0.0497; R_1 = 0.0831, $wR2$ = 0.1972 (I > 2θ(I)); R_1 = 0.1021, $wR2$ = 0.2079 (all data) and GOF = 1.039; Elemental analysis (%): Calcd. for $C_{75}H_{56.5}Cl_6Co_8N_{31.5}O_9$ (2227.14): C 40.45, H 2.56, N 19.81; found: C 39.90, H 2.95, N 19.34. IR (KBr pellets, cm^{-1}): 3444(m), 3070(m), 2377(w), 1666(s), 1573(s), 1535(s), 1473(s), 1361(s), 1274(m), 1197(s), 1143(m), 998(m), 921(vs), 885(m), 746(s), 644(m), 561(m).

(2) Solvent assignment for **2**:

The PLATON SQUEEZE procedure was used to treat regions of diffuse solvent which could not be modeled properly in terms of atomic sites. Their contribution to the diffraction pattern was removed and modified F^2 was written to a new HKL file. The number of located electrons, 724 in four voids per unit cell, is included in the formula, formula weight, calculated density, μ and F(000). There are four formula units in one unit cell. On base of charge balance considerations, volume/count_electrons analysis, TG analyses and elemental analyses, this residual electron density was assigned to five molecules of ethanol, and five molecules of water. So SQUEEZE removed these disordered units per unit cell. The TENTATIVE formula for **2** is $[Co_{16}(BTA)_{12}(BIC)_6Cl_8(EtOH)_3(H_2O)_2]\cdot(C_2H_5OH)_5(H_2O)_5$.

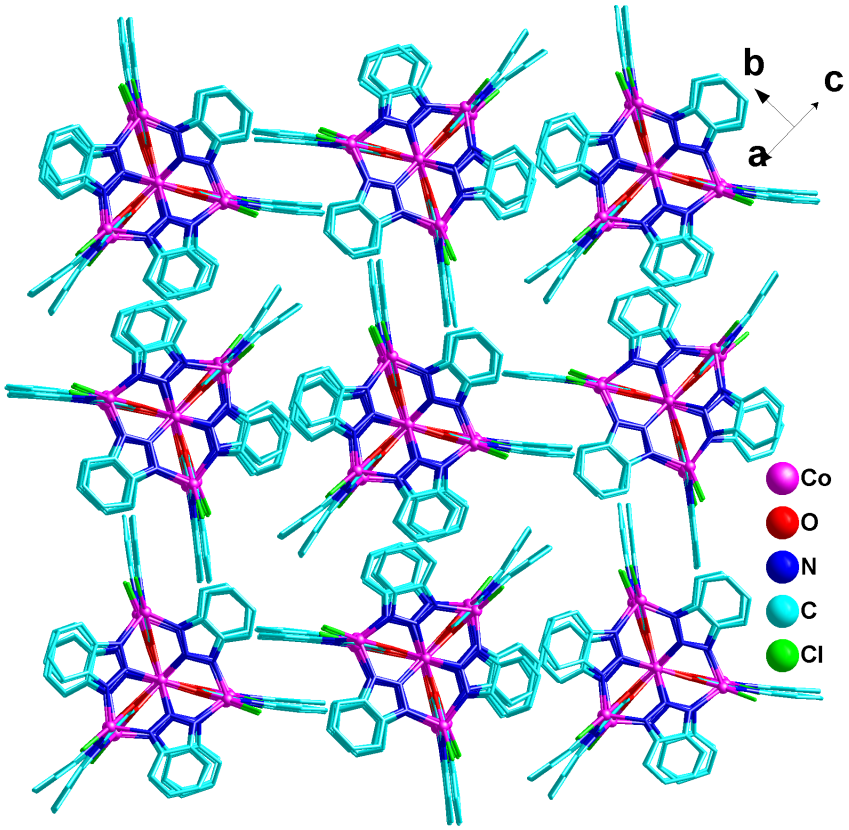
Crystal data for **2**: $C_{136}H_{134}Cl_8Co_{16}N_{48}O_{27}$, *Mr* = 4099.38; Monoclinic, $P2_1/c$; *a* = 30.195(5) Å, *b* = 20.367(4) Å, *c* = 33.896(4) Å, α = γ = 90°, β = 123.240(10)°; *V* = 17435(5) Å^3; *Z* = 4; D_{calc} = 1.562 g/cm^3; *T* = 113 K.; Reflections collected/unique = 174599 / 41136, R_{int} = 0.0653; R_1 = 0.0689, *wR2* = 0.1890 (I > 2θ(I)); R_1 = 0.0854, *wR2* = 0.2038 (all data) and *GOF* = 1.017; Elemental analysis (%): Calcd. for $C_{136}H_{134}Cl_8Co_{16}N_{48}O_{27}$ (4099.38): C 39.85, H 3.29, N 16.40; found: C 40.42, H 2.96, N 16.67. IR (KBr pellets, cm^{-1}): 3430(m), 1670(s), 1575(s), 1537(s), 1469(s), 1361(s), 1276(w), 1201(m), 1145(w), 995(w), 925 (w), 887(w), 790 (m), 748 (s), 644(w), 563(vw).

(3) Solvent assignment for **3**:

The PLATON SQUEEZE procedure was used to treat regions of diffuse solvent which could not be modeled properly in terms of atomic sites. Their contribution to the diffraction pattern was removed and modified F^2 was written to a new HKL file. The number of located electrons, 1537 in six voids per unit cell, is included in the formula, formula weight, calculated density, μ and *F*(000). There are four formula units in one unit cell. On base of charge balance considerations, volume/count_electrons analysis, TG analyses and elemental analyses, this residual electron density was assigned to four molecules of n-butanol, and twenty-one and half molecules of water. So SQUEEZE removed these disordered units per unit cell. The TENTATIVE formula for **3** is $[Co_{16}(BTA)_{12}(BIC)_6Cl_8(n\text{-}BuOH)(H_2O)_3]\cdot(n\text{-}BuOH)_4(H_2O)_{21.5}$.

Crystal data for **3**: $C_{140}H_{171}Cl_8Co_{16}N_{48}O_{41.5}$, *Mr* = 4416.71; Orthorhombic, $Pna2_1$; *a* = 34.484(10) Å, *b* = 20.624(6) Å, *c* = 23.922(7) Å, α = β = γ = 90°; *V* = 17013(9) Å^3; *Z* = 4; D_{calc} = 1.724 g/cm^3; *T* = 113 K.; Reflections collected/unique = 98194 / 30209, R_{int} = 0.1069; R_1 = 0.0758, *wR2* = 0.1840 (I > 2θ(I)); R_1 = 0.0905, *wR2* = 0.1961 (all data) and *GOF* = 1.012. Elemental analysis (%): Calcd. for $C_{140}H_{171}Cl_8Co_{16}N_{48}O_{41.5}$ (4416.71): C 38.07, H 3.90, N

15.22; found: C 37.49, H 3.45, N 14.74. IR (KBr pellets, cm^{-1}): 3407(m), 3068(w), 2960(m), 2869(w), 2385(vw), 1668(vs), 1575(vs), 1535(vs), 1471(vs), 1361(vs), 1276(m), 1203(s), 1147(w), 1066(w), 995(w), 923(w), 887(w), 788(s), 750(vs), 644(m), 561(w).



Scheme S1 The packing mode of complex **1**.

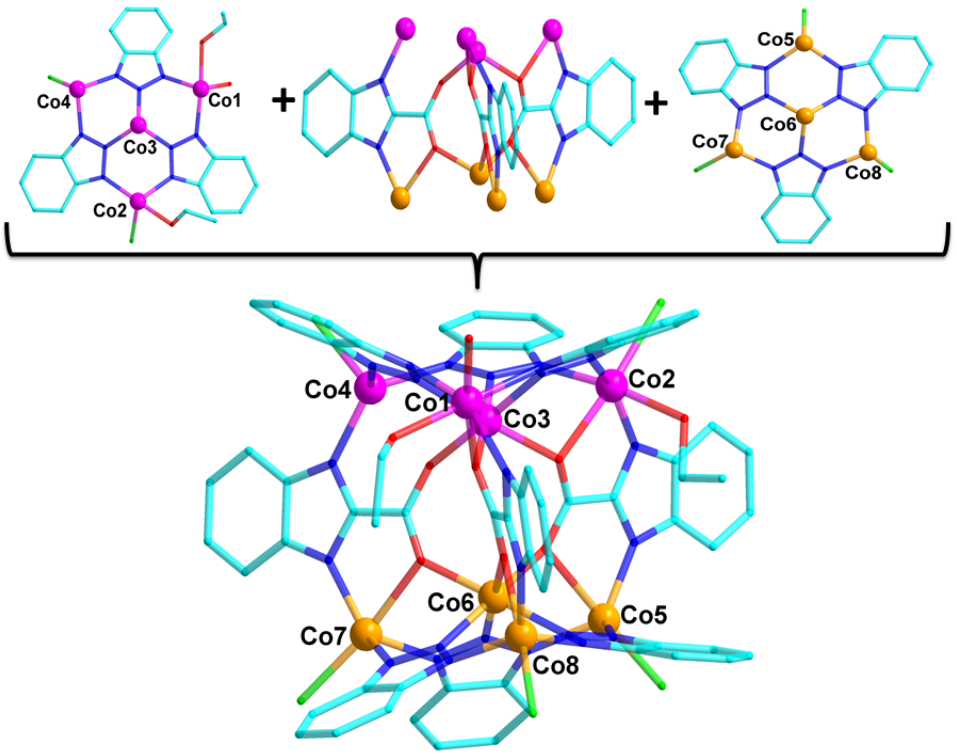


Fig. S1 The schematic constituent of the Co_8[a] building block in **2**.

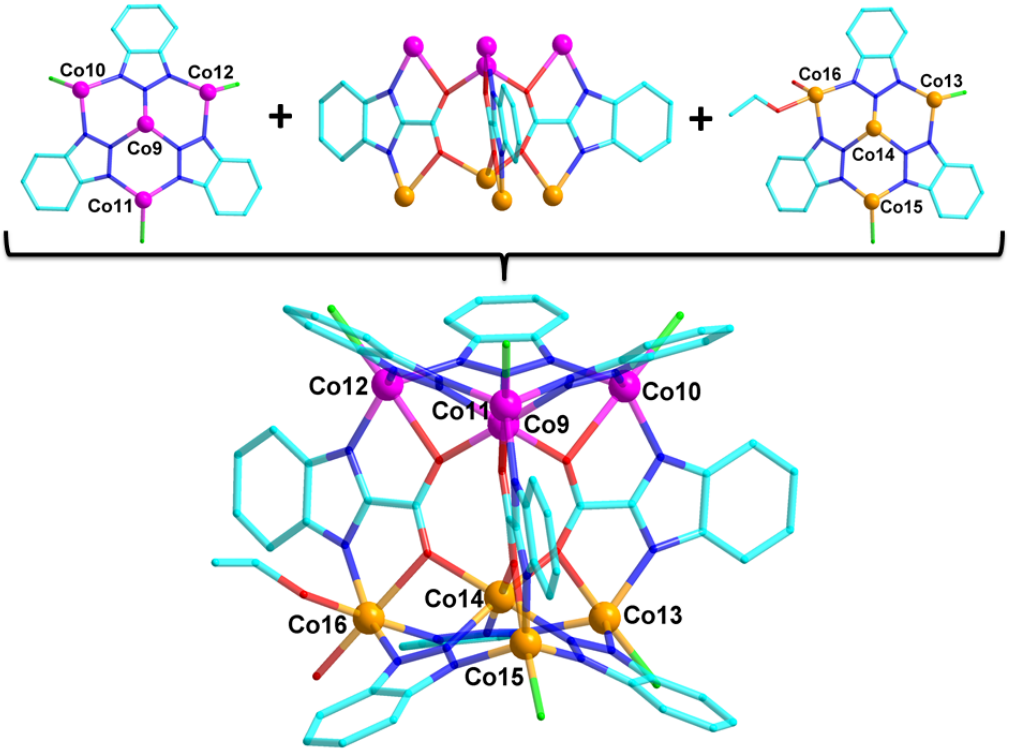


Fig. S2 The schematic constituent of the Co_8[b] building block in **2**.

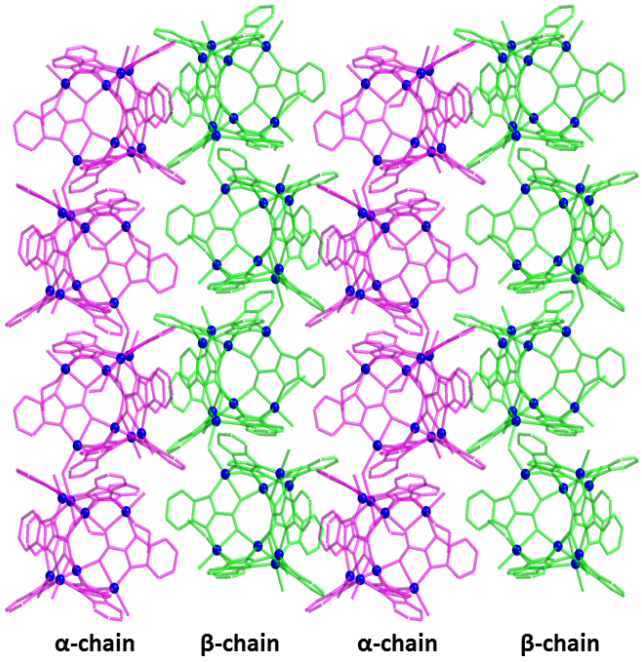


Fig. S3 The arrangement of the α-chain and β-chain along the *c* axis in **2.**

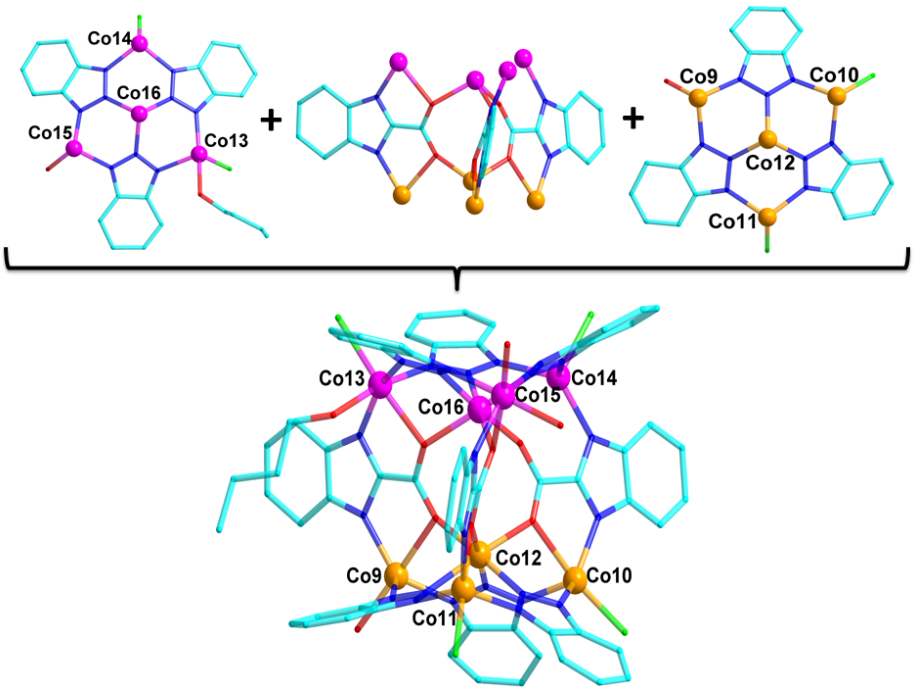


Fig. S4 The schematic constituent of the Co_8^a building block in **3**.

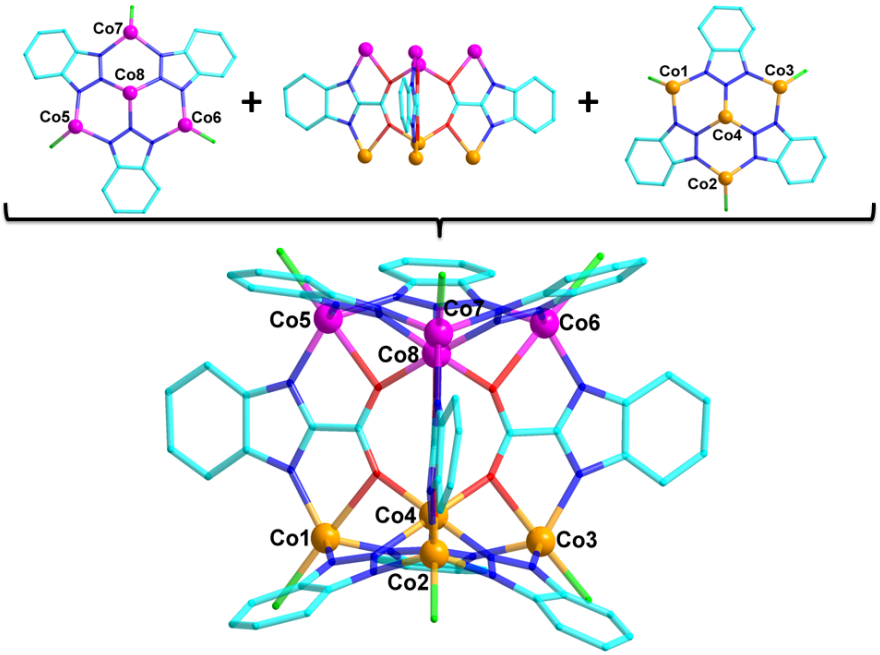


Fig. S5 The schematic constituent of the Co_8^b building block in **3**.

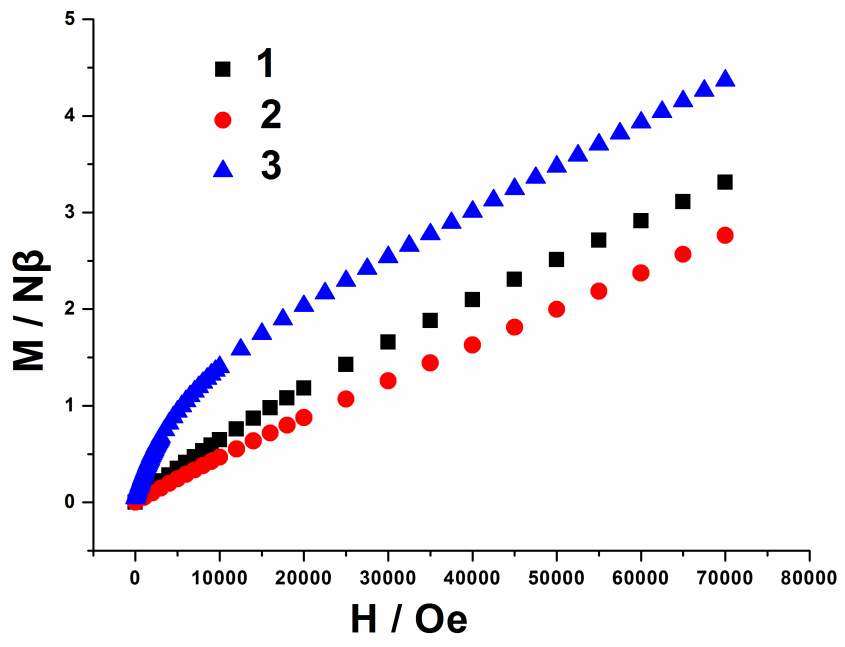


Fig. S6 Field dependence of the magnetization (*M*) of compounds **1-3** at 2 K (normalized to eight Co^{2+} ions).

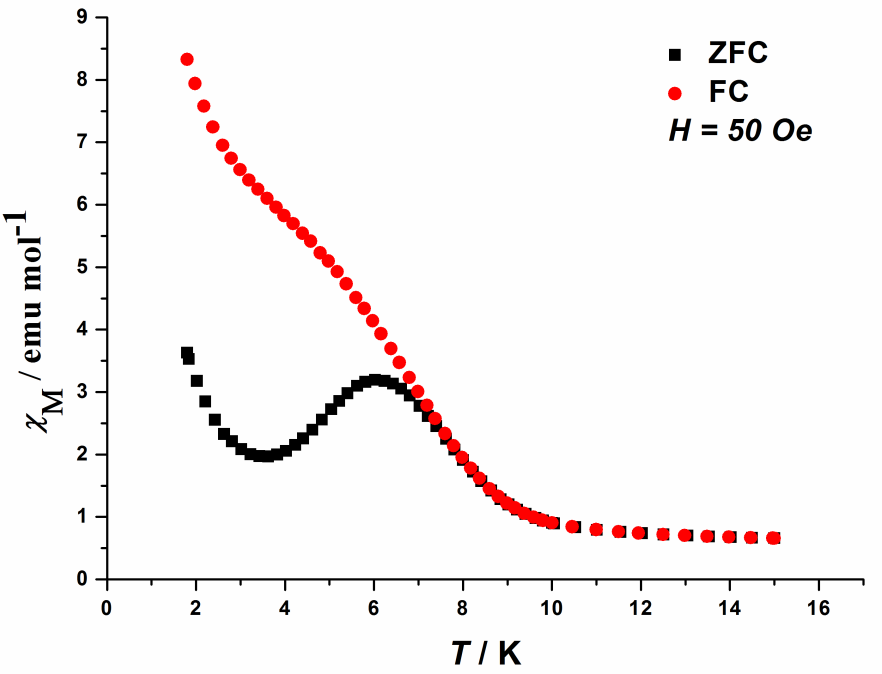


Fig. S7 FC and ZFC magnetization of **3** in the dc field of 50 Oe.

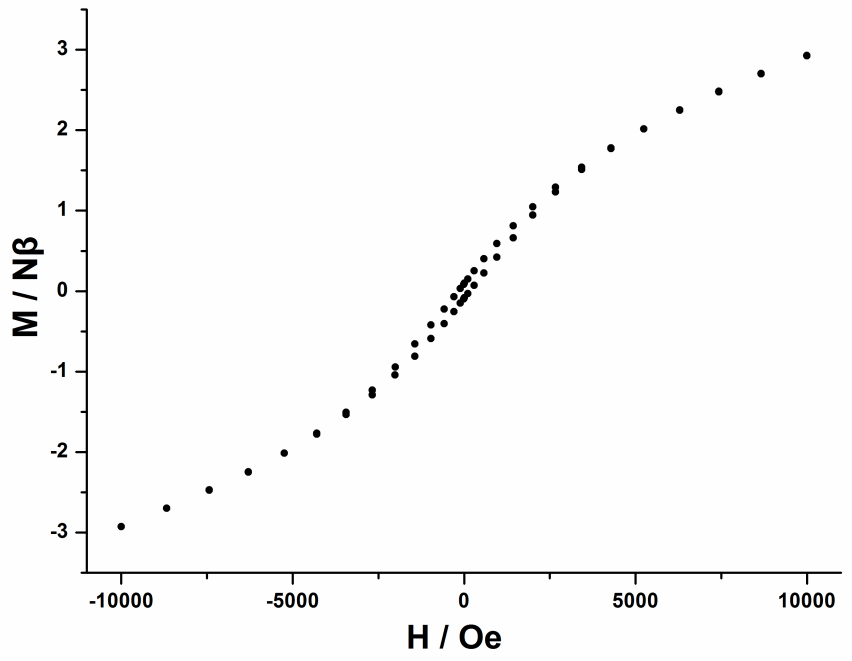


Fig. S8 Plots of hysteresis loop of **3** at 2K.

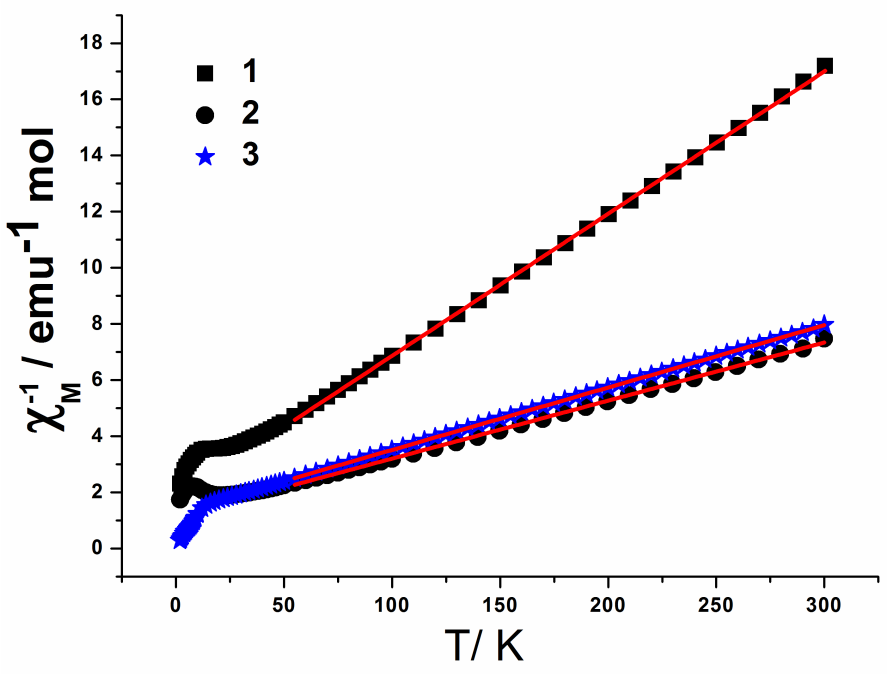


Fig. S9 The Curie-Weiss plots of **1-3**. Solid line represents the best fit.

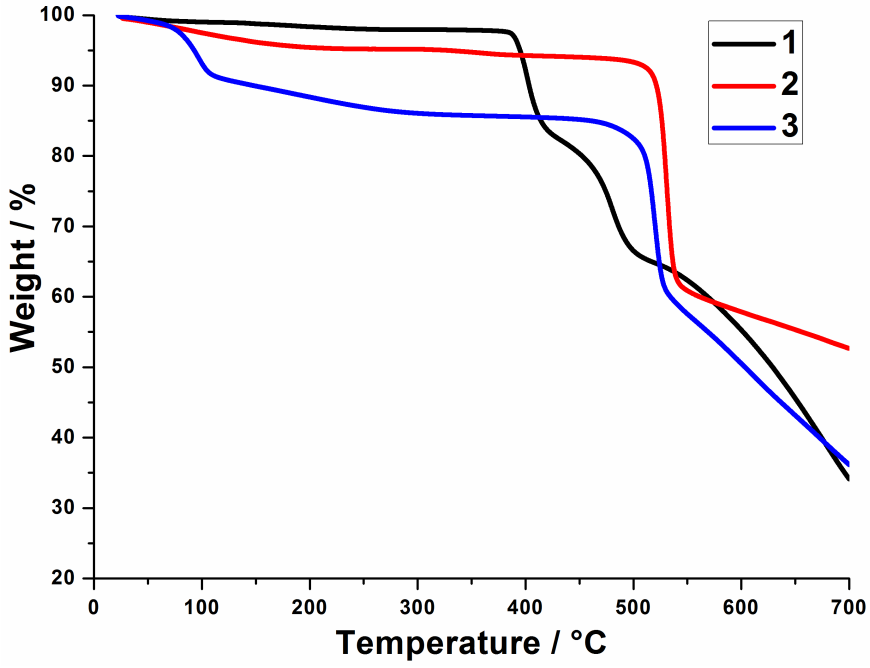


Fig. S10 TG curves of compounds **1-3.**

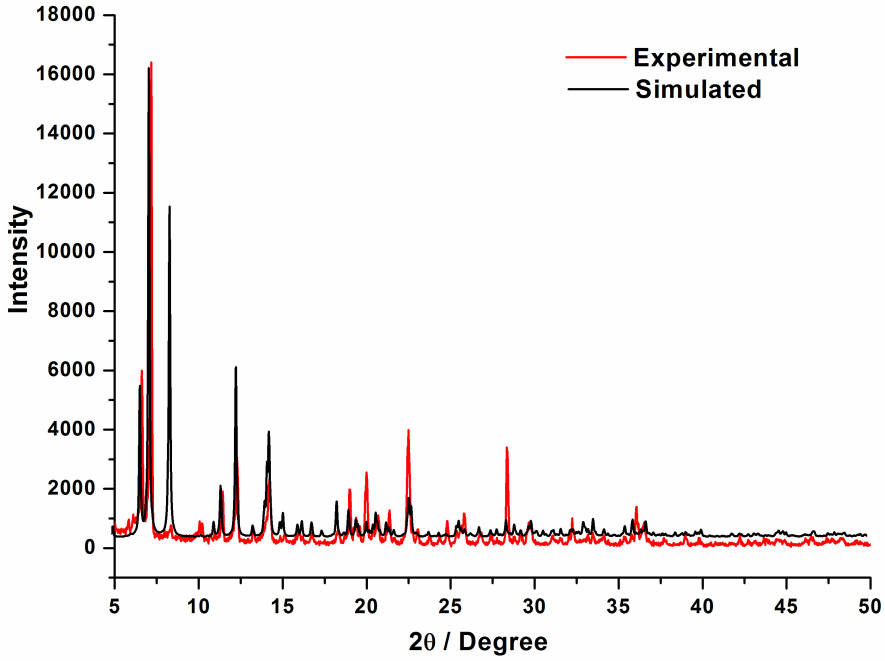


Fig. S11 XRPD pattern of **1**.

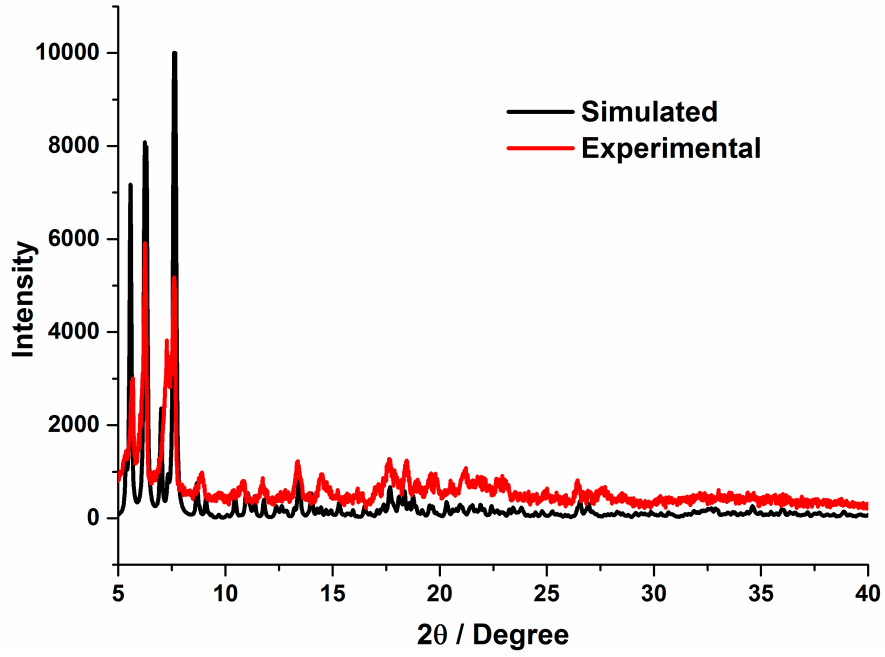


Fig. S12 XRPD pattern of **2**.

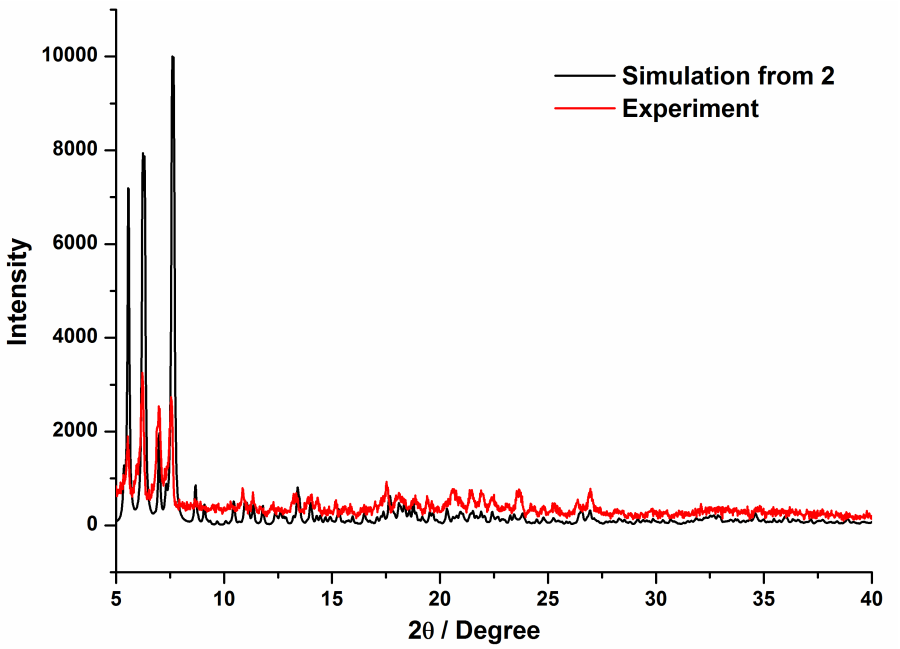


Fig. S13 XRPD patterns of the crystal from n-PrOH system.

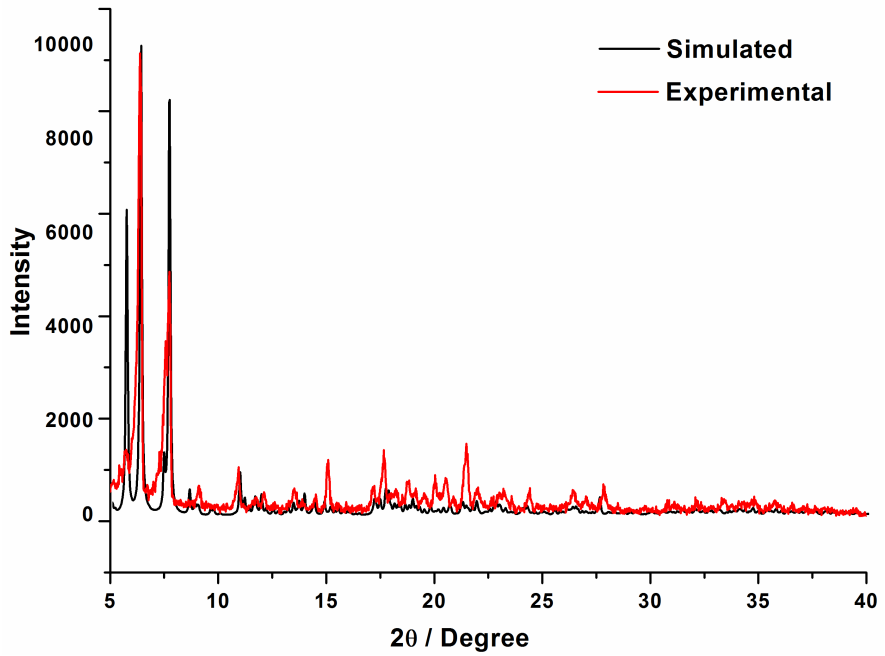


Fig. S14 XRPD pattern of **3**.

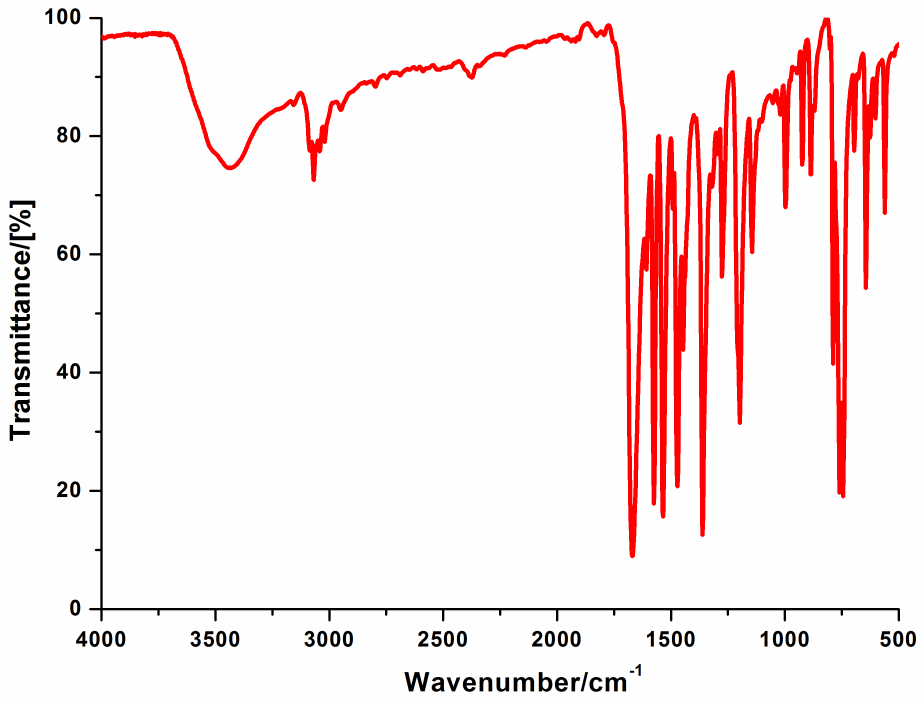


Fig. S15 IR spectrum of **1**.

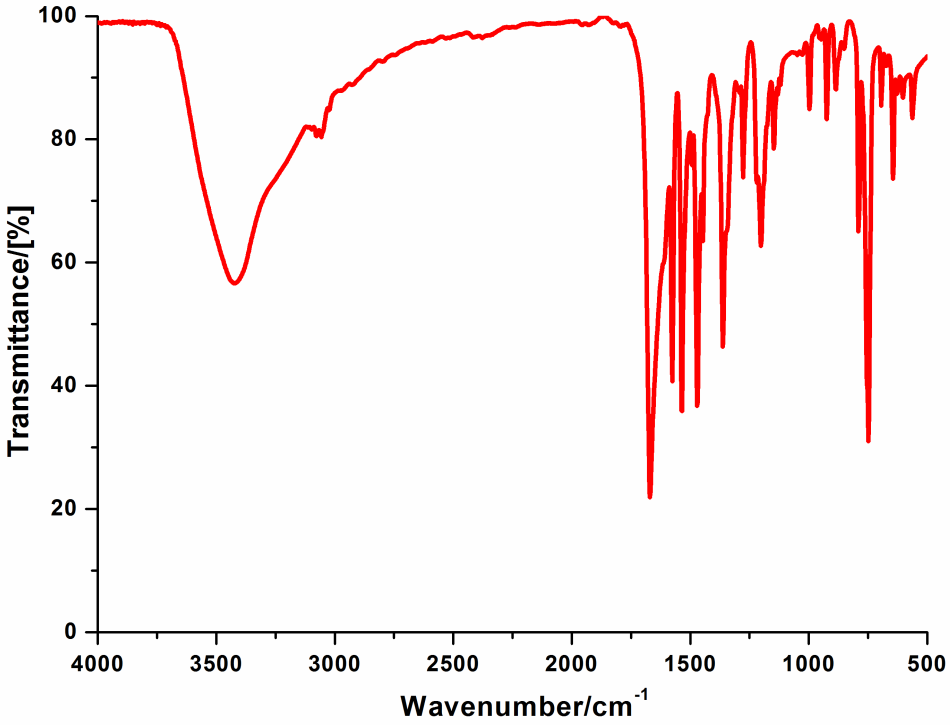


Fig. S16 IR spectrum of **2**.

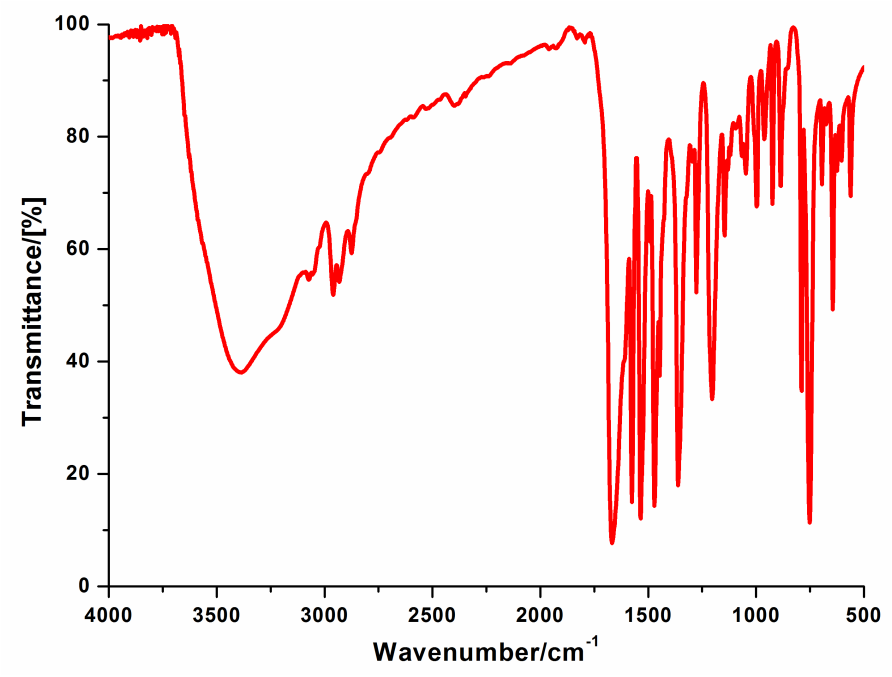


Fig. S17 IR spectrum of the crystal from n-PrOH system.

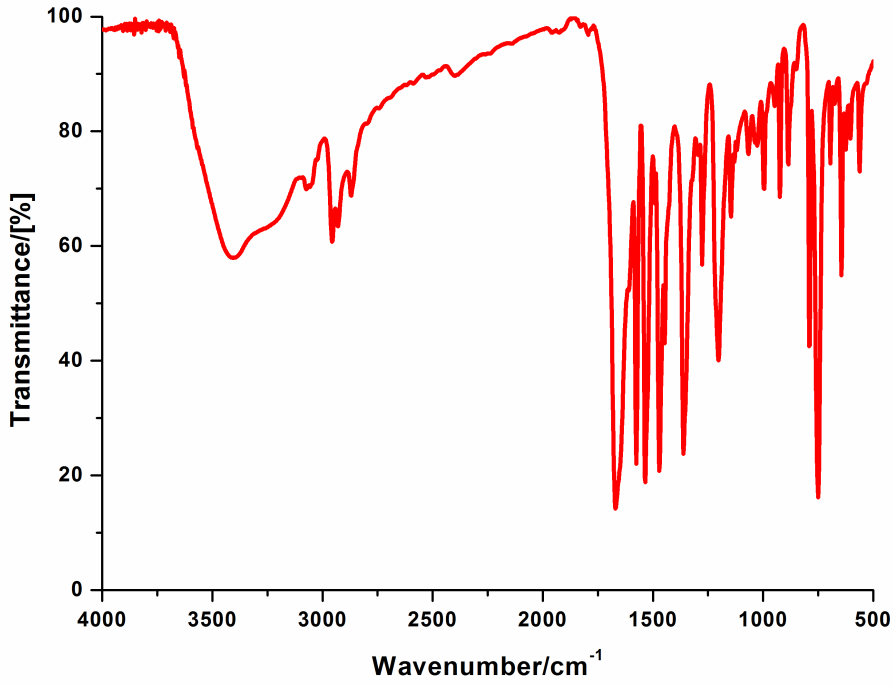


Fig. S18 IR spectrum of **3**.

Table S2 The selected bond lengths [Å] and angles [º] of complex **1**.

Co(1)-N(12)	2.061(5)	Co(1)-N(24)	2.073(4)
Co(1)-N(16)	2.097(5)	Co(1)-Cl(1)	2.2772(18)
Co(1)-O(3)	2.394(4)	Co(2)-N(10)	2.040(4)
Co(2)-N(22)	2.067(5)	Co(2)-N(21)	2.079(5)
Co(2)-Cl(2)	2.2770(17)	Co(2)-O(1)	2.390(3)
Co(3)-N(19)	2.022(5)	Co(3)-N(14)	2.106(6)
Co(3)-N(18)	2.120(6)	Co(3)-Cl(3)	2.2820(19)
Co(4)-O(1)	2.035(3)	Co(4)-O(3)	2.036(3)
Co(4)-O(5)	2.050(4)	Co(4)-N(17)	2.078(5)
Co(4)-N(23)	2.086(4)	Co(4)-N(20)	2.093(4)
Co(5)-N(13)	2.050(5)	Co(5)-N(1)	2.066(5)
Co(5)-N(7)	2.083(5)	Co(5)-Cl(4)	2.2586(17)
Co(5)-O(4)	2.390(4)	Co(6)-N(9)	2.064(5)
Co(6)-N(15)	2.075(5)	Co(6)-N(6)	2.082(5)
Co(6)-Cl(5)	2.275(2)	Co(6)-O(6)	2.392(4)
Co(7)-N(11)	2.071(4)	Co(7)-N(3)	2.071(5)
Co(7)-Cl(6)	2.2712(18)	Co(7)-N(4)	2.093(5)
Co(7)-O(2)	2.368(4)	Co(8)-O(6)	2.043(3)
Co(8)-O(4)	2.041(4)	Co(8)-N(5)	2.084(4)
Co(8)-O(2)	2.047(3)	Co(8)-N(8)	2.094(4)
Co(8)-N(2)	2.088(4)		
N(12)-Co(1)-N(24)	117.75(19)	N(12)-Co(1)-N(16)	128.77(18)
N(24)-Co(1)-N(16)	98.49(18)	N(12)-Co(1)-Cl(1)	100.90(14)
N(24)-Co(1)-Cl(1)	106.37(13)	N(16)-Co(1)-Cl(1)	102.04(14)

N(12)-Co(1)-O(3)	74.15(15)	N(24)-Co(1)-O(3)	80.22(15)
N(16)-Co(1)-O(3)	78.20(15)	Cl(1)-Co(1)-O(3)	173.22(10)
N(10)-Co(2)-N(22)	121.88(18)	N(10)-Co(2)-N(21)	125.36(19)
N(22)-Co(2)-N(21)	97.90(18)	N(10)-Co(2)-Cl(2)	100.02(13)
N(22)-Co(2)-Cl(2)	106.45(13)	N(21)-Co(2)-Cl(2)	102.72(13)
N(10)-Co(2)-O(1)	74.05(14)	N(22)-Co(2)-O(1)	79.26(15)
N(21)-Co(2)-O(1)	79.16(15)	Cl(2)-Co(2)-O(1)	173.52(10)
N(19)-Co(3)-N(14)	130.9(2)	N(19)-Co(3)-N(18)	97.6(2)
N(14)-Co(3)-N(18)	116.0(2)	N(19)-Co(3)-Cl(3)	103.35(14)
N(14)-Co(3)-Cl(3)	100.82(14)	N(18)-Co(3)-Cl(3)	105.64(13)
O(1)-Co(4)-O(3)	101.09(15)	O(1)-Co(4)-O(5)	98.64(15)
O(3)-Co(4)-O(5)	100.53(15)	O(1)-Co(4)-N(17)	176.90(17)
O(3)-Co(4)-N(17)	81.07(18)	O(5)-Co(4)-N(17)	83.09(16)
O(1)-Co(4)-N(23)	82.02(16)	O(3)-Co(4)-N(23)	82.52(15)
O(5)-Co(4)-N(23)	176.66(16)	N(17)-Co(4)-N(23)	96.11(17)
O(1)-Co(4)-N(20)	81.37(16)	O(3)-Co(4)-N(20)	176.87(17)
O(5)-Co(4)-N(20)	80.93(17)	N(17)-Co(4)-N(20)	96.4(2)
N(23)-Co(4)-N(20)	95.96(17)	N(13)-Co(5)-N(1)	124.6(2)
N(13)-Co(5)-N(7)	122.3(2)	N(1)-Co(5)-N(7)	98.06(18)
N(13)-Co(5)-Cl(4)	100.58(14)	N(1)-Co(5)-Cl(4)	104.80(13)
N(7)-Co(5)-Cl(4)	103.75(14)	N(13)-Co(5)-O(4)	74.35(15)
N(1)-Co(5)-O(4)	79.10(15)	N(7)-Co(5)-O(4)	78.74(15)
Cl(4)-Co(5)-O(4)	174.88(11)	N(9)-Co(6)-N(15)	126.5(2)
N(9)-Co(6)-N(6)	96.79(18)	N(15)-Co(6)-N(6)	122.40(18)
N(9)-Co(6)-Cl(5)	102.07(14)	N(15)-Co(6)-Cl(5)	99.45(14)
N(6)-Co(6)-Cl(5)	107.04(14)	N(9)-Co(6)-O(6)	80.50(15)

N(15)-Co(6)-O(6)	73.49(15)	N(6)-Co(6)-O(6)	79.57(15)
Cl(5)-Co(6)-O(6)	172.39(11)	N(3)-Co(7)-N(11)	116.1(2)
N(11)-Co(7)-N(4)	131.40(18)	N(3)-Co(7)-N(4)	97.96(17)
N(11)-Co(7)-Cl(6)	99.99(13)	N(3)-Co(7)-Cl(6)	108.06(14)
N(3)-Co(7)-O(2)	80.63(15)	N(4)-Co(7)-Cl(6)	100.99(14)
N(4)-Co(7)-O(2)	78.52(15)	N(11)-Co(7)-O(2)	74.45(14)
Cl(6)-Co(7)-O(2)	171.23(11)	O(4)-Co(8)-O(2)	101.34(16)
O(4)-Co(8)-O(6)	99.90(15)	O(4)-Co(8)-N(5)	176.91(16)
O(6)-Co(8)-O(2)	99.20(14)	O(2)-Co(8)-N(5)	80.74(17)
O(6)-Co(8)-N(5)	81.93(16)	O(6)-Co(8)-N(2)	177.15(17)
O(4)-Co(8)-N(2)	81.56(16)	N(5)-Co(8)-N(2)	96.49(17)
O(2)-Co(8)-N(2)	82.85(16)	O(6)-Co(8)-N(8)	81.59(15)
O(4)-Co(8)-N(8)	81.34(17)	N(5)-Co(8)-N(8)	96.52(19)
O(2)-Co(8)-N(8)	176.98(17)	N(2)-Co(8)-N(8)	96.25(17)

Table S2 The selected bond lengths [Å] and angles [º] of complex **2**.

Co(10)-N(15)	2.064(3)	Co(10)-N(6)	2.065(3)
Co(10)-N(7)	2.066(3)	Co(10)-Cl(2)	2.2910(12)
Co(10)-O(11)	2.391(3)	Co(9)-O(11)	2.044(3)
Co(9)-O(9)	2.048(3)	Co(9)-O(7)	2.056(3)
Co(9)-N(2)	2.089(3)	Co(9)-N(8)	2.089(3)
Co(9)-N(5)	2.114(3)	Co(12)-N(4)	2.036(3)
Co(12)-N(13)	2.038(4)	Co(12)-N(3)	2.087(3)
Co(12)-O(7)	2.324(3)	Co(12)-Cl(3)	2.3628(12)
Co(14)-O(10)	2.033(3)	Co(14)-N(20)	2.068(4)
Co(14)-N(17)	2.087(4)	Co(14)-O(12)	2.093(3)

Co(14)-N(23)	2.099(3)	Co(14)-O(8)	2.113(3)
Co(13)-N(14)	2.050(3)	Co(13)-N(24)	2.052(4)
Co(13)-N(16)	2.075(4)	Co(13)-O(12)	2.291(3)
Co(13)-Cl(3)#1	2.3804(12)	Co(11)-N(11)	2.069(4)
Co(11)-N(9)	2.081(4)	Co(11)-N(1)	2.094(4)
Co(11)-Cl(1)	2.2907(14)	Co(11)-O(9)	2.363(3)
Co(16)-O(30)	2.078(3)	Co(16)-N(18)	2.132(4)
Co(16)-N(19)	2.136(4)	Co(16)-N(12)	2.151(4)
Co(16)-O(13)	2.192(4)	Co(16)-O(8)	2.255(3)
Co(15)-N(22)	2.060(4)	Co(15)-N(10)	2.062(4)
Co(15)-N(21)	2.073(4)	Co(15)-Cl(4)	2.2708(13)
Co(6)-O(4)	2.038(3)	Co(6)-O(6)	2.055(3)
Co(6)-O(2)	2.076(3)	Co(6)-N(41)	2.085(3)
Co(6)-N(44)	2.099(3)	Co(6)-N(47)	2.113(3)
Co(3)-O(5)	2.038(3)	Co(3)-N(29)	2.071(3)
Co(3)-N(26)	2.089(3)	Co(3)-N(32)	2.090(3)
Co(3)-O(1)	2.118(3)	Co(3)-O(3)	2.142(3)
Co(2)-N(38)	2.111(3)	Co(2)-N(27)	2.124(3)
Co(2)-N(28)	2.139(3)	Co(2)-O(17)	2.190(3)
Co(2)-O(3)	2.234(3)	Co(2)-Cl(6)	2.4575(12)
Co(1)-O(15)	2.076(3)	Co(1)-N(30)	2.142(3)
Co(1)-N(36)	2.148(4)	Co(1)-N(33)	2.151(4)
Co(1)-O(20)	2.163(3)	Co(1)-O(1)	2.229(3)
Co(7)-N(45)	2.082(3)	Co(7)-N(35)	2.090(4)
Co(7)-N(40)	2.121(3)	Co(7)-Cl(7)	2.2978(12)
Co(7)-O(6)	2.311(3)	Co(8)-N(37)	2.030(4)

Co(8)-N(46)	2.042(3)	Co(8)-N(42)	2.055(3)
Co(8)-Cl(6)#2	2.3342(12)	Co(8)-O(2)	2.374(3)
Co(5)-N(39)	2.043(4)	Co(5)-N(48)	2.063(3)
Co(5)-N(43)	2.070(3)	Co(5)-Cl(8)	2.2814(12)
Co(4)-N(31)	2.058(4)	Co(4)-N(34)	2.060(3)
Co(4)-N(25)	2.071(3)	Co(4)-Cl(5)	2.2867(12)
Cl(6)-Co(8)#3	2.3342(12)	Cl(3)-Co(13)#4	2.3804(12)
N(15)-Co(10)-N(6)	120.04(14)	N(15)-Co(10)-N(7)	122.12(13)
N(6)-Co(10)-N(7)	101.99(13)	N(15)-Co(10)-Cl(2)	104.40(10)
N(6)-Co(10)-Cl(2)	100.88(10)	N(7)-Co(10)-Cl(2)	104.50(10)
N(15)-Co(10)-O(11)	74.52(12)	N(6)-Co(10)-O(11)	78.37(12)
N(7)-Co(10)-O(11)	77.50(11)	Cl(2)-Co(10)-O(11)	177.99(7)
O(11)-Co(9)-O(9)	100.35(12)	O(11)-Co(9)-O(7)	99.40(11)
O(9)-Co(9)-O(7)	98.28(12)	O(11)-Co(9)-N(2)	179.54(13)
O(9)-Co(9)-N(2)	79.21(13)	O(7)-Co(9)-N(2)	80.53(13)
O(11)-Co(9)-N(8)	81.30(12)	O(9)-Co(9)-N(8)	82.68(13)
O(7)-Co(9)-N(8)	178.67(14)	N(2)-Co(9)-N(8)	98.78(14)
O(11)-Co(9)-N(5)	80.55(13)	O(9)-Co(9)-N(5)	178.80(13)
O(7)-Co(9)-N(5)	82.33(12)	N(2)-Co(9)-N(5)	99.89(14)
N(8)-Co(9)-N(5)	96.69(13)	N(4)-Co(12)-N(13)	117.13(14)
N(4)-Co(12)-N(3)	106.41(13)	N(13)-Co(12)-N(3)	124.79(15)
N(4)-Co(12)-O(7)	80.94(12)	N(13)-Co(12)-O(7)	75.88(12)
N(3)-Co(12)-O(7)	79.41(12)	N(4)-Co(12)-Cl(3)	101.79(10)
N(13)-Co(12)-Cl(3)	103.01(10)	N(3)-Co(12)-Cl(3)	99.35(10)
O(7)-Co(12)-Cl(3)	177.24(8)	O(10)-Co(14)-N(20)	84.08(14)

O(10)-Co(14)-N(17)	178.60(14)	N(20)-Co(14)-N(17)	95.62(15)
O(10)-Co(14)-O(12)	99.36(11)	N(20)-Co(14)-O(12)	175.41(14)
N(17)-Co(14)-O(12)	80.87(13)	O(10)-Co(14)-N(23)	80.63(13)
N(20)-Co(14)-N(23)	96.40(14)	N(17)-Co(14)-N(23)	98.05(14)
O(12)-Co(14)-N(23)	81.24(13)	O(10)-Co(14)-O(8)	97.17(12)
N(20)-Co(14)-O(8)	81.65(13)	N(17)-Co(14)-O(8)	84.13(13)
O(12)-Co(14)-O(8)	100.85(12)	N(23)-Co(14)-O(8)	177.22(13)
N(14)-Co(13)-N(24)	109.90(14)	N(14)-Co(13)-N(16)	131.17(14)
N(24)-Co(13)-N(16)	106.68(14)	N(14)-Co(13)-O(12)	77.34(12)
N(24)-Co(13)-O(12)	82.00(13)	N(16)-Co(13)-O(12)	76.93(12)
N(14)-Co(13)-Cl(3)#1	100.52(10)	N(24)-Co(13)-Cl(3)#1	99.87(11)
N(16)-Co(13)-Cl(3)#1	103.90(11)	O(12)-Co(13)-Cl(3)#1	177.57(8)
N(11)-Co(11)-N(9)	116.47(14)	N(11)-Co(11)-N(1)	126.39(14)
N(9)-Co(11)-N(1)	101.64(14)	N(11)-Co(11)-Cl(1)	103.56(11)
N(9)-Co(11)-Cl(1)	103.01(11)	N(1)-Co(11)-Cl(1)	102.80(11)
N(11)-Co(11)-O(9)	74.88(12)	N(9)-Co(11)-O(9)	79.56(12)
N(1)-Co(11)-O(9)	76.78(12)	Cl(1)-Co(11)-O(9)	177.41(9)
O(30)-Co(16)-N(18)	95.49(14)	O(30)-Co(16)-N(19)	101.63(16)
N(18)-Co(16)-N(19)	95.03(15)	O(30)-Co(16)-N(12)	100.33(16)
N(18)-Co(16)-N(12)	96.70(16)	N(19)-Co(16)-N(12)	153.92(16)
O(30)-Co(16)-O(13)	88.61(15)	N(18)-Co(16)-O(13)	175.35(14)
N(19)-Co(16)-O(13)	81.97(15)	N(12)-Co(16)-O(13)	84.68(16)
O(30)-Co(16)-O(8)	175.64(15)	N(18)-Co(16)-O(8)	81.37(13)
N(19)-Co(16)-O(8)	81.72(13)	N(12)-Co(16)-O(8)	77.13(13)
O(13)-Co(16)-O(8)	94.65(13)	N(22)-Co(15)-N(10)	124.99(14)
N(22)-Co(15)-N(21)	100.24(14)	N(10)-Co(15)-N(21)	119.75(15)

N(22)-Co(15)-Cl(4)	101.45(11)	N(10)-Co(15)-Cl(4)	103.69(11)
N(21)-Co(15)-Cl(4)	103.53(11)	O(4)-Co(6)-O(6)	98.35(11)
O(4)-Co(6)-O(2)	100.89(12)	O(6)-Co(6)-O(2)	98.23(11)
O(4)-Co(6)-N(41)	176.43(12)	O(6)-Co(6)-N(41)	79.70(12)
O(2)-Co(6)-N(41)	82.40(13)	O(4)-Co(6)-N(44)	79.77(12)
O(6)-Co(6)-N(44)	82.53(12)	O(2)-Co(6)-N(44)	178.89(13)
N(41)-Co(6)-N(44)	96.96(13)	O(4)-Co(6)-N(47)	83.05(12)
O(6)-Co(6)-N(47)	178.60(12)	O(2)-Co(6)-N(47)	81.40(12)
N(41)-Co(6)-N(47)	98.90(13)	N(44)-Co(6)-N(47)	97.82(13)
O(5)-Co(3)-N(29)	178.78(13)	O(5)-Co(3)-N(26)	81.06(12)
N(29)-Co(3)-N(26)	98.75(13)	O(5)-Co(3)-N(32)	83.52(13)
N(29)-Co(3)-N(32)	95.31(14)	N(26)-Co(3)-N(32)	96.60(13)
O(5)-Co(3)-O(1)	95.91(11)	N(29)-Co(3)-O(1)	84.24(12)
N(26)-Co(3)-O(1)	176.50(12)	N(32)-Co(3)-O(1)	81.24(12)
O(5)-Co(3)-O(3)	98.47(11)	N(29)-Co(3)-O(3)	82.68(12)
N(26)-Co(3)-O(3)	82.10(12)	N(32)-Co(3)-O(3)	177.40(13)
O(1)-Co(3)-O(3)	100.17(11)	N(38)-Co(2)-N(27)	91.60(13)
N(38)-Co(2)-N(28)	155.44(14)	N(27)-Co(2)-N(28)	100.67(13)
N(38)-Co(2)-O(17)	82.77(13)	N(27)-Co(2)-O(17)	172.48(13)
N(28)-Co(2)-O(17)	82.84(13)	N(38)-Co(2)-O(3)	79.27(12)
N(27)-Co(2)-O(3)	79.90(12)	N(28)-Co(2)-O(3)	82.03(11)
O(17)-Co(2)-O(3)	94.10(12)	N(38)-Co(2)-Cl(6)	98.97(10)
N(27)-Co(2)-Cl(6)	92.71(10)	N(28)-Co(2)-Cl(6)	101.58(10)
O(17)-Co(2)-Cl(6)	93.09(11)	O(3)-Co(2)-Cl(6)	172.31(8)
O(15)-Co(1)-N(30)	92.08(13)	O(15)-Co(1)-N(36)	102.50(14)
N(30)-Co(1)-N(36)	98.38(14)	O(15)-Co(1)-N(33)	99.97(14)

N(30)-Co(1)-N(33)	94.63(13)	N(36)-Co(1)-N(33)	153.51(14)
O(15)-Co(1)-O(20)	91.55(14)	N(30)-Co(1)-O(20)	175.15(13)
N(36)-Co(1)-O(20)	83.97(14)	N(33)-Co(1)-O(20)	81.57(13)
O(15)-Co(1)-O(1)	173.00(12)	N(30)-Co(1)-O(1)	81.03(12)
N(36)-Co(1)-O(1)	77.45(12)	N(33)-Co(1)-O(1)	81.94(12)
O(20)-Co(1)-O(1)	95.40(12)	N(45)-Co(7)-N(35)	115.85(13)
N(45)-Co(7)-N(40)	96.66(13)	N(35)-Co(7)-N(40)	133.82(13)
N(45)-Co(7)-Cl(7)	105.21(10)	N(35)-Co(7)-Cl(7)	100.57(10)
N(40)-Co(7)-Cl(7)	101.35(10)	N(45)-Co(7)-O(6)	83.34(12)
N(35)-Co(7)-O(6)	74.59(12)	N(40)-Co(7)-O(6)	77.92(12)
Cl(7)-Co(7)-O(6)	171.43(8)	N(37)-Co(8)-N(46)	118.54(15)
N(37)-Co(8)-N(42)	119.05(15)	N(46)-Co(8)-N(42)	108.17(13)
N(37)-Co(8)-Cl(6)#2	104.29(11)	N(46)-Co(8)-Cl(6)#2	104.94(10)
N(42)-Co(8)-Cl(6)#2	98.76(10)	N(37)-Co(8)-O(2)	75.51(12)
N(46)-Co(8)-O(2)	77.70(12)	N(42)-Co(8)-O(2)	78.79(12)
Cl(6)#2-Co(8)-O(2)	176.92(8)	N(39)-Co(5)-N(48)	113.88(14)
N(39)-Co(5)-N(43)	125.64(14)	N(48)-Co(5)-N(43)	103.66(13)
N(39)-Co(5)-Cl(8)	106.06(10)	N(48)-Co(5)-Cl(8)	100.61(10)
N(43)-Co(5)-Cl(8)	103.85(10)	N(31)-Co(4)-N(34)	116.38(14)
N(31)-Co(4)-N(25)	101.62(13)	N(34)-Co(4)-N(25)	124.88(13)
N(31)-Co(4)-Cl(5)	102.85(11)	N(34)-Co(4)-Cl(5)	104.98(10)
N(25)-Co(4)-Cl(5)	103.50(10)		
Symmetry transformations used to generate equivalent atoms: #1: -x+2,y-1/2,-z+1/2; #2: -x+1,y-1/2,-z+1/2; #3: -x+1,y+1/2,-z+1/2; #4: -x+2,y+1/2,-z+1/2.			

Table S3 The selected bond lengths [Å] and angles [º] of complex **3**.

Co(1)-N(9)	2.033(8)	Co(1)-N(1)	2.058(8)
Co(1)-N(10)	2.060(8)	Co(1)-Cl(1)	2.346(3)
Co(1)-O(1)	2.353(6)	Co(2)-N(14)	2.049(7)
Co(2)-N(3)	2.081(9)	Co(2)-N(4)	2.124(7)
Co(2)-Cl(2)	2.305(3)	Co(2)-O(5)	2.328(6)
Co(3)-N(12)	2.057(7)	Co(3)-N(7)	2.055(7)
Co(3)-N(6)	2.086(7)	Co(3)-Cl(3)	2.293(3)
Co(3)-O(3)	2.357(6)	Co(4)-O(3)	2.057(6)
Co(4)-O(1)	2.057(7)	Co(4)-N(5)	2.063(8)
Co(4)-O(5)	2.086(6)	Co(4)-N(2)	2.123(7)
Co(4)-N(8)	2.128(7)	Co(5)-N(22)	2.048(8)
Co(5)-N(18)	2.082(8)	Co(5)-N(11)	2.090(9)
Co(5)-Cl(5)	2.292(4)	Co(5)-O(2)	2.337(7)
Co(6)-N(13)	2.041(8)	Co(6)-N(16)	2.049(7)
Co(6)-N(19)	2.070(8)	Co(6)-O(4)	2.296(6)
Co(6)-Cl(6)	2.382(2)	Co(7)-N(15)	2.048(8)
Co(7)-N(24)	2.073(9)	Co(7)-N(21)	2.094(8)
Co(7)-Cl(4)	2.291(3)	Co(7)-O(6)	2.375(7)
Co(8)-O(6)	2.052(7)	Co(8)-O(4)	2.070(6)
Co(8)-O(2)	2.092(7)	Co(8)-N(20)	2.092(8)
Co(8)-N(17)	2.111(7)	Co(8)-N(23)	2.116(8)
Co(9)-N(38)	2.049(7)	Co(9)-N(27)	2.069(7)
Co(9)-N(28)	2.072(7)	Co(9)-O(3W)	2.155(5)

Co(9)-O(11)	2.359(6)	Co(10)-N(25)	2.078(7)
Co(10)-N(34)	2.089(8)	Co(10)-N(33)	2.144(9)
Co(10)-Cl(7)	2.279(3)	Co(10)-O(7)	2.326(6)
Co(11)-N(36)	2.054(7)	Co(11)-N(30)	2.070(8)
Co(11)-N(31)	2.113(8)	Co(11)-O(9)	2.323(7)
Co(11)-Cl(6)	2.353(3)	Co(12)-O(11)	2.053(7)
Co(12)-O(9)	2.057(7)	Co(12)-O(7)	2.082(6)
Co(12)-N(26)	2.086(9)	Co(12)-N(32)	2.099(8)
Co(12)-N(29)	2.145(7)	Co(13)-N(43)	2.114(8)
Co(13)-N(39)	2.142(8)	Co(13)-O(13)	2.154(7)
Co(13)-N(40)	2.178(8)	Co(13)-O(12)	2.259(6)
Co(13)-Cl(1)#1	2.489(3)	Co(13)#2-Cl(1)	2.489(3)
Co(14)-N(46)	2.038(7)	Co(14)-N(35)	2.087(8)
Co(14)-N(45)	2.095(8)	Co(14)-Cl(8)	2.285(3)
Co(15)-O(1W)	2.080(7)	Co(15)-N(48)	2.113(9)
Co(15)-N(37)	2.152(8)	Co(15)-O(2W)	2.190(8)
Co(15)-O(10)	2.284(7)	Co(15)-N(42)	2.101(9)
Co(16)-N(41)	2.082(8)	Co(16)-O(8)	2.034(6)
Co(16)-N(44)	2.065(9)	Co(16)-N(47)	2.077(7)
Co(16)-O(10)	2.136(7)	Co(16)-O(12)	2.144(6)
N(9)-Co(1)-N(1)	107.7(3)	N(9)-Co(1)-N(10)	116.6(3)
N(1)-Co(1)-N(10)	121.3(3)	N(9)-Co(1)-Cl(1)	103.0(2)
N(1)-Co(1)-Cl(1)	96.7(2)	N(10)-Co(1)-Cl(1)	108.0(2)
N(9)-Co(1)-O(1)	78.2(3)	N(1)-Co(1)-O(1)	78.6(2)

N(10)-Co(1)-O(1)	75.2(3)	Cl(1)-Co(1)-O(1)	175.27(17)
N(14)-Co(2)-N(3)	118.9(3)	N(14)-Co(2)-N(4)	127.1(3)
N(3)-Co(2)-N(4)	100.9(3)	N(14)-Co(2)-Cl(2)	100.5(2)
N(3)-Co(2)-Cl(2)	103.4(2)	N(4)-Co(2)-Cl(2)	102.5(2)
N(14)-Co(2)-O(5)	74.6(2)	N(3)-Co(2)-O(5)	79.6(3)
N(4)-Co(2)-O(5)	80.6(2)	Cl(2)-Co(2)-O(5)	175.07(17)
N(12)-Co(3)-N(7)	122.9(3)	N(12)-Co(3)-N(6)	118.5(3)
N(7)-Co(3)-N(6)	102.8(3)	N(12)-Co(3)-Cl(3)	101.9(2)
N(7)-Co(3)-Cl(3)	101.0(2)	N(6)-Co(3)-Cl(3)	107.7(2)
N(12)-Co(3)-O(3)	75.2(2)	N(7)-Co(3)-O(3)	77.1(3)
N(6)-Co(3)-O(3)	77.9(3)	Cl(3)-Co(3)-O(3)	174.39(19)
O(3)-Co(4)-O(1)	98.8(3)	O(3)-Co(4)-N(5)	81.4(3)
O(1)-Co(4)-N(5)	179.3(3)	O(3)-Co(4)-O(5)	101.2(2)
O(1)-Co(4)-O(5)	98.7(3)	N(5)-Co(4)-O(5)	80.6(3)
O(3)-Co(4)-N(2)	178.6(3)	O(1)-Co(4)-N(2)	80.4(3)
N(5)-Co(4)-N(2)	99.4(3)	O(5)-Co(4)-N(2)	80.1(3)
O(3)-Co(4)-N(8)	80.2(3)	O(1)-Co(4)-N(8)	82.1(3)
N(5)-Co(4)-N(8)	98.6(3)	O(5)-Co(4)-N(8)	178.2(3)
N(2)-Co(4)-N(8)	98.5(3)	N(22)-Co(5)-N(18)	103.4(3)
N(22)-Co(5)-N(11)	121.2(3)	N(18)-Co(5)-N(11)	122.3(3)
N(22)-Co(5)-Cl(5)	103.4(3)	N(18)-Co(5)-Cl(5)	100.9(2)
N(11)-Co(5)-Cl(5)	102.0(3)	N(22)-Co(5)-O(2)	79.7(3)
N(18)-Co(5)-O(2)	77.9(3)	N(11)-Co(5)-O(2)	76.5(3)
Cl(5)-Co(5)-O(2)	176.91(19)	N(13)-Co(6)-N(16)	122.6(3)
N(13)-Co(6)-N(19)	118.1(3)	N(16)-Co(6)-N(19)	106.6(3)

N(13)-Co(6)-O(4)	77.1(2)	N(16)-Co(6)-O(4)	77.7(3)
N(19)-Co(6)-O(4)	79.6(3)	N(13)-Co(6)-Cl(6)	102.2(2)
N(16)-Co(6)-Cl(6)	105.1(2)	N(19)-Co(6)-Cl(6)	98.2(2)
O(4)-Co(6)-Cl(6)	176.90(19)	N(15)-Co(7)-N(24)	121.3(3)
N(15)-Co(7)-N(21)	120.1(3)	N(24)-Co(7)-N(21)	103.7(3)
N(15)-Co(7)-Cl(4)	103.3(2)	N(24)-Co(7)-Cl(4)	103.3(2)
N(21)-Co(7)-Cl(4)	102.3(2)	N(15)-Co(7)-O(6)	74.1(3)
N(24)-Co(7)-O(6)	79.1(3)	N(21)-Co(7)-O(6)	78.5(3)
Cl(4)-Co(7)-O(6)	177.2(2)	O(6)-Co(8)-O(4)	99.6(3)
O(6)-Co(8)-O(2)	100.2(3)	O(4)-Co(8)-O(2)	97.7(2)
O(6)-Co(8)-N(20)	80.0(3)	O(4)-Co(8)-N(20)	80.3(3)
O(2)-Co(8)-N(20)	178.0(3)	O(6)-Co(8)-N(17)	177.9(3)
O(4)-Co(8)-N(17)	81.6(3)	O(2)-Co(8)-N(17)	81.3(3)
N(20)-Co(8)-N(17)	98.6(3)	O(6)-Co(8)-N(23)	81.8(3)
O(4)-Co(8)-N(23)	178.4(2)	O(2)-Co(8)-N(23)	82.8(3)
N(20)-Co(8)-N(23)	99.2(3)	N(17)-Co(8)-N(23)	96.9(3)
N(38)-Co(9)-N(27)	136.7(3)	N(38)-Co(9)-N(28)	110.8(3)
N(27)-Co(9)-N(28)	101.2(3)	N(38)-Co(9)-O(3W)	103.4(3)
N(27)-Co(9)-O(3W)	100.1(3)	N(28)-Co(9)-O(3W)	98.0(3)
N(38)-Co(9)-O(11)	75.3(3)	N(27)-Co(9)-O(11)	82.7(3)
N(28)-Co(9)-O(11)	79.9(3)	O(3W)-Co(9)-O(11)	176.8(2)
N(25)-Co(10)-N(34)	112.6(3)	N(25)-Co(10)-N(33)	97.2(3)
N(34)-Co(10)-N(33)	134.6(3)	N(25)-Co(10)-Cl(7)	106.5(2)
N(34)-Co(10)-Cl(7)	101.7(2)	N(33)-Co(10)-Cl(7)	101.4(2)
N(25)-Co(10)-O(7)	82.0(2)	N(34)-Co(10)-O(7)	73.4(2)

N(33)-Co(10)-O(7)	78.1(3)	Cl(7)-Co(10)-O(7)	171.40(18)
N(36)-Co(11)-N(30)	123.2(3)	N(36)-Co(11)-N(31)	119.0(3)
N(30)-Co(11)-N(31)	105.9(3)	N(36)-Co(11)-O(9)	77.1(3)
N(30)-Co(11)-O(9)	78.0(3)	N(31)-Co(11)-O(9)	80.7(2)
N(36)-Co(11)-Cl(6)	102.6(2)	N(30)-Co(11)-Cl(6)	102.3(2)
N(31)-Co(11)-Cl(6)	99.3(2)	O(9)-Co(11)-Cl(6)	179.6(2)
O(11)-Co(12)-O(9)	100.1(3)	O(11)-Co(12)-O(7)	100.8(2)
O(9)-Co(12)-O(7)	100.1(3)	O(11)-Co(12)-N(26)	80.4(3)
O(9)-Co(12)-N(26)	178.1(3)	O(7)-Co(12)-N(26)	81.6(3)
O(11)-Co(12)-N(32)	179.0(3)	O(9)-Co(12)-N(32)	80.9(3)
O(7)-Co(12)-N(32)	79.5(3)	N(26)-Co(12)-N(32)	98.6(3)
O(11)-Co(12)-N(29)	82.3(3)	O(9)-Co(12)-N(29)	81.4(3)
O(7)-Co(12)-N(29)	176.2(3)	N(26)-Co(12)-N(29)	96.8(3)
N(32)-Co(12)-N(29)	97.4(3)	N(43)-Co(13)-N(39)	91.2(3)
N(43)-Co(13)-O(13)	171.0(3)	N(39)-Co(13)-O(13)	84.8(3)
N(43)-Co(13)-N(40)	101.1(3)	N(39)-Co(13)-N(40)	154.9(3)
O(13)-Co(13)-N(40)	79.7(3)	N(43)-Co(13)-O(12)	79.2(3)
N(39)-Co(13)-O(12)	79.3(2)	O(13)-Co(13)-O(12)	92.1(2)
N(40)-Co(13)-O(12)	81.6(2)	N(43)-Co(13)-Cl(1)#1	92.2(2)
N(39)-Co(13)-Cl(1)#1	97.3(2)	O(13)-Co(13)-Cl(1)#1	96.3(2)
N(40)-Co(13)-Cl(1)#1	103.94(19)	O(12)-Co(13)-Cl(1)#1	170.60(18)
N(46)-Co(14)-N(35) N(35)-Co(14)-N(45)	110.5(3) 127.6(3)	N(46)-Co(14)-N(45) N(46)-Co(14)-Cl(8)	103.3(3) 103.9(2)
N(35)-Co(14)-Cl(8)	107.8(2)	N(45)-Co(14)-Cl(8)	101.1(2)
O(1W)-Co(15)-N(42)	94.0(3)	O(1W)-Co(15)-N(48)	99.7(3)

N(42)-Co(15)-N(48)	93.6(3)	O(1W)-Co(15)-N(37)	102.7(3)
N(42)-Co(15)-N(37)	96.0(3)	N(48)-Co(15)-N(37)	154.9(3)
O(1W)-Co(15)-O(2W)	89.0(3)	N(42)-Co(15)-O(2W)	176.7(3)
N(48)-Co(15)-O(2W)	84.5(3)	N(37)-Co(15)-O(2W)	84.7(3)
O(1W)-Co(15)-O(10)	174.7(3)	N(42)-Co(15)-O(10)	81.0(3)
N(48)-Co(15)-O(10)	82.1(3)	N(37)-Co(15)-O(10)	76.6(3)
O(2W)-Co(15)-O(10)	96.1(3)	O(8)-Co(16)-N(44)	81.1(3)
O(8)-Co(16)-N(47)	83.7(3)	N(44)-Co(16)-N(47)	98.6(3)
O(8)-Co(16)-N(41)	177.3(3)	N(44)-Co(16)-N(41)	98.4(3)
N(47)-Co(16)-N(41)	93.8(3)	O(8)-Co(16)-O(10)	95.8(2)
N(44)-Co(16)-O(10)	176.7(3)	N(47)-Co(16)-O(10)	81.8(3)
N(41)-Co(16)-O(10)	84.8(3)	O(8)-Co(16)-O(12)	99.6(2)
N(44)-Co(16)-O(12)	82.1(3)	N(47)-Co(16)-O(12)	176.8(3)
N(41)-Co(16)-O(12)	83.0(3)	O(10)-Co(16)-O(12)	97.7(2)
Symmetry transformations used to generate equivalent atoms: #1: x,y-1,z; #2: x,y+1,z.			

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