Supplementary Materials

Hydrothermal Synthesis, Structure and Magnetic Properties of a Three-Dimensional Cobalt(II) – Aminophenyltetrazolate Coordination Polymer.

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Figures S1. ORTEP view of the building unit of $[Co_3(H_2O)_2(OH)_2(C_7N_5H_6)_4]$, showing the partial atom-labeling schemes and 50% thermal ellipsoids.

Figures S2. Infrared spectra of $[Co_3(H_2O)_2(OH)_2(C_7N_5H_6)_4]$.

Figures S3. TGA plot for $[Co_3(H_2O)_2(OH)_2(C_7N_5H_6)_4]$.

Figure S4. The field-dependent magnetization for $[Co_3(H_2O)_2(OH)_2(C_7N_5H_6)_4]$ at 300 K.

Figure S5. The temperature dependence of the inverse susceptibility for $[Co_3(H_2O)_2(OH)_2(C_7N_5H_6)_4]$. The red line through the data points is the fit to the Curie-Weiss law above 50 K.

Tables S1-S9. Tables of crystal data, atomic positional parameters and isotropic temperature factors, bond lengths and angles, anisotropic temperature factors, hydrogen atom positions, and hydrogen bond distances for $[Co_3(H_2O)_2(OH)_2(C_7N_5H_6)_4]$.

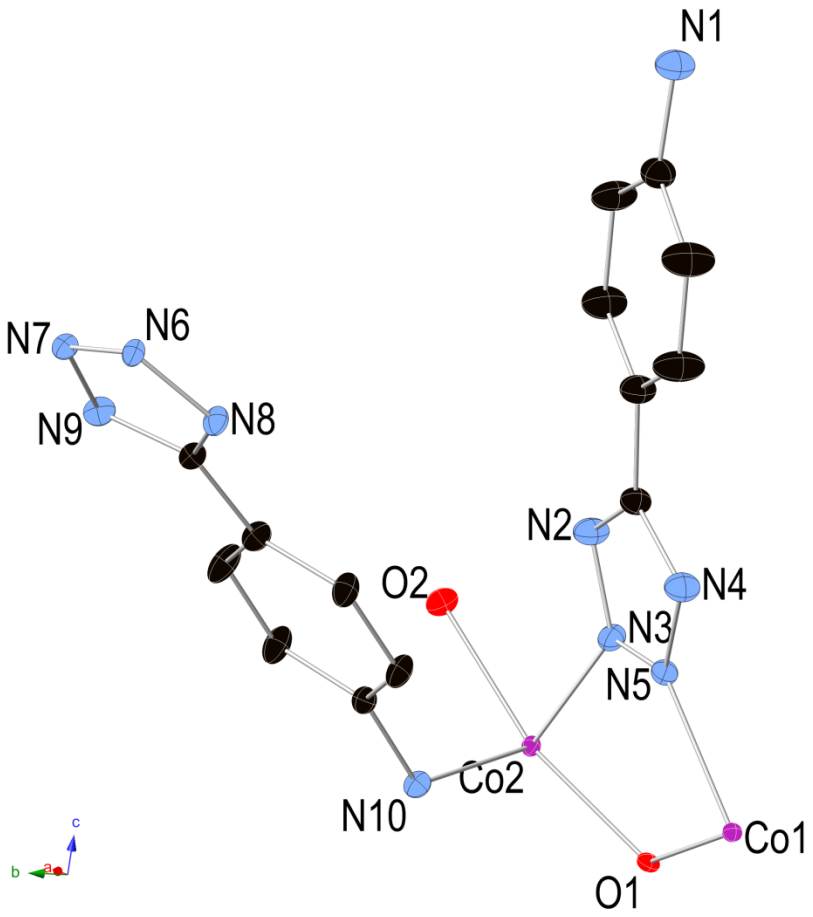

Figure S1. ORTEP view of compound $[Co_3(H_2O)_2(OH)_2(C_7N_5H_6)_4]$, showing the atom-labeling scheme and 50% thermal ellipsoids.

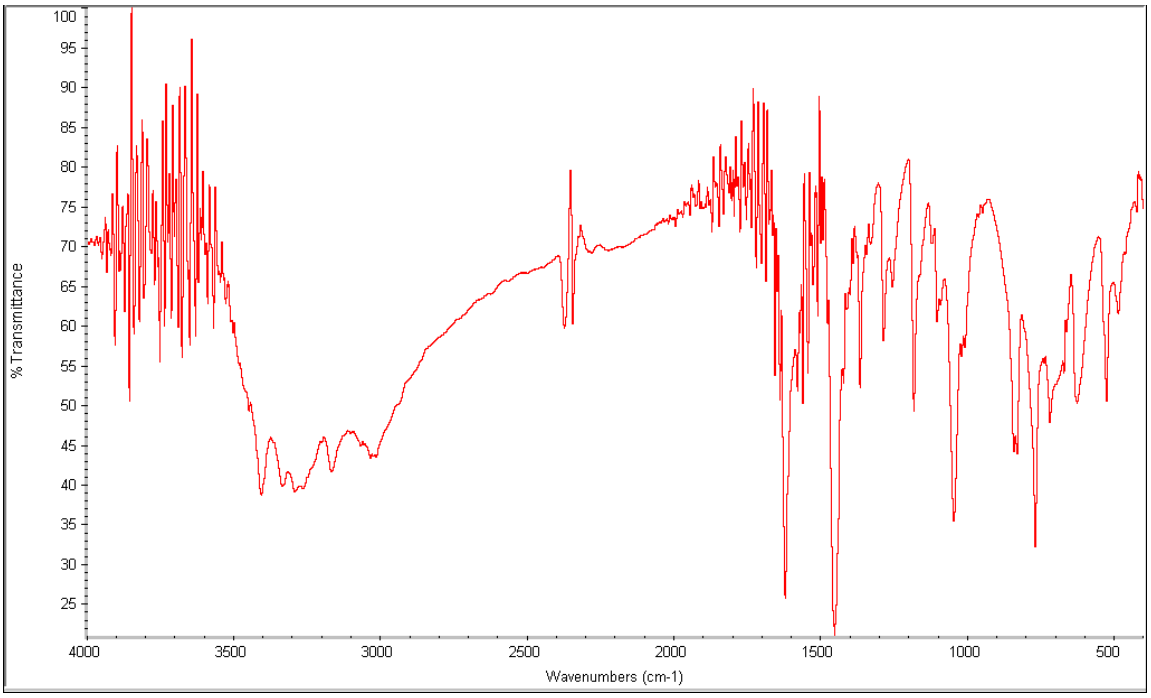

Figure S2. Infrared spectra of $[Co_3(H_2O)_2(OH)_2(C_7N_5H_6)_4]$.

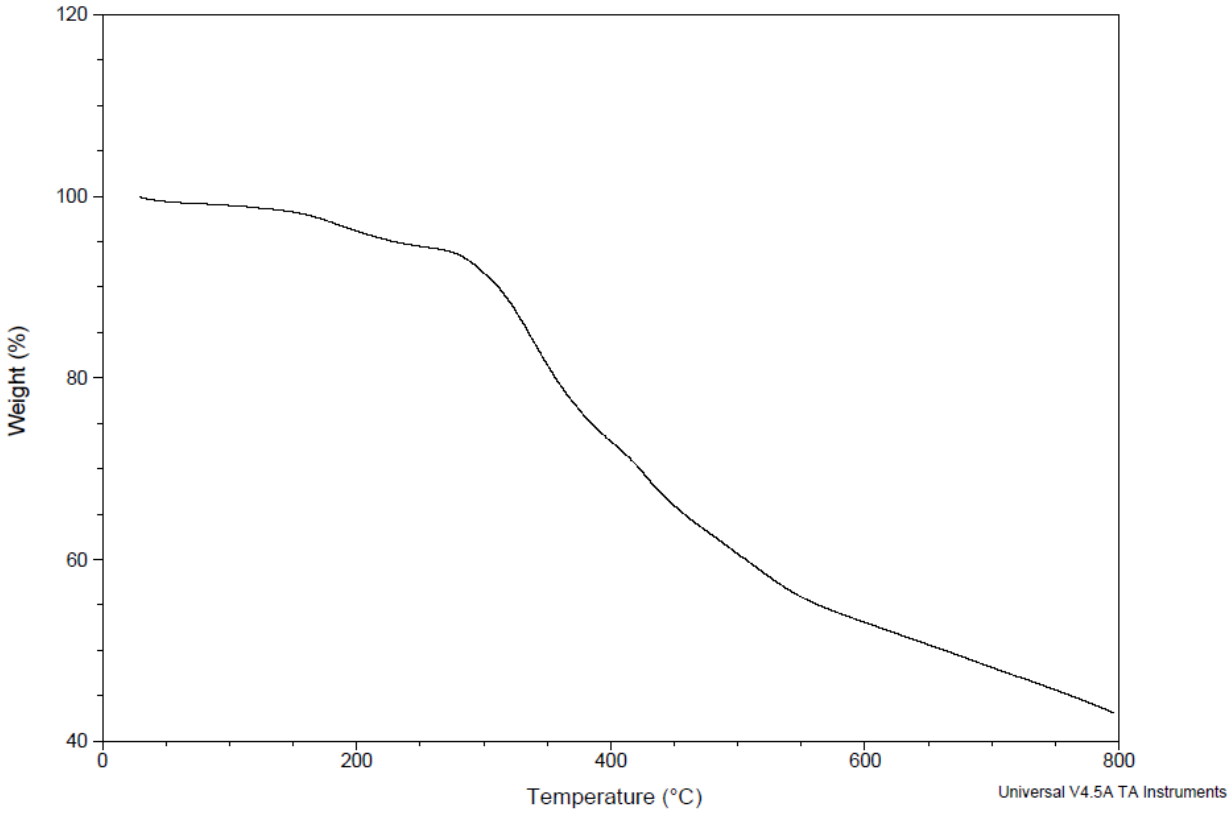

Figure S3. Thermogravimetric analysis profile for $[Co_3(H_2O)_2(OH)_2(C_7N_5H_6)_4]$ in the 25-800ºC range.

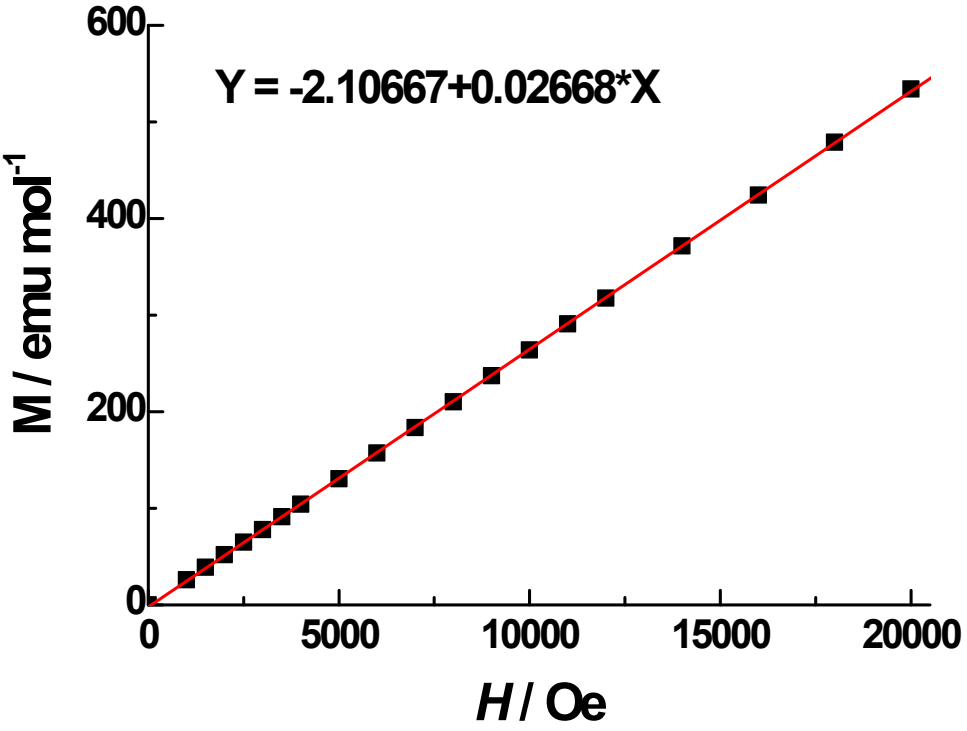

Figure S4. The field-dependent magnetization for $[Co_3(H_2O)_2(OH)_2(C_7N_5H_6)_4]$ at 300 K.

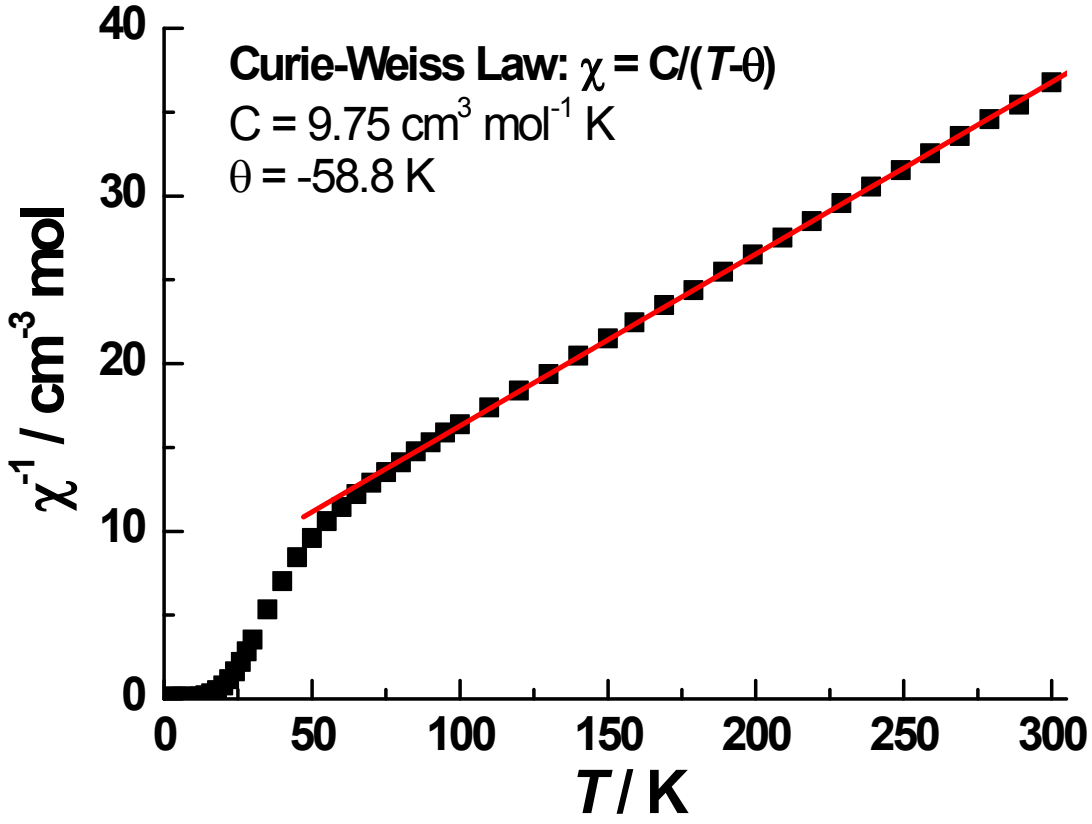

Figure S5. The temperature dependence of the inverse susceptibility for $[Co_3(H_2O)_2(OH)_2(C_7N_5H_6)_4]$. The red line through the data points is the fit to the Curie-Weiss law above 50 K.

Table S1. Sample and crystal data for $[Co_3(H_2O)_2(OH)_2(C_7N_4H_8)_4]$.

Identification code	$[Co_3(H_2O)_2(OH)_2(C_7N_4H_8)_4]$	
Chemical formula	$C_{28}H_{30}Co_3N_{20}O_4$	
Formula weight	887.51	
Temperature	90(2) K	
Wavelength	0.71073 Å	
Crystal size	0.131 x 0.136 x 0.176 mm	
Crystal system	Monoclinic	
Space group	P2(1)/n	
Unit cell dimensions	a = 6.6673(5) Å	α = 90°
	b = 21.2751(15) Å	β = 102.492(2)°
	c = 13.0771(9) Å	γ = 90°
Volume	1811.0(2) $Å^3$	
Z	2	
Density (calculated)	1.628 g/cm^3	
Absorption coefficient	1.424 mm^{-1}	
F(000)	902	

Table S2. Data collection and structure refinement for $[Co_3(H_2O)_2(OH)_2(C_7N_4H_8)_4]$.

Theta range for data collection	1.86 to 26.36°	
Index ranges	-8<=h<=6, -26<=k<=26, -16<=l<=16	
Reflections collected	21478	
Independent reflections	3708 [R(int) = 0.0225]	
Coverage of independent reflections	100.0%	
Absorption correction	Multi-scan	
Max. and min. transmission	0.8350 and 0.7880	
Refinement method	Full-matrix least-squares on F^2	
Refinement program	SHELXL-2013 (Sheldrick, 2013)	
Function minimized	$\Sigma\, w(F_o^2 - F_c^2)^2$	
Data / restraints / parameters	3708 / 7 / 271	
Goodness-of-fit on F^2	1.061	
Δ/σ_{max}	0.003	
Final R indices	3442 data; I>2σ(I)	R1 = 0.0232, wR2 = 0.0543
	all data	R1 = 0.0256, wR2 = 0.0552
Weighting scheme	$w=1/[\sigma^2(F_o^2)+(0.0219P)^2+1.7561P]$ where $P=(F_o^2+2F_c^2)/3$	
Largest diff. peak and hole	0.626 and -0.262 eÅ^{-3}	
R.M.S. deviation from mean	0.057 eÅ^{-3}	

Table S3. Atomic coordinates and equivalent isotropic atomic displacement parameters (Å^2) for $[Co_3(H_2O)_2(OH)_2(C_7N_4H_8)_4]$.

U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x/a	**y/b**	**z/c**	**U(eq)**
Co1	0.5	0.5	0.0	0.00631(7)
Co2	0.98249(3)	0.56695(2)	0.95344(2)	0.00686(6)
O1	0.21342(16)	0.51220(5)	0.05013(8)	0.0080(2)
O2	0.76923(18)	0.60969(6)	0.82694(9)	0.0137(2)
N1	0.2364(3)	0.58064(8)	0.25847(12)	0.0198(3)
N2	0.0758(2)	0.56393(7)	0.73302(11)	0.0165(3)
N3	0.1414(2)	0.54858(7)	0.83340(11)	0.0135(3)
N4	0.4103(2)	0.54462(7)	0.76477(11)	0.0164(3)
N5	0.3453(2)	0.53847(7)	0.85363(11)	0.0137(3)
N6	0.8158(2)	0.60539(6)	0.06103(10)	0.0101(3)
N7	0.6325(2)	0.58591(6)	0.06858(10)	0.0101(3)
N8	0.8684(2)	0.65639(6)	0.12200(11)	0.0120(3)
N9	0.5602(2)	0.62281(7)	0.13546(11)	0.0127(3)
N10	0.6601(2)	0.84430(6)	0.48558(11)	0.0106(3)
C1	0.2396(3)	0.58029(9)	0.36583(14)	0.0186(4)
C2	0.0561(3)	0.58174(10)	0.40109(14)	0.0236(4)
C3	0.4237(3)	0.57632(11)	0.43946(15)	0.0279(5)
C4	0.0582(3)	0.57715(10)	0.50691(15)	0.0234(4)
C5	0.4256(3)	0.57141(11)	0.54540(15)	0.0267(4)
C6	0.2426(3)	0.57091(9)	0.58060(14)	0.0184(4)
C7	0.2437(3)	0.56099(8)	0.69131(13)	0.0141(3)
C8	0.7083(2)	0.66605(8)	0.16696(12)	0.0113(3)
C9	0.6961(3)	0.71522(8)	0.24459(13)	0.0130(3)
C10	0.8614(3)	0.75462(8)	0.28424(14)	0.0152(3)
C11	0.5176(3)	0.72077(8)	0.28335(14)	0.0185(4)
C12	0.8512(3)	0.79749(8)	0.36306(13)	0.0148(3)
C13	0.5069(3)	0.76306(8)	0.36243(14)	0.0172(4)
C14	0.6749(3)	0.80112(7)	0.40355(13)	0.0114(3)

Table S4. Bond lengths (Å) for $[Co_3(H_2O)_2(OH)_2(C_7N_4H_8)_4]$.

Co1-N5	2.1315(14)	Co1-N5	2.1315(14)
Co1-N7	2.1407(14)	Co1-N7	2.1407(14)
Co1-O1	2.1655(11)	Co1-O1	2.1656(11)
Co2-N3	2.1116(14)	Co2-O1	2.1175(11)
Co2-O1	2.1252(11)	Co2-N6	2.1354(13)
Co2-O2	2.1372(12)	Co2-N10	2.2202(14)
O1-Co2	2.1253(11)	O1-H1	0.796(15)
O2-H2A	0.820(16)	O2-H2B	0.804(15)
N1-C1	1.400(2)	N1-H1A	0.909(16)
N1-H1B	0.918(16)	N2-N3	1.331(2)
N2-C7	1.349(2)	N3-N5	1.345(2)
N4-N5	1.3316(19)	N4-C7	1.348(2)
N6-N7	1.3142(19)	N6-N8	1.3473(19)
N7-N9	1.3400(19)	N7-Co1	2.1407(13)
N8-C8	1.341(2)	N9-C8	1.347(2)
N10-C14	1.432(2)	N10-Co2	2.2202(14)
N10-H10A	0.878(15)	N10-H10B	0.863(15)
C1-C3	1.389(3)	C1-C2	1.397(3)
C2-C4	1.384(3)	C2-H2	0.95
C3-C5	1.387(3)	C3-H3	0.95
C4-C6	1.394(3)	C4-H4	0.95
C5-C6	1.394(3)	C5-H5	0.95
C6-C7	1.462(2)	C8-C9	1.472(2)
C9-C10	1.392(2)	C9-C11	1.396(2)
C10-C12	1.389(2)	C10-H10	0.95
C11-C13	1.384(2)	C11-H11	0.95
C12-C14	1.392(2)	C12-H12	0.95
C13-C14	1.392(2)	C13-H13	0.95

Table S5. Bond angles (°) for $[Co_3(H_2O)_2(OH)_2(C_7N_4H_8)_4]$.

N5-Co1-N5	180.0	N5-Co1-N7	97.13(5)
N5-Co1-N7	82.88(5)	N5-Co1-N7	82.87(5)
N5-Co1-N7	97.12(5)	N7-Co1-N7	180.00(4)
N5-Co1-O1	86.48(5)	N5-Co1-O1	93.52(5)
N7-Co1-O1	94.71(5)	N7-Co1-O1	85.29(5)
N5-Co1-O1	93.52(5)	N5-Co1-O1	86.48(5)
N7-Co1-O1	85.29(5)	N7-Co1-O1	94.71(5)
O1-Co1-O1	180.0	N3-Co2-O1	85.71(5)
N3-Co2-O1	104.00(5)	O1-Co2-O1	86.64(4)
N3-Co2-N6	167.69(5)	O1-Co2-N6	103.42(5)
O1-Co2-N6	85.00(5)	N3-Co2-O2	81.96(5)
O1-Co2-O2	166.48(5)	O1-Co2-O2	90.99(5)
N6-Co2-O2	89.60(5)	N3-Co2-N10	88.01(5)
O1-Co2-N10	93.76(5)	O1-Co2-N10	167.98(5)
N6-Co2-N10	83.21(5)	O2-Co2-N10	91.32(5)
Co2-O1-Co2	93.36(4)	Co2-O1-Co1	117.41(5)
Co2-O1-Co1	118.47(5)	Co2-O1-H1	109.9(14)
Co2-O1-H1	105.6(14)	Co1-O1-H1	110.5(14)
Co2-O2-H2A	111.8(15)	Co2-O2-H2B	102.3(15)
H2A-O2-H2B	103.(2)	C1-N1-H1A	113.5(14)
C1-N1-H1B	115.1(14)	H1A-N1-H1B	114.6(19)
N3-N2-C7	105.24(14)	N2-N3-N5	109.62(13)
N2-N3-Co2	125.23(11)	N5-N3-Co2	122.12(10)
N5-N4-C7	105.88(14)	N4-N5-N3	108.58(13)
N4-N5-Co1	129.48(11)	N3-N5-Co1	120.67(10)
N7-N6-N8	109.69(12)	N7-N6-Co2	123.62(10)
N8-N6-Co2	126.33(10)	N6-N7-N9	109.61(12)
N6-N7-Co1	122.96(10)	N9-N7-Co1	126.84(10)
C8-N8-N6	104.64(13)	N7-N9-C8	104.87(13)
C14-N10-Co2	121.61(10)	C14-N10-H10A	109.4(13)
Co2-N10-H10A	107.8(13)	C14-N10-H10B	108.8(13)
Co2-N10-H10B	101.0(13)	H10A-N10-H10B	107.3(18)
C3-C1-C2	118.55(17)	C3-C1-N1	120.97(17)
C2-C1-N1	120.45(17)	C4-C2-C1	120.53(17)
C4-C2-H2	119.7	C1-C2-H2	119.7
C5-C3-C1	120.84(18)	C5-C3-H3	119.6
C1-C3-H3	119.6	C2-C4-C6	120.95(17)
C2-C4-H4	119.5	C6-C4-H4	119.5
C3-C5-C6	120.73(18)	C3-C5-H5	119.6
C6-C5-H5	119.6	C5-C6-C4	118.33(17)

C5-C6-C7	120.73(16)	C4-C6-C7	120.87(16)
N4-C7-N2	110.62(15)	N4-C7-C6	124.75(15)
N2-C7-C6	124.56(15)	N8-C8-N9	111.18(14)
N8-C8-C9	125.39(15)	N9-C8-C9	123.37(15)
C10-C9-C11	118.83(15)	C10-C9-C8	121.82(15)
C11-C9-C8	119.29(15)	C12-C10-C9	120.67(15)
C12-C10-H10	119.7	C9-C10-H10	119.7
C13-C11-C9	120.79(16)	C13-C11-H11	119.6
C9-C11-H11	119.6	C10-C12-C14	119.96(16)
C10-C12-H12	120.0	C14-C12-H12	120.0
C11-C13-C14	119.97(16)	C11-C13-H13	120.0
C14-C13-H13	120.0	C12-C14-C13	119.72(15)
C12-C14-N10	121.41(15)	C13-C14-N10	118.86(15)

Table S6. Torsion angles (°) for $[Co_3(H_2O)_2(OH)_2(C_7N_4H_8)_4]$.

C7-N2-N3-N5	1.93(18)	C7-N2-N3-Co2	162.45(12)
C7-N4-N5-N3	2.31(18)	C7-N4-N5-Co1	169.25(12)
N2-N3-N5-N4	-2.72(18)	Co2-N3-N5-N4	-163.95(11)
N2-N3-N5-Co1	-171.02(11)	Co2-N3-N5-Co1	27.75(17)
N8-N6-N7-N9	-0.79(17)	Co2-N6-N7-N9	-174.18(10)
N8-N6-N7-Co1	-172.53(10)	Co2-N6-N7-Co1	14.08(17)
N7-N6-N8-C8	0.51(17)	Co2-N6-N8-C8	173.68(11)
N6-N7-N9-C8	0.71(17)	Co1-N7-N9-C8	172.05(11)
C3-C1-C2-C4	-2.2(3)	N1-C1-C2-C4	175.65(19)
C2-C1-C3-C5	2.5(3)	N1-C1-C3-C5	-175.3(2)
C1-C2-C4-C6	-0.1(3)	C1-C3-C5-C6	-0.6(3)
C3-C5-C6-C4	-1.7(3)	C3-C5-C6-C7	175.4(2)
C2-C4-C6-C5	2.0(3)	C2-C4-C6-C7	-175.02(18)
N5-N4-C7-N2	-1.13(19)	N5-N4-C7-C6	-178.09(16)
N3-N2-C7-N4	-0.49(19)	N3-N2-C7-C6	176.48(16)
C5-C6-C7-N4	-8.0(3)	C4-C6-C7-N4	168.92(18)
C5-C6-C7-N2	175.41(18)	C4-C6-C7-N2	-7.6(3)
N6-N8-C8-N9	-0.06(18)	N6-N8-C8-C9	177.22(15)
N7-N9-C8-N8	-0.39(18)	N7-N9-C8-C9	-177.74(15)
N8-C8-C9-C10	-4.4(3)	N9-C8-C9-C10	172.54(16)
N8-C8-C9-C11	178.62(17)	N9-C8-C9-C11	-4.4(3)
C11-C9-C10-C12	1.8(3)	C8-C9-C10-C12	-175.19(16)
C10-C9-C11-C13	-2.3(3)	C8-C9-C11-C13	174.79(16)
C9-C10-C12-C14	0.3(3)	C9-C11-C13-C14	0.6(3)
C10-C12-C14-C13	-2.0(3)	C10-C12-C14-N10	179.32(15)
C11-C13-C14-C12	1.6(3)	C11-C13-C14-N10	-179.75(16)
Co2-N10-C14-C12	102.87(16)	Co2-N10-C14-C13	-75.80(18)

Table S7. Anisotropic atomic displacement parameters ($Å^2$) for $[Co_3(H_2O)_2(OH)_2(C_7N_4H_8)_4]$.
The anisotropic atomic 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}
Co1	0.00606(14)	0.00684(14)	0.00617(14)	-0.00008(11)	0.00161(10)	-0.00001(11)
Co2	0.00666(11)	0.00709(11)	0.00726(11)	0.00078(8)	0.00244(8)	0.00024(8)
O1	0.0087(5)	0.0095(5)	0.0060(5)	-0.0011(4)	0.0025(4)	-0.0001(4)
O2	0.0101(6)	0.0172(6)	0.0136(6)	0.0031(5)	0.0023(5)	-0.0002(5)
N1	0.0187(8)	0.0269(9)	0.0140(7)	0.0004(6)	0.0043(6)	0.0002(7)
N2	0.0168(7)	0.0216(8)	0.0114(7)	0.0015(6)	0.0037(6)	0.0005(6)
N3	0.0160(7)	0.0152(7)	0.0106(6)	0.0031(5)	0.0060(5)	0.0051(6)
N4	0.0163(7)	0.0204(8)	0.0132(7)	0.0011(6)	0.0050(6)	-0.0002(6)
N5	0.0198(7)	0.0134(7)	0.0093(6)	0.0007(5)	0.0061(6)	0.0039(6)
N6	0.0102(6)	0.0091(6)	0.0117(6)	-0.0023(5)	0.0042(5)	-0.0019(5)
N7	0.0100(6)	0.0102(6)	0.0105(6)	-0.0018(5)	0.0034(5)	0.0003(5)
N8	0.0135(7)	0.0100(6)	0.0135(7)	-0.0040(5)	0.0049(5)	-0.0015(5)
N9	0.0124(7)	0.0136(7)	0.0132(7)	-0.0048(5)	0.0049(5)	0.0000(5)
N10	0.0106(7)	0.0105(7)	0.0113(7)	-0.0024(5)	0.0037(5)	0.0005(5)
C1	0.0208(9)	0.0205(9)	0.0151(8)	0.0002(7)	0.0052(7)	-0.0002(7)
C2	0.0171(9)	0.0364(11)	0.0157(9)	0.0033(8)	0.0004(7)	0.0021(8)
C3	0.0177(9)	0.0488(13)	0.0188(9)	0.0026(9)	0.0074(8)	-0.0016(9)
C4	0.0168(9)	0.0373(11)	0.0177(9)	0.0027(8)	0.0071(7)	0.0028(8)
C5	0.0161(9)	0.0473(13)	0.0160(9)	0.0017(8)	0.0020(7)	-0.0006(9)
C6	0.0195(9)	0.0227(9)	0.0132(8)	0.0006(7)	0.0042(7)	0.0003(7)
C7	0.0126(8)	0.0169(8)	0.0126(8)	-0.0009(6)	0.0025(6)	-0.0006(6)
C8	0.0108(7)	0.0106(8)	0.0125(8)	-0.0018(6)	0.0022(6)	0.0009(6)
C9	0.0133(8)	0.0108(8)	0.0152(8)	-0.0038(6)	0.0038(6)	0.0011(6)
C10	0.0129(8)	0.0162(8)	0.0192(8)	-0.0044(7)	0.0091(7)	-0.0011(7)
C11	0.0117(8)	0.0180(9)	0.0263(10)	-0.0108(7)	0.0056(7)	-0.0046(7)
C12	0.0133(8)	0.0126(8)	0.0188(8)	-0.0051(7)	0.0043(7)	-0.0037(6)
C13	0.0132(8)	0.0171(9)	0.0235(9)	-0.0076(7)	0.0089(7)	-0.0013(7)
C14	0.0140(8)	0.0080(7)	0.0125(8)	-0.0012(6)	0.0034(6)	0.0021(6)

Table S8. Hydrogen atomic coordinates and isotropic atomic displacement parameters ($Å^2$) for $[Co_3(H_2O)_2(OH)_2(C_7N_4H_8)_4]$.

	x/a	y/b	z/c	U(eq)
H1	1.234(3)	0.5249(9)	1.1087(12)	0.01
H2A	0.666(3)	0.5882(9)	0.8080(16)	0.016
H2B	0.827(3)	0.6065(10)	0.7793(14)	0.016
H1A	1.127(3)	0.6013(10)	0.2196(16)	0.024
H1B	1.360(3)	0.5897(10)	0.2415(16)	0.024
H10A	0.784(2)	0.8538(9)	1.5208(14)	0.013
H10B	0.597(3)	0.8261(9)	1.5286(14)	0.013
H2	0.9290	0.5859	0.3520	0.028
H3	1.5499	0.5770	0.4169	0.033
H4	0.9323	0.5783	0.5297	0.028
H5	1.5530	0.5683	0.5945	0.032
H10	0.9823	0.7521	1.2571	0.018
H11	0.4020	0.6952	1.2551	0.022
H12	0.9646	0.8243	1.3893	0.018
H13	0.3850	0.7661	1.3886	0.021

Table S9. Hydrogen bond distances (Å) and angles (°) for $[Co_3(H_2O)_2(OH)_2(C_7N_4H_8)_4]$.

	Donor-H	Acceptor-H	Donor-Acceptor	Angle
O1-H1···N1	0.796(15)	2.286(15)	3.0636(19)	165.6
O2-H2B···N2	0.804(15)	2.090(18)	2.7784(19)	144.0
O2-H2A···N4	0.820(16)	1.914(16)	2.7317(19)	175.0