Supplementary Material (ESI) for Chemical Communications

Dehydration of the nanoporous coordination framework $Er^{III}[Co^{III}(CN)_6]\cdot 4(H_2O)$: single crystal to single crystal transformation and negative thermal expansion in $Er^{III}[Co^{III}(CN)_6]$

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SUPPLEMENTARY INFORMATION

Single Crystal X-ray Diffraction

Variable temperature single crystal X-ray diffraction data of **A·4H$_2$O** were collected on a Bruker-AXS SMART 1000 CCD diffractometer and data for **A**, from dehydration of the same crystal, were collected on a Bruker-Nonius APEX II-FR591 diffractometer. Both instruments were equipped with graphite-monochromated Mo-K_α radiation and Oxford Cryostreams nitrogen cryostreams. The sample was mounted with a thin film of grease to the interior of a 0.5 mm glass capillary. Data collection, integration of frame data and conversion to intensities corrected for Lorenz, polarization and absorption effects were performed using the programs smart and saint+ [BrukerAXS, SMART, SAINT and XPREP. Area detector control and data integration and reduction software. Bruker Analytical X-ray Instruments Inc.: Madison, Wisconsin, U.S.A., 1995] and sadabs [Sheldrick, G. M. SADABS. Empirical absorption correction program for area detector data. University of Göttingen, Germany, 1996]. Structure solutions, structural refinement, structure analyses and production of crystallographic tables were carried out using the programs shelxs-97 [Sheldrick, G. M. SHELXS-97. Program for crystal structure solution. University of Göttingen, Germany, 1997], shelxl-97 [Sheldrick, G. M. SHELXL-97. Program for crystal structure refinement. University of Göttingen, Germany, 1997], platon [Spek, A. L., *J. Appl. Cryst.* **2003**, *36*, 7-13.] and xcif97 [Sheldrick, G. M. SHELXCIF-97 Program for generation of crystallographic tables. University of Göttingen, Germany, 1997]. As it was not possible to locate all positions of hydrogen atoms in $Er^{III}[Co^{III}(CN)_6]\cdot 4(H_2O)$, these atoms were not used for structural refinement. All non-hydrogen atoms were refined with anisotropic displacement parameters. The cyanide C and N atoms were assigned by means of their displacement parameters, C was in all cases attached to Co and N to Er, respectively.

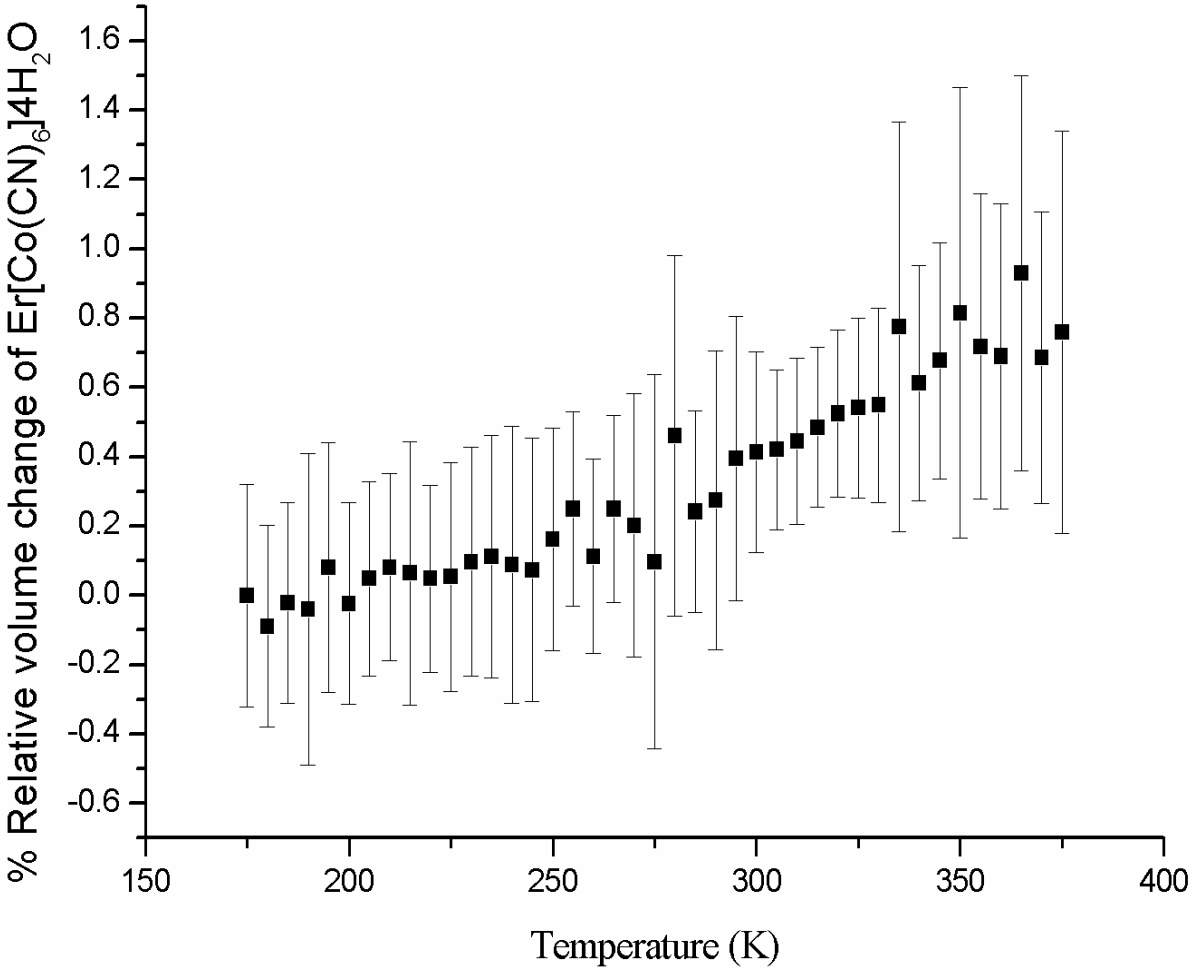

Fig. S1 Volume increase with temperature in $Er^{III}[Co^{III}(CN)_6]\cdot 4(H_2O)$ as determined by variable temperature single crystal X-ray diffraction. Error bars are ±1 e.s.d.

Thermogravimetry

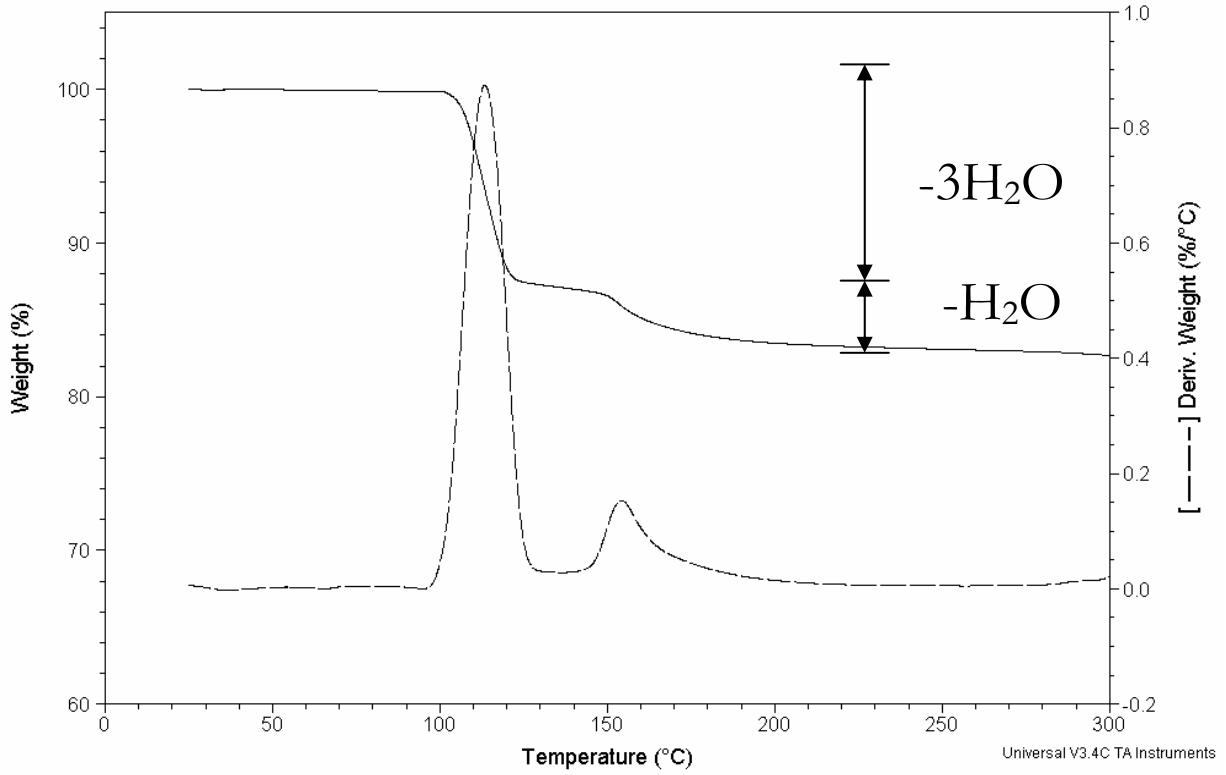

Fig. S2 Thermogravimetry of $Er^{III}[Co^{III}(CN)_6]\cdot 4(H_2O)$ under a dinitrogen atmosphere with a heating rate of 2 °C per minute.

Supplementary Material (ESI) for Chemical Communications

Full X-ray Crystallographic Tables

Table S1-1. Crystal data and structure refinement for **A**.

Identification code	er100	
Empirical formula	C6 Co Er N6	
Formula weight	382.31	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Hexagonal	
Space group	P 6_3/m m c	
Unit cell dimensions	a = 7.3887(2) Å	α= 90°.
	b = 7.3887(2) Å	β= 90°.
	c = 13.0436(7) Å	γ = 120°.
Volume	616.69(4) $Å^3$	
Z	2	
Density (calculated)	2.059 Mg/m^3	
Absorption coefficient	8.074 mm^{-1}	
F(000)	346	
Crystal size	0.25 x 0.22 x 0.11 mm^3	
Theta range for data collection	3.12 to 31.21°.	
Index ranges	-10<=h<=10, -10<=k<=10, -18<=l<=18	
Reflections collected	8106	
Independent reflections	415 [R(int) = 0.0173]	
Completeness to theta = 31.21°	97.6 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.410 and 0.2963	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	415 / 0 / 17	
Goodness-of-fit on F^2	1.268	
Final R indices [I>2sigma(I)]	R1 = 0.0103, wR2 = 0.0253	
R indices (all data)	R1 = 0.0117, wR2 = 0.0256	
Largest diff. peak and hole	0.754 and -0.537 e.$Å^{-3}$	

Table S1-2. Atomic coordinates (x 10^5) and equivalent isotropic displacement parameters ($Å^2$x 10^5) for **A**. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Er(1)	33330	66670	25000	689(6)
Co(1)	100000	100000	0	700(11)
C(1)	76040(30)	88020(15)	8431(13)	1160(30)
N(1)	61560(30)	80781(14)	13694(13)	1640(30)

Table S1-3. Bond lengths [Å] and angles [°] for **A**.

Er(1)-N(1)	2.3319(17)
Er(1)-N(1)#1	2.3319(17)
Er(1)-N(1)#2	2.3319(17)
Er(1)-N(1)#3	2.3319(17)
Er(1)-N(1)#4	2.3319(17)
Er(1)-N(1)#5	2.3319(17)
Co(1)-C(1)	1.8868(19)
Co(1)-C(1)#6	1.8868(19)
Co(1)-C(1)#7	1.8868(19)
Co(1)-C(1)#8	1.8868(19)
Co(1)-C(1)#9	1.8868(19)
Co(1)-C(1)#10	1.8868(19)
C(1)-N(1)	1.153(3)

N(1)-Er(1)-N(1)#1	78.46(9)
N(1)-Er(1)-N(1)#2	84.26(6)
N(1)#1-Er(1)-N(1)#2	134.43(3)
N(1)-Er(1)-N(1)#3	134.43(3)
N(1)#1-Er(1)-N(1)#3	84.26(6)
N(1)#2-Er(1)-N(1)#3	134.43(3)
N(1)-Er(1)-N(1)#4	84.26(6)
N(1)#1-Er(1)-N(1)#4	134.43(3)
N(1)#2-Er(1)-N(1)#4	84.26(6)
N(1)#3-Er(1)-N(1)#4	78.46(8)
N(1)-Er(1)-N(1)#5	134.43(3)
N(1)#1-Er(1)-N(1)#5	84.26(6)
N(1)#2-Er(1)-N(1)#5	78.46(9)
N(1)#3-Er(1)-N(1)#5	84.26(6)
N(1)#4-Er(1)-N(1)#5	134.43(3)
C(1)-Co(1)-C(1)#6	89.45(8)
C(1)-Co(1)-C(1)#7	89.45(8)
C(1)#6-Co(1)-C(1)#7	89.45(8)
C(1)-Co(1)-C(1)#8	90.55(8)
C(1)#6-Co(1)-C(1)#8	90.55(8)
C(1)#7-Co(1)-C(1)#8	180.0
C(1)-Co(1)-C(1)#9	180.0
C(1)#6-Co(1)-C(1)#9	90.55(8)

C(1)#7-Co(1)-C(1)#9	90.55(8)
C(1)#8-Co(1)-C(1)#9	89.45(8)
C(1)-Co(1)-C(1)#10	90.55(8)
C(1)#6-Co(1)-C(1)#10	180.0
C(1)#7-Co(1)-C(1)#10	90.55(8)
C(1)#8-Co(1)-C(1)#10	89.45(8)
C(1)#9-Co(1)-C(1)#10	89.45(8)
N(1)-C(1)-Co(1)	179.12(17)
C(1)-N(1)-Er(1)	177.31(16)

Symmetry transformations used to generate equivalent atoms:

#1 x,y,-z+1/2 #2 -x+y,-x+1,z #3 -y+1,x-y+1,-z+1/2

#4 -y+1,x-y+1,z #5 -x+y,-x+1,-z+1/2 #6 -y+2,x-y+1,z

#7 -x+y+1,-x+2,z #8 x-y+1,x,-z #9 -x+2,-y+2,-z

#10 y,-x+y+1,-z

Table S1-4. Anisotropic displacement parameters ($Å^2 x\ 10^5$) for **A**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U_{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U_{12}\ ]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Er(1)	764(7)	764(7)	540(9)	0	0	382(3)
Co(1)	746(16)	746(16)	610(20)	0	0	373(8)
C(1)	1240(90)	1320(60)	900(70)	-60(30)	-130(70)	620(40)
N(1)	1230(80)	2070(70)	1330(70)	40(30)	90(60)	610(40)

Table S2-1. Crystal data and structure refinement for **A**.

Identification code	er150	
Empirical formula	C6 Co Er N6	
Formula weight	382.31	
Temperature	150(2) K	
Wavelength	0.71073 Å	
Crystal system	Hexagonal	
Space group	P 6_3/m m c	
Unit cell dimensions	a = 7.3863(2) Å	α= 90°.
	b = 7.3863(2) Å	β= 90°.
	c = 13.0391(6) Å	γ = 120°.
Volume	616.07(4) $Å^3$	
Z	2	
Density (calculated)	2.061 Mg/m^3	
Absorption coefficient	8.082 mm^{-1}	
F(000)	346	
Crystal size	0.25 x 0.22 x 0.11 mm^3	
Theta range for data collection	3.12 to 31.22°.	
Index ranges	-10<=h<=10, -10<=k<=10, -18<=l<=18	
Reflections collected	8085	
Independent reflections	415 [R(int) = 0.0168]	
Completeness to theta = 31.22°	97.6 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.411 and 0.299	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	415 / 0 / 17	
Goodness-of-fit on F^2	1.263	
Final R indices [I>2sigma(I)]	R1 = 0.0100, wR2 = 0.0251	
R indices (all data)	R1 = 0.0113, wR2 = 0.0254	
Largest diff. peak and hole	0.700 and -0.496 $e.Å^{-3}$	

Table S2-2. Atomic coordinates (x 10^5) and equivalent isotropic displacement parameters ($Å^2$x 10^5) for **A**. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Er(1)	33330	66670	25000	814(6)
Co(1)	100000	100000	0	817(11)
C(1)	76030(30)	88014(15)	8420(13)	1380(30)
N(1)	61570(30)	80785(14)	13698(13)	2000(40)

Table S2-3. Bond lengths [Å] and angles [°] for **A**.

Er(1)-N(1)	2.3311(18)
Er(1)-N(1)#1	2.3311(17)
Er(1)-N(1)#2	2.3311(17)
Er(1)-N(1)#3	2.3311(17)
Er(1)-N(1)#4	2.3311(17)
Er(1)-N(1)#5	2.3311(17)
Co(1)-C(1)	1.8859(19)
Co(1)-C(1)#6	1.8860(19)
Co(1)-C(1)#7	1.8860(19)
Co(1)-C(1)#8	1.8860(19)
Co(1)-C(1)#9	1.8860(19)
Co(1)-C(1)#10	1.8860(19)
C(1)-N(1)	1.153(3)

N(1)-Er(1)-N(1)#1	78.42(9)
N(1)-Er(1)-N(1)#2	84.29(6)
N(1)#1-Er(1)-N(1)#2	134.41(3)
N(1)-Er(1)-N(1)#3	134.41(3)
N(1)#1-Er(1)-N(1)#3	84.29(6)
N(1)#2-Er(1)-N(1)#3	134.41(3)
N(1)-Er(1)-N(1)#4	84.29(6)
N(1)#1-Er(1)-N(1)#4	134.41(3)
N(1)#2-Er(1)-N(1)#4	84.29(6)
N(1)#3-Er(1)-N(1)#4	78.42(9)
N(1)-Er(1)-N(1)#5	134.41(3)
N(1)#1-Er(1)-N(1)#5	84.29(6)
N(1)#2-Er(1)-N(1)#5	78.42(9)
N(1)#3-Er(1)-N(1)#5	84.29(6)
N(1)#4-Er(1)-N(1)#5	134.41(3)
C(1)-Co(1)-C(1)#6	89.52(8)
C(1)-Co(1)-C(1)#7	90.48(8)
C(1)#6-Co(1)-C(1)#7	180.0
C(1)-Co(1)-C(1)#8	179.999(1)
C(1)#6-Co(1)-C(1)#8	90.48(8)
C(1)#7-Co(1)-C(1)#8	89.52(8)
C(1)-Co(1)-C(1)#9	90.48(8)
C(1)#6-Co(1)-C(1)#9	90.48(8)

C(1)#7-Co(1)-C(1)#9	89.52(8)
C(1)#8-Co(1)-C(1)#9	89.52(8)
C(1)-Co(1)-C(1)#10	89.52(8)
C(1)#6-Co(1)-C(1)#10	89.52(8)
C(1)#7-Co(1)-C(1)#10	90.48(8)
C(1)#8-Co(1)-C(1)#10	90.48(8)
C(1)#9-Co(1)-C(1)#10	180.0
N(1)-C(1)-Co(1)	178.95(17)
C(1)-N(1)-Er(1)	177.44(16)

Symmetry transformations used to generate equivalent atoms:

#1 x,y,-z+1/2 #2 -x+y,-x+1,z #3 -y+1,x-y+1,-z+1/2

#4 -y+1,x-y+1,z #5 -x+y,-x+1,-z+1/2 #6 -x+y+1,-x+2,z

#7 x-y+1,x,-z #8 -x+2,-y+2,-z #9 y,-x+y+1,-z

#10 -y+2,x-y+1,z

Table S2-4. Anisotropic displacement parameters ($Å^2 x\ 10^5$) for **A**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U_{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U_{12}\ ]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Er(1)	893(7)	893(7)	656(9)	0	0	446(3)
Co(1)	877(16)	877(16)	700(20)	0	0	438(8)
C(1)	1350(90)	1600(60)	1120(70)	-60(30)	-120(70)	680(40)
N(1)	1430(80)	2610(70)	1570(70)	110(30)	220(60)	710(40)

Table S3-1. Crystal data and structure refinement for **A**.

Identification code	er225	
Empirical formula	C6 Co Er N6	
Formula weight	382.31	
Temperature	225(2) K	
Wavelength	0.71073 Å	
Crystal system	Hexagonal	
Space group	P 6_3/m m c	
Unit cell dimensions	a = 7.3828(2) Å	α= 90°.
	b = 7.3828(2) Å	β= 90°.
	c = 13.0303(6) Å	γ = 120°.
Volume	615.07(4) $Å^3$	
Z	2	
Density (calculated)	2.064 Mg/m^3	
Absorption coefficient	8.095 mm^{-1}	
F(000)	346	
Crystal size	0.25 x 0.22 x 0.11 mm^3	
Theta range for data collection	3.13 to 31.24°.	
Index ranges	-10<=h<=10, -10<=k<=10, -18<=l<=18	
Reflections collected	8085	
Independent reflections	415 [R(int) = 0.0175]	
Completeness to theta = 31.24°	97.6 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.411 and 0.297	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	415 / 0 / 17	
Goodness-of-fit on F^2	1.248	
Final R indices [I>2sigma(I)]	R1 = 0.0099, wR2 = 0.0245	
R indices (all data)	R1 = 0.0115, wR2 = 0.0248	
Largest diff. peak and hole	0.528 and -0.485 $e.Å^{-3}$	

Table S3-2. Atomic coordinates (x 10^5) and equivalent isotropic displacement parameters ($Å^2$x 10^5) for **A**. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Er(1)	33330	66670	25000	1015(6)
Co(1)	100000	100000	0	1018(11)
C(1)	76030(30)	88016(16)	8427(14)	1750(40)
N(1)	61580(30)	80792(15)	13681(14)	2680(40)

Table S3-3. Bond lengths [Å] and angles [°] for **A**.

Er(1)-N(1)#1	2.3320(18)
Er(1)-N(1)#2	2.3320(18)
Er(1)-N(1)#3	2.3320(18)
Er(1)-N(1)#4	2.3320(18)
Er(1)-N(1)#5	2.3320(18)
Er(1)-N(1)	2.3320(18)
Co(1)-C(1)#6	1.885(2)
Co(1)-C(1)#7	1.885(2)
Co(1)-C(1)#8	1.885(2)
Co(1)-C(1)#9	1.885(2)
Co(1)-C(1)	1.885(2)
Co(1)-C(1)#10	1.885(2)
C(1)-N(1)	1.150(3)

N(1)#1-Er(1)-N(1)#2	134.43(3)
N(1)#1-Er(1)-N(1)#3	84.26(7)
N(1)#2-Er(1)-N(1)#3	134.43(3)
N(1)#1-Er(1)-N(1)#4	134.43(3)
N(1)#2-Er(1)-N(1)#4	84.26(7)
N(1)#3-Er(1)-N(1)#4	78.46(9)
N(1)#1-Er(1)-N(1)#5	84.26(7)
N(1)#2-Er(1)-N(1)#5	78.46(9)
N(1)#3-Er(1)-N(1)#5	84.26(7)
N(1)#4-Er(1)-N(1)#5	134.43(3)
N(1)#1-Er(1)-N(1)	78.47(9)
N(1)#2-Er(1)-N(1)	84.26(7)
N(1)#3-Er(1)-N(1)	134.43(3)
N(1)#4-Er(1)-N(1)	84.26(7)
N(1)#5-Er(1)-N(1)	134.43(3)
C(1)#6-Co(1)-C(1)#7	180.0
C(1)#6-Co(1)-C(1)#8	90.51(8)
C(1)#7-Co(1)-C(1)#8	89.49(8)
C(1)#6-Co(1)-C(1)#9	90.51(8)
C(1)#7-Co(1)-C(1)#9	89.49(8)
C(1)#8-Co(1)-C(1)#9	89.49(8)
C(1)#6-Co(1)-C(1)	89.49(8)
C(1)#7-Co(1)-C(1)	90.51(8)

C(1)#8-Co(1)-C(1)	180.0
C(1)#9-Co(1)-C(1)	90.51(8)
C(1)#6-Co(1)-C(1)#10	89.49(8)
C(1)#7-Co(1)-C(1)#10	90.51(8)
C(1)#8-Co(1)-C(1)#10	90.51(8)
C(1)#9-Co(1)-C(1)#10	180.0
C(1)-Co(1)-C(1)#10	89.49(8)
N(1)-C(1)-Co(1)	179.08(18)
C(1)-N(1)-Er(1)	177.31(17)

Symmetry transformations used to generate equivalent atoms:

#1 x,y,-z+1/2 #2 -x+y,-x+1,z #3 -y+1,x-y+1,-z+1/2

#4 -y+1,x-y+1,z #5 -x+y,-x+1,-z+1/2 #6 -x+y+1,-x+2,z

#7 x-y+1,x,-z #8 -x+2,-y+2,-z #9 y,-x+y+1,-z

#10 -y+2,x-y+1,z

Table S3-4. Anisotropic displacement parameters ($Å^2 x\ 10^5$) for **A**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U_{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U_{12}\ ]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Er(1)	1098(7)	1098(7)	848(9)	0	0	549(3)
Co(1)	1090(16)	1090(16)	870(20)	0	0	545(8)
C(1)	1690(90)	2020(70)	1430(80)	-20(30)	-40(70)	850(40)
N(1)	1870(90)	3580(80)	2030(80)	230(30)	460(70)	930(40)

Table S4-1. Crystal data and structure refinement for **A**.

Identification code	er300	
Empirical formula	C6 Co Er N6	
Formula weight	382.31	
Temperature	300(2) K	
Wavelength	0.71073 Å	
Crystal system	Hexagonal	
Space group	P 6_3/m m c	
Unit cell dimensions	a = 7.3782(2) Å	α= 90°.
	b = 7.3782(2) Å	β= 90°.
	c = 13.0222(6) Å	γ = 120°.
Volume	613.93(4) $Å^3$	
Z	2	
Density (calculated)	2.068 Mg/m^3	
Absorption coefficient	8.111 mm^{-1}	
F(000)	346	
Crystal size	0.25 x 0.22 x 0.11 mm^3	
Theta range for data collection	3.13 to 30.85°.	
Index ranges	-10<=h<=10, -10<=k<=10, -18<=l<=18	
Reflections collected	6345	
Independent reflections	405 [R(int) = 0.0185]	
Completeness to theta = 30.85°	98.3 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.411 and 0.309	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	405 / 0 / 17	
Goodness-of-fit on F^2	1.331	
Final R indices [I>2sigma(I)]	R1 = 0.0100, wR2 = 0.0262	
R indices (all data)	R1 = 0.0115, wR2 = 0.0265	
Largest diff. peak and hole	0.505 and -0.530 $e.Å^{-3}$	

Table S4-2. Atomic coordinates (x 10^5) and equivalent isotropic displacement parameters ($Å^2$x 10^5) for **A**. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Er(1)	33330	66670	25000	1238(7)
Co(1)	100000	100000	0	1218(13)
C(1)	75990(40)	87997(18)	8450(16)	2090(40)
N(1)	61550(30)	80776(17)	13684(16)	3340(50)

Table S4-3. Bond lengths [Å] and angles [°] for **A**.

Er(1)-N(1)#1	2.329(2)
Er(1)-N(1)#2	2.329(2)
Er(1)-N(1)#3	2.329(2)
Er(1)-N(1)#4	2.329(2)
Er(1)-N(1)#5	2.329(2)
Er(1)-N(1)	2.329(2)
Co(1)-C(1)#6	1.888(2)
Co(1)-C(1)#7	1.888(2)
Co(1)-C(1)#8	1.888(2)
Co(1)-C(1)#9	1.888(2)
Co(1)-C(1)#10	1.888(2)
Co(1)-C(1)	1.888(2)
C(1)-N(1)	1.147(3)

N(1)#1-Er(1)-N(1)#2	134.45(4)
N(1)#1-Er(1)-N(1)#3	84.22(8)
N(1)#2-Er(1)-N(1)#3	134.45(4)
N(1)#1-Er(1)-N(1)#4	134.45(4)
N(1)#2-Er(1)-N(1)#4	84.22(8)
N(1)#3-Er(1)-N(1)#4	78.52(11)
N(1)#1-Er(1)-N(1)#5	84.22(8)
N(1)#2-Er(1)-N(1)#5	78.52(11)
N(1)#3-Er(1)-N(1)#5	84.22(8)
N(1)#4-Er(1)-N(1)#5	134.45(4)
N(1)#1-Er(1)-N(1)	78.52(11)
N(1)#2-Er(1)-N(1)	84.22(8)
N(1)#3-Er(1)-N(1)	134.45(4)
N(1)#4-Er(1)-N(1)	84.22(8)
N(1)#5-Er(1)-N(1)	134.45(4)
C(1)#6-Co(1)-C(1)#7	89.45(9)
C(1)#6-Co(1)-C(1)#8	89.45(9)
C(1)#7-Co(1)-C(1)#8	89.45(9)
C(1)#6-Co(1)-C(1)#9	90.55(9)
C(1)#7-Co(1)-C(1)#9	90.55(9)
C(1)#8-Co(1)-C(1)#9	180.0
C(1)#6-Co(1)-C(1)#10	180.00(8)
C(1)#7-Co(1)-C(1)#10	90.55(9)

C(1)#8-Co(1)-C(1)#10	90.55(9)
C(1)#9-Co(1)-C(1)#10	89.45(9)
C(1)#6-Co(1)-C(1)	90.55(9)
C(1)#7-Co(1)-C(1)	180.0
C(1)#8-Co(1)-C(1)	90.55(9)
C(1)#9-Co(1)-C(1)	89.45(9)
C(1)#10-Co(1)-C(1)	89.45(9)
N(1)-C(1)-Co(1)	179.2(2)
C(1)-N(1)-Er(1)	177.2(2)

Symmetry transformations used to generate equivalent atoms:

#1 x,y,-z+1/2 #2 -x+y,-x+1,z #3 -y+1,x-y+1,-z+1/2

#4 -y+1,x-y+1,z #5 -x+y,-x+1,-z+1/2 #6 x-y+1,x,-z

#7 -x+2,-y+2,-z #8 y,-x+y+1,-z #9 -y+2,x-y+1,z

#10 -x+y+1,-x+2,z

Table S4-4. Anisotropic displacement parameters ($Å^2 x\ 10^5$) for **A**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U_{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U_{12}\ ]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Er(1)	1330(8)	1330(8)	1053(10)	0	0	665(4)
Co(1)	1312(18)	1312(18)	1030(30)	0	0	656(9)
C(1)	1910(100)	2470(80)	1720(90)	20(40)	50(80)	960(50)
N(1)	2240(110)	4510(110)	2510(100)	320(40)	630(80)	1120(50)

Table S5-1. Crystal data and structure refinement for **A**.

Identification code	er375	
Empirical formula	C6 Co Er N6	
Formula weight	382.31	
Temperature	375(2) K	
Wavelength	0.71073 Å	
Crystal system	Hexagonal	
Space group	P 6_3/m m c	
Unit cell dimensions	a = 7.3719(2) Å	α= 90°.
	b = 7.3719(2) Å	β= 90°.
	c = 13.0109(7) Å	γ = 120°.
Volume	612.35(4) $Å^3$	
Z	2	
Density (calculated)	2.073 Mg/m^3	
Absorption coefficient	8.132 mm^{-1}	
F(000)	346	
Crystal size	0.25 x 0.22 x 0.11 mm^3	
Theta range for data collection	3.13 to 31.10°.	
Index ranges	-10<=h<=10, -10<=k<=10, -18<=l<=18	
Reflections collected	7336	
Independent reflections	412 [R(int) = 0.0185]	
Completeness to theta = 31.10°	98.8 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.411 and 0.299	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	412 / 0 / 17	
Goodness-of-fit on F^2	1.305	
Final R indices [I>2sigma(I)]	R1 = 0.0105, wR2 = 0.0232	
R indices (all data)	R1 = 0.0124, wR2 = 0.0236	
Largest diff. peak and hole	0.445 and -0.551 $e.Å^{-3}$	

Table S5-2. Atomic coordinates (x 10^5) and equivalent isotropic displacement parameters ($Å^2$x 10^5) for **A**. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Er(1)	33330	66670	25000	1456(6)
Co(1)	100000	100000	0	1448(12)
C(1)	75960(30)	87981(17)	8451(15)	2490(40)
N(1)	61610(30)	80804(16)	13674(15)	4060(50)

Table S5-3. Bond lengths [Å] and angles [°] for **A**.

Er(1)-N(1)#1	2.3303(19)
Er(1)-N(1)#2	2.3303(19)
Er(1)-N(1)	2.330(2)
Er(1)-N(1)#3	2.3303(19)
Er(1)-N(1)#4	2.3303(19)
Er(1)-N(1)#5	2.3303(19)
Co(1)-C(1)#6	1.888(2)
Co(1)-C(1)#7	1.888(2)
Co(1)-C(1)#8	1.888(2)
Co(1)-C(1)	1.888(2)
Co(1)-C(1)#9	1.888(2)
Co(1)-C(1)#10	1.888(2)
C(1)-N(1)	1.141(3)

N(1)#1-Er(1)-N(1)#2	134.42(4)
N(1)#1-Er(1)-N(1)	78.46(10)
N(1)#2-Er(1)-N(1)	84.27(8)
N(1)#1-Er(1)-N(1)#3	84.27(8)
N(1)#2-Er(1)-N(1)#3	134.42(4)
N(1)-Er(1)-N(1)#3	134.42(4)
N(1)#1-Er(1)-N(1)#4	134.42(4)
N(1)#2-Er(1)-N(1)#4	84.27(8)
N(1)-Er(1)-N(1)#4	84.27(8)
N(1)#3-Er(1)-N(1)#4	78.46(10)
N(1)#1-Er(1)-N(1)#5	84.27(8)
N(1)#2-Er(1)-N(1)#5	78.46(10)
N(1)-Er(1)-N(1)#5	134.42(4)
N(1)#3-Er(1)-N(1)#5	84.27(8)
N(1)#4-Er(1)-N(1)#5	134.42(4)
C(1)#6-Co(1)-C(1)#7	180.0
C(1)#6-Co(1)-C(1)#8	90.51(9)
C(1)#7-Co(1)-C(1)#8	89.49(9)
C(1)#6-Co(1)-C(1)	89.49(9)
C(1)#7-Co(1)-C(1)	90.51(9)
C(1)#8-Co(1)-C(1)	180.0
C(1)#6-Co(1)-C(1)#9	90.51(9)
C(1)#7-Co(1)-C(1)#9	89.49(9)

C(1)#8-Co(1)-C(1)#9	89.49(9)
C(1)-Co(1)-C(1)#9	90.51(9)
C(1)#6-Co(1)-C(1)#10	89.49(9)
C(1)#7-Co(1)-C(1)#10	90.51(9)
C(1)#8-Co(1)-C(1)#10	90.51(9)
C(1)-Co(1)-C(1)#10	89.49(9)
C(1)#9-Co(1)-C(1)#10	180.0
N(1)-C(1)-Co(1)	179.07(19)
C(1)-N(1)-Er(1)	177.33(19)

Symmetry transformations used to generate equivalent atoms:

#1 x,y,-z+1/2 #2 -x+y,-x+1,z #3 -y+1,x-y+1,-z+1/2

#4 -y+1,x-y+1,z #5 -x+y,-x+1,-z+1/2 #6 -x+y+1,-x+2,z

#7 x-y+1,x,-z #8 -x+2,-y+2,-z #9 y,-x+y+1,-z

#10 -y+2,x-y+1,z

Table S5-4. Anisotropic displacement parameters ($Å^2 x\ 10^5$) for **A**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U_{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U_{12}\ ]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Er(1)	1543(7)	1543(7)	1282(9)	0	0	772(3)
Co(1)	1552(17)	1552(17)	1240(20)	0	0	776(8)
C(1)	2280(100)	2930(80)	2030(80)	80(40)	170(80)	1140(50)
N(1)	2650(100)	5510(110)	3080(90)	460(40)	910(80)	1320(50)

Table S6-1. Crystal data and structure refinement for **A.4(H_2O)**.

Identification code	er100w	
Empirical formula	C6 H8 Co Er N6 O4	
Formula weight	454.37	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	C m c m	
Unit cell dimensions	a = 7.2835(11) Å	α= 90°.
	b = 12.5836(19) Å	β= 90°.
	c = 13.462(2) Å	γ = 90°.
Volume	1233.8(3) $Å^3$	
Z	4	
Density (calculated)	2.446 Mg/m^3	
Absorption coefficient	8.115 mm^{-1}	
F(000)	852	
Crystal size	0.25 x 0.22 x 0.11 mm^3	
Theta range for data collection	3.03 to 27.96°.	
Index ranges	-9<=h<=9, -16<=k<=16, -17<=l<=17	
Reflections collected	4247	
Independent reflections	835 [R(int) = 0.0368]	
Completeness to theta = 27.96°	99.6 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.410 and 0.217	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	835 / 3 / 58	
Goodness-of-fit on F^2	1.172	
Final R indices [I>2sigma(I)]	R1 = 0.0272, wR2 = 0.0688	
R indices (all data)	R1 = 0.0297, wR2 = 0.0701	
Largest diff. peak and hole	2.009 and -1.670 $e.Å^{-3}$	

Table S6-2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^4) for **A.4(H_2O)**. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Er(1)	0	3249.8(3)	7500	74.9(14)
Co(1)	0	0	5000	82(2)
N(1)	0	2185(4)	5974(4)	139(11)
C(1)	0	1354(5)	5598(5)	119(12)
N(2)	2007(5)	4240(3)	6406(3)	148(8)
C(2)	3158(6)	4534(3)	5888(3)	131(9)
O(1)	2584(7)	2180(4)	7500	198(10)
O(2)	0	6556(4)	6002(4)	187(10)

Table S6-3. Bond lengths [Å] and angles [°] for **A.4(H_2O)**.

Er(1)-O(1)#1	2.314(5)
Er(1)-O(1)	2.314(5)
Er(1)-N(2)	2.421(4)
Er(1)-N(2)#2	2.421(4)
Er(1)-N(2)#3	2.421(4)
Er(1)-N(2)#1	2.421(4)
Er(1)-N(1)	2.453(5)
Er(1)-N(1)#2	2.453(5)
Co(1)-C(1)#4	1.884(6)
Co(1)-C(1)	1.884(6)
Co(1)-C(2)#5	1.890(5)
Co(1)-C(2)#6	1.890(5)
Co(1)-C(2)#7	1.890(5)
Co(1)-C(2)#8	1.890(5)
N(1)-C(1)	1.162(9)
N(2)-C(2)	1.151(6)
C(2)-Co(1)#9	1.890(5)
O(1)-H(1)	0.90(5)
O(2)-H(2)	0.90(5)
O(2)-H(3)	0.90(5)

O(1)#1-Er(1)-O(1)	108.8(3)
O(1)#1-Er(1)-N(2)	142.24(9)
O(1)-Er(1)-N(2)	78.96(14)
O(1)#1-Er(1)-N(2)#2	142.24(9)
O(1)-Er(1)-N(2)#2	78.96(14)
N(2)-Er(1)-N(2)#2	74.98(18)
O(1)#1-Er(1)-N(2)#3	78.96(14)
O(1)-Er(1)-N(2)#3	142.24(9)
N(2)-Er(1)-N(2)#3	74.29(19)
N(2)#2-Er(1)-N(2)#3	118.04(19)
O(1)#1-Er(1)-N(2)#1	78.96(14)
O(1)-Er(1)-N(2)#1	142.24(9)
N(2)-Er(1)-N(2)#1	118.04(19)
N(2)#2-Er(1)-N(2)#1	74.29(19)
N(2)#3-Er(1)-N(2)#1	74.98(18)
O(1)#1-Er(1)-N(1)	71.47(9)

O(1)-Er(1)-N(1)	71.47(9)
N(2)-Er(1)-N(1)	76.78(14)
N(2)#2-Er(1)-N(1)	142.28(10)
N(2)#3-Er(1)-N(1)	76.78(14)
N(2)#1-Er(1)-N(1)	142.28(10)
O(1)#1-Er(1)-N(1)#2	71.47(9)
O(1)-Er(1)-N(1)#2	71.47(9)
N(2)-Er(1)-N(1)#2	142.28(10)
N(2)#2-Er(1)-N(1)#2	76.78(14)
N(2)#3-Er(1)-N(1)#2	142.28(10)
N(2)#1-Er(1)-N(1)#2	76.78(14)
N(1)-Er(1)-N(1)#2	113.8(3)
C(1)#4-Co(1)-C(1)	180.0
C(1)#4-Co(1)-C(2)#5	89.41(19)
C(1)-Co(1)-C(2)#5	90.59(19)
C(1)#4-Co(1)-C(2)#6	90.59(19)
C(1)-Co(1)-C(2)#6	89.41(19)
C(2)#5-Co(1)-C(2)#6	180.0
C(1)#4-Co(1)-C(2)#7	89.41(19)
C(1)-Co(1)-C(2)#7	90.59(19)
C(2)#5-Co(1)-C(2)#7	90.4(3)
C(2)#6-Co(1)-C(2)#7	89.6(3)
C(1)#4-Co(1)-C(2)#8	90.59(19)
C(1)-Co(1)-C(2)#8	89.41(19)
C(2)#5-Co(1)-C(2)#8	89.6(3)
C(2)#6-Co(1)-C(2)#8	90.4(3)
C(2)#7-Co(1)-C(2)#8	180.0
C(1)-N(1)-Er(1)	148.9(5)
N(1)-C(1)-Co(1)	179.5(6)
C(2)-N(2)-Er(1)	166.8(4)
N(2)-C(2)-Co(1)#9	178.0(4)
Er(1)-O(1)-H(1)	126(4)
H(2)-O(2)-H(3)	126(8)

Symmetry transformations used to generate equivalent atoms:

#1 -x,y,-z+3/2 #2 x,y,-z+3/2 #3 -x,y,z #4 -x,-y,-z+1

#5 -x+1/2,y-1/2,z #6 x-1/2,-y+1/2,-z+1 #7 x-1/2,y-1/2,z

#8 -x+1/2,-y+1/2,-z+1 #9 x+1/2,y+1/2,z

Table S6-4. Anisotropic displacement parameters ($Å^2 x\ 10^4$) for **A.4(H_2O)**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U_{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U_{12}\ ]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Er(1)	56(2)	79(2)	89(2)	0	0	0
Co(1)	66(5)	73(5)	106(6)	1(4)	0	0
N(1)	130(30)	140(30)	140(30)	-30(20)	0	0
C(1)	110(30)	140(30)	100(30)	30(20)	0	0
N(2)	108(18)	196(19)	140(18)	4(15)	-11(15)	-35(15)
C(2)	140(20)	110(20)	150(20)	-4(16)	-22(17)	18(16)
O(1)	170(20)	280(30)	150(20)	0	0	70(20)
O(2)	190(30)	190(20)	180(20)	10(20)	0	0

Table S6-5. Hydrogen coordinates (x 10^3) and isotropic displacement parameters ($Å^2$x 10^3) for **A.4(H_2O)**.

	x	y	z	U(eq)
H(1)	342(8)	212(5)	701(4)	30
H(2)	0	695(6)	544(5)	28
H(3)	0	584(4)	604(7)	28

Table S6-6. Hydrogen bonds for **A.4(H_2O)** [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(1)-H(1)...O(2)#10	0.90(5)	1.92(5)	2.789(5)	162(6)
O(2)-H(2)...N(1)#11	0.90(5)	2.19(5)	3.095(8)	176(8)
O(2)-H(3)...N(2)	0.90(5)	2.54(4)	3.306(6)	143(2)

Symmetry transformations used to generate equivalent atoms:

#1 -x,y,-z+3/2 #2 x,y,-z+3/2 #3 -x,y,z #4 -x,-y,-z+1

#5 -x+1/2,y-1/2,z #6 x-1/2,-y+1/2,-z+1 #7 x-1/2,y-1/2,z

#8 -x+1/2,-y+1/2,-z+1 #9 x+1/2,y+1/2,z #10 x+1/2,y-1/2,z

#11 -x,-y+1,-z+1

Table S7-1. Crystal data and structure refinement for **A.4(H_2O)**.

Identification code	er150w	
Empirical formula	C6 H8 Co Er N6 O4	
Formula weight	454.37	
Temperature	150(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	C m c m	
Unit cell dimensions	a = 7.2858(12) Å	α= 90°.
	b = 12.601(2) Å	β= 90°.
	c = 13.469(2) Å	γ = 90°.
Volume	1236.5(3) $Å^3$	
Z	4	
Density (calculated)	2.441 Mg/m^3	
Absorption coefficient	8.097 mm^{-1}	
F(000)	852	
Crystal size	0.25 x 0.22 x 0.11 mm^3	
Theta range for data collection	3.02 to 27.94°.	
Index ranges	-9<=h<=9, -16<=k<=16, -17<=l<=17	
Reflections collected	4247	
Independent reflections	833 [R(int) = 0.0371]	
Completeness to theta = 27.94°	99.3 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.410 and 0.214	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	833 / 3 / 58	
Goodness-of-fit on F^2	1.190	
Final R indices [I>2sigma(I)]	R1 = 0.0282, wR2 = 0.0717	
R indices (all data)	R1 = 0.0310, wR2 = 0.0740	
Largest diff. peak and hole	2.526 and -1.418 $e.Å^{-3}$	

Table S7-2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^4) for **A.4(H_2O)**. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Er(1)	0	3249.7(3)	7500	84.9(15)
Co(1)	0	0	5000	91(3)
N(1)	0	2178(5)	5985(4)	163(11)
C(1)	0	1351(5)	5607(5)	132(12)
N(2)	2009(6)	4237(3)	6407(3)	167(8)
C(2)	3155(6)	4532(3)	5886(3)	138(9)
O(1)	2587(8)	2186(4)	7500	227(11)
O(2)	0	6558(4)	6004(4)	229(11)

Table S7-3. Bond lengths [Å] and angles [°] for **A.4(H_2O)**.

Er(1)-O(1)	2.313(5)
Er(1)-O(1)#1	2.313(5)
Er(1)-N(2)	2.420(4)
Er(1)-N(2)#2	2.420(4)
Er(1)-N(2)#3	2.420(4)
Er(1)-N(2)#1	2.420(4)
Er(1)-N(1)	2.447(6)
Er(1)-N(1)#2	2.447(6)
Co(1)-C(1)	1.889(7)
Co(1)-C(1)#4	1.889(7)
Co(1)-C(2)#5	1.892(5)
Co(1)-C(2)#6	1.892(5)
Co(1)-C(2)#7	1.892(5)
Co(1)-C(2)#8	1.892(5)
N(1)-C(1)	1.160(9)
N(2)-C(2)	1.152(6)
C(2)-Co(1)#9	1.892(5)
O(1)-H(1)	0.94(5)
O(2)-H(2)	0.95(5)
O(2)-H(3)	0.95(5)
O(1)-Er(1)-O(1)#1	109.1(3)
O(1)-Er(1)-N(2)	78.75(15)
O(1)#1-Er(1)-N(2)	142.26(10)
O(1)-Er(1)-N(2)#2	78.75(15)
O(1)#1-Er(1)-N(2)#2	142.26(10)
N(2)-Er(1)-N(2)#2	74.92(19)
O(1)-Er(1)-N(2)#3	142.26(10)
O(1)#1-Er(1)-N(2)#3	78.75(15)
N(2)-Er(1)-N(2)#3	74.4(2)
N(2)#2-Er(1)-N(2)#3	118.1(2)
O(1)-Er(1)-N(2)#1	142.26(10)
O(1)#1-Er(1)-N(2)#1	78.75(15)
N(2)-Er(1)-N(2)#1	118.1(2)
N(2)#2-Er(1)-N(2)#1	74.4(2)
N(2)#3-Er(1)-N(2)#1	74.92(19)
O(1)-Er(1)-N(1)	71.34(10)

O(1)#1-Er(1)-N(1)	71.34(10)
N(2)-Er(1)-N(1)	77.09(14)
N(2)#2-Er(1)-N(1)	142.27(10)
N(2)#3-Er(1)-N(1)	77.09(14)
N(2)#1-Er(1)-N(1)	142.27(10)
O(1)-Er(1)-N(1)#2	71.34(10)
O(1)#1-Er(1)-N(1)#2	71.34(10)
N(2)-Er(1)-N(1)#2	142.27(10)
N(2)#2-Er(1)-N(1)#2	77.09(14)
N(2)#3-Er(1)-N(1)#2	142.27(10)
N(2)#1-Er(1)-N(1)#2	77.09(14)
N(1)-Er(1)-N(1)#2	113.0(3)
C(1)-Co(1)-C(1)#4	180.0
C(1)-Co(1)-C(2)#5	90.4(2)
C(1)#4-Co(1)-C(2)#5	89.6(2)
C(1)-Co(1)-C(2)#6	89.6(2)
C(1)#4-Co(1)-C(2)#6	90.4(2)
C(2)#5-Co(1)-C(2)#6	180.0(2)
C(1)-Co(1)-C(2)#7	90.4(2)
C(1)#4-Co(1)-C(2)#7	89.6(2)
C(2)#5-Co(1)-C(2)#7	90.5(3)
C(2)#6-Co(1)-C(2)#7	89.5(3)
C(1)-Co(1)-C(2)#8	89.6(2)
C(1)#4-Co(1)-C(2)#8	90.4(2)
C(2)#5-Co(1)-C(2)#8	89.5(3)
C(2)#6-Co(1)-C(2)#8	90.5(3)
C(2)#7-Co(1)-C(2)#8	180.0
C(1)-N(1)-Er(1)	149.5(5)
N(1)-C(1)-Co(1)	179.6(6)
C(2)-N(2)-Er(1)	167.1(4)
N(2)-C(2)-Co(1)#9	178.4(4)
Er(1)-O(1)-H(1)	124(4)
H(2)-O(2)-H(3)	115(8)

Symmetry transformations used to generate equivalent atoms:

#1 -x,y,-z+3/2 #2 x,y,-z+3/2 #3 -x,y,z #4 -x,-y,-z+1

#5 -x+1/2,y-1/2,z #6 x-1/2,-y+1/2,-z+1 #7 x-1/2,y-1/2,z

#8 -x+1/2,-y+1/2,-z+1 #9 x+1/2,y+1/2,z

Table S7-4. Anisotropic displacement parameters ($Å^2 x\ 10^4$) for **A.4(H_2O)**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U_{11} + ... + 2\ h\ k\ a^*\ b^*\ U_{12}\ ]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Er(1)	70(2)	90(2)	95(2)	0	0	0
Co(1)	84(5)	84(5)	106(6)	1(4)	0	0
N(1)	180(30)	150(30)	160(30)	-30(20)	0	0
C(1)	90(30)	170(30)	140(30)	20(20)	0	0
N(2)	114(18)	210(20)	177(19)	21(16)	-5(15)	-45(15)
C(2)	140(20)	120(20)	160(20)	-1(16)	-17(17)	7(16)
O(1)	180(30)	350(30)	150(20)	0	0	120(20)
O(2)	230(30)	240(30)	210(30)	10(20)	0	0

Table S7-5. Hydrogen coordinates (x 10^3) and isotropic displacement parameters ($Å^2$x 10^3) for **A.4(H_2O)**.

	x	y	z	U(eq)
H(1)	344(8)	215(5)	697(4)	34
H(2)	0	689(7)	537(5)	34
H(3)	0	581(4)	598(7)	34

Table S7-6. Hydrogen bonds for **A.4(H_2O)** [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(1)-H(1)...O(2)#10	0.94(5)	1.89(5)	2.789(6)	159(6)
O(2)-H(2)...N(1)#11	0.95(5)	2.17(5)	3.117(8)	173(8)
O(2)-H(3)...N(2)	0.95(5)	2.53(5)	3.315(6)	141(3)

Symmetry transformations used to generate equivalent atoms:

#1 -x,y,-z+3/2 #2 x,y,-z+3/2 #3 -x,y,z #4 -x,-y,-z+1

#5 -x+1/2,y-1/2,z #6 x-1/2,-y+1/2,-z+1 #7 x-1/2,y-1/2,z

#8 -x+1/2,-y+1/2,-z+1 #9 x+1/2,y+1/2,z #10 x+1/2,y-1/2,z

#11 -x,-y+1,-z+1

Table S8-1. Crystal data and structure refinement for **A.4(H_2O)**.

Identification code	er225w	
Empirical formula	C6 H8 Co Er N6 O4	
Formula weight	454.37	
Temperature	225(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	C m c m	
Unit cell dimensions	a = 7.2828(12) Å	α= 90°.
	b = 12.623(2) Å	β= 90°.
	c = 13.471(2) Å	γ = 90°.
Volume	1238.4(3) $Å^3$	
Z	4	
Density (calculated)	2.437 Mg/m^3	
Absorption coefficient	8.085 mm^{-1}	
F(000)	852	
Crystal size	0.25 x 0.22 x 0.11 mm^3	
Theta range for data collection	3.02 to 27.93°.	
Index ranges	-9<=h<=9, -16<=k<=16, -17<=l<=17	
Reflections collected	4255	
Independent reflections	834 [R(int) = 0.0366]	
Completeness to theta = 27.93°	99.3 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.411 and 0.218	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	834 / 3 / 58	
Goodness-of-fit on F^2	1.149	
Final R indices [I>2sigma(I)]	R1 = 0.0287, wR2 = 0.0742	
R indices (all data)	R1 = 0.0321, wR2 = 0.0765	
Largest diff. peak and hole	2.178 and -0.862 $e.Å^{-3}$	

Table S8-2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^4) for **A.4(H_2O)**. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Er(1)	0	3249.4(3)	7500	106.6(16)
Co(1)	0	0	5000	110(3)
N(1)	0	2172(5)	5991(5)	212(13)
C(1)	0	1343(5)	5611(5)	170(13)
N(2)	2007(6)	4235(3)	6403(3)	215(9)
C(2)	3151(7)	4530(4)	5883(4)	158(9)
O(1)	2590(8)	2192(5)	7500	298(13)
O(2)	0	6561(5)	6000(5)	301(13)

Table S8-3. Bond lengths [Å] and angles [°] for **A.4(H_2O)**.

Er(1)-O(1)	2.311(6)
Er(1)-O(1)#1	2.311(6)
Er(1)-N(2)#2	2.423(4)
Er(1)-N(2)#3	2.423(4)
Er(1)-N(2)#1	2.423(4)
Er(1)-N(2)	2.423(4)
Er(1)-N(1)	2.446(6)
Er(1)-N(1)#2	2.446(6)
Co(1)-C(1)#4	1.885(7)
Co(1)-C(1)	1.885(7)
Co(1)-C(2)#5	1.892(5)
Co(1)-C(2)#6	1.892(5)
Co(1)-C(2)#7	1.892(5)
Co(1)-C(2)#8	1.892(5)
N(1)-C(1)	1.164(10)
N(2)-C(2)	1.150(7)
C(2)-Co(1)#9	1.892(5)
O(1)-H(1)	0.98(5)
O(2)-H(2)	0.99(5)
O(2)-H(3)	0.99(5)
O(1)-Er(1)-O(1)#1	109.4(3)
O(1)-Er(1)-N(2)#2	78.71(17)
O(1)#1-Er(1)-N(2)#2	142.12(11)
O(1)-Er(1)-N(2)#3	142.12(11)
O(1)#1-Er(1)-N(2)#3	78.71(17)
N(2)#2-Er(1)-N(2)#3	118.2(2)
O(1)-Er(1)-N(2)#1	142.12(11)
O(1)#1-Er(1)-N(2)#1	78.71(17)
N(2)#2-Er(1)-N(2)#1	74.2(2)
N(2)#3-Er(1)-N(2)#1	75.2(2)
O(1)-Er(1)-N(2)	78.71(17)
O(1)#1-Er(1)-N(2)	142.12(11)
N(2)#2-Er(1)-N(2)	75.2(2)
N(2)#3-Er(1)-N(2)	74.2(2)
N(2)#1-Er(1)-N(2)	118.2(2)
O(1)-Er(1)-N(1)	71.26(11)

O(1)#1-Er(1)-N(1)	71.26(12)
N(2)#2-Er(1)-N(1)	142.43(11)
N(2)#3-Er(1)-N(1)	77.22(16)
N(2)#1-Er(1)-N(1)	142.43(11)
N(2)-Er(1)-N(1)	77.22(16)
O(1)-Er(1)-N(1)#2	71.26(11)
O(1)#1-Er(1)-N(1)#2	71.26(12)
N(2)#2-Er(1)-N(1)#2	77.22(16)
N(2)#3-Er(1)-N(1)#2	142.43(11)
N(2)#1-Er(1)-N(1)#2	77.22(16)
N(2)-Er(1)-N(1)#2	142.43(11)
N(1)-Er(1)-N(1)#2	112.4(3)
C(1)#4-Co(1)-C(1)	179.999(1)
C(1)#4-Co(1)-C(2)#5	89.6(2)
C(1)-Co(1)-C(2)#5	90.4(2)
C(1)#4-Co(1)-C(2)#6	90.4(2)
C(1)-Co(1)-C(2)#6	89.6(2)
C(2)#5-Co(1)-C(2)#6	180.000(1)
C(1)#4-Co(1)-C(2)#7	89.6(2)
C(1)-Co(1)-C(2)#7	90.4(2)
C(2)#5-Co(1)-C(2)#7	90.7(3)
C(2)#6-Co(1)-C(2)#7	89.3(3)
C(1)#4-Co(1)-C(2)#8	90.4(2)
C(1)-Co(1)-C(2)#8	89.6(2)
C(2)#5-Co(1)-C(2)#8	89.3(3)
C(2)#6-Co(1)-C(2)#8	90.7(3)
C(2)#7-Co(1)-C(2)#8	180.0
C(1)-N(1)-Er(1)	149.8(6)
N(1)-C(1)-Co(1)	179.9(6)
C(2)-N(2)-Er(1)	167.0(4)
N(2)-C(2)-Co(1)#9	178.5(4)
Er(1)-O(1)-H(1)	127(4)
H(2)-O(2)-H(3)	123(9)

Symmetry transformations used to generate equivalent atoms:

#1 -x,y,-z+3/2 #2 x,y,-z+3/2 #3 -x,y,z #4 -x,-y,-z+1

#5 -x+1/2,y-1/2,z #6 x-1/2,-y+1/2,-z+1 #7 x-1/2,y-1/2,z

#8 -x+1/2,-y+1/2,-z+1 #9 x+1/2,y+1/2,z

Table S8-4. Anisotropic displacement parameters ($Å^2 x\ 10^4$) for **A.4(H_2O)**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U_{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U_{12}\ ]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Er(1)	90(2)	112(2)	118(2)	0	0	0
Co(1)	103(6)	99(6)	130(6)	-3(4)	0	0
N(1)	220(30)	200(30)	210(30)	-80(30)	0	0
C(1)	170(30)	150(30)	180(30)	40(30)	0	0
N(2)	190(20)	270(20)	180(20)	32(17)	-1(17)	-51(17)
C(2)	170(20)	140(20)	170(20)	6(17)	-30(18)	-16(17)
O(1)	240(30)	410(30)	240(30)	0	0	160(30)
O(2)	320(30)	310(30)	270(30)	-10(20)	0	0

Table S8-5. Hydrogen coordinates (x 10^3) and isotropic displacement parameters ($Å^2$x 10^3) for **A.4(H_2O)**.

	x	y	z	U(eq)
H(1)	352(9)	214(6)	698(5)	45
H(2)	0	693(8)	535(6)	45
H(3)	0	578(4)	606(8)	45

Table S8-6. Hydrogen bonds for **A.4(H_2O)** [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(1)-H(1)...O(2)#10	0.98(5)	1.85(6)	2.793(6)	161(7)
O(2)-H(2)...N(1)#11	0.99(5)	2.14(5)	3.123(9)	176(9)
O(2)-H(3)...N(2)	0.99(5)	2.48(5)	3.324(7)	143.1(19)

Symmetry transformations used to generate equivalent atoms:

#1 -x,y,-z+3/2 #2 x,y,-z+3/2 #3 -x,y,z #4 -x,-y,-z+1

#5 -x+1/2,y-1/2,z #6 x-1/2,-y+1/2,-z+1 #7 x-1/2,y-1/2,z

#8 -x+1/2,-y+1/2,-z+1 #9 x+1/2,y+1/2,z #10 x+1/2,y-1/2,z

#11 -x,-y+1,-z+1

Table S9-1. Crystal data and structure refinement for **A.4(H_2O)**.

Identification code	er300w	
Empirical formula	C6 H8 Co Er N6 O4	
Formula weight	454.37	
Temperature	300(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	C m c m	
Unit cell dimensions	a = 7.2765(10) Å	α= 90°.
	b = 12.6476(18) Å	β= 90°.
	c = 13.4804(18) Å	γ = 90°.
Volume	1240.6(3) $Å^3$	
Z	4	
Density (calculated)	2.433 Mg/m^3	
Absorption coefficient	8.071 mm^{-1}	
F(000)	852	
Crystal size	0.25 x 0.22 x 0.11 mm^3	
Theta range for data collection	3.02 to 27.96°.	
Index ranges	-9<=h<=9, -16<=k<=16, -17<=l<=17	
Reflections collected	4264	
Independent reflections	836 [R(int) = 0.0374]	
Completeness to theta = 27.96°	99.3 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.412 and 0.215	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	836 / 3 / 58	
Goodness-of-fit on F^2	1.148	
Final R indices [I>2sigma(I)]	R1 = 0.0275, wR2 = 0.0714	
R indices (all data)	R1 = 0.0311, wR2 = 0.0735	
Largest diff. peak and hole	2.425 and -0.791 $e.Å^{-3}$	

Table S9-2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^4) for **A.4(H_2O)**. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Er(1)	0	3248.1(3)	7500	123.2(15)
Co(1)	0	0	5000	124(3)
N(1)	0	2160(5)	5997(5)	237(12)
C(1)	0	1342(5)	5619(5)	185(13)
N(2)	2012(6)	4232(3)	6400(3)	253(9)
C(2)	3157(7)	4528(3)	5880(3)	181(9)
O(1)	2606(8)	2195(5)	7500	342(13)
O(2)	0	6558(5)	5991(5)	375(14)

Table S9-3. Bond lengths [Å] and angles [°] for **A.4(H_2O)**.

Er(1)-O(1)	2.317(5)
Er(1)-O(1)#1	2.317(5)
Er(1)-N(2)	2.427(4)
Er(1)-N(2)#2	2.427(4)
Er(1)-N(2)#3	2.427(4)
Er(1)-N(2)#1	2.427(4)
Er(1)-N(1)#2	2.450(6)
Er(1)-N(1)	2.450(6)
Co(1)-C(2)#4	1.887(5)
Co(1)-C(2)#5	1.887(5)
Co(1)-C(2)#6	1.887(5)
Co(1)-C(2)#7	1.887(5)
Co(1)-C(1)#8	1.891(7)
Co(1)-C(1)	1.891(7)
N(1)-C(1)	1.153(9)
N(2)-C(2)	1.151(6)
C(2)-Co(1)#9	1.887(5)
O(1)-H(1)	0.95(5)
O(2)-H(2)	0.96(5)
O(2)-H(3)	0.96(5)
O(1)-Er(1)-O(1)#1	109.8(3)
O(1)-Er(1)-N(2)	78.54(17)
O(1)#1-Er(1)-N(2)	142.04(11)
O(1)-Er(1)-N(2)#2	78.54(17)
O(1)#1-Er(1)-N(2)#2	142.04(11)
N(2)-Er(1)-N(2)#2	75.3(2)
O(1)-Er(1)-N(2)#3	142.04(11)
O(1)#1-Er(1)-N(2)#3	78.54(17)
N(2)-Er(1)-N(2)#3	74.2(2)
N(2)#2-Er(1)-N(2)#3	118.3(2)
O(1)-Er(1)-N(2)#1	142.04(11)
O(1)#1-Er(1)-N(2)#1	78.54(17)
N(2)-Er(1)-N(2)#1	118.3(2)
N(2)#2-Er(1)-N(2)#1	74.2(2)
N(2)#3-Er(1)-N(2)#1	75.3(2)
O(1)-Er(1)-N(1)#2	71.15(11)

O(1)#1-Er(1)-N(1)#2	71.15(11)
N(2)-Er(1)-N(1)#2	142.51(11)
N(2)#2-Er(1)-N(1)#2	77.47(16)
N(2)#3-Er(1)-N(1)#2	142.51(11)
N(2)#1-Er(1)-N(1)#2	77.47(16)
O(1)-Er(1)-N(1)	71.15(11)
O(1)#1-Er(1)-N(1)	71.15(11)
N(2)-Er(1)-N(1)	77.47(16)
N(2)#2-Er(1)-N(1)	142.51(11)
N(2)#3-Er(1)-N(1)	77.47(16)
N(2)#1-Er(1)-N(1)	142.51(11)
N(1)#2-Er(1)-N(1)	111.6(3)
C(2)#4-Co(1)-C(2)#5	180.0(2)
C(2)#4-Co(1)-C(2)#6	89.4(3)
C(2)#5-Co(1)-C(2)#6	90.6(3)
C(2)#4-Co(1)-C(2)#7	90.6(3)
C(2)#5-Co(1)-C(2)#7	89.4(3)
C(2)#6-Co(1)-C(2)#7	180.0
C(2)#4-Co(1)-C(1)#8	89.6(2)
C(2)#5-Co(1)-C(1)#8	90.4(2)
C(2)#6-Co(1)-C(1)#8	90.4(2)
C(2)#7-Co(1)-C(1)#8	89.6(2)
C(2)#4-Co(1)-C(1)	90.4(2)
C(2)#5-Co(1)-C(1)	89.6(2)
C(2)#6-Co(1)-C(1)	89.6(2)
C(2)#7-Co(1)-C(1)	90.4(2)
C(1)#8-Co(1)-C(1)	180.0
C(1)-N(1)-Er(1)	150.4(6)
N(1)-C(1)-Co(1)	179.9(6)
C(2)-N(2)-Er(1)	167.2(4)
N(2)-C(2)-Co(1)#9	178.5(4)
Er(1)-O(1)-H(1)	125(5)
H(2)-O(2)-H(3)	128(10)

Symmetry transformations used to generate equivalent atoms:

#1 -x,y,-z+3/2 #2 x,y,-z+3/2 #3 -x,y,z #4 -x+1/2,y-1/2,z

#5 x-1/2,-y+1/2,-z+1 #6 -x+1/2,-y+1/2,-z+1 #7 x-1/2,y-1/2,z

#8 -x,-y,-z+1 #9 x+1/2,y+1/2,z

Table S9-4. Anisotropic displacement parameters ($Å^2 x\ 10^4$) for **A.4(H_2O)**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U_{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U_{12}\ ]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Er(1)	103(2)	132(2)	134(2)	0	0	0
Co(1)	111(5)	113(5)	148(6)	0(4)	0	0
N(1)	290(30)	190(30)	240(30)	-70(20)	0	0
C(1)	180(30)	200(30)	180(30)	10(30)	0	0
N(2)	190(20)	330(20)	240(20)	43(17)	32(17)	-58(17)
C(2)	200(20)	160(20)	180(20)	17(16)	-18(18)	8(17)
O(1)	290(30)	480(30)	260(30)	0	0	210(30)
O(2)	400(40)	380(30)	340(30)	0(30)	0	0

Table S9-5. Hydrogen coordinates (x 10^3) and isotropic displacement parameters ($Å^2$x 10^3) for **A.4(H_2O)**.

	x	y	z	U(eq)
H(1)	338(10)	207(6)	694(5)	51
H(2)	0	693(8)	537(6)	56
H(3)	0	581(5)	610(9)	56

Table S9-6. Hydrogen bonds for **A.4(H_2O)** [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(1)-H(1)...O(2)#10	0.95(5)	1.86(5)	2.797(6)	168(7)
O(2)-H(2)...N(1)#11	0.96(5)	2.18(5)	3.132(9)	177(10)
O(2)-H(3)...N(2)	0.96(5)	2.51(5)	3.331(7)	144.2(10)

Symmetry transformations used to generate equivalent atoms:

#1 -x,y,-z+3/2 #2 x,y,-z+3/2 #3 -x,y,z #4 -x+1/2,y-1/2,z

#5 x-1/2,-y+1/2,-z+1 #6 -x+1/2,-y+1/2,-z+1 #7 x-1/2,y-1/2,z

#8 -x,-y,-z+1 #9 x+1/2,y+1/2,z #10 x+1/2,y-1/2,z

#11 -x,-y+1,-z+1

Table S10-1. Crystal data and structure refinement for **A.4(H_2O)**.

Identification code	er375w	
Empirical formula	C6 H8 Co Er N6 O4	
Formula weight	454.37	
Temperature	375(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	C m c m	
Unit cell dimensions	a = 7.275(3) Å	α= 90°.
	b = 12.687(5) Å	β= 90°.
	c = 13.487(5) Å	γ = 90°.
Volume	1244.8(8) $Å^3$	
Z	4	
Density (calculated)	2.425 Mg/m^3	
Absorption coefficient	8.044 mm^{-1}	
F(000)	852	
Crystal size	0.25 x 0.22 x 0.11 mm^3	
Theta range for data collection	3.02 to 28.01°.	
Index ranges	-9<=h<=9, -16<=k<=16, -17<=l<=17	
Reflections collected	4247	
Independent reflections	839 [R(int) = 0.0590]	
Completeness to theta = 28.01°	99.1 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.413 and 0.199	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	839 / 0 / 51	
Goodness-of-fit on F^2	1.238	
Final R indices [I>2sigma(I)]	R1 = 0.0426, wR2 = 0.1079	
R indices (all data)	R1 = 0.0495, wR2 = 0.1139	
Largest diff. peak and hole	1.535 and -1.418 $e.Å^{-3}$	

Table S10-2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^4) for **A.4(H_2O)**. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Er(1)	0	3246.0(4)	7500	161(2)
Co(1)	0	0	5000	165(4)
N(1)	0	2141(7)	6012(7)	300(20)
C(1)	0	1326(7)	5622(8)	208(19)
N(2)	2014(10)	4220(5)	6396(5)	314(15)
C(2)	3158(10)	4518(5)	5879(5)	217(14)
O(1)	2612(13)	2198(8)	7500	460(20)
O(2)	0	6546(7)	5974(8)	490(20)

Table S10-3. Bond lengths [Å] and angles [°] for **A.4(H_2O)**.

Er(1)-O(1)#1	2.319(9)
Er(1)-O(1)	2.319(9)
Er(1)-N(2)	2.427(7)
Er(1)-N(2)#2	2.427(7)
Er(1)-N(2)#3	2.427(7)
Er(1)-N(2)#1	2.427(7)
Er(1)-N(1)#2	2.448(9)
Er(1)-N(1)	2.448(9)
Co(1)-C(1)	1.880(9)
Co(1)-C(1)#4	1.880(9)
Co(1)-C(2)#5	1.891(7)
Co(1)-C(2)#6	1.891(7)
Co(1)-C(2)#7	1.891(7)
Co(1)-C(2)#8	1.891(7)
N(1)-C(1)	1.160(14)
N(2)-C(2)	1.150(10)
C(2)-Co(1)#9	1.891(7)
O(1)-H(1)	0.9776
O(2)-H(2)	0.9811
O(2)-H(3)	0.9828

O(1)#1-Er(1)-O(1)	110.0(6)
O(1)#1-Er(1)-N(2)	141.86(17)
O(1)-Er(1)-N(2)	78.3(3)
O(1)#1-Er(1)-N(2)#2	141.86(17)
O(1)-Er(1)-N(2)#2	78.3(3)
N(2)-Er(1)-N(2)#2	75.7(3)
O(1)#1-Er(1)-N(2)#3	78.3(3)
O(1)-Er(1)-N(2)#3	141.86(17)
N(2)-Er(1)-N(2)#3	74.3(3)
N(2)#2-Er(1)-N(2)#3	118.8(3)
O(1)#1-Er(1)-N(2)#1	78.3(3)
O(1)-Er(1)-N(2)#1	141.86(17)
N(2)-Er(1)-N(2)#1	118.8(3)
N(2)#2-Er(1)-N(2)#1	74.3(3)
N(2)#3-Er(1)-N(2)#1	75.7(3)
O(1)#1-Er(1)-N(1)#2	70.83(19)

O(1)-Er(1)-N(1)#2	70.83(19)
N(2)-Er(1)-N(1)#2	142.61(17)
N(2)#2-Er(1)-N(1)#2	77.8(3)
N(2)#3-Er(1)-N(1)#2	142.61(17)
N(2)#1-Er(1)-N(1)#2	77.8(3)
O(1)#1-Er(1)-N(1)	70.83(19)
O(1)-Er(1)-N(1)	70.83(18)
N(2)-Er(1)-N(1)	77.8(3)
N(2)#2-Er(1)-N(1)	142.61(17)
N(2)#3-Er(1)-N(1)	77.8(3)
N(2)#1-Er(1)-N(1)	142.61(18)
N(1)#2-Er(1)-N(1)	110.1(5)
C(1)-Co(1)-C(1)#4	179.998(1)
C(1)-Co(1)-C(2)#5	90.5(3)
C(1)#4-Co(1)-C(2)#5	89.5(3)
C(1)-Co(1)-C(2)#6	89.5(3)
C(1)#4-Co(1)-C(2)#6	90.5(3)
C(2)#5-Co(1)-C(2)#6	180.000(1)
C(1)-Co(1)-C(2)#7	90.5(3)
C(1)#4-Co(1)-C(2)#7	89.5(3)
C(2)#5-Co(1)-C(2)#7	90.3(4)
C(2)#6-Co(1)-C(2)#7	89.7(4)
C(1)-Co(1)-C(2)#8	89.5(3)
C(1)#4-Co(1)-C(2)#8	90.5(3)
C(2)#5-Co(1)-C(2)#8	89.7(4)
C(2)#6-Co(1)-C(2)#8	90.3(4)
C(2)#7-Co(1)-C(2)#8	180.000(1)
C(1)-N(1)-Er(1)	151.9(9)
N(1)-C(1)-Co(1)	179.5(10)
C(2)-N(2)-Er(1)	167.6(6)
N(2)-C(2)-Co(1)#9	178.5(7)
Er(1)-O(1)-H(1)	121.6
H(2)-O(2)-H(3)	111.2

Symmetry transformations used to generate equivalent atoms:

#1 -x,y,-z+3/2 #2 x,y,-z+3/2 #3 -x,y,z #4 -x,-y,-z+1

#5 -x+1/2,y-1/2,z #6 x-1/2,-y+1/2,-z+1 #7 x-1/2,y-1/2,z

#8 -x+1/2,-y+1/2,-z+1 #9 x+1/2,y+1/2,z

Table S10-4. Anisotropic displacement parameters ($Å^2 x\ 10^4$) for **A.4(H_2O)**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U_{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U_{12}\ ]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Er(1)	154(3)	160(3)	170(3)	0	0	0
Co(1)	169(9)	144(8)	183(9)	8(6)	0	0
N(1)	370(50)	230(40)	310(50)	-100(40)	0	0
C(1)	270(50)	140(40)	220(50)	-30(40)	0	0
N(2)	340(40)	330(30)	280(30)	60(30)	20(30)	-30(30)
C(2)	210(30)	200(30)	240(40)	30(30)	0(30)	-50(30)
O(1)	410(50)	590(60)	380(50)	0	0	250(50)
O(2)	470(60)	560(60)	440(60)	-20(50)	0	0

Table S10-5. Hydrogen coordinates (x 10^3) and isotropic displacement parameters ($Å^2$x 10^3) for **A.4(H_2O)**.

	x	y	z	U(eq)
H(1)	349	221	695	69
H(2)	0	686	531	74
H(3)	0	577	594	74

Table S10-6. Hydrogen bonds for **A.4(H_2O)** [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(1)-H(1)...O(2)#10	0.98	1.91	2.817(10)	152.8
O(2)-H(2)...N(1)#11	0.98	2.19	3.154(14)	168.9
O(2)-H(3)...N(2)	0.98	2.53	3.344(10)	139.8

Symmetry transformations used to generate equivalent atoms:

#1 -x,y,-z+3/2 #2 x,y,-z+3/2 #3 -x,y,z #4 -x,-y,-z+1

#5 -x+1/2,y-1/2,z #6 x-1/2,-y+1/2,-z+1 #7 x-1/2,y-1/2,z

#8 -x+1/2,-y+1/2,-z+1 #9 x+1/2,y+1/2,z #10 x+1/2,y-1/2,z

#11 -x,-y+1,-z+1