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Poly[[tetraaqua(μ_4-imidazole-4,5-dicarboxylato)(μ_3-imidazole-4,5-dicarboxylato)-μ_3-sulfato-μ_2-sulfato-cobalt(II)dierbium(III)] monohydrate]

Feng Sun

School of Chemistry and Environment, South China Normal University, Guangzhou 510631, People's Republic of China
Correspondence e-mail: fengsun1974@yahoo.com.cn

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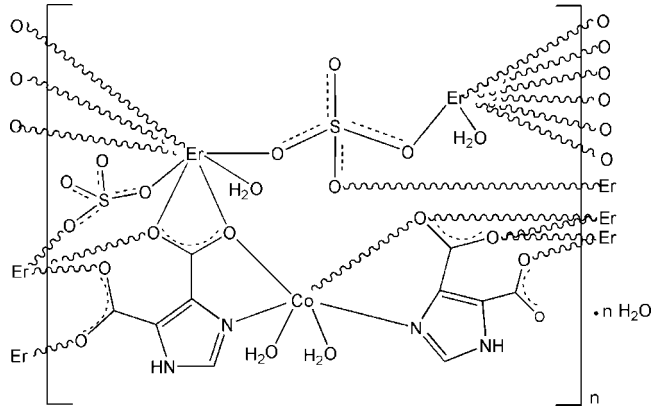
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.007 Å; R factor = 0.023; wR factor = 0.055; data-to-parameter ratio = 10.4.

The asymmetric unit of the title compound, $\{[CoEr_2(C_5H_2N_2O_4)_2(SO_4)_2(H_2O)_4]\cdot H_2O\}_n$, contains a Co^{II} ion, two Er^{III} ions, two imidazole-4,5-dicarboxylate (imdc) ligands, two SO_4^{2-} anions, four coordinated water molecules and one uncoordinated water molecule. The Co^{II} ion is six-coordinated by two O atoms from two coordinated water molecules and two O atoms and two N atoms from two imdc ligands in a slightly distorted octahedral geometry. Both Er^{III} ions are eight-coordinated in a bicapped trigonal–prismatic coordination geometry. One Er^{III} ion is coordinated by four O atoms from two imidazole-4,5-dicarboxylate ligands, three O atoms from three SO_4^{2-} anions and one water O atom; the other Er^{III} ion is bonded to five O atoms from three imdc ligands, two O atoms from two SO_4^{2-} anions as well as one coordinated water molecule. The coordinated metal units are connected by bridging imdc ligands and sulfate ions, generating a two-dimensional heterometallic layer. The two-dimensional layers are stacked along the b axis *via* N—H···O, O—H···O and C—H···O hydrogen-bonding interactions between water molecules, SO_4^{2-} anions, and imdc ligands, generating a three-dimensional framework.

Related literature

For applications of lanthanide–transition metal complexes similar to the title compound, see: Cheng *et al.* (2006); Kuang *et al.* (2007). For related structures, see: Sun *et al.* (2006); Zhu *et al.* (2010).



Experimental

Crystal data

$[CoEr_2(C_5H_2N_2O_4)_2(SO_4)_2(H_2O)_4]\cdot H_2O$
M_r = 983.84
Triclinic, $P\overline{1}$
a = 9.0512 (5) Å
b = 10.6827 (6) Å
c = 12.8945 (8) Å
α = 92.955 (1)°
β = 97.054 (1)°
γ = 108.612 (1)°
V = 1167.17 (12) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 8.12 mm^{-1}
T = 296 K
0.20 × 0.18 × 0.15 mm

Data collection

Bruker APEXII area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.215, T_{max} = 0.296
6026 measured reflections
4123 independent reflections
3820 reflections with $I > 2\sigma(I)$
R_{int} = 0.017

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.023
$wR(F^2)$ = 0.055
S = 1.03
4123 reflections
397 parameters
12 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.87 e Å^{-3}
$\Delta\rho_{min}$ = −1.35 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O8^{i}	0.86 (5)	1.95 (5)	2.806 (6)	176 (7)
O1W—H1W···O8^{ii}	0.82 (5)	2.08 (5)	2.885 (6)	166 (5)
N4—H2···O3^{iii}	0.86 (4)	1.93 (3)	2.785 (5)	172 (7)
O1W—H2W···O3^{ii}	0.82 (5)	2.01 (4)	2.822 (5)	170 (4)
O1W—H2W···O4^{ii}	0.82 (5)	2.58 (5)	3.048 (5)	118 (5)
O2W—H3W···O16^{iv}	0.81 (4)	1.92 (5)	2.730 (5)	176 (8)
O2W—H4W···O3^{ii}	0.80 (4)	2.49 (5)	2.897 (5)	113 (4)
O3W—H5W···O5W	0.82 (7)	1.89 (7)	2.692 (7)	169 (7)
O3W—H6W···O6^{v}	0.81 (3)	2.57 (4)	3.336 (6)	158 (8)
O4W—H7W···O5W	0.82 (4)	1.98 (4)	2.752 (6)	158 (6)
O4W—H8W···O2W	0.81 (5)	2.57 (7)	3.167 (6)	132 (6)
O5W—H9W···O8^{vi}	0.85 (5)	1.90 (5)	2.737 (6)	169 (5)
O5W—H10W···O16^{iv}	0.86 (5)	1.97 (6)	2.787 (6)	159 (7)
C3—H3···O6^{iii}	0.93	2.46	3.224 (7)	140

Symmetry codes: (i) $-x+1, -y, -z+1$; (ii) $-x, -y, -z$; (iii) $x+1, y+1, z$; (iv) $-x+1, -y+1, -z$; (v) $-x, -y, -z+1$; (vi) $x, y+1, z$.

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine

structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: PV2354).

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supporting information

Acta Cryst. (2010). E**66**, m1615–m1616 [https://doi.org/10.1107/S1600536810047203]

Poly[[tetraaqua(μ_4-imidazole-4,5-dicarboxylato)(μ_3-imidazole-4,5-dicarboxylato)-μ_3-sulfato-μ_2-sulfato-cobalt(II)dierbium(III)] monohydrate]

Feng Sun

S1. Comment

In the past few years, there has been a tremendous increase of interset in lanthanide-transition metal heterometallic complexs with bridging multifunctionnal organic ligands because of their impressive topological structures as well aso due to their versatile applications in ion exchange, magnetism, bimetallic catalysis and luminescent probes (Cheng *et al.*, 2006; Kuang *et al.*, 2007; Sun *et al.*, 2006; Zhu *et al.*, 2010). As an extension of this research, the structure of the title compound, a new heterometallic coordination polymer, (I), has been determined which is presented in this artcle.

The asymmetric unite of the title compound (Fig. 1), contains a Co^{II} ion, two Er^{III} ions, two imidazole-4,5-dicarboxylate (imdc) ligands, two SO_4^{2-} anions, four coordinated water molecules and one lattice water molecule. The Co^{II} ion is six-coordinated with two O atoms from two coordinated water molecules, two O atoms and two N atoms from two imdc ligands, to give a slightly distorted octahedral geometry. Both Er^{III} ions are eight-coordinated in a bicapped trigonal prismatic coordination geometry. One Er^{III} ion is coordinated by four O atoms from two idmc ligands, three O atoms from three SO_4^{2-} anions and one water molecule; the other Er^{III} ion is bonded to five O atoms from three imidazole-4, 5-dicarboxylate ligands, two O atoms from two SO_4^{2-} anions as well as one coordinated water molecule. These metal coordination units are connected by bridging imdc ligands and sulfate anions, generating a two-dimensional heterometallic layer. The two-dimensional layers are stacked along *b* axis *via* hydrogen-bonding interactions between water molecules, SO_4^{2-} anions, and imdc ligands to generate the three-dimensional framework (Tab. 1 and Fig. 2).

S2. Experimental

A mixture of $CoSO_4.7H_2O$ (0.141 g, 0.5 mmol), Er_2O_3 (0.098 g, 0.25 mmol), imidazole-4,5-dicarboxylic acid (0.156 g, 1 mmol), and H_2O (7 ml) was sealed in a 20 ml Teflon-lined reaction vessel at 443 K for 5 days then slowly cooled to room temperature. The product was collected by filtration, washed with water and air-dried. Red block crystals suitable for X-ray analysis were obtained.

S3. Refinement

H atoms bonded to C atoms were positioned geometrically and refined as riding, with C—H = 0.93 Å and U_{iso}(H) = 1.2 U_{eq}(C). H atoms bonded to N atoms and H atoms of water molecules were found from difference Fourier maps and refined isotropically with restraints: N—H = 0.87 Å, O—H = 0.82 or 0.86 Å and U_{iso}(H) = 1.5 U_{eq}(N, O). In the final difference map, the largest residual electron density and the deepest hole are located at 0.96 and 0.85 Å, respectively from Er2.

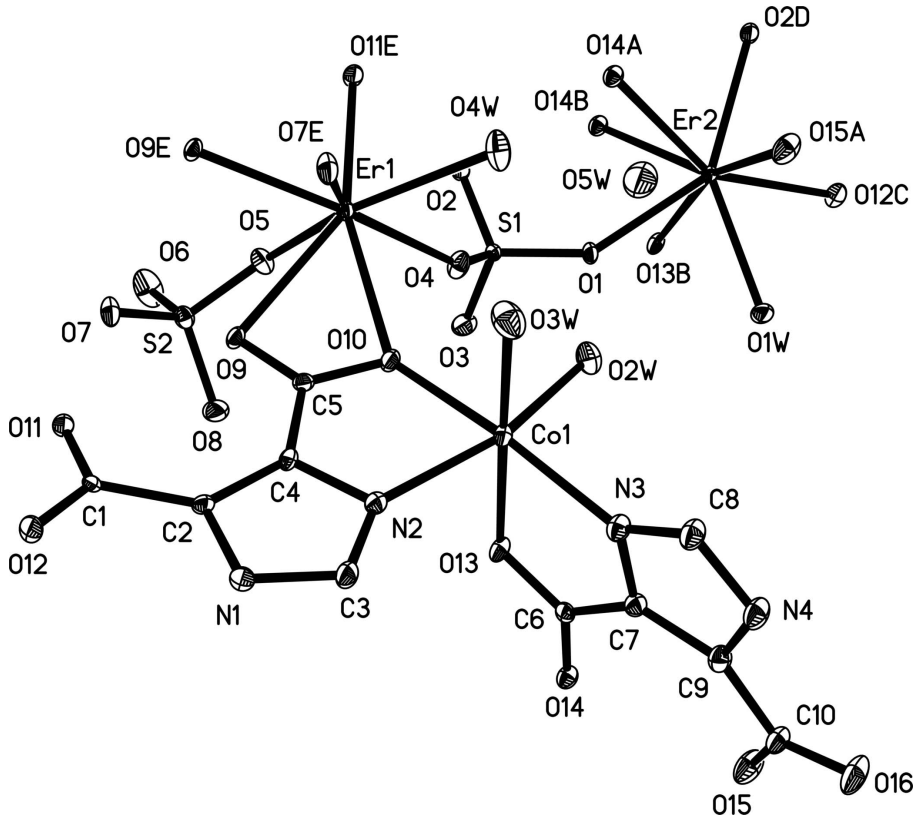

Figure 1

The molecular structure showing the atomic-numbering scheme and displacement ellipsoids drawn at the 30% probability level. Symmetry codes: (A) -1 + *x*, *y*, *z*; (B) -*x*, -*y*, -*z*; (C) -1 + *x*, *y*, -1 + *z*; (D) -1 - *x*, -*y*, -*z*; (E) -*x*, -*y*, 1 - *z*.

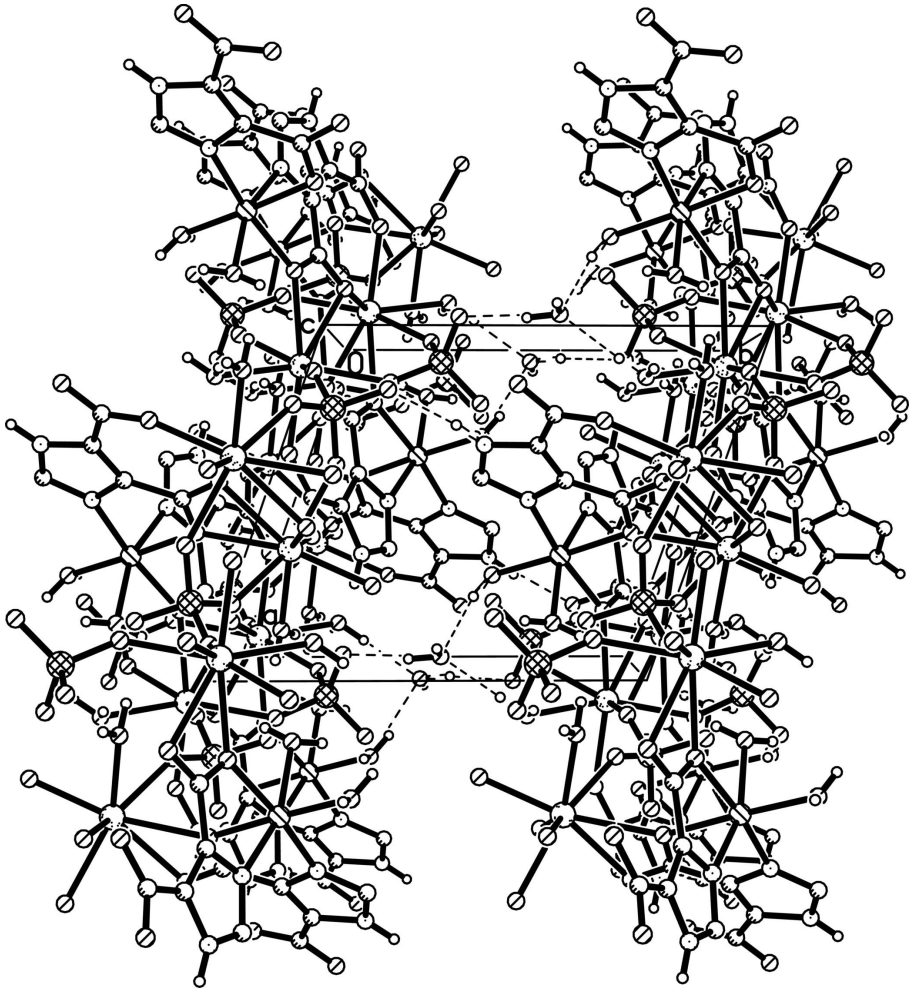

Figure 2

A view of the three-dimensional structure of the title compound, the hydrogen bonding interactions showed as broken lines.

Poly[[tetraaqua(μ_4-imidazole-4,5-dicarboxylato)(μ_3-imidazole- 4,5-dicarboxylato)-μ_3-sulfato-μ_2-sulfato-cobalt(II)dierbium(III)] monohydrate]

Crystal data

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Hall symbol: -P 1
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$b = 10.6827$ (6) Å
$c = 12.8945$ (8) Å
$\alpha = 92.955$ (1)°
$\beta = 97.054$ (1)°
$\gamma = 108.612$ (1)°
$V = 1167.17$ (12) Å^3
$Z = 2$
$F(000) = 930$
$D_x = 2.799$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 4400 reflections
$\theta = 2.4$–28.0°
$\mu = 8.12$ mm^{-1}
$T = 296$ K
Block, red
0.20 × 0.18 × 0.15 mm

Data collection

Bruker APEXII area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scan
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.215, T_{max} = 0.296
6026 measured reflections
4123 independent reflections
3820 reflections with $I > 2\sigma(I)$
R_{int} = 0.017
θ_{max} = 25.2°, θ_{min} = 1.6°
h = −10→5
k = −12→12
l = −15→15

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.023
$wR(F^2)$ = 0.055
S = 1.03
4123 reflections
397 parameters
12 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0283P)^2 + 1.940P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.87 e Å^{-3}
$\Delta\rho_{min}$ = −1.35 e Å^{-3}

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2, conventional R-factors R are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating R-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	y	z	U_{iso}*/U_{eq}
Er1	−0.09070 (2)	0.049642 (19)	0.366467 (14)	0.01288 (7)
Er2	−0.37193 (2)	0.088827 (18)	−0.105666 (14)	0.01193 (7)
Co1	0.34879 (7)	0.28628 (6)	0.27282 (4)	0.01585 (14)
S1	−0.22681 (13)	−0.07707 (11)	0.09734 (8)	0.0129 (2)
S2	−0.07687 (14)	−0.27513 (11)	0.40191 (9)	0.0170 (2)
C1	0.4802 (5)	0.0827 (4)	0.6454 (3)	0.0145 (9)
C2	0.5054 (5)	0.1537 (4)	0.5507 (3)	0.0152 (9)
C3	0.6350 (6)	0.2989 (5)	0.4510 (4)	0.0212 (10)
H3	0.7175	0.3621	0.4271	0.025*
C4	0.4062 (5)	0.1634 (4)	0.4630 (3)	0.0150 (9)
C5	0.2387 (5)	0.1004 (4)	0.4232 (3)	0.0144 (9)
C6	0.5165 (5)	0.1950 (4)	0.1209 (3)	0.0144 (9)
C7	0.5691 (6)	0.3402 (5)	0.1209 (4)	0.0177 (10)
C8	0.5776 (6)	0.5343 (5)	0.1817 (4)	0.0235 (11)
H8	0.5609	0.6028	0.2209	0.028*

C9	0.6679 (6)	0.4298 (4)	0.0658 (4)	0.0196 (10)
C10	0.7520 (6)	0.4192 (5)	−0.0250 (4)	0.0218 (11)
N1	0.6495 (5)	0.2411 (4)	0.5397 (3)	0.0190 (9)
N2	0.4904 (5)	0.2554 (4)	0.4025 (3)	0.0169 (8)
N3	0.5133 (5)	0.4078 (4)	0.1927 (3)	0.0189 (9)
N4	0.6703 (5)	0.5521 (4)	0.1067 (3)	0.0249 (9)
O1	−0.2200 (4)	0.0083 (3)	0.0104 (2)	0.0208 (7)
O2	−0.3866 (4)	−0.1266 (3)	0.1256 (3)	0.0224 (7)
O3	−0.1750 (4)	−0.1884 (3)	0.0667 (3)	0.0245 (8)
O4	−0.1162 (4)	0.0023 (3)	0.1883 (2)	0.0229 (8)
O5	−0.1393 (4)	−0.1746 (3)	0.3560 (2)	0.0218 (7)
O6	−0.1995 (5)	−0.4018 (4)	0.3964 (3)	0.0407 (10)
O7	−0.0089 (4)	−0.2307 (3)	0.5147 (2)	0.0235 (8)
O8	0.0526 (4)	−0.2828 (4)	0.3446 (3)	0.0278 (8)
O9	0.1450 (4)	0.0157 (3)	0.4693 (2)	0.0171 (7)
O10	0.1848 (4)	0.1367 (3)	0.3383 (2)	0.0182 (7)
O11	0.3504 (4)	−0.0057 (3)	0.6478 (2)	0.0183 (7)
O12	0.5935 (4)	0.1177 (3)	0.7192 (2)	0.0235 (8)
O13	0.4190 (4)	0.1442 (3)	0.1823 (2)	0.0178 (7)
O14	0.5640 (4)	0.1192 (3)	0.0648 (2)	0.0164 (7)
O15	0.7324 (5)	0.3048 (3)	−0.0682 (3)	0.0322 (9)
O16	0.8340 (5)	0.5232 (3)	−0.0549 (3)	0.0367 (10)
H2	0.726 (7)	0.631 (3)	0.097 (5)	0.055*
H1	0.739 (4)	0.250 (6)	0.576 (5)	0.055*
O1W	−0.1359 (4)	0.1275 (4)	−0.1711 (3)	0.0261 (8)
H1W	−0.120 (7)	0.159 (6)	−0.227 (3)	0.039*
H2W	−0.050 (4)	0.140 (6)	−0.135 (4)	0.039*
O2W	0.1566 (5)	0.2533 (4)	0.1512 (3)	0.0285 (8)
H3W	0.164 (8)	0.320 (4)	0.122 (4)	0.043*
H4W	0.121 (7)	0.182 (3)	0.118 (4)	0.043*
O3W	0.2893 (6)	0.4288 (4)	0.3606 (3)	0.0376 (10)
H5W	0.226 (7)	0.456 (7)	0.326 (5)	0.056*
H6W	0.290 (9)	0.416 (7)	0.422 (2)	0.056*
O4W	−0.1271 (5)	0.2319 (4)	0.2783 (3)	0.0366 (10)
H7W	−0.072 (7)	0.310 (3)	0.286 (5)	0.055*
H8W	−0.106 (8)	0.223 (7)	0.220 (3)	0.055*
O5W	0.0527 (6)	0.4842 (4)	0.2458 (3)	0.0433 (11)
H9W	0.044 (9)	0.557 (4)	0.269 (5)	0.065*
H10W	0.079 (9)	0.499 (7)	0.185 (3)	0.065*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Er1	0.01014 (12)	0.01703 (11)	0.01108 (11)	0.00352 (8)	0.00105 (8)	0.00507 (8)
Er2	0.01019 (12)	0.01510 (11)	0.01112 (11)	0.00425 (8)	0.00202 (8)	0.00503 (8)
Co1	0.0167 (3)	0.0187 (3)	0.0132 (3)	0.0060 (3)	0.0037 (2)	0.0058 (2)
S1	0.0105 (6)	0.0177 (5)	0.0113 (5)	0.0056 (4)	0.0012 (4)	0.0046 (4)
S2	0.0165 (6)	0.0160 (5)	0.0170 (5)	0.0042 (5)	−0.0009 (5)	0.0020 (4)

C1	0.014 (2)	0.024 (2)	0.010 (2)	0.013 (2)	0.0026 (18)	0.0040 (18)
C2	0.009 (2)	0.021 (2)	0.015 (2)	0.0033 (19)	0.0025 (18)	0.0037 (18)
C3	0.017 (3)	0.025 (3)	0.021 (2)	0.003 (2)	0.005 (2)	0.010 (2)
C4	0.017 (3)	0.021 (2)	0.009 (2)	0.007 (2)	0.0039 (18)	0.0029 (17)
C5	0.013 (2)	0.021 (2)	0.012 (2)	0.0077 (19)	0.0023 (18)	0.0007 (18)
C6	0.010 (2)	0.018 (2)	0.013 (2)	0.0030 (19)	−0.0023 (18)	0.0039 (18)
C7	0.015 (2)	0.019 (2)	0.018 (2)	0.0043 (19)	0.0024 (19)	0.0044 (18)
C8	0.031 (3)	0.018 (2)	0.023 (2)	0.007 (2)	0.011 (2)	0.0044 (19)
C9	0.020 (3)	0.016 (2)	0.021 (2)	0.003 (2)	0.004 (2)	0.0038 (19)
C10	0.022 (3)	0.019 (2)	0.023 (2)	0.003 (2)	0.009 (2)	0.006 (2)
N1	0.008 (2)	0.026 (2)	0.0180 (19)	0.0005 (17)	−0.0027 (16)	0.0045 (17)
N2	0.014 (2)	0.021 (2)	0.0164 (19)	0.0049 (16)	0.0034 (16)	0.0049 (16)
N3	0.023 (2)	0.016 (2)	0.0168 (19)	0.0049 (17)	0.0050 (17)	0.0012 (15)
N4	0.030 (3)	0.016 (2)	0.027 (2)	0.0035 (19)	0.0112 (19)	0.0055 (18)
O1	0.0156 (18)	0.0305 (19)	0.0197 (16)	0.0097 (15)	0.0039 (14)	0.0155 (14)
O2	0.0127 (18)	0.0340 (19)	0.0241 (17)	0.0097 (15)	0.0060 (14)	0.0164 (15)
O3	0.028 (2)	0.0163 (17)	0.0333 (19)	0.0085 (15)	0.0146 (16)	0.0047 (14)
O4	0.0192 (19)	0.0291 (19)	0.0143 (16)	0.0004 (15)	−0.0006 (14)	0.0032 (14)
O5	0.0226 (19)	0.0201 (17)	0.0219 (17)	0.0079 (15)	−0.0028 (14)	0.0022 (14)
O6	0.030 (2)	0.023 (2)	0.054 (3)	−0.0059 (17)	−0.0115 (19)	0.0110 (18)
O7	0.034 (2)	0.0225 (18)	0.0148 (16)	0.0116 (16)	0.0009 (15)	0.0048 (13)
O8	0.026 (2)	0.044 (2)	0.0189 (17)	0.0186 (17)	0.0052 (15)	0.0015 (15)
O9	0.0104 (16)	0.0256 (18)	0.0136 (15)	0.0025 (14)	0.0031 (13)	0.0080 (13)
O10	0.0124 (17)	0.0270 (18)	0.0146 (15)	0.0044 (14)	0.0032 (13)	0.0082 (13)
O11	0.0102 (17)	0.0265 (18)	0.0170 (16)	0.0035 (14)	0.0018 (13)	0.0079 (13)
O12	0.0103 (17)	0.038 (2)	0.0179 (16)	0.0024 (15)	−0.0020 (14)	0.0098 (15)
O13	0.0208 (18)	0.0150 (16)	0.0169 (15)	0.0024 (14)	0.0082 (14)	0.0045 (13)
O14	0.0190 (18)	0.0136 (15)	0.0161 (15)	0.0036 (13)	0.0051 (13)	0.0014 (12)
O15	0.041 (2)	0.0173 (18)	0.036 (2)	0.0022 (16)	0.0194 (18)	0.0018 (15)
O16	0.050 (3)	0.0216 (19)	0.040 (2)	0.0056 (18)	0.026 (2)	0.0105 (16)
O1W	0.0148 (19)	0.046 (2)	0.0222 (18)	0.0137 (17)	0.0050 (15)	0.0139 (17)
O2W	0.032 (2)	0.030 (2)	0.0228 (19)	0.0108 (19)	−0.0028 (16)	0.0054 (16)
O3W	0.052 (3)	0.035 (2)	0.031 (2)	0.024 (2)	0.001 (2)	0.0002 (18)
O4W	0.047 (3)	0.025 (2)	0.033 (2)	0.0063 (19)	−0.001 (2)	0.0113 (18)
O5W	0.063 (3)	0.035 (2)	0.043 (2)	0.025 (2)	0.025 (2)	0.009 (2)

Geometric parameters (Å, º)

Er1—O11^{i}	2.227 (3)	C3—H3	0.9300
Er1—O7^{i}	2.268 (3)	C4—N2	1.380 (6)
Er1—O5	2.286 (3)	C4—C5	1.462 (6)
Er1—O4	2.294 (3)	C5—O9	1.258 (5)
Er1—O9^{i}	2.324 (3)	C5—O10	1.272 (5)
Er1—O4W	2.396 (4)	C6—O14	1.267 (5)
Er1—O10	2.447 (3)	C6—O13	1.269 (5)
Er1—O9	2.508 (3)	C6—C7	1.470 (6)
Er1—C5	2.848 (4)	C6—Er2^{v}	2.879 (4)
Er2—O15^{ii}	2.198 (3)	C7—C9	1.378 (7)

Er2—O12^{iii}	2.291 (3)	C7—N3	1.383 (6)
Er2—O1	2.292 (3)	C8—N3	1.313 (6)
Er2—O1W	2.316 (4)	C8—N4	1.338 (6)
Er2—O2^{iv}	2.333 (3)	C8—H8	0.9300
Er2—O14^{ii}	2.373 (3)	C9—N4	1.376 (6)
Er2—O14^{v}	2.474 (3)	C9—C10	1.492 (7)
Er2—O13^{v}	2.514 (3)	C10—O16	1.234 (6)
Er2—C6^{v}	2.879 (4)	C10—O15	1.266 (6)
Er2—Er2^{iv}	3.9596 (4)	N1—H1	0.86 (5)
Co1—N3	2.062 (4)	N4—H2	0.86 (4)
Co1—N2	2.085 (4)	O2—Er2^{iv}	2.333 (3)
Co1—O3W	2.093 (4)	O7—Er1^{i}	2.268 (3)
Co1—O10	2.099 (3)	O9—Er1^{i}	2.324 (3)
Co1—O2W	2.120 (4)	O11—Er1^{i}	2.227 (3)
Co1—O13	2.165 (3)	O12—Er2^{vi}	2.291 (3)
S1—O3	1.464 (3)	O13—Er2^{v}	2.514 (3)
S1—O4	1.471 (3)	O14—Er2^{vii}	2.373 (3)
S1—O2	1.471 (3)	O14—Er2^{v}	2.474 (3)
S1—O1	1.477 (3)	O15—Er2^{vii}	2.198 (3)
S2—O6	1.443 (4)	O1W—H1W	0.82 (5)
S2—O5	1.481 (3)	O1W—H2W	0.82 (5)
S2—O8	1.482 (4)	O2W—H3W	0.81 (4)
S2—O7	1.497 (3)	O2W—H4W	0.80 (4)
C1—O11	1.255 (6)	O3W—H5W	0.82 (7)
C1—O12	1.256 (5)	O3W—H6W	0.81 (3)
C1—C2	1.474 (6)	O4W—H7W	0.82 (4)
C2—N1	1.369 (6)	O4W—H8W	0.81 (5)
C2—C4	1.385 (6)	O5W—H9W	0.85 (5)
C3—N2	1.304 (6)	O5W—H10W	0.86 (5)
C3—N1	1.339 (6)		

O11^{i}—Er1—O7^{i}	103.78 (12)	O2W—Co1—O13	87.26 (13)
O11^{i}—Er1—O5	87.24 (12)	O3—S1—O4	108.4 (2)
O7^{i}—Er1—O5	140.03 (11)	O3—S1—O2	110.1 (2)
O11^{i}—Er1—O4	89.33 (12)	O4—S1—O2	109.7 (2)
O7^{i}—Er1—O4	137.77 (12)	O3—S1—O1	109.2 (2)
O5—Er1—O4	79.46 (12)	O4—S1—O1	107.83 (19)
O11^{i}—Er1—O9^{i}	77.27 (11)	O2—S1—O1	111.55 (19)
O7^{i}—Er1—O9^{i}	71.65 (11)	O6—S2—O5	111.1 (2)
O5—Er1—O9^{i}	73.70 (11)	O6—S2—O8	112.1 (2)
O4—Er1—O9^{i}	150.39 (11)	O5—S2—O8	107.4 (2)
O11^{i}—Er1—O4W	77.71 (14)	O6—S2—O7	108.6 (2)
O7^{i}—Er1—O4W	73.79 (12)	O5—S2—O7	109.60 (18)
O5—Er1—O4W	145.94 (13)	O8—S2—O7	107.9 (2)
O4—Er1—O4W	70.10 (13)	O11—C1—O12	124.8 (4)
O9^{i}—Er1—O4W	130.42 (13)	O11—C1—C2	119.4 (4)
O11^{i}—Er1—O10	162.82 (11)	O12—C1—C2	115.8 (4)
O7^{i}—Er1—O10	77.34 (12)	N1—C2—C4	104.3 (4)

O5—Er1—O10	102.96 (12)	N1—C2—C1	121.7 (4)
O4—Er1—O10	79.20 (11)	C4—C2—C1	133.7 (4)
O9^{i}—Er1—O10	118.64 (10)	N2—C3—N1	111.4 (4)
O4W—Er1—O10	86.33 (13)	N2—C3—H3	124.3
O11^{i}—Er1—O9	145.10 (10)	N1—C3—H3	124.3
O7^{i}—Er1—O9	75.86 (11)	N2—C4—C2	109.5 (4)
O5—Er1—O9	73.80 (11)	N2—C4—C5	115.7 (4)
O4—Er1—O9	114.74 (11)	C2—C4—C5	134.8 (4)
O9^{i}—Er1—O9	69.47 (12)	O9—C5—O10	118.6 (4)
O4W—Er1—O9	132.82 (13)	O9—C5—C4	123.8 (4)
O10—Er1—O9	52.05 (10)	O10—C5—C4	117.6 (4)
O11^{i}—Er1—C5	169.83 (11)	O9—C5—Er1	61.7 (2)
O7^{i}—Er1—C5	71.00 (13)	O10—C5—Er1	58.9 (2)
O5—Er1—C5	91.51 (12)	C4—C5—Er1	163.6 (3)
O4—Er1—C5	100.37 (12)	O14—C6—O13	118.8 (4)
O9^{i}—Er1—C5	92.68 (11)	O14—C6—C7	124.0 (4)
O4W—Er1—C5	108.36 (14)	O13—C6—C7	117.2 (4)
O10—Er1—C5	26.44 (11)	O14—C6—Er2^{v}	58.8 (2)
O9—Er1—C5	26.19 (11)	O13—C6—Er2^{v}	60.7 (2)
O15^{ii}—Er2—O12^{iii}	89.96 (13)	C7—C6—Er2^{v}	172.0 (3)
O15^{ii}—Er2—O1	102.94 (13)	C9—C7—N3	109.4 (4)
O12^{iii}—Er2—O1	139.27 (12)	C9—C7—C6	134.6 (4)
O15^{ii}—Er2—O1W	79.51 (14)	N3—C7—C6	116.0 (4)
O12^{iii}—Er2—O1W	69.98 (12)	N3—C8—N4	111.3 (4)
O1—Er2—O1W	74.63 (12)	N3—C8—H8	124.3
O15^{ii}—Er2—O2^{iv}	85.40 (13)	N4—C8—H8	124.3
O12^{iii}—Er2—O2^{iv}	78.38 (12)	N4—C9—C7	104.8 (4)
O1—Er2—O2^{iv}	140.26 (11)	N4—C9—C10	120.1 (4)
O1W—Er2—O2^{iv}	144.73 (11)	C7—C9—C10	134.9 (4)
O15^{ii}—Er2—O14^{ii}	77.81 (12)	O16—C10—O15	124.0 (5)
O12^{iii}—Er2—O14^{ii}	149.10 (12)	O16—C10—C9	117.7 (4)
O1—Er2—O14^{ii}	71.57 (11)	O15—C10—C9	118.3 (4)
O1W—Er2—O14^{ii}	133.35 (12)	C3—N1—C2	108.8 (4)
O2^{iv}—Er2—O14^{ii}	72.50 (11)	C3—N1—H1	123 (5)
O15^{ii}—Er2—O14^{v}	146.41 (12)	C2—N1—H1	127 (5)
O12^{iii}—Er2—O14^{v}	111.88 (11)	C3—N2—C4	106.0 (4)
O1—Er2—O14^{v}	77.45 (11)	C3—N2—Co1	141.3 (3)
O1W—Er2—O14^{v}	131.03 (12)	C4—N2—Co1	112.6 (3)
O2^{iv}—Er2—O14^{v}	75.04 (11)	C8—N3—C7	106.0 (4)
O14^{ii}—Er2—O14^{v}	70.43 (11)	C8—N3—Co1	139.7 (3)
O15^{ii}—Er2—O13^{v}	161.49 (12)	C7—N3—Co1	114.1 (3)
O12^{iii}—Er2—O13^{v}	80.41 (11)	C8—N4—C9	108.5 (4)
O1—Er2—O13^{v}	75.46 (11)	C8—N4—H2	120 (4)
O1W—Er2—O13^{v}	82.34 (12)	C9—N4—H2	131 (4)
O2^{iv}—Er2—O13^{v}	107.80 (11)	S1—O1—Er2	143.0 (2)
O14^{ii}—Er2—O13^{v}	118.04 (10)	S1—O2—Er2^{iv}	142.13 (19)
O14^{v}—Er2—O13^{v}	51.89 (10)	S1—O4—Er1	142.7 (2)
O15^{ii}—Er2—C6^{v}	171.02 (13)	S2—O5—Er1	141.0 (2)

O12^{iii}—Er2—C6^{v}	98.50 (12)	S2—O7—Er1^{i}	143.41 (19)
O1—Er2—C6^{v}	72.49 (12)	C5—O9—Er1^{i}	143.6 (3)
O1W—Er2—C6^{v}	106.14 (13)	C5—O9—Er1	92.2 (3)
O2^{iv}—Er2—C6^{v}	93.33 (12)	Er1^{i}—O9—Er1	110.53 (12)
O14^{ii}—Er2—C6^{v}	93.33 (11)	C5—O10—Co1	115.3 (3)
O14^{v}—Er2—C6^{v}	26.00 (11)	C5—O10—Er1	94.6 (3)
O13^{v}—Er2—C6^{v}	26.10 (11)	Co1—O10—Er1	144.42 (15)
O15^{ii}—Er2—Er2^{iv}	113.19 (9)	C1—O11—Er1^{i}	144.9 (3)
O12^{iii}—Er2—Er2^{iv}	138.32 (8)	C1—O12—Er2^{vi}	136.0 (3)
O1—Er2—Er2^{iv}	71.02 (8)	C6—O13—Co1	114.4 (3)
O1W—Er2—Er2^{iv}	145.23 (8)	C6—O13—Er2^{v}	93.2 (3)
O2^{iv}—Er2—Er2^{iv}	70.03 (8)	Co1—O13—Er2^{v}	150.77 (15)
O14^{ii}—Er2—Er2^{iv}	36.06 (7)	C6—O14—Er2^{vii}	141.8 (3)
O14^{v}—Er2—Er2^{iv}	34.37 (7)	C6—O14—Er2^{v}	95.2 (3)
O13^{v}—Er2—Er2^{iv}	84.04 (7)	Er2^{vii}—O14—Er2^{v}	109.57 (11)
C6^{v}—Er2—Er2^{iv}	58.22 (9)	C10—O15—Er2^{vii}	158.3 (3)
N3—Co1—N2	102.00 (15)	Er2—O1W—H1W	123 (4)
N3—Co1—O3W	100.19 (16)	Er2—O1W—H2W	125 (4)
N2—Co1—O3W	92.08 (15)	H1W—O1W—H2W	108 (6)
N3—Co1—O10	170.48 (14)	Co1—O2W—H3W	111 (5)
N2—Co1—O10	78.70 (13)	Co1—O2W—H4W	119 (5)
O3W—Co1—O10	89.25 (16)	H3W—O2W—H4W	119 (6)
N3—Co1—O2W	95.07 (15)	Co1—O3W—H5W	112 (5)
N2—Co1—O2W	160.56 (15)	Co1—O3W—H6W	113 (5)
O3W—Co1—O2W	94.00 (16)	H5W—O3W—H6W	126 (7)
O10—Co1—O2W	82.93 (14)	Er1—O4W—H7W	130 (5)
N3—Co1—O13	77.96 (13)	Er1—O4W—H8W	107 (5)
N2—Co1—O13	87.28 (14)	H7W—O4W—H8W	91 (7)
O3W—Co1—O13	177.87 (16)	H9W—O5W—H10W	104 (7)
O10—Co1—O13	92.62 (12)		

Symmetry codes: (i) −*x*, −*y*, −*z*+1; (ii) *x*−1, *y*, *z*; (iii) *x*−1, *y*, *z*−1; (iv) −*x*−1, −*y*, −*z*; (v) −*x*, −*y*, −*z*; (vi) *x*+1, *y*, *z*+1; (vii) *x*+1, *y*, *z*.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O8^{viii}	0.86 (5)	1.95 (5)	2.806 (6)	176 (7)
O1*W*—H1*W*···O8^{v}	0.82 (5)	2.08 (5)	2.885 (6)	166 (5)
N4—H2···O3^{ix}	0.86 (4)	1.93 (3)	2.785 (5)	172 (7)
O1*W*—H2*W*···O3^{v}	0.82 (5)	2.01 (4)	2.822 (5)	170 (4)
O1*W*—H2*W*···O4^{v}	0.82 (5)	2.58 (5)	3.048 (5)	118 (5)
O2*W*—H3*W*···O16^{x}	0.81 (4)	1.92 (5)	2.730 (5)	176 (8)
O2*W*—H4*W*···O3^{v}	0.80 (4)	2.49 (5)	2.897 (5)	113 (4)
O3*W*—H5*W*···O5*W*	0.82 (7)	1.89 (7)	2.692 (7)	169 (7)
O3*W*—H6*W*···O6^{i}	0.81 (3)	2.57 (4)	3.336 (6)	158 (8)
O4*W*—H7*W*···O5*W*	0.82 (4)	1.98 (4)	2.752 (6)	158 (6)
O4*W*—H8*W*···O2*W*	0.81 (5)	2.57 (7)	3.167 (6)	132 (6)
O5*W*—H9*W*···O8^{xi}	0.85 (5)	1.90 (5)	2.737 (6)	169 (5)

O5*W*—H10*W*···O16^{x}	0.86 (5)	1.97 (6)	2.787 (6)	159 (7)
C3—H3···O6^{ix}	0.93	2.46	3.224 (7)	140

Symmetry codes: (i) −*x*, −*y*, −*z*+1; (v) −*x*, −*y*, −*z*; (viii) −*x*+1, −*y*, −*z*+1; (ix) *x*+1, *y*+1, *z*; (x) −*x*+1, −*y*+1, −*z*; (xi) *x*, *y*+1, *z*.