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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)digadolinium(III)] monohydrate]

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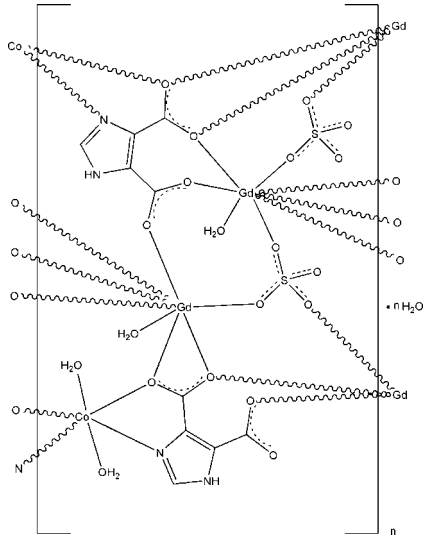
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.006 Å; R factor = 0.022; wR factor = 0.054; data-to-parameter ratio = 10.6.

The asymmetric unit of the title compound, $\{[CoGd_2(C_5H_2N_2O_4)_2(SO_4)_2(H_2O)_4]\cdot H_2O\}_n$, contains one Co^{II} ion, two Gd^{III} ions, two imidazole-4,5-dicarboxylate 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, as well as two O atoms and two N atoms from two imidazole-4,5-dicarboxylate ligands, giving a slightly distorted octahedral geometry. Both Gd^{III} ions are eight-coordinated in a distorted bicapped trigonal–prismatic geometry. One Gd^{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 a water O atom; the other Gd^{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 a water O atom. These metal coordination units are connected by bridging imidazole-4,5-dicarboxylate and sulfate ligands, generating a heterometallic layer parallel to the *ac* plane. The layers are stacked along the *b* axis *via* N—H···O, O—H···O, and C—H···O hydrogen-bonding interactions, generating a three-dimensional framework.

Related literature

For applications of lanthanide–transition metal heterometallic complexes with bridging multifunctional organic ligands, see: Cheng *et al.* (2006); Kuang *et al.* (2007); Sun *et al.* (2006); Zhu *et al.* (2010).



Experimental

Crystal data

$[CoGd_2(C_5H_2N_2O_4)_2(SO_4)_2(H_2O)_4]\cdot H_2O$
M_r = 963.82
Triclinic, $P\overline{1}$
a = 9.0916 (5) Å
b = 10.7714 (6) Å
c = 12.9736 (7) Å
α = 93.119 (1)°
β = 96.416 (1)°
γ = 108.840 (1)°
V = 1189.35 (11) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 6.48 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} = 0.284, T_{max} = 0.378
6174 measured reflections
4208 independent reflections
3790 reflections with $I > 2\sigma(I)$
R_{int} = 0.016

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.022
$wR(F^2)$ = 0.054
S = 1.02
4208 reflections
397 parameters
17 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.79 e Å^{-3}
$\Delta\rho_{min}$ = −0.81 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O1^{i}	0.87 (4)	1.96 (4)	2.820 (5)	172 (5)
O1W—H1W···O5W^{ii}	0.81 (4)	1.95 (3)	2.745 (5)	169 (6)
N3—H2···O14^{iii}	0.87 (3)	1.93 (3)	2.787 (4)	169 (4)
O2W—H3W···O1^{i}	0.80 (3)	2.09 (4)	2.878 (5)	171 (5)
O2W—H4W···O14^{i}	0.81 (4)	2.04 (4)	2.842 (5)	172 (5)
O2W—H4W···O15^{i}	0.81 (4)	2.52 (4)	3.035 (5)	123 (4)
O3W—H5W···O12^{iv}	0.82 (3)	1.95 (4)	2.734 (4)	162 (5)
O3W—H6W···O14^{v}	0.83 (3)	2.41 (4)	2.919 (4)	120 (3)
O4W—H7W···O3^{vi}	0.82 (3)	2.49 (3)	3.306 (6)	174 (6)
O4W—H8W···O5W^{iii}	0.82 (5)	1.89 (5)	2.700 (6)	175 (6)
O5W—H9W···O12^{v}	0.85 (4)	1.99 (4)	2.797 (6)	161 (5)
O5W—H10W···O1^{i}	0.85 (5)	1.93 (5)	2.728 (5)	157 (6)
C3—H3···O3^{vii}	0.93	2.44	3.193 (5)	138

Symmetry codes: (i) $x-1, y, z$; (ii) $x+1, y+1, z$; (iii) $x, y+1, z$; (iv) $-x+1, -y+2, -z$; (v) $-x+1, -y+1, -z$; (vi) $-x+1, -y+1, -z+1$; (vii) $-x+1, -y, -z+1$.

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: *XP* in *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: HP2018).

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supporting information

Acta Cryst. (2011). E**67**, m1741–m1742 [https://doi.org/10.1107/S160053681104726X]

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

Li-Cai Zhu

S1. Comment

In the past few years, lanthanide-transition metal heterometallic complexs with bridging multifunctionnal organic ligands are of increasing interest, not only because of their impressive topological structures, but also due to their versatile applications in ion exchange, magnetism, bimetallic catalysis and luminescent probe(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 one Co^{II} ion, two Gd^{III} ions, two imidazole-4, 5-dicarboxylate ligands, two SO_4^{2-} anions, four coordinated water molecules and one uncoordinated 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 imidazole-4, 5-dicarboxylate ligands, giving a slightly distorted octahedral geometry. Both Gd^{III} ions are eight-coordinated in a bicapped trigonal prismatic coordination geometry. One Gd^{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 molecule; the other Gd^{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 imidazole-4, 5-dicarboxylate and sulfate ligands, generating a two-dimensional heterometallic layer. The two-dimensional layers are stacked along *b* axis *via* N—H···O, O—H···O, and C—H···O hydrogen-bonding interactions to generate the three-dimensional framework(Table 1 and Fig. 2).

S2. Experimental

A mixture of $CoSO_4.7H_2O$(0.141 g, 0.5 mmol), Gd_2O_3(0.09 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 a restraint of N—H = 0.87 Å, O—H = 0.82 or 0.86 Å and U_{iso}(H) = 1.5 U_{eq}(N, O).

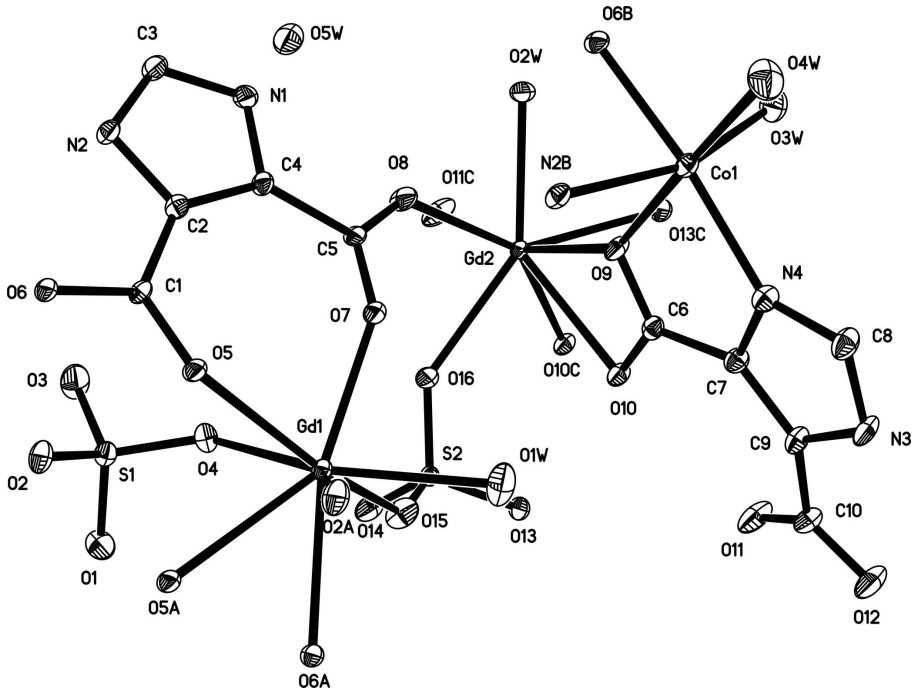

Figure 1

The molecular structure showing the atomic-numbering scheme and displacement ellipsoids drawn at the 30% probability level. Symmetry codes: (A) 2 - *x*, 1 - *y*, 1 - *z*; (B) 1 - *x*, 1 - *y*, 1 - *z*; (C) 1 - *x*, 1 - *y*, -*z*.

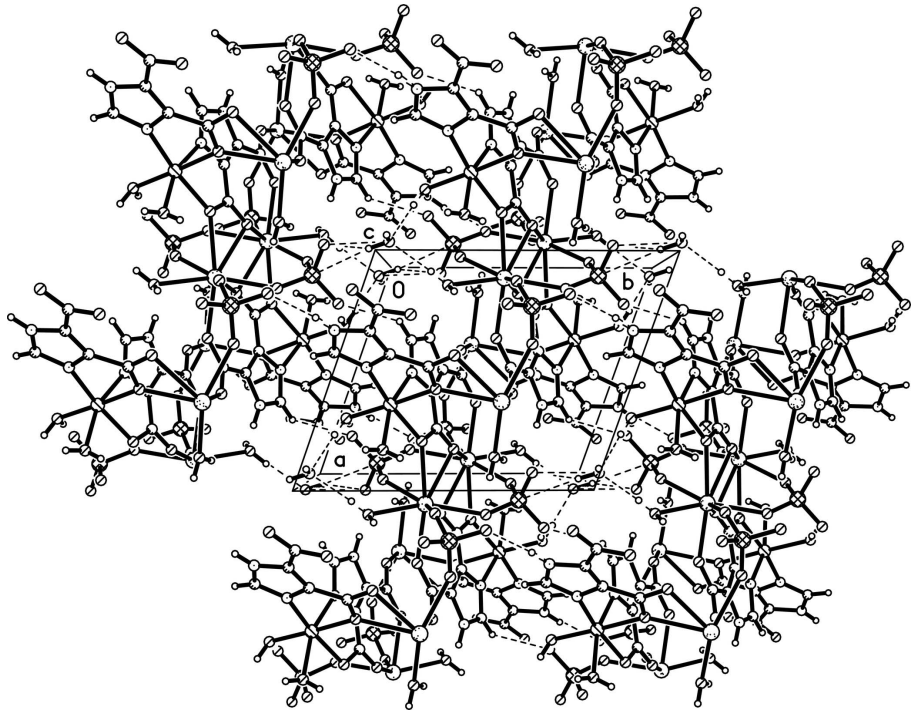

Figure 2

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)digadolinium(III)] monohydrate]

Crystal data

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Hall symbol: -P 1
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$b = 10.7714$ (6) Å
$c = 12.9736$ (7) Å
$\alpha = 93.119$ (1)°
$\beta = 96.416$ (1)°
$\gamma = 108.840$ (1)°
$V = 1189.35$ (11) Å^3
$Z = 2$
$F(000) = 914$
$D_x = 2.691$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 4033 reflections
$\theta = 2.4$–27.9°
$\mu = 6.48$ 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)
$T_{min} = 0.284$, $T_{max} = 0.378$
6174 measured reflections
4208 independent reflections
3790 reflections with $I > 2\sigma(I)$
$R_{int} = 0.016$
$\theta_{max} = 25.2°$, $\theta_{min} = 1.6°$
$h = -10\rightarrow8$
$k = -9\rightarrow12$
$l = -14\rightarrow15$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.022$
$wR(F^2) = 0.054$
$S = 1.02$
4208 reflections
397 parameters
17 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
$w = 1/[\sigma^2(F_o^2) + (0.0292P)^2 + 0.3497P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.002$
$\Delta\rho_{max} = 0.79$ e Å^{-3}
$\Delta\rho_{min} = -0.81$ 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 (Å^2)

	x	y	z	U_{iso}*/U_{eq}
Gd1	0.90952 (2)	0.549083 (19)	0.364770 (14)	0.01526 (7)

Gd2	0.37043 (2)	0.410578 (19)	0.108204 (14)	0.01441 (7)
Co1	0.35411 (7)	0.78823 (6)	0.27426 (4)	0.01829 (13)
S1	0.92233 (13)	0.22231 (10)	0.40357 (8)	0.0196 (2)
S2	0.77447 (12)	0.42234 (10)	0.09511 (7)	0.0157 (2)
C1	0.7564 (5)	0.3980 (4)	0.5774 (3)	0.0152 (9)
C2	0.5906 (5)	0.3349 (4)	0.5377 (3)	0.0175 (9)
C3	0.3614 (5)	0.1987 (4)	0.5498 (3)	0.0224 (10)
H3	0.2790	0.1358	0.5738	0.027*
C4	0.4925 (5)	0.3440 (4)	0.4526 (3)	0.0176 (9)
C5	0.5166 (5)	0.4170 (4)	0.3574 (3)	0.0179 (9)
C6	0.5196 (5)	0.6976 (4)	0.1215 (3)	0.0183 (9)
C7	0.5717 (5)	0.8417 (4)	0.1198 (3)	0.0198 (9)
C8	0.5810 (6)	1.0356 (4)	0.1824 (3)	0.0262 (11)
H8	0.5656	1.1038	0.2221	0.031*
C9	0.6687 (5)	0.9312 (4)	0.0646 (3)	0.0212 (10)
C10	0.7527 (5)	0.9224 (4)	−0.0265 (3)	0.0253 (10)
N1	0.3480 (4)	0.2571 (4)	0.4626 (3)	0.0219 (8)
N2	0.5066 (4)	0.2422 (3)	0.5971 (3)	0.0188 (8)
N3	0.6720 (5)	1.0523 (3)	0.1057 (3)	0.0251 (9)
N4	0.5169 (4)	0.9092 (3)	0.1936 (3)	0.0209 (8)
O1	1.0507 (4)	0.2115 (3)	0.3471 (2)	0.0307 (8)
O2	0.9891 (4)	0.2677 (3)	0.5141 (2)	0.0260 (7)
O3	0.7976 (4)	0.0979 (3)	0.3993 (3)	0.0429 (10)
O4	0.8622 (4)	0.3220 (3)	0.3559 (2)	0.0236 (7)
O5	0.8508 (3)	0.4831 (3)	0.5314 (2)	0.0191 (6)
O6	0.8087 (3)	0.3626 (3)	0.6615 (2)	0.0195 (6)
O7	0.6446 (3)	0.5035 (3)	0.3536 (2)	0.0227 (7)
O8	0.4026 (4)	0.3819 (3)	0.2864 (2)	0.0291 (8)
O9	0.4237 (4)	0.6481 (3)	0.1835 (2)	0.0216 (7)
O10	0.5663 (3)	0.6222 (3)	0.0648 (2)	0.0201 (7)
O11	0.7322 (4)	0.8084 (3)	−0.0689 (3)	0.0373 (9)
O12	0.8336 (4)	1.0256 (3)	−0.0559 (3)	0.0371 (9)
O13	0.7800 (4)	0.5049 (3)	0.0081 (2)	0.0261 (7)
O14	0.8239 (4)	0.3108 (3)	0.0655 (2)	0.0302 (8)
O15	0.8852 (4)	0.5027 (3)	0.1839 (2)	0.0315 (8)
O16	0.6158 (4)	0.3748 (3)	0.1261 (2)	0.0296 (8)
H1	0.260 (4)	0.251 (5)	0.426 (3)	0.044*
H2	0.725 (5)	1.128 (3)	0.087 (4)	0.044*
O1W	0.8720 (5)	0.7325 (3)	0.2745 (3)	0.0411 (9)
H1W	0.931 (6)	0.807 (3)	0.275 (4)	0.062*
H2W	0.843 (7)	0.703 (5)	0.216 (2)	0.062*
O2W	0.1300 (4)	0.3676 (4)	0.1756 (3)	0.0301 (8)
H3W	0.115 (5)	0.331 (5)	0.227 (2)	0.045*
H4W	0.046 (4)	0.359 (5)	0.143 (3)	0.045*
O3W	0.1637 (4)	0.7554 (3)	0.1538 (2)	0.0305 (8)
H5W	0.166 (7)	0.811 (3)	0.113 (3)	0.046*
H6W	0.131 (6)	0.686 (3)	0.114 (3)	0.046*
O4W	0.2924 (5)	0.9293 (4)	0.3611 (3)	0.0402 (9)

H7W	0.267 (6)	0.916 (6)	0.419 (2)	0.060*
H8W	0.221 (5)	0.949 (6)	0.330 (4)	0.060*
O5W	0.0564 (5)	−0.0166 (4)	0.2481 (3)	0.0440 (10)
H9W	0.079 (7)	−0.006 (5)	0.187 (2)	0.066*
H10W	0.028 (7)	0.046 (4)	0.271 (4)	0.066*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Gd1	0.01463 (12)	0.01957 (12)	0.01160 (11)	0.00505 (9)	0.00226 (8)	0.00460 (8)
Gd2	0.01453 (12)	0.01764 (12)	0.01186 (11)	0.00550 (9)	0.00300 (8)	0.00492 (8)
Co1	0.0212 (3)	0.0206 (3)	0.0141 (3)	0.0069 (2)	0.0050 (2)	0.0054 (2)
S1	0.0214 (6)	0.0180 (5)	0.0181 (5)	0.0053 (4)	0.0011 (4)	0.0022 (4)
S2	0.0164 (5)	0.0211 (5)	0.0111 (5)	0.0077 (4)	0.0024 (4)	0.0041 (4)
C1	0.020 (2)	0.017 (2)	0.0083 (19)	0.0053 (18)	0.0044 (17)	0.0013 (16)
C2	0.022 (2)	0.021 (2)	0.0102 (19)	0.0082 (18)	0.0032 (17)	0.0004 (17)
C3	0.021 (2)	0.024 (2)	0.020 (2)	0.0035 (19)	0.0038 (19)	0.0055 (18)
C4	0.018 (2)	0.021 (2)	0.013 (2)	0.0056 (18)	0.0011 (17)	0.0031 (17)
C5	0.017 (2)	0.029 (2)	0.010 (2)	0.0095 (19)	0.0058 (17)	0.0057 (17)
C6	0.018 (2)	0.020 (2)	0.015 (2)	0.0039 (18)	−0.0011 (18)	0.0041 (18)
C7	0.023 (2)	0.018 (2)	0.018 (2)	0.0057 (18)	0.0050 (18)	0.0017 (17)
C8	0.038 (3)	0.017 (2)	0.025 (2)	0.009 (2)	0.012 (2)	0.0031 (19)
C9	0.026 (3)	0.014 (2)	0.021 (2)	0.0034 (18)	0.0045 (19)	0.0031 (18)
C10	0.027 (3)	0.024 (3)	0.023 (2)	0.003 (2)	0.010 (2)	0.005 (2)
N1	0.016 (2)	0.031 (2)	0.0177 (19)	0.0067 (17)	0.0005 (15)	0.0044 (16)
N2	0.020 (2)	0.0204 (19)	0.0142 (17)	0.0039 (15)	0.0035 (15)	0.0047 (14)
N3	0.035 (2)	0.0154 (19)	0.025 (2)	0.0043 (17)	0.0127 (18)	0.0081 (16)
N4	0.024 (2)	0.0188 (19)	0.0185 (18)	0.0050 (16)	0.0045 (16)	0.0011 (15)
O1	0.033 (2)	0.046 (2)	0.0184 (16)	0.0199 (16)	0.0057 (14)	0.0000 (15)
O2	0.037 (2)	0.0269 (17)	0.0154 (15)	0.0120 (15)	0.0022 (14)	0.0038 (13)
O3	0.031 (2)	0.0262 (19)	0.057 (2)	−0.0065 (15)	−0.0102 (18)	0.0148 (17)
O4	0.0266 (18)	0.0222 (16)	0.0229 (16)	0.0107 (14)	−0.0012 (14)	0.0020 (13)
O5	0.0160 (16)	0.0252 (16)	0.0149 (14)	0.0041 (13)	0.0030 (12)	0.0064 (12)
O6	0.0167 (16)	0.0296 (17)	0.0125 (14)	0.0070 (13)	0.0029 (12)	0.0074 (12)
O7	0.0161 (16)	0.0295 (17)	0.0225 (16)	0.0057 (13)	0.0029 (13)	0.0122 (13)
O8	0.0191 (17)	0.048 (2)	0.0167 (16)	0.0052 (15)	0.0010 (13)	0.0133 (15)
O9	0.0276 (18)	0.0182 (15)	0.0193 (15)	0.0049 (13)	0.0105 (13)	0.0067 (12)
O10	0.0246 (17)	0.0149 (15)	0.0209 (15)	0.0048 (13)	0.0084 (13)	0.0036 (12)
O11	0.053 (2)	0.0187 (18)	0.037 (2)	0.0021 (16)	0.0258 (18)	0.0011 (15)
O12	0.050 (2)	0.0236 (18)	0.039 (2)	0.0061 (16)	0.0248 (18)	0.0103 (15)
O13	0.0230 (18)	0.042 (2)	0.0184 (16)	0.0142 (15)	0.0053 (13)	0.0170 (14)
O14	0.039 (2)	0.0200 (17)	0.0346 (18)	0.0095 (15)	0.0187 (16)	0.0038 (14)
O15	0.035 (2)	0.0346 (19)	0.0158 (16)	0.0001 (15)	0.0002 (14)	−0.0013 (14)
O16	0.0236 (18)	0.045 (2)	0.0275 (17)	0.0164 (15)	0.0122 (14)	0.0208 (15)
O1W	0.053 (3)	0.029 (2)	0.035 (2)	0.0081 (18)	−0.0066 (19)	0.0089 (16)
O2W	0.0199 (18)	0.049 (2)	0.0271 (18)	0.0154 (16)	0.0092 (14)	0.0182 (16)
O3W	0.035 (2)	0.0295 (18)	0.0251 (17)	0.0100 (16)	−0.0016 (15)	0.0045 (14)
O4W	0.055 (3)	0.041 (2)	0.032 (2)	0.0265 (19)	0.0098 (18)	0.0015 (18)

O5W	0.063 (3)	0.040 (2)	0.043 (2)	0.028 (2)	0.026 (2)	0.0114 (18)

Geometric parameters (Å, º)

Gd1—O7	2.283 (3)	C3—N2	1.314 (5)
Gd1—O2^{i}	2.319 (3)	C3—N1	1.336 (5)
Gd1—O4	2.337 (3)	C3—H3	0.9300
Gd1—O15	2.343 (3)	C4—N1	1.370 (5)
Gd1—O5	2.375 (3)	C4—C5	1.498 (5)
Gd1—O1W	2.447 (3)	C5—O7	1.242 (5)
Gd1—O6^{i}	2.498 (3)	C5—O8	1.249 (5)
Gd1—O5^{i}	2.562 (3)	C6—O9	1.263 (5)
Gd1—C1^{i}	2.905 (4)	C6—O10	1.268 (5)
Gd1—Gd1^{i}	4.0465 (4)	C6—C7	1.471 (6)
Gd2—O11^{ii}	2.244 (3)	C7—C9	1.373 (6)
Gd2—O13^{ii}	2.338 (3)	C7—N4	1.399 (5)
Gd2—O8	2.348 (3)	C8—N4	1.320 (5)
Gd2—O2W	2.361 (3)	C8—N3	1.347 (6)
Gd2—O16	2.373 (3)	C8—H8	0.9300
Gd2—O10^{ii}	2.414 (3)	C9—N3	1.372 (5)
Gd2—O10	2.535 (3)	C9—C10	1.493 (6)
Gd2—O9	2.561 (3)	C10—O12	1.226 (5)
Gd2—C6	2.934 (4)	C10—O11	1.265 (5)
Gd2—Gd2^{ii}	4.0349 (4)	N1—H1	0.87 (4)
Co1—N4	2.058 (4)	N2—Co1^{iii}	2.086 (3)
Co1—N2^{iii}	2.086 (3)	N3—H2	0.87 (3)
Co1—O6^{iii}	2.096 (3)	O2—Gd1^{i}	2.319 (3)
Co1—O4W	2.097 (4)	O5—Gd1^{i}	2.562 (3)
Co1—O3W	2.122 (3)	O6—Co1^{iii}	2.096 (3)
Co1—O9	2.157 (3)	O6—Gd1^{i}	2.498 (3)
S1—O3	1.443 (3)	O10—Gd2^{ii}	2.414 (3)
S1—O1	1.478 (3)	O11—Gd2^{ii}	2.244 (3)
S1—O2	1.483 (3)	O13—Gd2^{ii}	2.338 (3)
S1—O4	1.486 (3)	O1W—H1W	0.81 (4)
S2—O14	1.459 (3)	O1W—H2W	0.789 (19)
S2—O15	1.469 (3)	O2W—H3W	0.80 (3)
S2—O13	1.470 (3)	O2W—H4W	0.81 (4)
S2—O16	1.476 (3)	O3W—H5W	0.82 (3)
C1—O5	1.264 (5)	O3W—H6W	0.83 (3)
C1—O6	1.269 (5)	O4W—H7W	0.82 (3)
C1—C2	1.458 (6)	O4W—H8W	0.82 (5)
C1—Gd1^{i}	2.905 (4)	O5W—H9W	0.85 (4)
C2—C4	1.369 (6)	O5W—H10W	0.85 (5)
C2—N2	1.377 (5)		

O7—Gd1—O2^{i}	103.56 (11)	O4W—Co1—O3W	93.45 (14)
O7—Gd1—O4	87.61 (10)	N4—Co1—O9	78.00 (12)
O2^{i}—Gd1—O4	139.04 (10)	N2^{iii}—Co1—O9	87.71 (13)

O7—Gd1—O15	90.06 (11)	O6^{iii}—Co1—O9	91.82 (11)
O2^{i}—Gd1—O15	137.61 (11)	O4W—Co1—O9	178.18 (14)
O4—Gd1—O15	80.42 (11)	O3W—Co1—O9	87.04 (13)
O7—Gd1—O5	76.05 (10)	O3—S1—O1	112.2 (2)
O2^{i}—Gd1—O5	71.43 (10)	O3—S1—O2	108.8 (2)
O4—Gd1—O5	73.46 (10)	O1—S1—O2	107.78 (19)
O15—Gd1—O5	150.71 (11)	O3—S1—O4	110.53 (19)
O7—Gd1—O1W	77.94 (12)	O1—S1—O4	107.51 (18)
O2^{i}—Gd1—O1W	74.57 (11)	O2—S1—O4	110.02 (17)
O4—Gd1—O1W	146.18 (11)	O14—S2—O15	108.6 (2)
O15—Gd1—O1W	69.33 (12)	O14—S2—O13	109.56 (18)
O5—Gd1—O1W	130.26 (12)	O15—S2—O13	107.94 (19)
O7—Gd1—O6^{i}	164.37 (9)	O14—S2—O16	110.07 (19)
O2^{i}—Gd1—O6^{i}	76.75 (10)	O15—S2—O16	109.10 (19)
O4—Gd1—O6^{i}	102.43 (10)	O13—S2—O16	111.47 (17)
O15—Gd1—O6^{i}	80.01 (10)	O5—C1—O6	118.6 (4)
O5—Gd1—O6^{i}	118.09 (9)	O5—C1—C2	123.7 (3)
O1W—Gd1—O6^{i}	87.23 (12)	O6—C1—C2	117.7 (3)
O7—Gd1—O5^{i}	144.56 (9)	O5—C1—Gd1^{i}	61.8 (2)
O2^{i}—Gd1—O5^{i}	75.17 (10)	O6—C1—Gd1^{i}	58.9 (2)
O4—Gd1—O5^{i}	73.51 (10)	C2—C1—Gd1^{i}	163.6 (3)
O15—Gd1—O5^{i}	115.09 (11)	C4—C2—N2	109.0 (4)
O5—Gd1—O5^{i}	69.99 (11)	C4—C2—C1	135.5 (4)
O1W—Gd1—O5^{i}	132.85 (11)	N2—C2—C1	115.5 (3)
O6^{i}—Gd1—O5^{i}	50.97 (9)	N2—C3—N1	110.9 (4)
O7—Gd1—C1^{i}	168.66 (10)	N2—C3—H3	124.5
O2^{i}—Gd1—C1^{i}	70.40 (11)	N1—C3—H3	124.5
O4—Gd1—C1^{i}	91.09 (11)	C2—C4—N1	105.5 (3)
O15—Gd1—C1^{i}	100.83 (11)	C2—C4—C5	133.9 (4)
O5—Gd1—C1^{i}	92.78 (10)	N1—C4—C5	120.4 (4)
O1W—Gd1—C1^{i}	108.73 (12)	O7—C5—O8	125.4 (4)
O6^{i}—Gd1—C1^{i}	25.79 (9)	O7—C5—C4	119.5 (4)
O5^{i}—Gd1—C1^{i}	25.77 (10)	O8—C5—C4	115.1 (4)
O7—Gd1—Gd1^{i}	111.99 (7)	O9—C6—O10	119.1 (4)
O2^{i}—Gd1—Gd1^{i}	69.58 (7)	O9—C6—C7	117.3 (4)
O4—Gd1—Gd1^{i}	69.70 (7)	O10—C6—C7	123.6 (4)
O15—Gd1—Gd1^{i}	141.31 (9)	O9—C6—Gd2	60.5 (2)
O5—Gd1—Gd1^{i}	36.51 (7)	O10—C6—Gd2	59.4 (2)
O1W—Gd1—Gd1^{i}	144.09 (9)	C7—C6—Gd2	171.4 (3)
O6^{i}—Gd1—Gd1^{i}	82.97 (6)	C9—C7—N4	109.2 (4)
O5^{i}—Gd1—Gd1^{i}	33.48 (6)	C9—C7—C6	135.5 (4)
C1^{i}—Gd1—Gd1^{i}	57.20 (7)	N4—C7—C6	115.3 (4)
O11^{ii}—Gd2—O13^{ii}	104.05 (12)	N4—C8—N3	110.6 (4)
O11^{ii}—Gd2—O8	90.51 (12)	N4—C8—H8	124.7
O13^{ii}—Gd2—O8	138.78 (11)	N3—C8—H8	124.7
O11^{ii}—Gd2—O2W	79.70 (13)	N3—C9—C7	105.2 (4)
O13^{ii}—Gd2—O2W	75.63 (11)	N3—C9—C10	119.4 (4)
O8—Gd2—O2W	69.29 (11)	C7—C9—C10	135.2 (4)

O11^{ii}—Gd2—O16	85.00 (13)	O12—C10—O11	125.0 (4)
O13^{ii}—Gd2—O16	139.36 (10)	O12—C10—C9	117.9 (4)
O8—Gd2—O16	79.29 (11)	O11—C10—C9	117.1 (4)
O2W—Gd2—O16	144.68 (10)	C3—N1—C4	108.3 (3)
O11^{ii}—Gd2—O10^{ii}	76.41 (10)	C3—N1—H1	125 (4)
O13^{ii}—Gd2—O10^{ii}	71.52 (10)	C4—N1—H1	126 (4)
O8—Gd2—O10^{ii}	149.64 (11)	C3—N2—C2	106.3 (3)
O2W—Gd2—O10^{ii}	132.68 (11)	C3—N2—Co1^{iii}	140.8 (3)
O16—Gd2—O10^{ii}	72.45 (10)	C2—N2—Co1^{iii}	112.8 (3)
O11^{ii}—Gd2—O10	145.26 (11)	C8—N3—C9	109.0 (4)
O13^{ii}—Gd2—O10	76.33 (10)	C8—N3—H2	125 (4)
O8—Gd2—O10	112.31 (10)	C9—N3—H2	126 (4)
O2W—Gd2—O10	131.93 (11)	C8—N4—C7	106.0 (4)
O16—Gd2—O10	74.61 (10)	C8—N4—Co1	139.7 (3)
O10^{ii}—Gd2—O10	70.80 (11)	C7—N4—Co1	114.0 (3)
O11^{ii}—Gd2—O9	163.85 (11)	S1—O2—Gd1^{i}	144.35 (18)
O13^{ii}—Gd2—O9	74.78 (10)	S1—O4—Gd1	141.43 (18)
O8—Gd2—O9	80.86 (10)	C1—O5—Gd1	143.6 (3)
O2W—Gd2—O9	84.47 (11)	C1—O5—Gd1^{i}	92.4 (2)
O16—Gd2—O9	106.54 (11)	Gd1—O5—Gd1^{i}	110.01 (11)
O10^{ii}—Gd2—O9	117.44 (9)	C1—O6—Co1^{iii}	115.4 (3)
O10—Gd2—O9	50.71 (9)	C1—O6—Gd1^{i}	95.3 (2)
O11^{ii}—Gd2—C6	169.70 (11)	Co1^{iii}—O6—Gd1^{i}	143.17 (13)
O13^{ii}—Gd2—C6	71.59 (11)	C5—O7—Gd1	145.3 (3)
O8—Gd2—C6	98.84 (11)	C5—O8—Gd2	134.4 (3)
O2W—Gd2—C6	107.59 (12)	C6—O9—Co1	115.0 (3)
O16—Gd2—C6	92.46 (12)	C6—O9—Gd2	94.1 (2)
O10^{ii}—Gd2—C6	93.30 (11)	Co1—O9—Gd2	149.36 (13)
O10—Gd2—C6	25.50 (10)	C6—O10—Gd2^{ii}	142.3 (3)
O9—Gd2—C6	25.43 (10)	C6—O10—Gd2	95.1 (2)
O11^{ii}—Gd2—Gd2^{ii}	112.07 (8)	Gd2^{ii}—O10—Gd2	109.20 (11)
O13^{ii}—Gd2—Gd2^{ii}	70.24 (7)	C10—O11—Gd2^{ii}	159.9 (3)
O8—Gd2—Gd2^{ii}	139.01 (7)	S2—O13—Gd2^{ii}	144.17 (19)
O2W—Gd2—Gd2^{ii}	145.64 (8)	S2—O15—Gd1	141.6 (2)
O16—Gd2—Gd2^{ii}	69.68 (7)	S2—O16—Gd2	142.69 (18)
O10^{ii}—Gd2—Gd2^{ii}	36.40 (6)	Gd1—O1W—H1W	130 (4)
O10—Gd2—Gd2^{ii}	34.41 (6)	Gd1—O1W—H2W	104 (4)
O9—Gd2—Gd2^{ii}	82.98 (6)	H1W—O1W—H2W	108 (3)
C6—Gd2—Gd2^{ii}	57.82 (8)	Gd2—O2W—H3W	122 (4)
N4—Co1—N2^{iii}	102.68 (14)	Gd2—O2W—H4W	127 (3)
N4—Co1—O6^{iii}	169.67 (13)	H3W—O2W—H4W	108 (3)
N2^{iii}—Co1—O6^{iii}	78.43 (12)	Co1—O3W—H5W	120 (4)
N4—Co1—O4W	100.20 (15)	Co1—O3W—H6W	121 (4)
N2^{iii}—Co1—O4W	92.40 (14)	H5W—O3W—H6W	102 (3)
O6^{iii}—Co1—O4W	89.98 (14)	Co1—O4W—H7W	121 (4)
N4—Co1—O3W	94.51 (14)	Co1—O4W—H8W	113 (4)

N2^{iii}—Co1—O3W	160.56 (13)	H7W—O4W—H8W	104 (3)
O6^{iii}—Co1—O3W	83.04 (12)	H9W—O5W—H10W	110 (3)

Symmetry codes: (i) −*x*+2, −*y*+1, −*z*+1; (ii) −*x*+1, −*y*+1, −*z*; (iii) −*x*+1, −*y*+1, −*z*+1.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O1^{iv}	0.87 (4)	1.96 (4)	2.820 (5)	172 (5)
O1*W*—H1*W*···O5*W*^{v}	0.81 (4)	1.95 (3)	2.745 (5)	169 (6)
N3—H2···O14^{vi}	0.87 (3)	1.93 (3)	2.787 (4)	169 (4)
O2*W*—H3*W*···O1^{iv}	0.80 (3)	2.09 (4)	2.878 (5)	171 (5)
O2*W*—H4*W*···O14^{iv}	0.81 (4)	2.04 (4)	2.842 (5)	172 (5)
O2*W*—H4*W*···O15^{iv}	0.81 (4)	2.52 (4)	3.035 (5)	123 (4)
O3*W*—H5*W*···O12^{vii}	0.82 (3)	1.95 (4)	2.734 (4)	162 (5)
O3*W*—H6*W*···O14^{ii}	0.83 (3)	2.41 (4)	2.919 (4)	120 (3)
O4*W*—H7*W*···O3^{iii}	0.82 (3)	2.49 (3)	3.306 (6)	174 (6)
O4*W*—H8*W*···O5*W*^{vi}	0.82 (5)	1.89 (5)	2.700 (6)	175 (6)
O5*W*—H9*W*···O12^{ii}	0.85 (4)	1.99 (4)	2.797 (6)	161 (5)
O5*W*—H10*W*···O1^{iv}	0.85 (5)	1.93 (5)	2.728 (5)	157 (6)
C3—H3···O3^{viii}	0.93	2.44	3.193 (5)	138

Symmetry codes: (ii) −*x*+1, −*y*+1, −*z*; (iii) −*x*+1, −*y*+1, −*z*+1; (iv) *x*−1, *y*, *z*; (v) *x*+1, *y*+1, *z*; (vi) *x*, *y*+1, *z*; (vii) −*x*+1, −*y*+2, −*z*; (viii) −*x*+1, −*y*, −*z*+1.