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A one-dimensional triaquaeuropium(III)–1*H*,3*H*-benzimidazol-3-ium-5,6-dicarboxylate–sulfate polymeric structure

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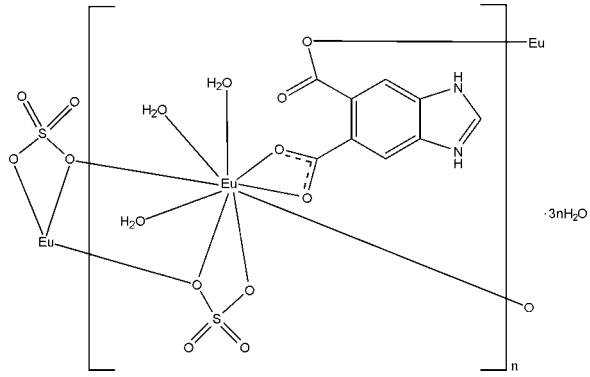
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.008 Å; R factor = 0.036; wR factor = 0.097; data-to-parameter ratio = 11.5.

In the title coordination polymer, *catena*-poly[[[triaquaeuropium(III)]-bis(μ-1*H*,3*H*-benzimidazol-3-ium-5,6-dicarboxylato-$\kappa^3O^5,O^{5'}:O^6$)-[triaquaeuropium(III)]-di-μ-sulfato-$\kappa^3O:O,O';\kappa^3O,O':O'$] hexahydrate], $\{[Eu_2(C_9H_5N_2O_4)_2(SO_4)_2(H_2O)_6]\cdot 6H_2O\}_n$, the 1*H*,3*H*-benzimidazol-3-ium-5,6-dicarboxylate ligand is protonated at the imidazole group (H_2bdc). The Eu^{III} ion is coordinated by nine O atoms from two H_2bdc ligands, two sulfate anions and three water molecules, displaying a bicapped trigonal prismatic geometry. The carboxylate groups of the H_2bdc ligands and the sulfate anions link the Eu^{III} ions, forming a chain along [010]. These chains are further connected by N—H···O and O—H···O hydrogen bonds and π–π interactions between the imidazole and benzene rings [centroid–centroid distances = 3.997 (4), 3.829 (4) and 3.573 (4) Å] into a three-dimensional supramolecular network.

Related literature

For background to 1*H*-benzimidazole-5,6-dicarboxylate complexes, see: Wang *et al.* (2010); Wei *et al.* (2008); Xie *et al.* (2010); Yao *et al.* (2008).



Experimental

Crystal data

$[Eu_2(C_9H_5N_2O_4)_2(SO_4)_2(H_2O)_6]\cdot 6H_2O$
M_r = 1122.58
Triclinic, $P\overline{1}$
a = 7.1261 (16) Å
b = 9.581 (2) Å
c = 12.424 (3) Å
α = 100.496 (3)°
β = 98.060 (3)°
γ = 94.979 (3)°
V = 820.3 (3) Å^3
Z = 1
Mo $K\alpha$ radiation
μ = 4.03 mm^{-1}
T = 298 K
0.30 × 0.26 × 0.20 mm

Data collection

Bruker APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
T_{min} = 0.310, T_{max} = 0.446
4076 measured reflections
2841 independent reflections
2669 reflections with $I > 2\sigma(I)$
R_{int} = 0.024

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.097
S = 1.02
2841 reflections
248 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 1.82 e Å^{-3}
$\Delta\rho_{min}$ = −2.51 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1W—H1W···O4^{i}	0.84	1.90	2.717 (6)	165
O1W—H2W···O7^{ii}	0.84	2.24	3.049 (6)	163
O2W—H3W···O5^{ii}	0.84	1.96	2.775 (6)	162
O2W—H4W···O3^{iii}	0.85	1.85	2.659 (6)	159
O3W—H5W···O4W^{iii}	0.84	2.07	2.810 (6)	146
O3W—H6W···O2^{iv}	0.85	2.10	2.864 (6)	149
O4W—H7W···O5^{ii}	0.86	2.34	3.045 (6)	139
O4W—H8W···O1	0.84	2.04	2.869 (6)	168
O5W—H9W···O6W	0.84	2.03	2.864 (8)	171
O5W—H10W···O6^{v}	0.84	2.01	2.790 (7)	154
O6W—H11W···O6^{vi}	0.84	2.37	3.165 (8)	158
O6W—H12W···O5^{ii}	0.85	2.20	2.895 (7)	139
O6W—H12W···O1W	0.85	2.46	3.060 (7)	129
N1—H1A···O5W^{vii}	0.86 (8)	1.96 (8)	2.752 (8)	153 (7)
N1—H1A···O4W^{vii}	0.86 (8)	2.48 (8)	2.989 (7)	119 (6)
N2—H2···O6W^{viii}	0.86	1.91	2.734 (7)	161

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

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; program(s) used to solve

structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEPIII* (Burnett & Johnson, 1996) and *PLATON* (Spek, 2009); 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: HY2456).

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A one-dimensional triaquaeuropium(III)–1*H*,3*H*-benzimidazol-3-ium-5,6-dicarboxylate–sulfate polymeric structure

Xia Cai, Jing-Jun Lin, Hao-Zhao Chen, Lai-Chen Chen and Rong-Hua Zeng

S1. Comment

In recent years, research on coordination polymers has made considerable progress in the fields of supramolecular chemistry and crystal engineering, because of their intriguing structural motifs and functional properties, such as molecular adsorption, magnetism and luminescence. Ligands play a key role in the construction of coordination polymers with fascinating topology, intriguing architectures and useful physical-chemical properties. Benzimidazole-5,6-dicarboxylic acid (H_3bdc) is a potential bifunctional ligand with carboxylate and N-donor functional groups and has been used to prepare such metal-organic complexes in possession of multidimensional networks and interesting properties (Wang *et al.*, 2010; Wei *et al.*, 2008; Xie *et al.*, 2010; Yao *et al.*, 2008). Recently, we obtained the title coordination polymer, which was synthesized by the hydrothermal reaction of Eu_2O_3 with H_3bdc in an aqueous solution.

The title compound has a polymeric chain architecture. As shown in Fig. 1, the Eu^{III} ion is in a bicapped trigonal-prismatic geometry, defined by nine O atoms from two 1*H*,3*H*-benzimidazol-3-ium-5,6-dicarboxylate ligands (H_2bdc), which are protonated at the imidazole groups, two sulfate anions and three water molecules. The H_2bdc ligands and sulfate anions link the Eu^{III} ions into a chain along [0 1 0] (Fig. 2). The adjacent Eu···Eu separations are 4.272 (4) and 6.663 (5) Å. The Eu—O bond lengths range from 2.376 (4) to 2.610 (4) Å and O—Eu—O bond angles vary from 52.01 (1) to 143.68 (1) °. The chains are further connected by N—H···O and O—H···O hydrogen bonds (Table 1) and π–π interactions between the imidazole and benzene rings [centroid–centroid distances = 3.997 (4), 3.829 (4) and 3.573 (4) Å] into a three-dimensional supramolecular network.

S2. Experimental

A mixture of Eu_2O_3 (0.352 g, 1 mmol), H_3bdc (0.206 g, 1 mmol), water (10 ml) in the presence of H_2SO_4 (0.038 g, 0.385 mmol) was stirred vigorously for 30 min and then sealed in a 20 ml Teflon-lined stainless-steel autoclave. The autoclave was heated and maintained at 443 K for 3 days, and then cooled to room temperature at 5 K h^{-1}. Colorless block crystals of the title compound were obtained.

S3. Refinement

Water H atoms were tentatively located in difference Fourier maps and were refined with distance restraints of O—H = 0.84 and H···H = 1.35 Å, and with U_{iso}(H) = 1.5U_{eq}(O). H atoms bound to C and N atoms were positioned geometrically and refined as riding atoms, with C—H = 0.93 and N—H = 0.86 Å and with U_{iso}(H) = 1.2U_{eq}(C, N). H1A atom attached to N1 was refined with U_{iso}(H) = 0.035 $Å^2$. The highest residual electron density was found at 1.00 Å from Eu1 atom and the deepest hole at 0.97 Å from Eu1 atom.

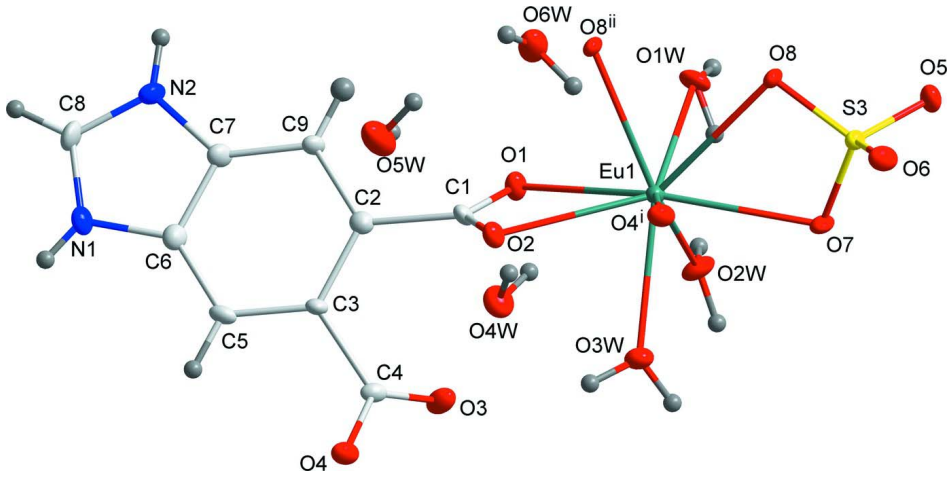

Figure 1

The asymmetric unit of the title compound. Displacement ellipsoids are drawn at the 30% probability level. [Symmetry codes: (i) 2-x, -y, -z; (ii) 2-x, 1-y, -z.]

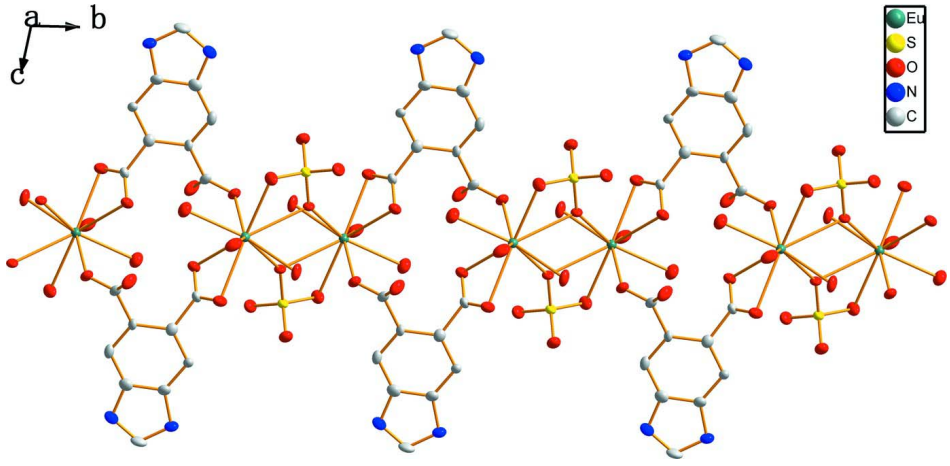

Figure 2

A view of the chain structure along [0 1 0].

catena-poly[[[triaquaeuropium(III)]-bis(*μ*-1*H*,3*H*-benzimidazol-3-ium-5,6-dicarboxylato-$\kappa^3O^5,O^{5'}$:O^6)-[triaquaeuropium(III)]-di-*μ*-sulfato-κ^3O:O,O';κ^3O,O':O'] hexahydrate]

Crystal data

$[Eu_2(C_9H_5N_2O_4)_2(SO_4)_2(H_2O)_6]\cdot 6H_2O$
$M_r = 1122.58$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 7.1261\ (16)$ Å
$b = 9.581\ (2)$ Å
$c = 12.424\ (3)$ Å
$\alpha = 100.496\ (3)°$
$\beta = 98.060\ (3)°$
$\gamma = 94.979\ (3)°$
$V = 820.3\ (3)$ Å^3
$Z = 1$
$F(000) = 552$
$D_x = 2.273$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 3240 reflections
$\theta = 2.5–25.2°$
$\mu = 4.03$ mm^{-1}
$T = 298$ K
Block, colorless
0.30 × 0.26 × 0.20 mm

Data collection

Bruker APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
T_{min} = 0.310, T_{max} = 0.446
4076 measured reflections
2841 independent reflections
2669 reflections with $I > 2\sigma(I)$
R_{int} = 0.024
θ_{max} = 25.2°, θ_{min} = 1.7°
h = −8→8
k = −10→11
l = −14→14

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.097
S = 1.02
2841 reflections
248 parameters
0 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
$w = 1/[\sigma^2(F_o^2) + (0.0656P)^2 + 2.2735P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 1.82 e Å^{-3}
$\Delta\rho_{min}$ = −2.51 e Å^{-3}

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Eu1	0.82011 (3)	0.30949 (3)	−0.00038 (2)	0.01547 (13)
S3	0.7557 (2)	0.48078 (15)	−0.19659 (11)	0.0178 (3)
O1	0.8381 (6)	0.2686 (5)	0.1916 (3)	0.0245 (9)
O2	1.0266 (6)	0.1509 (4)	0.0920 (3)	0.0235 (9)
O7	0.6411 (6)	0.3533 (5)	−0.1756 (3)	0.0255 (9)
O8	0.9029 (5)	0.5245 (4)	−0.0939 (3)	0.0197 (8)
O5	0.6331 (6)	0.5948 (5)	−0.2072 (3)	0.0274 (9)
O6	0.8483 (7)	0.4467 (5)	−0.2935 (3)	0.0286 (10)
N1	1.3014 (7)	−0.0260 (6)	0.5455 (4)	0.0249 (11)
N2	1.2981 (7)	0.2039 (6)	0.5675 (4)	0.0251 (11)
H2	1.3174	0.2932	0.5979	0.030*
C1	0.9614 (8)	0.1832 (6)	0.1807 (5)	0.0190 (12)
C2	1.0383 (8)	0.1201 (6)	0.2791 (5)	0.0194 (12)
C3	1.0338 (8)	−0.0312 (6)	0.2662 (4)	0.0164 (11)
C5	1.1219 (8)	−0.0927 (6)	0.3485 (5)	0.0198 (12)
H5	1.1239	−0.1911	0.3393	0.024*
C6	1.2079 (8)	−0.0005 (6)	0.4462 (5)	0.0218 (12)
C7	1.2050 (8)	0.1468 (6)	0.4603 (5)	0.0213 (12)
C8	1.3518 (9)	0.0977 (7)	0.6146 (5)	0.0274 (14)
H8	1.4162	0.1086	0.6866	0.033*
C9	1.1232 (8)	0.2109 (6)	0.3771 (4)	0.0189 (11)
H9	1.1250	0.3095	0.3864	0.023*
O4W	0.5121 (7)	0.1310 (5)	0.2584 (4)	0.0352 (11)
H8W	0.6008	0.1653	0.2294	0.053*

H7W	0.4457	0.2009	0.2736	0.053*
O6W	0.7298 (9)	0.5166 (6)	0.3452 (4)	0.0439 (13)
H11W	0.8442	0.5054	0.3395	0.066*
H12W	0.6655	0.4779	0.2826	0.09 (4)*
O5W	0.6913 (11)	0.3173 (6)	0.4890 (5)	0.0644 (19)
H9W	0.6934	0.3808	0.4506	0.097*
H10W	0.7710	0.3559	0.5453	0.097*
O3W	0.7114 (6)	0.0596 (4)	−0.0781 (4)	0.0283 (10)
H5W	0.6097	0.0179	−0.1180	0.042*
H6W	0.7713	−0.0084	−0.0605	0.042*
O1W	0.7080 (6)	0.5224 (4)	0.0984 (4)	0.0266 (9)
H2W	0.6011	0.5504	0.1051	0.040*
H1W	0.7804	0.5996	0.1181	0.040*
O2W	0.4946 (6)	0.2615 (5)	0.0214 (4)	0.0308 (10)
H4W	0.4110	0.1952	−0.0161	0.046*
H3W	0.4346	0.3063	0.0678	0.046*
C4	0.9079 (8)	−0.1258 (6)	0.1673 (4)	0.0179 (11)
O4	0.9655 (6)	−0.2426 (4)	0.1255 (3)	0.0226 (9)
O3	0.7505 (6)	−0.0878 (5)	0.1382 (4)	0.0290 (10)
H1A	1.323 (11)	−0.109 (9)	0.557 (6)	0.035*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Eu1	0.01833 (18)	0.01343 (19)	0.01383 (18)	0.00052 (11)	0.00124 (11)	0.00220 (12)
S3	0.0222 (7)	0.0163 (7)	0.0138 (6)	−0.0006 (5)	0.0006 (5)	0.0030 (5)
O1	0.031 (2)	0.026 (2)	0.018 (2)	0.0101 (18)	0.0039 (17)	0.0053 (17)
O2	0.032 (2)	0.022 (2)	0.018 (2)	0.0070 (18)	0.0074 (17)	0.0046 (17)
O7	0.027 (2)	0.021 (2)	0.024 (2)	−0.0095 (17)	−0.0053 (17)	0.0065 (17)
O8	0.021 (2)	0.020 (2)	0.0140 (19)	−0.0041 (16)	−0.0042 (15)	0.0017 (16)
O5	0.034 (2)	0.023 (2)	0.024 (2)	0.0087 (18)	−0.0010 (18)	0.0051 (18)
O6	0.042 (3)	0.025 (2)	0.018 (2)	0.0020 (19)	0.0083 (18)	0.0016 (17)
N1	0.029 (3)	0.027 (3)	0.021 (3)	0.005 (2)	0.004 (2)	0.011 (2)
N2	0.033 (3)	0.022 (3)	0.016 (2)	−0.003 (2)	0.002 (2)	−0.001 (2)
C1	0.026 (3)	0.013 (3)	0.018 (3)	0.001 (2)	0.001 (2)	0.004 (2)
C2	0.018 (3)	0.020 (3)	0.020 (3)	0.000 (2)	0.004 (2)	0.004 (2)
C3	0.019 (3)	0.013 (3)	0.017 (3)	−0.001 (2)	0.003 (2)	0.002 (2)
C5	0.024 (3)	0.013 (3)	0.024 (3)	0.002 (2)	0.007 (2)	0.002 (2)
C6	0.024 (3)	0.022 (3)	0.020 (3)	0.000 (2)	0.005 (2)	0.007 (2)
C7	0.025 (3)	0.022 (3)	0.015 (3)	−0.002 (2)	0.005 (2)	0.002 (2)
C8	0.028 (3)	0.039 (4)	0.013 (3)	0.001 (3)	−0.002 (2)	0.007 (3)
C9	0.025 (3)	0.015 (3)	0.016 (3)	−0.001 (2)	0.005 (2)	0.002 (2)
O4W	0.035 (2)	0.037 (3)	0.039 (3)	0.003 (2)	0.012 (2)	0.014 (2)
O6W	0.067 (4)	0.036 (3)	0.024 (3)	0.016 (3)	−0.003 (2)	−0.002 (2)
O5W	0.123 (6)	0.031 (3)	0.033 (3)	0.003 (3)	−0.006 (3)	0.007 (2)
O3W	0.030 (2)	0.019 (2)	0.032 (2)	−0.0014 (18)	−0.0022 (18)	0.0008 (18)
O1W	0.024 (2)	0.014 (2)	0.043 (3)	0.0046 (16)	0.0111 (19)	0.0037 (18)
O2W	0.023 (2)	0.035 (3)	0.028 (2)	−0.0041 (18)	0.0029 (18)	−0.0072 (19)

C4	0.024 (3)	0.015 (3)	0.015 (3)	−0.003 (2)	0.007 (2)	0.002 (2)
O4	0.030 (2)	0.019 (2)	0.019 (2)	0.0003 (17)	0.0081 (17)	−0.0012 (16)
O3	0.024 (2)	0.025 (2)	0.032 (2)	0.0055 (18)	−0.0039 (18)	−0.0061 (19)

Geometric parameters (Å, º)

Eu1—O4^{i}	2.374 (4)	C3—C5	1.375 (8)
Eu1—O2W	2.387 (4)	C3—C4	1.510 (8)
Eu1—O3W	2.427 (4)	C5—C6	1.392 (8)
Eu1—O8^{ii}	2.434 (4)	C5—H5	0.9300
Eu1—O1W	2.439 (4)	C6—C7	1.392 (9)
Eu1—O1	2.474 (4)	C7—C9	1.381 (8)
Eu1—O2	2.518 (4)	C8—H8	0.9300
Eu1—O8	2.607 (4)	C9—H9	0.9300
S3—O6	1.451 (4)	O4W—H8W	0.8415
S3—O5	1.470 (4)	O4W—H7W	0.8612
S3—O7	1.493 (4)	O6W—H11W	0.8423
S3—O8	1.502 (4)	O6W—H12W	0.8471
O1—C1	1.256 (7)	O5W—H9W	0.8390
O2—C1	1.252 (7)	O5W—H10W	0.8403
N1—C8	1.319 (8)	O3W—H5W	0.8408
N1—C6	1.390 (8)	O3W—H6W	0.8534
N1—H1A	0.86 (8)	O1W—H2W	0.8393
N2—C8	1.322 (8)	O1W—H1W	0.8396
N2—C7	1.392 (7)	O2W—H4W	0.8507
N2—H2	0.8600	O2W—H3W	0.8434
C1—C2	1.517 (8)	C4—O3	1.235 (7)
C2—C9	1.387 (8)	C4—O4	1.272 (7)
C2—C3	1.426 (8)		

O4^{i}—Eu1—O2W	140.91 (14)	C8—N1—C6	108.3 (5)
O4^{i}—Eu1—O3W	76.22 (15)	C8—N1—H1A	127 (5)
O2W—Eu1—O3W	71.09 (15)	C6—N1—H1A	124 (5)
O4^{i}—Eu1—O8^{ii}	81.63 (13)	C8—N2—C7	108.3 (5)
O2W—Eu1—O8^{ii}	137.26 (14)	C8—N2—H2	125.8
O3W—Eu1—O8^{ii}	143.77 (14)	C7—N2—H2	125.8
O4^{i}—Eu1—O1W	140.46 (14)	O2—C1—O1	122.2 (5)
O2W—Eu1—O1W	69.33 (15)	O2—C1—C2	118.8 (5)
O3W—Eu1—O1W	140.36 (14)	O1—C1—C2	119.0 (5)
O8^{ii}—Eu1—O1W	71.68 (14)	C9—C2—C3	121.4 (5)
O4^{i}—Eu1—O1	126.79 (14)	C9—C2—C1	119.3 (5)
O2W—Eu1—O1	75.86 (15)	C3—C2—C1	119.1 (5)
O3W—Eu1—O1	92.05 (14)	C5—C3—C2	121.3 (5)
O8^{ii}—Eu1—O1	78.65 (13)	C5—C3—C4	119.1 (5)
O1W—Eu1—O1	76.39 (14)	C2—C3—C4	119.1 (5)
O4^{i}—Eu1—O2	75.47 (14)	C3—C5—C6	116.7 (5)
O2W—Eu1—O2	111.08 (15)	C3—C5—H5	121.6
O3W—Eu1—O2	69.40 (14)	C6—C5—H5	121.6

O8^{ii}—Eu1—O2	77.54 (13)	N1—C6—C5	131.7 (6)
O1W—Eu1—O2	124.10 (14)	N1—C6—C7	106.4 (5)
O1—Eu1—O2	52.20 (13)	C5—C6—C7	121.8 (5)
O4^{i}—Eu1—O8	71.41 (13)	C9—C7—N2	131.6 (6)
O2W—Eu1—O8	116.64 (14)	C9—C7—C6	122.3 (5)
O3W—Eu1—O8	131.57 (13)	N2—C7—C6	106.2 (5)
O8^{ii}—Eu1—O8	64.15 (14)	N1—C8—N2	110.7 (5)
O1W—Eu1—O8	70.87 (13)	N1—C8—H8	124.6
O1—Eu1—O8	136.26 (13)	N2—C8—H8	124.6
O2—Eu1—O8	131.95 (13)	C7—C9—C2	116.4 (5)
O4^{i}—Eu1—Eu1^{ii}	73.90 (10)	C7—C9—H9	121.8
O2W—Eu1—Eu1^{ii}	133.79 (11)	C2—C9—H9	121.8
O3W—Eu1—Eu1^{ii}	149.81 (11)	H8W—O4W—H7W	104.3
O8^{ii}—Eu1—Eu1^{ii}	33.30 (9)	H11W—O6W—H12W	105.6
O1W—Eu1—Eu1^{ii}	67.72 (10)	H9W—O5W—H10W	101.4
O1—Eu1—Eu1^{ii}	109.19 (10)	Eu1—O3W—H5W	132.6
O2—Eu1—Eu1^{ii}	106.55 (10)	Eu1—O3W—H6W	122.9
O8—Eu1—Eu1^{ii}	30.84 (8)	H5W—O3W—H6W	104.1
O6—S3—O5	111.0 (3)	Eu1—O1W—H2W	135.5
O6—S3—O7	112.3 (3)	Eu1—O1W—H1W	120.5
O5—S3—O7	109.6 (3)	H2W—O1W—H1W	101.5
O6—S3—O8	110.1 (3)	Eu1—O2W—H4W	128.4
O5—S3—O8	110.2 (2)	Eu1—O2W—H3W	128.4
O7—S3—O8	103.5 (2)	H4W—O2W—H3W	103.2
C1—O1—Eu1	93.8 (3)	O3—C4—O4	125.0 (5)
C1—O2—Eu1	91.8 (3)	O3—C4—C3	116.9 (5)
S3—O8—Eu1^{ii}	146.0 (2)	O4—C4—C3	117.9 (5)
S3—O8—Eu1	97.84 (18)	C4—O4—Eu1^{i}	135.3 (4)
Eu1^{ii}—O8—Eu1	115.85 (14)		

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*W*—H1*W*···O4^{iii}	0.84	1.90	2.717 (6)	165
O1*W*—H2*W*···O7^{iv}	0.84	2.24	3.049 (6)	163
O2*W*—H3*W*···O5^{iv}	0.84	1.96	2.775 (6)	162
O2*W*—H4*W*···O3^{v}	0.85	1.85	2.659 (6)	159
O3*W*—H5*W*···O4*W*^{v}	0.84	2.07	2.810 (6)	146
O3*W*—H6*W*···O2^{i}	0.85	2.10	2.864 (6)	149
O4*W*—H7*W*···O5^{iv}	0.86	2.34	3.045 (6)	139
O4*W*—H8*W*···O1	0.84	2.04	2.869 (6)	168
O5*W*—H9*W*···O6*W*	0.84	2.03	2.864 (8)	171
O5*W*—H10*W*···O6^{vi}	0.84	2.01	2.790 (7)	154
O6*W*—H11*W*···O6^{ii}	0.84	2.37	3.165 (8)	158
O6*W*—H12*W*···O5^{iv}	0.85	2.20	2.895 (7)	139
O6*W*—H12*W*···O1*W*	0.85	2.46	3.060 (7)	129

N1—H1*A*···O5*W*^{vii}	0.86 (8)	1.96 (8)	2.752 (8)	153 (7)
N1—H1*A*···O4*W*^{vii}	0.86 (8)	2.48 (8)	2.989 (7)	119 (6)
N2—H2···O6*W*^{viii}	0.86	1.91	2.734 (7)	161

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