

Acta Crystallographica Section E

Structure Reports

Online

ISSN 1600-5368

Poly[tetraaquabis(μ_4 -thiophene-2,5-dicarboxylato)(μ_2 -thiophene-2,5-dicarboxylato)dieuropium(III)]

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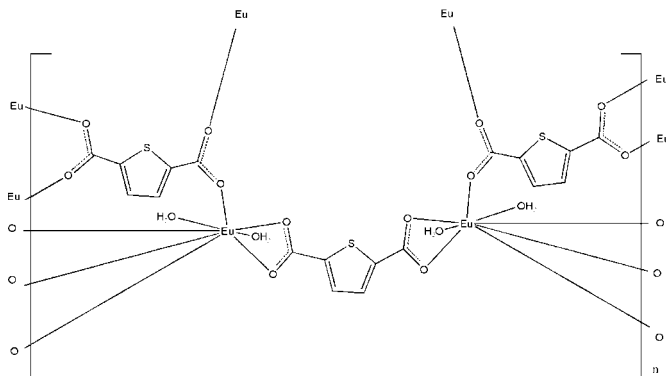
Received 23 May 2012; accepted 28 June 2012

Key indicators: single-crystal X-ray study; $T = 295$ K; mean $\sigma(\text{C}-\text{C}) = 0.008$ Å; R factor = 0.035; wR factor = 0.090; data-to-parameter ratio = 14.6.

The three-dimensional coordination polymer, $[\text{Eu}_2(\text{C}_6\text{H}_2\text{O}_4\text{S})_3(\text{H}_2\text{O})_4]_n$, has been synthesized under hydrothermal conditions. The asymmetric unit comprises one Eu^{3+} cation, two aqua ligands and one and a half thiophene-2,5-dicarboxylate anions (the half-anion being completed by a twofold rotation axis). The Eu^{3+} cation is eight-coordinated in a distorted dodecahedral geometry. The crystal structure features $\text{O}-\text{H}\cdots\text{O}$ hydrogen bonds.

Related literature

For the structures and potential applications of metal hybrid compounds, see: Bo *et al.* (2008). For a number of lanthanide coordination polymers based on pyridinedicarboxylic acid, see: Xu *et al.* (2011). For metal-organic framework structures formed by $4f$ metals and thiophene-2,5-dicarboxylate anions, see: Huang *et al.* (2009).



Experimental

Crystal data

$[\text{Eu}_2(\text{C}_6\text{H}_2\text{O}_4\text{S})_3(\text{H}_2\text{O})_4]$
 $M_r = 886.44$
 Monoclinic, $C2/c$
 $a = 25.366$ (8) Å
 $b = 5.8326$ (14) Å
 $c = 19.008$ (6) Å
 $\beta = 124.136$ (4)°
 $V = 2327.7$ (12) Å³
 $Z = 4$
 Mo $K\alpha$ radiation
 $\mu = 5.69$ mm⁻¹
 $T = 295$ K
 $0.22 \times 0.12 \times 0.11$ mm

Data collection

Bruker SMART APEXII CCD diffractometer
 Absorption correction: multi-scan (*SADABS*; Bruker, 2004)
 $T_{\min} = 0.445$, $T_{\max} = 0.535$
 8572 measured reflections
 2634 independent reflections
 2290 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.061$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.035$
 $wR(F^2) = 0.090$
 $S = 1.00$
 2634 reflections
 180 parameters
 H atoms treated by a mixture of independent and constrained refinement
 $\Delta\rho_{\text{max}} = 1.97$ e Å⁻³
 $\Delta\rho_{\text{min}} = -1.74$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{O7}-\text{H7A}\cdots\text{O4}^{\text{i}}$	0.85	2.11	2.915 (6)	158
$\text{O7}-\text{H7A}\cdots\text{O3}^{\text{ii}}$	0.85	2.53	3.073 (5)	123
$\text{O7}-\text{H7B}\cdots\text{O5}^{\text{iii}}$	0.85	2.03	2.833 (5)	158
$\text{O8}-\text{H8B}\cdots\text{O6}^{\text{iii}}$	0.85	2.10	2.846 (5)	147
$\text{O8}-\text{H8A}\cdots\text{O5}^{\text{iv}}$	0.85	2.46	2.919 (5)	115

Symmetry codes: (i) $-x + \frac{3}{2}, y + \frac{1}{2}, -z + \frac{3}{2}$; (ii) $x, y + 1, z$; (iii) $-x + 2, -y + 1, -z + 2$; (iv) $-x + 2, -y, -z + 2$.

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: *DIAMOND* (Brandenburg, 1999); software used to prepare material for publication: *enCIFer* (Allen *et al.*, 2004) and *PLATON* (Spek, 2009).

This work was supported financially by the Doctoral Fund Project of Shandong Province (BS2009SF019) and the National Natural Science Foundation of China (grants Nos. 21076063 and 20963007).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: RK2364).

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supporting information

Acta Cryst. (2012). E68, m1024 [https://doi.org/10.1107/S1600536812029546]

Poly[tetraaquabis(μ_4 -thiophene-2,5-dicarboxylato)(μ_2 -thiophene-2,5-dicarboxylato)dieuropium(III)]

Xi-Gang Du, Jun Zhang and Jia-Jia Li

S1. Comment

The design and synthesis of metal-hybrid compounds have attracted considerable interest due to their intriguing topological structures and potential applications as functional materials in luminescence, magnetism, host-guest chemistry, catalysis and gas adsorption and separation (Bo *et al.*, 2008). In recent years, a number of lanthanide coordination polymers based on pyridinedicarboxylic acid have been synthesized under hydrothermal conditions (Xu *et al.*, 2011). By contrast with these lanthanide complexes containing only rigid pyridinedicarboxylic ligands, the high-dimensional coordination complexes of 4f metal-organic frameworks formed by H_2tdc (thiophene-2,5-dicarboxylic acid) are still scarce (Huang *et al.*, 2009). Herein, we report a new structure derived from thiophene-2,5-dicarboxylic acid (Scheme 1), namely $[Eu_2(tdc)_3(H_2O)_4]_n$.

A view of the coordination environment of the Eu^{3+} with atom labeling is illustrated in Fig. 1. The Hydrogen-bond are listed in Table 1. The Eu—O bond lengths range from 2.336 (2) Å to 2.493 (1) Å, and the bond angles of O—Eu—O are in the range of 51.87 (11)° to 156.27 (13)°. In structure, *tdc* ligand adopt two different coordination modes, constructing an ordered three-dimensional lanthanide framework (Fig. 2).

S2. Experimental

All chemicals and solvents except $Eu(NO_3)_3$ were purchased and used as received without further purification. $Eu(NO_3)_3$ was prepared by dissolving Eu_2O_3 with concentrated HNO_3 and then evaporating at 373 K until crystal film formed. A mixture of $Eu(NO_3)_3$ (0.3 mmol), KSCN (0.15 mmol), H_2tdc (0.3 mmol) and deionized water (8.0 ml) in a 23 ml teflon-lined autoclave and kept under autogenous pressure at 443 K for 5 days and then cooling to room temperature at a rate of 5 K h^{-1} . Colourless crystals were isolated by filtration.

S3. Refinement

All hydrogen atoms were positioned geometrically and treated as riding, with C—H = 0.93 Å (CH) and $U_{iso}(H) = 1.2U_{eq}(C)$, with C—H = 0.97 Å (CH_2) and $U_{iso}(H) = 1.2U_{eq}(C)$, and with C—H = 0.96 Å (CH_3) and $U_{iso}(H) = 1.5U_{eq}(C)$

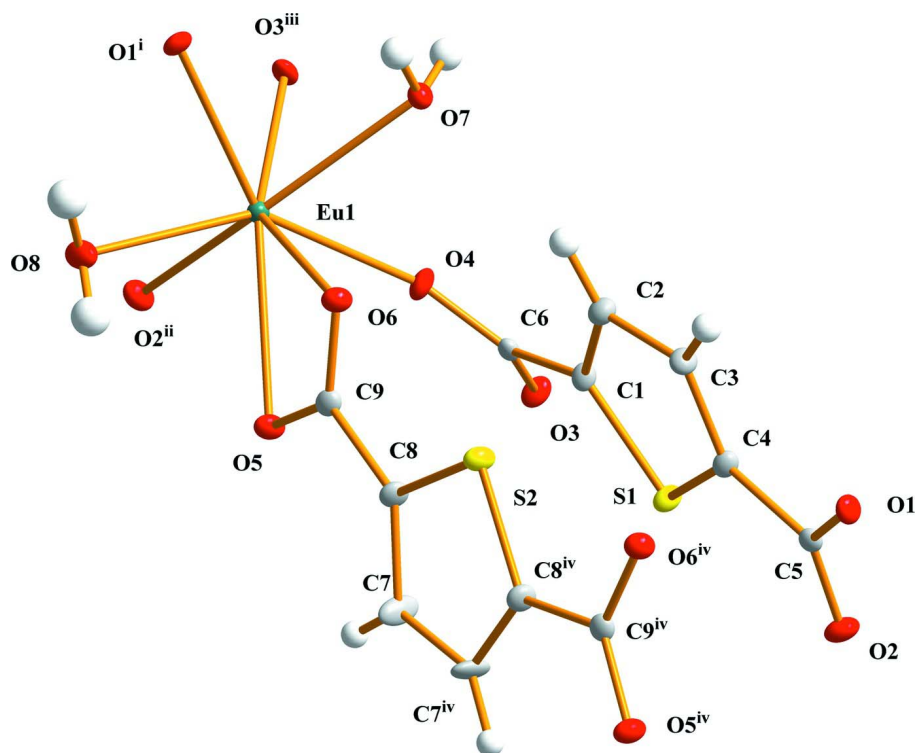


Figure 1

The coordination environment of the Eu^{3+} with the atom numbering scheme. Displacement ellipsoids are presented at 30% probability level. Symmetry codes: (i) $x, 1-y, 1/2+z$; (ii) $x, -y, 1/2+z$; (iii) $3/2-x, 1/2+y, 3/2-z$; (iv) $2-x, y, 1/2-z$;

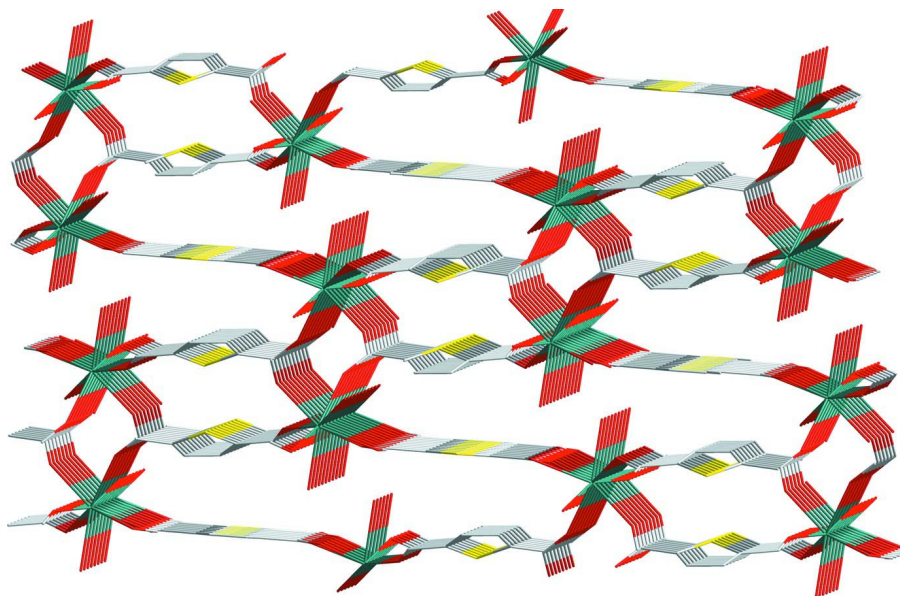


Figure 2

Three-dimensional architecture in the crystal structure of title compound. All the hydrogen atoms are omitted for clarity.

Poly[tetraaquabis(μ_4 -thiophene-2,5-dicarboxylato)(μ_2 -thiophene-2,5-dicarboxylato)dieuropium(III)]

Crystal data

[Eu₂(C₆H₂O₄S)₃(H₂O)₄] $M_r = 886.44$ Monoclinic, $C2/c$ Hall symbol: $-C\ 2yc$ $a = 25.366\ (8)\ \text{\AA}$ $b = 5.8326\ (14)\ \text{\AA}$ $c = 19.008\ (6)\ \text{\AA}$ $\beta = 124.136\ (4)^\circ$ $V = 2327.7\ (12)\ \text{\AA}^3$ $Z = 4$ $F(000) = 1696$ $D_x = 2.530\ \text{Mg m}^{-3}$ Mo $K\alpha$ radiation, $\lambda = 0.71073\ \text{\AA}$

Cell parameters from 8572 reflections

 $\theta = 2.6\text{--}27.5^\circ$ $\mu = 5.69\ \text{mm}^{-1}$ $T = 295\ \text{K}$

Block, colourless

 $0.22 \times 0.12 \times 0.11\ \text{mm}$

Data collection

Bruker SMART APEXII CCD

diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

 φ and ω scansAbsorption correction: multi-scan
(*SADABS*; Bruker, 2004) $T_{\min} = 0.445$, $T_{\max} = 0.535$

8572 measured reflections

2634 independent reflections

2290 reflections with $I > 2\sigma(I)$ $R_{\text{int}} = 0.061$ $\theta_{\max} = 27.5^\circ$, $\theta_{\min} = 2.6^\circ$ $h = -32 \rightarrow 32$ $k = -7 \rightarrow 7$ $l = -24 \rightarrow 24$

Refinement

Refinement on F^2

Least-squares matrix: full

 $R[F^2 > 2\sigma(F^2)] = 0.035$ $wR(F^2) = 0.090$ $S = 1.00$

2634 reflections

180 parameters

0 restraints

Primary atom site location: structure-invariant
direct methodsSecondary atom site location: difference Fourier
mapHydrogen site location: inferred from
neighbouring sitesH atoms treated by a mixture of independent
and constrained refinement $w = 1/[\sigma^2(F_o^2) + (0.0272P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$ $(\Delta/\sigma)_{\max} = 0.026$ $\Delta\rho_{\max} = 1.97\ \text{e}\ \text{\AA}^{-3}$ $\Delta\rho_{\min} = -1.74\ \text{e}\ \text{\AA}^{-3}$

Special details

Geometry. All s.u.'s (except the s.u. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell s.u.'s are taken into account individually in the estimation of s.u.'s in distances, angles and torsion angles; correlations between s.u.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell s.u.'s is used for estimating s.u.'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 (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Eu1	0.866707 (10)	0.33845 (4)	0.887181 (14)	0.01268 (11)
S1	0.80798 (6)	0.0059 (2)	0.56308 (7)	0.0174 (3)
S2	1.0000	0.3059 (3)	0.7500	0.0186 (4)

O1	0.89384 (19)	0.3300 (5)	0.4736 (2)	0.0174 (8)
O2	0.84987 (18)	-0.0175 (6)	0.4448 (2)	0.0222 (8)
O3	0.73304 (15)	-0.0491 (6)	0.6396 (2)	0.0183 (7)
O4	0.79280 (18)	0.1905 (6)	0.7483 (2)	0.0197 (8)
O5	0.92823 (17)	0.0273 (6)	0.8657 (2)	0.0188 (7)
O6	0.94444 (17)	0.3894 (6)	0.8480 (2)	0.0186 (7)
O7	0.83645 (19)	0.6714 (5)	0.7928 (2)	0.0175 (8)
H7A	0.7974	0.7025	0.7705	0.026*
H7B	0.8592	0.7858	0.8214	0.026*
O8	0.96903 (18)	0.2934 (7)	1.0254 (2)	0.0254 (9)
H8B	0.9831	0.4248	1.0475	0.038*
H8A	0.9956	0.2279	1.0181	0.038*
C1	0.8071 (2)	0.1795 (8)	0.6351 (3)	0.0144 (10)
C2	0.8346 (2)	0.3894 (9)	0.6426 (3)	0.0185 (10)
H2	0.8382	0.5055	0.6786	0.022*
C3	0.8565 (2)	0.4072 (9)	0.5900 (3)	0.0171 (10)
H3	0.8758	0.5383	0.5866	0.021*
C4	0.8467 (2)	0.2123 (9)	0.5438 (3)	0.0154 (10)
C5	0.8649 (2)	0.1712 (7)	0.4835 (3)	0.0135 (10)
C6	0.7759 (2)	0.1015 (8)	0.6773 (3)	0.0139 (9)
C7	0.9866 (3)	-0.1143 (10)	0.7733 (4)	0.0283 (13)
C8	0.9766 (2)	0.1034 (9)	0.7912 (3)	0.0172 (10)
C9	0.9486 (2)	0.1754 (8)	0.8384 (3)	0.0153 (11)
H7	0.976 (3)	-0.227 (10)	0.794 (3)	0.018*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Eu1	0.01266 (17)	0.01346 (19)	0.01289 (17)	0.00158 (7)	0.00776 (14)	0.00075 (7)
S1	0.0208 (6)	0.0165 (6)	0.0195 (6)	-0.0051 (5)	0.0142 (5)	-0.0040 (5)
S2	0.0227 (9)	0.0160 (8)	0.0265 (9)	0.000	0.0195 (8)	0.000
O1	0.020 (2)	0.020 (2)	0.0183 (19)	-0.0001 (13)	0.0144 (18)	0.0045 (13)
O2	0.0246 (19)	0.0203 (19)	0.0277 (18)	-0.0023 (15)	0.0183 (17)	-0.0077 (15)
O3	0.0154 (16)	0.0226 (18)	0.0193 (16)	-0.0090 (14)	0.0112 (15)	-0.0068 (15)
O4	0.023 (2)	0.026 (2)	0.0136 (17)	-0.0048 (14)	0.0122 (17)	-0.0045 (14)
O5	0.0225 (18)	0.0167 (18)	0.0263 (18)	0.0018 (14)	0.0193 (16)	0.0025 (15)
O6	0.0195 (18)	0.0171 (18)	0.0240 (18)	0.0007 (14)	0.0150 (16)	-0.0003 (15)
O7	0.019 (2)	0.016 (2)	0.0163 (18)	0.0006 (12)	0.0093 (17)	0.0015 (12)
O8	0.0196 (19)	0.0235 (18)	0.0209 (19)	0.0019 (15)	0.0039 (17)	-0.0051 (16)
C1	0.012 (2)	0.018 (3)	0.014 (2)	-0.0042 (17)	0.007 (2)	-0.0008 (17)
C2	0.020 (3)	0.019 (2)	0.018 (2)	-0.002 (2)	0.011 (2)	-0.003 (2)
C3	0.022 (3)	0.013 (2)	0.020 (2)	-0.0036 (19)	0.013 (2)	0.000 (2)
C4	0.012 (2)	0.020 (2)	0.016 (2)	-0.0009 (19)	0.009 (2)	-0.001 (2)
C5	0.010 (2)	0.015 (3)	0.014 (2)	0.0018 (16)	0.006 (2)	0.0016 (17)
C6	0.012 (2)	0.016 (2)	0.013 (2)	0.0052 (19)	0.0073 (19)	0.0038 (19)
C7	0.050 (4)	0.016 (2)	0.044 (3)	-0.008 (3)	0.042 (3)	-0.002 (3)
C8	0.018 (2)	0.020 (2)	0.022 (2)	0.001 (2)	0.016 (2)	0.000 (2)
C9	0.010 (2)	0.020 (3)	0.015 (2)	-0.0005 (17)	0.006 (2)	-0.0012 (18)

Geometric parameters (Å, °)

Eu1—O2 ⁱ	2.326 (3)	O4—C6	1.275 (6)
Eu1—O1 ⁱⁱ	2.375 (3)	O5—C9	1.259 (6)
Eu1—O3 ⁱⁱⁱ	2.376 (3)	O6—C9	1.274 (5)
Eu1—O4	2.382 (4)	O7—H7A	0.8500
Eu1—O7	2.456 (3)	O7—H7B	0.8500
Eu1—O8	2.461 (4)	O8—H8B	0.8500
Eu1—O6	2.486 (4)	O8—H8A	0.8501
Eu1—O5	2.572 (3)	C1—C2	1.376 (7)
S1—C1	1.713 (5)	C1—C6	1.480 (7)
S1—C4	1.718 (5)	C2—C3	1.392 (7)
S2—C8 ^{iv}	1.697 (5)	C2—H2	0.9300
S2—C8	1.697 (5)	C3—C4	1.372 (7)
O1—C5	1.260 (6)	C3—H3	0.9300
O1—Eu1 ^v	2.375 (3)	C4—C5	1.476 (7)
O2—C5	1.258 (5)	C7—C8	1.373 (8)
O2—Eu1 ^{vi}	2.326 (3)	C7—C7 ^{iv}	1.389 (11)
O3—C6	1.262 (6)	C7—H7	0.87 (6)
O3—Eu1 ^{vii}	2.376 (3)	C8—C9	1.484 (7)
O2 ⁱ —Eu1—O1 ⁱⁱ	112.82 (13)	C9—O6—Eu1	94.0 (3)
O2 ⁱ —Eu1—O3 ⁱⁱⁱ	82.43 (12)	Eu1—O7—H7A	109.4
O1 ⁱⁱ —Eu1—O3 ⁱⁱⁱ	77.54 (13)	Eu1—O7—H7B	109.4
O2 ⁱ —Eu1—O4	89.55 (13)	H7A—O7—H7B	109.5
O1 ⁱⁱ —Eu1—O4	143.48 (13)	Eu1—O8—H8B	109.3
O3 ⁱⁱⁱ —Eu1—O4	77.34 (13)	Eu1—O8—H8A	109.3
O2 ⁱ —Eu1—O7	156.27 (13)	H8B—O8—H8A	109.5
O1 ⁱⁱ —Eu1—O7	73.27 (14)	C2—C1—C6	127.7 (5)
O3 ⁱⁱⁱ —Eu1—O7	76.49 (12)	C2—C1—S1	112.1 (4)
O4—Eu1—O7	75.39 (12)	C6—C1—S1	120.2 (3)
O2 ⁱ —Eu1—O8	76.92 (13)	C1—C2—C3	112.0 (5)
O1 ⁱⁱ —Eu1—O8	68.02 (13)	C1—C2—H2	124.0
O3 ⁱⁱⁱ —Eu1—O8	128.08 (13)	C3—C2—H2	124.0
O4—Eu1—O8	147.93 (13)	C4—C3—C2	113.4 (5)
O7—Eu1—O8	125.05 (13)	C4—C3—H3	123.3
O2 ⁱ —Eu1—O6	128.58 (12)	C2—C3—H3	123.3
O1 ⁱⁱ —Eu1—O6	98.00 (13)	C3—C4—C5	127.6 (5)
O3 ⁱⁱⁱ —Eu1—O6	146.20 (12)	C3—C4—S1	111.3 (4)
O4—Eu1—O6	88.55 (12)	C5—C4—S1	121.1 (4)
O7—Eu1—O6	70.23 (13)	O2—C5—O1	124.5 (5)
O8—Eu1—O6	78.11 (13)	O2—C5—C4	118.1 (4)
O2 ⁱ —Eu1—O5	78.18 (12)	O1—C5—C4	117.3 (4)
O1 ⁱⁱ —Eu1—O5	135.91 (12)	O3—C6—O4	123.7 (5)
O3 ⁱⁱⁱ —Eu1—O5	145.99 (12)	O3—C6—C1	117.3 (4)
O4—Eu1—O5	74.85 (12)	O4—C6—C1	119.0 (4)
O7—Eu1—O5	114.24 (12)	C8—C7—C7 ^{iv}	112.4 (3)
O8—Eu1—O5	73.97 (12)	C8—C7—H7	116 (4)

O6—Eu1—O5	51.87 (11)	C7 ^{iv} —C7—H7	131 (4)
C1—S1—C4	91.2 (2)	C7—C8—C9	128.9 (5)
C8 ^{iv} —S2—C8	91.8 (4)	C7—C8—S2	111.7 (4)
C5—O1—Eu1 ^v	137.3 (3)	C9—C8—S2	119.4 (4)
C5—O2—Eu1 ^{vi}	154.6 (3)	O5—C9—O6	121.7 (5)
C6—O3—Eu1 ^{vii}	142.1 (3)	O5—C9—C8	120.1 (4)
C6—O4—Eu1	155.3 (3)	O6—C9—C8	118.1 (4)
C9—O5—Eu1	90.4 (3)		
O2 ⁱ —Eu1—O4—C6	-109.1 (8)	C1—S1—C4—C5	179.0 (4)
O1 ⁱⁱ —Eu1—O4—C6	121.1 (8)	Eu1 ^{vi} —O2—C5—O1	40.7 (11)
O3 ⁱⁱⁱ —Eu1—O4—C6	168.6 (8)	Eu1 ^{vi} —O2—C5—C4	-140.3 (6)
O7—Eu1—O4—C6	89.5 (8)	Eu1 ^v —O1—C5—O2	91.7 (6)
O8—Eu1—O4—C6	-45.1 (9)	Eu1 ^v —O1—C5—C4	-87.3 (6)
O6—Eu1—O4—C6	19.5 (8)	C3—C4—C5—O2	-177.7 (5)
O5—Eu1—O4—C6	-31.2 (8)	S1—C4—C5—O2	1.7 (7)
O2 ⁱ —Eu1—O5—C9	-174.6 (3)	C3—C4—C5—O1	1.4 (8)
O1 ⁱⁱ —Eu1—O5—C9	-63.9 (3)	S1—C4—C5—O1	-179.2 (4)
O3 ⁱⁱⁱ —Eu1—O5—C9	128.8 (3)	Eu1 ^{vii} —O3—C6—O4	36.1 (8)
O4—Eu1—O5—C9	92.6 (3)	Eu1 ^{vii} —O3—C6—C1	-142.9 (4)
O7—Eu1—O5—C9	26.7 (3)	Eu1—O4—C6—O3	140.6 (6)
O8—Eu1—O5—C9	-95.0 (3)	Eu1—O4—C6—C1	-40.4 (10)
O6—Eu1—O5—C9	-7.7 (3)	C2—C1—C6—O3	152.4 (5)
O2 ⁱ —Eu1—O6—C9	24.1 (3)	S1—C1—C6—O3	-24.0 (6)
O1 ⁱⁱ —Eu1—O6—C9	151.9 (3)	C2—C1—C6—O4	-26.7 (8)
O3 ⁱⁱⁱ —Eu1—O6—C9	-128.6 (3)	S1—C1—C6—O4	156.9 (4)
O4—Eu1—O6—C9	-64.1 (3)	C7 ^{iv} —C7—C8—C9	179.4 (7)
O7—Eu1—O6—C9	-139.1 (3)	C7 ^{iv} —C7—C8—S2	0.3 (9)
O8—Eu1—O6—C9	86.5 (3)	C8 ^{iv} —S2—C8—C7	-0.1 (3)
O5—Eu1—O6—C9	7.7 (3)	C8 ^{iv} —S2—C8—C9	-179.3 (5)
C4—S1—C1—C2	1.0 (4)	Eu1—O5—C9—O6	14.0 (5)
C4—S1—C1—C6	177.9 (4)	Eu1—O5—C9—C8	-164.0 (4)
C6—C1—C2—C3	-176.9 (5)	Eu1—O6—C9—O5	-14.6 (5)
S1—C1—C2—C3	-0.2 (6)	Eu1—O6—C9—C8	163.5 (4)
C1—C2—C3—C4	-1.0 (7)	C7—C8—C9—O5	-2.5 (8)
C2—C3—C4—C5	-178.9 (5)	S2—C8—C9—O5	176.5 (4)
C2—C3—C4—S1	1.7 (6)	C7—C8—C9—O6	179.4 (6)
C1—S1—C4—C3	-1.5 (4)	S2—C8—C9—O6	-1.6 (6)

Symmetry codes: (i) $x, -y, z+1/2$; (ii) $x, -y+1, z+1/2$; (iii) $-x+3/2, y+1/2, -z+3/2$; (iv) $-x+2, y, -z+3/2$; (v) $x, -y+1, z-1/2$; (vi) $x, -y, z-1/2$; (vii) $-x+3/2, y-1/2, -z+3/2$.

Hydrogen-bond geometry ($\text{\AA}, ^\circ$)

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O7—H7A \cdots O4 ⁱⁱⁱ	0.85	2.11	2.915 (6)	158
O7—H7A \cdots O3 ^{viii}	0.85	2.53	3.073 (5)	123
O7—H7B \cdots O5 ^{viii}	0.85	2.03	2.833 (5)	158

O8—H8B···O6 ^{ix}	0.85	2.10	2.846 (5)	147
O8—H8A···O5 ^x	0.85	2.46	2.919 (5)	115

Symmetry codes: (iii) $-x+3/2, y+1/2, -z+3/2$; (viii) $x, y+1, z$; (ix) $-x+2, -y+1, -z+2$; (x) $-x+2, -y, -z+2$.