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Europium(III) sulfate hydroxide

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(S–O) = 0.005 Å
R factor = 0.022
wR factor = 0.052
Data-to-parameter ratio = 10.3

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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$Eu(SO_4)(OH)$ was obtained hydrothermally from an aqueous solution of europium(III) nitrate, trimethylamine and sulfuric acid. The structure features nine-coordinated europium with sulfate and hydroxide anions acting as bridging ligands.

Comment

Over the past few decades, the synthesis of new three-dimensional frameworks has received great attention, because of their functional applications in catalysis, ion-exchange and optical devices. As the building elements of open-frameworks, not only silicon but also germanium oxoanions have been chosen to synthesize new frameworks (Li *et al.*, 1998; Lin *et al.*2003; Plévert *et al.*, 2001; Xu, Fan, Chino *et al.*, 2004; Xu, Fan, Elangovan *et al.*, 2004). In the past few years, an important advance in the synthesis of inorganic materials has been achieved by the study of lanthanide frameworks (Zhang *et al.*, 2004; Yuan *et al.*, 2004; Xu *et al.*, 2006; Doran *et al.*, 2002). In this work, we designed and synthesized the title compound, europium(III) sulfate hydroxide, which features a three-dimensional framework.

Similar to $La(SO_4)(OH)$ (Zhang *et al.*, 2004), the framework of the title compound features EuO_9 polyhedra and SO_4 tetrahedra. As shown in Fig. 1, the asymmetric unit contains one Eu^{3+} ion, one SO_4^{2-} group and one hydroxide group. The coordination about Eu is achieved by six bridging sulfate ions;

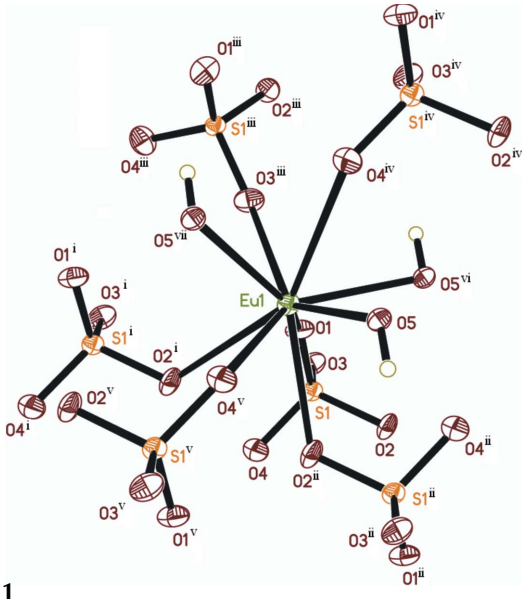

Figure 1
Part of the polymeric structure of the title compound, showing the coordination of Eu. Displacement ellipsoids are drawn at the 70% probability level. [Symmetry codes: (i) $x-\frac{1}{2}, -y+\frac{3}{2}, z+\frac{1}{2}$; (ii) $-x, -y+1, -z$; (iii) $x-1, y, z$; (iv) $-x+1, -y+1, -z$; (v) $x, y, z+1$; (vi) $-x+1, -y+1, -z+1$; (vii) $-x, -y+1, -z+1$.]

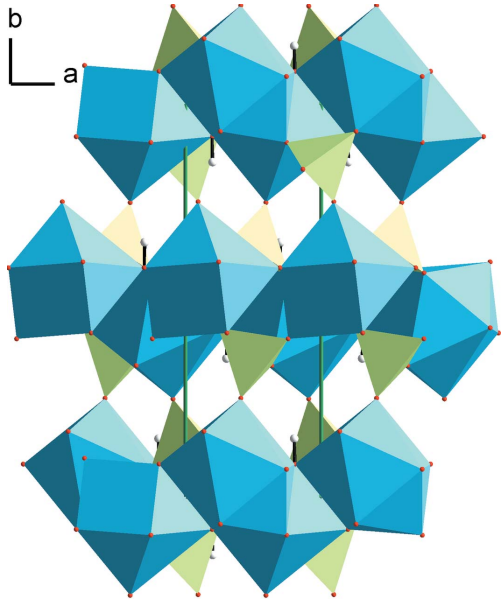

Figure 2
The crystal packing of $Eu(SO_4)(OH)$ in a view along the *c* axis.

each S atom makes four S—O—Eu linkages through bridging O atoms. The coordination is completed by three hydroxide ions, which act as bridging ligands between three Eu^{3+} ions.

The Eu atom has typical geometrical parameters (Table 1); the Eu–O and O—Eu—O bond distances and bond angles are in agreement with those found in other reported rare-earth compounds (Zhang *et al.*, 2004; Yuan *et al.*, 2004). The geometry of the sulfate ions is unexceptional. Fig. 2 shows the three-dimensional arrangement in the crystal structure, displaying the way in which the different Eu ions are connected by bridging sulfate and hydroxide groups, yielding a layered structure.

Experimental

The title compound was synthesized hydrothermally from a mixture of $Eu(NO_3)_3{\cdot}6H_2O$ (Shanghai Chemical Reagent Factory), H_2SO_4 (Tianjin Kermel Chemical Reagents Development Center), water and trimethylamine (Beijing Yili Chemical Reagents Factory). In a typical synthesis, $Eu(NO_3)_3{\cdot}6H_2O$ (0.45 g) was dissolved in a mixture of trimethylamine (0.74 g) and water (3.5 g) followed by the addition of H_2SO_4 (98%, 0.03 g) with constant stirring. The mixture was kept in a 25 ml Teflon-lined steel autoclave at 453 K for 6 d. The autoclave was cooled slowly to room temperature, and then the product was filtered off, washed with distilled water and dried at room temperature. Colorless block-shaped crystals of the title compound were obtained.

Crystal data

$Eu(SO_4)(OH)$
M_r = 265.03
Monoclinic, $P2_1/n$
a = 4.4195 (8) Å
b = 12.280 (2) Å
c = 6.7919 (12) Å
β = 106.389 (2)°
V = 353.64 (11) Å^3
Z = 4
D_x = 4.978 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 18.20 mm^{-1}
T = 293 (2) K
Block, colorless
0.09 × 0.09 × 0.06 mm

Data collection

Bruker APEX2 CCD diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003)
T_{min} = 0.291, T_{max} = 0.408
(expected range = 0.239–0.335)
1879 measured reflections
701 independent reflections
644 reflections with $I > 2\sigma(I)$
R_{int} = 0.026
θ_{max} = 26.0°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.022
$wR(F^2)$ = 0.052
S = 1.04
701 reflections
68 parameters
Only H-atom coordinates refined
$w = 1/[\sigma^2(F_o^2) + (0.0301P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 1.56 e Å^{-3}
$\Delta\rho_{min}$ = −0.89 e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.0147 (9)

Table 1
Selected geometric parameters (Å, °).

Eu1—O3^{i}	2.332 (4)	Eu1—O4^{vi}	2.578 (5)
Eu1—O5	2.393 (4)	Eu1—O4^{vii}	2.782 (4)
Eu1—O5^{ii}	2.397 (4)	S1—O1	1.455 (4)
Eu1—O1	2.450 (4)	S1—O3	1.457 (5)
Eu1—O2^{iii}	2.498 (5)	S1—O4	1.469 (4)
Eu1—O2^{iv}	2.501 (4)	S1—O2	1.500 (4)
Eu1—O5^{v}	2.503 (4)		
O3^{i}—Eu1—O5	135.42 (15)	O1—S1—O4	111.9 (3)
O5^{ii}—Eu1—O1	71.56 (15)	O3—S1—O4	109.5 (3)
O5^{ii}—Eu1—O2^{iii}	139.03 (14)	O1—S1—O2	108.9 (3)
O5—Eu1—O4^{vii}	59.28 (14)	O3—S1—O2	108.5 (2)
O1—S1—O3	110.7 (2)	O4—S1—O2	107.3 (3)

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

The highest peak in the difference map is 0.88 (2) Å from atom Eu1. The H atom was located in a difference Fourier map and the positional parameters were refined [O—H = 0.84 (2) Å].

Data collection: *APEX2* (Bruker, 2005); cell refinement: *SAINT* (Bruker, 2005); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

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