Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Cerium(III) hydroxide sulfate, $Ce(OH)SO_4$

Yan Yang,[a,b] Li-Hong Zhu,[c] Ming-Hua Zeng[a] and Xiao-Long Feng[d]*

[a]Department of Chemistry, Guangxi Normal University, Guilin, Guangxi 541000, People's Republic of China, [b]Department of Chemistry, Yulin Normal College, Yulin, Guangxi 537000, People's Republic of China, [c]Department of Chemistry, Huanggang Normal College, Huangzhou, Hubei 441000, People's Republic of China, and [d]Instrumental Analysis and Research Center, Sun Yat-Sen University, 135 West Xingang Road, Guangzhou 510275, People's Republic of China

Correspondence e-mail: pusfxl@zsu.edu.cn

Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(S–O) = 0.003 Å
R factor = 0.015
wR factor = 0.040
Data-to-parameter ratio = 12.1

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

The title compound has been hydrothermally synthesized. The coordination environment of the Ce^{III} atom consists of six sulfate groups and three OH groups. The crystal structure consists of an infinite three-dimensional framework.

Received 2 February 2005
Accepted 16 February 2005
Online 26 February 2005

Comment

Although a number of hydrous lanthanide sulfate complexes have been reported in the past, structural information on anhydrous lanthanide sulfates is still limited (Wickleder, 1999, 2000). Only a few structures of hydroxide sulfates have been reported (Zhang *et al.*, 2004). We report here the structure of cerium hydroxide sulfate, (I).

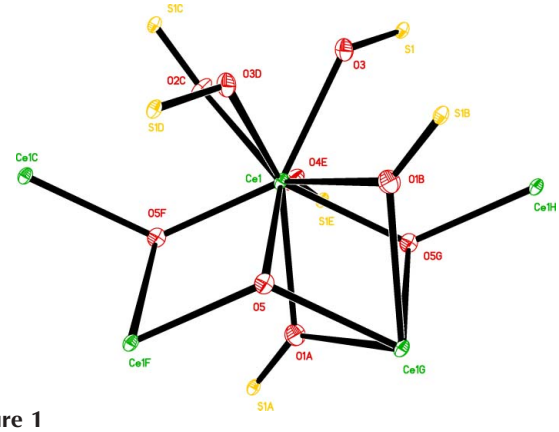

Figure 1
Perspective view of the coordination mode of the cerium ion. [Symmetry codes: (*A*) $x, y, 1+z$; (*B*) $2-x, -y, 1-z$; (*C*) $x-1, y, z$; (*D*) $1-x, 2-y, 1-z$; (*E*) $x\frac{3}{2}-y, \frac{1}{2}+z$; (*F*) $1-x, 2-y, 2-z$; (*G*) $2-x, 2-y, 2-z$; (*H*) $1+x, y, z$.]

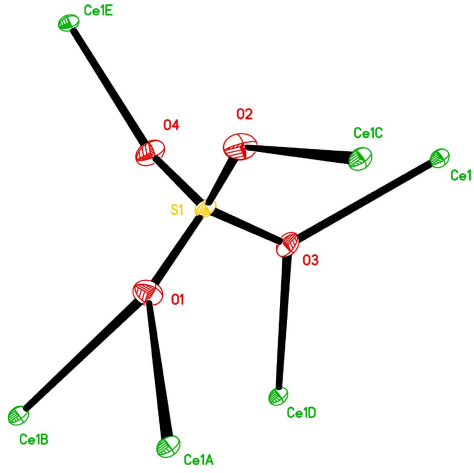

Figure 2
Perspective view of the coordination mode of the sulfate group. [Symmetry Codes: (*A*) $2-x, 2-y, 1-z$; (*B*) $x, y, z-1$; (*C*) $1+x, y, z$; (*D*) $1-x, 2-y, 1-z$; (*E*) $x, \frac{3}{2}-y, z-\frac{1}{2}$.]

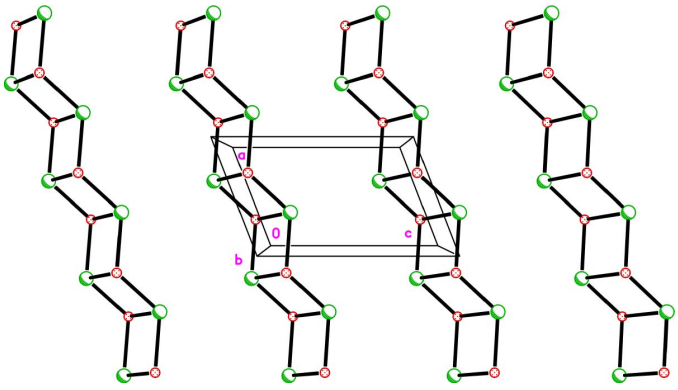

Figure 3
The chains formed by cerium (green circles) and hydroxide (red circles, showing O atoms only). H atoms have been omitted.

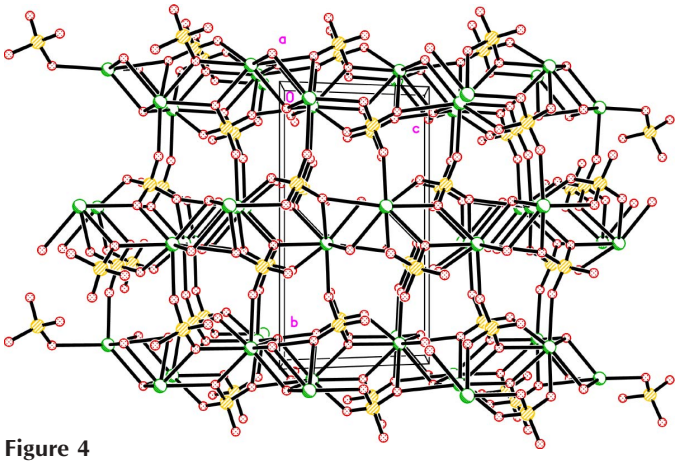

Figure 4
Packing diagram of compound (I). H atoms have been omitted.

In (I), each cerium ion is coordinated by nine O atoms, of which six are from six different sulfate groups, while the other three are from three μ_3-OH groups (Fig. 1). All O atoms of the sulfate group take part in the coordination (Fig. 2). The S atom makes four S—O—Ce linkages through two two-coordinate O atoms (S—O—Ce) and two three-coordinate O atoms (S—μ_3-O—Ce_2).

Compound (I) is, in fact, isostructural with lanthanum(III) hydroxide sulfate (Zhang *et al.*, 2004). In the structure, one OH group links three different cerium ions, which form cerium–hydroxide chains (Fig. 3). The chains are linked by sulfate groups into an infinite three-dimensional framework (Fig. 4). In the structure, the H atom of the OH group forms a weak O—H···O hydrogen bond with one O atom of a sulfate group (Table 2).

Experimental

A mixture of $Ce(NO_3)_3{\cdot}6H_2O$ (0.217 g, 0.5 mmol), $Na_2SO_4{\cdot}10H_2O$ (0.161 g, 0.5 mmol), NaOH (0.040 g, 2 mmol) and H_2O (15 ml) was stirred in air for 20 min and transferred to a 25 ml Teflon-lined stainless steel reactor and heated at 443 K for 4 d. After being cooled slowly at a rate of 6 K h^{-1} to room temperature, colorless crystals suitable for X-ray diffraction analysis were obtained.

Crystal data

$Ce(OH)(SO_4)$	D_x = 4.463 Mg m^{-3}
M_r = 253.19	Mo $K\alpha$ radiation
Monoclinic, $P2_1/c$	Cell parameters from 995 reflections
a = 4.5079 (13) Å	θ = 3.1–27.0°
b = 12.556 (4) Å	μ = 12.52 mm^{-1}
c = 7.135 (2) Å	T = 293 (2) K
β = 111.094 (4)°	Block, colorless
V = 376.8 (2) $Å^3$	0.19 × 0.14 × 0.11 mm
Z = 4	

Data collection

Bruker SMART 1000 CCD diffractometer	820 independent reflections
ω scans	795 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	R_{int} = 0.021
T_{min} = 0.148, T_{max} = 0.251	θ_{max} = 27.0°
3082 measured reflections	$h = -5 \rightarrow 5$
	$k = -16 \rightarrow 16$
	$l = -9 \rightarrow 8$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0217P)^2 + 0.2357P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.015	$(\Delta/\sigma)_{max}$ = 0.001
$wR(F^2)$ = 0.040	$\Delta\rho_{max}$ = 0.94 e $Å^{-3}$
S = 1.23	$\Delta\rho_{min}$ = −0.66 e $Å^{-3}$
820 reflections	
68 parameters	
All H-atom parameters refined	

Table 1
Selected geometric parameters (Å, °).

Ce1—O4^{i}	2.410 (3)	Ce1—O1^{vii}	2.839 (3)
Ce1—O5^{ii}	2.459 (2)	Ce1—Ce1^{iv}	3.7370 (8)
Ce1—O5	2.481 (2)	Ce1—Ce1^{ii}	3.9677 (9)
Ce1—O2^{iii}	2.530 (2)	S1—O2	1.455 (2)
Ce1—O5^{iv}	2.558 (3)	S1—O4	1.459 (2)
Ce1—O3^{v}	2.567 (2)	S1—O1	1.473 (2)
Ce1—O3	2.571 (3)	S1—O3	1.495 (2)
Ce1—O1^{vi}	2.661 (3)		
Ce1^{ii}—O5—Ce1	106.86 (9)	Ce1—O5—Ce1^{iv}	95.72 (8)
Ce1^{ii}—O5—Ce1^{iv}	127.93 (10)		

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

Table 2
Hydrogen-bonding geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O5—H5···O2^{viii}	0.76 (5)	2.52 (5)	3.241 (4)	159 (4)

Symmetry code: (viii) $2-x, \frac{1}{2}+y, \frac{3}{2}-z$.

The H atom was located in a difference map and refined isotropically.

Data collection: *SMART* (Bruker, 1999); cell refinement: *SAINT-Plus* (Bruker, 1999); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXTL* (Bruker, 1999); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

References

Bruker (1999). *SMART* (Version 5.054), *SAINT-Plus* (Version 6.45) and *SHELXTL* (Version 6.14). Bruker AXS Inc., Madison, Wisconsin, USA.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.

Wickleder, M. S. (1999). *Z. Anorg. Allg. Chem.* **625**, 1548–1555.
Wickleder, M. S. (2000). *Z. Anorg. Allg. Chem.* **626**, 1468–1472.
Zhang, Q., Lu, C., Yang, W., Chen, S. & Yu, Y. (2004). *Inorg. Chem. Commun.* **7**, 889–892.