

## Redetermination of dicerium(III) tris(sulfate) tetrahydrate

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Key indicators: single-crystal X-ray study;  $T = 293$  K; mean  $\sigma(\text{Ce}-\text{O}) = 0.003$  Å;  $R$  factor = 0.027;  $wR$  factor = 0.067; data-to-parameter ratio = 10.2.

$\text{Ce}_2(\text{SO}_4)_3(\text{H}_2\text{O})_4$  was obtained hydrothermally from an aqueous solution of cerium(III) oxide, trimethylamine and sulfuric acid. The precision of the structure determination has been significantly improved compared with the previous result [Dereigne (1972). *Bull. Soc. Fr. Mineral. Cristallogr.* **95**, 269–280]. The coordination about the two Ce atoms is achieved by seven and six bridging O atoms from sulfate anions. Each S atom makes four S—O—Ce linkages through bridging O atoms. The coordination sphere of each Ce is completed by two water molecules, which act as terminal ligands.

### Related literature

For related literature, see: Doran *et al.* (2002); Li *et al.* (1998); Plévert *et al.* (2001); Shi (1987); Xu, Cheng & You (2006); Xu, Ding *et al.* (2006); Yuan *et al.* (2004); Zhang *et al.* (2004). For the previous structure determination, see: Dereigne (1972).

### Experimental

#### Crystal data

$\text{Ce}_2(\text{SO}_4)_3(\text{H}_2\text{O})_4$	$V = 1272.5$ (2) Å <sup>3</sup>
$M_r = 640.48$	$Z = 4$
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation
$a = 13.1257$ (14) Å	$\mu = 7.65$ mm <sup>-1</sup>
$b = 7.2520$ (8) Å	$T = 293$ (2) K
$c = 13.3823$ (14) Å	$0.13 \times 0.12 \times 0.10$ mm
$\beta = 92.5720$ (10)°	

#### Data collection

Bruker APEX2 CCD diffractometer	5923 measured reflections
Absorption correction: multi-scan (SADABS; Sheldrick, 2003)	2201 independent reflections
$T_{\min} = 0.437$ , $T_{\max} = 0.515$ (expected range = 0.394–0.466)	2071 reflections with $I > 2\sigma(I)$
	$R_{\text{int}} = 0.032$

#### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.027$	16 restraints
$wR(F^2) = 0.067$	Only H-atom coordinates refined
$S = 1.09$	$\Delta\rho_{\text{max}} = 1.12$ e Å <sup>-3</sup>
2201 reflections	$\Delta\rho_{\text{min}} = -2.16$ e Å <sup>-3</sup>
215 parameters	

Table 1

Selected geometric parameters (Å, °).

Ce1—O10	2.449 (2)	Ce2—O1 <sup>iii</sup>	2.354 (3)
Ce1—O7	2.465 (3)	Ce2—O4 <sup>iv</sup>	2.430 (3)
Ce1—O12 <sup>i</sup>	2.476 (4)	Ce2—O5 <sup>iii</sup>	2.470 (3)
Ce1—O11 <sup>ii</sup>	2.517 (3)	Ce2—O6 <sup>v</sup>	2.489 (3)
Ce1—O4W	2.524 (3)	Ce2—O3W	2.494 (3)
Ce1—O3	2.547 (3)	Ce2—O2W	2.497 (3)
Ce1—O3 <sup>i</sup>	2.621 (3)	Ce2—O9	2.529 (4)
Ce1—O1W	2.647 (3)	Ce2—O8	2.659 (3)
Ce1—O11	2.710 (3)		
O10—Ce1—O3	150.11 (9)	O3—Ce1—O11	53.24 (9)

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

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

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: FI2049).

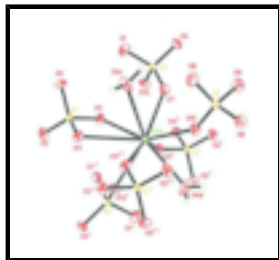
### References

- Bruker (2005). SAINT and APEX2. Bruker AXS Inc., Madison, Wisconsin, USA.
- Dereigne, A. (1972). *Bull. Soc. Fr. Mineral. Cristallogr.* **95**, 269–280.
- Doran, M., Norquist, A. & O'Hare, D. (2002). *Chem. Commun.* pp. 2946–2947.
- Li, H., Eddaoudi, M., Richardson, D. A. & Yaghi, O. M. (1998). *J. Am. Chem. Soc.* **120**, 8567–8568.
- Plévert, J., Gentz, T. M., Laine, A., Li, H., Young, V. G., Yaghi, O. M. & O'Keeffe, M. (2001). *J. Am. Chem. Soc.* **123**, 12706–12707.
- Sheldrick, G. M. (1997a). SHELXS97 and SHELXL97. University of Göttingen, Germany.
- Sheldrick, G. M. (1997b). SHELXTL. Version 5.10. Bruker AXS Inc., Madison, Wisconsin, USA.
- Sheldrick, G. M. (2003). SADABS. University of Göttingen, Germany.
- Shi, B. (1987). *Jiegouhuaxue*, **6**, 70–72.
- Xu, Y., Cheng, L. & You, W. (2006). *Inorg. Chem.* **45**, 7705–7708.
- Xu, Y., Ding, S.-H., Zhou, G.-P. & Liu, Y.-G. (2006). *Acta Cryst.* **E62**, m1749–m1750.
- Yuan, Y., Song, J. & Mao, J. (2004). *Inorg. Chem. Commun.* **7**, 24–26.
- Zhang, Q., Lu, C., Yang, W., Chen, S. & Yu, Y. (2004). *Inorg. Chem. Commun.* **7**, 889–892.

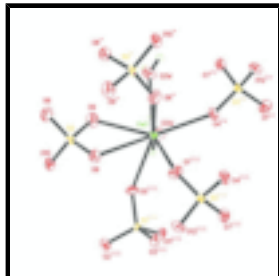




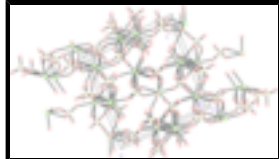
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