Acta Crystallographica Section E
Structure Reports
Online

ISSN 1600-5368

Tetrasodium(I) pentaoxalatodicerate(III) dihydrate

Hui Lu,[a] Yun-Long Fu,[a] Jun-Ying Yang[a] and Seik Weng Ng[b]*

[a]School of Chemistry and Materials Science, Shanxi Normal University, Linfen 041004, People's Republic of China, and [b]Department of Chemistry, University of Malaya, 50603 Kuala Lumpur, Malaysia

Correspondence e-mail: seikweng@um.edu.my

Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.006 Å
R factor = 0.026
wR factor = 0.083
Data-to-parameter ratio = 13.2

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

The Ce atom in the title compound, $Na_4[Ce_2(C_2O_4)_5]\cdot 2H_2O$, is chelated by five oxalate groups in a bicapped square-antiprismatic geometry; one oxalate ligand is located on a centre of inversion. All oxalate groups function in a μ_2-bridging mode, resulting in a three-dimensional network architecture.

Received 14 December 2006
Accepted 15 December 2006

Comment

The preceeding paper reports the structure of tetrasodium pentaoxalatodilanthanate dihydrate (Lu *et al.*, 2007). The cerium analog is isostructural, the compound crystallizing with similar unit-cell dimensions. The Ce atom in $[(H_2O)_2Na_4][(C_2O_4)_5Ce_2]$ has a bicapped square-antiprismatic geometry; water molecules in the three-dimensional polyanionic network interact through hydrogen bonds (Table 2). One oxalate ligand is located on a centre of inversion.

Experimental

A mixture of cerium(III) nitrate x-hydrate (0.217 g, 0.5 mmol), oxalic acid dihydrate ((0.252 g, 2 mmol), nicotinic acid (0.123 g, 1 mmol), sodium hydroxide (0.200 g, 5 mmol) and water (10 ml) was placed in a 15-ml Teflon-lined stainless-steel Parr bomb. The bomb was heated at 433 K for 72 h. Colourless crystals were isolated from the cool solution in about 50% yield.

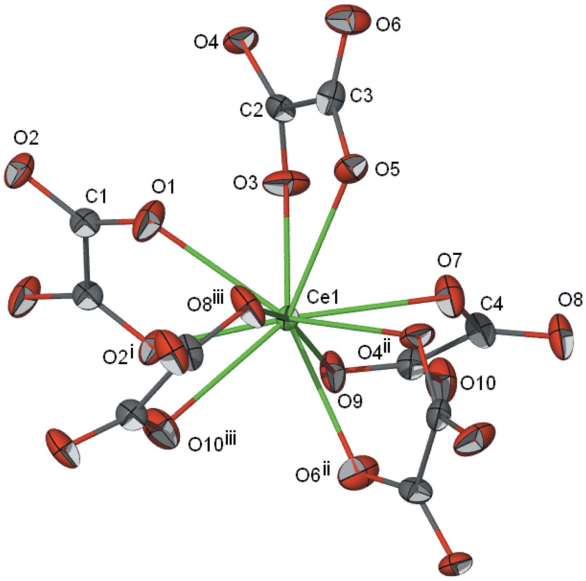

Figure 1
Fig. 1. Displacement ellipsoid plot of the polyanion of $[(H_2O)_2Na_4]^{4+}$ $[(C_2O_4)_5Ce_2]^{4-}$ at the 50% probability level; the sodium cations and water molecule are not shown. Symmetry codes are given in Table 1.

doi:10.1107/S1600536806054560

Crystal data

$Na_4[Ce_2(C_2O_4)_5]\cdot 2H_2O$
$M_r = 848.33$
Monoclinic, $P2_1/n$
$a = 7.8378\ (6)$ Å
$b = 11.647\ (1)$ Å
$c = 11.938\ (1)$ Å
$\beta = 101.030\ (1)°$
$V = 1069.7\ (2)$ Å^3

$Z = 2$
$D_x = 2.634$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 4.39$ mm^{-1}
$T = 293\ (2)$ K
Block, colourless
$0.14 \times 0.06 \times 0.05$ mm

Data collection

Bruker APEX area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.578$, $T_{max} = 0.810$

6885 measured reflections
2369 independent reflections
2131 reflections with $I > 2\sigma(I)$
$R_{int} = 0.030$
$\theta_{max} = 27.5°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.026$
$wR(F^2) = 0.083$
$S = 1.08$
2369 reflections
180 parameters

All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.05P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.89$ e Å^{-3}
$\Delta\rho_{min} = -0.71$ e Å^{-3}

Table 1
Selected bond lengths (Å).

Ce1—O1	2.537 (3)	Ce1—O6^{ii}	2.532 (3)
Ce1—O2^{i}	2.560 (3)	Ce1—O7	2.535 (3)
Ce1—O3	2.526 (3)	Ce1—O8^{iii}	2.548 (3)
Ce1—O4^{ii}	2.688 (3)	Ce1—O9	2.649 (3)
Ce1—O5	2.596 (3)	Ce1—O10^{iii}	2.677 (3)

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

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

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
O1w—H1$\cdots$O3^{iv}	0.85 (1)	2.02 (2)	2.848 (5)	166 (8)
O1w—H2$\cdots$O6^{v}	0.85 (1)	1.99 (3)	2.813 (5)	161 (8)

Symmetry codes: (iv) $-x+1, -y+1, -z$; (v) $-x+2, -y+1, -z$.

The water H atoms were located in a difference Fourier map and were refined with distance restraints of O–H 0.85 (1) and H$\cdots$H 1.39 (1) Å. Their displacement parameters were freely refined.

Data collection: *SMART* (Bruker, 2003); cell refinement: *SAINT* (Bruker, 2003); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2006).

We thank the Natural Scientific Foundation Committee of Shanxi Province (No. 20041031) and the University of Malaya for generously supporting this study.

References

Barbour, L. J. (2001). *J. Supramol. Chem.* **1**, 189–191.
Bruker (2003). *SAINT* (Version 6.36A) and *SMART* (Version 6.36A). Bruker AXS Inc., Madison, Winsonsin, USA.
Lu, H., Fu, Y.-L., Yang, J.-Y. & Ng, S. W. (2007). Acta Cryst. E**63**, m316–m318.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Westrip, S. P. (2006). *publCIF*. In preparation.