Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Cerium triborate, CeB_3O_6

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Received 13 September 2004
Accepted 29 September 2004
Online 9 October 2004

Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(O–B) = 0.007 Å
R factor = 0.031
wR factor = 0.086
Data-to-parameter ratio = 13.1

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

CeB_3O_6 crystallizes in the monoclinic space group $I2/a$ and is a member of the isostructural series $RE B_3O_6$ (RE = La, Pr, Nd, Sm, Eu, Gd, Tb). The structure consists of chains of $[B_6O_{12}]_n^{6-}$ building units, that run parallel to the c axis, and tenfold coordinated Ce^{3+}.

Comment

The binary rare earth oxoborates of general composition $RE B_3O_6$, that are structurally characterized for RE = La (Ysker & Hoffmann, 1970; Abdullaev *et al.*, 1981), RE = Pr (Sieke *et al.*, 2002), RE = Nd (Pakhomov *et al.*, 1972), RE = Sm and Gd (Abdullaev *et al.*, 1975), RE = Eu (Goriounova *et al.*, 2004) and RE = Tb (Goriounova *et al.*, 2003), form an isostructural series and crystallize in the monoclinic space group $I2/a$ (No. 15). For RE = Tb, a further structural modification with orthorhombic symmetry is known (Nikelski & Schleid, 2003), $RE B_3O_6$ with RE = Dy–Lu are also found to adopt this latter structure type (Emme *et al.*, 2004). Synthesis conditions for single crystals of CeB_3O_6 were established during systematic investigations of crystal-growth conditions for binary rare earth borates in our group.

CeB_3O_6 is a member of the isostructural series of $RE B_3O_6$ with monoclinic symmetry $I2/a$. Its structure consists of infinite chains running along the c axis of the structure, which are built of $[B_6O_{12}]_n^{6-}$ structural units (Fig. 1). Tenfold coordinated Ce atoms link the borate chains into a three-dimensional framework. For a more detailed description of the special features of the complex borate polyanion and the Ce coordination, the reader is referred to the isostructural EuB_3O_6 (Goriounova *et al.*, 2004).

Experimental

Crystals of CeB_3O_6 were grown in the pseudo-ternary system Ce_2O_3—B_2O_3—SrO. A homogenized powder mixture of $Ce_2(CO_3)_3{\cdot}5H_2O$ (99.9%, Alfa Aesar), H_3BO_3 (99.8%, Merck) and $SrCO_3$ (98%, Merck) in a ratio of 1 mol% $Ce_2(CO_3)_3{\cdot}5H_2O$/40 mol% H_3BO_3/1.5 mol% $SrCO_3$ was heated in a covered platinum crucible to 1373 K and subsequently cooled with a cooling rate of about 2.0 K h^{-1} to 1173 K. Transparent green single crystals of the title compound were mechanically separated from the strontium borate flux.

Crystal data

CeB_3O_6
M_r = 268.55
Monoclinic, $I2/a$
a = 6.4468 (2) Å
b = 8.1266 (3) Å
c = 7.9300 (2) Å
β = 93.639 (6)°
V = 414.62 (2) Å^3
Z = 4
D_x = 4.302 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 25 reflections
θ = 10.9–22.1°
μ = 10.92 mm^{-1}
T = 293 (2) K
Parallelepiped, green
0.25 × 0.22 × 0.20 mm

Data collection

Nonius MACH3 four-circle diffractometer
$\omega/2\theta$ scans
Absorption correction: ψ scan (*MolEN*; Fair, 1990)
T_{min} = 0.082, T_{max} = 0.113
669 measured reflections
628 independent reflections
620 reflections with $I > 2\sigma(I)$

R_{int} = 0.022
θ_{max} = 30.4°
$h = -9 \rightarrow 9$
$k = 0 \rightarrow 11$
$l = 0 \rightarrow 11$
3 standard reflections
every 100 reflections
frequency: 60 min
intensity decay: 2.4%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.031
$wR(F^2)$ = 0.086
S = 1.19
628 reflections
48 parameters

$w = 1/[\sigma^2(F_o^2) + (0.0553P)^2 + 8.1518P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 2.75 e Å^{-3}
$\Delta\rho_{min}$ = −2.58 e Å^{-3}
Extinction correction: *SHELXL*97
Extinction coefficient: 0.0045 (12)

Table 1
Selected geometric parameters (Å, °).

Ce—O2	2.399 (4)	B1—O1^{iii}	1.416 (7)
Ce—O2^{i}	2.534 (4)	B1—O2	1.328 (7)
Ce—O3	2.586 (4)	B2—O1^{iv}	1.486 (7)
Ce—O1	2.597 (4)	B2—O3^{v}	1.456 (6)
Ce—O1^{ii}	2.828 (4)		
O2—B1—O3^{vi}	126.0 (5)	O3—B2—O1^{vii}	103.7 (2)
O2—B1—O1^{iii}	116.8 (5)	O3^{v}—B2—O1^{iv}	103.7 (2)
O3^{vi}—B1—O1^{iii}	117.2 (5)	O3—B2—O1^{iv}	111.5 (2)
O3^{v}—B2—O3	117.9 (7)	O1^{iv}—B2—O1^{vii}	108.4 (6)
O3^{v}—B2—O1^{vii}	111.5 (2)		

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

Because most of the REB$_3$O$_6$ structures are described in space group $I2/a$, we also used this non-standard setting. The highest peak and deepest hole are located 0.69 and 0.91 Å, respectively, from Ce.

Data collection: *MACH*3 *Server Software* (Enraf–Nonius, 1993); cell refinement: *MACH*3 *Server Software*; data reduction: *MolEN* (Fair, 1990); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ATOMS* (Dowty, 2002); software used to prepare material for publication: *SHELXL*97.

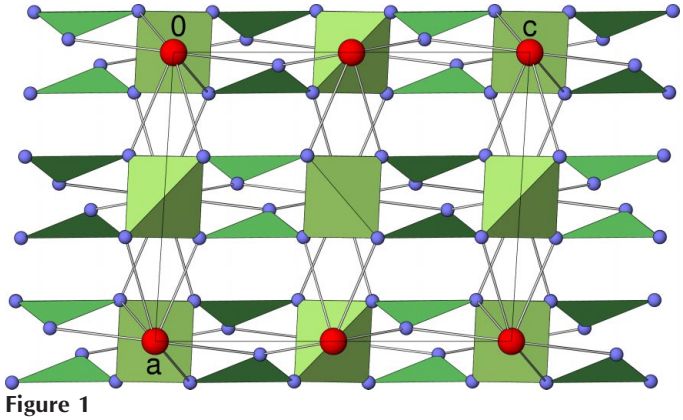

Figure 1
Projection of the structure of the title compound along [010]. Ce atoms are shown as red spheres, O atoms as small blue spheres, [BO$_4$] groups (olive) and [BO$_3$] (green) are represented as polyhedra.

This work was supported by the Deutsche Forschungsgemeinschaft, Graduiertenkolleg 549 'Azentrische Kristalle'.

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