Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Europium triborate, EuB_3O_6

Alexandra Goriounova, Peter Held,* Petra Becker and Ladislav Bohatý

Institut für Kristallographie, Universität zu Köln, Zülpicher Straße 49b, D-50674 Köln, Germany

Correspondence e-mail: peter.held@uni-koeln.de

Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(O–B) = 0.005 Å
R factor = 0.047
wR factor = 0.106
Data-to-parameter ratio = 25.5

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

Received 10 September 2004
Accepted 29 September 2004
Online 9 October 2004

Europium triborate, EuB_3O_6, has been grown from a strontium borate flux. It crystallizes in the space group $I2/a$ and is a member of the isostructural series REB_3O_6 (RE = La, Ce, Pr, Nd, Sm, Gd, Tb). Its structure consists of chains of $[B_6O_{12}]_n^{6-}$ building units, that run parallel to the c axis, and tenfold coordinated Eu^{3+}.

Comment

The binary rare earth oxoborates REB_3O_6 (RE = La, Ce, Pr, Nd, Sm, Gd, Tb) are known to form an isostructural series and crystallize in the monoclinic space group $I2/a$ (Ysker & Hoffmann, 1970; Abdullaev *et al.*, 1975, 1981; Goriounova *et al.*, 2003, 2004; Sieke *et al.*, 2002; Pakhomov *et al.*, 1972). For RE = Tb, a further structural modification with orthorhombic symmetry is known (Nikelski & Schleid, 2003) that was also found for REB_3O_6 with the smaller lanthanides Dy–Lu (Emme *et al.*, 2004). The crystal structure of EuB_3O_6 is reported here for the first time.

In the course of systematic investigations of crystal-growth conditions for binary rare earth borates, methods of synthesis from ternary systems were established that led to single crystals of EuB_3O_6.

EuB_3O_6 is a member of the isostructural series of REB_3O_6 with monoclinic symmetry $I2/a$ (No. 15). Its structure consists of infinite chains that are built of $[B_6O_{12}]_n^{6-}$ structural units that run along the c axis of the structure (Fig. 1). Eu is tenfold coordinated to oxygen and links the borate chains into a three-dimensional framework (Fig. 2). The complex borate polyanion is composed of $[BO_4]$ tetrahedra that are connected *via* two $[BO_3]$ triangles at a time to the adjacent $[BO_4]$ tetrahedra on both sides (Fig. 3). Each $[BO_3]$ is connected to two $[BO_4]$, the bridging O atoms belong also to the coordination polyhedron of one Eu. The non-bridging O atoms of the $[BO_3]$

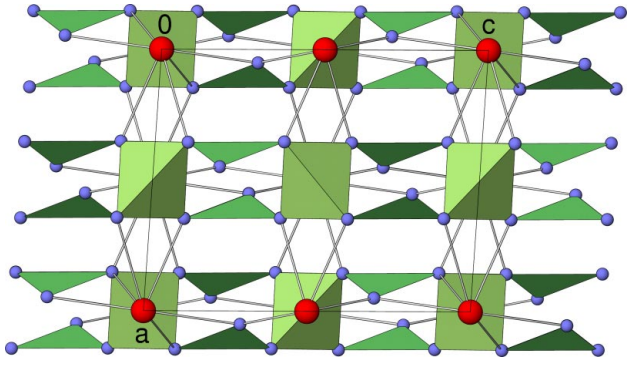

Figure 1
Projection of the structure of the title compound along [010]. Eu atoms are shown as red spheres, O atoms as small blue spheres, $[BO_4]$ groups (olive) and $[BO_3]$ (green) are represented as polyhedra.

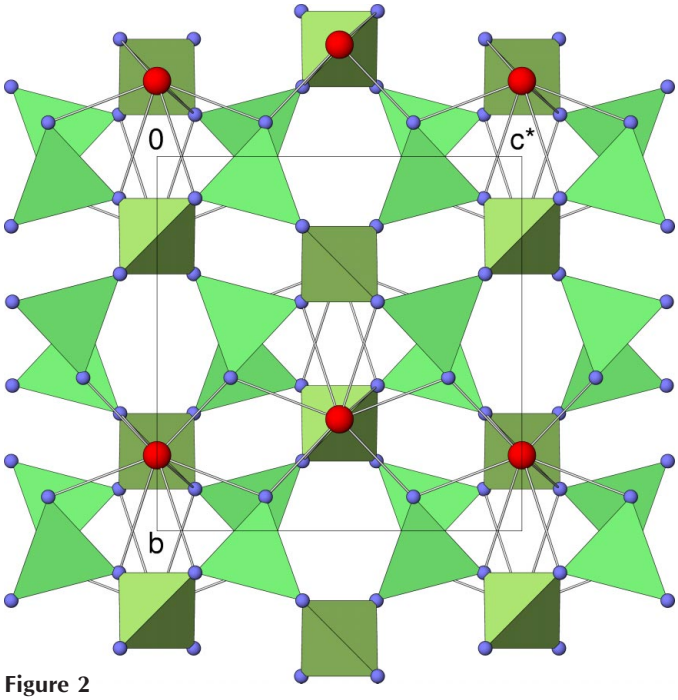

Figure 2
Projection of the structure of the title compound along [100]. Eu atoms are shown as red spheres, O atoms as small blue spheres, [BO_4] groups (olive) and [BO_3] (green) are represented as polyhedra.

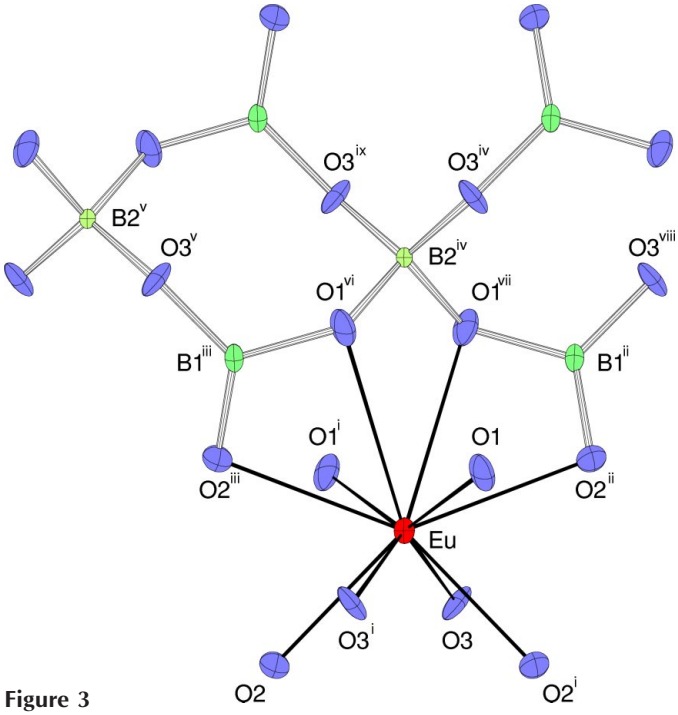

Figure 3
*ORTEP*III projection (Burnett & Johnson, 1996) of the tenfold Eu coordination and the main features of the borate chains of the title compound with the atom-numbering scheme (projection along [100]). Atoms are shown as 75% probability ellipsoids. [Symmetry codes: (i) $\frac{1}{2}-x, y, 1-z$; (ii) $x, -y, z+\frac{1}{2}$; (iii) $\frac{1}{2}-x, \frac{1}{2}-y, \frac{1}{2}-z$; (iv) $x-\frac{1}{2}, 1-y, z$; (v) $x-\frac{1}{2}, y+\frac{1}{2}, z-\frac{1}{2}$; (vi) $-x, 1-y, 1-z$; (vii) $x+\frac{1}{2}, 1-y, z$; (viii) $1-x, y+\frac{1}{2}, \frac{3}{2}-z$; (ix) $1-x, 1-y, 1-z$.]

groups coordinate two Eu simultaneously, each. The irregular [EuO_{10}] coordination polyhedra are connected *via* edges to infinite chains along the *c* axis. The B—O distances of the [BO_3] group range from 1.322 (6) to 1.415 (5) Å. The [BO_3] triangles are substantially distorted with a B—O distance of the non-bridging atom O2 that is significantly shorter than the B—O distances of the bridging atoms O1 and O3. B—O distances of the [BO_4] tetrahedron range from 1.451 (5) to 1.478 (5) Å and fit well into the range of B—O distances found for many other borate structures [see, for comparison, *e.g.* Zobetz (1982) and Zobetz (1990)].

Experimental

Crystals of EuB_3O_6 were grown in the pseudo-ternary system Eu_2O_3—B_2O_3—SrO. A homogenized powder mixture of Eu_2O_3 (99.9%, Meldform metals), H_3BO_3 (99.8%, Merck) and SrO (98%, Merck) in a ratio of 1 mol% Eu_2O_3/40 mol% H_3BO_3/1.5 mol% SrO 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 colorless single crystals of the title compound were mechanically separated from the strontium borate flux.

Crystal data

EuB_3O_6
M_r = 280.38
Monoclinic, $I2/a$
a = 6.2830 (9) Å
b = 8.0331 (6) Å
c = 7.8406 (7) Å
β = 93.70 (1)°
V = 394.91 (7) Å^3
Z = 4
D_x = 4.716 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 25 reflections
θ = 24.8–30.1°
μ = 15.82 mm^{-1}
T = 293 (2) K
Parallelepiped, colourless
0.18 × 0.15 × 0.13 mm

Data collection

Nonius MACH3 four-circle diffractometer
$\omega/2\theta$ scans
Absorption correction: ψ scan (*MolEN*; Fair, 1990)
T_{min} = 0.068, T_{max} = 0.128
4454 measured reflections
1222 independent reflections
1140 reflections with $I > 2\sigma(I)$
R_{int} = 0.070
θ_{max} = 39.9°
$h = -11 \rightarrow 11$
$k = -14 \rightarrow 14$
$l = -14 \rightarrow 14$
3 standard reflections
every 100 reflections
frequency: 60 min
intensity decay: 1.0%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.107
S = 1.09
1222 reflections
48 parameters
$w = 1/[\sigma^2(F_o^2) + (0.0606P)^2 + 3.5865P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 4.50 e Å^{-3}
$\Delta\rho_{min}$ = −3.86 e Å^{-3}
Extinction correction: *SHELXL*97
Extinction coefficient: 0.0093 (13)

Table 1
Selected geometric parameters (Å, °).

Eu—O2	2.338 (3)	B1—O1^{iii}	1.415 (5)
Eu—O3	2.492 (4)	B1—O2	1.322 (6)
Eu—O2^{i}	2.499 (3)	B1—O3^{iv}	1.388 (6)
Eu—O1	2.518 (4)	B2—O1^{v}	1.478 (5)
Eu—O1^{ii}	2.789 (4)	B2—O3^{vi}	1.451 (5)
O2—B1—O3^{iv}	126.6 (4)	O3—B2—O1^{vii}	102.5 (2)
O2—B1—O1^{iii}	116.7 (4)	O3^{vi}—B2—O1^{v}	102.5 (2)
O3^{iv}—B1—O1^{iii}	116.7 (4)	O3—B2—O1^{v}	113.1 (2)
O3^{vi}—B2—O3	117.6 (5)	O1^{vii}—B2—O1^{v}	107.9 (5)
O3^{vi}—B2—O1^{vii}	113.1 (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) $1-x, -y, 1-z$; (v) $1+x, y, z$; (vi) $\frac{3}{2}-x, y, 1-z$; (vii) $\frac{1}{2}-x, y, 1-z$.

Because most of the $RE B_3O_6$ structures are described in space group *I*2/*a*, we also used this non-standard setting. The highest peak and deepest hole are located 0.65 and 0.58 Å, respectively, from Eu.

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.

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

References

Abdullaev, G. K., Mamedov, Kh. S. & Dzhafarov, G. G. (1975). *Sov. Phys. Crystallogr.* **20**, 161–163.
Abdullaev, G. K., Mamedov, Kh. S. & Dzhafarov, G. G. (1981). *Sov. Phys. Crystallogr.* **26**, 473–474.
Burnett, M. N. & Johnson, C. K. (1996). *ORTEP*III. Report ORNL-6895. Oak Ridge National Laboratory, Tennessee, USA.
Dowty, E. (2002). *ATOMS*. Version 6.0. Shape Software, 521 Hidden Valley Road, Kingsport, TN 37663, USA.
Emme, H., Nikelski, T., Schleid, T., Pöttgen, R., Möller, M. H. & Huppertz, H. (2004). *Z. Naturforsch. Teil B*, **59**, 202–215.
Enraf–Nonius (1993). MACH3 Server Software. OpenVMS version. Enraf–Nonius, Delft, The Netherlands.
Fair, C. K. (1990). *MolEN*. Enraf–Nonius, Delft, The Netherlands.
Goriounova, A., Held, P., Becker, P. & Bohatý, L. (2003). *Acta Cryst.* E**59**, i83–i85.
Goriounova, A., Held, P., Becker, P. & Bohatý, L. (2004). *Acta Cryst.* E**60**, i134–i135.
Nikelski, T. & Schleid, T. (2003). *Z. Anorg. Allg. Chem.* **629**, 1017–1022.
Pakhomov, V. I., Sil'nitskaya, G. I., Medvedev, A. V. & Dzhurinskii, B. F. (1972). *Inorg. Mater.* **8**, 1107–1110.
Sheldrick, G. M. (1997). *SHELXS*97 and *SHELXL*97. University of Göttingen, Germany.
Sieke, C., Nikelski, T. & Schleid, T. (2002). *Z. Anorg. Allg. Chem.* **628**, 819–823.
Ysker, J. St & Hoffmann, W. (1970). *Naturwissenschaften*, **57**, 129–130.
Zobetz, E. (1982). *Z. Kristallogr.* **160**, 81–92.
Zobetz, E. (1990). *Z. Kristallogr.* **191**, 45–57.