

$\text{Na}_3\text{Sc}_2(\text{BO}_3)_3$ Yang Zhang,^a Ning Ye^{a*} and
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Key indicators

Single-crystal X-ray study

 $T = 293 \text{ K}$ Mean $\sigma(\text{O}-\text{B}) = 0.002 \text{ \AA}$ R factor = 0.019 wR factor = 0.055

Data-to-parameter ratio = 11.3

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

Single crystals of trisodium discandium trisborate have been grown by slowly cooling a NaBO_2 -containing melt from 1273 K to room temperature. The title compound adopts a new structure type and contains distorted ScO_6 octahedra, NaO_8 polyhedra and triangular BO_3 groups as simple building units. Two ScO_6 octahedra share triangular faces along the c axis, forming an $[\text{Sc}_2\text{O}_9]$ dimer. By sharing corners and edges with the other building units, the three-dimensional framework is accomplished. All atoms except O1 are in special positions: Sc (site symmetry 3.), Na (.2), O2 (.2) and B (.2).

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Comment

The title compound, $\text{Na}_3\text{Sc}_2(\text{BO}_3)_3$ (I), was found from analysis of phase equilibria in the system $\text{Na}_2\text{O}-\text{Sc}_2\text{O}_3-\text{B}_2\text{O}_3$, in which the monoclinic compound NaScB_2O_5 has been reported previously (Becker & Held, 2001). Although $\text{Na}_3\text{La}_2(\text{BO}_3)_3$ (Zhang *et al.*, 2001), which can be considered as a shortite $[\text{Na}_2\text{Ca}_2(\text{CO}_3)_3]$ derivative (Dickens *et al.*, 1971), is of the same formula type as compound (I), the latter adopts a new structure type. As shown in Figs. 1 and 2, the structure contains distorted ScO_6 octahedra (3. symmetry), NaO_8 polyhedra (.2 symmetry) and triangular BO_3 groups (.2

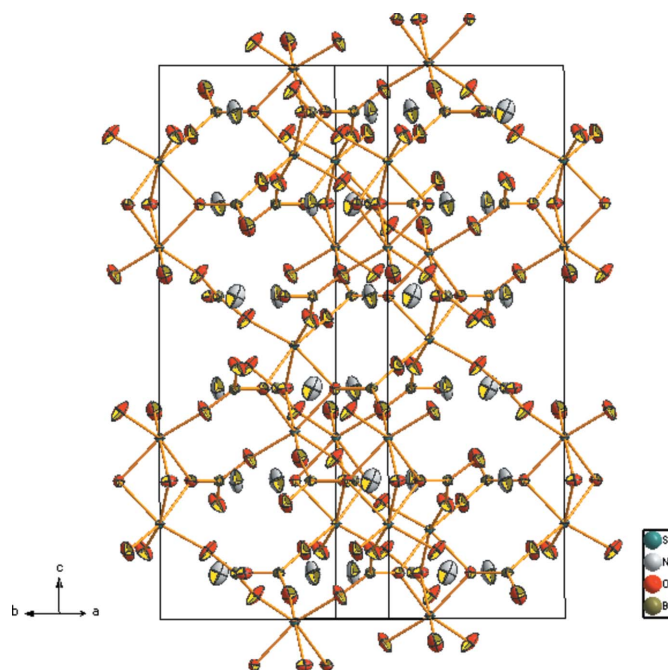


Figure 1

The structure of (I) in a projection approximately along the $[\bar{1}\bar{1}0]$ direction with displacement ellipsoids drawn at the 85% probability level. Na—O bonds have been omitted for clarity.

symmetry). Selected bond lengths and angles for these single building units are listed in Table 1.

The six O atoms around the Sc atom are distorted from an ideal octahedron along the threefold axis. The Sc–O bonds can be classified into two groups with different bond lengths of 2.0146 (11) Å for Sc–O1 and 2.1816 (11) Å for Sc–O2, which extend in opposite directions along the threefold axis. Two ScO₆ octahedra share a triangular face containing three O2 atoms, forming an [Sc₂O₉] group along the *c* axis. These groups are linked by planar BO₃ triangles by sharing vertices, forming a three-dimensional network. The Na atoms are located in the vacancies of the network and are eightfold-coordinated by O atoms with bond lengths ranging from 2.4302 (14) to 2.8220 (12) Å. The average B–O bond length of 1.368 (2) Å, as well as the O–B–O angles of essentially 120°, indicate a nearly ideal trigonal symmetry, which is in good agreement with the results of geometric studies for the triangular BO₃ group (Zobetz, 1982).

Experimental

Single crystals of compound (I) were grown using a NaBO₂ flux. The ratio of the mixture for crystal growth was 1:5:5 of Sc₂O₃ (Sinopharm Reagent, 99.99%), B₂O₃ (Tongya Materials, 99.8%) and Na₂CO₃ (Hongguang Materials, 99.8%). The mixture was heated in a Pt crucible to 1273 K, held at this temperature for several hours, and then cooled at a rate of 3 K h⁻¹ from 1273 to 973 K. The remaining flux attached to the crystals was readily dissolved in distilled water and block-shaped crystals were obtained with an average size of 0.6 mm. An endothermic signal in DTA (differential thermal analysis) experiments indicates decomposition of the compound at 1313 K. In the X-ray diffraction pattern of material quenched from 1333 K to room temperature, reflections are assignable solely to ScBO₃ (Keszler & Sun, 1998), indicating that the material decomposes to form ScBO₃ and a liquid at 1313 K.

Crystal data

Na ₃ Sc ₂ (BO ₃) ₃	$D_x = 2.614 \text{ Mg m}^{-3}$
$M_r = 335.32$	Mo $K\alpha$ radiation
Trigonal, $R\bar{3}c$	$\mu = 1.77 \text{ mm}^{-1}$
$a = 8.6128 (6) \text{ \AA}$	$T = 293 (2) \text{ K}$
$c = 19.897 (2) \text{ \AA}$	Block, colourless
$V = 1278.24 (18) \text{ \AA}^3$	$0.3 \times 0.2 \times 0.15 \text{ mm}$
$Z = 6$	

Data collection

Rigaku Mercury CCD diffractometer	2758 measured reflections
ω scans	329 independent reflections
Absorption correction: multi-scan (<i>CrystalClear</i> ; Rigaku, 2000)	326 reflections with $I > 2\sigma(I)$
$T_{\min} = 0.723$, $T_{\max} = 0.850$ (expected range = 0.652–0.766)	$R_{\text{int}} = 0.020$
	$\theta_{\text{max}} = 27.5^\circ$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0181P)^2 + 2.8185P]$
$R[F^2 > 2\sigma(F^2)] = 0.019$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.055$	$(\Delta/\sigma)_{\text{max}} < 0.001$
$S = 1.40$	$\Delta\rho_{\text{max}} = 0.30 \text{ e \AA}^{-3}$
329 reflections	$\Delta\rho_{\text{min}} = -0.48 \text{ e \AA}^{-3}$
29 parameters	Extinction correction: <i>SHELXL97</i>
	Extinction coefficient: 0.0145 (11)

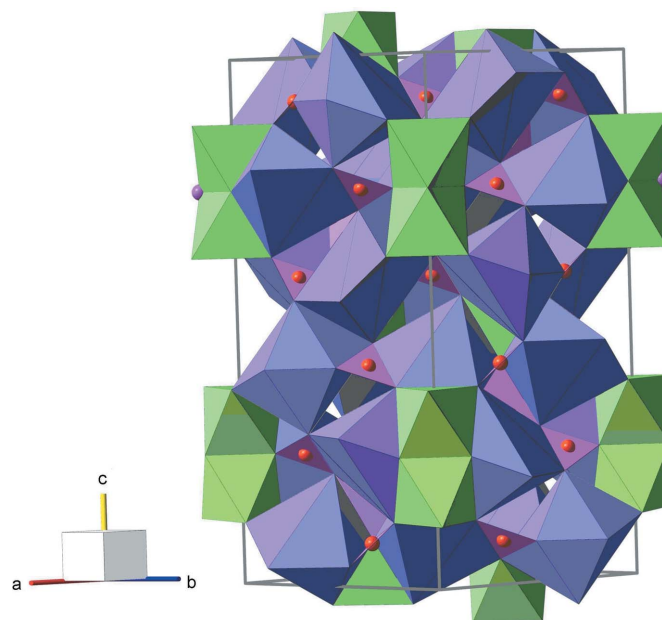


Figure 2

Polyhedral representation of (I) in a projection along [110]. ScO₆ octahedra are green, NaO₈ polyhedra are cyan and BO₃ triangles are mauve.

Table 1

Selected geometric parameters (Å, °).

Sc–O1	2.0146 (11)	Na–O1 ⁱⁱ	2.7644 (13)
Sc–O2	2.1816 (11)	Na–O1 ⁱⁱⁱ	2.8220 (12)
Na–O1 ⁱ	2.4302 (14)	B–O2	1.382 (3)
Na–O2	2.5037 (8)	B–O1 ^{iv}	1.3624 (15)
O1 ^{iv} –B–O1 ^v	119.94 (19)	O1 ^{iv} –B–O2	120.03 (9)

Symmetry codes: (i) $-x + 2, -y + 1, -z$; (ii) $-x + y + 1, -x + 1, z$; (iii) $x - y + 1, x, -z$; (iv) $y, -x + y, -z$; (v) $-y + \frac{4}{3}, -x + \frac{2}{3}, z + \frac{1}{6}$.

Data collection: *CrystalClear* (Rigaku, 2000); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *Balls and Sticks* (Kang & Ozawa, 2002) and *DIAMOND* (Brandenburg, 2004); software used to prepare material for publication: *enCIFer* (Allen *et al.*, 2004).

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References

- Allen, F. H., Johnson, O., Shields, G. P., Smith, B. R. & Towler, M. (2004). *J. Appl. Cryst.* **37**, 335–338.
- Becker, P. & Held, P. (2001). *Z. Kristallogr. New Cryst. Struct.* **216**, 35.
- Brandenburg, K. (2004). *DIAMOND*. Version 3.0. Crystal Impact GbR, Bonn, Germany.
- Dickens, B., Hyman, A. & Brown, W. E. (1971). *J. Res. Natl Bur. Stand.* **75**, 129–135.
- Kang, S. J. & Ozawa, T. C. (2002). *Balls and Sticks*. Version 1.51. (URL: <http://www.softbug.com/toycrate/bs/>).

Keszler, D. A. & Sun, H. (1988). *Acta. Cryst. C* **44**, 1505–1507.

Rigaku (2000). *CrystalClear*. Version 1.3. Rigaku Corporation, Tokyo, Japan.

Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.

Zhang, G. C., Wu, Y. C., Fu, P. Z., Wang, G. F., Pan, S. L. & Chen, C. T. (2001). *Chem. Lett.* **30**, 456–457.

Zobetz, E. (1982). *Z. Kristallogr.* **160**, 81–92.