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Crystal structure of dibarium pentaborate chloride, $Ba_2B_5O_9Cl$

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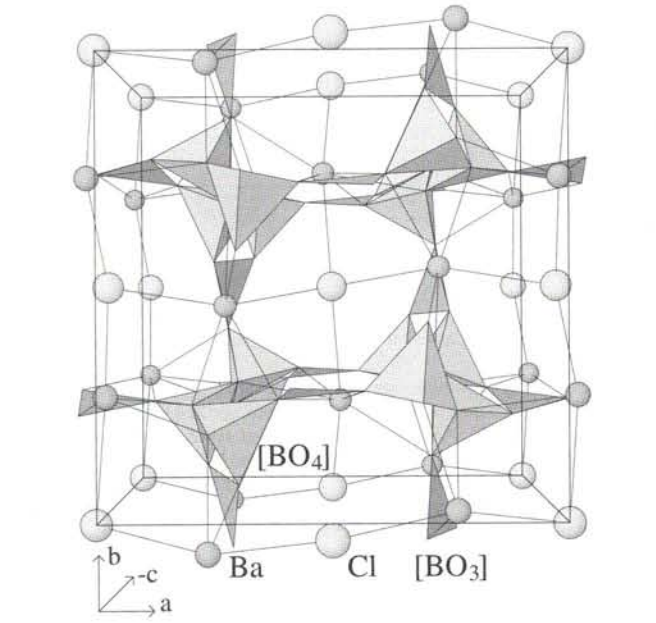

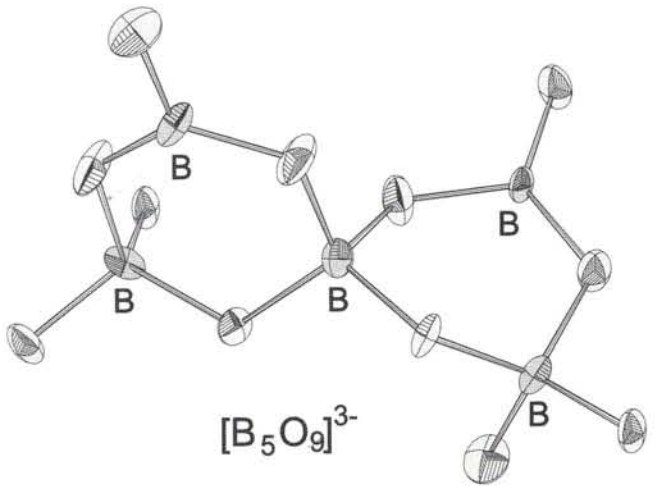

Abstract

$B_5Ba_2ClO_9$, orthorhombic, *Pnn*2 (No. 34), $a = 11.6358(9)$ Å, $b = 11.583(1)$ Å, $c = 6.6823(7)$ Å, $V = 900.6$ Å^3, $Z = 4$, $R_{gt}(F) = 0.020$, $wR_{ref}(F^2) = 0.054$, $T = 293$ K.

Source of material

The dibarium pentaborate chloride was synthesized using the method described for $Sr_2B_5O_9Cl$ [1]. Single crystals with dimensions up to $2 \times 1 \times 1$ mm^3 were grown from $BaCl_2$ flux in a temperature range between 1273 K and 1173 K.

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Discussion

Dibarium pentaborate chloride is isostructural to $Ca_2B_5O_9Br$ [2,3] and $Eu_2B_5O_9X$ (with X = Cl, Br) [4,5]. The structure consists of Ba^{2+} cations, Cl^- and $B_5O_9^{3-}$ anions. The pentaborate group is formed by a series of three corner-linked $[BO_4]$ tetrahedra, additionally two neighbouring tetrahedra each are bridged by one planar $[BO_3]$ group ($[BO_3]$:$[BO_4]$=2:3). Using the description for polyanions in anhydrous borates introduced in [6] and modified in [7], the borate polyanions ("fundamental building block") in $Ba_2B_5O_9Cl$ can be depicted as 2D3T:<D2T><D2T>. Sharing common oxygen atoms, the main structure unit is composed of the pentaborate groups to form wave-like, infinite chains of $[BO_4]$ tetrahedra parallel to the *c* axis. The chains are interlinked along the *a* and *b* axis via $[BO_3]$ groups of the pentaborate units. The result is a three dimensional framework of $[B_5O_9]_\infty^{3-}$ parts with large channels, in which the Cl^- anions are placed in maximum distance. The Cl^- is separated from the anionic $[B_5O_9]_\infty^{3-}$ structure part by Ba^{2+} cations, which coordinate the chlorine in form of a distorted tetrahedra. The $[ClBa_4]$ tetrahedra are linked to another four ones to form the cationic part $[ClBa_2]_\infty^{3+}$ of the structure. Both symmetrically independent Ba^{2+} cations are surrounded by seven oxygen and two chlorine atoms. The interaction between the Ba^{2+} cations and the next neighbourhood seems to be spatially limited because of the special arrangement of the $[B_5O_9]_\infty^{3-}$ and $[ClBa_2]_\infty^{3+}$ framework.

Table 1. Data collection and handling.

Crystal:	colourless prism, size 0.24 × 0.24 × 0.24 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	90.17 cm^{-1}
Diffractometer, scan mode:	Enraf-Nonius MACH3, $\omega/2\theta$
$2\theta_{max}$:	61.04°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	8152, 2740
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\,\sigma(I_{obs})$, 2636
$N(param)_{refined}$:	156
Programs:	MolEN [8], SHELXL-97 [9], ATOMS [10]

Table 2. Atomic coordinates and displacement parameters (in Å^2).

Atom	Site	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Ba(1)	4*c*	0.26853(2)	0.98071(2)	0.99472(3)	0.0115(1)	0.0081(1)	0.0062(1)	0.00000(7)	0.0007(1)	–0.00107(8)
Ba(2)	4*c*	0.45669(2)	0.74525(2)	0.64915(5)	0.0074(1)	0.0122(1)	0.0071(1)	0.00046(7)	–0.00069(8)	–0.00127(8)
Cl(1)	2*b*	1/2	0	0.7676(3)	0.0135(7)	0.0132(6)	0.0280(7)	–0.0028(6)	0	0
Cl(2)	2*a*	1/2	1/2	0.5056(4)	0.0121(6)	0.0132(6)	0.0389(8)	–0.0004(5)	0	0
O(1)	4*c*	0.1928(3)	0.7608(2)	0.0558(4)	0.006(1)	0.009(1)	0.003(1)	0.002(1)	–0.0012(9)	0.0000(8)
O(2)	4*c*	0.2486(3)	0.1201(3)	0.3082(4)	0.019(1)	0.005(1)	0.005(1)	–0.003(1)	0.000(1)	0.0001(9)
O(3)	4*c*	0.0620(3)	0.7083(3)	0.7995(4)	0.006(1)	0.019(1)	0.008(1)	–0.003(1)	–0.003(1)	0.004(1)
O(4)	4*c*	0.2335(2)	0.8179(3)	0.7125(4)	0.006(1)	0.009(1)	0.003(1)	–0.0017(9)	0.0017(8)	0.0006(9)
O(5)	4*c*	0.2064(3)	0.0850(2)	0.6498(4)	0.016(1)	0.006(1)	0.005(1)	–0.001(1)	0.002(1)	–0.001(1)
O(6)	4*c*	0.0757(2)	0.7954(3)	0.4781(5)	0.007(1)	0.020(1)	0.005(1)	–0.001(1)	–0.001(1)	0.003(1)
O(7)	4*c*	0.3941(3)	0.7687(3)	0.0958(4)	0.005(1)	0.015(1)	0.011(1)	–0.001(1)	–0.0004(9)	0.0016(9)
O(8)	4*c*	0.2695(3)	0.7299(2)	0.3922(4)	0.012(1)	0.006(1)	0.003(1)	0.001(1)	0.0004(9)	0.0005(9)
O(9)	4*c*	0.2258(3)	0.9303(3)	0.4063(4)	0.021(2)	0.004(1)	0.006(1)	–0.001(1)	0.0011(9)	–0.0004(9)
B(1)	4*c*	0.2850(4)	0.7129(4)	0.1779(6)	0.006(2)	0.008(2)	0.004(2)	0.001(1)	–0.001(1)	–0.000(1)
B(2)	4*c*	0.2262(4)	0.0420(4)	0.4626(5)	0.007(2)	0.007(2)	0.002(2)	0.001(1)	–0.000(1)	0.001(1)
B(3)	4*c*	0.1861(4)	0.7288(4)	0.8432(6)	0.008(2)	0.007(2)	0.004(2)	–0.000(1)	0.000(1)	0.001(1)
B(4)	4*c*	0.0108(4)	0.7484(3)	0.6289(7)	0.006(2)	0.010(2)	0.005(2)	0.002(1)	–0.002(2)	–0.001(1)
B(5)	4*c*	0.2014(3)	0.8187(3)	0.4986(7)	0.004(2)	0.005(2)	0.006(1)	–0.001(1)	0.004(2)	–0.001(1)

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