Aristarainite: Na$_2$Mg[B$_5$O$_9$(OH)$_4$]$_2$·4H$_2$O: a sheet structure with chains of hexaborate polyanions

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Abstract

The rare sodium magnesium borate mineral aristarainite from Salta, Argentina, is monoclinic, space group $P2_1/a$, with $a = 18.886(4)$, $b = 7.521(2)$, $c = 7.815(1)$ Å, $\beta = 97.72(1)^\circ$, $Z = 2$. The atomic positions, including those of hydrogens, were determined by the symbolic addition method and difference Fourier syntheses, and refined by the method of least squares to an $R$ factor of 0.036 for 1941 reflections, measured on a single crystal automatic diffractometer. The chemical composition has been revised to Na$_5$O·MgO·6B$_2$O$_5$·8H$_2$O, as opposed to Na$_4$O·MgO·6B$_2$O$_5$·10H$_2$O reported by Hurlbut and Erd (1974).

Aristarainite contains the hexaborate polyanion $[B_5O_9(OH)_{i-4}]^{6-}$, consisting of three borate triangles and three borate tetrahedra sharing corners. These polyanions are linked into infinite chains, $[B_5O_9(OH)_{i-4}]^{6-}$, parallel to the $b$ axis, by sharing a common oxygen corner between a borate tetrahedron and a borate triangle belonging to two different but adjacent polyanions. Aristarainite provides the first example of such chains. Mg and Na, respectively, in octahedral and distorted square-pyramidal coordination, bind these chains into sheets parallel to (001), which in turn are cross-linked by hydrogen bonds. The average bond distances (Å) are: Mg–O, 2.094; Na–O, 2.509; B–O tetrahedral, 1.471; triangular, 1.363; O–H, 0.89; H⋯O, 1.91; and O–H⋯O, 2.782. The average B–O bond, involving the oxygen bonded to three tetrahedrally coordinated borons, is significantly longer (1.517 Å) than the average tetrahedral B–O bond. All hydrogens are involved in hydrogen bonding except those belonging to one water molecule bonded solely to Na.

Introduction

Aristarainite, a new hydrated sodium magnesium borate from the Tinealayu borax deposit, Salta, Argentina, was first described by Hurlbut and Erd (1974), who named the mineral after L. F. Aristarain of Argentina for his contributions to borate mineralogy. At Tinealayu, it occurs in a matrix of borax and kernite, in association with halite and other borates, mecallisterite, rivadavaite, excurrite, ameghinitte, kernakovite, probertite, ulyeite, ginorite, tincalocnite, and the borosilicate sarsleite.

Two of these borates, mecallisterite and rivadavaite, contain the isolated borate polyanion, $[B_5O_9(OH)_{i-4}]^{6-}$, consisting of three borate tetrahedra and three borate triangles sharing corners (Dal Negro et al., 1969; Dal Negro et al., 1973). This polyanion has also been found in aksaite (Dal Negro et al., 1971). These polyanions are polymerized into sheets in the structures of tunellite (Clark, 1964), and strontioginorite (Koerner et al., 1970). Following Christ's (1960), the isolated hexaborate polyanions can polymerize into chains by splitting out water molecules. Aristarainite provides the first example of such a polymerized chain of hexaborate polyanions.

Chemical composition

The chemical composition of aristarainite was reported by Hurlbut and Erd (1974) as Na$_5$O·MgO·6B$_2$O$_5$·10H$_2$O, with two formula units in the unit cell (space group $P2_1/a$). The structure determination indicates the presence of two independent water molecules and four different hydroxyl groups, resulting in a revised chemical formula, Na$_5$O·MgO·6B$_2$O$_5$·8H$_2$O. The calculated density for this composition (2.005 g cm$^{-3}$) is slightly less than the measured value (2.027 g cm$^{-3}$). A three-dimensional difference Fourier synthesis, calculated following the final refinement of the structure, was completely featureless, thus confirming the chemical composition of aristarainite reported here.