Lovdarite, $K_4Na_{12}(Be_{8}Si_{28}O_{72}) \cdot 18 \text{H}_2\text{O}$, a zeolite-like mineral: structural features and OD character

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Abstract: The crystal structure of lovdarite, a beryllio-silicate from Lovozero, is determined and refined to $R = 0.082$, using 1517 independent reflections; the space group is $Pma2_1$, with $a = 39.576(1)$, $b = 6.9308(2)$, $c = 7.1526(3)$ Å. The crystal chemical formula derived in the structural study is $K_4Na_{12}(Be_{8}Si_{28}O_{72}) \cdot 18 \text{H}_2\text{O}$.

The loverdarite structure may be described as a three-dimensional framework of silicon and beryllium tetrahedra with alkali cations and water molecules in the cavities. The most outstanding feature of the structure is the arrangement of five tetrahedra in two three-membered rings, sharing a tetrahedron. Lovdarite is the first recorded example of a framework silicate containing three-membered rings: strain is released by the presence of a beryllium cation in each ring.

The OD character of loverdarite — evident from its peculiar diffraction pattern — is discussed on the basis of the structural results; an indication is given of the building layers and possible MDO polytypes are derived.

Key-words: lovdarite, crystal structure, zeolite-like mineral, polytypism, OD theory.

Introduction

Lovedarite was first found in a pegmatite vein from the Yubileynaya deposit, on Mount Karnasurt in the Lovozero pluton (USSR), and has been described by Men’shikov et al. (1973). These authors indicate that the new mineral should be "classified as a zeolitic hydrous alkali-beryllium tectosilicate", with chemical composition (Na,K,Ca)$_4(\text{Be,Al})_2\text{Si}_6\text{O}_{18}$ \cdot 4 $\text{H}_2\text{O}$, space group $P2_12_12_1$ and unit cell parameters $a = 38.789$, $b = 6.776$, $c = 7.012$ Å. More recently, chemical, crystallographic, morphological and optical data have been presented by Khomyakov et al. (1975). These new chemical data match perfectly with those presented by Men’shikov et al. (1973) and point to the following chemical formula: $K_4Na_{13}$ ($\text{Si}_{12}\text{AlBe}_8\text{O}_{72}) \cdot 19.5 \text{H}_2\text{O}$. As regards the crystallographic features, Khomyakov et al. (1975), on the basis of the diffraction patterns, maintain that the structure of lovedarite is partially disordered and should be classified as an OD structure; furthermore they state "that the real periods of lovedarite lattice are $a = 78.88$, $b = 6.91$, $c = 7.15$ Å", thus doubling the $a$ parameter given by Men’shikov et al. (1973).

A very short account of the most important features of the crystal structure of lovedarite was presented in a poster at the 12th International Congress of Crystallography (Merlino, 1981). Since then, the structure-type of lovedarite has been outlined in various reviews and compilations. Moreover, a synthetic analogue has been prepared and its structure analysed through the Rietveld refinement of X-ray powder data (Ueda et al., 1986).

It is the aim of the present paper to give a detailed description of the refined crystal structure of lovedarite, and to discuss its OD character; an indication of the building layers is given and the possible OD sequences are derived from the X-ray diffraction data.

Experimental

A careful scrutiny of the diffraction pattern of a number of crystals of lovedarite, kindly supplied by A. P. Khomyakov, shows that all specimens present the same diffraction pattern as regards the reflections $hkl$ with $l = 2n$ (indices are given on the basis of the unit cell proposed by Men’shikov et al. (1973).