STRUCTURAL INVESTIGATIONS ON BREDIGITE (Ca7Mg(SiO4)4) FROM THE HATRURIM COMPLEX

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Bredigite (idealized chemical composition Ca₇Mg(SiO₄)₄) is a rare mineral that has been described from petrological settings related to pyrometamorphism. It has been observed, for example, in contact-metamorphized rocks or in altered carbonate-silicate xenoliths within volcanites based on siliceous limestone-dolomite protoliths.

In pyrometamorphic rocks of the Hatrurim Complex, consisting of products of combustion metamorphism, the existence of small bredigite grains, mainly in larnite rocks, was repeatedly noted (SOKOL et al., 2010). The Hatrurim Complex is distributed over a wide area along the Dead Sea rift zone in the territories of Israel, Palestine and Jordan. Its formation was driven by combustion processes of a sedimentary protolith, however, its detailed genesis is still under discussion (SOKOL et al., 2010; VAPNIK & NOVIKOV, 2013).

Bredigite samples from ternesite-gazeevite-larnite pyrometamorphic rocks of the Hatrurim Complex have been studied by electron probe microanalysis as well as single-crystal diffraction using synchrotron radiation (X06DA beamline at the Swiss Light Source, Paul-Scherrer-Institute). They are characterized by a relatively uniform composition. The empirical formula calculated on the basis of 16 oxygen atoms per formula unit is:

 $(Ca_{7.006}Na_{0.015}Ba_{0.014})_{\Sigma 7.035}Mg_{0.938}(Si_{4.000}P_{0.014})_{\Sigma 4.014}O_{16}.$

Basic crystallographic data of a sample studied by X-ray diffraction are as follows: orthorhombic symmetry, space group *Pnnm*, a = 18.38102(17) Å, b = 6.74936(7) Å, c = 10.90328(11) Å, V = 1352.66(2) Å³, Z = 4. Structure solution and subsequent least-squares refinements resulted in a residual of R(|F|) = 0.023 for 2584 independent observed reflections with I > $2\sigma(I)$ and 149 parameters. To the best of our knowledge this is the first detailed structural investigation on natural bredigite. In contrast to previous studies on samples retrieved from metallurgical slags there was no need to describe the structure in the acentric space group *Pnn2* (MOORE & ARAKI, 1976).

Furthermore, the problem of barium incorporation into the bredigite structure is discussed. Data on the composition of Ba-bearing bredigites from pyrometamorphic rocks of the Hatrurim Complex from Jordan with simplified formula Ba_{0.7}Ca_{13.3}Mg₂(SiO₄)₈ (based on 32 oxygen atoms) are provided for the first time, pointing out perspectives of finding new Ba-bearing minerals isostructural with bredigite in nature.

MOORE, P.B., ARAKI, T. (1976): Am. Mineral., 61, 74-87.

SOKOL, E., NOVIKOV, I., ZATEEVA, S., VAPNIK, Y., SHAGNAM, R., KOZMENKO, O. (2010): Basin Res., 22, 414-438.

VAPNIK, Y., NOVIKOV, I. (2013): Basin Res., 25, 115-120.