A green dumortierite from Kutná Hora region, Czech Republic: spectroscopic and structural study

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INTRODUCTION

Cempírek (2003) and Cempírek & Novák (2003) made overview of small abyssal pegmatites on the eastern part of the Moldanubicum (Gföhl Unit), Bohemian Massif, Czech Republic. The Kuklík and Miskovice pegmatites near Kutná Hora are the most evolved pegmatites in the region. Besides the tournaline with significantly increased content of Al, they contain several types of green to greenish-blue dumortierite. Losert (1956) first noticed the reversed optical orientation of the mineral in the Kuklík pegmatite. Cempírek (2003) found low concentrations of most of the other elements than Al and Si in green dumortierite from both pegmatites.

Losert (1956) and Cempírek (2003) described a general internal structure of the pegmatites and their mineral assemblages. The border zone consists of coarse-grained quartz + oligoclase + K-feldspar + tourmaline (I) + muscovite. The core zone is rich in quartz and black to dark green tourmaline (I) with rims of blue tourmaline (II) (olenite-foitite, Cempírek & Novák 2003) and abundant colorless to green dumortierite (poor in Fe and Ti). It represents the latest primary Al,B-rich phase in the pegmatite (Cempírek 2003).

Absorption spectroscopy

Optical spectra were examined using dumortierite single crystal double-polished thin sections (thickness 40-25 μ m), cut perpendicularly to the three crystallographic axes. Spectra for each sample were measured over a range of 180° in steps of 10°.

Absorption spectra in the visible range show three, strongly polarized absorption bands at 12000, 16700 and 24400 cm⁻¹(ca. 830, 600 and 410 nm). In the infrared region, strongly polarized OH-stretching vibration at 3500 cm⁻¹, weak stretching vibration at 3530 cm⁻¹ and OH-bending vibration overtone at 4410 cm⁻¹ are the most important features.

Absorption bands in the visible spectra can be interpreted as intervalence charge transfer absorption of Fe^{2+} - Ti^{4+} or Fe^{2+} - Fe^{3+} in M(1) and/or M(4) octahedra, in which the substitution of minor Fe and Ti is usual. The absorption band at 24400 cm⁻¹ is uncommon in the dumortierite structure, and is responsible for bluish-green color of Kutná Hora crystals, as the absorption window left is about at 20000 cm-1 (500 nm). Also, the other important feature responsible



for the color is a low content of absorbing cations, which is reflected in low values of linear absorption coefficients in studied samples. This well corresponds with earlier EMP data (Cempírek, 2003) showing only 0.012 apfu (Fe + Ti) to be present.

The OH-stretching vibrations at 3500 and 3530 cm⁻¹ in IR region suggest the only one site hosting OH. The indistinct peak splitting can be attributed to local different nearest-neighbor environment, e.g. slight substitution of Al for Si in oxygen-binding tetrahedra. The polarization of the peaks suggest the [T(2), M(1)]-coordinated O(7) site as a possible host for OH groups.



Structure

The preliminary crystal structure refinement provided formula $(Al_{0.82} \square_{0.18})$ $(Al_{5.98} \square_{0.02})$ Si₂(Si_{0.87}Al_{0.13}) B O₁₆ [O_{1.14}(OH)_{0.86}], with *a* = 11.7992(24), *b* = 20.1957(40), *c* = 4.6970(9) Å. The structural formula, although imprecise (refinement R=2.77), show the expected substitutions in M(1) octahedra and T(2) tetrahedra. However, the Al/Si ratio is still lower than values detected by EMP (Cempírek, 2003). The significant OH content calculated to fit the stoichiometry seems to fit well to the spectroscopic observations, with OH occupying O(7) site.

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