

## STRUCTURE AND COLOR OF THE JACK CREEK DUMORTIERITE (MONTANA, USA) USING SPECTROSCOPIC APPROACHES

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A blue dumortierite sample from the Jack Creek hydrothermal system (Boulder Basin, Montana, USA) (FOIT et al., 1989) was studied using Fourier-transform infrared spectroscopy (FTIR), electron paramagnetic resonance (EPR) spectroscopy, near UV-visible-near Infrared spectroscopy, X-ray absorption near edge spectroscopy (XANES) and Mössbauer spectroscopy.

FTIR spectroscopy shows for the OH groups the existence of various environments, which are related to substitutions and/or vacancies in the M1 octahedral site. Mössbauer spectroscopy consistently reveals the presence of Fe<sup>2+</sup> and Fe<sup>3+</sup> in octahedral sites, Fe<sup>3+</sup> being dominantly represented. The strong and sharp signal observed at 0.113 T in the EPR spectra of pink dumortierite samples with low Fe content (Lincoln Hill and Louvincourt) (FUCHS et al., 2004) and related to a site with a pure axial distortion, [i. e., a site symmetry with a n-fold ( $n \geq 3$ ) rotation axis, corresponding to the A11 site in dumortierite] is not present in the Jack Creek sample. In contrast, the signals observed at 0.16 T correspond to more distorted sites (ABRAGAM & BLEANEY, 1970). This rhombic signal can be related to Fe<sup>3+</sup> ions located in tetrahedral or in distorted octahedral sites (A12, A13 or A14).

EPR and XANES also indicate that a fraction of the Fe atoms are not isolated but concentrated in magnetic domains. Optical spectroscopy indicates an important contribution of intervalence charge transfer transitions (IVCT), the most important between Fe<sup>2+</sup> and Fe<sup>3+</sup> and a smaller contribution between Fe<sup>2+</sup> and Ti<sup>4+</sup>. These transitions are responsible for the blue color of the Jack Creek Dumortierite sample.

Based on the XANES study of the Jack Creek (Montana) sample Ti seems to be mainly restricted to the M1 site (95%). Ab initio XANES (using FEFF) calculations at the Fe K-edge suggest that Fe is located mainly in the A12, A13 and A14 sites (having the highest energy and shorter average Al-O distances). Thermodynamically, Fe would preferentially partition toward the A11 site. But, a temperature dependence of different site distortion could explain this apparent discrepancy as for Fe in olivine.

### References

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