Synthesis and Characterization of a Cubic Iron Hydroxy Boracite

Stephanie C. Neumair[a], Johanna S. Knyrim[b], Oliver Oeckler[c], Reinhard Kaindl[d], and Hubert Huppertz[a]

[a] Institut für Allgemeine, Anorganische und Theoretische Chemie, Leopold-Franzens-Universität Innsbruck, Innrain 52a, 6020 Innsbruck, Austria
[b] Süd-Chemie AG, BU Performance Packaging, Ostenriederstraße 15, 85368 Moosburg, Germany
[c] Department Chemie, Ludwig-Maximilians-Universität München, Butenandtstraße 5 – 13, 81377 München, Germany
[d] Institut für Mineralogie und Petrographie, Leopold-Franzens-Universität Innsbruck, Innrain 52f, 6020 Innsbruck, Austria

Reprint requests to H. Huppertz. E-mail: Hubert.Huppertz@uibk.ac.at

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The cubic iron hydroxy boracite $Fe_3B_7O_{13}OH \cdot 1.5\,H_2O$ was synthesized from Fe_2O_3 and B_2O_3 under high-pressure/high-temperature conditions of 3 GPa and 960 °C in a modified Walker-type multianvil apparatus. The crystal structure was determined at room temperature by X-ray diffraction on single crystals. It crystallizes in the cubic space group $F\bar{4}3c$ ($Z = 8$) with the parameters $a = 1222.4(2)$ pm, $V = 1.826(4)$ nm^3, $R_1 = 0.0362$, and $wR_2 = 0.0726$ (all data). The B-O network is similar to that of other cubic boracites.

Key words: Borate, Crystal Structure, Hydroxy Boracite, High Pressure