

High-pressure Synthesis and Characterization of the Fluoride Borate $\text{Tm}_5(\text{BO}_3)_2\text{F}_9$

Almut Haberer^a, Michael Enders^a, Reinhard Kaindl^b, and Hubert Huppertz^a

^a Institut für Allgemeine, Anorganische und Theoretische Chemie, Leopold-Franzens-Universität Innsbruck, Innrain 52a, 6020 Innsbruck, Austria

^b Institut für Mineralogie und Petrographie, Leopold-Franzens-Universität Innsbruck, Innrain 52, 6020 Innsbruck, Austria

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

Z. Naturforsch. **2010**, *65b*, 1213 – 1218; received June 17, 2010

The rare earth fluoride borate $\text{Tm}_5(\text{BO}_3)_2\text{F}_9$ was synthesized from Tm_2O_3 , B_2O_3 , and TmF_3 under high-pressure/high-temperature conditions of 5 GPa and 900 °C in a Walker-type multianvil apparatus. The single-crystal structure determination revealed that $\text{Tm}_5(\text{BO}_3)_2\text{F}_9$ is isotypic to the compounds $\text{RE}_5(\text{BO}_3)_2\text{F}_9$ ($\text{RE} = \text{Er}, \text{Yb}$). $\text{Tm}_5(\text{BO}_3)_2\text{F}_9$ crystallizes in the space group $C2/c$ ($Z = 4$) with the parameters $a = 2030.9(4)$, $b = 606.2(2)$, $c = 822.6(2)$ pm, $\beta = 100.5(1)^\circ$, $V = 995.7(3) \text{ \AA}^3$, $R_1 = 0.0341$, and $wR_2 = 0.0724$ (all data). The structure is composed of isolated BO_3 groups, ninefold coordinated thulium cations, and fluoride anions. Infrared and Raman spectroscopic data of $\text{Tm}_5(\text{BO}_3)_2\text{F}_9$ are compared to the data of $\text{RE}_5(\text{BO}_3)_2\text{F}_9$ ($\text{RE} = \text{Er}, \text{Yb}$).

Key words: Rare Earth, Fluoride, Borate, High Pressure, Crystal Structure