

High-pressure Synthesis and Crystal Structure of the Borate $\text{Sc}_3\text{B}_5\text{O}_{12}$

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Dedicated to Professor Hubert Schmidbaur on the occasion of his 75th birthday

The rare-earth borate $\text{Sc}_3\text{B}_5\text{O}_{12}$ was synthesized under high-pressure / high-temperature conditions of 6 GPa and 1100 °C in a Walker-type multianvil apparatus. The single-crystal structure determination revealed an isotypy to $RE_3\text{B}_5\text{O}_{12}$ ($RE = \text{Er-Lu}$). $\text{Sc}_3\text{B}_5\text{O}_{12}$ crystallizes in the rare space group $Pmna$ ($Z = 4$) with the parameters $a = 1245.4(3)$, $b = 443.46(9)$, $c = 1222.1(2)$ pm, $V = 0.675(1)$ nm³, $R_1 = 0.0520$, and $wR_2 = 0.0860$ (all data). The structure of $\text{Sc}_3\text{B}_5\text{O}_{12}$ is composed of layers of condensed BO_4 tetrahedra, separated by eight-fold coordinated scandium ions.

Key words: Borate, Crystal Structure