Synthesis and Crystal Structure of the High-pressure Iron Borate
\(\beta\)-FeB\(_2\)O\(_4\)

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The iron borate \(\beta\)-FeB\(_2\)O\(_4\) was synthesized under high-pressure/high-temperature conditions of 8 GPa and 1030 °C. The structure of \(\beta\)-FeB\(_2\)O\(_4\) is isotypic to HP-NiB\(_2\)O\(_4\), representing the second example of a borate in which every BO\(_4\) tetrahedron shares a common edge with a second one. \(\beta\)-FeB\(_2\)O\(_4\) crystallizes in the space group \(C2/c\) \((Z = 4)\) with the parameters \(a = 950.0(2)\) pm, \(b = 562.9(2)\) pm, \(c = 443.7(1)\) pm, \(\beta = 108.50(3)\)°, \(V = 0.22495(8)\) nm\(^3\), \(R1 = 0.0293\), and \(wR2 = 0.0647\) (all data). The structure consists of layers of BO\(_4\) tetrahedra, connected \(\text{via}\) strings of edge-sharing FeO\(_6\) octahedra. A ligand field splitting of \(\Delta_0 \approx 8860\) cm\(^{-1}\) is estimated from polarized single-crystal electronic absorption spectra of \(\beta\)-FeB\(_2\)O\(_4\). The tetragonal distortion of the ligand field in the [Fe\(_{\text{II}}\)O\(_6\)] chromophore amounts to \(-(8/3)d\sigma \approx 2900\) cm\(^{-1}\). In the range of 16000 cm\(^{-1}\) \(\leq \tilde{\nu} \leq 24000\) cm\(^{-1}\), rather strong spin-forbidden transitions within the [Fe\(_{\text{II}}\)O\(_6\)] chromophore are observed.

Key words: Borate, High Pressure, Crystal Structure