Synthesis and Crystal Structure of the Praseodymium Orthoborate \( \lambda \)-PrBO\(_3\)

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Z. Naturforsch. 2010, 65b, 1206 – 1212; received May 18, 2010

The praseodymium orthoborate \( \lambda \)-PrBO\(_3\) was synthesized from Pr\(_6\)O\(_{11}\), B\(_2\)O\(_3\), and PrF\(_3\) under high-pressure / high-temperature conditions of 3 GPa and 800 °C in a Walker-type multianvil apparatus. The crystal structure was determined on the basis of single-crystal X-ray diffraction data, collected at room temperature. The title compound crystallizes in the orthorhombic aragonite-type structure, space group \( Pnma \), with the lattice parameters \( a = 577.1(2) \), \( b = 506.7(2) \), \( c = 813.3(2) \) pm, and \( V = 0.2378(2) \) nm\(^3\), with \( R_1 = 0.0400 \) and \( wR_2 = 0.0495 \) (all data). Within the trigonal-planar BO\(_3\) groups, the average B–O distance is 137.2 pm. The praseodymium atoms are ninefold coordinated by oxygen atoms.

Key words: High Pressure, Crystal Structure, Multianvil, Orthoborate, Aragonite