

β -CaB₄O₇: A New Polymorph Synthesized under High-Pressure/High-Temperature Conditions

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A new oxoborate β -CaB₄O₇ has been synthesized under high-pressure/high-temperature conditions from calcium oxide and boron oxide with a Walker-type multianvil apparatus at 7.7 GPa and 1100 °C. Single crystal X-ray structure determination of β -CaB₄O₇ revealed: $Pmn2_1$, $a = 1058.4(1)$, $b = 436.9(1)$, $c = 419.4(1)$ pm, $Z = 2$, $R1 = 0.0305$, $wR2 = 0.0587$ (all data). The compound is isotypic to the known oxoborates SrB₄O₇, PbB₄O₇, and EuB₄O₇ exhibiting a network structure of linked BO₄ tetrahedra. As a prominent feature of the tetrahedral network an oxygen atom is coordinated to three boron atoms. The relation of the crystal structure of the high-pressure phase β -CaB₄O₇ to the normal-pressure phase α -CaB₄O₇ as well as the relation to the isotypic phases MB₄O₇ (M = Sr, Pb, Eu) are discussed. The results of IR-spectroscopic investigations on β -CaB₄O₇ are also presented.

Key words: High-Pressure, Multianvil, β -CaB₄O₇, Borates, Crystal Structure