Rietveld Refinement of the Crystal Structure of α-Be_3N_2 and the Experimental Determination of Optical Band Gaps for Mg_3N_2, Ca_3N_2 and $CaMg_2N_2$

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Z. Naturforsch. **58b,** 159 – 162 (2003); received October 15, 2002

α-Be_3N_2 powder was obtained by reacting Be metal with dry, flowing N_2 at 1600 K. The product contained 5.9(7) wt.% of BeO. The anti-bixbyite structure suggested earlier was verified through Rietveld refinement on the basis of X-ray powder data ($Ia\bar{3}$ (#206); $a = 814.518(6)$ pm). The optical band gaps of α-Be_3N_2, Mg_3N_2 and Ca_3N_2 are compared with newly measured values for Mg_3N_2, Ca_3N_2 and $CaMg_2N_2$.

Key words: Beryllium Nitride, Optical Band Gap, Rietveld Refinement, Structure Elucidation