Syntheses and Crystal Structures of the New Ternary Barium Halide Hydrides Ba_2H_3X (X = Cl or Br)

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Single crystals of the isotypic hydrides Ba_2H_3X (X = Cl or Br) were obtained by solid-state reactions of Ba, NaCl, $NaNH_2$ and metallic Na, or Ba, NH_4Br and Na, respectively, in sealed, silica-jacketed stainless-steel ampoules. The crystal structures of the new compounds were determined by means of single crystal X-ray diffraction. Ba_2H_3Cl and Ba_2H_3Br crystallize in a stuffed *anti* CdI_2 structure and adopt the space group $P\bar{3}m1$ (No. 164) with the lattice parameters a = 443.00(6), c = 723.00(14) pm and a = 444.92(4), c = 754.48(14) pm, respectively. The hydride positions are derived by crystallographic reasoning and with the help of EUTAX calculations. The results are compared with known data for binary and ternary alkaline earth metal hydrides.

Key words: Barium, Bromide, Chloride, Hydride, Synthesis, Structure Elucidation