New Calcium Hydride Halides with Familiar Structures.
Syntheses and Crystal Structures of Ca$_7$H$_{12}$Cl$_2$ and Ca$_2$H$_3$Br

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Single crystals of Ca$_7$H$_{12}$Cl$_2$ and Ca$_2$H$_3$Br were obtained by reacting stoichiometric amounts of CaH$_2$ and CaX$_2$ ($X = \text{Cl, Br}$) at 1300 K in the presence of surplus Ca metal for 13 h in silica-jacketed Nb ampoules. The crystal structures of the new compounds were determined by means of single-crystal X-ray diffraction. Ca$_7$H$_{12}$Cl$_2$ crystallizes isotypical to Ba$_7$Cl$_2$F$_{12}$ and Sr$_7$H$_{12}$Cl$_2$ in the hexagonal space group $P\bar{6}$ (no. 174) with the lattice parameters $a = 936.51(8)$, $c = 368.65(2)$ pm, while Ca$_2$H$_3$Br crystallizes in a stuffed anti-CdI$_2$ structure isotypical to Ba$_2$H$_3$Cl and therefore adopts the space group $P\bar{3}m1$ (no. 164) with the lattice parameters $a = 391.37(6)$ and $c = 697.04(13)$ pm. The structural results are corroborated by EUTAX calculations on the title compounds and the comparison of these results to those for CaH$_2$, CaX$_2$ and CaHX ($X = \text{Cl, Br}$). Similar calculations on the hypothetical compound “Ca$_7$H$_{12}$Br$_2$” give a possible explanation for the preferred formation of the compound Ca$_2$H$_3$Br.

Key words: Calcium, Halide, Hydride, Structure Elucidation, EUTAX Calculations