$Ba_5(Al/Ga)_5(Sn/Pb)$: Neue Verbindungen an der Zintl-Grenze

$Ba_5(Al/Ga)_5(Sn/Pb)$: New Compounds at the Zintl Border

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The new isotypic intermetallic phases $Ba_5M^{III}_5M^{IV}$ (M^{III} = Al, Ga; M^{IV} = Sn, Pb) have been synthesized from stoichiometric amounts of the elements at maximum temperatures of 900 to 1000 °C. They crystallize in the hexagonal space group *P*6*m*2 (Ba_5Al_5Sn: $a = 605.05(8)$, $c = 1109.0(2)$ pm, $R1 = 0.0137$; Ba_5Ga_5Sn: $a = 599.45(5)$, $c = 1086.00(7)$ pm, $R1 = 0.0485$; Ba_5Al_5Pb: $a = 606.9(2)$, $c = 1112.0(4)$ pm, $R1 = 0.0409$ and Ba_5Ga_5Pb: $a = 601.76(7)$, $c = 1091.51(13)$ pm, $R1 = 0.0295$), forming a new structure type. Similar to the Zintl phases Ba_2M^{IV} (Co_2Si structure type, orthorhombic, space group *Pnma*; Ba_2Sn: $a = 861.52(14)$, $b = 569.85(9)$, $c = 1056.9(2)$ pm, $R1 = 0.0217$ and Ba_2Pb: $a = 865.12(13)$, $b = 569.1(2)$, $c = 1061.8(2)$ pm, $R1 = 0.0470$), these new ternary phases contain isolated M^{IV} atoms (coordinated by 11 Ba atoms). In addition, sheets of 3- and 4-bonded Al/Ga atoms similar to those in Ba_3Al_5 are present. In accordance with this, a formal subdivision of $Ba_5M^{III}_5M^{IV}$ into $Ba_3M^{III}_5 \cdot Ba_2M^{IV}$ can be performed to describe the observed intergrowth or chemical twinning of two different binary intermetallics to give the new ternary compounds. Beyond structural aspects, also the nature of the chemical bonding (as studied by FP-LAPW calculations) in these new, non-electron precise compounds in the vicinity of the Zintl border can be interpreted in this vein.

Key words: Zintl Phases, Laves Phases, Crystal Structure, Band Structure Calculation