$Sr_{14}[Al_4]_2[Ge]_3$: Eine Zintl-Phase mit isolierten $[Ge]^{4-}$- und $[Al_4]^{8-}$-Anionen

$Sr_{14}[Al_4]_2[Ge]_3$: A Zintl Phase with Isolated $[Ge]^{4-}$ and $[Al_4]^{8-}$ Anions

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The new ternary intermetallic compound $Sr_{14}[Al_4]_2[Ge]_3$ was synthesized from stoichiometric ratios of the elements. The crystal structure (trigonal, space group $R\bar{3}$, a = 1196.58(2), c = 4010.33(7) pm, Z = 6, $R1$ = 0.0574) was determined using single crystal X-ray data. The structure contains two crystallographically independent tetrahedral $[Al_4]$ anions with Al-Al distances in the range from 269.7 to 273.6 pm. Taking into account the Zintl concept and the isosteric analogy to white phosphorus, their formal charge is −8. Both of these tetrahedra are surrounded by 16 Sr cations. The three isolated Ge^{4-} anions per formula unit (isosteric to the noble gases) are coordinated by nine Sr cations. According to the ionic description $Sr_{14}[Al_4]_2[Ge]_3 \mapsto 14Sr^{2+} + 2[Al_4]^{8-} + 3[Ge]^{4-}$ the title compound is an electron-precise Zintl phase. This interpretation is supported by the results of a FP-LAPW band structure calculation, which show a distinct minimum of the total density of states at the Fermi level. Attempts to synthesize the analogous compounds in the systems Sr-Ga-Ge and Ca-Ga-Ge resulted in the formation of new members of the $Ca_{11}Ga_7$ structure type family. In the case of Ca-Al-Ge only the stable binary border compounds Ca_2Ge and $CaAl_2$ were formed in respective experiments.

Key words: Aluminium, Germanium, Zintl Phases, Band Structure Calculation