

Sr₃Al₂Ge₄, Ca₁₀Al₆Ge₉ und Ca₂₀Al₆Ge₁₃. Neue Aluminium-Germanide

Sr₃Al₂Ge₄, Ca₁₀Al₆Ge₉ and Ca₂₀Al₆Ge₁₃. New Aluminium Germanides

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In the ternary systems Ca-Al-Ge and Sr-Al-Ge three germanides with new structure types have been synthesized from stoichiometric ratios of the elements. Their crystal structures were determined using single crystal X-ray data. In the structure of Sr₃Al₂Ge₄ (monoclinic, space group *C2/m*, *a* = 1267.6(4), *b* = 416.2(2), *c* = 887.4(3) pm, β = 110.37(2)°, *Z* = 2, *R*1 = 0.0354) Al-Ge sheets with Al in tetrahedral (*i. e.* Al⁺) and Ge in threefold ψ -tetrahedral (*i. e.* Ge[−]) coordination against Ge are present. Thus, the compound can be classified as an electron precise Zintl phase. This finding is verified by the result of a band structure calculation (within the FP-LAPW approach), that shows a distinct minimum of the total density of states at the Fermi level. The structure of Ca₁₀Al₆Ge₉ (trigonal, space group *R $\bar{3}m$* , *a* = 1398.45(14), *c* = 2107.4(3) pm, *Z* = 6, *R*1 = 0.0613) contains complicated sheets of trigonal planar building units [AlGe₃] and [AlGe₄] tetrahedra. The compound Ca₂₀[Al₃Ge₆]₂[Ge] (hexagonal, space group *P6₃/m*, *a* = 1600.9(2), *c* = 458.48(7) pm, *Z* = 1, *R*1 = 0.0282) shows two planar trimers of [AlGe₃] triangles of formula [Al₃Ge₆] besides isolated Ge atoms (*i. e.* Ge^{4−}). The overall electron count of the latter compounds, that contain trigonal planar coordinated Al atoms and considerable multiple bond character of the Al-Ge bonds, shows a very small deviation from the Zintl concept, comparable to the one observed in other aluminium-germanides like SrAlGe.

Key words: Aluminium, Germanium, Zintl Phases