

BaCu₆Ge₂S₈ – Ein Thiogermanat als Variante der Li₃Bi-Struktur

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BaCu₆Ge₂S₈ was synthesized by direct reaction of the elements at 750°C and characterized by X-ray single crystal techniques. The thiogermanate crystallizes in a new orthorhombic structure type ($a = 6.122(1)$ Å, $b = 12.084(3)$ Å, $c = 17.614(5)$ Å; *Pbcm*, $Z = 4$). Isolated [GeS₄]⁴⁻ tetrahedra form a slightly distorted cubic face-centered (fcc) arrangement. Ba and Cu atoms each occupy half the octahedral gaps (*OG*) of this “tetrahedra packing”. Further Cu atoms fill the tetrahedral gaps (*TG*) completely. The compound can be written as Ba₂^(1/2OG)(Cu₂)₂^(1/2OG)Cu₈^(TG)(GeS₄)₄. Thus the structure of BaCu₆Ge₂S₈ can be derived from the Li₃Bi type. The sulfur coordination of the metal atoms (Cu tetrahedral or trigonal, Ba with CN 8) are realized by the spatial orientation of the [GeS₄]⁴⁻ tetrahedra. Their centers nearly maintain the fcc-arrangement. This structure interpretation of BaCu₆Ge₂S₈ from the viewpoint of a “filled tetrahedra packing” is discussed for further known thiogermanate compounds.

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