Au_3SnCuP_{10} and Au_3SnP_7: Preparation and Crystal Structures of Au_3Sn Heterocluster Polyphosphides

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Dedicated to Professor Wolfgang Jeitschko on the occasion of his 70th birthday

The formation of Au_3Sn heteroclusters completes the homologous series of M_3Sn clusters observed for transition metal main-group polyphosphides. Au_3SnCuP_{10} is cubic, space group $F\bar{4}3m$ (No. 216) with lattice parameter $a = 10.3953(5)$ Å. The structure refinement yielded $R1 = 0.0353$ and $wR2 = 0.0726$ for 154 F^2 values and 13 variables. Disordered Au_3Sn heteroclusters occupy all octahedral, and adamantane like P_{10} cages one half of the tetrahedral voids of a face-centred cubic (fcc) arrangement of copper. Ordered and orientationally disordered Au_3Sn heteroclusters have been observed for Au_3SnP_7, embedded in a $^1_\infty[P_7]$ polyphosphide unit formed by six-membered phosphorus rings in chair conformation which are linked by a P-bridge. Au_3SnP_7 is monoclinic, space group $P2_1/m$ (No. 11) with lattice parameters of $a = 6.219(2)$, $b = 10.836(2)$, $c = 6.318(2)$ Å, $\beta = 108.65(2)^\circ$, $V = 403.4(2)$ Å^3, $R1 = 0.0412$ and $wR2 = 0.0745$, 1261 F^2 values and 56 variables. Au_3SnP_7 with disordered Au_3Sn clusters has slightly larger lattice parameters of $a = 6.343(3)$, $b = 10.955(3)$, $c = 6.372(3)$ Å, $\beta = 108.63(2)^\circ$, $V = 419.6(2)$ Å^3, $R1 = 0.0324$ and $wR2 = 0.0691$, 1131 F^2 values and 58 variables.

Key words: Polyphosphides, Heterocluster, Structure Determination