

Structure

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Synthesis, Crystal Structure, Phase Relations and Chemical Bonding Analysis of the New Nowotny Chimney-Ladder Compound $\text{ZrBi}_{1.62}$.

— The new title compound is synthesized from the elements (quartz tube, 780 °C, 48 h) and characterized by single crystal XRD, powder XRD, DTA, SEM, and quantum chemical DFT calculations. The compound crystallizes in the superspace group pair $W:P4/nnc:q-1q1 \rightarrow P:4_1/amd:1-1ss$. Two hypothetical commensurate approximants of the $\text{ZrBi}_{1.62}$ structure are Zr_3Bi_5 (tetragonal space group $P4n2$, $Z = 4$) and $\text{Zr}_8\text{Bi}_{13}$ (tetragonal space group $P4c2$, $Z = 4$). The calculated electron density of states indicates metallic behavior of the compound. — (BOSTROEM*, M.; LIND, H.; LIDIN, S.; NIEWA, R.; GRIN, Y.; Solid State Sci. 8 (2006) 10, 1173-1180; MPI Chem. Phys. fester Stoffe, D-01187 Dresden, Germany; Eng.) — W. Pewestorf