The Crystal Structure of WC Type ZrTe. Advantages in Chemical Bonding as Contrasted to NiAs Type ZrTe

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Single crystals of WC type ZrTe were prepared from the elements. A single crystal structure determination of this structure type was performed for the first time: ZrTe (WC) crystallizes in the hexagonal space group $P\bar{6}m2$ (No. 187), $hP2$, $Z = 1$, $a = 377.06(5)$, $c = 386.05(8)$ pm; 84 reflections, 5 variables, $R(F) = 0.037$. The distinctions in bonding for ZrTe (WC) and a hypothetical stoichiometric ZrTe crystallizing in the NiAs type structure were analyzed on the basis of extended Hückel calculations. Heteronuclear interactions contribute most strongly to the stability of both structures. Attractive Zr-Zr interactions energetically favour ZrTe (WC) relative to ZrTe (NiAs). The Fermi level of ZrTe (WC) resides in a local minimum of the DOS, whereas that of ZrTe (NiAs) intersects a local DOS maximum, and is pushed up by about 0.5 eV, expressing the decisive destabilization of NiAs type ZrTe. As a consequence, metal deficiency is observed for ZrTe (NiAs), in contrast to ZrTe (WC).