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 *P6m2* (No. 187), *hP*2, $Z = 1$, $a = 377.06(5)$, $c = 386.05(8)$ 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*).