Pt-Dumbbells in Ba_3Pt_2: Interplay of Geometric and Relativistic Effects on Pt–Pt Bonding

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Ba_3Pt_2 has been synthesized by reaction of a 3 : 2 mixture of Ba and Pt at 1223 K in argon, and characterized by single-crystal X-ray structure determination and electrical resistivity measurements. Ba_3Pt_2 crystallizes in the Er_3Ni_2 structure type (space group $R\bar{3}$ with $a = 962.40(6)$, $c = 1860.6(1)$ pm, $Z = 9$, $R(F)_{N'} = 0.063$, $N'(hkl) = 777$), and is isotypic to Ca_3Pt_2 and Sr_3Pt_2. The Pt atoms occur in pairs at a distance of 303 pm. According to the analysis of the Electron Localization Function and the Crystal Orbital Hamilton Population obtained from DFT band structure calculations, covalent bonding can be assumed in the Pt-dumbbells, although it is weaker in Ba_3Pt_2 than in Ca_3Pt_2. The peculiarities of the platinum compounds due to relativistic effects are elaborated by a comparison with theoretical results for Ca_3Pd_2. Ba_3Pt_2 exhibits metallic conductivity ($\rho_{270} = 0.7$ m$\Omega \cdot$ cm), which is in accordance with band structure calculations.

Key words: Barium, Band Structure Calculation, Crystal Structure, Intermetallic Compound, Platinum