Preparation, Characterization and Crystal Structure of the Room Temperature Phase of $[(CH_3)(C_6H_5)_3P]_2[ZnBr_4]$: A Member of the A_2BX_4 Family

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Z. Naturforsch. **62a,** 549 – 554 (2007); received March 21, 2007

The compound bis(methyltriphenylphosphonium) tetrabromozincate(II), $[C_{19}H_{18}P]_2[ZnBr_4]$, $M_r = 939.640$, has a monoclinic unit cell, space group $P2_1$. The lattice parameters are $a = 9.7693(4)$ Å, $b = 12.5508(4)$ Å, $c = 16.5372(6)$ Å, $\alpha = 90.00°$, $\beta = 105.2670(11)°$, $\gamma = 90.00°$, $V = 1956.11(11)$ Å^3, $Z = 2$, $D_x = 1.595$ mg m^{-3} at $T = 298$ K. The structure consists of one distorted $[ZnBr_4]^{2-}$ tetrahedron and two $[(CH_3)(C_6H_5)_3P]^+$ cations. Differential scanning calorimetry indicates a continuous second-order transition at (276 ± 2) K that may be classified as a commensurate to incommensurate transformation. A first-order transition to a higher symmetry is associated with a four-fold rotation of the $[ZnBr_4]^{2-}$ ion and a change of entropy $\Delta S = 22.92$ J/(K · mol) at $T = (362 \pm 3)$ K.

Dilatometric measurements showed a decrease of the lattice parameters in the temperature range 230 – 260 K, confirmed the transition at (276 ± 2) K, and indicated the presence of a third transition at 282 K.

Key words: Crystal Structure; Phase Transition; Commensurate-Incommensurate.
PACS numbers: 61.10.i, 64.70.Kb, 61.44.Fw.