Pseudo-symmetries of the Phases of $(Et_4N)_2ZnBr_4$

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The phase sequence of $(Et_4N)_2ZnBr_4$ has been determined based on thermal analysis. Below the decomposition point (572 K) four phases are distinguished.

The structures of three of the phases have been determined from 4-circle diffraction data at 240 (neutrons), 299 and 373 K (X-rays), respectively. The multiply twinned low-temperature phase (at 240 K) is characterized by a pseudo-orthorhombic lattice (monoclinic, P1a1, a = 17.6120(9) Å, b = 8.8195(4) Å, c = 16.1062(6) Å and β = 89.94(2)°), whereas the room-temperature phase (299 K: $P42_1c$, a = 8.9874(6) Å and c = 15.9774 Å) and the first high-temperature phase (373 K: $P4_2/nmc$, a = 9.145(4) Å and c = 15.835(8) Å) belong to the tetragonal crystal system. The transitions between the three phases are essentially connected with a stepwise ordering of the Et_4N^+ ions, whereas the positions of the heavy atoms change only slightly. Three ^{81}Br NQR lines are observed between 77 and 204 K.

Key words: $(Et_4N)_2ZnBr_4$; Twinning; Pseudo-symmetry; Structures.