Refinement of the Crystal Structure of Cronstedtite-3T

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Abstract: The crystal structure of cronstedtite-3T from Kutná Hora (Bohemia, Czechoslovakia), space group $P3_1$, was refined to R_w(all) = 3.1% for 1336 independent diffractions. There are two and three independent tetrahedral and octahedral positions, respectively, in this structure. The tetrahedra are occupied by 0.75 Si and 0.25 Fe while the octahedra are uniformly occupied by Fe. The refinement process was hindered by two problems: a " strong " superposition structure (all atoms of the octahedral sheets, i.e., ÷ 70% of the total diffraction power contribute almost solely to the family diffractions with mod(h – k, 3) = 0), and a slight disorder of the investigated crystal. The first problem was resolved by a preliminary block-diagonal refinement procedure where the atoms coinciding in the superposition structure were separated into individual blocks. The second problem was resolved by including two scale factors into the final full-matrix refinement: one for family diffractions, the other for the remaining ones which are characteristic for this polytype.

Key Words: Cronstedtite • Order-disorder (OD) • Polytypism

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