

Preparation, crystal structure and characterization of α -NaSbP₂S₆ and β -NaSbP₂S₆ phases

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The new phases α -NaSbP₂S₆ and β -NaSbP₂S₆ were synthesized by ceramic and reactive flux methods at 773 K. The structures of α -NaSbP₂S₆ and β -NaSbP₂S₆ were determined by the single-crystal X-ray diffraction technique. α -NaSbP₂S₆ crystallizes in the monoclinic space group P2₁/c with $a = 11.231(2)$ Å, $b = 7.2807(15)$ Å, $c = 11.640(2)$ Å, $\beta = 108.99(3)^\circ$, $V = 900.0(3)$ Å³ and $z = 4$. β -NaSbP₂S₆ crystallizes in the monoclinic space group P2₁ with $a = 6.6167(13)$ Å, $b = 7.3993(15)$ Å, $c = 9.895(2)$ Å, $\beta = 92.12(3)^\circ$, $V = 484.10(17)$ Å³ and $z = 2$. The α - and β -phases of NaSbP₂S₆ are closely related, the main difference lies in the stacking of the [Sb[P₂S₆]]_n- layers. The structure of α -NaSbP₂S₆ consists of two condensed layers (MPS3 type) to give an ABAB... sequence with Na⁺ cations located in the interlayer space. The packing of β -NaSbP₂S₆ is formed by monolayers of [Sb[P₂S₆]]_n- stacked in an AA... fashion separated by a layer of Na⁺ cations. Both phases are derivatives of the M1+M3+P2Q6 family. The op