

Light-induced alteration of arsenic sulfides: A new product with an orthorhombic crystal structure

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ABSTRACT

The crystal structure of a new light-induced alteration product obtained from a natural non-stoichiometric arsenic sulfide (original chemical formula $\text{As}_4\text{S}_{4.35}$) was solved in the space group *Pccn*, and refined to a final *R* index of 9.89%. Unit-cell parameters are: $a = 19.352(7)$, $b = 10.166(3)$, $c = 8.697(4)$ Å, $V = 1711(1)$ Å³; $Z = 8$. The structural refinement results yielded a chemical formula close to As_4S_5 . The structure consists of discrete, covalently bonded As_4S_5 molecules, which are held together by van der Waals forces. The molecular packing is similar to that of the original crystal, which, in turn, is the same as to that of $\beta\text{-As}_4\text{S}_4$. The phase originated from a continuous, room-temperature, light-induced alteration process that does not require a complete rearrangement of the molecular packing and therefore does not imply the loss of coherency between crystalline domains.

Keywords: XRD data, arsenic sulfide, crystal structure, light-induced alteration, molecular packing