

Alacranite, As₈S₉: structural study of the holotype and re-assignment of the original chemical formula

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ABSTRACT

Alacranite from the type locality (Uzon caldera, Kamchatka, Russian Federation) was submitted for structural analysis. A single crystal was selected and the following lattice parameters were determined: $a = 9.942(4)$, $b = 9.601(2)$, $c = 9.178(3)$ Å, $\beta = 101.94(3)^\circ$, $V = 857.1(5)$ Å³. The crystal structure was solved in the $P2/c$ space group using direct methods and refined to $R = 6.79\%$ for 472 observed reflections. The structure of alacranite consists of an ordered sequence of As₄S₄ and As₄S₅ cage-like molecules, with a molecular packing closely resembling that found in the β -As₄S₄ phase. Both As-As and As-S intramolecular distances are in the range usually observed for covalent bonds. The structural model confirms the chemical formula As₈S₉ for alacranite, and accounts for differences in the unit-cell parameters of alacranite compared to those of the natural analogue of β -As₄S₄. This latter mineral, therefore, should receive a new name.