

Preparation and Crystal Structure of $\text{Cs}_4\text{Nb}_2\text{S}_{11}$

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The new polychalcogenide $\text{Cs}_4\text{Nb}_2\text{S}_{11}$ was prepared from the melt. $\text{Cs}_4\text{Nb}_2\text{S}_{11}$ is orthorhombic, *oP68*, s.g. *Pca2₁* (No.29), *Z* = 4 with *a* = 13.775(9) Å, *b* = 8.043(9) Å, *c* = 18.306(5) Å. The crystal structure was determined from diffractometer data and refined to a conventional *R* of 0.052 (1104 Fo's, 154 variables). It is characterized by asymmetric discrete binuclear moieties $[\text{Nb}_2\text{S}_{11}]^{4-}$ which are separated by the alkali cations. Each Nb atom is side-on coordinated by two S_2^{2-} groups, one bridging and one terminal sulfide ligand. Nb-S bond lengths are 2.15(1) Å to 2.22(1) Å (terminal) and 2.44(1) Å to 2.51(1) Å (others). A further longer Nb-S bond (2.86(1) Å and 2.90(1) Å, resp.) expands the coordination of the two crystallographically independent transition metal atoms to distorted pentagonal bipyramidal configurations. The Nb-Nb-distance is 3.517(3) Å. The anionic groups are arranged in hexagonal close packed slabs running parallel to (001). The atomic arrangement corresponds to that of $\text{K}_4\text{Ta}_2\text{S}_{11}$.

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