Low Dimensional Materials: Syntheses, Structures, and Optical Properties of Rb_2CuTaS_4 , $Rb_2CuTaSe_4$, $RbCu_2TaSe_4$, $K_3Ag_3Ta_2Se_8$, and $Rb_3AgTa_2Se_{12}$

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Z. Naturforsch. **59b**, 1006 – 1014 (2004); received July 14, 2004

Dedicated to Professor Kurt O. Klepp on the occasion of his 60th birthday

The new compounds Rb₂CuTaS₄ (1), Rb₂CuTaSe₄ (2), RbCu₂TaSe₄ (3), K₃Ag₃Ta₂Se₈ (4), and Rb₃AgTa₂Se₁₂ (5) have been synthesized by the reactive flux method at 773 or 873 K. Their crystal structures were determined by single crystal X-ray diffraction. Crystal data for 1: space group Fddd, a = 5.598(1), b = 13.512(4), c = 23.854(5) Å, Z = 8; Crystal data for 2: space group Fddd, a = 5.782(1), b = 13.924(3), c = 24.653(5) Å, Z = 8; Crystal data for 3: space group C2cm, a = 5.7218(3), b = 19.2463(13), c = 7.7456(5) Å, Z = 4; Crystal data for 4: space group C2/c, $a = 25.1374(19), b = 6.1007(3), c = 14.4030(11) \text{ Å}, \beta = 119.703(8)^{\circ}, Z = 4$; Crystal data for 5: space group $P2_1/n$, a = 9.8186(6), b = 13.7462(11), c = 15.7368(9) Å, $\beta = 96.681(7)^{\circ}$, Z = 4. The compounds 1 and 2 are built up of ${}^{1}_{\infty}$ [CuTaQ₄]²⁻ anionic chains which are formed by edge-sharing CuO₄ and TaO₄ tetrahedra. The rubidium cations are located between the chains, Compound 3 consists of $_{\infty}^{2}$ [Cu₂TaSe₄] – anionic layers separated by rubidium cations. The anionic layers are formed by \(^1\) CuTaSe₄\(^1\)²⁻ chains which are connected by CuSe₄ tetrahedra that share common edges with the TaSe₄ tetrahedra of neighboring chains. In compound $4\frac{1}{\infty}[Ag_3Ta_2Se_8]^{3-}$ anionic chains are found which are separated by potassium cations. These chains are formed by successive corner sharing of AgSe₄ tetrahedra and edge sharing between AgSe₄ and TaSe₄ tetrahedra. All three structures are closely related with the sulvanite (Cu₃VS₄) structure type. Compound 5 contains a one dimensional $\frac{1}{\infty}[AgTa_2Se_{12}]^{3-}$ anionic chain formed by interconnection of AgSe₄ tetrahedra and $[Ta_2Se_{11}]$ units. In the structure three monoselenide, three diselenide, and one triselenide anions are found. Raman and far-IR spectroscopic data of compounds 1 and 4 were collected and an interpretation is presented.

Key words: Tantalum Compound, Quaternary Chalcogenides, Crystal Structures, Flux Reaction, Optical Properties