

K₄Ti₃Te₉ – A New Pseudo One-Dimensional Polyanionic Alkali Chalcogenometallate(IV)

Andreas Kolb and Kurt O. Klepp

Department of General and Inorganic Chemistry, University of Linz,
Altenbergerstr. 69, A-4040 Linz, Austria

Reprint requests to Prof. Kurt O. Klepp. E-mail: kurt.klepp@jku.at

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Lustrous black needle shaped single crystals of K₄Ti₃Te₉ were obtained by reacting K₂Te with the corresponding elemental components at 1000 °C. K₄Ti₃Te₉ is monoclinic, *mP*64, s. g. *P*2₁/*c* (No. 14), *Z* = 4 with *a* = 9.052(2), *b* = 8.088(1), *c* = 29.465(9) Å, *β* = 92.35(1)°. The crystal structure was determined from diffractometer data and refined to a conventional *R* value of 0.035 (2840 *F*_o's, 146 variables). The compound contains undulating polyanionic chains built up by severely distorted TiTe₆ octahedra sharing opposite faces which run parallel to [100] and are arranged in a hexagonal rod packing. The translation period comprises three octahedra. The most striking feature of this compound is the formation of two ditelluride groups per formula unit with unusually long Te-Te distances of 2.960(2) and 3.025(2) Å, respectively. All other Te-Te distances start at 3.2 Å. The nearest homonuclear neighbours of the two pairs are at 3.215(2) and 3.333(2) Å apart. Ti-Te bond lengths range from 2.700(3) to 2.841(3) Å with an average value of 2.772(4) Å for all three crystallographically independent titanium atoms. The alkali cations are irregularly coordinated by 7 to 9 tellurium atoms.

Key words: Chalcogenides, Polyanionic Chains, Group IVa Metal Compounds