Preparation and Crystal Structure of Na_4TiSe_4. A Selenotitanate with Discrete Tetrahedral Anions

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Red crystals of Na_4TiSe_4 were obtained by reacting an intimate mixture of Na_2Se, Ti and Se at 750°Ç. Na_4TiSe_4 is monoclinic, space group *I2/a* with a = 24.027(6), b = 7.346(4), c = 21.572(6) Å, β = 104.52(2)°, Z = 16. Its crystal structure was determined from diffractometer data (AgKα-radiation) and refined to a conventional R of 0.036 for 2673 F_o's and 158 variables. The crystal structure is of a new type, characterized by the presence of discrete tetrahedral complex anions, $[TiSe_4]^{4-}$, which are arranged in slabs parallel to (100). The average Ti-Se bond length is 2.385(1) Å. The Na^+ cations are in different chalcogen environments with distorted octahedral, square pyramidal or planar configurations, respectively.