Preparation and Crystal Structure of Na$_4$TiSe$_4$.
A Selenotitanate with Discrete Tetrahedral Anions

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Red crystals of Na$_4$TiSe$_4$ were obtained by reacting an intimate mixture of Na$_2$Se, Ti and Se at 750°C. Na$_4$TiSe$_4$ is monoclinic, space group $I2/a$ with $a = 24.027(6)$, $b = 7.346(4)$, $c = 21.572(6)$ Å, $\beta = 104.52(2)^\circ$, $Z = 16$. Its crystal structure was determined from diffractometer data (AgK$\alpha$-radiation) and refined to a conventional $R$ of 0.036 for 2673 $F_0$'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.