

TiFe₃Te₃ [1]; TiMo₃Se₃ [2]

Structural features: Infinite columns of face-sharing Fe₆ octahedra parallel to [001]; Te above the octahedron faces. Ultimate condensation of Fe₆Te₈ clusters (a Fe₆ octahedron surrounded by a Te₈ cube). See Fig. IV.51.

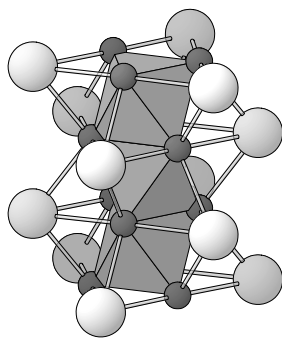


Fig. IV.51. **TiFe₃Te₃**

Arrangement of Fe₆ octahedra (Fe atoms small) and Te atoms (large).

Klepp K., Boller H. (1979) [1]

Fe₃Te₃Ti

$a = 0.935$, $c = 0.4223$ nm, $c/a = 0.452$, $V = 0.3197$ nm³, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Fe1	6h	$m..$	0.1493	0.1701	$\frac{1}{4}$		bicapped square prism Fe ₆ Te ₄
Te2	6h	$m..$	0.357	0.0462	$\frac{1}{4}$		4-vertex polyhedron Fe ₄
Ti3	2c	$-6..$	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$		tricapped trigonal prism Te ₉

Transformation from published data: $y, x, -z$; origin shift $0\ 0\ \frac{1}{2}$

Experimental: single crystal, diffractometer, X-rays, $R = 0.048$

Remarks: The same data are quoted in [3], where refinements on powder neutron diffraction data collected at 6 and 154 K are reported (magnetic structure determined).

References: [1] Klepp K., Boller H. (1979), Monatsh. Chem. 110, 677-684. [2] Potel M., Chevrel R., Sergent M. (1980), Acta Crystallogr. B 36, 1545-1548. [3] Bronger W., Klepp K., Müller P. (1985), J. Less-Common Met. 106, 301-303.