

Co_{0.33}NbS₂ [2]; Mn_{0.33}NbS₂ [5]; Fe_{0.33}TiS₂ [3]

Structural features: Close-packed S layers in BBCC stacking; Nb in trigonal prismatic, Co in octahedral voids. Infinite slabs of edge-linked NbS₆ trigonal prisms are interconnected via CoS₆ octahedra to form a 3D-framework. Ordering variant of Nb_{1.25}S₂. See Fig. IV.37.

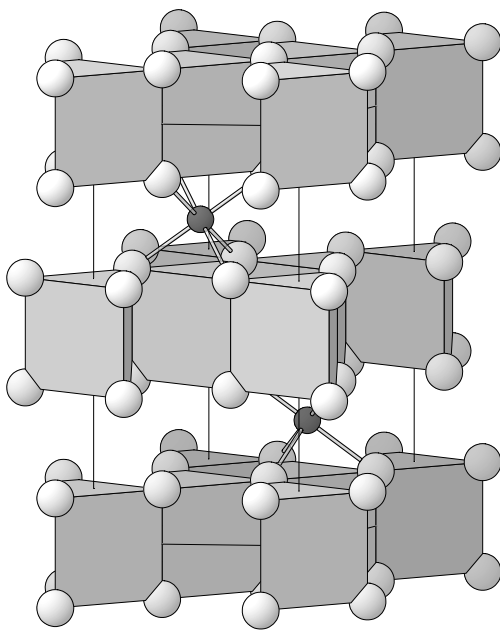


Fig. IV.37. Co_{0.33}NbS₂

Arrangement of NbS₆ trigonal prisms and CoS₆ octahedra (Co atoms small, S atoms large).

Parkin S.S.P. et al. (1983) [1]

Co_{0.95}Nb₃S₆

$a = 0.5749$, $c = 1.1886$ nm, $c/a = 2.067$, $V = 0.3402$ nm³, $Z = 2$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
S1	12i	1	0.3322	0.0009	0.1306		4-vertex polyhedron CoNb ₃
Nb2	4f	3..	1/3	2/3	0.5056		trigonal prism S ₆
Co3	2c	3.2	1/3	2/3	1/4	0.949	8-vertex polyhedron S ₆ Nb ₂
Nb4	2a	32.	0	0	0		trigonal prism S ₆

Transformation from published data: $-x, -y, -z$

Experimental: single crystal, diffractometer, neutrons, $R = 0.070$

Remarks: Two additional partly occupied Co sites are reported in [4]. The description of Fe_{0.33}TiS₂ in space group (163) *P*-31c in [3] does not take into consideration all symmetry elements of the proposed structure. In [3] (Fe_{0.33}TiS₂) the Wyckoff position of the second Ti site is misprinted as 2f instead of 4f.

References: [1] Parkin S.S.P., Marseglia E.A., Brown P.J. (1983), J. Phys. C: Solid State Phys. 16, 2765-2778. [2] Van Den Berg J.M., Cossee P. (1968), Inorg. Chim. Acta 2, 143-148. [3] Takahashi T., Yamada O. (1973), J. Solid State Chem. 7, 25-30. [4] Van Laar B., Rietveld H.M., Ijdo D.J.W. (1971), J. Solid State Chem. 3, 154-160. [5] Anzenhofer K., Van Den Berg J.M., Cossee P., Helle J.N. (1970), J. Phys. Chem. Solids 31, 1057-1067.