

$\text{Ag}_{0.6}\text{NbS}_2$  $hP10$  $(186) P6_3mc - b^5$  **$\text{Ag}_{0.6}\text{NbS}_2$  It [1]**

Structural features: Close-packed S layers in BBCC stacking; Nb in trigonal prismatic, Ag in tetrahedral voids (partial disorder for the latter).  $\text{NbS}_6$  trigonal prisms share edges to form infinite slabs.

Van Der Lee A. et al. (1991) [1]

 $\text{Ag}_{0.60}\text{NbS}_2$  $a = 0.3355$ ,  $c = 1.431$  nm,  $c/a = 4.265$ ,  $V = 0.1395$  nm<sup>3</sup>,  $Z = 2$ 

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
Ag1	$2b$	$3m.$	$\frac{1}{3}$	$\frac{2}{3}$	0.0	0.27	7-vertex polyhedron $\text{Ag}_3\text{S}_4$
S2	$2b$	$3m.$	$\frac{1}{3}$	$\frac{2}{3}$	0.161		7-vertex polyhedron $\text{Ag}_4\text{Nb}_3$
S3	$2b$	$3m.$	$\frac{1}{3}$	$\frac{2}{3}$	0.3773		7-vertex polyhedron $\text{Ag}_4\text{Nb}_3$
Ag4	$2b$	$3m.$	$\frac{1}{3}$	$\frac{2}{3}$	0.5414	0.33	7-vertex polyhedron $\text{Ag}_3\text{S}_4$
Nb5	$2b$	$3m.$	$\frac{1}{3}$	$\frac{2}{3}$	0.7689		trigonal prism $\text{S}_6$

Transformation from published data:  $-x, -y, -z$ ; origin shift 0 0 0.4811Experimental: single crystal, diffractometer, X-rays,  $R = 0.044$ ,  $T = 100$  K

Remarks: Phase stable at  $T < 124$  K. Average structure; the incommensurately modulated superstructure was refined in superspace group  $P:P6_3mc:6mm$ . Short interatomic distances for partly occupied site(s).

References: [1] Van Der Lee A., Van Smaalen S., Wiegers G.A., De Boer J.L. (1991), Phys. Rev. B: Condens. Matter 43, 9420-9431.