

$\text{Ta}_9\text{Ni}_2\text{S}_6$	$hP17$	(189) $P\text{-}62m - \text{kgf}^2c$
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**$\text{Ni}_2\text{Ta}_9\text{S}_6$**  [1]

Structural features: Infinite columns of base-linked  $\text{NiTa}_6\text{Ta}_3$  tricapped trigonal prisms share the capping atoms to form a 3D-framework; S in large channels parallel to [001].

Harbrecht B., Franzen H.F. (1985) [1]

$\text{Ni}_2\text{S}_6\text{Ta}_9$

$a = 1.0127$ ,  $c = 0.3367$  nm,  $c/a = 0.332$ ,  $V = 0.2990$  nm<sup>3</sup>,  $Z = 1$

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
Ta1	$6k$	$m..$	0.19683	0.4603	$\frac{1}{2}$		square pyramid $\text{S}_3\text{Ni}_2$
S2	$3g$	$m2m$	0.7316	0	$\frac{1}{2}$		4-vertex polyhedron $\text{Ta}_4$
S3	$3f$	$m2m$	0.2953	0	0		5-vertex polyhedron $\text{Ta}_5$
Ta4	$3f$	$m2m$	0.5466	0	0		15-vertex polyhedron $\text{S}_3\text{Ni}_2\text{Ta}_{10}$
Ni5	$2c$	$-6..$	$\frac{1}{3}$	$\frac{2}{3}$	0		trigonal prism $\text{Ta}_6$

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

Experimental: single crystal, diffractometer, X-rays,  $R = 0.031$

Remarks: The same paper was also published as [2]. For  $\text{Fe}_2\text{Ta}_9\text{S}_6$  and  $\text{Co}_2\text{Ta}_9\text{S}_6$  (isotypic according to [1]) a superstructure with double cell volume was later reported [4]. In [3] the  $c$ -parameter is misprinted as 3.367 nm instead of 0.3367 nm.

References: [1] Harbrecht B., Franzen H.F. (1985), J. Less-Common Met. 113, 349-360. [2] Harbrecht B., Franzen H.F. (1986), J. Less-Common Met. 115, 177-189. [3] (1986), Structure Reports 52A, 59. [4] Harbrecht B. (1986), J. Less-Common Met. 124, 125-134.