

TaSe ₂	<i>hP</i> 12	(186) $P6_3mc - b^4a^2$
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TaSe₂ 4s(c) [1]

Structural features: Close-packed Se layers in AABBAACC stacking; Ta in trigonal prismatic voids (stacking sequence AbA BcB AcA CbC). Layer structure with sandwiches consisting of three sublayers (Se-Ta-Se). Infinite slabs of edge-linked TaSe₆ trigonal prisms share edges in hc stacking.

Huisman R., Jellinek F. (1969) [1]

Se₂Ta

$a = 0.3436$, $c = 2.5532$ nm, $c/a = 7.431$, $V = 0.2611$ nm³, $Z = 4$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Ta1	2 <i>b</i>	3 <i>m.</i>	$\frac{1}{3}$	$\frac{2}{3}$	0.05		anticuboctahedron Se ₆ Ta ₆
Se2	2 <i>b</i>	3 <i>m.</i>	$\frac{1}{3}$	$\frac{2}{3}$	0.236		non-coplanar triangle Ta ₃
Se3	2 <i>b</i>	3 <i>m.</i>	$\frac{1}{3}$	$\frac{2}{3}$	0.371		non-coplanar triangle Ta ₃
Ta4	2 <i>b</i>	3 <i>m.</i>	$\frac{1}{3}$	$\frac{2}{3}$	0.797		anticuboctahedron Se ₆ Ta ₆
Se5	2 <i>a</i>	3 <i>m.</i>	0	0	0.0		non-coplanar triangle Ta ₃
Se6	2 <i>a</i>	3 <i>m.</i>	0	0	0.128		non-coplanar triangle Ta ₃

Transformation from published data: -*x*, -*y*, -*z*; origin shift 0 0 0.822

Experimental: powder, diffractometer, X-rays, R_B = 0.157

Remarks: Phase stable at T < 1043 K.

References: [1] Huisman R., Jellinek F. (1969), J. Less-Common Met. 17, 111-117.