

TaSe <sub>2</sub>	<i>hP</i> 156	(176) $P6_3/m - i^{10}h^4f^2ba$
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**TaSe<sub>2</sub> 4s(b) rt [1]**

Structural features: Close-packed Se layers in BBCBCCBC stacking; Ta in trigonal prismatic and octahedral voids (BaB CaB CaC BaC). Layer structure with two kinds of sandwich consisting of three sublayers each (Se-Ta-Se for both). The largest deviation from the ideal structure is observed for Ta in octahedral coordination.

Lüdecke J. et al. (1999) [1]

Se<sub>2</sub>Ta

$a = 1.24579$ ,  $c = 2.51495$  nm,  $c/a = 2.019$ ,  $V = 3.3803$  nm<sup>3</sup>,  $Z = 52$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Se1	12 <i>i</i>	1	0.0257	0.5894	0.1838		non-coplanar triangle Ta <sub>3</sub>
Se2	12 <i>i</i>	1	0.0509	0.175	0.0706		non-coplanar triangle Ta <sub>3</sub>
Se3	12 <i>i</i>	1	0.1028	0.3597	0.18366		non-coplanar triangle Ta <sub>3</sub>
Ta4	12 <i>i</i>	1	0.1519	0.5172	0.00401		octahedron Se <sub>6</sub>
Se5	12 <i>i</i>	1	0.1803	0.129	0.1846		non-coplanar triangle Ta <sub>3</sub>
Ta6	12 <i>i</i>	1	0.2172	0.2867	0.00003		octahedron Se <sub>6</sub>
Se7	12 <i>i</i>	1	0.2863	0.4842	0.06254		non-coplanar triangle Ta <sub>3</sub>
Se8	12 <i>i</i>	1	0.354	0.2513	0.06905		non-coplanar triangle Ta <sub>3</sub>
Se9	12 <i>i</i>	1	0.4352	0.0281	0.06198		non-coplanar triangle Ta <sub>3</sub>
Se10	12 <i>i</i>	1	0.4875	0.2055	0.18408		non-coplanar triangle Ta <sub>3</sub>
Ta11	6 <i>h</i>	<i>m</i> ..	0.157	0.5416	<sup>1</sup> / <sub>4</sub>		trigonal prism Se <sub>6</sub>
Ta12	6 <i>h</i>	<i>m</i> ..	0.2322	0.3068	<sup>1</sup> / <sub>4</sub>		trigonal prism Se <sub>6</sub>
Ta13	6 <i>h</i>	<i>m</i> ..	0.3116	0.0795	<sup>1</sup> / <sub>4</sub>		trigonal prism Se <sub>6</sub>
Ta14	6 <i>h</i>	<i>m</i> ..	0.615	0.1516	<sup>1</sup> / <sub>4</sub>		trigonal prism Se <sub>6</sub>
Se15	4 <i>f</i>	3..	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.1835		non-coplanar triangle Ta <sub>3</sub>
Se16	4 <i>f</i>	3..	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.56147		non-coplanar triangle Ta <sub>3</sub>
Ta17	2 <i>b</i>	-3..	0	0	0		octahedron Se <sub>6</sub>
Ta18	2 <i>a</i>	-6..	0	0	<sup>1</sup> / <sub>4</sub>		trigonal prism Se <sub>6</sub>

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

Experimental: single crystal, diffractometer, X-rays, R = 0.071

Remarks: Phase stable at 75 < T < 410 K. Refinement in (3+2)D-superspace.

References: [1] Lüdecke J., Van Smaalen S., Spijkerman A., De Boer J.L., Wiegers G.A. (1999), Phys. Rev. B: Condens. Matter 59, 6063-6071.