

CaTa₄O₁₁*hP*32(182) *P*6₃22 – *ig*²*fdc***CaTa₄O₁₁** [2], calciotantiteStructural features: Infinite layers of edge-linked TaO₇ pentagonal bipyramids share vertices with TaO₆ octahedra to form a 3D-framework. See Fig. IV.38.

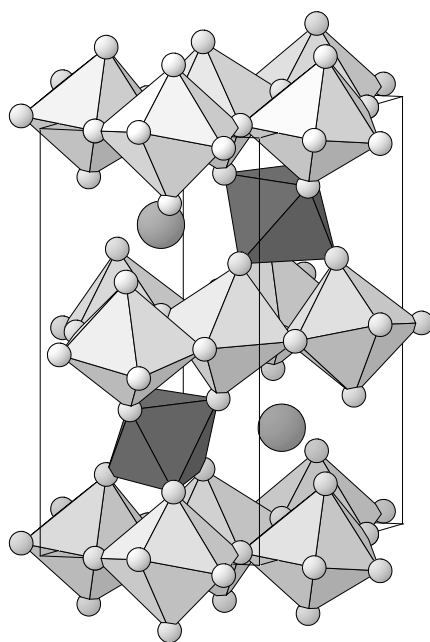
Isobe M. et al. (1975) [1]

CaO₁₁Ta₄ $a = 0.62173$, $c = 1.2271$ nm, $c/a = 1.974$, $V = 0.4108$ nm³, $Z = 2$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	12 <i>i</i>	1	0.43	0.059	0.344		non-colinear Ta ₂
O2	6 <i>g</i>	.2.	0.25	0	0		non-colinear Ta ₂
Ta3	6 <i>g</i>	.2.	0.6411	0	0		pentagonal bipyramid O ₇
O4	4 <i>f</i>	3..	$\frac{1}{3}$	$\frac{2}{3}$	0.038		non-coplanar triangle Ta ₃
Ta5	2 <i>d</i>	3.2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{3}{4}$		octahedron O ₆
Ca6	2 <i>c</i>	3.2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$		8-vertex polyhedron O ₈

Transformation from published data: origin shift 0 0 $\frac{1}{2}$

Experimental: single crystal, diffractometer, X-rays, R = 0.032

Fig. IV.38. **CaTa₄O₁₁**Arrangement of TaO₆ octahedra (dark), TaO₇ pentagonal bipyramids (light) (O atoms small) and Ca atoms (large).

References: [1] Isobe M., Marumo F., Iwai S., Kimura M. (1975), Acta Crystallogr. B 31, 908-910. [2] Jahnberg L. (1970), J. Solid State Chem. 1, 454-462.