

CeTa<sub>7</sub>O<sub>19</sub>*hP*54(188) *P*-6*c*2 – *l*<sup>3</sup>khgca**(Ce,Ta)Ta<sub>6</sub>O<sub>19</sub>** [1]

Structural features: TaO<sub>7</sub> pentagonal bipyramids share edges and vertices to form double slabs, which are interconnected via distorted TaO<sub>8</sub> cubes to form a 3D-framework.

Johnson A.W.S., Gatehouse B.M. (1980) [1]

CeO<sub>19</sub>Ta<sub>7</sub>*a* = 0.6226, *c* = 1.9976 nm, *c/a* = 3.208, *V* = 0.6706 nm<sup>3</sup>, *Z* = 2

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Ta1	12 <i>l</i>	1	0.02727	0.33333	0.1562		pentagonal bipyramid O <sub>7</sub>
O2	12 <i>l</i>	1	0.06467	0.33333	0.059		single atom Ta
O3	12 <i>l</i>	1	0.42567	0.33333	0.156		non-colinear Ta <sub>2</sub>
O4	6 <i>k</i>	<i>m</i> ..	0.06267	0.33333	<sup>1</sup> / <sub>4</sub>		non-colinear Ta <sub>2</sub>
O5	4 <i>h</i>	3..	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.131		non-coplanar triangle Ta <sub>3</sub>
O6	4 <i>g</i>	3..	0	0	0.131		non-coplanar triangle Ta <sub>3</sub>
Ta7	2 <i>c</i>	3.2	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0		octahedron O <sub>6</sub>
Ce8	2 <i>a</i>	3.2	0	0	0		octahedron O <sub>6</sub>

Transformation from published data: origin shift <sup>1</sup>/<sub>3</sub> <sup>2</sup>/<sub>3</sub> <sup>1</sup>/<sub>2</sub>

Experimental: thin film, electron diffraction

Remarks: Supersedes a refinement in space group (193) *P*6<sub>3</sub>/*mcm* with partial disorder Ce/Ta [2]; the lower symmetry was confirmed by convergent-beam electron diffraction. We derived the atom coordinates in space group (188) *P*-6*c*2 from those reported in [2].

References: [1] Johnson A.W.S., Gatehouse B.M. (1980), Acta Crystallogr. B 36, 523-526. [2] Gatehouse B.M. (1979), J. Solid State Chem. 27, 209-213.