

Cu<sub>3</sub>Ta<sub>7</sub>O<sub>19</sub>*hP*58(176) *P*6<sub>3</sub>/*m* – i<sup>3</sup>hgfeb**Cu<sub>3</sub>Ta<sub>7</sub>O<sub>19</sub>** [1]

Structural features: Double infinite slabs of edge-linked TaO<sub>7</sub> pentagonal bipyramids (common vertices between the slabs) share vertices with TaO<sub>6</sub> octahedra to form a 3D-framework; Cu in linear coordination.

Jahnberg L., Sundberg M. (1992) [1]

Cu<sub>3</sub>O<sub>19</sub>Ta<sub>7</sub>*a* = 0.62323, *c* = 2.0156 nm, *c/a* = 3.234, *V* = 0.6780 nm<sup>3</sup>, *Z* = 2

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	12 <i>i</i>	1	0.03	0.27	0.057		non-coplanar triangle CuTa <sub>2</sub>
Ta2	12 <i>i</i>	1	0.03	0.34	0.156		pentagonal bipyramid O <sub>7</sub>
O3	12 <i>i</i>	1	0.42	0.34	0.156		non-collinear Ta <sub>2</sub>
O4	6 <i>h</i>	<i>m</i> ..	0.06	0.36	<sup>1</sup> / <sub>4</sub>		non-collinear Ta <sub>2</sub>
Cu5	6 <i>g</i>	-1	<sup>1</sup> / <sub>2</sub>	0	0		colinear O <sub>2</sub>
O6	4 <i>f</i>	3..	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.14		non-coplanar triangle Ta <sub>3</sub>
O7	4 <i>e</i>	3..	0	0	0.164		non-coplanar triangle Ta <sub>3</sub>
Ta8	2 <i>b</i>	-3..	0	0	0		octahedron O <sub>6</sub>

Transformation from published data: origin shift 0 0 <sup>1</sup>/<sub>2</sub>

Experimental: polycrystalline sample, electron diffraction

References: [1] Jahnberg L., Sundberg M. (1992), J. Solid State Chem. 100, 212-219.