

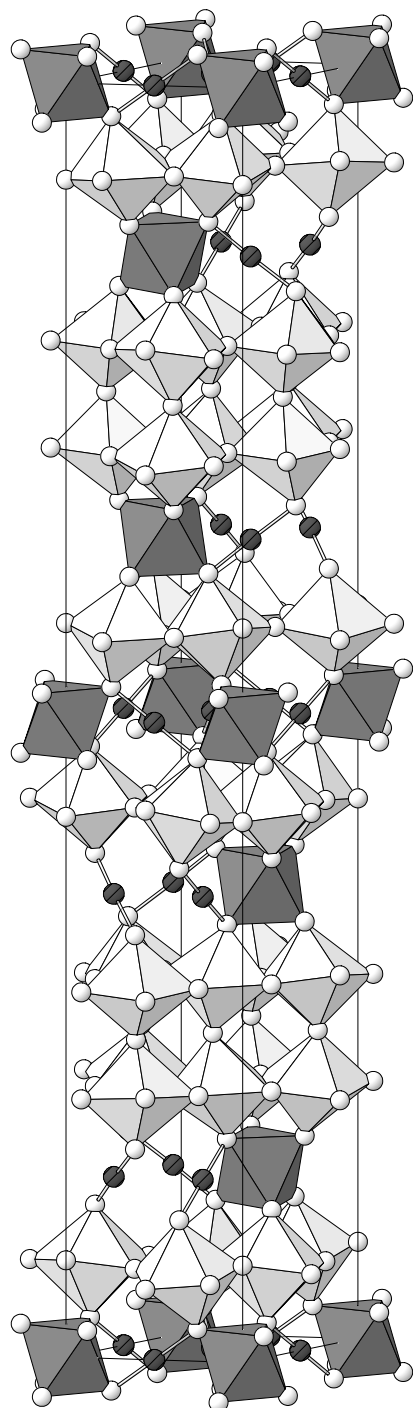
$\text{Cu}_7\text{Ta}_{15}\text{O}_{41}$ [1]

Fig. IV.84. **$\text{Cu}_7\text{Ta}_{15}\text{O}_{41}$**

Arrangement of TaO_6 octahedra (dark), TaO_7 pentagonal bipyramids (light) (O atoms light) and Cu atoms (dark; partly occupied sites).

Structural features: Double and simple infinite slabs of edge-linked TaO₇ pentagonal bipyramids (common vertices between the slabs) share vertices with TaO₆ octahedra to form a 3D-framework; Cu in linear coordination. See Fig. IV.84.

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

Cu₇O₄₁Ta₁₅

$a = 0.62262$, $c = 4.4877$ nm, $c/a = 7.208$, $V = 1.5066$ nm³, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Ta1	12i	1	0.0	0.36	0.208		pentagonal bipyramid O ₇
O2	12i	1	0.06	0.43	0.166		non-coplanar triangle Ta ₂ Cu
O3	12i	1	0.23	0.27	0.026		non-coplanar triangle CuTa ₂
O4	12i	1	0.25	0.25	0.208		non-colinear Ta ₂
Ta5	12i	1	0.3	0.33	0.069		pentagonal bipyramid O ₇
O6	12i	1	0.3	0.39	0.112		non-coplanar triangle CuTa ₂
Cu7	12i	1	0.33	0.17	0.139	0.778	non-colinear O ₂
O8	12i	1	0.42	0.09	0.069		non-colinear Ta ₂
O9	6h	$m..$	0.41	0.04	$\frac{1}{4}$		non-colinear Ta ₂
Cu10	6g	-1	$\frac{1}{2}$	0	0	0.778	colinear O ₂
O11	4f	3..	$\frac{1}{3}$	$\frac{2}{3}$	0.062		non-coplanar triangle Ta ₃
Ta12	4f	3..	$\frac{1}{3}$	$\frac{2}{3}$	0.139		octahedron O ₆
O13	4f	3..	$\frac{1}{3}$	$\frac{2}{3}$	0.212		non-coplanar triangle Ta ₃
O14	4f	3..	$\frac{1}{3}$	$\frac{2}{3}$	0.701		non-coplanar triangle Ta ₃
O15	4e	3..	0	0	0.076		non-coplanar triangle Ta ₃
Ta16	2b	-3..	0	0	0		octahedron O ₆

Transformation from published data: $y, x, -z$; origin shift $0\ 0\ \frac{1}{2}$

Experimental: polycrystalline sample, electron diffraction

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