

$\text{Ba}_5(\text{Ta}_{0.5}\text{Ru}_{0.5})_2\text{O}_9\text{Cl}_2$  $hP36$  $(182) P6_322 - \text{ihf}^3\text{ed}$ **Ba<sub>5</sub>RuTaO<sub>9</sub>Cl<sub>2</sub>** [1]

Structural features: Double perovskite-type slabs (three close-packed BaO<sub>3</sub> layers, (Ta,Ru) in octahedral (O<sub>6</sub>) voids) alternate with two hexagon-mesh BaCl layers along [001]. Units of two face-linked (Ta,Ru)O<sub>6</sub> octahedra.

Wilkens J., Müller Buschbaum H. (1991) [1]

 $\text{Ba}_5\text{Cl}_2\text{O}_9\text{Ru}_{0.94}\text{Ta}_{1.06}$  $a = 0.58985$ ,  $c = 2.4739$  nm,  $c/a = 4.194$ ,  $V = 0.7454$  nm<sup>3</sup>,  $Z = 2$ 

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
O1	12i	1	0.329	0.141	0.1555		single atom Ta
O2	6h	..2	0.149	0.298	$\frac{1}{4}$		non-colinear Ta <sub>2</sub>
Cl3	4f	3..	$\frac{1}{3}$	$\frac{2}{3}$	0.0486		colinear Ba <sub>2</sub>
Ba4	4f	3..	$\frac{1}{3}$	$\frac{2}{3}$	0.1699		10-vertex polyhedron O <sub>9</sub> Cl
Ba5	4f	3..	$\frac{1}{3}$	$\frac{2}{3}$	0.5757		monocapped trigonal prism O <sub>3</sub> Cl <sub>4</sub>
M6	4e	3..	0	0	0.1905		octahedron O <sub>6</sub>
Ba7	2d	3.2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{3}{4}$		anticuboctahedron O <sub>12</sub>

 $\text{M6} = 0.53\text{Ta} + 0.47\text{Ru}$ 

Experimental: single crystal, diffractometer, X-rays, R = 0.051

Remarks: When relevant, we changed the last digit of the atom coordinates to respect the symmetry conditions for special positions.

References: [1] Wilkens J., Müller Buschbaum H. (1991), J. Less-Common Met. 171, 255-262.