

BaTa ₂ O ₆	<i>hP33</i>	(189) <i>P</i> -62 <i>m</i> – li ² gf ²
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Ba_{0.5-x}TaO_{3-x} [1]

Structural features: Triple infinite chains of vertex-linked TaO₆ octahedra (partly ordered O vacancies).

Gray I., Millman A.P. (1960) [1]

BaO₆Ta₂

$a = 0.896$, $c = 0.779$ nm, $c/a = 0.869$, $V = 0.5416$ nm³, $Z = 3$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	12 <i>l</i>	1	0.18	0.47	0.26	0.75	single atom Ta
Ta2	6 <i>i</i>	<i>..m</i>	0.23	0	0.26		octahedron O ₆
O3	6 <i>i</i>	<i>..m</i>	0.84	0	0.26	0.5	non-colinear Ta ₂
O4	3 <i>g</i>	<i>m2m</i>	0.23	0	¹ / ₂		colinear Ta ₂
O5	3 <i>f</i>	<i>m2m</i>	0.23	0	0		colinear Ta ₂
Ba6	3 <i>f</i>	<i>m2m</i>	0.63	0	0		non-coplanar square O ₄

Transformation from published data: origin shift 0 0 ¹/₂

Experimental: single crystal, precession photographs, X-rays, R = 0.240

Remarks: Ba_{0.44}(Ta⁴⁺)_{0.74}(Ta⁵⁺)_{0.26}O_{2.57}. Tentative structure in disagreement with the observed fix cation ratio Ba/Ta = 0.44. We assume that in table 1 of [1] the number of O is misprinted so that the total number per cell is 21 instead of 18 (given in the text); we assigned an arbitrary value to the occupancy of site O1.

References: [1] Gray I., Millman A.P. (1960), Nature (London) 188, 1099-1100.