

BaHgRuO₅ [1]

Structural features: Hg₃Ru₃O₁₅ units (rings formed by three RuO₅ trigonal bipyramids interconnected via O-Hg-O linear units) in a Mg-type (h.c.p.) arrangement. See Fig. IV.71.

Hansen T. et al. (1995) [1]

BaHgO₅Ru

$a = 1.0176$, $c = 0.84121$ nm, $c/a = 0.827$, $V = 0.7544$ nm³, $Z = 6$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	12i	1	0.114	0.356	0.093		single atom Ru
Ru2	6h	$m..$	0.0124	0.343	$\frac{1}{4}$		trigonal bipyramid O ₅
O3	6h	$m..$	0.12	0.569	$\frac{1}{4}$		non-colinear RuHg
O4	6h	$m..$	0.229	0.107	$\frac{1}{4}$		non-colinear HgRu
Hg5	6h	$m..$	0.3336	0.3216	$\frac{1}{4}$		non-colinear O ₂
O6	6h	$m..$	0.492	0.179	$\frac{1}{4}$		single atom Ru
Ba7	4f	3..	$\frac{1}{3}$	$\frac{2}{3}$	0.0165		tricapped trigonal prism O ₉
Ba8	2b	-3..	0	0	0		icosahedron O ₁₂

Transformation from published data: $y, x, -z$

Experimental: powder, diffractometer, X-rays, $R_B = 0.040$

Remarks: In table 5 of [1] the Wyckoff positions are misprinted as $2a$, $4b$, $6c$ and $12d$ instead of $2b$, $4f$, $6h$ and $12i$, respectively.

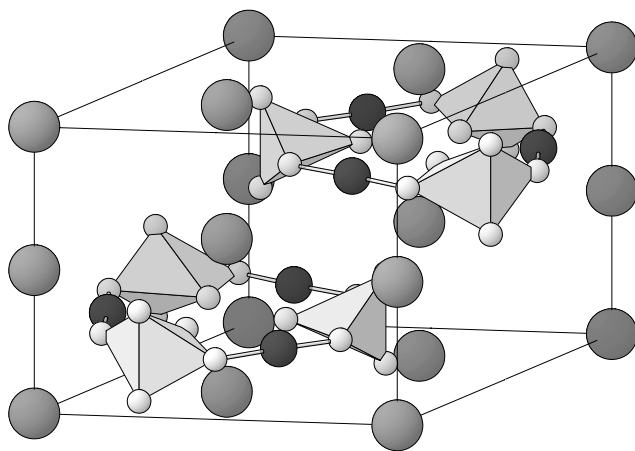


Fig. IV.71. **BaHgRuO₅**

Arrangement of Hg₃Ru₃O₁₅ units (three RuO₅ trigonal bipyramids, Hg atoms dark, O atoms light) and Ba atoms (large). For clarity, atoms located in the cell but belonging to units with the central atom in a neighboring cell are omitted.

References: [1] Hansen T., Le Bail A., Lalignat Y. (1995), J. Solid State Chem. 120, 223-230.