

BaHgO <sub>2</sub>	<i>hP24</i>	(182) <i>P6<sub>3</sub>22</i> – ihfā
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**BaHgO<sub>2</sub>** [1]

Structural features: Close-packed O layers in BBCC stacking; Ba in trigonal prismatic, Hg in linear voids. Infinite slabs of edge-linked BaO<sub>6</sub> trigonal prisms are interconnected via O-Hg-O linear units to form a 3D-framework.

Soll M., Müller Buschbaum H. (1990) [1]

BaHgO<sub>2</sub>

$a = 0.69038$ ,  $c = 1.197$  nm,  $c/a = 1.734$ ,  $V = 0.4941$  nm<sup>3</sup>,  $Z = 6$

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
O1	12 <i>i</i>	1	0.029	0.342	0.104		single atom Hg
Hg2	6 <i>h</i>	..2	0.1716	0.3432	$\frac{1}{4}$		non-colinear O <sub>2</sub>
Ba3	4 <i>f</i>	3..	$\frac{1}{3}$	$\frac{2}{3}$	0.5353		trigonal prism O <sub>6</sub>
Ba4	2 <i>a</i>	32.	0	0	0		trigonal prism O <sub>6</sub>

Experimental: single crystal, diffractometer, X-rays

References: [1] Soll M., Müller Buschbaum H. (1990), J. Less-Common Met. 162, 169-174.