

NaHg ₂ IO ₂	<i>hP</i> 18	(180) <i>P</i> 6 ₂ 22 – jfda
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NaHg₂O₂I [2]

Structural features: Infinite -Hg-O- chains with linear O-Hg-O segments; chains in consecutive layers perpendicular to [001] are rotated by 60°.

Aurivillius K. (1964) [1]

Hg₂INaO₂

$a = 0.6667$, $c = 1.0054$ nm, $c/a = 1.508$, $V = 0.3870$ nm³, $Z = 3$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	6 <i>j</i>	..2	0.1521	0.3042	$\frac{1}{2}$		tetrahedron Hg ₂ Na ₂
Hg2	6 <i>f</i>	2..	$\frac{1}{2}$	0	0.1667		colinear O ₂
I3	3 <i>d</i>	222	$\frac{1}{2}$	0	$\frac{1}{2}$		octahedron Hg ₆
Na4	3 <i>a</i>	222	0	0	0		tetrahedron O ₄

Transformation from published data: origin shift 0 0 $\frac{1}{2}$

Experimental: single crystal, Weissenberg photographs, X-rays, R = 0.104

References: [1] Aurivillius K. (1964), Acta Chem. Scand. 18, 1305-1306. [2] Aurivillius K. (1960), Acta Chem. Scand. 14, 2196-2215.