

AgI	<i>hP24</i>	(186) $P6_3mc - b^6a^6$
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# **AgI 12H** [1]

Structural features: Close-packed I layers in  $h_5c$  stacking; Ag in tetrahedral voids (same stacking position as the preceding I layer).  $AgI_4$  tetrahedra share vertices to form a 3D-framework.

Prager P.R. (1974) [1]

AgI

$a = 0.4592$ ,  $c = 4.506$  nm,  $c/a = 9.813$ ,  $V = 0.8229$  nm<sup>3</sup>,  $Z = 12$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
I1	<i>2b</i>	<i>3m.</i>	$\frac{1}{3}$	$\frac{2}{3}$	0.08333		tetrahedron Ag <sub>4</sub>
Ag2	<i>2b</i>	<i>3m.</i>	$\frac{1}{3}$	$\frac{2}{3}$	0.14583		tetrahedron I <sub>4</sub>
I3	<i>2b</i>	<i>3m.</i>	$\frac{1}{3}$	$\frac{2}{3}$	0.25		tetrahedron Ag <sub>4</sub>
Ag4	<i>2b</i>	<i>3m.</i>	$\frac{1}{3}$	$\frac{2}{3}$	0.3125		tetrahedron I <sub>4</sub>
I5	<i>2b</i>	<i>3m.</i>	$\frac{1}{3}$	$\frac{2}{3}$	0.41667		tetrahedron Ag <sub>4</sub>
Ag6	<i>2b</i>	<i>3m.</i>	$\frac{1}{3}$	$\frac{2}{3}$	0.47917		tetrahedron I <sub>4</sub>
I7	<i>2a</i>	<i>3m.</i>	0	0	0.0		tetrahedron Ag <sub>4</sub>
Ag8	<i>2a</i>	<i>3m.</i>	0	0	0.0625		tetrahedron I <sub>4</sub>
I9	<i>2a</i>	<i>3m.</i>	0	0	0.16667		tetrahedron Ag <sub>4</sub>
Ag10	<i>2a</i>	<i>3m.</i>	0	0	0.22917		tetrahedron I <sub>4</sub>
I11	<i>2a</i>	<i>3m.</i>	0	0	0.33333		tetrahedron Ag <sub>4</sub>
Ag12	<i>2a</i>	<i>3m.</i>	0	0	0.39583		tetrahedron I <sub>4</sub>

Transformation from published data: origin shift 0 0 0.08333

Experimental: single crystal, precession photographs, X-rays

Remarks: Zhdanov notation (2111)<sub>2</sub>; idealized coordinates.

References: [1] Prager P.R. (1974), Acta Crystallogr. A 30, 369-373.