

AgYbPb	<i>hP9</i>	(187) <i>P-6m2</i> – ihgfc
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# **YbAgPb** [1]

Structural features: 3D-framework of fused AgYb<sub>6</sub> and PbYb<sub>6</sub> trigonal prisms. Substitution derivative of AlB<sub>2</sub>.

Merlo F. et al. (1996) [1]

AgPbYb

$a = 0.4873$ ,  $c = 1.1017$  nm,  $c/a = 2.261$ ,  $V = 0.2266$  nm<sup>3</sup>,  $Z = 3$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Yb1	2 <i>i</i>	3 <i>m</i> .	$\frac{2}{3}$	$\frac{1}{3}$	0.1659		bicapped hexagonal prism Ag <sub>6</sub> Pb <sub>6</sub> Yb <sub>2</sub>
Pb2	2 <i>h</i>	3 <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.3478		pentacapped trigonal prism Ag <sub>4</sub> Yb <sub>6</sub> Pb
Ag3	2 <i>g</i>	3 <i>m</i> .	0	0	0.3063		10-vertex polyhedron Pb <sub>4</sub> Yb <sub>6</sub>
Yb4	1 <i>f</i>	-6 <i>m2</i>	$\frac{2}{3}$	$\frac{1}{3}$	$\frac{1}{2}$		bicapped hexagonal prism Pb <sub>6</sub> Ag <sub>6</sub> Yb <sub>2</sub>
Ag5	1 <i>c</i>	-6 <i>m2</i>	$\frac{1}{3}$	$\frac{2}{3}$	0		pentacapped trigonal prism Pb <sub>5</sub> Yb <sub>6</sub>
Pb6	1 <i>a</i>	-6 <i>m2</i>	0	0	0		pentacapped trigonal prism Ag <sub>5</sub> Yb <sub>6</sub>

Transformation from published data: origin shift  $\frac{1}{3} \frac{2}{3} \frac{1}{2}$

Experimental: single crystal, diffractometer, X-rays, R = 0.068

References: [1] Merlo F., Pani M., Fornasini M.L. (1996), J. Alloys Compd. 232, 289-295.