

Co <sub>2</sub> As	<i>hP</i> 36	(189) <i>P</i> -62 <i>m</i> – k <sup>2</sup> jg <sup>2</sup> f <sup>3</sup> ca
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**Co<sub>2</sub>As α** [1]; FePdP [3]

Structural features: Infinite columns of base-linked AsCo<sub>6</sub>Co<sub>3</sub> tricapped trigonal prisms share atoms to form a 3D-framework (a framework of edge-linked trigonal prisms with tubes of edge-linked prism columns centered by a single prism column shifted by  $c/2$  in channels parallel to [001]).

Artigas M. et al. (1991) [1]

AsCo<sub>2</sub>

$a = 1.19867$ ,  $c = 0.35875$  nm,  $c/a = 0.299$ ,  $V = 0.4464$  nm<sup>3</sup>,  $Z = 12$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
As1	6 <i>k</i>	<i>m</i> ..	0.1602	0.3372	$\frac{1}{2}$		tricapped trigonal prism Co <sub>9</sub>
Co2	6 <i>k</i>	<i>m</i> ..	0.1703	0.5395	$\frac{1}{2}$		14-vertex polyhedron As <sub>5</sub> Co <sub>9</sub>
Co3	6 <i>j</i>	<i>m</i> ..	0.2901	0.4645	0		cuboctahedron As <sub>4</sub> Co <sub>8</sub>
Co4	3 <i>g</i>	<i>m</i> 2 <i>m</i>	0.124	0	$\frac{1}{2}$		cuboctahedron As <sub>4</sub> Co <sub>8</sub>
Co5	3 <i>g</i>	<i>m</i> 2 <i>m</i>	0.621	0	$\frac{1}{2}$		cuboctahedron As <sub>4</sub> Co <sub>8</sub>
Co6	3 <i>f</i>	<i>m</i> 2 <i>m</i>	0.299	0	0		pseudo Frank-Kasper As <sub>6</sub> Co <sub>12</sub>
As7	3 <i>f</i>	<i>m</i> 2 <i>m</i>	0.5029	0	0		tricapped trigonal prism Co <sub>9</sub>
Co8	3 <i>f</i>	<i>m</i> 2 <i>m</i>	0.803	0	0		pseudo Frank-Kasper As <sub>6</sub> Co <sub>12</sub>
As9	2 <i>c</i>	-6..	$\frac{1}{3}$	$\frac{2}{3}$	0		tricapped trigonal prism Co <sub>9</sub>
As10	1 <i>a</i>	-62 <i>m</i>	0	0	0		tricapped trigonal prism Co <sub>9</sub>

Experimental: powder, diffractometer, X-rays,  $R_B = 0.057$

Remarks: Phase stable at  $T < 725$  K. Structure identical to the model called H<sub>12</sub> in [4]. An additional, partly occupied site is reported in [2]. Partial ordering of Fe and Pd is reported for FePdP [3].

References: [1] Artigas M., Bacmann M., Fruchart D., Fruchart R., Soubeyroux J.L., Wolfers P. (1991), C. R. Acad. Sci., Ser. II 313, 635-640. [2] Lindeberg I., Andersson Y. (1991), J. Less-Common Met. 175, 163-169. [3] Artigas M., Bacmann M., Fruchart D., Wolfers P., Fruchart R. (1991), J. Alloys Compd. 176, 105-114. [4] Artigas M., Fruchart D., Boursier D., Fruchart R. (1990), C. R. Acad. Sci., Ser. II 310, 1621-1627.