

Co ₂ As	<i>hP</i> 38	(189) <i>P</i> -62 <i>m</i> – k ² jg ² Γ ³ dca
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Co₂As α [1]

Structural features: Structure intermediate between Fe₂P and ideal α-Co₂As.

Lindeberg I., Andersson Y. (1991) [1]

AsCo₂

a = 1.19821, *c* = 0.35822 nm, *c/a* = 0.299, *V* = 0.4454 nm³, *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> ..	0.1611	0.3345	1/2		tricapped trigonal prism Co ₉
Co2	6 <i>k</i>	<i>m</i> ..	0.1687	0.5379	1/2		single atom As
Co3	6 <i>j</i>	<i>m</i> ..	0.2833	0.4594	0		tetrahedron As ₄
Co4	3 <i>g</i>	<i>m</i> 2 <i>m</i>	0.1275	0	1/2		tetrahedron As ₄
Co5	3 <i>g</i>	<i>m</i> 2 <i>m</i>	0.6251	0	1/2		cuboctahedron As ₄ Co ₈
Co6	3 <i>f</i>	<i>m</i> 2 <i>m</i>	0.3061	0	0		pseudo Frank-Kasper As ₆ Co ₁₂
As7	3 <i>f</i>	<i>m</i> 2 <i>m</i>	0.4989	0	0		tricapped trigonal prism Co ₉
Co8	3 <i>f</i>	<i>m</i> 2 <i>m</i>	0.797	0	0		pseudo Frank-Kasper As ₆ Co ₁₂
As9	2 <i>d</i>	-6..	1/3	2/3	1/2	0.13	trigonal bipyramid As ₂ Co ₃
As10	2 <i>c</i>	-6..	1/3	2/3	0	0.87	colinear As ₂
As11	1 <i>a</i>	-62 <i>m</i>	0	0	0		tricapped trigonal prism Co ₉

Transformation from published data: origin shift 0 0 1/2

Experimental: single crystal, diffractometer, X-rays, R = 0.089

Remarks: Phase stable at T < 725 K. Short interatomic distances: d(Co2-As9) = 0.180 nm, explained by the occurrence of twinning or stacking faults. Short interatomic distances for partly occupied site(s).

References: [1] Lindeberg I., Andersson Y. (1991), J. Less-Common Met. 175, 163-169.