

CoZn₁₃ Structure:

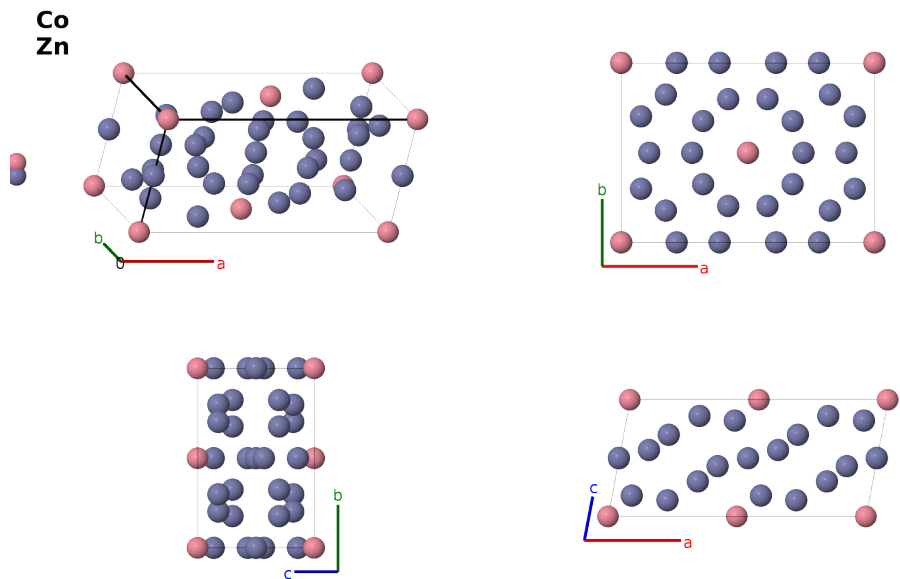
AB13_mC28_12_a_c2i2j-001

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<https://aflow.org/prototype-encyclopedia/6H3E>

https://aflow.org/prototype-encyclopedia/AB13_mC28_12_a_c2i2j-001



Prototype	CoZn ₁₃
AFLOW prototype label	AB13_mC28_12_a_c2i2j-001
ICSD	102736
CCDC	1660706
Pearson symbol	mC28
Space group number	12
Space group symbol	$C2/m$
AFLOW prototype command	<pre>aflow --proto=AB13_mC28_12_a_c2i2j-001 --params=a, b/a, c/a, β, x_3, z_3, x_4, z_4, x_5, y_5, z_5, x_6, y_6, z_6</pre>

Other compounds with this structure

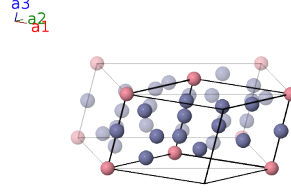
FeZn₁₃, MnZn₁₃

- (Brown, 1962) state that the transition metal in this structure may be either on the (2a) or (2c) Wyckoff site. We arbitrarily place it on the (2a) site.

- The coordinates of the Zn-II atom given in (Brown, 1962) are not consistent with Figure 5 and Table 4 in that paper, and the Co-Zn-II distance is much too small. By shifting the x -coordinate by $1/2$, from 0.111 to 0.611, we obtain excellent agreement with both figure and table.

Base-centered Monoclinic primitive vectors

$$\begin{aligned}\mathbf{a}_1 &= \frac{1}{2}a \hat{\mathbf{x}} - \frac{1}{2}b \hat{\mathbf{y}} \\ \mathbf{a}_2 &= \frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{2}b \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \cos \beta \hat{\mathbf{x}} + c \sin \beta \hat{\mathbf{z}}\end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= 0$	$=$	0	(2a)	Co I
$\mathbf{B}_2$	$= \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2}c \cos \beta \hat{\mathbf{x}} + \frac{1}{2}c \sin \beta \hat{\mathbf{z}}$	(2c)	Zn I
$\mathbf{B}_3$	$= x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$(ax_3 + cz_3 \cos \beta) \hat{\mathbf{x}} + cz_3 \sin \beta \hat{\mathbf{z}}$	(4i)	Zn II
$\mathbf{B}_4$	$= -x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$-(ax_3 + cz_3 \cos \beta) \hat{\mathbf{x}} - cz_3 \sin \beta \hat{\mathbf{z}}$	(4i)	Zn II
$\mathbf{B}_5$	$= x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$(ax_4 + cz_4 \cos \beta) \hat{\mathbf{x}} + cz_4 \sin \beta \hat{\mathbf{z}}$	(4i)	Zn III
$\mathbf{B}_6$	$= -x_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$-(ax_4 + cz_4 \cos \beta) \hat{\mathbf{x}} - cz_4 \sin \beta \hat{\mathbf{z}}$	(4i)	Zn III
$\mathbf{B}_7$	$= (x_5 - y_5) \mathbf{a}_1 + (x_5 + y_5) \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$(ax_5 + cz_5 \cos \beta) \hat{\mathbf{x}} + by_5 \hat{\mathbf{y}} + cz_5 \sin \beta \hat{\mathbf{z}}$	(8j)	Zn IV
$\mathbf{B}_8$	$= -(x_5 + y_5) \mathbf{a}_1 - (x_5 - y_5) \mathbf{a}_2 - z_5 \mathbf{a}_3$	$=$	$-(ax_5 + cz_5 \cos \beta) \hat{\mathbf{x}} + by_5 \hat{\mathbf{y}} - cz_5 \sin \beta \hat{\mathbf{z}}$	(8j)	Zn IV
$\mathbf{B}_9$	$= -(x_5 - y_5) \mathbf{a}_1 - (x_5 + y_5) \mathbf{a}_2 - z_5 \mathbf{a}_3$	$=$	$-(ax_5 + cz_5 \cos \beta) \hat{\mathbf{x}} - by_5 \hat{\mathbf{y}} - cz_5 \sin \beta \hat{\mathbf{z}}$	(8j)	Zn IV
$\mathbf{B}_{10}$	$= (x_5 + y_5) \mathbf{a}_1 + (x_5 - y_5) \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$(ax_5 + cz_5 \cos \beta) \hat{\mathbf{x}} - by_5 \hat{\mathbf{y}} + cz_5 \sin \beta \hat{\mathbf{z}}$	(8j)	Zn IV
$\mathbf{B}_{11}$	$= (x_6 - y_6) \mathbf{a}_1 + (x_6 + y_6) \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$(ax_6 + cz_6 \cos \beta) \hat{\mathbf{x}} + by_6 \hat{\mathbf{y}} + cz_6 \sin \beta \hat{\mathbf{z}}$	(8j)	Zn V
$\mathbf{B}_{12}$	$= -(x_6 + y_6) \mathbf{a}_1 - (x_6 - y_6) \mathbf{a}_2 - z_6 \mathbf{a}_3$	$=$	$-(ax_6 + cz_6 \cos \beta) \hat{\mathbf{x}} + by_6 \hat{\mathbf{y}} - cz_6 \sin \beta \hat{\mathbf{z}}$	(8j)	Zn V
$\mathbf{B}_{13}$	$= -(x_6 - y_6) \mathbf{a}_1 - (x_6 + y_6) \mathbf{a}_2 - z_6 \mathbf{a}_3$	$=$	$-(ax_6 + cz_6 \cos \beta) \hat{\mathbf{x}} - by_6 \hat{\mathbf{y}} - cz_6 \sin \beta \hat{\mathbf{z}}$	(8j)	Zn V
$\mathbf{B}_{14}$	$= (x_6 + y_6) \mathbf{a}_1 + (x_6 - y_6) \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$(ax_6 + cz_6 \cos \beta) \hat{\mathbf{x}} - by_6 \hat{\mathbf{y}} + cz_6 \sin \beta \hat{\mathbf{z}}$	(8j)	Zn V

References

- [1] P. J. Brown, *The structure of the ζ -phase in the transition metal-zinc alloy systems*, Acta Cryst. **15**, 608–612 (1962), doi:10.1107/S0365110X62001528.

Found in

- [1] W. B. Pearson, *A Handbook of Lattice Spacings and Structures of Metals and Alloys, Volume 2, International Series of Monographs on Metal Physics and Physical Metallurgy*, vol. 8 (Pergamon Press, Oxford, London, Edinburgh, New York, Toronto, Sydney, Paris, Braunschweig, 1967).

First cited in

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