

Spinel (Co₃O₄, *D*7₂) Structure: A3B4_cF56_227_ad_e-001

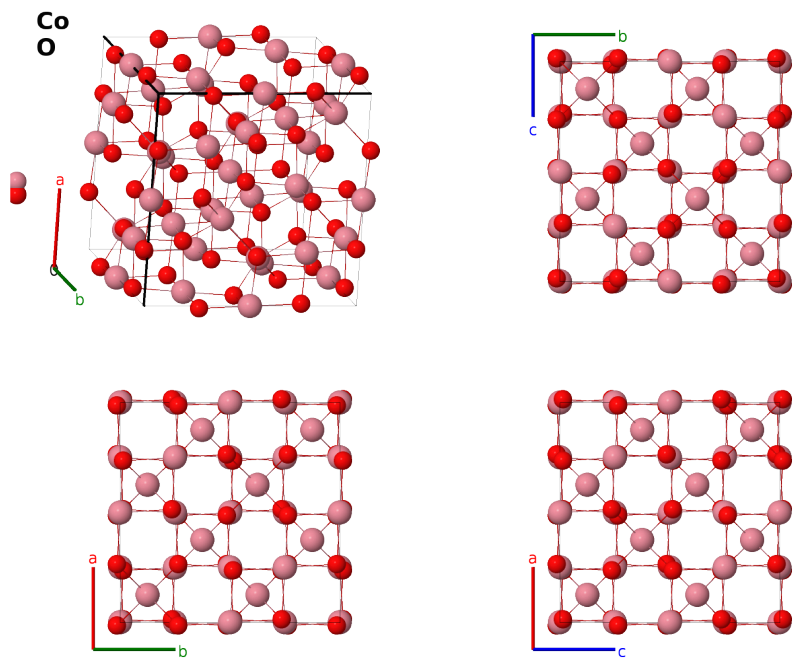
This structure previously used the label(s) **A3B4_cF56_227_ad_e**. Calls to these addresses will be redirected here.

Cite this page as:

- H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettl, M. Esters, X. Campilongo, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*, Comput. Mater. Sci. **240**, 112988 (2024), doi: 10.1016/j.commatsci.2024.112988.
- D. Hicks, M. J. Mehl, M. Esters, C. Oses, O. Levy, G. L. W. Hart, C. Toher, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 3*, Comput. Mater. Sci. **199**, 110450 (2021), doi: 10.1016/j.commatsci.2021.110450.

<https://aflow.org/prototype-encyclopedia/SV6X>

https://aflow.org/prototype-encyclopedia/A3B4_cF56_227_ad_e-001



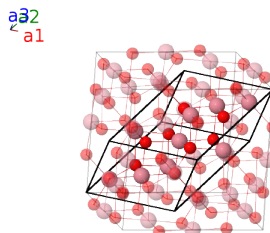
Prototype	Co ₃ O ₄
AFLOW prototype label	A3B4_cF56_227_ad_e-001
<i>Strukturbericht</i> designation	<i>D</i> 7 ₂
Mineral name	spinel
ICSD	24210
CCDC	1600256
Pearson symbol	cF56
Space group number	227
Space group symbol	<i>Fd</i> $\bar{3}$ <i>m</i>
AFLOW prototype command	<code>aflow --proto=A3B4_cF56_227_ad_e-001</code> <code>--params=<i>a</i>, <i>x</i>₃</code>

Other compounds with this structure

NiCo₂O₄, Co₃S₄, Fe₃O₄, γ -Si₃N₄, NiCo₂S₄, FeNi₂S₄

- The binary $D7_2$ and ternary $H1_1$ spinel structures are for all intents and purposes identical. We could use $D7_2$ for the binary spinels and $H1_1$ for the ternaries, but historically this has not been the case. We dual-list this structure only to keep the historical record intact.
- (Hahn, 1955) has an extensive list of ternary spinels and inverse spinels.

Face-centered Cubic primitive vectors

$$\begin{aligned} \mathbf{a}_1 &= \frac{1}{2}a\hat{\mathbf{y}} + \frac{1}{2}a\hat{\mathbf{z}} \\ \mathbf{a}_2 &= \frac{1}{2}a\hat{\mathbf{x}} + \frac{1}{2}a\hat{\mathbf{z}} \\ \mathbf{a}_3 &= \frac{1}{2}a\hat{\mathbf{x}} + \frac{1}{2}a\hat{\mathbf{y}} \end{aligned}$$


Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= \frac{1}{8}\mathbf{a}_1 + \frac{1}{8}\mathbf{a}_2 + \frac{1}{8}\mathbf{a}_3$	$=$	$\frac{1}{8}a\hat{\mathbf{x}} + \frac{1}{8}a\hat{\mathbf{y}} + \frac{1}{8}a\hat{\mathbf{z}}$	(8a)	Co I
$\mathbf{B}_2$	$= \frac{7}{8}\mathbf{a}_1 + \frac{7}{8}\mathbf{a}_2 + \frac{7}{8}\mathbf{a}_3$	$=$	$\frac{7}{8}a\hat{\mathbf{x}} + \frac{7}{8}a\hat{\mathbf{y}} + \frac{7}{8}a\hat{\mathbf{z}}$	(8a)	Co I
$\mathbf{B}_3$	$= \frac{1}{2}\mathbf{a}_1 + \frac{1}{2}\mathbf{a}_2 + \frac{1}{2}\mathbf{a}_3$	$=$	$\frac{1}{2}a\hat{\mathbf{x}} + \frac{1}{2}a\hat{\mathbf{y}} + \frac{1}{2}a\hat{\mathbf{z}}$	(16d)	Co II
$\mathbf{B}_4$	$= \frac{1}{2}\mathbf{a}_1 + \frac{1}{2}\mathbf{a}_2$	$=$	$\frac{1}{4}a\hat{\mathbf{x}} + \frac{1}{4}a\hat{\mathbf{y}} + \frac{1}{2}a\hat{\mathbf{z}}$	(16d)	Co II
$\mathbf{B}_5$	$= \frac{1}{2}\mathbf{a}_1 + \frac{1}{2}\mathbf{a}_3$	$=$	$\frac{1}{4}a\hat{\mathbf{x}} + \frac{1}{2}a\hat{\mathbf{y}} + \frac{1}{4}a\hat{\mathbf{z}}$	(16d)	Co II
$\mathbf{B}_6$	$= \frac{1}{2}\mathbf{a}_2 + \frac{1}{2}\mathbf{a}_3$	$=$	$\frac{1}{2}a\hat{\mathbf{x}} + \frac{1}{4}a\hat{\mathbf{y}} + \frac{1}{4}a\hat{\mathbf{z}}$	(16d)	Co II
$\mathbf{B}_7$	$= x_3\mathbf{a}_1 + x_3\mathbf{a}_2 + x_3\mathbf{a}_3$	$=$	$ax_3\hat{\mathbf{x}} + ax_3\hat{\mathbf{y}} + ax_3\hat{\mathbf{z}}$	(32e)	O I
$\mathbf{B}_8$	$= x_3\mathbf{a}_1 + x_3\mathbf{a}_2 - (3x_3 - \frac{1}{2})\mathbf{a}_3$	$=$	$-a(x_3 - \frac{1}{4})\hat{\mathbf{x}} - a(x_3 - \frac{1}{4})\hat{\mathbf{y}} + ax_3\hat{\mathbf{z}}$	(32e)	O I
$\mathbf{B}_9$	$= x_3\mathbf{a}_1 - (3x_3 - \frac{1}{2})\mathbf{a}_2 + x_3\mathbf{a}_3$	$=$	$-a(x_3 - \frac{1}{4})\hat{\mathbf{x}} + ax_3\hat{\mathbf{y}} - a(x_3 - \frac{1}{4})\hat{\mathbf{z}}$	(32e)	O I
$\mathbf{B}_{10}$	$= -(3x_3 - \frac{1}{2})\mathbf{a}_1 + x_3\mathbf{a}_2 + x_3\mathbf{a}_3$	$=$	$ax_3\hat{\mathbf{x}} - a(x_3 - \frac{1}{4})\hat{\mathbf{y}} - a(x_3 - \frac{1}{4})\hat{\mathbf{z}}$	(32e)	O I
$\mathbf{B}_{11}$	$= -x_3\mathbf{a}_1 - x_3\mathbf{a}_2 + (3x_3 + \frac{1}{2})\mathbf{a}_3$	$=$	$a(x_3 + \frac{1}{4})\hat{\mathbf{x}} + a(x_3 + \frac{1}{4})\hat{\mathbf{y}} - ax_3\hat{\mathbf{z}}$	(32e)	O I
$\mathbf{B}_{12}$	$= -x_3\mathbf{a}_1 - x_3\mathbf{a}_2 - x_3\mathbf{a}_3$	$=$	$-ax_3\hat{\mathbf{x}} - ax_3\hat{\mathbf{y}} - ax_3\hat{\mathbf{z}}$	(32e)	O I
$\mathbf{B}_{13}$	$= -x_3\mathbf{a}_1 + (3x_3 + \frac{1}{2})\mathbf{a}_2 - x_3\mathbf{a}_3$	$=$	$a(x_3 + \frac{1}{4})\hat{\mathbf{x}} - ax_3\hat{\mathbf{y}} + a(x_3 + \frac{1}{4})\hat{\mathbf{z}}$	(32e)	O I
$\mathbf{B}_{14}$	$= (3x_3 + \frac{1}{2})\mathbf{a}_1 - x_3\mathbf{a}_2 - x_3\mathbf{a}_3$	$=$	$-ax_3\hat{\mathbf{x}} + a(x_3 + \frac{1}{4})\hat{\mathbf{y}} + a(x_3 + \frac{1}{4})\hat{\mathbf{z}}$	(32e)	O I

References

- [1] O. Knop, K. I. G. Reid, Sutarno, and Y. Nakagawa, *Chalkogenides of the transition elements. VI. X-Ray, neutron, and magnetic investigation of the spinels Co₃O₄, NiCo₂O₄, Co₃S₄, and NiCo₂S₄*, Can. J. Chem. **46**, 3463–3476 (1968), doi:10.1139/v68-576.
- [2] H. Hahn, G. Frank, W. Klingler, A. D. Störger, and G. Störger, *Chalkogenide. VI. Über Ternäre Chalkogenide des Aluminiums, Galliums und Indiums mit Zink, Cadmium und Quecksilber*, Z. Anorganische und Allgemeine Chemie **279**, 241–270 (1955), doi:10.1002/zaac.19552790502.

First cited in

D. Hicks, M. J. Mehl, E. Gossett, C. Toher, O. Levy, R. M. Hanson, G. Hart, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 2*, Comput. Mater. Sci. **161**, S1 (2019). doi: 10.1016/j.commatsci.2018.10.043