

Model of Ferrite Structure (cI16): AB4C3_cI16_229_a_c_b-001

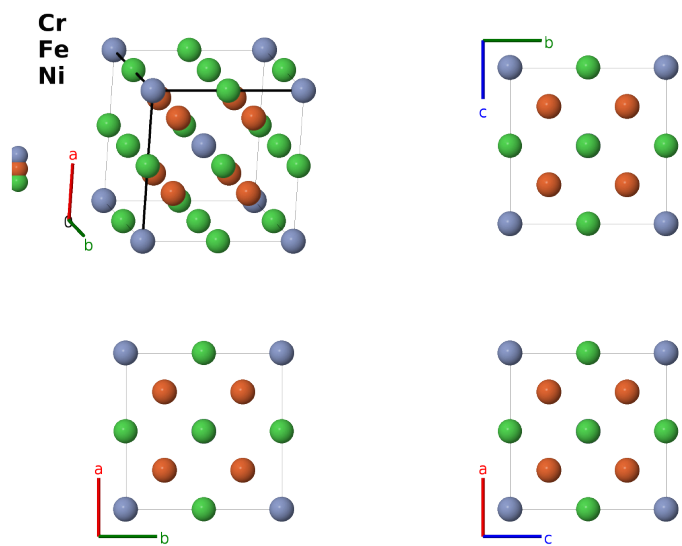
This structure previously used the label(s) **AB4C3_cI16_229_a_c_b**. Calls to these addresses will be redirected here.

Cite this page as:

- H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettel, 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/YRPB>

https://aflow.org/prototype-encyclopedia/AB4C3_cI16_229_a_c_b-001

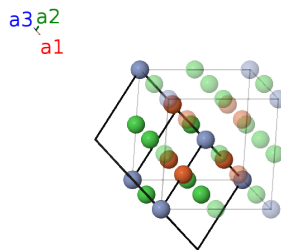


Prototype	CrFe ₄ Ni ₃
AFLOW prototype label	AB4C3_cI16_229_a_c_b-001
Pearson symbol	cI16
Space group number	229
Space group symbol	$Im\bar{3}m$
AFLOW prototype command	<code>aflow --proto=AB4C3_cI16_229_a_c_b-001 --params=a</code>

- Ferritic steels are alloys of iron and other metals with an averaged body-centered cubic structure. This model represents one approximation for a ferritic steel. It is not meant to represent a real steel, and the selection of atom types for each Wyckoff position is arbitrary. If we replace the chromium atoms by nickel, this becomes the CsCl (*B2*) with $a_{B2} = 1/4 a$. If we replace both the nickel and chromium atoms by iron, then the structure becomes a body-centered cubic lattice (*A2*) again with $a_{A2} = 1/4 a$.

Body-centered Cubic primitive vectors

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



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$=$	0	$=$	0	$(2a)$ Cr I
$\mathbf{B}_2$	$=$	$\frac{1}{2}\mathbf{a}_2 + \frac{1}{2}\mathbf{a}_3$	$=$	$\frac{1}{2}a\hat{\mathbf{x}}$	$(6b)$ Ni I
$\mathbf{B}_3$	$=$	$\frac{1}{2}\mathbf{a}_1 + \frac{1}{2}\mathbf{a}_3$	$=$	$\frac{1}{2}a\hat{\mathbf{y}}$	$(6b)$ Ni I
$\mathbf{B}_4$	$=$	$\frac{1}{2}\mathbf{a}_1 + \frac{1}{2}\mathbf{a}_2$	$=$	$\frac{1}{2}a\hat{\mathbf{z}}$	$(6b)$ Ni I
$\mathbf{B}_5$	$=$	$\frac{1}{2}\mathbf{a}_1 + \frac{1}{2}\mathbf{a}_2 + \frac{1}{2}\mathbf{a}_3$	$=$	$\frac{1}{4}a\hat{\mathbf{x}} + \frac{1}{4}a\hat{\mathbf{y}} + \frac{1}{4}a\hat{\mathbf{z}}$	$(8c)$ Fe I
$\mathbf{B}_6$	$=$	$\frac{1}{2}\mathbf{a}_3$	$=$	$\frac{1}{4}a\hat{\mathbf{x}} + \frac{1}{4}a\hat{\mathbf{y}} - \frac{1}{4}a\hat{\mathbf{z}}$	$(8c)$ Fe I
$\mathbf{B}_7$	$=$	$\frac{1}{2}\mathbf{a}_2$	$=$	$\frac{1}{4}a\hat{\mathbf{x}} - \frac{1}{4}a\hat{\mathbf{y}} + \frac{1}{4}a\hat{\mathbf{z}}$	$(8c)$ Fe I
$\mathbf{B}_8$	$=$	$\frac{1}{2}\mathbf{a}_1$	$=$	$-\frac{1}{4}a\hat{\mathbf{x}} + \frac{1}{4}a\hat{\mathbf{y}} + \frac{1}{4}a\hat{\mathbf{z}}$	$(8c)$ Fe I

References

- [1] M. J. Mehl, D. Hicks, C. Toher, O. Levy, R. M. Hanson, G. Hart, and S. Curtarolo, *The AFLOW library of crystallographic prototypes: part 1*, Comput. Mater. Sci. **136**, S1–S828 (2017), doi:10.1016/j.commatsci.2017.01.017.

First cited in

M. J. Mehl, D. Hicks, C. Toher, O. Levy, R. M. Hanson, G. L. W. Hart, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 1*, Comput. Mater. Sci. **136**, S1-828 (2017). doi: 10.1016/j.commatsci.2017.01.017