

Model of Austenite Structure (cI32): AB12C3_cI32_229_a_h_b-001

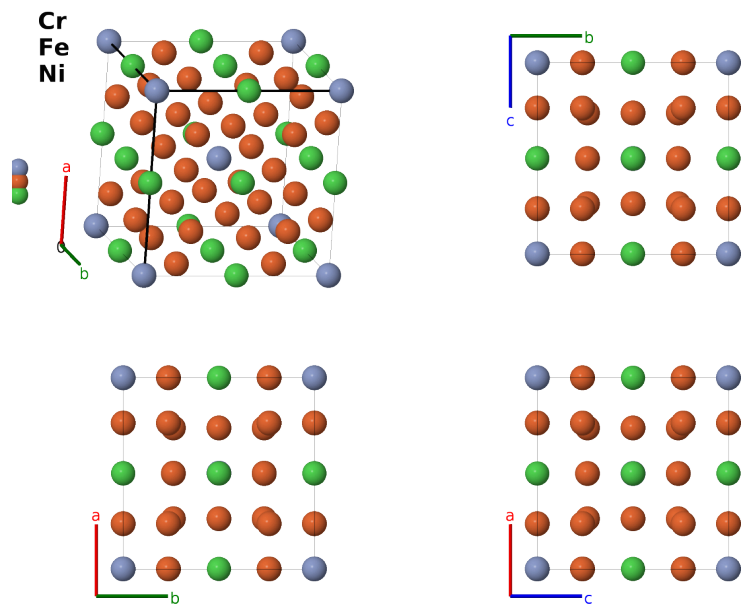
This structure previously used the label(s) **AB12C3_cI32_229_a_h_b**. Calls to these addresses will be redirected here.

Cite this page as:

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<https://aflow.org/prototype-encyclopedia/L6PB>

https://aflow.org/prototype-encyclopedia/AB12C3_cI32_229_a_h_b-001

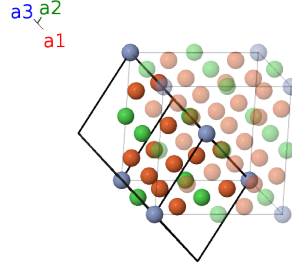


Prototype	CrFe ₁₂ Ni ₃
AFLOW prototype label	AB12C3_cI32_229_a_h_b-001
Pearson symbol	cI32
Space group number	229
Space group symbol	$Im\bar{3}m$
AFLOW prototype command	<code>aflow --proto=AB12C3_cI32_229_a_h_b-001 --params=a, y₃</code>

- Austenitic steels are alloys of iron and other metals with an averaged face-centered cubic structure. This model represents one approximation for an austenite steel. If we set $y_3 = 1/4$, the atoms are on the sites of an fcc lattice.

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
$\mathbf{B}_5$	$2y_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + y_3 \mathbf{a}_3$	$=$	$ay_3 \hat{\mathbf{y}} + ay_3 \hat{\mathbf{z}}$	(24h)	Fe I
$\mathbf{B}_6$	$y_3 \mathbf{a}_2 - y_3 \mathbf{a}_3$	$=$	$-ay_3 \hat{\mathbf{y}} + ay_3 \hat{\mathbf{z}}$	(24h)	Fe I
$\mathbf{B}_7$	$-y_3 \mathbf{a}_2 + y_3 \mathbf{a}_3$	$=$	$ay_3 \hat{\mathbf{y}} - ay_3 \hat{\mathbf{z}}$	(24h)	Fe I
$\mathbf{B}_8$	$-2y_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 - y_3 \mathbf{a}_3$	$=$	$-ay_3 \hat{\mathbf{y}} - ay_3 \hat{\mathbf{z}}$	(24h)	Fe I
$\mathbf{B}_9$	$y_3 \mathbf{a}_1 + 2y_3 \mathbf{a}_2 + y_3 \mathbf{a}_3$	$=$	$ay_3 \hat{\mathbf{x}} + ay_3 \hat{\mathbf{z}}$	(24h)	Fe I
$\mathbf{B}_{10}$	$-y_3 \mathbf{a}_1 + y_3 \mathbf{a}_3$	$=$	$ay_3 \hat{\mathbf{x}} - ay_3 \hat{\mathbf{z}}$	(24h)	Fe I
$\mathbf{B}_{11}$	$y_3 \mathbf{a}_1 - y_3 \mathbf{a}_3$	$=$	$-ay_3 \hat{\mathbf{x}} + ay_3 \hat{\mathbf{z}}$	(24h)	Fe I
$\mathbf{B}_{12}$	$-y_3 \mathbf{a}_1 - 2y_3 \mathbf{a}_2 - y_3 \mathbf{a}_3$	$=$	$-ay_3 \hat{\mathbf{x}} - ay_3 \hat{\mathbf{z}}$	(24h)	Fe I
$\mathbf{B}_{13}$	$y_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + 2y_3 \mathbf{a}_3$	$=$	$ay_3 \hat{\mathbf{x}} + ay_3 \hat{\mathbf{y}}$	(24h)	Fe I
$\mathbf{B}_{14}$	$y_3 \mathbf{a}_1 - y_3 \mathbf{a}_2$	$=$	$-ay_3 \hat{\mathbf{x}} + ay_3 \hat{\mathbf{y}}$	(24h)	Fe I
$\mathbf{B}_{15}$	$-y_3 \mathbf{a}_1 + y_3 \mathbf{a}_2$	$=$	$ay_3 \hat{\mathbf{x}} - ay_3 \hat{\mathbf{y}}$	(24h)	Fe I
$\mathbf{B}_{16}$	$-y_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 - 2y_3 \mathbf{a}_3$	$=$	$-ay_3 \hat{\mathbf{x}} - ay_3 \hat{\mathbf{y}}$	(24h)	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.

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