# Model of Austenite Structure (cF108): AB18C8_cF108_225_a_eh_f-001

This structure previously used the label(s) `AB18C8_cF108_225_a_eh_f`. Calls to these addresses will be redirected here.

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- 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.

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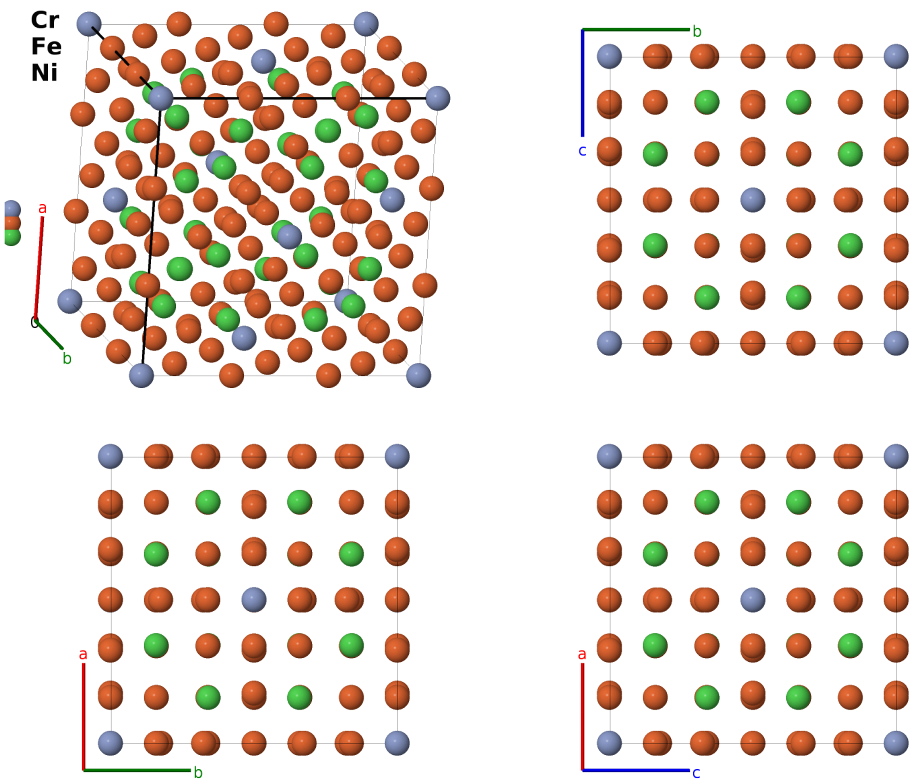
https://aflow.org/prototype-encyclopedia/VR5Q

https://aflow.org/prototype-encyclopedia/AB18C8_cF108_225_a_eh_f-001




| | |
|---|---|
| **Prototype** | $CrFe_{18}MoNi_8$ |
| **AFLOW prototype label** | AB18C8_cF108_225_a_eh_f-001 |
| **Pearson symbol** | cF108 |
| **Space group number** | 225 |
| **Space group symbol** | $Fm\bar{3}m$ |
| **AFLOW prototype command** | `aflow --proto=AB18C8_cF108_225_a_eh_f-001` `--params=`$a, x_2, x_3, y_4$ |

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- 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 $x_2 = 1/3$, $x_3 = 2/3$, and $y_4 = 2/3$, the atoms are on the sites of an fcc lattice with lattice constant $a_{fcc} = a/3$.

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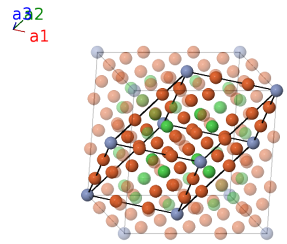
### Face-centered Cubic primitive vectors

$$
\begin{aligned}
\mathbf{a_1} &= \tfrac{1}{2}a\,\mathbf{\hat{y}} + \tfrac{1}{2}a\,\mathbf{\hat{z}} \\
\mathbf{a_2} &= \tfrac{1}{2}a\,\mathbf{\hat{x}} + \tfrac{1}{2}a\,\mathbf{\hat{z}} \\
\mathbf{a_3} &= \tfrac{1}{2}a\,\mathbf{\hat{x}} + \tfrac{1}{2}a\,\mathbf{\hat{y}}
\end{aligned}
$$

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### Basis vectors

| | | Lattice coordinates | | Cartesian coordinates | Wyckoff position | Atom type |
|---|---|---|---|---|---|---|
| $\mathbf{B_1}$ | = | $0$ | = | $0$ | (4a) | Cr I |
| $\mathbf{B_2}$ | = | $-x_2\,\mathbf{a}_1 + x_2\,\mathbf{a}_2 + x_2\,\mathbf{a}_3$ | = | $a x_2\,\mathbf{\hat{x}}$ | (24e) | Fe I |
| $\mathbf{B_3}$ | = | $x_2\,\mathbf{a}_1 - x_2\,\mathbf{a}_2 - x_2\,\mathbf{a}_3$ | = | $-a x_2\,\mathbf{\hat{x}}$ | (24e) | Fe I |
| $\mathbf{B_4}$ | = | $x_2\,\mathbf{a}_1 - x_2\,\mathbf{a}_2 + x_2\,\mathbf{a}_3$ | = | $a x_2\,\mathbf{\hat{y}}$ | (24e) | Fe I |
| $\mathbf{B_5}$ | = | $-x_2\,\mathbf{a}_1 + x_2\,\mathbf{a}_2 - x_2\,\mathbf{a}_3$ | = | $-a x_2\,\mathbf{\hat{y}}$ | (24e) | Fe I |
| $\mathbf{B_6}$ | = | $x_2\,\mathbf{a}_1 + x_2\,\mathbf{a}_2 - x_2\,\mathbf{a}_3$ | = | $a x_2\,\mathbf{\hat{z}}$ | (24e) | Fe I |
| $\mathbf{B_7}$ | = | $-x_2\,\mathbf{a}_1 - x_2\,\mathbf{a}_2 + x_2\,\mathbf{a}_3$ | = | $-a x_2\,\mathbf{\hat{z}}$ | (24e) | Fe I |
| $\mathbf{B_8}$ | = | $x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + x_3\,\mathbf{a}_3$ | = | $a x_3\,\mathbf{\hat{x}} + a x_3\,\mathbf{\hat{y}} + a x_3\,\mathbf{\hat{z}}$ | (32f) | Ni I |
| $\mathbf{B_9}$ | = | $x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 - 3x_3\,\mathbf{a}_3$ | = | $-a x_3\,\mathbf{\hat{x}} - a x_3\,\mathbf{\hat{y}} + a x_3\,\mathbf{\hat{z}}$ | (32f) | Ni I |
| $\mathbf{B_{10}}$ | = | $x_3\,\mathbf{a}_1 - 3x_3\,\mathbf{a}_2 + x_3\,\mathbf{a}_3$ | = | $-a x_3\,\mathbf{\hat{x}} + a x_3\,\mathbf{\hat{y}} - a x_3\,\mathbf{\hat{z}}$ | (32f) | Ni I |
| $\mathbf{B_{11}}$ | = | $-3x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + x_3\,\mathbf{a}_3$ | = | $a x_3\,\mathbf{\hat{x}} - a x_3\,\mathbf{\hat{y}} - a x_3\,\mathbf{\hat{z}}$ | (32f) | Ni I |
| $\mathbf{B_{12}}$ | = | $-x_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 + 3x_3\,\mathbf{a}_3$ | = | $a x_3\,\mathbf{\hat{x}} + a x_3\,\mathbf{\hat{y}} - a x_3\,\mathbf{\hat{z}}$ | (32f) | Ni I |
| $\mathbf{B_{13}}$ | = | $-x_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 - x_3\,\mathbf{a}_3$ | = | $-a x_3\,\mathbf{\hat{x}} - a x_3\,\mathbf{\hat{y}} - a x_3\,\mathbf{\hat{z}}$ | (32f) | Ni I |
| $\mathbf{B_{14}}$ | = | $-x_3\,\mathbf{a}_1 + 3x_3\,\mathbf{a}_2 - x_3\,\mathbf{a}_3$ | = | $a x_3\,\mathbf{\hat{x}} - a x_3\,\mathbf{\hat{y}} + a x_3\,\mathbf{\hat{z}}$ | (32f) | Ni I |
| $\mathbf{B_{15}}$ | = | $3x_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 - x_3\,\mathbf{a}_3$ | = | $-a x_3\,\mathbf{\hat{x}} + a x_3\,\mathbf{\hat{y}} + a x_3\,\mathbf{\hat{z}}$ | (32f) | Ni I |
| $\mathbf{B_{16}}$ | = | $2y_4\,\mathbf{a}_1$ | = | $a y_4\,\mathbf{\hat{y}} + a y_4\,\mathbf{\hat{z}}$ | (48h) | Fe II |
| $\mathbf{B_{17}}$ | = | $2y_4\,\mathbf{a}_2 - 2y_4\,\mathbf{a}_3$ | = | $-a y_4\,\mathbf{\hat{y}} + a y_4\,\mathbf{\hat{z}}$ | (48h) | Fe II |
| $\mathbf{B_{18}}$ | = | $-2y_4\,\mathbf{a}_2 + 2y_4\,\mathbf{a}_3$ | = | $a y_4\,\mathbf{\hat{y}} - a y_4\,\mathbf{\hat{z}}$ | (48h) | Fe II |
| $\mathbf{B_{19}}$ | = | $-2y_4\,\mathbf{a}_1$ | = | $-a y_4\,\mathbf{\hat{y}} - a y_4\,\mathbf{\hat{z}}$ | (48h) | Fe II |
| $\mathbf{B_{20}}$ | = | $2y_4\,\mathbf{a}_2$ | = | $a y_4\,\mathbf{\hat{x}} + a y_4\,\mathbf{\hat{z}}$ | (48h) | Fe II |
| $\mathbf{B_{21}}$ | = | $-2y_4\,\mathbf{a}_1 + 2y_4\,\mathbf{a}_3$ | = | $a y_4\,\mathbf{\hat{x}} - a y_4\,\mathbf{\hat{z}}$ | (48h) | Fe II |
| $\mathbf{B_{22}}$ | = | $2y_4\,\mathbf{a}_1 - 2y_4\,\mathbf{a}_3$ | = | $-a y_4\,\mathbf{\hat{x}} + a y_4\,\mathbf{\hat{z}}$ | (48h) | Fe II |
| $\mathbf{B_{23}}$ | = | $-2y_4\,\mathbf{a}_2$ | = | $-a y_4\,\mathbf{\hat{x}} - a y_4\,\mathbf{\hat{z}}$ | (48h) | Fe II |
| $\mathbf{B_{24}}$ | = | $2y_4\,\mathbf{a}_3$ | = | $a y_4\,\mathbf{\hat{x}} + a y_4\,\mathbf{\hat{y}}$ | (48h) | Fe II |
| $\mathbf{B_{25}}$ | = | $2y_4\,\mathbf{a}_1 - 2y_4\,\mathbf{a}_2$ | = | $-a y_4\,\mathbf{\hat{x}} + a y_4\,\mathbf{\hat{y}}$ | (48h) | Fe II |
| $\mathbf{B_{26}}$ | = | $-2y_4\,\mathbf{a}_1 + 2y_4\,\mathbf{a}_2$ | = | $a y_4\,\mathbf{\hat{x}} - a y_4\,\mathbf{\hat{y}}$ | (48h) | Fe II |
| $\mathbf{B_{27}}$ | = | $-2y_4\,\mathbf{a}_3$ | = | $-a y_4\,\mathbf{\hat{x}} - a y_4\,\mathbf{\hat{y}}$ | (48h) | Fe II |

## 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

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