

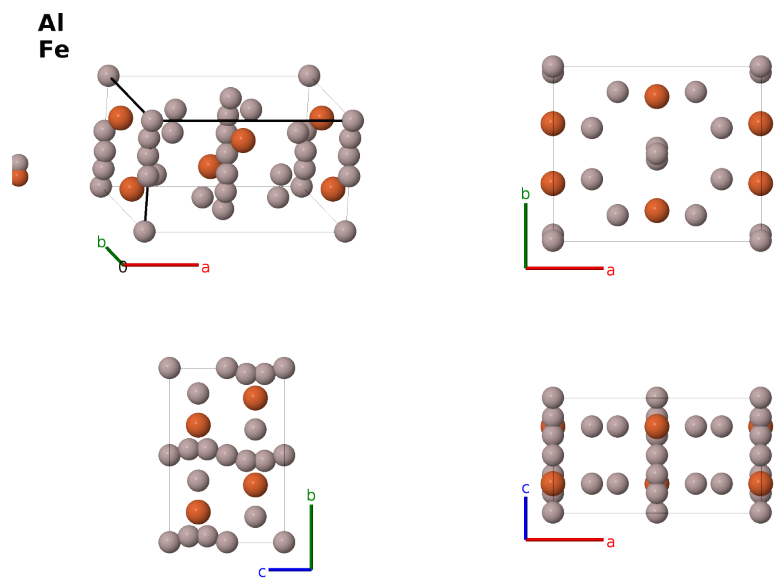
η -Fe₂Al₅ Structure: A5B_oC24_63_afg_c-001

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/US2Q>

https://aflow.org/prototype-encyclopedia/A5B_oC24_63_afg_c-001

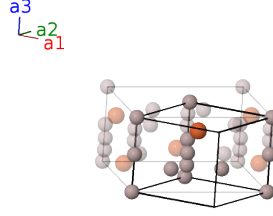


Prototype	Al ₅ Fe ₂
AFLOW prototype label	A5B_oC24_63_afg_c-001
ICSD	105132
CCDC	1663029
Pearson symbol	oC24
Space group number	63
Space group symbol	<i>Cmcm</i>
AFLOW prototype command	<code>aflow --proto=A5B_oC24_63_afg_c-001</code> <code>--params=a, b/a, c/a, y₂, y₃, z₃, x₄, y₄</code>

- The Al-I (4a) sites are occupied 34% of the time, while the Al-III (8g) sites are 24% occupied, giving a stoichiometry near Fe₂Al₅.
- We have shifted the origin to move the Al-I atom from the (4b) site in (Burkhardt, 1994) to the (4a) site.

Base-centered Orthorhombic primitive vectors

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



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	=	0	=	0	(4a) Al I
$\mathbf{B}_2$	=	$\frac{1}{2} \mathbf{a}_3$	=	$\frac{1}{2}c \hat{\mathbf{z}}$	(4a) Al I
$\mathbf{B}_3$	=	$-y_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	=	$by_2 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(4c) Fe I
$\mathbf{B}_4$	=	$y_2 \mathbf{a}_1 - y_2 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	=	$-by_2 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(4c) Fe I
$\mathbf{B}_5$	=	$-y_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	=	$by_3 \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(8f) Al II
$\mathbf{B}_6$	=	$y_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$	=	$-by_3 \hat{\mathbf{y}} + c(z_3 + \frac{1}{2}) \hat{\mathbf{z}}$	(8f) Al II
$\mathbf{B}_7$	=	$-y_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 - (z_3 - \frac{1}{2}) \mathbf{a}_3$	=	$by_3 \hat{\mathbf{y}} - c(z_3 - \frac{1}{2}) \hat{\mathbf{z}}$	(8f) Al II
$\mathbf{B}_8$	=	$y_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 - z_3 \mathbf{a}_3$	=	$-by_3 \hat{\mathbf{y}} - cz_3 \hat{\mathbf{z}}$	(8f) Al II
$\mathbf{B}_9$	=	$(x_4 - y_4) \mathbf{a}_1 + (x_4 + y_4) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	=	$ax_4 \hat{\mathbf{x}} + by_4 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(8g) Al III
$\mathbf{B}_{10}$	=	$-(x_4 - y_4) \mathbf{a}_1 - (x_4 + y_4) \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	=	$-ax_4 \hat{\mathbf{x}} - by_4 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(8g) Al III
$\mathbf{B}_{11}$	=	$-(x_4 + y_4) \mathbf{a}_1 - (x_4 - y_4) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	=	$-ax_4 \hat{\mathbf{x}} + by_4 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(8g) Al III
$\mathbf{B}_{12}$	=	$(x_4 + y_4) \mathbf{a}_1 + (x_4 - y_4) \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	=	$ax_4 \hat{\mathbf{x}} - by_4 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(8g) Al III

References

- [1] U. Burkhardt, Y. Grin, M. Ellner, and K. Peters, *Structure refinement of the iron-aluminium phase with the approximate composition Fe_2Al_5* , Acta Crystallogr. Sect. B **50**, 313–316 (1994), doi:10.1107/S0108768193013989.

Found in

- [1] T. Tsukahara, N. Takata, S. Kobayashi, and M. Takeyama, *Mechanical Properties of Fe_2Al_5 and FeAl_3 Intermetallic Phases at Ambient Temperature*, Tetsu-to-Hagane **102**, 29–35 (2016), doi:10.2355/tetsutohagane.TETSU-2015-063.

First cited in

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