

Al₁₃Fe₄ Structure: A13B4_mC102_12_ah8i5j_4ij-001

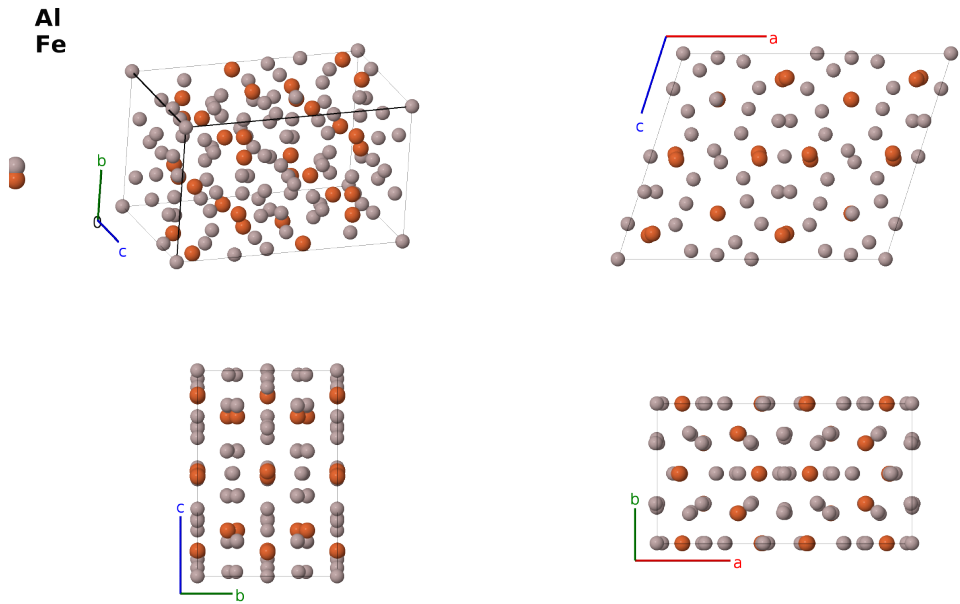
This structure previously used the label(s) **A13B4_mC102_12_dg8i5j_4ij**. Calls to these addresses will be redirected here.

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<https://aflow.org/prototype-encyclopedia/U8YR>

https://aflow.org/prototype-encyclopedia/A13B4_mC102_12_ah8i5j_4ij-001

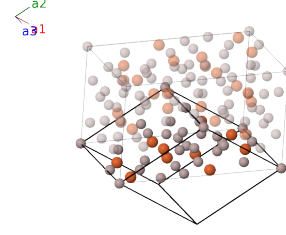


Prototype	Al ₁₃ Fe ₄
AFLOW prototype label	A13B4_mC102_12_ah8i5j_4ij-001
ICSD	57795
CCDC	1621838
Pearson symbol	mC102
Space group number	12
Space group symbol	<i>C</i> 2/ <i>m</i>
AFLOW prototype command	<pre>aflow --proto=A13B4_mC102_12_ah8i5j_4ij-001 --params=a,b/a,c/a,β,y₂,x₃,z₃,x₄,z₄,x₅,z₅,x₆,z₆,x₇,z₇,x₈,z₈,x₉,z₉,x₁₀,z₁₀,x₁₁, z₁₁,x₁₂,z₁₂,x₁₃,z₁₃,x₁₄,z₁₄,x₁₅,y₁₅,z₁₅,x₁₆,y₁₆,z₁₆,x₁₇,y₁₇,z₁₇,x₁₈,y₁₈,z₁₈,x₁₉,y₁₉,z₁₉, x₂₀,y₂₀,z₂₀</pre>

- The Al-IV site is only occupied 70% of the time. This makes the stoichiometry Al_{12.8}Fe₄, which (Black, 1955ab) rounds to Al₁₃Fe₄.

Base-centered Monoclinic primitive vectors

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



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$=$	0	$=$	0	(2a) Al I
$\mathbf{B}_2$	$=$	$-y_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2}c \cos \beta \hat{\mathbf{x}} + by_2 \hat{\mathbf{y}} + \frac{1}{2}c \sin \beta \hat{\mathbf{z}}$	(4h) Al II
$\mathbf{B}_3$	$=$	$y_2 \mathbf{a}_1 - y_2 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2}c \cos \beta \hat{\mathbf{x}} - by_2 \hat{\mathbf{y}} + \frac{1}{2}c \sin \beta \hat{\mathbf{z}}$	(4h) Al II
$\mathbf{B}_4$	$=$	$x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$(ax_3 + cz_3 \cos \beta) \hat{\mathbf{x}} + cz_3 \sin \beta \hat{\mathbf{z}}$	(4i) Al III
$\mathbf{B}_5$	$=$	$-x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$-(ax_3 + cz_3 \cos \beta) \hat{\mathbf{x}} - cz_3 \sin \beta \hat{\mathbf{z}}$	(4i) Al III
$\mathbf{B}_6$	$=$	$x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$(ax_4 + cz_4 \cos \beta) \hat{\mathbf{x}} + cz_4 \sin \beta \hat{\mathbf{z}}$	(4i) Al IV
$\mathbf{B}_7$	$=$	$-x_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$-(ax_4 + cz_4 \cos \beta) \hat{\mathbf{x}} - cz_4 \sin \beta \hat{\mathbf{z}}$	(4i) Al IV
$\mathbf{B}_8$	$=$	$x_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$(ax_5 + cz_5 \cos \beta) \hat{\mathbf{x}} + cz_5 \sin \beta \hat{\mathbf{z}}$	(4i) Al V
$\mathbf{B}_9$	$=$	$-x_5 \mathbf{a}_1 - x_5 \mathbf{a}_2 - z_5 \mathbf{a}_3$	$=$	$-(ax_5 + cz_5 \cos \beta) \hat{\mathbf{x}} - cz_5 \sin \beta \hat{\mathbf{z}}$	(4i) Al V
$\mathbf{B}_{10}$	$=$	$x_6 \mathbf{a}_1 + x_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$(ax_6 + cz_6 \cos \beta) \hat{\mathbf{x}} + cz_6 \sin \beta \hat{\mathbf{z}}$	(4i) Al VI
$\mathbf{B}_{11}$	$=$	$-x_6 \mathbf{a}_1 - x_6 \mathbf{a}_2 - z_6 \mathbf{a}_3$	$=$	$-(ax_6 + cz_6 \cos \beta) \hat{\mathbf{x}} - cz_6 \sin \beta \hat{\mathbf{z}}$	(4i) Al VI
$\mathbf{B}_{12}$	$=$	$x_7 \mathbf{a}_1 + x_7 \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$(ax_7 + cz_7 \cos \beta) \hat{\mathbf{x}} + cz_7 \sin \beta \hat{\mathbf{z}}$	(4i) Al VII
$\mathbf{B}_{13}$	$=$	$-x_7 \mathbf{a}_1 - x_7 \mathbf{a}_2 - z_7 \mathbf{a}_3$	$=$	$-(ax_7 + cz_7 \cos \beta) \hat{\mathbf{x}} - cz_7 \sin \beta \hat{\mathbf{z}}$	(4i) Al VII
$\mathbf{B}_{14}$	$=$	$x_8 \mathbf{a}_1 + x_8 \mathbf{a}_2 + z_8 \mathbf{a}_3$	$=$	$(ax_8 + cz_8 \cos \beta) \hat{\mathbf{x}} + cz_8 \sin \beta \hat{\mathbf{z}}$	(4i) Al VIII
$\mathbf{B}_{15}$	$=$	$-x_8 \mathbf{a}_1 - x_8 \mathbf{a}_2 - z_8 \mathbf{a}_3$	$=$	$-(ax_8 + cz_8 \cos \beta) \hat{\mathbf{x}} - cz_8 \sin \beta \hat{\mathbf{z}}$	(4i) Al VIII
$\mathbf{B}_{16}$	$=$	$x_9 \mathbf{a}_1 + x_9 \mathbf{a}_2 + z_9 \mathbf{a}_3$	$=$	$(ax_9 + cz_9 \cos \beta) \hat{\mathbf{x}} + cz_9 \sin \beta \hat{\mathbf{z}}$	(4i) Al IX
$\mathbf{B}_{17}$	$=$	$-x_9 \mathbf{a}_1 - x_9 \mathbf{a}_2 - z_9 \mathbf{a}_3$	$=$	$-(ax_9 + cz_9 \cos \beta) \hat{\mathbf{x}} - cz_9 \sin \beta \hat{\mathbf{z}}$	(4i) Al IX
$\mathbf{B}_{18}$	$=$	$x_{10} \mathbf{a}_1 + x_{10} \mathbf{a}_2 + z_{10} \mathbf{a}_3$	$=$	$(ax_{10} + cz_{10} \cos \beta) \hat{\mathbf{x}} + cz_{10} \sin \beta \hat{\mathbf{z}}$	(4i) Al X
$\mathbf{B}_{19}$	$=$	$-x_{10} \mathbf{a}_1 - x_{10} \mathbf{a}_2 - z_{10} \mathbf{a}_3$	$=$	$-(ax_{10} + cz_{10} \cos \beta) \hat{\mathbf{x}} - cz_{10} \sin \beta \hat{\mathbf{z}}$	(4i) Al X
$\mathbf{B}_{20}$	$=$	$x_{11} \mathbf{a}_1 + x_{11} \mathbf{a}_2 + z_{11} \mathbf{a}_3$	$=$	$(ax_{11} + cz_{11} \cos \beta) \hat{\mathbf{x}} + cz_{11} \sin \beta \hat{\mathbf{z}}$	(4i) Fe I
$\mathbf{B}_{21}$	$=$	$-x_{11} \mathbf{a}_1 - x_{11} \mathbf{a}_2 - z_{11} \mathbf{a}_3$	$=$	$-(ax_{11} + cz_{11} \cos \beta) \hat{\mathbf{x}} - cz_{11} \sin \beta \hat{\mathbf{z}}$	(4i) Fe I
$\mathbf{B}_{22}$	$=$	$x_{12} \mathbf{a}_1 + x_{12} \mathbf{a}_2 + z_{12} \mathbf{a}_3$	$=$	$(ax_{12} + cz_{12} \cos \beta) \hat{\mathbf{x}} + cz_{12} \sin \beta \hat{\mathbf{z}}$	(4i) Fe II
$\mathbf{B}_{23}$	$=$	$-x_{12} \mathbf{a}_1 - x_{12} \mathbf{a}_2 - z_{12} \mathbf{a}_3$	$=$	$-(ax_{12} + cz_{12} \cos \beta) \hat{\mathbf{x}} - cz_{12} \sin \beta \hat{\mathbf{z}}$	(4i) Fe II
$\mathbf{B}_{24}$	$=$	$x_{13} \mathbf{a}_1 + x_{13} \mathbf{a}_2 + z_{13} \mathbf{a}_3$	$=$	$(ax_{13} + cz_{13} \cos \beta) \hat{\mathbf{x}} + cz_{13} \sin \beta \hat{\mathbf{z}}$	(4i) Fe III
$\mathbf{B}_{25}$	$=$	$-x_{13} \mathbf{a}_1 - x_{13} \mathbf{a}_2 - z_{13} \mathbf{a}_3$	$=$	$-(ax_{13} + cz_{13} \cos \beta) \hat{\mathbf{x}} - cz_{13} \sin \beta \hat{\mathbf{z}}$	(4i) Fe III
$\mathbf{B}_{26}$	$=$	$x_{14} \mathbf{a}_1 + x_{14} \mathbf{a}_2 + z_{14} \mathbf{a}_3$	$=$	$(ax_{14} + cz_{14} \cos \beta) \hat{\mathbf{x}} + cz_{14} \sin \beta \hat{\mathbf{z}}$	(4i) Fe IV
$\mathbf{B}_{27}$	$=$	$-x_{14} \mathbf{a}_1 - x_{14} \mathbf{a}_2 - z_{14} \mathbf{a}_3$	$=$	$-(ax_{14} + cz_{14} \cos \beta) \hat{\mathbf{x}} - cz_{14} \sin \beta \hat{\mathbf{z}}$	(4i) Fe IV
$\mathbf{B}_{28}$	$=$	$(x_{15} - y_{15}) \mathbf{a}_1 +$ $(x_{15} + y_{15}) \mathbf{a}_2 + z_{15} \mathbf{a}_3$	$=$	$(ax_{15} + cz_{15} \cos \beta) \hat{\mathbf{x}} + by_{15} \hat{\mathbf{y}} + cz_{15} \sin \beta \hat{\mathbf{z}}$	(8j) Al XI

References

- [1] P. J. Black, *The Structure of $FeAl_3.I$* , *Acta Cryst.***8**, 43 – 48(1955), *doi* : 10.1107/S0365110X5500011X.
- [2] P. J. Black, *The Structure of $FeAl_3.II$* , *Acta Cryst.***8**, 175 – 182(1955), *doi* : 10.1107/S0365110X62001103.

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