$Al_{13}Fe_4$ Structure: A13B4_mC102_12_ah8i5j_4ij-001

This structure originally had the label `A13B4_mC102_12_dg8i5j_4ij`. Calls to that address will be redirected here.

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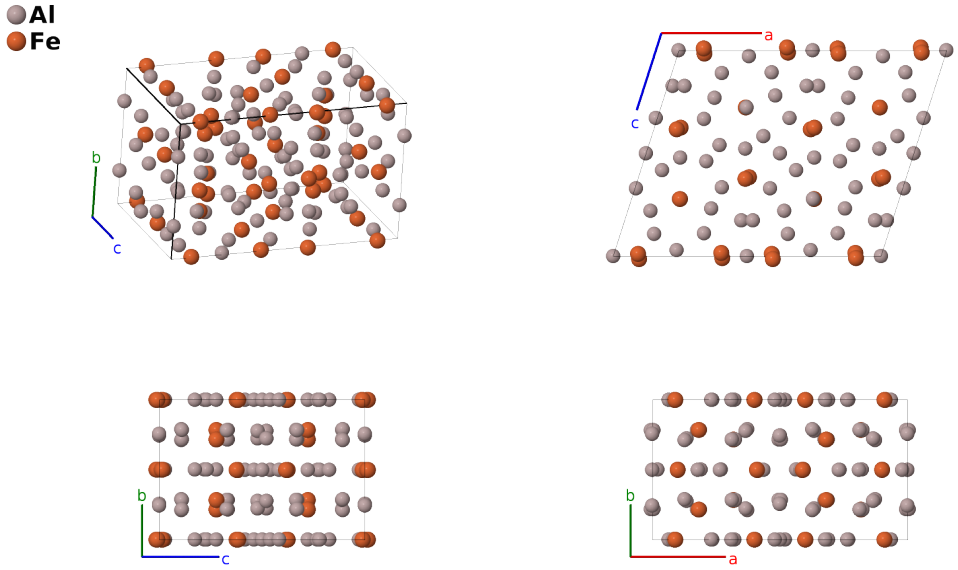
https://aflow.org/p/U8YR

https://aflow.org/p/A13B4_mC102_12_ah8i5j_4ij-001

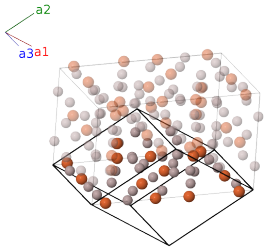


Prototype	$Al_{13}Fe_4$
AFLOW prototype label	A13B4_mC102_12_ah8i5j_4ij-001
ICSD	57795
Pearson symbol	mC102
Space group number	12
Space group symbol	$C2/m$
AFLOW prototype command	`aflow --proto=A13B4_mC102_12_ah8i5j_4ij-001 --params=`$a, b/a, c/a, \beta, y_2, x_3, z_3, x_4, z_4, x_5, z_5, x_6, z_6, x_7, z_7, x_8, z_8, x_9, z_9, x_{10}, z_{10}, x_{11}, z_{11}, x_{12}, z_{12}, x_{13}, z_{13}, x_{14}, z_{14}, x_{15}, y_{15}, z_{15}, x_{16}, y_{16}, z_{16}, x_{17}, y_{17}, z_{17}, x_{18}, y_{18}, z_{18}, x_{19}, y_{19}, z_{19}, x_{20}, y_{20}, z_{20}$

- The Al-IV site is only occupied 70% of the time. This makes the stoichiometry $Al_{12.8}Fe_4$, which (Black, 1955ab) rounds to $Al_{13}Fe_4$.

Base-centered Monoclinic primitive vectors

$$
\begin{aligned}
\mathbf{a_1} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{1}{2}b\,\hat{\mathbf{y}} \\
\mathbf{a_2} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}b\,\hat{\mathbf{y}} \\
\mathbf{a_3} &= c\cos\beta\,\hat{\mathbf{x}} + c\sin\beta\,\hat{\mathbf{z}}
\end{aligned}
$$



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
$\mathbf{B_{29}}$	=	$-(x_{15} + y_{15})\,\mathbf{a}_1 - (x_{15} - y_{15})\,\mathbf{a}_2 - z_{15}\,\mathbf{a}_3$	=	$-(ax_{15} + cz_{15}\cos\beta)\,\hat{\mathbf{x}} + by_{15}\,\hat{\mathbf{y}} - cz_{15}\sin\beta\,\hat{\mathbf{z}}$	(8j)	Al XI

$$\mathbf{B_{30}} = -(x_{15}-y_{15})\,\mathbf{a}_1 - (x_{15}+y_{15})\,\mathbf{a}_2 - z_{15}\,\mathbf{a}_3 = -(ax_{15}+cz_{15}\cos\beta)\,\hat{\mathbf{x}} - by_{15}\,\hat{\mathbf{y}} - cz_{15}\sin\beta\,\hat{\mathbf{z}} \quad (8j) \quad \text{Al XI}$$

$$\mathbf{B_{31}} = (x_{15}+y_{15})\,\mathbf{a}_1 + (x_{15}-y_{15})\,\mathbf{a}_2 + z_{15}\,\mathbf{a}_3 = (ax_{15}+cz_{15}\cos\beta)\,\hat{\mathbf{x}} - by_{15}\,\hat{\mathbf{y}} + cz_{15}\sin\beta\,\hat{\mathbf{z}} \quad (8j) \quad \text{Al XI}$$

$$\mathbf{B_{32}} = (x_{16}-y_{16})\,\mathbf{a}_1 + (x_{16}+y_{16})\,\mathbf{a}_2 + z_{16}\,\mathbf{a}_3 = (ax_{16}+cz_{16}\cos\beta)\,\hat{\mathbf{x}} + by_{16}\,\hat{\mathbf{y}} + cz_{16}\sin\beta\,\hat{\mathbf{z}} \quad (8j) \quad \text{Al XII}$$

$$\mathbf{B_{33}} = -(x_{16}+y_{16})\,\mathbf{a}_1 - (x_{16}-y_{16})\,\mathbf{a}_2 - z_{16}\,\mathbf{a}_3 = -(ax_{16}+cz_{16}\cos\beta)\,\hat{\mathbf{x}} + by_{16}\,\hat{\mathbf{y}} - cz_{16}\sin\beta\,\hat{\mathbf{z}} \quad (8j) \quad \text{Al XII}$$

$$\mathbf{B_{34}} = -(x_{16}-y_{16})\,\mathbf{a}_1 - (x_{16}+y_{16})\,\mathbf{a}_2 - z_{16}\,\mathbf{a}_3 = -(ax_{16}+cz_{16}\cos\beta)\,\hat{\mathbf{x}} - by_{16}\,\hat{\mathbf{y}} - cz_{16}\sin\beta\,\hat{\mathbf{z}} \quad (8j) \quad \text{Al XII}$$

$$\mathbf{B_{35}} = (x_{16}+y_{16})\,\mathbf{a}_1 + (x_{16}-y_{16})\,\mathbf{a}_2 + z_{16}\,\mathbf{a}_3 = (ax_{16}+cz_{16}\cos\beta)\,\hat{\mathbf{x}} - by_{16}\,\hat{\mathbf{y}} + cz_{16}\sin\beta\,\hat{\mathbf{z}} \quad (8j) \quad \text{Al XII}$$

$$\mathbf{B_{36}} = (x_{17}-y_{17})\,\mathbf{a}_1 + (x_{17}+y_{17})\,\mathbf{a}_2 + z_{17}\,\mathbf{a}_3 = (ax_{17}+cz_{17}\cos\beta)\,\hat{\mathbf{x}} + by_{17}\,\hat{\mathbf{y}} + cz_{17}\sin\beta\,\hat{\mathbf{z}} \quad (8j) \quad \text{Al XIII}$$

$$\mathbf{B_{37}} = -(x_{17}+y_{17})\,\mathbf{a}_1 - (x_{17}-y_{17})\,\mathbf{a}_2 - z_{17}\,\mathbf{a}_3 = -(ax_{17}+cz_{17}\cos\beta)\,\hat{\mathbf{x}} + by_{17}\,\hat{\mathbf{y}} - cz_{17}\sin\beta\,\hat{\mathbf{z}} \quad (8j) \quad \text{Al XIII}$$

$$\mathbf{B_{38}} = -(x_{17}-y_{17})\,\mathbf{a}_1 - (x_{17}+y_{17})\,\mathbf{a}_2 - z_{17}\,\mathbf{a}_3 = -(ax_{17}+cz_{17}\cos\beta)\,\hat{\mathbf{x}} - by_{17}\,\hat{\mathbf{y}} - cz_{17}\sin\beta\,\hat{\mathbf{z}} \quad (8j) \quad \text{Al XIII}$$

$$\mathbf{B_{39}} = (x_{17}+y_{17})\,\mathbf{a}_1 + (x_{17}-y_{17})\,\mathbf{a}_2 + z_{17}\,\mathbf{a}_3 = (ax_{17}+cz_{17}\cos\beta)\,\hat{\mathbf{x}} - by_{17}\,\hat{\mathbf{y}} + cz_{17}\sin\beta\,\hat{\mathbf{z}} \quad (8j) \quad \text{Al XIII}$$

$$\mathbf{B_{40}} = (x_{18}-y_{18})\,\mathbf{a}_1 + (x_{18}+y_{18})\,\mathbf{a}_2 + z_{18}\,\mathbf{a}_3 = (ax_{18}+cz_{18}\cos\beta)\,\hat{\mathbf{x}} + by_{18}\,\hat{\mathbf{y}} + cz_{18}\sin\beta\,\hat{\mathbf{z}} \quad (8j) \quad \text{Al XIV}$$

$$\mathbf{B_{41}} = -(x_{18}+y_{18})\,\mathbf{a}_1 - (x_{18}-y_{18})\,\mathbf{a}_2 - z_{18}\,\mathbf{a}_3 = -(ax_{18}+cz_{18}\cos\beta)\,\hat{\mathbf{x}} + by_{18}\,\hat{\mathbf{y}} - cz_{18}\sin\beta\,\hat{\mathbf{z}} \quad (8j) \quad \text{Al XIV}$$

$$\mathbf{B_{42}} = -(x_{18}-y_{18})\,\mathbf{a}_1 - (x_{18}+y_{18})\,\mathbf{a}_2 - z_{18}\,\mathbf{a}_3 = -(ax_{18}+cz_{18}\cos\beta)\,\hat{\mathbf{x}} - by_{18}\,\hat{\mathbf{y}} - cz_{18}\sin\beta\,\hat{\mathbf{z}} \quad (8j) \quad \text{Al XIV}$$

$$\mathbf{B_{43}} = (x_{18}+y_{18})\,\mathbf{a}_1 + (x_{18}-y_{18})\,\mathbf{a}_2 + z_{18}\,\mathbf{a}_3 = (ax_{18}+cz_{18}\cos\beta)\,\hat{\mathbf{x}} - by_{18}\,\hat{\mathbf{y}} + cz_{18}\sin\beta\,\hat{\mathbf{z}} \quad (8j) \quad \text{Al XIV}$$

$$\mathbf{B_{44}} = (x_{19}-y_{19})\,\mathbf{a}_1 + (x_{19}+y_{19})\,\mathbf{a}_2 + z_{19}\,\mathbf{a}_3 = (ax_{19}+cz_{19}\cos\beta)\,\hat{\mathbf{x}} + by_{19}\,\hat{\mathbf{y}} + cz_{19}\sin\beta\,\hat{\mathbf{z}} \quad (8j) \quad \text{Al XV}$$

$$\mathbf{B_{45}} = -(x_{19}+y_{19})\,\mathbf{a}_1 - (x_{19}-y_{19})\,\mathbf{a}_2 - z_{19}\,\mathbf{a}_3 = -(ax_{19}+cz_{19}\cos\beta)\,\hat{\mathbf{x}} + by_{19}\,\hat{\mathbf{y}} - cz_{19}\sin\beta\,\hat{\mathbf{z}} \quad (8j) \quad \text{Al XV}$$

$$\mathbf{B_{46}} = -(x_{19}-y_{19})\,\mathbf{a}_1 - (x_{19}+y_{19})\,\mathbf{a}_2 - z_{19}\,\mathbf{a}_3 = -(ax_{19}+cz_{19}\cos\beta)\,\hat{\mathbf{x}} - by_{19}\,\hat{\mathbf{y}} - cz_{19}\sin\beta\,\hat{\mathbf{z}} \quad (8j) \quad \text{Al XV}$$

$$\mathbf{B_{47}} = (x_{19}+y_{19})\,\mathbf{a}_1 + (x_{19}-y_{19})\,\mathbf{a}_2 + z_{19}\,\mathbf{a}_3 = (ax_{19}+cz_{19}\cos\beta)\,\hat{\mathbf{x}} - by_{19}\,\hat{\mathbf{y}} + cz_{19}\sin\beta\,\hat{\mathbf{z}} \quad (8j) \quad \text{Al XV}$$

$$\mathbf{B_{48}} = (x_{20}-y_{20})\,\mathbf{a}_1 + (x_{20}+y_{20})\,\mathbf{a}_2 + z_{20}\,\mathbf{a}_3 = (ax_{20}+cz_{20}\cos\beta)\,\hat{\mathbf{x}} + by_{20}\,\hat{\mathbf{y}} + cz_{20}\sin\beta\,\hat{\mathbf{z}} \quad (8j) \quad \text{Fe V}$$

$$\mathbf{B_{49}} = -(x_{20}+y_{20})\,\mathbf{a}_1 - (x_{20}-y_{20})\,\mathbf{a}_2 - z_{20}\,\mathbf{a}_3 = -(ax_{20}+cz_{20}\cos\beta)\,\hat{\mathbf{x}} + by_{20}\,\hat{\mathbf{y}} - cz_{20}\sin\beta\,\hat{\mathbf{z}} \quad (8j) \quad \text{Fe V}$$

$$\mathbf{B_{50}} = -(x_{20}-y_{20})\,\mathbf{a}_1 - (x_{20}+y_{20})\,\mathbf{a}_2 - z_{20}\,\mathbf{a}_3 = -(ax_{20}+cz_{20}\cos\beta)\,\hat{\mathbf{x}} - by_{20}\,\hat{\mathbf{y}} - cz_{20}\sin\beta\,\hat{\mathbf{z}} \quad (8j) \quad \text{Fe V}$$

$$\mathbf{B_{51}} = (x_{20}+y_{20})\,\mathbf{a}_1 + (x_{20}-y_{20})\,\mathbf{a}_2 + z_{20}\,\mathbf{a}_3 = (ax_{20}+cz_{20}\cos\beta)\,\hat{\mathbf{x}} - by_{20}\,\hat{\mathbf{y}} + cz_{20}\sin\beta\,\hat{\mathbf{z}} \quad (8j) \quad \text{Fe V}$$

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.