

ζ -Fe₂N Structure: A2B_oP12_60_d_c-001

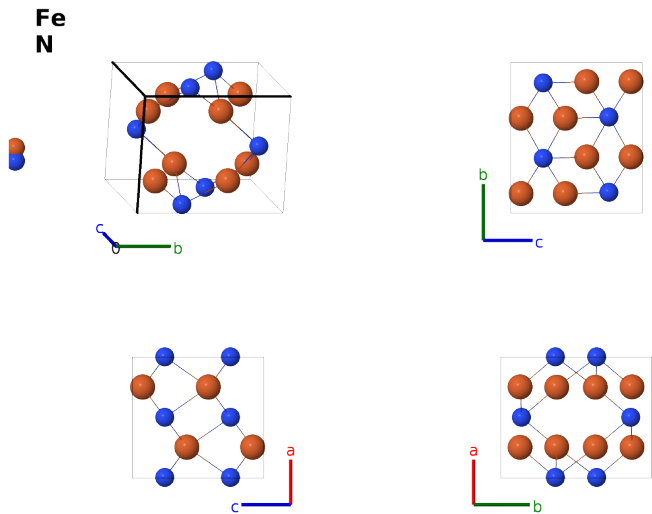
This structure previously used the label(s) **A2B_oP12_60_d_c.Fe2N**. Calls to these addresses will be redirected here.

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<https://aflow.org/prototype-encyclopedia/5GP6>

https://aflow.org/prototype-encyclopedia/A2B_oP12_60_d_c-001



Prototype	Fe ₂ N
AFLOW prototype label	A2B_oP12_60_d_c-001
ICSD	81732
CCDC	1641860
Pearson symbol	oP12
Space group number	60
Space group symbol	<i>Pbcn</i>
AFLOW prototype command	<code>aflow --proto=A2B_oP12_60_d_c-001</code> <code>--params=a, b/a, c/a, y₁, x₂, y₂, z₂</code>

Other compounds with this structure

Mo₂C, Mo₂N, Ru₂C, V₂C, V₂N, β W₂C

- Fe₂N can also be found in the η -Fe₂N/ β -V₂N ($L'3_2$) structure. It has also been reported in the $L'3_0$ structure
- This structure has the same AFLOW label as α -PbO₂, but in that case the lead site is only 49% occupied, so that composition is actually closer to PbO₄.

- The structures are generated by the same symmetry operations with different sets of parameters (`--params`) specified in their corresponding CIF files.

Simple Orthorhombic primitive vectors



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= y_1 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$by_1 \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(4c)	N I
$\mathbf{B}_2$	$= \frac{1}{2} \mathbf{a}_1 - (y_1 - \frac{1}{2}) \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} - b (y_1 - \frac{1}{2}) \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(4c)	N I
$\mathbf{B}_3$	$= -y_1 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$-by_1 \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(4c)	N I
$\mathbf{B}_4$	$= \frac{1}{2} \mathbf{a}_1 + (y_1 + \frac{1}{2}) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + b (y_1 + \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(4c)	N I
$\mathbf{B}_5$	$= x_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$ax_2 \hat{\mathbf{x}} + by_2 \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$	(8d)	Fe I
$\mathbf{B}_6$	$= -(x_2 - \frac{1}{2}) \mathbf{a}_1 - (y_2 - \frac{1}{2}) \mathbf{a}_2 + (z_2 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_2 - \frac{1}{2}) \hat{\mathbf{x}} - b(y_2 - \frac{1}{2}) \hat{\mathbf{y}} + c(z_2 + \frac{1}{2}) \hat{\mathbf{z}}$	(8d)	Fe I
$\mathbf{B}_7$	$= -x_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 - (z_2 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_2 \hat{\mathbf{x}} + by_2 \hat{\mathbf{y}} - c(z_2 - \frac{1}{2}) \hat{\mathbf{z}}$	(8d)	Fe I
$\mathbf{B}_8$	$= (x_2 + \frac{1}{2}) \mathbf{a}_1 - (y_2 - \frac{1}{2}) \mathbf{a}_2 - z_2 \mathbf{a}_3$	$=$	$a(x_2 + \frac{1}{2}) \hat{\mathbf{x}} - b(y_2 - \frac{1}{2}) \hat{\mathbf{y}} - cz_2 \hat{\mathbf{z}}$	(8d)	Fe I
$\mathbf{B}_9$	$= -x_2 \mathbf{a}_1 - y_2 \mathbf{a}_2 - z_2 \mathbf{a}_3$	$=$	$-ax_2 \hat{\mathbf{x}} - by_2 \hat{\mathbf{y}} - cz_2 \hat{\mathbf{z}}$	(8d)	Fe I
$\mathbf{B}_{10}$	$= (x_2 + \frac{1}{2}) \mathbf{a}_1 + (y_2 + \frac{1}{2}) \mathbf{a}_2 - (z_2 - \frac{1}{2}) \mathbf{a}_3$	$=$	$a(x_2 + \frac{1}{2}) \hat{\mathbf{x}} + b(y_2 + \frac{1}{2}) \hat{\mathbf{y}} - c(z_2 - \frac{1}{2}) \hat{\mathbf{z}}$	(8d)	Fe I
$\mathbf{B}_{11}$	$= x_2 \mathbf{a}_1 - y_2 \mathbf{a}_2 + (z_2 + \frac{1}{2}) \mathbf{a}_3$	$=$	$ax_2 \hat{\mathbf{x}} - by_2 \hat{\mathbf{y}} + c(z_2 + \frac{1}{2}) \hat{\mathbf{z}}$	(8d)	Fe I
$\mathbf{B}_{12}$	$= -(x_2 - \frac{1}{2}) \mathbf{a}_1 + (y_2 + \frac{1}{2}) \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$-a(x_2 - \frac{1}{2}) \hat{\mathbf{x}} + b(y_2 + \frac{1}{2}) \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$	(8d)	Fe I

References

- [1] D. Rechenbach and H. Jacobs, *Structure determination of ζ -Fe₂N by neutron and synchrotron powder diffraction* **235**, 15–22 (1996), doi:10.1016/0925-8388(95)02097-7.

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