

η -Fe₂C Structure:

AB2_oP6_58_a_g-002

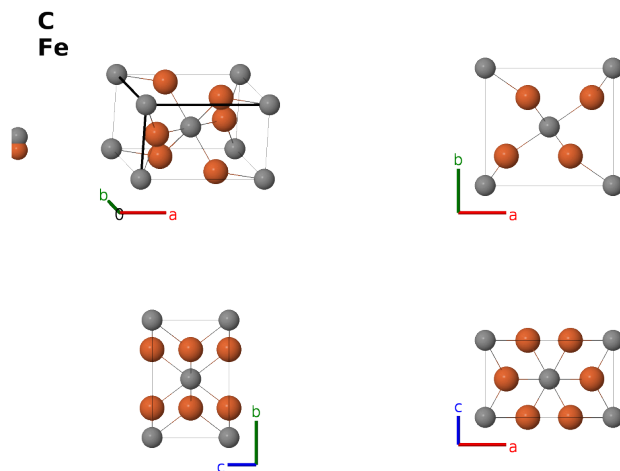
This structure previously used the label(s) **AB2_oP6_58_a_g.eta-Fe2C**. Calls to these addresses will be redirected here.

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<https://aflow.org/prototype-encyclopedia/FF5Q>

https://aflow.org/prototype-encyclopedia/AB2_oP6_58_a_g-002



Prototype	Fe ₂ C
AFLOW prototype label	AB2_oP6_58_a_g-002
ICSD	76826
CCDC	1637348
Pearson symbol	oP6
Space group number	58
Space group symbol	<i>Pnnm</i>
AFLOW prototype command	<code>aflow --proto=AB2_oP6_58_a_g-002 --params=a, b/a, c/a, x₂, y₂</code>

Other compounds with this structure

C₂Si, Co₂C, Co₂N, N₂Al, N₂Os, Pd₂B, Pd₂N, Rh₂C

- Classified as bcc-related by Hellner and Schwarz (Westbrook, 1995), Vol. I, Chap. 13.
- Hydrophilite (CaCl₂, C35), η -Fe₂C, and marcasite (FeS₂, C18) have the same AFLOW prototype label, AB2_oP6_58_a_g. They are generated by the same symmetry operations with different sets of parameters (`--params`) specified in their corresponding CIF files.

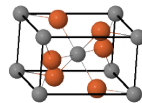
Simple Orthorhombic primitive vectors



$$\mathbf{a}_1 = a \hat{\mathbf{x}}$$

$$\mathbf{a}_2 = b \hat{\mathbf{y}}$$

$$\mathbf{a}_3 = c \hat{\mathbf{z}}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	=	0	=	0	(2a) C I
$\mathbf{B}_2$	=	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	=	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} b \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(2a) C I
$\mathbf{B}_3$	=	$x_2 \mathbf{a}_1 + y_2 \mathbf{a}_2$	=	$ax_2 \hat{\mathbf{x}} + by_2 \hat{\mathbf{y}}$	(4g) Fe I
$\mathbf{B}_4$	=	$-x_2 \mathbf{a}_1 - y_2 \mathbf{a}_2$	=	$-ax_2 \hat{\mathbf{x}} - by_2 \hat{\mathbf{y}}$	(4g) Fe I
$\mathbf{B}_5$	=	$-(x_2 - \frac{1}{2}) \mathbf{a}_1 + (y_2 + \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	=	$-a(x_2 - \frac{1}{2}) \hat{\mathbf{x}} + b(y_2 + \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4g) Fe I
$\mathbf{B}_6$	=	$(x_2 + \frac{1}{2}) \mathbf{a}_1 - (y_2 - \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	=	$a(x_2 + \frac{1}{2}) \hat{\mathbf{x}} - b(y_2 - \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4g) Fe I

References

- [1] Y. Hirotsu and S. Nagakura, *Crystal structure and morphology of the carbide precipitated from martensitic high carbon steel during the first stage of tempering*, Acta Metall. **20**, 645–655 (1972), doi:10.1016/0001-6160(72)90020-X.
- [2] J. H. Westbrook and R. L. Fleischer, eds., *Intermetallic Compounds – Principles and Practice* (John Wiley & Sons, Ltd., Chichester, England, 1995). Two Volumes.

First cited in

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