η-Fe_2C Structure: AB2_oP6_58_a_g-002

This structure originally had the label `AB2_oP6_58_a_g.eta-Fe2C`. Calls to that address will be redirected here.

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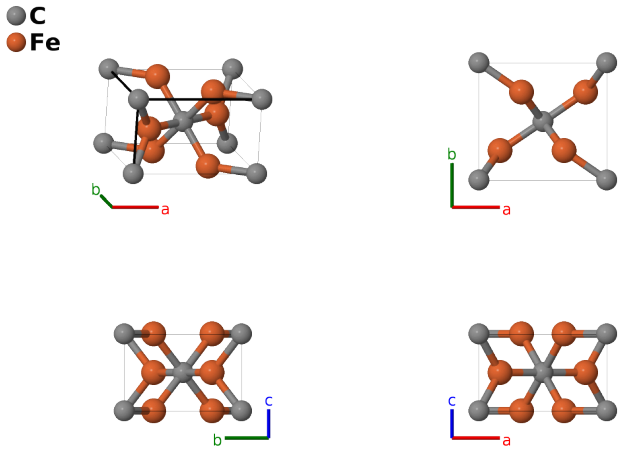
https://aflow.org/p/FF5Q

https://aflow.org/p/AB2_oP6_58_a_g-002

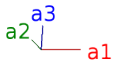


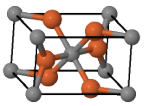
Prototype	Fe_2C
AFLOW prototype label	AB2_oP6_58_a_g-002
ICSD	76826
Pearson symbol	oP6
Space group number	58
Space group symbol	*Pnnm*
AFLOW prototype command	`aflow --proto=AB2_oP6_58_a_g-002 --params=`$a, b/a, c/a, x_2, y_2$

- Classified as bcc-related by Hellner and Schwarz (Westbrook, 1995), Vol. I, Chap. 13.
- Hydrophilite ($CaCl_2$, $C35$), η–Fe_2C, and marcasite (FeS_2, $C18$) 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
$\mathbf{B_5}$	=	$-\left(x_2 - \frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_2 + \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-a\left(x_2 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + b\left(y_2 + \frac{1}{2}\right)\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4g)	Fe I
$\mathbf{B_6}$	=	$\left(x_2 + \frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_2 - \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$a\left(x_2 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - b\left(y_2 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(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.