η-carbide (Fe_3W_3C, $E9_3$) Structure: AB3C3_cF112_227_c_de_f-001

This structure previously used the label(s) `AB3C3_cF112_227_c_de_f`. Calls to these addresses will be redirected here.

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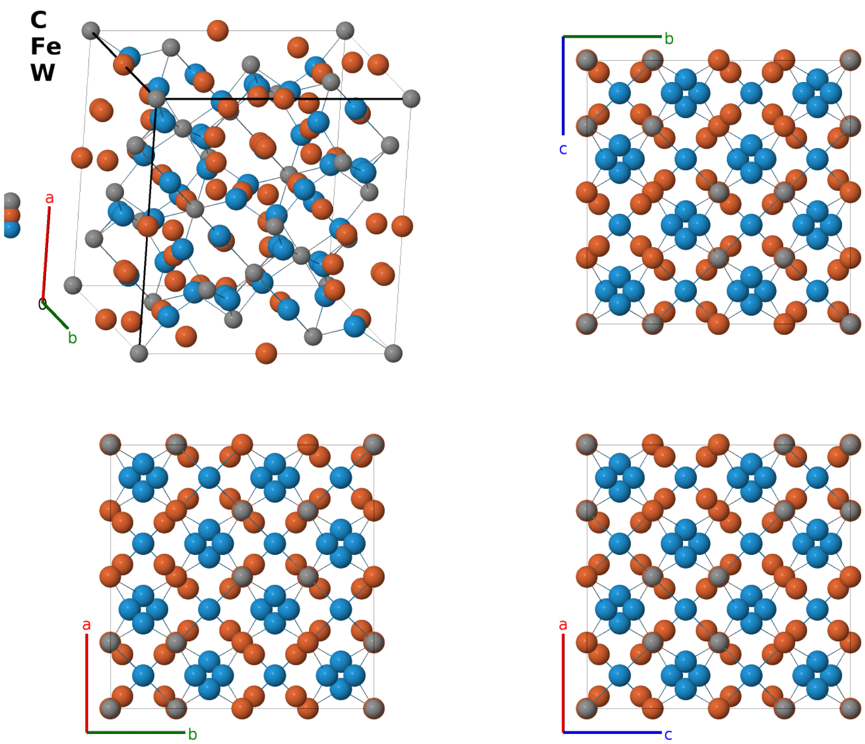
https://aflow.org/prototype-encyclopedia/WVM5

https://aflow.org/prototype-encyclopedia/AB3C3_cF112_227_c_de_f-001



Prototype	CFe_3W_3
AFLOW prototype label	AB3C3_cF112_227_c_de_f-001
***Strukturbericht* designation**	$E9_3$
Mineral name	η-carbide
ICSD	43230
CCDC	1612753
Pearson symbol	cF112
Space group number	227
Space group symbol	$Fd\bar{3}m$

AFLOW prototype command `aflow --proto=AB3C3_cF112_227_c_de_f-001`
`--params=`a, x_3, x_4

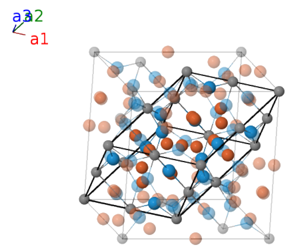
Other compounds with this structure

Cr_3Nb_3C, Fe_3Mo_3C, Fe_4Mo_2C, Fe_6W_6C, Hf_5Zn_3C, Mn_3Mo_3C, Mn_3Ni_3Si, Mn_3Ti_3O, Mn_3W_3C, Mo_3Ni_3C, Mo_4Co_2C, Mo_4Co_2C, Mo_4Ni_2C, Nb_2ZnC_x, Nb_2ZnC_x, $Nb_4Rh_2C_x$, Ni_3W_3C, Ni_5W_6C, Ti_2ZnC_x, Ti_2ZnC_x, Ti_4Pt_2O, Ti_4Rh_2O, V_3Zr_3C, W_3Co_3C, W_4Co_2C, Zn_2ZnN_x, Zr_2ZnC_x, Zr_4Pt_2O

- Experimentally, the (48f) site is a random mixture of composition $W_{2/3}Fe_{1/3}$. We use W for this site in the pictures above.
- In many compounds the carbon sites has vacancies, which accounts for the varying stoichiometries in the compounds list.
- Ti_4Co_2O is an ordered form of this structure with a different stoichiometry.

Face-centered Cubic primitive vectors

$$\mathbf{a_1} = \frac{1}{2}a\,\mathbf{\hat{y}} + \frac{1}{2}a\,\mathbf{\hat{z}}$$
$$\mathbf{a_2} = \frac{1}{2}a\,\mathbf{\hat{x}} + \frac{1}{2}a\,\mathbf{\hat{z}}$$
$$\mathbf{a_3} = \frac{1}{2}a\,\mathbf{\hat{x}} + \frac{1}{2}a\,\mathbf{\hat{y}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(16c)	C I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\mathbf{\hat{x}} + \frac{1}{4}a\,\mathbf{\hat{y}}$	(16c)	C I
$\mathbf{B_3}$	=	$\frac{1}{2}\,\mathbf{a}_2$	=	$\frac{1}{4}a\,\mathbf{\hat{x}} + \frac{1}{4}a\,\mathbf{\hat{z}}$	(16c)	C I
$\mathbf{B_4}$	=	$\frac{1}{2}\,\mathbf{a}_1$	=	$\frac{1}{4}a\,\mathbf{\hat{y}} + \frac{1}{4}a\,\mathbf{\hat{z}}$	(16c)	C I
$\mathbf{B_5}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\mathbf{\hat{x}} + \frac{1}{2}a\,\mathbf{\hat{y}} + \frac{1}{2}a\,\mathbf{\hat{z}}$	(16d)	Fe I
$\mathbf{B_6}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2$	=	$\frac{1}{4}a\,\mathbf{\hat{x}} + \frac{1}{4}a\,\mathbf{\hat{y}} + \frac{1}{2}a\,\mathbf{\hat{z}}$	(16d)	Fe I
$\mathbf{B_7}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\mathbf{\hat{x}} + \frac{1}{2}a\,\mathbf{\hat{y}} + \frac{1}{4}a\,\mathbf{\hat{z}}$	(16d)	Fe I
$\mathbf{B_8}$	=	$\frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\mathbf{\hat{x}} + \frac{1}{4}a\,\mathbf{\hat{y}} + \frac{1}{4}a\,\mathbf{\hat{z}}$	(16d)	Fe I
$\mathbf{B_9}$	=	$x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + x_3\,\mathbf{a}_3$	=	$ax_3\,\mathbf{\hat{x}} + ax_3\,\mathbf{\hat{y}} + ax_3\,\mathbf{\hat{z}}$	(32e)	Fe II
$\mathbf{B_{10}}$	=	$x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 - \left(3x_3 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_3 - \frac{1}{4}\right)\,\mathbf{\hat{x}} - a\left(x_3 - \frac{1}{4}\right)\,\mathbf{\hat{y}} + ax_3\,\mathbf{\hat{z}}$	(32e)	Fe II
$\mathbf{B_{11}}$	=	$x_3\,\mathbf{a}_1 - \left(3x_3 - \frac{1}{2}\right)\,\mathbf{a}_2 + x_3\,\mathbf{a}_3$	=	$-a\left(x_3 - \frac{1}{4}\right)\,\mathbf{\hat{x}} + ax_3\,\mathbf{\hat{y}} - a\left(x_3 - \frac{1}{4}\right)\,\mathbf{\hat{z}}$	(32e)	Fe II
$\mathbf{B_{12}}$	=	$-\left(3x_3 - \frac{1}{2}\right)\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + x_3\,\mathbf{a}_3$	=	$ax_3\,\mathbf{\hat{x}} - a\left(x_3 - \frac{1}{4}\right)\,\mathbf{\hat{y}} - a\left(x_3 - \frac{1}{4}\right)\,\mathbf{\hat{z}}$	(32e)	Fe II
$\mathbf{B_{13}}$	=	$-x_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 + \left(3x_3 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(x_3 + \frac{1}{4}\right)\,\mathbf{\hat{x}} + a\left(x_3 + \frac{1}{4}\right)\,\mathbf{\hat{y}} - ax_3\,\mathbf{\hat{z}}$	(32e)	Fe II
$\mathbf{B_{14}}$	=	$-x_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 - x_3\,\mathbf{a}_3$	=	$-ax_3\,\mathbf{\hat{x}} - ax_3\,\mathbf{\hat{y}} - ax_3\,\mathbf{\hat{z}}$	(32e)	Fe II
$\mathbf{B_{15}}$	=	$-x_3\,\mathbf{a}_1 + \left(3x_3 + \frac{1}{2}\right)\,\mathbf{a}_2 - x_3\,\mathbf{a}_3$	=	$a\left(x_3 + \frac{1}{4}\right)\,\mathbf{\hat{x}} - ax_3\,\mathbf{\hat{y}} + a\left(x_3 + \frac{1}{4}\right)\,\mathbf{\hat{z}}$	(32e)	Fe II
$\mathbf{B_{16}}$	=	$\left(3x_3 + \frac{1}{2}\right)\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 - x_3\,\mathbf{a}_3$	=	$-ax_3\,\mathbf{\hat{x}} + a\left(x_3 + \frac{1}{4}\right)\,\mathbf{\hat{y}} + a\left(x_3 + \frac{1}{4}\right)\,\mathbf{\hat{z}}$	(32e)	Fe II
$\mathbf{B_{17}}$	=	$-\left(x_4 - \frac{1}{4}\right)\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 + x_4\,\mathbf{a}_3$	=	$ax_4\,\mathbf{\hat{x}} + \frac{1}{8}a\,\mathbf{\hat{y}} + \frac{1}{8}a\,\mathbf{\hat{z}}$	(48f)	W I

$\mathbf{B_{18}}$	$=$	$x_4\,\mathbf{a}_1-\left(x_4-\frac{1}{4}\right)\,\mathbf{a}_2-\left(x_4-\frac{1}{4}\right)\,\mathbf{a}_3$	$=$	$-a\left(x_4-\frac{1}{4}\right)\,\hat{\mathbf{x}}+\frac{1}{8}a\,\hat{\mathbf{y}}+\frac{1}{8}a\,\hat{\mathbf{z}}$	(48f)	W I
$\mathbf{B_{19}}$	$=$	$x_4\,\mathbf{a}_1-\left(x_4-\frac{1}{4}\right)\,\mathbf{a}_2+x_4\,\mathbf{a}_3$	$=$	$\frac{1}{8}a\,\hat{\mathbf{x}}+ax_4\,\hat{\mathbf{y}}+\frac{1}{8}a\,\hat{\mathbf{z}}$	(48f)	W I
$\mathbf{B_{20}}$	$=$	$-\left(x_4-\frac{1}{4}\right)\,\mathbf{a}_1+x_4\,\mathbf{a}_2-\left(x_4-\frac{1}{4}\right)\,\mathbf{a}_3$	$=$	$\frac{1}{8}a\,\hat{\mathbf{x}}-a\left(x_4-\frac{1}{4}\right)\,\hat{\mathbf{y}}+\frac{1}{8}a\,\hat{\mathbf{z}}$	(48f)	W I
$\mathbf{B_{21}}$	$=$	$x_4\,\mathbf{a}_1+x_4\,\mathbf{a}_2-\left(x_4-\frac{1}{4}\right)\,\mathbf{a}_3$	$=$	$\frac{1}{8}a\,\hat{\mathbf{x}}+\frac{1}{8}a\,\hat{\mathbf{y}}+ax_4\,\hat{\mathbf{z}}$	(48f)	W I
$\mathbf{B_{22}}$	$=$	$-\left(x_4-\frac{1}{4}\right)\,\mathbf{a}_1-\left(x_4-\frac{1}{4}\right)\,\mathbf{a}_2+x_4\,\mathbf{a}_3$	$=$	$\frac{1}{8}a\,\hat{\mathbf{x}}+\frac{1}{8}a\,\hat{\mathbf{y}}-a\left(x_4-\frac{1}{4}\right)\,\hat{\mathbf{z}}$	(48f)	W I
$\mathbf{B_{23}}$	$=$	$\left(x_4+\frac{3}{4}\right)\,\mathbf{a}_1-x_4\,\mathbf{a}_2+\left(x_4+\frac{3}{4}\right)\,\mathbf{a}_3$	$=$	$\frac{3}{8}a\,\hat{\mathbf{x}}+a\left(x_4+\frac{3}{4}\right)\,\hat{\mathbf{y}}+\frac{3}{8}a\,\hat{\mathbf{z}}$	(48f)	W I
$\mathbf{B_{24}}$	$=$	$-x_4\,\mathbf{a}_1+\left(x_4+\frac{3}{4}\right)\,\mathbf{a}_2-x_4\,\mathbf{a}_3$	$=$	$\frac{3}{8}a\,\hat{\mathbf{x}}-ax_4\,\hat{\mathbf{y}}+\frac{3}{8}a\,\hat{\mathbf{z}}$	(48f)	W I
$\mathbf{B_{25}}$	$=$	$-x_4\,\mathbf{a}_1+\left(x_4+\frac{3}{4}\right)\,\mathbf{a}_2+\left(x_4+\frac{3}{4}\right)\,\mathbf{a}_3$	$=$	$a\left(x_4+\frac{3}{4}\right)\,\hat{\mathbf{x}}+\frac{3}{8}a\,\hat{\mathbf{y}}+\frac{3}{8}a\,\hat{\mathbf{z}}$	(48f)	W I
$\mathbf{B_{26}}$	$=$	$\left(x_4+\frac{3}{4}\right)\,\mathbf{a}_1-x_4\,\mathbf{a}_2-x_4\,\mathbf{a}_3$	$=$	$-ax_4\,\hat{\mathbf{x}}+\frac{3}{8}a\,\hat{\mathbf{y}}+\frac{3}{8}a\,\hat{\mathbf{z}}$	(48f)	W I
$\mathbf{B_{27}}$	$=$	$-x_4\,\mathbf{a}_1-x_4\,\mathbf{a}_2+\left(x_4+\frac{3}{4}\right)\,\mathbf{a}_3$	$=$	$\frac{3}{8}a\,\hat{\mathbf{x}}+\frac{3}{8}a\,\hat{\mathbf{y}}-ax_4\,\hat{\mathbf{z}}$	(48f)	W I
$\mathbf{B_{28}}$	$=$	$\left(x_4+\frac{3}{4}\right)\,\mathbf{a}_1+\left(x_4+\frac{3}{4}\right)\,\mathbf{a}_2-x_4\,\mathbf{a}_3$	$=$	$\frac{3}{8}a\,\hat{\mathbf{x}}+\frac{3}{8}a\,\hat{\mathbf{y}}+a\left(x_4+\frac{3}{4}\right)\,\hat{\mathbf{z}}$	(48f)	W I

References

[1] Q.-B. Yang and S. Andersson, *Application of coincidence site lattices for crystal structure description. Part I:* $\Sigma = 3$, Acta Crystallogr. Sect. B **43**, 1–14 (1987), doi:10.1107/S0108768187098380.

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