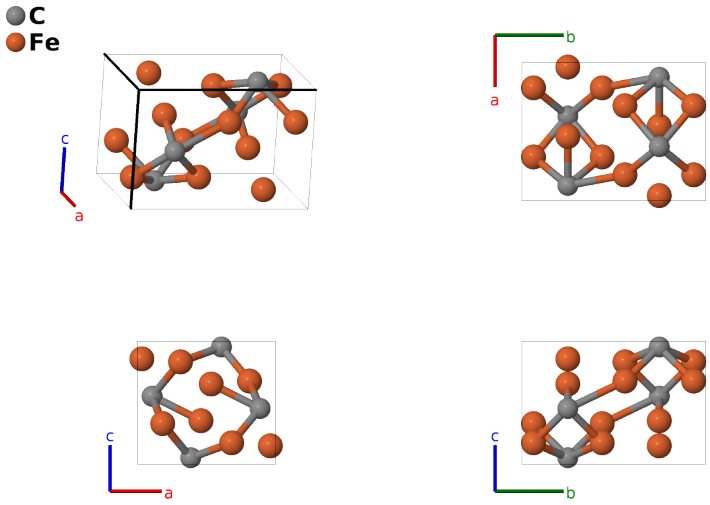
Cementite (Fe_3C, $D0_{11}$) Structure: AB3_oP16_62_c_cd-001

This structure originally had the label `AB3_oP16_62_c_cd`. Calls to that address will be redirected here.

Cite this page as: M. J. Mehl, D. Hicks, C. Toher, O. Levy, R. M. Hanson, G. Hart, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 1*, Comput. Mater. Sci. **136**, S1-828 (2017). doi: 10.1016/j.commatsci.2017.01.017

https://aflow.org/p/KYLC

https://aflow.org/p/AB3_oP16_62_c_cd-001



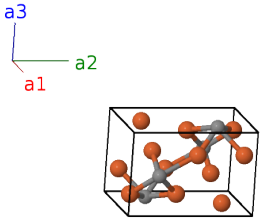
Prototype	CFe_3
AFLOW prototype label	AB3_oP16_62_c_cd-001
***Strukturbericht* designation**	$D0_{11}$
Mineral name	cementite
ICSD	16593
Pearson symbol	oP16
Space group number	62
Space group symbol	*Pnma*
AFLOW prototype command	`aflow --proto=AB3_oP16_62_c_cd-001 --params=`$a, b/a, c/a, x_1, z_1, x_2, z_2, x_3, y_3, z_3$

Other compounds with this structure
Co_3B, Co_3C, La_3Co, Mn_3C, Ni_3B, Ni_3C, Ni_3Y, Pd_3B, Pd_3P, Pd_3Si, Pt_3Si (HT)

- Cementite ($D0_{11}$, Fe_3C) and orthorhombic ClF_3 share the same AFLOW prototype label, AB3_oP16_oP16_c_cd. 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
$\mathbf{B_1}$	=	$x_1\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + z_1\,\mathbf{a}_3$	=	$ax_1\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} + cz_1\,\hat{\mathbf{z}}$	(4c)	C I
$\mathbf{B_2}$	=	$-\left(x_1 - \frac{1}{2}\right)\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 + \left(z_1 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_1 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} + c\left(z_1 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4c)	C I
$\mathbf{B_3}$	=	$-x_1\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 - z_1\,\mathbf{a}_3$	=	$-ax_1\,\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} - cz_1\,\hat{\mathbf{z}}$	(4c)	C I
$\mathbf{B_4}$	=	$\left(x_1 + \frac{1}{2}\right)\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 - \left(z_1 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(x_1 + \frac{1}{2}\right)\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} - c\left(z_1 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4c)	C I
$\mathbf{B_5}$	=	$x_2\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$ax_2\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(4c)	Fe I
$\mathbf{B_6}$	=	$-\left(x_2 - \frac{1}{2}\right)\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 + \left(z_2 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_2 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} + c\left(z_2 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4c)	Fe I
$\mathbf{B_7}$	=	$-x_2\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 - z_2\,\mathbf{a}_3$	=	$-ax_2\,\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} - cz_2\,\hat{\mathbf{z}}$	(4c)	Fe I
$\mathbf{B_8}$	=	$\left(x_2 + \frac{1}{2}\right)\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 - \left(z_2 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(x_2 + \frac{1}{2}\right)\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} - c\left(z_2 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4c)	Fe I
$\mathbf{B_9}$	=	$x_3\,\mathbf{a}_1 + y_3\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} + by_3\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(8d)	Fe II
$\mathbf{B_{10}}$	=	$-\left(x_3 - \frac{1}{2}\right)\,\mathbf{a}_1 - y_3\,\mathbf{a}_2 + \left(z_3 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_3 - \frac{1}{2}\right)\,\hat{\mathbf{x}} - by_3\,\hat{\mathbf{y}} + c\left(z_3 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8d)	Fe II
$\mathbf{B_{11}}$	=	$-x_3\,\mathbf{a}_1 + \left(y_3 + \frac{1}{2}\right)\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} + b\left(y_3 + \frac{1}{2}\right)\,\hat{\mathbf{y}} - cz_3\,\hat{\mathbf{z}}$	(8d)	Fe II
$\mathbf{B_{12}}$	=	$\left(x_3 + \frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_3 - \frac{1}{2}\right)\,\mathbf{a}_2 - \left(z_3 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(x_3 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - b\left(y_3 - \frac{1}{2}\right)\,\hat{\mathbf{y}} - c\left(z_3 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8d)	Fe II
$\mathbf{B_{13}}$	=	$-x_3\,\mathbf{a}_1 - y_3\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} - by_3\,\hat{\mathbf{y}} - cz_3\,\hat{\mathbf{z}}$	(8d)	Fe II
$\mathbf{B_{14}}$	=	$\left(x_3 + \frac{1}{2}\right)\,\mathbf{a}_1 + y_3\,\mathbf{a}_2 - \left(z_3 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(x_3 + \frac{1}{2}\right)\,\hat{\mathbf{x}} + by_3\,\hat{\mathbf{y}} - c\left(z_3 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8d)	Fe II
$\mathbf{B_{15}}$	=	$x_3\,\mathbf{a}_1 - \left(y_3 - \frac{1}{2}\right)\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} - b\left(y_3 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(8d)	Fe II
$\mathbf{B_{16}}$	=	$-\left(x_3 - \frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_3 + \frac{1}{2}\right)\,\mathbf{a}_2 + \left(z_3 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_3 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + b\left(y_3 + \frac{1}{2}\right)\,\hat{\mathbf{y}} + c\left(z_3 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8d)	Fe II

References

[1] F. H. Herbstein and J. Smuts, *Comparison of X-ray and neutron-diffraction refinements of the structure of cementite Fe_3C*, Acta Cryst. **17**, 1331–1332 (1964), doi:10.1107/S0365110X64003346.

Found in

[1] R. T. Downs and M. Hall-Wallace, *The American Mineralogist Crystal Structure Database*, Am. Mineral. **88**, 247–250 (2003).