Fe_4C Structure: AB4_cP5_215_a_e-001

This structure originally had the label `AB4_cP5_215_a_e`. Calls to that address will be redirected here.

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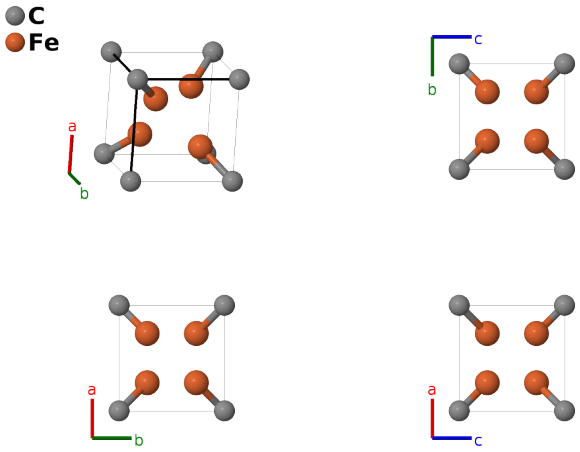
https://aflow.org/p/WNQX

https://aflow.org/p/AB4_cP5_215_a_e-001



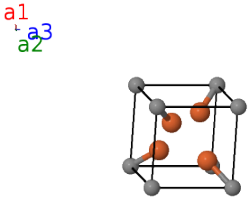
Prototype	CFe_4
AFLOW prototype label	AB4_cP5_215_a_e-001
ICSD	44729
Pearson symbol	cP5
Space group number	215
Space group symbol	$P\bar{4}3m$
AFLOW prototype command	`aflow --proto=AB4_cP5_215_a_e-001 --params=`a, x_2

Other compounds with this structure
Co_4N, Fe_4N, Mn_4N

- When $x_2 = 1/4$ the iron atoms are at the positions of the face-centered cubic lattice. In Fe_4C, x_2 is about 0.265.

Simple Cubic primitive vectors

$$\mathbf{a_1} = a\,\hat{\mathbf{x}}$$
$$\mathbf{a_2} = a\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = a\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(1a)	C I
$\mathbf{B_2}$	=	$x_2\,\mathbf{a}_1 + x_2\,\mathbf{a}_2 + x_2\,\mathbf{a}_3$	=	$ax_2\,\hat{\mathbf{x}} + ax_2\,\hat{\mathbf{y}} + ax_2\,\hat{\mathbf{z}}$	(4e)	Fe I
$\mathbf{B_3}$	=	$-x_2\,\mathbf{a}_1 - x_2\,\mathbf{a}_2 + x_2\,\mathbf{a}_3$	=	$-ax_2\,\hat{\mathbf{x}} - ax_2\,\hat{\mathbf{y}} + ax_2\,\hat{\mathbf{z}}$	(4e)	Fe I
$\mathbf{B_4}$	=	$-x_2\,\mathbf{a}_1 + x_2\,\mathbf{a}_2 - x_2\,\mathbf{a}_3$	=	$-ax_2\,\hat{\mathbf{x}} + ax_2\,\hat{\mathbf{y}} - ax_2\,\hat{\mathbf{z}}$	(4e)	Fe I
$\mathbf{B_5}$	=	$x_2\,\mathbf{a}_1 - x_2\,\mathbf{a}_2 - x_2\,\mathbf{a}_3$	=	$ax_2\,\hat{\mathbf{x}} - ax_2\,\hat{\mathbf{y}} - ax_2\,\hat{\mathbf{z}}$	(4e)	Fe I

References

[1] Z. G. Pinsker and S. V. Kaverin, *Electron-Diffraction Determination of the Structure of Iron Carbide Fe_4C*, Sov. Physics-Crystallogr., translated from Kristallografiya **1**, 48–53 (1956).

Found in

[1] P. Villars and L. Calvert, *Pearson's Handbook of Crystallographic Data for Intermetallic Phases* (ASM International, Materials Park, OH, 1991), 2nd edn.