$ThFe_2SiC$ Structure: AB2CD_oC20_63_a_f_c_c-001

This structure previously used the label(s) `AB2CD_oC20_63_b_f_c_c`. Calls to these addresses will be redirected here.

Cite this page as:

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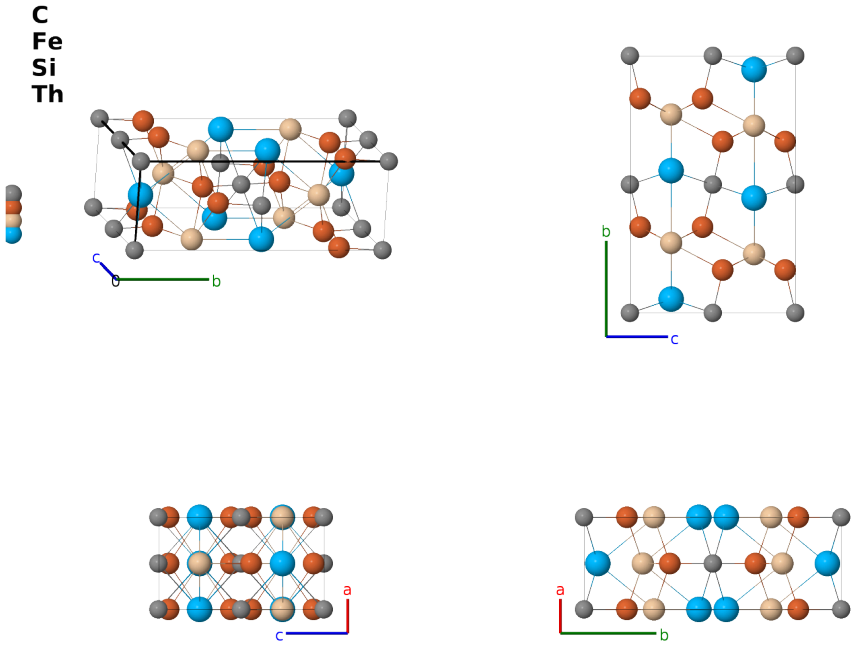
https://aflow.org/prototype-encyclopedia/UF5S

https://aflow.org/prototype-encyclopedia/AB2CD_oC20_63_a_f_c_c-001



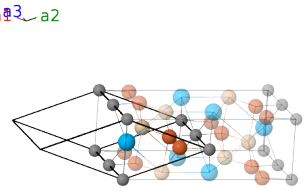
Prototype	CFe_2SiTh
AFLOW prototype label	AB2CD_oC20_63_a_f_c_c-001
ICSD	75133
CCDC	1635799
Pearson symbol	oC20
Space group number	63
Space group symbol	$Cmcm$
AFLOW prototype command	`aflow --proto=AB2CD_oC20_63_a_f_c_c-001 --params=`$a, b/a, c/a, y_2, y_3, y_4, z_4$

Other compounds with this structure
$ErFe_2SiC$, $GdFe_2SiC$, $HoFe_2SiC$, $LuFe_2SiC$, $SmFe_2SiC$, $TbFe_2SiC$, $TmFe_2SiC$, UFe_2SiC, YFe_2SiC

- This structure is a "filled" version of the Re_3B structure, with carbon atoms sitting in the (4b) Wyckoff positions. This is the quaternary version of the structure. The ternary version, where one of the (4c) Wyckoff positions has the same atom type as the (8f) site, is designated the the V_3AsC structure.
- (Witte, 1994) does not designate a prototype for this structure, but as they only give full crystallographic data for the $ThFe_2SiC$ structure we will use this as the prototype.
- (Witte, 1994) lists the occupation of each site as Th (100.2%), Fe (97.7%), Si (96.0%), and C (97.0%), indicating that there are vacancies on the Fe, Si, and C sites, and that some of the Th atoms are either interstitial or occuping the other (4c) site or the (8f) site.

Base-centered Orthorhombic primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(4a)	C I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}c\,\hat{\mathbf{z}}$	(4a)	C I
$\mathbf{B_3}$	=	$-y_2\,\mathbf{a}_1 + y_2\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$by_2\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(4c)	Si I
$\mathbf{B_4}$	=	$y_2\,\mathbf{a}_1 - y_2\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$-by_2\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(4c)	Si I
$\mathbf{B_5}$	=	$-y_3\,\mathbf{a}_1 + y_3\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$by_3\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(4c)	Th I
$\mathbf{B_6}$	=	$y_3\,\mathbf{a}_1 - y_3\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$-by_3\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(4c)	Th I
$\mathbf{B_7}$	=	$-y_4\,\mathbf{a}_1 + y_4\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$by_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(8f)	Fe I
$\mathbf{B_8}$	=	$y_4\,\mathbf{a}_1 - y_4\,\mathbf{a}_2 + \left(z_4 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-by_4\,\hat{\mathbf{y}} + c\left(z_4 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8f)	Fe I
$\mathbf{B_9}$	=	$-y_4\,\mathbf{a}_1 + y_4\,\mathbf{a}_2 - \left(z_4 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$by_4\,\hat{\mathbf{y}} - c\left(z_4 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8f)	Fe I
$\mathbf{B_{10}}$	=	$y_4\,\mathbf{a}_1 - y_4\,\mathbf{a}_2 - z_4\,\mathbf{a}_3$	=	$-by_4\,\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$	(8f)	Fe I

References

[1] A. M. Witte and W. Jeitschko, *Carbides with Filled Re_3B-Type Structure*, J. Solid State Chem. **112**, 232–236 (1994), doi:10.1006/jssc.1994.1297.

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