SiF_4 ($D1_2$) Structure: A4B_cI10_217_c_a-001

This structure previously used the label(s) `A4B_cI10_217_c_a`. Calls to these addresses will be redirected here.

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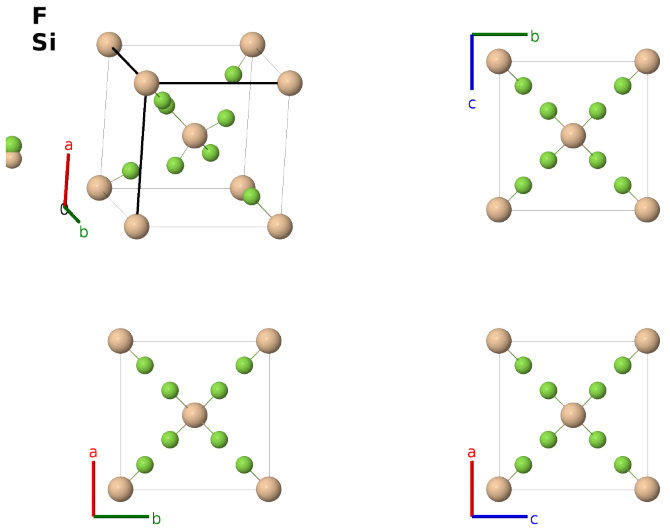
https://aflow.org/prototype-encyclopedia/WBME

https://aflow.org/prototype-encyclopedia/A4B_cI10_217_c_a-001

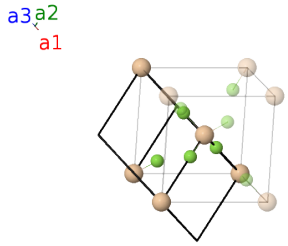


Prototype	F_4Si
AFLOW prototype label	A4B_cI10_217_c_a-001
***Strukturbericht* designation**	$D1_2$
ICSD	14122
CCDC	1595523
Pearson symbol	cI10
Space group number	217
Space group symbol	$I\bar{4}3m$
AFLOW prototype command	`aflow --proto=A4B_cI10_217_c_a-001 --params=`a, x_2

- We determined the lattice constant for this structure from the internal coordinates and the Si-F bond length given in (Atoji, 1954).

Body-centered Cubic primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(2a)	Si I
$\mathbf{B_2}$	=	$2x_2\,\mathbf{a}_1 + 2x_2\,\mathbf{a}_2 + 2x_2\,\mathbf{a}_3$	=	$ax_2\,\hat{\mathbf{x}} + ax_2\,\hat{\mathbf{y}} + ax_2\,\hat{\mathbf{z}}$	(8c)	F I
$\mathbf{B_3}$	=	$-2x_2\,\mathbf{a}_3$	=	$-ax_2\,\hat{\mathbf{x}} - ax_2\,\hat{\mathbf{y}} + ax_2\,\hat{\mathbf{z}}$	(8c)	F I
$\mathbf{B_4}$	=	$-2x_2\,\mathbf{a}_2$	=	$-ax_2\,\hat{\mathbf{x}} + ax_2\,\hat{\mathbf{y}} - ax_2\,\hat{\mathbf{z}}$	(8c)	F I
$\mathbf{B_5}$	=	$-2x_2\,\mathbf{a}_1$	=	$ax_2\,\hat{\mathbf{x}} - ax_2\,\hat{\mathbf{y}} - ax_2\,\hat{\mathbf{z}}$	(8c)	F I

References

[1] M. Atoji and W. N. Lipscomb, *The structure of SiF_4*, Acta Cryst. **7**, 597 (1954), doi:10.1107/S0365110X5400196X.

First cited in

M. J. Mehl, D. Hicks, C. Toher, O. Levy, R. M. Hanson, G. L. W. 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