$CrSi_2$ ($C40$) Structure: AB2_hP9_180_c_i-001

This structure previously used the label(s) `AB2_hP9_180_d_j`. Calls to these addresses will be redirected here.

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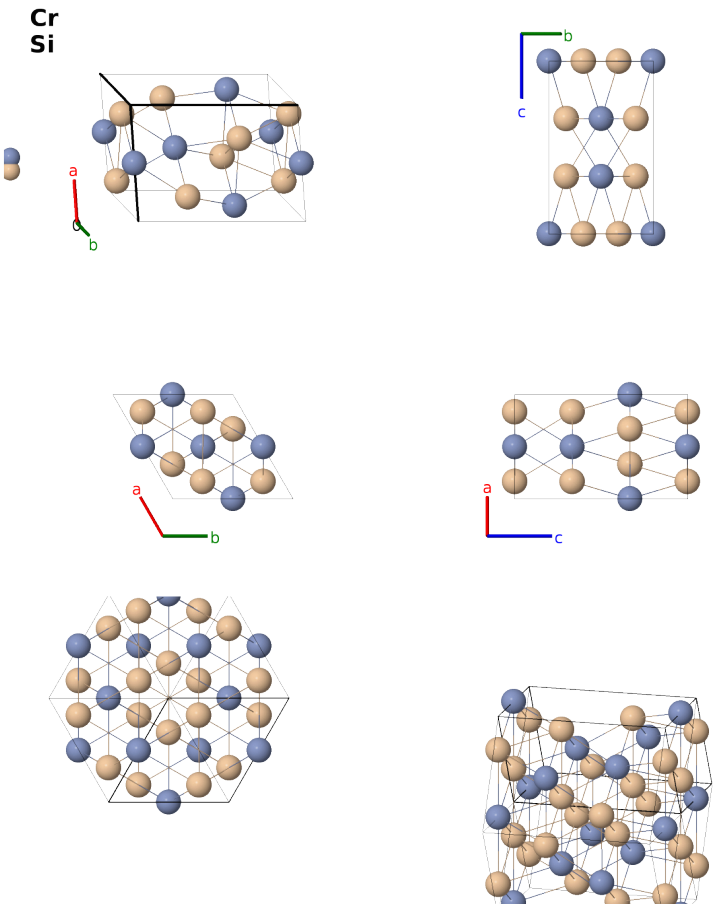
https://aflow.org/prototype-encyclopedia/3K6M

https://aflow.org/prototype-encyclopedia/AB2_hP9_180_c_i-001



Prototype	$CrSi_2$
AFLOW prototype label	AB2_hP9_180_c_i-001
***Strukturbericht* designation**	$C40$
ICSD	161434
CCDC	1677806
Pearson symbol	hP9
Space group number	180

Space group symbol $P6_222$

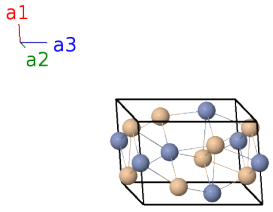
AFLOW prototype command `aflow --proto=AB2_hP9_180_c_i-001 --params=`$a, c/a, x_2$

Other compounds with this structure
$HfSn_2$, $MoSi_2$, $NbGe_2$, $TaGe_2$, $TaSi_2$, VGe_2, VSi_2, WSi_2

- This compound can also be found in the enantiomorphic space group $P6_422$ #181.

Hexagonal primitive vectors

$$\mathbf{a_1} = \frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,\hat{\mathbf{y}}$$
$$\mathbf{a_2} = \frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$\frac{1}{2}\,\mathbf{a}_1$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{4}a\,\hat{\mathbf{y}}$	(3c)	Cr I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_2 + \frac{2}{3}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{4}a\,\hat{\mathbf{y}} + \frac{2}{3}c\,\hat{\mathbf{z}}$	(3c)	Cr I
$\mathbf{B_3}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + \frac{1}{3}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{3}c\,\hat{\mathbf{z}}$	(3c)	Cr I
$\mathbf{B_4}$	=	$x_2\,\mathbf{a}_1 + 2x_2\,\mathbf{a}_2$	=	$\frac{3}{2}ax_2\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_2\,\hat{\mathbf{y}}$	(6i)	Si I
$\mathbf{B_5}$	=	$-2x_2\,\mathbf{a}_1 - x_2\,\mathbf{a}_2 + \frac{2}{3}\,\mathbf{a}_3$	=	$-\frac{3}{2}ax_2\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_2\,\hat{\mathbf{y}} + \frac{2}{3}c\,\hat{\mathbf{z}}$	(6i)	Si I
$\mathbf{B_6}$	=	$x_2\,\mathbf{a}_1 - x_2\,\mathbf{a}_2 + \frac{1}{3}\,\mathbf{a}_3$	=	$-\sqrt{3}ax_2\,\hat{\mathbf{y}} + \frac{1}{3}c\,\hat{\mathbf{z}}$	(6i)	Si I
$\mathbf{B_7}$	=	$-x_2\,\mathbf{a}_1 - 2x_2\,\mathbf{a}_2$	=	$-\frac{3}{2}ax_2\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_2\,\hat{\mathbf{y}}$	(6i)	Si I
$\mathbf{B_8}$	=	$2x_2\,\mathbf{a}_1 + x_2\,\mathbf{a}_2 + \frac{2}{3}\,\mathbf{a}_3$	=	$\frac{3}{2}ax_2\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_2\,\hat{\mathbf{y}} + \frac{2}{3}c\,\hat{\mathbf{z}}$	(6i)	Si I
$\mathbf{B_9}$	=	$-x_2\,\mathbf{a}_1 + x_2\,\mathbf{a}_2 + \frac{1}{3}\,\mathbf{a}_3$	=	$\sqrt{3}ax_2\,\hat{\mathbf{y}} + \frac{1}{3}c\,\hat{\mathbf{z}}$	(6i)	Si I

References

[1] T. Dasgupta, J. Etourneau, B. Chevalier, S. F. Matar, and A. M. Umarji, *Structural, thermal, and electrical properties of $CrSi_2$*, J. Appl. Phys. **103**, 113516 (2008), doi:10.1063/1.2917347.

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