Sc-V (High-Pressure) Structure: A_hP6_178_a-001

This structure originally had the label `A_hP6_178_a`. Calls to that address will be redirected here.

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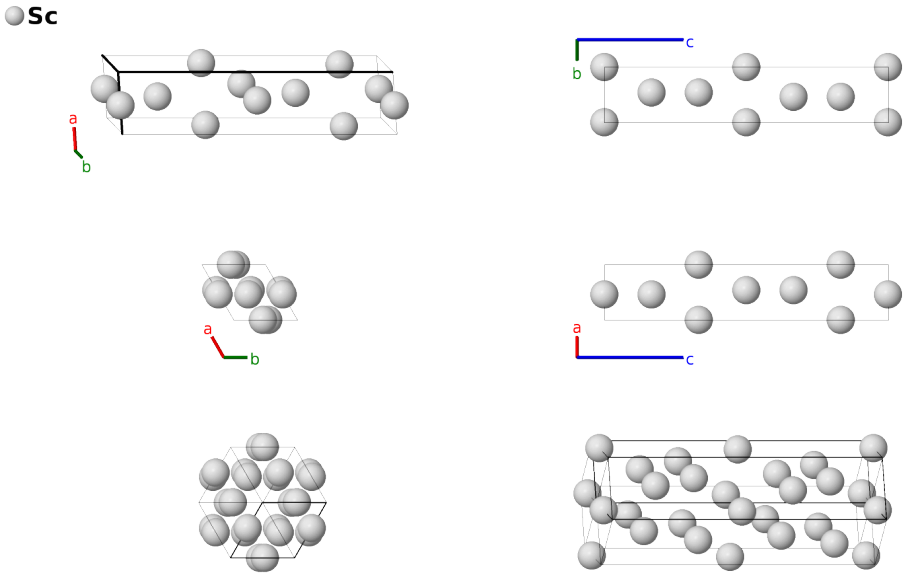
https://aflow.org/p/Z993

https://aflow.org/p/A_hP6_178_a-001

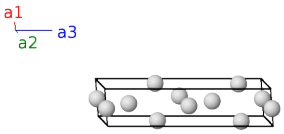


Prototype	Sc
AFLOW prototype label	A_hP6_178_a-001
ICSD	153837
Pearson symbol	hP6
Space group number	178
Space group symbol	$P6_122$
AFLOW prototype command	`aflow --proto=A_hP6_178_a-001 --params=`$a, c/a, x_1$

- This high pressure phase of scandium becomes stable at 240 GPa. We use the experimental data at 242 GPa and 297K. This chiral structure could also have been presented in the enantiomorphic space group $P6_522$ #179.

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
$\mathbf{B_1}$	=	$x_1\,\mathbf{a}_1$	=	$\frac{1}{2}ax_1\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_1\,\hat{\mathbf{y}}$	(6a)	Sc I
$\mathbf{B_2}$	=	$x_1\,\mathbf{a}_2 + \frac{1}{3}\,\mathbf{a}_3$	=	$\frac{1}{2}ax_1\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_1\,\hat{\mathbf{y}} + \frac{1}{3}c\,\hat{\mathbf{z}}$	(6a)	Sc I
$\mathbf{B_3}$	=	$-x_1\,\mathbf{a}_1 - x_1\,\mathbf{a}_2 + \frac{2}{3}\,\mathbf{a}_3$	=	$-ax_1\,\hat{\mathbf{x}} + \frac{2}{3}c\,\hat{\mathbf{z}}$	(6a)	Sc I
$\mathbf{B_4}$	=	$-x_1\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_3$	=	$-\frac{1}{2}ax_1\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_1\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(6a)	Sc I
$\mathbf{B_5}$	=	$-x_1\,\mathbf{a}_2 + \frac{5}{6}\,\mathbf{a}_3$	=	$-\frac{1}{2}ax_1\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_1\,\hat{\mathbf{y}} + \frac{5}{6}c\,\hat{\mathbf{z}}$	(6a)	Sc I
$\mathbf{B_6}$	=	$x_1\,\mathbf{a}_1 + x_1\,\mathbf{a}_2 + \frac{1}{6}\,\mathbf{a}_3$	=	$ax_1\,\hat{\mathbf{x}} + \frac{1}{6}c\,\hat{\mathbf{z}}$	(6a)	Sc I

References

[1] Y. Akahama, H. Fujihisa, and H. Kawamura, *New Helical Chain Structure for Scandium at 240 GPa*, Phys. Rev. Lett. **94**, 195503 (2005), doi:10.1103/PhysRevLett.94.195503.