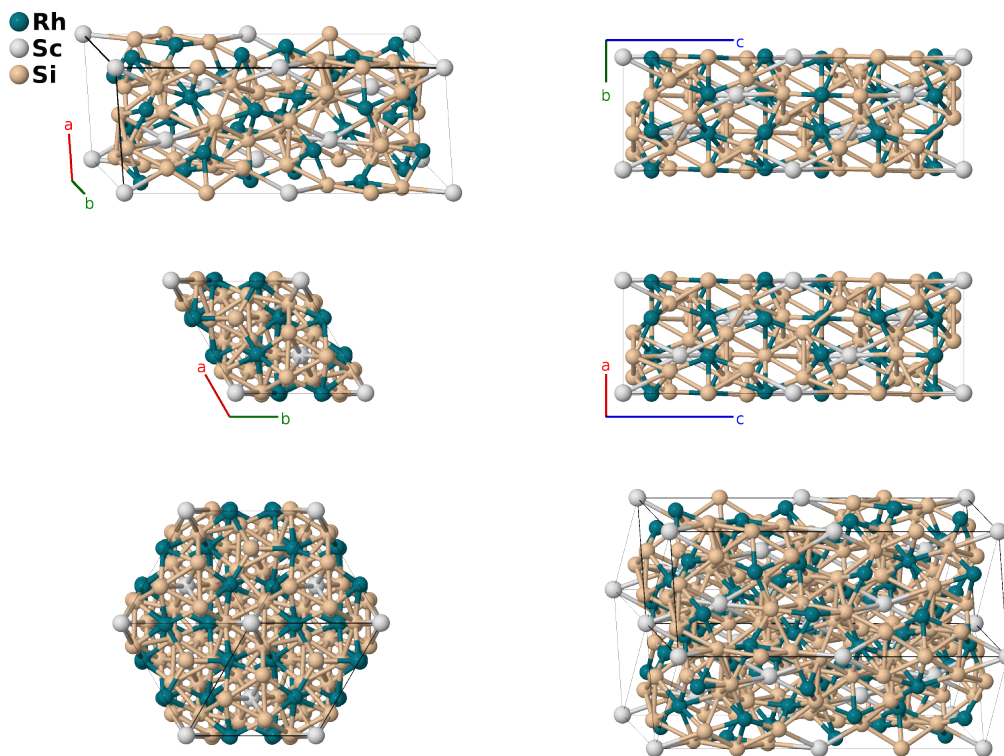


ScRh₃Si₇ Structure: A3BC7_hR22_167_e_b_af-001

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<https://aflow.org/p/NS5K>

https://aflow.org/p/A3BC7_hR22_167_e_b_af-001



Prototype	Rh ₃ ScSi ₇
AFLOW prototype label	A3BC7_hR22_167_e_b_af-001
ICSD	15243
Pearson symbol	hR22
Space group number	167
Space group symbol	$R\bar{3}c$
AFLOW prototype command	<code>aflow --proto=A3BC7_hR22_167_e_b_af-001 --params=a, c/a, x₃, x₄, y₄, z₄</code>

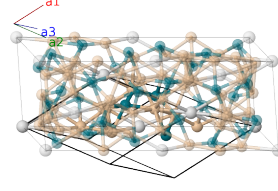
Other compounds with this structure

CeAu₃Al₇, NdAu₃Al₇, PrAu₃Al₇, ScIr₃Si₇, SmAu₃Al₇, YbIr₃Ge₇, YbIr₃Si₇, YbRh₃Si₇

- Hexagonal settings of this structure can be obtained with the option `--hex`.

Rhombohedral primitive vectors

$$\begin{aligned}\mathbf{a}_1 &= \frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + \frac{1}{3}c \hat{\mathbf{z}} \\ \mathbf{a}_2 &= \frac{1}{\sqrt{3}}a \hat{\mathbf{y}} + \frac{1}{3}c \hat{\mathbf{z}} \\ \mathbf{a}_3 &= -\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + \frac{1}{3}c \hat{\mathbf{z}}\end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
\mathbf{B}_1	$= \frac{1}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{4}c \hat{\mathbf{z}}$	(2a)	Si I
\mathbf{B}_2	$= \frac{3}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{3}{4}c \hat{\mathbf{z}}$	(2a)	Si I
\mathbf{B}_3	$= 0$	$=$	0	(2b)	Sc I
\mathbf{B}_4	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2}c \hat{\mathbf{z}}$	(2b)	Sc I
\mathbf{B}_5	$= x_3 \mathbf{a}_1 - (x_3 - \frac{1}{2}) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{8}a (4x_3 - 1) \hat{\mathbf{x}} - \frac{\sqrt{3}}{8}a (4x_3 - 1) \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(6e)	Rh I
\mathbf{B}_6	$= \frac{1}{4} \mathbf{a}_1 + x_3 \mathbf{a}_2 - (x_3 - \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{8}a (4x_3 - 1) \hat{\mathbf{x}} + \frac{\sqrt{3}}{8}a (4x_3 - 1) \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(6e)	Rh I
\mathbf{B}_7	$= -(x_3 - \frac{1}{2}) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + x_3 \mathbf{a}_3$	$=$	$-a (x_3 - \frac{1}{4}) \hat{\mathbf{x}} + \frac{1}{4}c \hat{\mathbf{z}}$	(6e)	Rh I
\mathbf{B}_8	$= -x_3 \mathbf{a}_1 + (x_3 + \frac{1}{2}) \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$-\frac{1}{8}a (4x_3 + 3) \hat{\mathbf{x}} + \frac{\sqrt{3}}{24}a (12x_3 + 1) \hat{\mathbf{y}} + \frac{5}{12}c \hat{\mathbf{z}}$	(6e)	Rh I
\mathbf{B}_9	$= \frac{3}{4} \mathbf{a}_1 - x_3 \mathbf{a}_2 + (x_3 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-\frac{1}{8}a (4x_3 - 1) \hat{\mathbf{x}} - \frac{\sqrt{3}}{24}a (12x_3 + 5) \hat{\mathbf{y}} + \frac{5}{12}c \hat{\mathbf{z}}$	(6e)	Rh I
\mathbf{B}_{10}	$= (x_3 + \frac{1}{2}) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - x_3 \mathbf{a}_3$	$=$	$a (x_3 + \frac{1}{4}) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + \frac{5}{12}c \hat{\mathbf{z}}$	(6e)	Rh I
\mathbf{B}_{11}	$= x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$\frac{1}{2}a (x_4 - z_4) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a (x_4 - 2y_4 + z_4) \hat{\mathbf{y}} + \frac{1}{3}c (x_4 + y_4 + z_4) \hat{\mathbf{z}}$	(12f)	Si II
\mathbf{B}_{12}	$= z_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + y_4 \mathbf{a}_3$	$=$	$-\frac{1}{2}a (y_4 - z_4) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a (2x_4 - y_4 - z_4) \hat{\mathbf{y}} + \frac{1}{3}c (x_4 + y_4 + z_4) \hat{\mathbf{z}}$	(12f)	Si II
\mathbf{B}_{13}	$= y_4 \mathbf{a}_1 + z_4 \mathbf{a}_2 + x_4 \mathbf{a}_3$	$=$	$-\frac{1}{2}a (x_4 - y_4) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a (x_4 + y_4 - 2z_4) \hat{\mathbf{y}} + \frac{1}{3}c (x_4 + y_4 + z_4) \hat{\mathbf{z}}$	(12f)	Si II
\mathbf{B}_{14}	$= -(z_4 - \frac{1}{2}) \mathbf{a}_1 - (y_4 - \frac{1}{2}) \mathbf{a}_2 - (x_4 - \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2}a (x_4 - z_4) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a (x_4 - 2y_4 + z_4) \hat{\mathbf{y}} - \frac{1}{6}c (2x_4 + 2y_4 + 2z_4 - 3) \hat{\mathbf{z}}$	(12f)	Si II
\mathbf{B}_{15}	$= -(y_4 - \frac{1}{2}) \mathbf{a}_1 - (x_4 - \frac{1}{2}) \mathbf{a}_2 - (z_4 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-\frac{1}{2}a (y_4 - z_4) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a (2x_4 - y_4 - z_4) \hat{\mathbf{y}} - \frac{1}{6}c (2x_4 + 2y_4 + 2z_4 - 3) \hat{\mathbf{z}}$	(12f)	Si II
\mathbf{B}_{16}	$= -(x_4 - \frac{1}{2}) \mathbf{a}_1 - (z_4 - \frac{1}{2}) \mathbf{a}_2 - (y_4 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-\frac{1}{2}a (x_4 - y_4) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a (x_4 + y_4 - 2z_4) \hat{\mathbf{y}} - \frac{1}{6}c (2x_4 + 2y_4 + 2z_4 - 3) \hat{\mathbf{z}}$	(12f)	Si II
\mathbf{B}_{17}	$= -x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$-\frac{1}{2}a (x_4 - z_4) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a (x_4 - 2y_4 + z_4) \hat{\mathbf{y}} - \frac{1}{3}c (x_4 + y_4 + z_4) \hat{\mathbf{z}}$	(12f)	Si II
\mathbf{B}_{18}	$= -z_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 - y_4 \mathbf{a}_3$	$=$	$\frac{1}{2}a (y_4 - z_4) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a (2x_4 - y_4 - z_4) \hat{\mathbf{y}} - \frac{1}{3}c (x_4 + y_4 + z_4) \hat{\mathbf{z}}$	(12f)	Si II
\mathbf{B}_{19}	$= -y_4 \mathbf{a}_1 - z_4 \mathbf{a}_2 - x_4 \mathbf{a}_3$	$=$	$\frac{1}{2}a (x_4 - y_4) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a (x_4 + y_4 - 2z_4) \hat{\mathbf{y}} - \frac{1}{3}c (x_4 + y_4 + z_4) \hat{\mathbf{z}}$	(12f)	Si II
\mathbf{B}_{20}	$= (z_4 + \frac{1}{2}) \mathbf{a}_1 + (y_4 + \frac{1}{2}) \mathbf{a}_2 + (x_4 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-\frac{1}{2}a (x_4 - z_4) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a (x_4 - 2y_4 + z_4) \hat{\mathbf{y}} + \frac{1}{6}c (2x_4 + 2y_4 + 2z_4 + 3) \hat{\mathbf{z}}$	(12f)	Si II
\mathbf{B}_{21}	$= (y_4 + \frac{1}{2}) \mathbf{a}_1 + (x_4 + \frac{1}{2}) \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2}a (y_4 - z_4) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a (2x_4 - y_4 - z_4) \hat{\mathbf{y}} + \frac{1}{6}c (2x_4 + 2y_4 + 2z_4 + 3) \hat{\mathbf{z}}$	(12f)	Si II
\mathbf{B}_{22}	$= (x_4 + \frac{1}{2}) \mathbf{a}_1 + (z_4 + \frac{1}{2}) \mathbf{a}_2 + (y_4 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2}a (x_4 - y_4) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a (x_4 + y_4 - 2z_4) \hat{\mathbf{y}} + \frac{1}{6}c (2x_4 + 2y_4 + 2z_4 + 3) \hat{\mathbf{z}}$	(12f)	Si II

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