

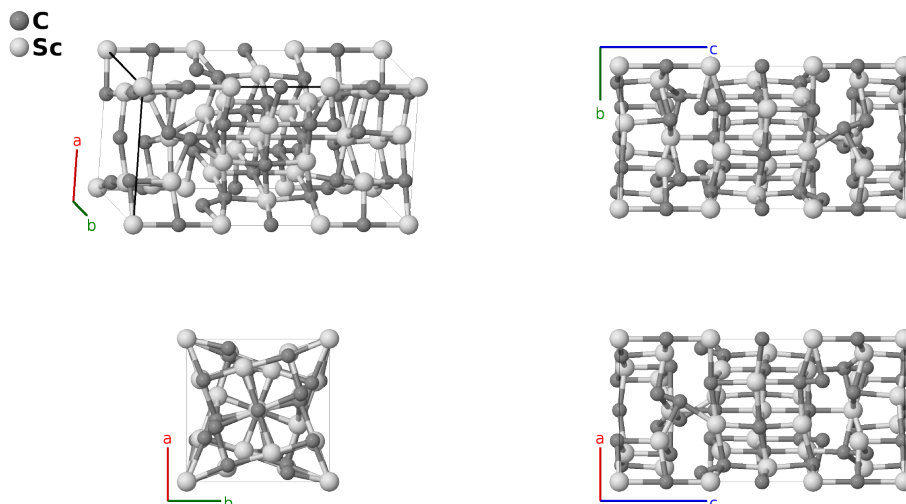
C₁₉Sc₁₅ Structure: A19B15_tP68_114_ac4e_bc3e-001

This structure originally had the label A19B15_tP68_114_bc4e_ac3e. Calls to that address will be redirected here.

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

https://aflow.org/p/A19B15_tP68_114_ac4e_bc3e-001



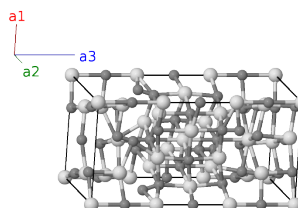
Prototype	C ₁₉ Sc ₁₅
AFLOW prototype label	A19B15_tP68_114_ac4e_bc3e-001
ICSD	42631
Pearson symbol	tP68
Space group number	114
Space group symbol	$P\bar{4}2_1c$
AFLOW prototype command	aflow --proto=A19B15_tP68_114_ac4e_bc3e-001 --params=a, c/a, z ₃ , z ₄ , x ₅ , y ₅ , z ₅ , x ₆ , y ₆ , z ₆ , x ₇ , y ₇ , z ₇ , x ₈ , y ₈ , z ₈ , x ₉ , y ₉ , z ₉ , x ₁₀ , y ₁₀ , z ₁₀ , x ₁₁ , y ₁₁ , z ₁₁

Other compounds with this structure

C₁₉Er₁₅, C₁₉Lu₁₅, C₁₉Tm₁₅, C₁₉Y₁₅, C₁₉Yb₁₅

Simple Tetragonal primitive vectors

$$\begin{aligned} \mathbf{a}_1 &= a \hat{x} \\ \mathbf{a}_2 &= a \hat{y} \\ \mathbf{a}_3 &= c \hat{z} \end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
\mathbf{B}_1	$= 0$	$=$	0	(2a)	C I
\mathbf{B}_2	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(2a)	C I
\mathbf{B}_3	$= \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} c \hat{\mathbf{z}}$	(2b)	Sc I
\mathbf{B}_4	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}}$	(2b)	Sc I
\mathbf{B}_5	$= z_3 \mathbf{a}_3$	$=$	$cz_3 \hat{\mathbf{z}}$	(4c)	C II
\mathbf{B}_6	$= -z_3 \mathbf{a}_3$	$=$	$-cz_3 \hat{\mathbf{z}}$	(4c)	C II
\mathbf{B}_7	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 - (z_3 - \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} - c (z_3 - \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	C II
\mathbf{B}_8	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} + c (z_3 + \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	C II
\mathbf{B}_9	$= z_4 \mathbf{a}_3$	$=$	$cz_4 \hat{\mathbf{z}}$	(4c)	Sc II
\mathbf{B}_{10}	$= -z_4 \mathbf{a}_3$	$=$	$-cz_4 \hat{\mathbf{z}}$	(4c)	Sc II
\mathbf{B}_{11}	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 - (z_4 - \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} - c (z_4 - \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	Sc II
\mathbf{B}_{12}	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} + c (z_4 + \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	Sc II
\mathbf{B}_{13}	$= x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$ax_5 \hat{\mathbf{x}} + ay_5 \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(8e)	C III
\mathbf{B}_{14}	$= -x_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$-ax_5 \hat{\mathbf{x}} - ay_5 \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(8e)	C III
\mathbf{B}_{15}	$= y_5 \mathbf{a}_1 - x_5 \mathbf{a}_2 - z_5 \mathbf{a}_3$	$=$	$ay_5 \hat{\mathbf{x}} - ax_5 \hat{\mathbf{y}} - cz_5 \hat{\mathbf{z}}$	(8e)	C III
\mathbf{B}_{16}	$= -y_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 - z_5 \mathbf{a}_3$	$=$	$-ay_5 \hat{\mathbf{x}} + ax_5 \hat{\mathbf{y}} - cz_5 \hat{\mathbf{z}}$	(8e)	C III
\mathbf{B}_{17}	$= -(x_5 - \frac{1}{2}) \mathbf{a}_1 + (y_5 + \frac{1}{2}) \mathbf{a}_2 - (z_5 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-a (x_5 - \frac{1}{2}) \hat{\mathbf{x}} + a (y_5 + \frac{1}{2}) \hat{\mathbf{y}} - c (z_5 - \frac{1}{2}) \hat{\mathbf{z}}$	(8e)	C III
\mathbf{B}_{18}	$= (x_5 + \frac{1}{2}) \mathbf{a}_1 - (y_5 - \frac{1}{2}) \mathbf{a}_2 - (z_5 - \frac{1}{2}) \mathbf{a}_3$	$=$	$a (x_5 + \frac{1}{2}) \hat{\mathbf{x}} - a (y_5 - \frac{1}{2}) \hat{\mathbf{y}} - c (z_5 - \frac{1}{2}) \hat{\mathbf{z}}$	(8e)	C III
\mathbf{B}_{19}	$= -(y_5 - \frac{1}{2}) \mathbf{a}_1 - (x_5 - \frac{1}{2}) \mathbf{a}_2 + (z_5 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a (y_5 - \frac{1}{2}) \hat{\mathbf{x}} - a (x_5 - \frac{1}{2}) \hat{\mathbf{y}} + c (z_5 + \frac{1}{2}) \hat{\mathbf{z}}$	(8e)	C III
\mathbf{B}_{20}	$= (y_5 + \frac{1}{2}) \mathbf{a}_1 + (x_5 + \frac{1}{2}) \mathbf{a}_2 + (z_5 + \frac{1}{2}) \mathbf{a}_3$	$=$	$a (y_5 + \frac{1}{2}) \hat{\mathbf{x}} + a (x_5 + \frac{1}{2}) \hat{\mathbf{y}} + c (z_5 + \frac{1}{2}) \hat{\mathbf{z}}$	(8e)	C III
\mathbf{B}_{21}	$= x_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$ax_6 \hat{\mathbf{x}} + ay_6 \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}}$	(8e)	C IV
\mathbf{B}_{22}	$= -x_6 \mathbf{a}_1 - y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$-ax_6 \hat{\mathbf{x}} - ay_6 \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}}$	(8e)	C IV
\mathbf{B}_{23}	$= y_6 \mathbf{a}_1 - x_6 \mathbf{a}_2 - z_6 \mathbf{a}_3$	$=$	$ay_6 \hat{\mathbf{x}} - ax_6 \hat{\mathbf{y}} - cz_6 \hat{\mathbf{z}}$	(8e)	C IV
\mathbf{B}_{24}	$= -y_6 \mathbf{a}_1 + x_6 \mathbf{a}_2 - z_6 \mathbf{a}_3$	$=$	$-ay_6 \hat{\mathbf{x}} + ax_6 \hat{\mathbf{y}} - cz_6 \hat{\mathbf{z}}$	(8e)	C IV
\mathbf{B}_{25}	$= -(x_6 - \frac{1}{2}) \mathbf{a}_1 + (y_6 + \frac{1}{2}) \mathbf{a}_2 - (z_6 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-a (x_6 - \frac{1}{2}) \hat{\mathbf{x}} + a (y_6 + \frac{1}{2}) \hat{\mathbf{y}} - c (z_6 - \frac{1}{2}) \hat{\mathbf{z}}$	(8e)	C IV
\mathbf{B}_{26}	$= (x_6 + \frac{1}{2}) \mathbf{a}_1 - (y_6 - \frac{1}{2}) \mathbf{a}_2 - (z_6 - \frac{1}{2}) \mathbf{a}_3$	$=$	$a (x_6 + \frac{1}{2}) \hat{\mathbf{x}} - a (y_6 - \frac{1}{2}) \hat{\mathbf{y}} - c (z_6 - \frac{1}{2}) \hat{\mathbf{z}}$	(8e)	C IV
\mathbf{B}_{27}	$= -(y_6 - \frac{1}{2}) \mathbf{a}_1 - (x_6 - \frac{1}{2}) \mathbf{a}_2 + (z_6 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a (y_6 - \frac{1}{2}) \hat{\mathbf{x}} - a (x_6 - \frac{1}{2}) \hat{\mathbf{y}} + c (z_6 + \frac{1}{2}) \hat{\mathbf{z}}$	(8e)	C IV
\mathbf{B}_{28}	$= (y_6 + \frac{1}{2}) \mathbf{a}_1 + (x_6 + \frac{1}{2}) \mathbf{a}_2 + (z_6 + \frac{1}{2}) \mathbf{a}_3$	$=$	$a (y_6 + \frac{1}{2}) \hat{\mathbf{x}} + a (x_6 + \frac{1}{2}) \hat{\mathbf{y}} + c (z_6 + \frac{1}{2}) \hat{\mathbf{z}}$	(8e)	C IV
\mathbf{B}_{29}	$= x_7 \mathbf{a}_1 + y_7 \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$ax_7 \hat{\mathbf{x}} + ay_7 \hat{\mathbf{y}} + cz_7 \hat{\mathbf{z}}$	(8e)	C V
\mathbf{B}_{30}	$= -x_7 \mathbf{a}_1 - y_7 \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$-ax_7 \hat{\mathbf{x}} - ay_7 \hat{\mathbf{y}} + cz_7 \hat{\mathbf{z}}$	(8e)	C V
\mathbf{B}_{31}	$= y_7 \mathbf{a}_1 - x_7 \mathbf{a}_2 - z_7 \mathbf{a}_3$	$=$	$ay_7 \hat{\mathbf{x}} - ax_7 \hat{\mathbf{y}} - cz_7 \hat{\mathbf{z}}$	(8e)	C V
\mathbf{B}_{32}	$= -y_7 \mathbf{a}_1 + x_7 \mathbf{a}_2 - z_7 \mathbf{a}_3$	$=$	$-ay_7 \hat{\mathbf{x}} + ax_7 \hat{\mathbf{y}} - cz_7 \hat{\mathbf{z}}$	(8e)	C V

$$\begin{aligned}
\mathbf{B}_{62} &= -x_{11} \mathbf{a}_1 - y_{11} \mathbf{a}_2 + z_{11} \mathbf{a}_3 &= & -ax_{11} \hat{\mathbf{x}} - ay_{11} \hat{\mathbf{y}} + cz_{11} \hat{\mathbf{z}} & (8e) & \text{Sc V} \\
\mathbf{B}_{63} &= y_{11} \mathbf{a}_1 - x_{11} \mathbf{a}_2 - z_{11} \mathbf{a}_3 &= & ay_{11} \hat{\mathbf{x}} - ax_{11} \hat{\mathbf{y}} - cz_{11} \hat{\mathbf{z}} & (8e) & \text{Sc V} \\
\mathbf{B}_{64} &= -y_{11} \mathbf{a}_1 + x_{11} \mathbf{a}_2 - z_{11} \mathbf{a}_3 &= & -ay_{11} \hat{\mathbf{x}} + ax_{11} \hat{\mathbf{y}} - cz_{11} \hat{\mathbf{z}} & (8e) & \text{Sc V} \\
\mathbf{B}_{65} &= -\left(x_{11} - \frac{1}{2}\right) \mathbf{a}_1 + \left(y_{11} + \frac{1}{2}\right) \mathbf{a}_2 - &= & -a\left(x_{11} - \frac{1}{2}\right) \hat{\mathbf{x}} + a\left(y_{11} + \frac{1}{2}\right) \hat{\mathbf{y}} - & (8e) & \text{Sc V} \\
&\quad \left(z_{11} - \frac{1}{2}\right) \mathbf{a}_3 && c\left(z_{11} - \frac{1}{2}\right) \hat{\mathbf{z}} \\
\mathbf{B}_{66} &= \left(x_{11} + \frac{1}{2}\right) \mathbf{a}_1 - \left(y_{11} - \frac{1}{2}\right) \mathbf{a}_2 - &= & a\left(x_{11} + \frac{1}{2}\right) \hat{\mathbf{x}} - a\left(y_{11} - \frac{1}{2}\right) \hat{\mathbf{y}} - & (8e) & \text{Sc V} \\
&\quad \left(z_{11} - \frac{1}{2}\right) \mathbf{a}_3 && c\left(z_{11} - \frac{1}{2}\right) \hat{\mathbf{z}} \\
\mathbf{B}_{67} &= -\left(y_{11} - \frac{1}{2}\right) \mathbf{a}_1 - \left(x_{11} - \frac{1}{2}\right) \mathbf{a}_2 + &= & -a\left(y_{11} - \frac{1}{2}\right) \hat{\mathbf{x}} - a\left(x_{11} - \frac{1}{2}\right) \hat{\mathbf{y}} + & (8e) & \text{Sc V} \\
&\quad \left(z_{11} + \frac{1}{2}\right) \mathbf{a}_3 && c\left(z_{11} + \frac{1}{2}\right) \hat{\mathbf{z}} \\
\mathbf{B}_{68} &= \left(y_{11} + \frac{1}{2}\right) \mathbf{a}_1 + \left(x_{11} + \frac{1}{2}\right) \mathbf{a}_2 + &= & a\left(y_{11} + \frac{1}{2}\right) \hat{\mathbf{x}} + a\left(x_{11} + \frac{1}{2}\right) \hat{\mathbf{y}} + & (8e) & \text{Sc V} \\
&\quad \left(z_{11} + \frac{1}{2}\right) \mathbf{a}_3 && c\left(z_{11} + \frac{1}{2}\right) \hat{\mathbf{z}}
\end{aligned}$$

References

- [1] H. Jedlicka, H. Nowotny, and F. Benesovsky, *Zum System Scandium-Kohlenstoff, 2. Mitt.: Kristallstruktur des C-reichen Carbids*, *Monatsh. Chem.* **102**, 389–403 (1971), doi:10.1007/BF00909332.