

C₁₉Sc₁₅ Structure: A19B15_tP68_114_ac4e_bc3e-001

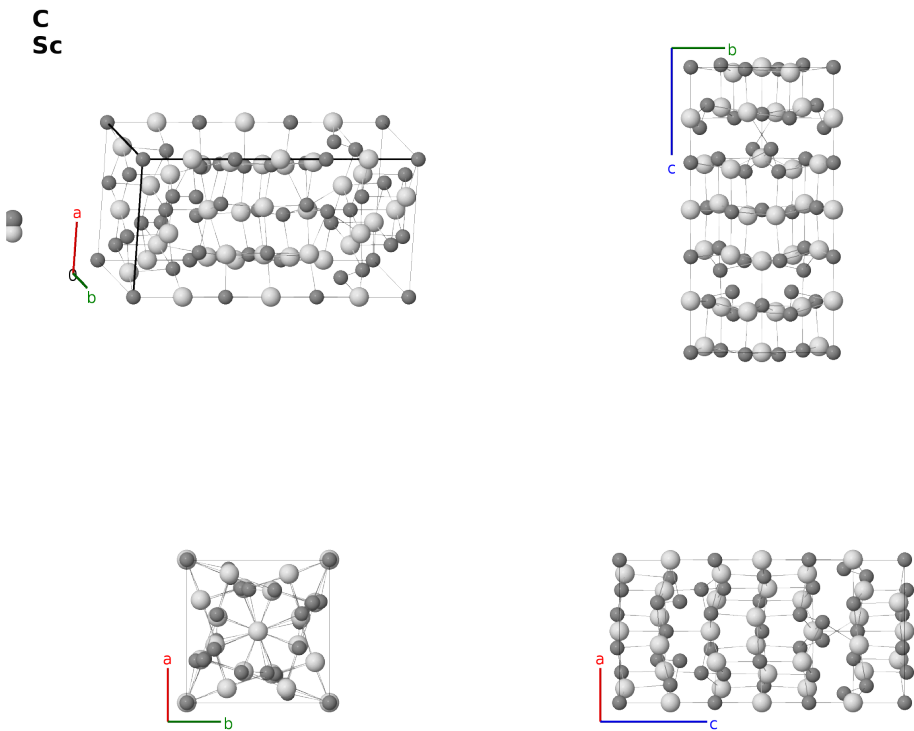
This structure previously used the label(s) **A19B15_tP68_114_bc4e_ac3e**. Calls to these addresses will be redirected here.

Cite this page as:

- H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettel, M. Esters, X. Campilongo, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*, Comput. Mater. Sci. **240**, 112988 (2024), doi: 10.1016/j.commatsci.2024.112988.
- D. Hicks, M. J. Mehl, M. Esters, C. Osos, O. Levy, G. L. W. Hart, C. Toher, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 3*, Comput. Mater. Sci. **199**, 110450 (2021), doi: 10.1016/j.commatsci.2021.110450.

<https://aflow.org/prototype-encyclopedia/PVAV>

https://aflow.org/prototype-encyclopedia/A19B15_tP68_114_ac4e_bc3e-001



Prototype	C ₁₉ Sc ₁₅
AFLOW prototype label	A19B15_tP68_114_ac4e_bc3e-001
ICSD	42631
CCDC	1612277
Pearson symbol	tP68
Space group number	114
Space group symbol	$P\bar{4}_21c$

AFLOW prototype command `aflow --proto=A19B15_tP68_114_ac4e_bc3e-001`
 `--params=a, c/a, z3, z4, x5, y5, z5, x6, y6, z6, x7, y7, z7, x8, y8, z8, x9, y9, z9, x10, y10, z10,`
 `x11, y11, z11`

Other compounds with this structure

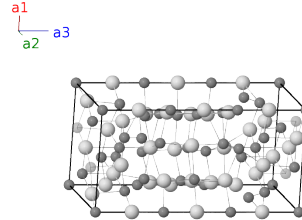
C₁₉Er₁₅, C₁₉Lu₁₅, C₁₉Tm₁₅, C₁₉Y₁₅, C₁₉Yb₁₅

Simple Tetragonal primitive vectors

$$\mathbf{a}_1 = a \hat{\mathbf{x}}$$

$$\mathbf{a}_2 = a \hat{\mathbf{y}}$$

$$\mathbf{a}_3 = c \hat{\mathbf{z}}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$=$	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
$\mathbf{B}_5$	$=$	$z_3 \mathbf{a}_3$	$=$	$c z_3 \hat{\mathbf{z}}$	(4c) C II
$\mathbf{B}_6$	$=$	$-z_3 \mathbf{a}_3$	$=$	$-c z_3 \hat{\mathbf{z}}$	(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
$\mathbf{B}_9$	$=$	$z_4 \mathbf{a}_3$	$=$	$c z_4 \hat{\mathbf{z}}$	(4c) Sc II
$\mathbf{B}_{10}$	$=$	$-z_4 \mathbf{a}_3$	$=$	$-c z_4 \hat{\mathbf{z}}$	(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
$\mathbf{B}_{13}$	$=$	$x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$a x_5 \hat{\mathbf{x}} + a y_5 \hat{\mathbf{y}} + c z_5 \hat{\mathbf{z}}$	(8e) C III
$\mathbf{B}_{14}$	$=$	$-x_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$-a x_5 \hat{\mathbf{x}} - a y_5 \hat{\mathbf{y}} + c z_5 \hat{\mathbf{z}}$	(8e) C III
$\mathbf{B}_{15}$	$=$	$y_5 \mathbf{a}_1 - x_5 \mathbf{a}_2 - z_5 \mathbf{a}_3$	$=$	$a y_5 \hat{\mathbf{x}} - a x_5 \hat{\mathbf{y}} - c z_5 \hat{\mathbf{z}}$	(8e) C III
$\mathbf{B}_{16}$	$=$	$-y_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 - z_5 \mathbf{a}_3$	$=$	$-a y_5 \hat{\mathbf{x}} + a x_5 \hat{\mathbf{y}} - c z_5 \hat{\mathbf{z}}$	(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

$$\begin{aligned}
\mathbf{B}_{51} &= -\left(y_9 - \frac{1}{2}\right) \mathbf{a}_1 - \left(x_9 - \frac{1}{2}\right) \mathbf{a}_2 + \left(z_9 + \frac{1}{2}\right) \mathbf{a}_3 &= -a\left(y_9 - \frac{1}{2}\right) \hat{\mathbf{x}} - a\left(x_9 - \frac{1}{2}\right) \hat{\mathbf{y}} + c\left(z_9 + \frac{1}{2}\right) \hat{\mathbf{z}} &(8e) &\text{Sc III} \\
\mathbf{B}_{52} &= \left(y_9 + \frac{1}{2}\right) \mathbf{a}_1 + \left(x_9 + \frac{1}{2}\right) \mathbf{a}_2 + \left(z_9 + \frac{1}{2}\right) \mathbf{a}_3 &= a\left(y_9 + \frac{1}{2}\right) \hat{\mathbf{x}} + a\left(x_9 + \frac{1}{2}\right) \hat{\mathbf{y}} + c\left(z_9 + \frac{1}{2}\right) \hat{\mathbf{z}} &(8e) &\text{Sc III} \\
\mathbf{B}_{53} &= x_{10} \mathbf{a}_1 + y_{10} \mathbf{a}_2 + z_{10} \mathbf{a}_3 &= ax_{10} \hat{\mathbf{x}} + ay_{10} \hat{\mathbf{y}} + cz_{10} \hat{\mathbf{z}} &(8e) &\text{Sc IV} \\
\mathbf{B}_{54} &= -x_{10} \mathbf{a}_1 - y_{10} \mathbf{a}_2 + z_{10} \mathbf{a}_3 &= -ax_{10} \hat{\mathbf{x}} - ay_{10} \hat{\mathbf{y}} + cz_{10} \hat{\mathbf{z}} &(8e) &\text{Sc IV} \\
\mathbf{B}_{55} &= y_{10} \mathbf{a}_1 - x_{10} \mathbf{a}_2 - z_{10} \mathbf{a}_3 &= ay_{10} \hat{\mathbf{x}} - ax_{10} \hat{\mathbf{y}} - cz_{10} \hat{\mathbf{z}} &(8e) &\text{Sc IV} \\
\mathbf{B}_{56} &= -y_{10} \mathbf{a}_1 + x_{10} \mathbf{a}_2 - z_{10} \mathbf{a}_3 &= -ay_{10} \hat{\mathbf{x}} + ax_{10} \hat{\mathbf{y}} - cz_{10} \hat{\mathbf{z}} &(8e) &\text{Sc IV} \\
\mathbf{B}_{57} &= -\left(x_{10} - \frac{1}{2}\right) \mathbf{a}_1 + \left(y_{10} + \frac{1}{2}\right) \mathbf{a}_2 - \left(z_{10} - \frac{1}{2}\right) \mathbf{a}_3 &= -a\left(x_{10} - \frac{1}{2}\right) \hat{\mathbf{x}} + a\left(y_{10} + \frac{1}{2}\right) \hat{\mathbf{y}} - c\left(z_{10} - \frac{1}{2}\right) \hat{\mathbf{z}} &(8e) &\text{Sc IV} \\
\mathbf{B}_{58} &= \left(x_{10} + \frac{1}{2}\right) \mathbf{a}_1 - \left(y_{10} - \frac{1}{2}\right) \mathbf{a}_2 - \left(z_{10} - \frac{1}{2}\right) \mathbf{a}_3 &= a\left(x_{10} + \frac{1}{2}\right) \hat{\mathbf{x}} - a\left(y_{10} - \frac{1}{2}\right) \hat{\mathbf{y}} - c\left(z_{10} - \frac{1}{2}\right) \hat{\mathbf{z}} &(8e) &\text{Sc IV} \\
\mathbf{B}_{59} &= -\left(y_{10} - \frac{1}{2}\right) \mathbf{a}_1 - \left(x_{10} - \frac{1}{2}\right) \mathbf{a}_2 + \left(z_{10} + \frac{1}{2}\right) \mathbf{a}_3 &= -a\left(y_{10} - \frac{1}{2}\right) \hat{\mathbf{x}} - a\left(x_{10} - \frac{1}{2}\right) \hat{\mathbf{y}} + c\left(z_{10} + \frac{1}{2}\right) \hat{\mathbf{z}} &(8e) &\text{Sc IV} \\
\mathbf{B}_{60} &= \left(y_{10} + \frac{1}{2}\right) \mathbf{a}_1 + \left(x_{10} + \frac{1}{2}\right) \mathbf{a}_2 + \left(z_{10} + \frac{1}{2}\right) \mathbf{a}_3 &= a\left(y_{10} + \frac{1}{2}\right) \hat{\mathbf{x}} + a\left(x_{10} + \frac{1}{2}\right) \hat{\mathbf{y}} + c\left(z_{10} + \frac{1}{2}\right) \hat{\mathbf{z}} &(8e) &\text{Sc IV} \\
\mathbf{B}_{61} &= 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}_{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 - \left(z_{11} - \frac{1}{2}\right) \mathbf{a}_3 &= -a\left(x_{11} - \frac{1}{2}\right) \hat{\mathbf{x}} + a\left(y_{11} + \frac{1}{2}\right) \hat{\mathbf{y}} - c\left(z_{11} - \frac{1}{2}\right) \hat{\mathbf{z}} &(8e) &\text{Sc V} \\
\mathbf{B}_{66} &= \left(x_{11} + \frac{1}{2}\right) \mathbf{a}_1 - \left(y_{11} - \frac{1}{2}\right) \mathbf{a}_2 - \left(z_{11} - \frac{1}{2}\right) \mathbf{a}_3 &= a\left(x_{11} + \frac{1}{2}\right) \hat{\mathbf{x}} - a\left(y_{11} - \frac{1}{2}\right) \hat{\mathbf{y}} - c\left(z_{11} - \frac{1}{2}\right) \hat{\mathbf{z}} &(8e) &\text{Sc V} \\
\mathbf{B}_{67} &= -\left(y_{11} - \frac{1}{2}\right) \mathbf{a}_1 - \left(x_{11} - \frac{1}{2}\right) \mathbf{a}_2 + \left(z_{11} + \frac{1}{2}\right) \mathbf{a}_3 &= -a\left(y_{11} - \frac{1}{2}\right) \hat{\mathbf{x}} - a\left(x_{11} - \frac{1}{2}\right) \hat{\mathbf{y}} + c\left(z_{11} + \frac{1}{2}\right) \hat{\mathbf{z}} &(8e) &\text{Sc V} \\
\mathbf{B}_{68} &= \left(y_{11} + \frac{1}{2}\right) \mathbf{a}_1 + \left(x_{11} + \frac{1}{2}\right) \mathbf{a}_2 + \left(z_{11} + \frac{1}{2}\right) \mathbf{a}_3 &= a\left(y_{11} + \frac{1}{2}\right) \hat{\mathbf{x}} + a\left(x_{11} + \frac{1}{2}\right) \hat{\mathbf{y}} + c\left(z_{11} + \frac{1}{2}\right) \hat{\mathbf{z}} &(8e) &\text{Sc V}
\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.

First cited in

D. Hicks, M. J. Mehl, M. Esters, C. Osos, O. Levy, G. L. W. Hart, C. Toher, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 3*, Comput. Mater. Sci. **199**, 110450 (2021), doi: 10.1016/j.commatsci.2021.110450.