

V₆C₅ Structure:

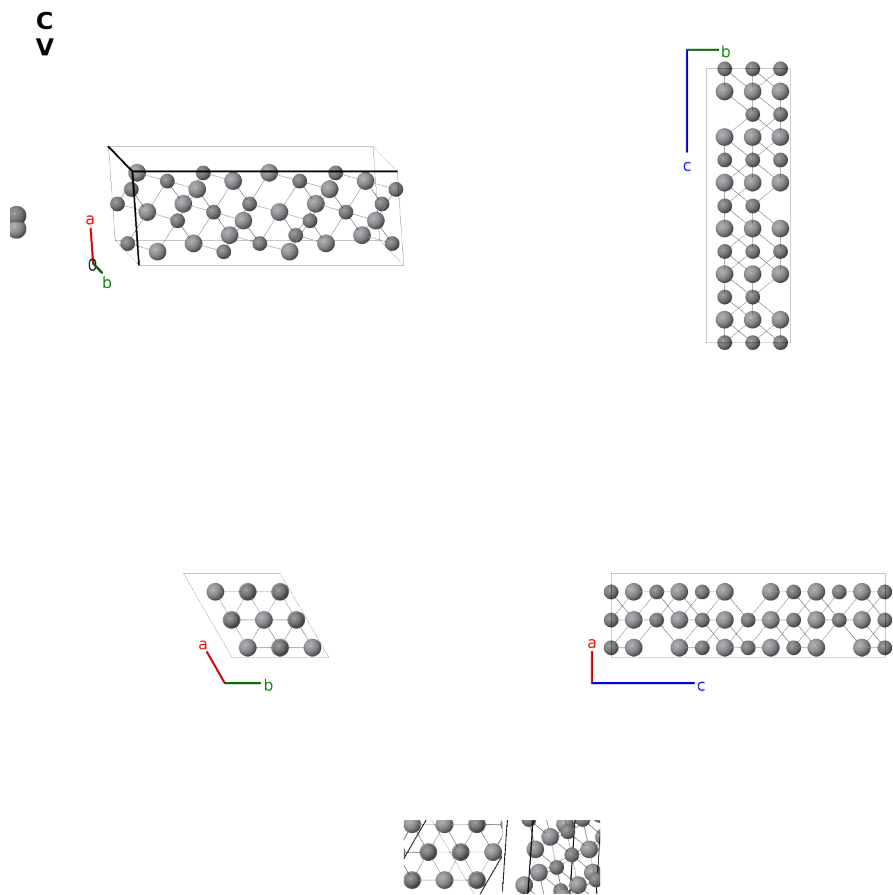
A5B6_hP33_151_3a2b_3c-001

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- 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/V1KT>

https://aflow.org/prototype-encyclopedia/A5B6_hP33_151_3a2b_3c-001

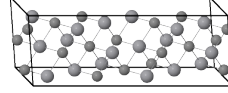


Prototype	C ₅ V ₆
AFLOW prototype label	A5B6_hP33_151_3a2b_3c-001
ICSD	654841
CCDC	1765779
Pearson symbol	hP33
Space group number	151
Space group symbol	$P3_112$
AFLOW prototype command	<code>aflow --proto=A5B6_hP33_151_3a2b_3c-001</code> <code>--params=a, c/a, x₁, x₂, x₃, x₄, x₅, x₆, y₆, z₆, x₇, y₇, z₇, x₈, y₈, z₈</code>

- This is the CuPt ($L1_1$) structure with one of every six carbon atoms removed. Placing carbon atoms on another (3a) site with $x = 1/9$ will restore the $L1_1$ structure.
- (Venables, 1968) put this structure in space group $P3_1$ #144 or its enantiomorph $P3_2$ #145. (Cenzual, 1991) showed that with the given coordinates the space group is actually $P3_1$ #151.

Trigonal (Hexagonal) primitive vectors

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



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= x_1 \mathbf{a}_1 - x_1 \mathbf{a}_2 + \frac{1}{3} \mathbf{a}_3$	$=$	$-\sqrt{3}ax_1 \hat{\mathbf{y}} + \frac{1}{3}c \hat{\mathbf{z}}$	(3a)	C I
$\mathbf{B}_2$	$= x_1 \mathbf{a}_1 + 2x_1 \mathbf{a}_2 + \frac{2}{3} \mathbf{a}_3$	$=$	$\frac{3}{2}ax_1 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_1 \hat{\mathbf{y}} + \frac{2}{3}c \hat{\mathbf{z}}$	(3a)	C I
$\mathbf{B}_3$	$= -2x_1 \mathbf{a}_1 - x_1 \mathbf{a}_2$	$=$	$-\frac{3}{2}ax_1 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_1 \hat{\mathbf{y}}$	(3a)	C I
$\mathbf{B}_4$	$= x_2 \mathbf{a}_1 - x_2 \mathbf{a}_2 + \frac{1}{3} \mathbf{a}_3$	$=$	$-\sqrt{3}ax_2 \hat{\mathbf{y}} + \frac{1}{3}c \hat{\mathbf{z}}$	(3a)	C II
$\mathbf{B}_5$	$= x_2 \mathbf{a}_1 + 2x_2 \mathbf{a}_2 + \frac{2}{3} \mathbf{a}_3$	$=$	$\frac{3}{2}ax_2 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_2 \hat{\mathbf{y}} + \frac{2}{3}c \hat{\mathbf{z}}$	(3a)	C II
$\mathbf{B}_6$	$= -2x_2 \mathbf{a}_1 - x_2 \mathbf{a}_2$	$=$	$-\frac{3}{2}ax_2 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_2 \hat{\mathbf{y}}$	(3a)	C II
$\mathbf{B}_7$	$= x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 + \frac{1}{3} \mathbf{a}_3$	$=$	$-\sqrt{3}ax_3 \hat{\mathbf{y}} + \frac{1}{3}c \hat{\mathbf{z}}$	(3a)	C III
$\mathbf{B}_8$	$= x_3 \mathbf{a}_1 + 2x_3 \mathbf{a}_2 + \frac{2}{3} \mathbf{a}_3$	$=$	$\frac{3}{2}ax_3 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_3 \hat{\mathbf{y}} + \frac{2}{3}c \hat{\mathbf{z}}$	(3a)	C III
$\mathbf{B}_9$	$= -2x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2$	$=$	$-\frac{3}{2}ax_3 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_3 \hat{\mathbf{y}}$	(3a)	C III
$\mathbf{B}_{10}$	$= x_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 + \frac{5}{6} \mathbf{a}_3$	$=$	$-\sqrt{3}ax_4 \hat{\mathbf{y}} + \frac{5}{6}c \hat{\mathbf{z}}$	(3b)	C IV
$\mathbf{B}_{11}$	$= x_4 \mathbf{a}_1 + 2x_4 \mathbf{a}_2 + \frac{1}{6} \mathbf{a}_3$	$=$	$\frac{3}{2}ax_4 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_4 \hat{\mathbf{y}} + \frac{1}{6}c \hat{\mathbf{z}}$	(3b)	C IV
$\mathbf{B}_{12}$	$= -2x_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-\frac{3}{2}ax_4 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_4 \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(3b)	C IV
$\mathbf{B}_{13}$	$= x_5 \mathbf{a}_1 - x_5 \mathbf{a}_2 + \frac{5}{6} \mathbf{a}_3$	$=$	$-\sqrt{3}ax_5 \hat{\mathbf{y}} + \frac{5}{6}c \hat{\mathbf{z}}$	(3b)	C V
$\mathbf{B}_{14}$	$= x_5 \mathbf{a}_1 + 2x_5 \mathbf{a}_2 + \frac{1}{6} \mathbf{a}_3$	$=$	$\frac{3}{2}ax_5 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_5 \hat{\mathbf{y}} + \frac{1}{6}c \hat{\mathbf{z}}$	(3b)	C V
$\mathbf{B}_{15}$	$= -2x_5 \mathbf{a}_1 - x_5 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-\frac{3}{2}ax_5 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_5 \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(3b)	C V
$\mathbf{B}_{16}$	$= x_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_6 + y_6) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a(x_6 - y_6) \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}}$	(6c)	V I
$\mathbf{B}_{17}$	$= -y_6 \mathbf{a}_1 + (x_6 - y_6) \mathbf{a}_2 + (z_6 + \frac{1}{3}) \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_6 - 2y_6) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_6 \hat{\mathbf{y}} + c(z_6 + \frac{1}{3}) \hat{\mathbf{z}}$	(6c)	V I
$\mathbf{B}_{18}$	$= -(x_6 - y_6) \mathbf{a}_1 - x_6 \mathbf{a}_2 + (z_6 + \frac{2}{3}) \mathbf{a}_3$	$=$	$-\frac{1}{2}a(2x_6 - y_6) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_6 \hat{\mathbf{y}} + \frac{1}{3}c(3z_6 + 2) \hat{\mathbf{z}}$	(6c)	V I
$\mathbf{B}_{19}$	$= -y_6 \mathbf{a}_1 - x_6 \mathbf{a}_2 - (z_6 - \frac{2}{3}) \mathbf{a}_3$	$=$	$-\frac{1}{2}a(x_6 + y_6) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a(x_6 - y_6) \hat{\mathbf{y}} - \frac{1}{3}c(3z_6 - 2) \hat{\mathbf{z}}$	(6c)	V I
$\mathbf{B}_{20}$	$= -(x_6 - y_6) \mathbf{a}_1 + y_6 \mathbf{a}_2 - (z_6 - \frac{1}{3}) \mathbf{a}_3$	$=$	$\frac{1}{2}a(-x_6 + 2y_6) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_6 \hat{\mathbf{y}} - c(z_6 - \frac{1}{3}) \hat{\mathbf{z}}$	(6c)	V I

$$\begin{aligned}
\mathbf{B}_{21} &= x_6 \mathbf{a}_1 + (x_6 - y_6) \mathbf{a}_2 - z_6 \mathbf{a}_3 &= \frac{1}{2}a(2x_6 - y_6) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_6 \hat{\mathbf{y}} - cz_6 \hat{\mathbf{z}} &(6c) & \text{V I} \\
\mathbf{B}_{22} &= x_7 \mathbf{a}_1 + y_7 \mathbf{a}_2 + z_7 \mathbf{a}_3 &= \frac{1}{2}a(x_7 + y_7) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a(x_7 - y_7) \hat{\mathbf{y}} + cz_7 \hat{\mathbf{z}} &(6c) & \text{V II} \\
\mathbf{B}_{23} &= -y_7 \mathbf{a}_1 + (x_7 - y_7) \mathbf{a}_2 + (z_7 + \frac{1}{3}) \mathbf{a}_3 &= \frac{1}{2}a(x_7 - 2y_7) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_7 \hat{\mathbf{y}} + c(z_7 + \frac{1}{3}) \hat{\mathbf{z}} &(6c) & \text{V II} \\
\mathbf{B}_{24} &= -(x_7 - y_7) \mathbf{a}_1 - x_7 \mathbf{a}_2 + (z_7 + \frac{2}{3}) \mathbf{a}_3 &= -\frac{1}{2}a(2x_7 - y_7) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_7 \hat{\mathbf{y}} + \frac{1}{3}c(3z_7 + 2) \hat{\mathbf{z}} &(6c) & \text{V II} \\
\mathbf{B}_{25} &= -y_7 \mathbf{a}_1 - x_7 \mathbf{a}_2 - (z_7 - \frac{2}{3}) \mathbf{a}_3 &= -\frac{1}{2}a(x_7 + y_7) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a(x_7 - y_7) \hat{\mathbf{y}} - \frac{1}{3}c(3z_7 - 2) \hat{\mathbf{z}} &(6c) & \text{V II} \\
\mathbf{B}_{26} &= -(x_7 - y_7) \mathbf{a}_1 + y_7 \mathbf{a}_2 - (z_7 - \frac{1}{3}) \mathbf{a}_3 &= \frac{1}{2}a(-x_7 + 2y_7) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_7 \hat{\mathbf{y}} - c(z_7 - \frac{1}{3}) \hat{\mathbf{z}} &(6c) & \text{V II} \\
\mathbf{B}_{27} &= x_7 \mathbf{a}_1 + (x_7 - y_7) \mathbf{a}_2 - z_7 \mathbf{a}_3 &= \frac{1}{2}a(2x_7 - y_7) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_7 \hat{\mathbf{y}} - cz_7 \hat{\mathbf{z}} &(6c) & \text{V II} \\
\mathbf{B}_{28} &= x_8 \mathbf{a}_1 + y_8 \mathbf{a}_2 + z_8 \mathbf{a}_3 &= \frac{1}{2}a(x_8 + y_8) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a(x_8 - y_8) \hat{\mathbf{y}} + cz_8 \hat{\mathbf{z}} &(6c) & \text{V III} \\
\mathbf{B}_{29} &= -y_8 \mathbf{a}_1 + (x_8 - y_8) \mathbf{a}_2 + (z_8 + \frac{1}{3}) \mathbf{a}_3 &= \frac{1}{2}a(x_8 - 2y_8) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_8 \hat{\mathbf{y}} + c(z_8 + \frac{1}{3}) \hat{\mathbf{z}} &(6c) & \text{V III} \\
\mathbf{B}_{30} &= -(x_8 - y_8) \mathbf{a}_1 - x_8 \mathbf{a}_2 + (z_8 + \frac{2}{3}) \mathbf{a}_3 &= -\frac{1}{2}a(2x_8 - y_8) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_8 \hat{\mathbf{y}} + \frac{1}{3}c(3z_8 + 2) \hat{\mathbf{z}} &(6c) & \text{V III} \\
\mathbf{B}_{31} &= -y_8 \mathbf{a}_1 - x_8 \mathbf{a}_2 - (z_8 - \frac{2}{3}) \mathbf{a}_3 &= -\frac{1}{2}a(x_8 + y_8) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a(x_8 - y_8) \hat{\mathbf{y}} - \frac{1}{3}c(3z_8 - 2) \hat{\mathbf{z}} &(6c) & \text{V III} \\
\mathbf{B}_{32} &= -(x_8 - y_8) \mathbf{a}_1 + y_8 \mathbf{a}_2 - (z_8 - \frac{1}{3}) \mathbf{a}_3 &= \frac{1}{2}a(-x_8 + 2y_8) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_8 \hat{\mathbf{y}} - c(z_8 - \frac{1}{3}) \hat{\mathbf{z}} &(6c) & \text{V III} \\
\mathbf{B}_{33} &= x_8 \mathbf{a}_1 + (x_8 - y_8) \mathbf{a}_2 - z_8 \mathbf{a}_3 &= \frac{1}{2}a(2x_8 - y_8) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_8 \hat{\mathbf{y}} - cz_8 \hat{\mathbf{z}} &(6c) & \text{V III}
\end{aligned}$$

References

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Found in

- [1] K. Cenzual, L. M. Gelato, M. Penzo, and E. Parthé, *Inorganic structure types with revised space groups. I*, Acta Crystallogr. Sect. B **47**, 433–439 (1991), doi:10.1107/S0108768191000903.

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