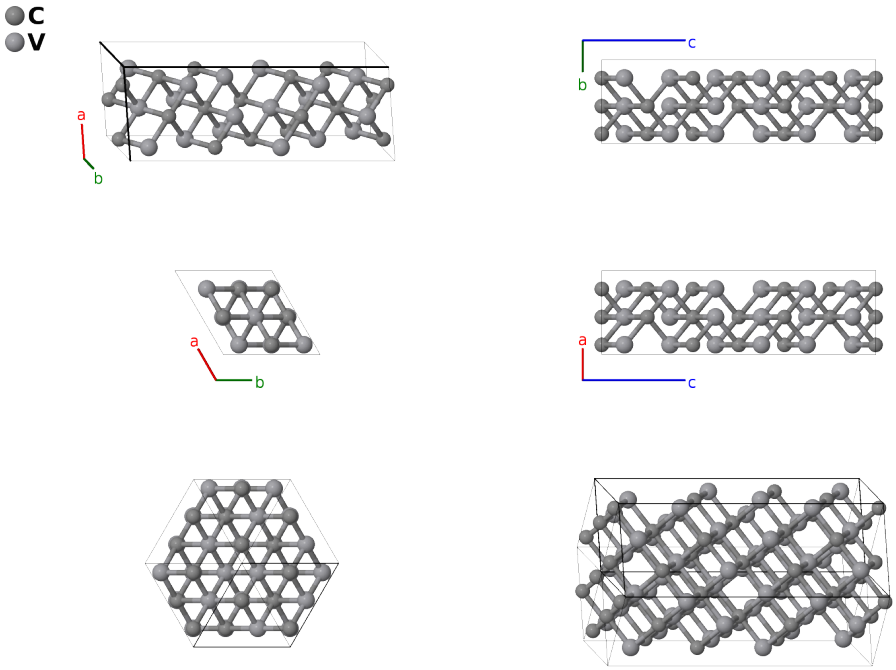
V_6C_5 Structure: A5B6_hP33_151_3a2b_3c-001

Cite this page as: H. Eckert, S. Divilov, A. Zettel, M. J. Mehl, D. Hicks, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*. In preparation.

https://aflow.org/p/V1KT

https://aflow.org/p/A5B6_hP33_151_3a2b_3c-001

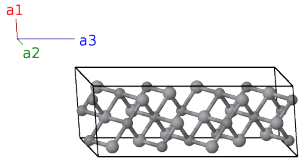


Prototype	C_5V_6
AFLOW prototype label	A5B6_hP33_151_3a2b_3c-001
ICSD	654841
Pearson symbol	hP33
Space group number	151
Space group symbol	$P3_112$
AFLOW prototype command	`aflow --proto=A5B6_hP33_151_3a2b_3c-001 --params=`$a, c/a, x_1, x_2, x_3, x_4, x_5, x_6, y_6, z_6, x_7, y_7, z_7, x_8, y_8, z_8$

- 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 $P3_112$ #151.

Trigonal (Hexagonal) primitive vectors

$$
\begin{aligned}
\mathbf{a_1} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}a\,\hat{\mathbf{y}} \\
\mathbf{a_2} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}a\,\hat{\mathbf{y}} \\
\mathbf{a_3} &= c\,\hat{\mathbf{z}}
\end{aligned}
$$



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
$\mathbf{B_{17}}$	=	$-y_6\,\mathbf{a}_1 + (x_6 - y_6)\,\mathbf{a}_2 + \left(z_6 + \frac{1}{3}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_6 - 2y_6)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_6\,\hat{\mathbf{y}} + c\left(z_6 + \frac{1}{3}\right)\,\hat{\mathbf{z}}$	(6c)	V I
$\mathbf{B_{18}}$	=	$-(x_6 - y_6)\,\mathbf{a}_1 - x_6\,\mathbf{a}_2 + \left(z_6 + \frac{2}{3}\right)\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(2x_6 - y_6)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_6\,\hat{\mathbf{y}} + \frac{1}{3}c\,(3z_6 + 2)\,\hat{\mathbf{z}}$	(6c)	V I
$\mathbf{B_{19}}$	=	$-y_6\,\mathbf{a}_1 - x_6\,\mathbf{a}_2 - \left(z_6 - \frac{2}{3}\right)\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(x_6 + y_6)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,(x_6 - y_6)\,\hat{\mathbf{y}} - \frac{1}{3}c\,(3z_6 - 2)\,\hat{\mathbf{z}}$	(6c)	V I
$\mathbf{B_{20}}$	=	$-(x_6 - y_6)\,\mathbf{a}_1 + y_6\,\mathbf{a}_2 - \left(z_6 - \frac{1}{3}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(-x_6 + 2y_6)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_6\,\hat{\mathbf{y}} - c\left(z_6 - \frac{1}{3}\right)\,\hat{\mathbf{z}}$	(6c)	V I
$\mathbf{B_{21}}$	=	$x_6\,\mathbf{a}_1 + (x_6 - y_6)\,\mathbf{a}_2 - z_6\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(2x_6 - y_6)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_6\,\hat{\mathbf{y}} - cz_6\,\hat{\mathbf{z}}$	(6c)	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)	V II
$\mathbf{B_{23}}$	=	$-y_7\,\mathbf{a}_1 + (x_7 - y_7)\,\mathbf{a}_2 + \left(z_7 + \frac{1}{3}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_7 - 2y_7)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_7\,\hat{\mathbf{y}} + c\left(z_7 + \frac{1}{3}\right)\,\hat{\mathbf{z}}$	(6c)	V II
$\mathbf{B_{24}}$	=	$-(x_7 - y_7)\,\mathbf{a}_1 - x_7\,\mathbf{a}_2 + \left(z_7 + \frac{2}{3}\right)\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(2x_7 - y_7)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_7\,\hat{\mathbf{y}} + \frac{1}{3}c\,(3z_7 + 2)\,\hat{\mathbf{z}}$	(6c)	V II
$\mathbf{B_{25}}$	=	$-y_7\,\mathbf{a}_1 - x_7\,\mathbf{a}_2 - \left(z_7 - \frac{2}{3}\right)\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(x_7 + y_7)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,(x_7 - y_7)\,\hat{\mathbf{y}} - \frac{1}{3}c\,(3z_7 - 2)\,\hat{\mathbf{z}}$	(6c)	V II
$\mathbf{B_{26}}$	=	$-(x_7 - y_7)\,\mathbf{a}_1 + y_7\,\mathbf{a}_2 - \left(z_7 - \frac{1}{3}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(-x_7 + 2y_7)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_7\,\hat{\mathbf{y}} - c\left(z_7 - \frac{1}{3}\right)\,\hat{\mathbf{z}}$	(6c)	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)	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)	V III
$\mathbf{B_{29}}$	=	$-y_8\,\mathbf{a}_1 + (x_8 - y_8)\,\mathbf{a}_2 + \left(z_8 + \frac{1}{3}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_8 - 2y_8)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_8\,\hat{\mathbf{y}} + c\left(z_8 + \frac{1}{3}\right)\,\hat{\mathbf{z}}$	(6c)	V III
$\mathbf{B_{30}}$	=	$-(x_8 - y_8)\,\mathbf{a}_1 - x_8\,\mathbf{a}_2 + \left(z_8 + \frac{2}{3}\right)\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(2x_8 - y_8)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_8\,\hat{\mathbf{y}} + \frac{1}{3}c\,(3z_8 + 2)\,\hat{\mathbf{z}}$	(6c)	V III
$\mathbf{B_{31}}$	=	$-y_8\,\mathbf{a}_1 - x_8\,\mathbf{a}_2 - \left(z_8 - \frac{2}{3}\right)\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(x_8 + y_8)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,(x_8 - y_8)\,\hat{\mathbf{y}} - \frac{1}{3}c\,(3z_8 - 2)\,\hat{\mathbf{z}}$	(6c)	V III
$\mathbf{B_{32}}$	=	$-(x_8 - y_8)\,\mathbf{a}_1 + y_8\,\mathbf{a}_2 - \left(z_8 - \frac{1}{3}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(-x_8 + 2y_8)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_8\,\hat{\mathbf{y}} - c\left(z_8 - \frac{1}{3}\right)\,\hat{\mathbf{z}}$	(6c)	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)	V III

References

[1] J. D. Venables, D. Kahn, and R. G. Lye, *Structure of the ordered compound V_6C_5*, Phil. Mag. **18**, 177–192 (1968), doi:10.1080/14786436808227320.

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.