KB_6H_6 Structure: A6B6C_cF104_202_h_h_c-001

This structure originally had the label `A6B6C_cF104_202_h_h_c`. Calls to that address will be redirected here.

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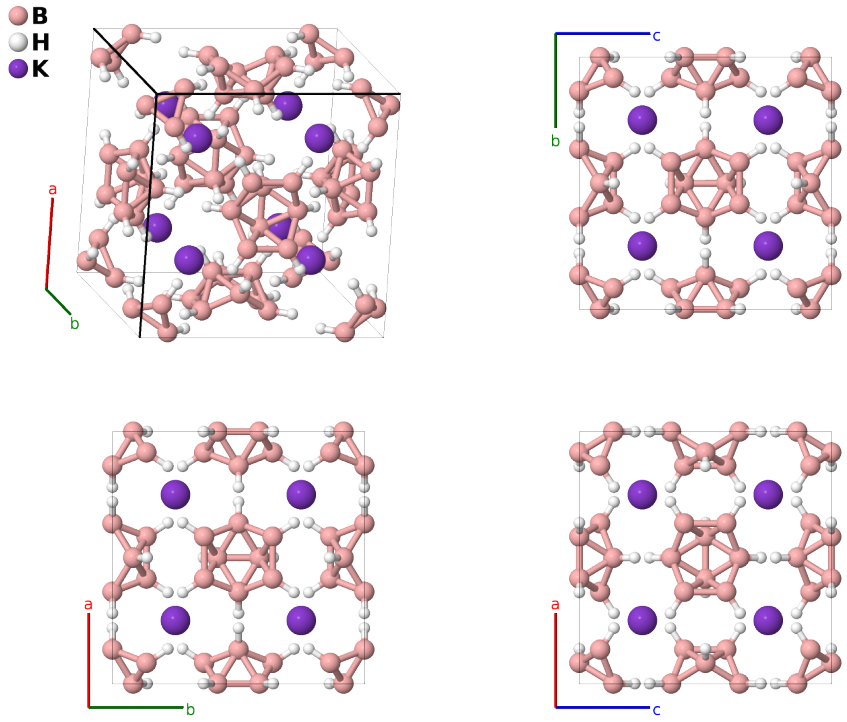
https://aflow.org/p/PZB0

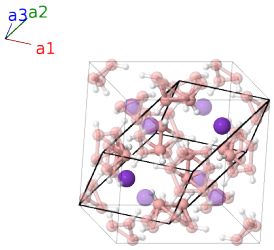
https://aflow.org/p/A6B6C_cF104_202_h_h_c-001



Prototype	B_6H_6K
AFLOW prototype label	A6B6C_cF104_202_h_h_c-001
ICSD	36148
Pearson symbol	cF104
Space group number	202
Space group symbol	$Fm\overline{3}$
AFLOW prototype command	`aflow --proto=A6B6C_cF104_202_h_h_c-001 --params=`a, y_2, z_2, y_3, z_3

Face-centered Cubic primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} + \frac{1}{4}a\,\hat{\mathbf{z}}$	(8c)	K I
$\mathbf{B_2}$	=	$\frac{3}{4}\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{3}{4}a\,\hat{\mathbf{x}} + \frac{3}{4}a\,\hat{\mathbf{y}} + \frac{3}{4}a\,\hat{\mathbf{z}}$	(8c)	K I
$\mathbf{B_3}$	=	$(y_2+z_2)\,\mathbf{a}_1 - (y_2-z_2)\,\mathbf{a}_2 + (y_2-z_2)\,\mathbf{a}_3$	=	$ay_2\,\hat{\mathbf{y}} + az_2\,\hat{\mathbf{z}}$	(48h)	B I
$\mathbf{B_4}$	=	$-(y_2-z_2)\,\mathbf{a}_1 + (y_2+z_2)\,\mathbf{a}_2 - (y_2+z_2)\,\mathbf{a}_3$	=	$-ay_2\,\hat{\mathbf{y}} + az_2\,\hat{\mathbf{z}}$	(48h)	B I
$\mathbf{B_5}$	=	$(y_2-z_2)\,\mathbf{a}_1 - (y_2+z_2)\,\mathbf{a}_2 + (y_2+z_2)\,\mathbf{a}_3$	=	$ay_2\,\hat{\mathbf{y}} - az_2\,\hat{\mathbf{z}}$	(48h)	B I
$\mathbf{B_6}$	=	$-(y_2+z_2)\,\mathbf{a}_1 + (y_2-z_2)\,\mathbf{a}_2 - (y_2-z_2)\,\mathbf{a}_3$	=	$-ay_2\,\hat{\mathbf{y}} - az_2\,\hat{\mathbf{z}}$	(48h)	B I
$\mathbf{B_7}$	=	$(y_2-z_2)\,\mathbf{a}_1 + (y_2+z_2)\,\mathbf{a}_2 - (y_2-z_2)\,\mathbf{a}_3$	=	$az_2\,\hat{\mathbf{x}} + ay_2\,\hat{\mathbf{z}}$	(48h)	B I
$\mathbf{B_8}$	=	$-(y_2+z_2)\,\mathbf{a}_1 - (y_2-z_2)\,\mathbf{a}_2 + (y_2+z_2)\,\mathbf{a}_3$	=	$az_2\,\hat{\mathbf{x}} - ay_2\,\hat{\mathbf{z}}$	(48h)	B I
$\mathbf{B_9}$	=	$(y_2+z_2)\,\mathbf{a}_1 + (y_2-z_2)\,\mathbf{a}_2 - (y_2+z_2)\,\mathbf{a}_3$	=	$-az_2\,\hat{\mathbf{x}} + ay_2\,\hat{\mathbf{z}}$	(48h)	B I
$\mathbf{B_{10}}$	=	$-(y_2-z_2)\,\mathbf{a}_1 - (y_2+z_2)\,\mathbf{a}_2 + (y_2-z_2)\,\mathbf{a}_3$	=	$-az_2\,\hat{\mathbf{x}} - ay_2\,\hat{\mathbf{z}}$	(48h)	B I
$\mathbf{B_{11}}$	=	$-(y_2-z_2)\,\mathbf{a}_1 + (y_2-z_2)\,\mathbf{a}_2 + (y_2+z_2)\,\mathbf{a}_3$	=	$ay_2\,\hat{\mathbf{x}} + az_2\,\hat{\mathbf{y}}$	(48h)	B I
$\mathbf{B_{12}}$	=	$(y_2+z_2)\,\mathbf{a}_1 - (y_2+z_2)\,\mathbf{a}_2 - (y_2-z_2)\,\mathbf{a}_3$	=	$-ay_2\,\hat{\mathbf{x}} + az_2\,\hat{\mathbf{y}}$	(48h)	B I
$\mathbf{B_{13}}$	=	$-(y_2+z_2)\,\mathbf{a}_1 + (y_2+z_2)\,\mathbf{a}_2 + (y_2-z_2)\,\mathbf{a}_3$	=	$ay_2\,\hat{\mathbf{x}} - az_2\,\hat{\mathbf{y}}$	(48h)	B I
$\mathbf{B_{14}}$	=	$(y_2-z_2)\,\mathbf{a}_1 - (y_2-z_2)\,\mathbf{a}_2 - (y_2+z_2)\,\mathbf{a}_3$	=	$-ay_2\,\hat{\mathbf{x}} - az_2\,\hat{\mathbf{y}}$	(48h)	B I
$\mathbf{B_{15}}$	=	$(y_3+z_3)\,\mathbf{a}_1 - (y_3-z_3)\,\mathbf{a}_2 + (y_3-z_3)\,\mathbf{a}_3$	=	$ay_3\,\hat{\mathbf{y}} + az_3\,\hat{\mathbf{z}}$	(48h)	H I
$\mathbf{B_{16}}$	=	$-(y_3-z_3)\,\mathbf{a}_1 + (y_3+z_3)\,\mathbf{a}_2 - (y_3+z_3)\,\mathbf{a}_3$	=	$-ay_3\,\hat{\mathbf{y}} + az_3\,\hat{\mathbf{z}}$	(48h)	H I
$\mathbf{B_{17}}$	=	$(y_3-z_3)\,\mathbf{a}_1 - (y_3+z_3)\,\mathbf{a}_2 + (y_3+z_3)\,\mathbf{a}_3$	=	$ay_3\,\hat{\mathbf{y}} - az_3\,\hat{\mathbf{z}}$	(48h)	H I
$\mathbf{B_{18}}$	=	$-(y_3+z_3)\,\mathbf{a}_1 + (y_3-z_3)\,\mathbf{a}_2 - (y_3-z_3)\,\mathbf{a}_3$	=	$-ay_3\,\hat{\mathbf{y}} - az_3\,\hat{\mathbf{z}}$	(48h)	H I

$\mathbf{B_{19}}$	=	$(y_3 - z_3)\ \mathbf{a}_1 + (y_3 + z_3)\ \mathbf{a}_2 - (y_3 - z_3)\ \mathbf{a}_3$	=	$az_3\,\hat{\mathbf{x}} + ay_3\,\hat{\mathbf{z}}$	(48h)	H I
$\mathbf{B_{20}}$	=	$-(y_3 + z_3)\ \mathbf{a}_1 - (y_3 - z_3)\ \mathbf{a}_2 + (y_3 + z_3)\ \mathbf{a}_3$	=	$az_3\,\hat{\mathbf{x}} - ay_3\,\hat{\mathbf{z}}$	(48h)	H I
$\mathbf{B_{21}}$	=	$(y_3 + z_3)\ \mathbf{a}_1 + (y_3 - z_3)\ \mathbf{a}_2 - (y_3 + z_3)\ \mathbf{a}_3$	=	$-az_3\,\hat{\mathbf{x}} + ay_3\,\hat{\mathbf{z}}$	(48h)	H I
$\mathbf{B_{22}}$	=	$-(y_3 - z_3)\ \mathbf{a}_1 - (y_3 + z_3)\ \mathbf{a}_2 + (y_3 - z_3)\ \mathbf{a}_3$	=	$-az_3\,\hat{\mathbf{x}} - ay_3\,\hat{\mathbf{z}}$	(48h)	H I
$\mathbf{B_{23}}$	=	$-(y_3 - z_3)\ \mathbf{a}_1 + (y_3 - z_3)\ \mathbf{a}_2 + (y_3 + z_3)\ \mathbf{a}_3$	=	$ay_3\,\hat{\mathbf{x}} + az_3\,\hat{\mathbf{y}}$	(48h)	H I
$\mathbf{B_{24}}$	=	$(y_3 + z_3)\ \mathbf{a}_1 - (y_3 + z_3)\ \mathbf{a}_2 - (y_3 - z_3)\ \mathbf{a}_3$	=	$-ay_3\,\hat{\mathbf{x}} + az_3\,\hat{\mathbf{y}}$	(48h)	H I
$\mathbf{B_{25}}$	=	$-(y_3 + z_3)\ \mathbf{a}_1 + (y_3 + z_3)\ \mathbf{a}_2 + (y_3 - z_3)\ \mathbf{a}_3$	=	$ay_3\,\hat{\mathbf{x}} - az_3\,\hat{\mathbf{y}}$	(48h)	H I
$\mathbf{B_{26}}$	=	$(y_3 - z_3)\ \mathbf{a}_1 - (y_3 - z_3)\ \mathbf{a}_2 - (y_3 + z_3)\ \mathbf{a}_3$	=	$-ay_3\,\hat{\mathbf{x}} - az_3\,\hat{\mathbf{y}}$	(48h)	H I

References

[1] J. A. Wunderlich and W. N. Lipscomb, *Structure of $B_{12}H_{12}^{-2}$ Ion*, J. Am. Chem. Soc. **82**, 4427–4428 (1960), doi:10.1021/ja01501a076.

Found in

[1] P. Villars and K. Cenzual, *Pearson's Crystal Data – Crystal Structure Database for Inorganic Compounds* (2013). ASM International.