High-Pressure CuBi Structure: AB_oP8_51_ef_af-001

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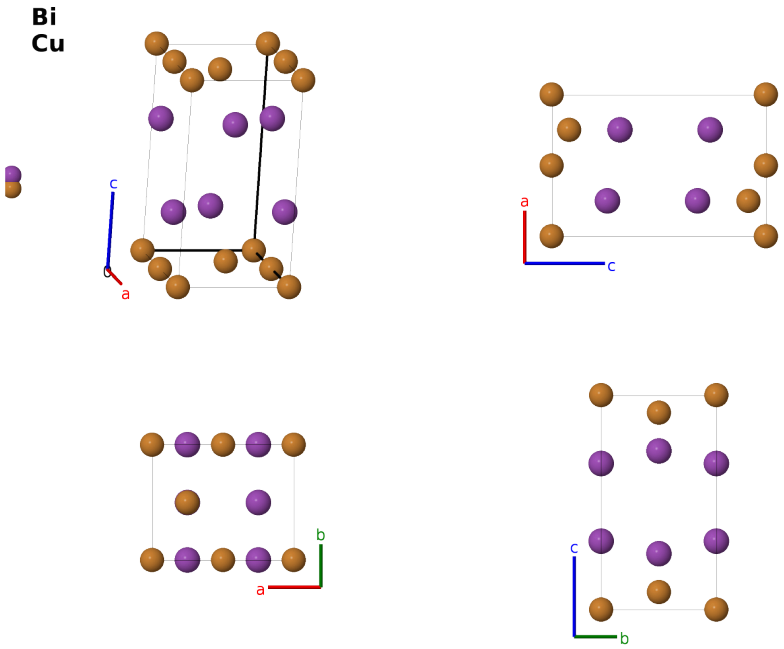
https://aflow.org/prototype-encyclopedia/TKGJ

https://aflow.org/prototype-encyclopedia/AB_oP8_51_ef_af-001

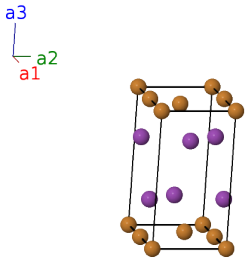


Prototype	BiCu
AFLOW prototype label	AB_oP8_51_ef_af-001
ICSD	253703
CCDC	1927357
Pearson symbol	oP8
Space group number	51
Space group symbol	*Pmma*
AFLOW prototype command	`aflow --proto=AB_oP8_51_ef_af-001 --params=`$a, b/a, c/a, z_2, z_3, z_4$

- This is a high-pressure phase of CuBi, prepared at $P = 5$ GPa and $T = 720$ K. Under ambient conditions CuBi is in the rock salt ($B1$) structure.

Simple Orthorhombic primitive vectors

$$\mathbf{a_1} = a\,\hat{\mathbf{x}}$$
$$\mathbf{a_2} = b\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(2a)	Cu I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_1$	=	$\frac{1}{2}a\,\hat{\mathbf{x}}$	(2a)	Cu I
$\mathbf{B_3}$	=	$\frac{1}{4}\,\mathbf{a}_1 + z_2\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + cz_2\,\hat{\mathbf{z}}$	(2e)	Bi I
$\mathbf{B_4}$	=	$\frac{3}{4}\,\mathbf{a}_1 - z_2\,\mathbf{a}_3$	=	$\frac{3}{4}a\,\hat{\mathbf{x}} - cz_2\,\hat{\mathbf{z}}$	(2e)	Bi I
$\mathbf{B_5}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{2}b\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(2f)	Bi II
$\mathbf{B_6}$	=	$\frac{3}{4}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$	=	$\frac{3}{4}a\,\hat{\mathbf{x}} + \frac{1}{2}b\,\hat{\mathbf{y}} - cz_3\,\hat{\mathbf{z}}$	(2f)	Bi II
$\mathbf{B_7}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{2}b\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(2f)	Cu II
$\mathbf{B_8}$	=	$\frac{3}{4}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 - z_4\,\mathbf{a}_3$	=	$\frac{3}{4}a\,\hat{\mathbf{x}} + \frac{1}{2}b\,\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$	(2f)	Cu II

References

[1] K. Guo, L. Akselrud, M. Bobnar, U. Burkhardt, M. Schmidt, J.-T. Zhao, U. Schwarz, and Y. Grin, *Weak Interactions under Pressure: hp-CuBi and Its Analogues*, Angew. Chem. Int. Ed. **56**, 5620–5624 (2017), doi:10.1002/anie.201700712.

Found in

[1] ICSD, Inorganic Crystal Structure Database. ID 253703.

First cited in

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