Bi_2CdO_4 Structure: A2BC4_tI112_141_gh_f_ghi-001

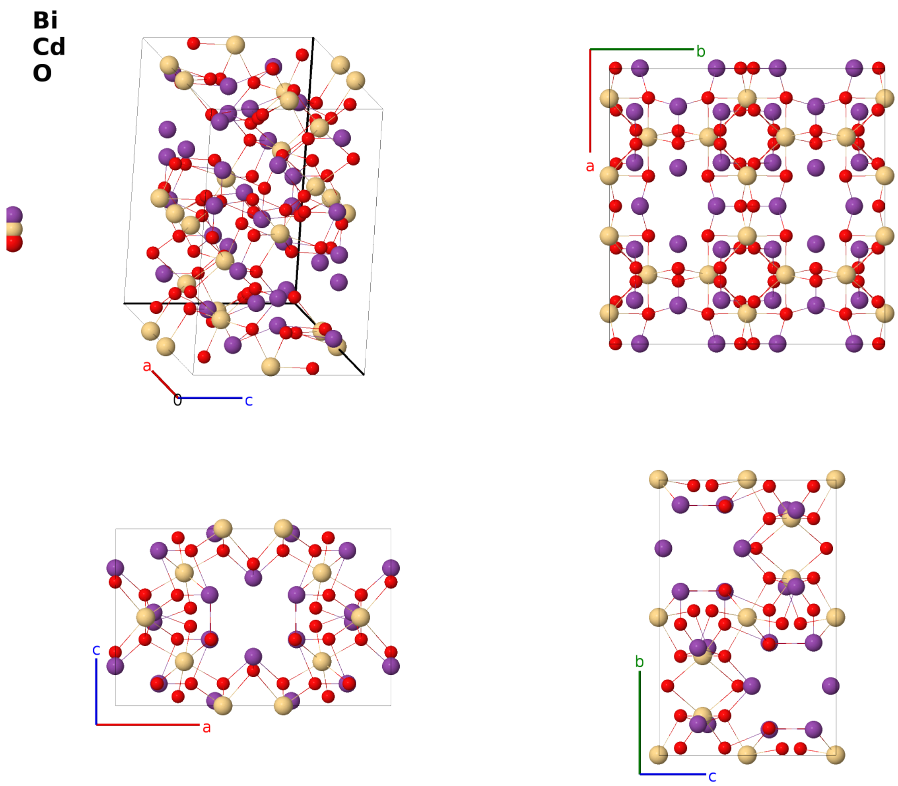
Cite this page as:

- 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. Oses, 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/K32G

https://aflow.org/prototype-encyclopedia/A2BC4_tI112_141_gh_f_ghi-001



Prototype	Bi_2CdO_4
AFLOW prototype label	A2BC4_tI112_141_gh_f_ghi-001
ICSD	89453
CCDC	1649125
Pearson symbol	tI112
Space group number	141
Space group symbol	$I4_1/amd$
AFLOW prototype command	`aflow --proto=A2BC4_tI112_141_gh_f_ghi-001 --params=`$a, c/a, x_1, x_2, x_3, y_4, z_4, y_5, z_5, x_6, y_6, z_6$

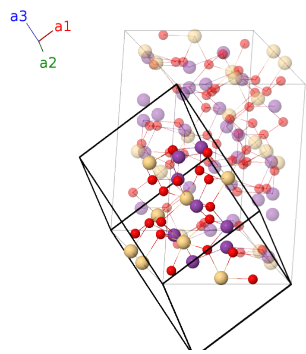
Other compounds with this structure

Li_2WO_4

- (Kirik, 1999) give the coordinates of the oxygen atoms on the (32g) Wyckoff position as (0.1575,0.09252,0.875), however the correct value for x should be 1/4-y = 0.15748. We made this minor correction to maintain the symmetry. In practice, the error is less than the measurement error in the sample.
- When the bismuth on the (16g) or (16h) site is replaced by another atomic species this becomes the quaternary $BiYCdO_4$ structure. Both forms are given the Bi_2CdO_4 structure type in the ICSD.

Body-centered Tetragonal primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$x_1\,\mathbf{a}_2 + x_1\,\mathbf{a}_3$	=	$ax_1\,\mathbf{\hat{x}}$	(16f)	Cd I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_1 - x_1\,\mathbf{a}_2 - \left(x_1 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_1\,\mathbf{\hat{x}} + \frac{1}{2}a\,\mathbf{\hat{y}}$	(16f)	Cd I
$\mathbf{B_3}$	=	$x_1\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + x_1\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\mathbf{\hat{x}} + a\left(x_1 - \frac{1}{4}\right)\,\mathbf{\hat{y}} + \frac{1}{4}c\,\mathbf{\hat{z}}$	(16f)	Cd I
$\mathbf{B_4}$	=	$-x_1\,\mathbf{a}_1 - \left(x_1 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\mathbf{\hat{x}} - a\left(x_1 - \frac{1}{4}\right)\,\mathbf{\hat{y}} - \frac{1}{4}c\,\mathbf{\hat{z}}$	(16f)	Cd I
$\mathbf{B_5}$	=	$-x_1\,\mathbf{a}_2 - x_1\,\mathbf{a}_3$	=	$-ax_1\,\mathbf{\hat{x}}$	(16f)	Cd I
$\mathbf{B_6}$	=	$\frac{1}{2}\,\mathbf{a}_1 + x_1\,\mathbf{a}_2 + \left(x_1 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$ax_1\,\mathbf{\hat{x}} + \frac{1}{2}a\,\mathbf{\hat{y}}$	(16f)	Cd I
$\mathbf{B_7}$	=	$-x_1\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 - x_1\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\mathbf{\hat{x}} - a\left(x_1 + \frac{1}{4}\right)\,\mathbf{\hat{y}} + \frac{1}{4}c\,\mathbf{\hat{z}}$	(16f)	Cd I
$\mathbf{B_8}$	=	$x_1\,\mathbf{a}_1 + \left(x_1 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\mathbf{\hat{x}} + a\left(x_1 + \frac{1}{4}\right)\,\mathbf{\hat{y}} - \frac{1}{4}c\,\mathbf{\hat{z}}$	(16f)	Cd I
$\mathbf{B_9}$	=	$\left(x_2 + \frac{1}{8}\right)\,\mathbf{a}_1 + \left(x_2 + \frac{7}{8}\right)\,\mathbf{a}_2 + \left(2x_2 + \frac{1}{4}\right)\,\mathbf{a}_3$	=	$a\left(x_2 + \frac{1}{2}\right)\,\mathbf{\hat{x}} + a\left(x_2 - \frac{1}{4}\right)\,\mathbf{\hat{y}} + \frac{3}{8}c\,\mathbf{\hat{z}}$	(16g)	Bi I
$\mathbf{B_{10}}$	=	$-\left(x_2 - \frac{1}{8}\right)\,\mathbf{a}_1 - \left(x_2 - \frac{7}{8}\right)\,\mathbf{a}_2 - \left(2x_2 - \frac{1}{4}\right)\,\mathbf{a}_3$	=	$-a\left(x_2 - \frac{1}{2}\right)\,\mathbf{\hat{x}} - a\left(x_2 + \frac{1}{4}\right)\,\mathbf{\hat{y}} + \frac{3}{8}c\,\mathbf{\hat{z}}$	(16g)	Bi I
$\mathbf{B_{11}}$	=	$\left(x_2 + \frac{7}{8}\right)\,\mathbf{a}_1 - \left(x_2 - \frac{1}{8}\right)\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$-ax_2\,\mathbf{\hat{x}} + a\left(x_2 + \frac{3}{4}\right)\,\mathbf{\hat{y}} + \frac{1}{8}c\,\mathbf{\hat{z}}$	(16g)	Bi I
$\mathbf{B_{12}}$	=	$-\left(x_2 - \frac{7}{8}\right)\,\mathbf{a}_1 + \left(x_2 + \frac{1}{8}\right)\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$ax_2\,\mathbf{\hat{x}} - a\left(x_2 - \frac{3}{4}\right)\,\mathbf{\hat{y}} + \frac{1}{8}c\,\mathbf{\hat{z}}$	(16g)	Bi I
$\mathbf{B_{13}}$	=	$-\left(x_2 - \frac{7}{8}\right)\,\mathbf{a}_1 - \left(x_2 - \frac{1}{8}\right)\,\mathbf{a}_2 - \left(2x_2 - \frac{3}{4}\right)\,\mathbf{a}_3$	=	$-ax_2\,\mathbf{\hat{x}} - a\left(x_2 - \frac{3}{4}\right)\,\mathbf{\hat{y}} + \frac{1}{8}c\,\mathbf{\hat{z}}$	(16g)	Bi I
$\mathbf{B_{14}}$	=	$\left(x_2 + \frac{7}{8}\right)\,\mathbf{a}_1 + \left(x_2 + \frac{1}{8}\right)\,\mathbf{a}_2 + \left(2x_2 + \frac{3}{4}\right)\,\mathbf{a}_3$	=	$ax_2\,\mathbf{\hat{x}} + a\left(x_2 + \frac{3}{4}\right)\,\mathbf{\hat{y}} + \frac{1}{8}c\,\mathbf{\hat{z}}$	(16g)	Bi I
$\mathbf{B_{15}}$	=	$-\left(x_2 - \frac{1}{8}\right)\,\mathbf{a}_1 + \left(x_2 + \frac{7}{8}\right)\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$a\left(x_2 + \frac{1}{2}\right)\,\mathbf{\hat{x}} - a\left(x_2 + \frac{1}{4}\right)\,\mathbf{\hat{y}} + \frac{3}{8}c\,\mathbf{\hat{z}}$	(16g)	Bi I
$\mathbf{B_{16}}$	=	$\left(x_2 + \frac{1}{8}\right)\,\mathbf{a}_1 - \left(x_2 - \frac{7}{8}\right)\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$-a\left(x_2 - \frac{1}{2}\right)\,\mathbf{\hat{x}} + a\left(x_2 - \frac{1}{4}\right)\,\mathbf{\hat{y}} + \frac{3}{8}c\,\mathbf{\hat{z}}$	(16g)	Bi I

$\mathbf{B_{17}}$	=	$\left(x_3+\frac{1}{8}\right)\,\mathbf{a}_1+\left(x_3+\frac{7}{8}\right)\,\mathbf{a}_2+\left(2x_3+\frac{1}{4}\right)\,\mathbf{a}_3$	=	$a\left(x_3+\frac{1}{2}\right)\,\mathbf{\hat{x}}+a\left(x_3-\frac{1}{4}\right)\,\mathbf{\hat{y}}+\frac{3}{8}c\,\mathbf{\hat{z}}$	(16g)	O I
$\mathbf{B_{18}}$	=	$-\left(x_3-\frac{1}{8}\right)\,\mathbf{a}_1-\left(x_3-\frac{7}{8}\right)\,\mathbf{a}_2-\left(2x_3-\frac{1}{4}\right)\,\mathbf{a}_3$	=	$-a\left(x_3-\frac{1}{2}\right)\,\mathbf{\hat{x}}-a\left(x_3+\frac{1}{4}\right)\,\mathbf{\hat{y}}+\frac{3}{8}c\,\mathbf{\hat{z}}$	(16g)	O I
$\mathbf{B_{19}}$	=	$\left(x_3+\frac{7}{8}\right)\,\mathbf{a}_1-\left(x_3-\frac{1}{8}\right)\,\mathbf{a}_2+\frac{3}{4}\,\mathbf{a}_3$	=	$-ax_3\,\mathbf{\hat{x}}+a\left(x_3+\frac{3}{4}\right)\,\mathbf{\hat{y}}+\frac{1}{8}c\,\mathbf{\hat{z}}$	(16g)	O I
$\mathbf{B_{20}}$	=	$-\left(x_3-\frac{7}{8}\right)\,\mathbf{a}_1+\left(x_3+\frac{1}{8}\right)\,\mathbf{a}_2+\frac{3}{4}\,\mathbf{a}_3$	=	$ax_3\,\mathbf{\hat{x}}-a\left(x_3-\frac{3}{4}\right)\,\mathbf{\hat{y}}+\frac{1}{8}c\,\mathbf{\hat{z}}$	(16g)	O I
$\mathbf{B_{21}}$	=	$-\left(x_3-\frac{7}{8}\right)\,\mathbf{a}_1-\left(x_3-\frac{1}{8}\right)\,\mathbf{a}_2-\left(2x_3-\frac{3}{4}\right)\,\mathbf{a}_3$	=	$-ax_3\,\mathbf{\hat{x}}-a\left(x_3-\frac{3}{4}\right)\,\mathbf{\hat{y}}+\frac{1}{8}c\,\mathbf{\hat{z}}$	(16g)	O I
$\mathbf{B_{22}}$	=	$\left(x_3+\frac{7}{8}\right)\,\mathbf{a}_1+\left(x_3+\frac{1}{8}\right)\,\mathbf{a}_2+\left(2x_3+\frac{3}{4}\right)\,\mathbf{a}_3$	=	$ax_3\,\mathbf{\hat{x}}+a\left(x_3+\frac{3}{4}\right)\,\mathbf{\hat{y}}+\frac{1}{8}c\,\mathbf{\hat{z}}$	(16g)	O I
$\mathbf{B_{23}}$	=	$-\left(x_3-\frac{1}{8}\right)\,\mathbf{a}_1+\left(x_3+\frac{7}{8}\right)\,\mathbf{a}_2+\frac{1}{4}\,\mathbf{a}_3$	=	$a\left(x_3+\frac{1}{2}\right)\,\mathbf{\hat{x}}-a\left(x_3+\frac{1}{4}\right)\,\mathbf{\hat{y}}+\frac{3}{8}c\,\mathbf{\hat{z}}$	(16g)	O I
$\mathbf{B_{24}}$	=	$\left(x_3+\frac{1}{8}\right)\,\mathbf{a}_1-\left(x_3-\frac{7}{8}\right)\,\mathbf{a}_2+\frac{1}{4}\,\mathbf{a}_3$	=	$-a\left(x_3-\frac{1}{2}\right)\,\mathbf{\hat{x}}+a\left(x_3-\frac{1}{4}\right)\,\mathbf{\hat{y}}+\frac{3}{8}c\,\mathbf{\hat{z}}$	(16g)	O I
$\mathbf{B_{25}}$	=	$\left(y_4+z_4\right)\,\mathbf{a}_1+z_4\,\mathbf{a}_2+y_4\,\mathbf{a}_3$	=	$ay_4\,\mathbf{\hat{y}}+cz_4\,\mathbf{\hat{z}}$	(16h)	Bi II
$\mathbf{B_{26}}$	=	$\left(-y_4+z_4+\frac{1}{2}\right)\,\mathbf{a}_1+z_4\,\mathbf{a}_2-\left(y_4-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(y_4-\frac{1}{2}\right)\,\mathbf{\hat{y}}+cz_4\,\mathbf{\hat{z}}$	(16h)	Bi II
$\mathbf{B_{27}}$	=	$z_4\,\mathbf{a}_1+\left(-y_4+z_4+\frac{1}{2}\right)\,\mathbf{a}_2-y_4\,\mathbf{a}_3$	=	$-a\left(y_4-\frac{1}{4}\right)\,\mathbf{\hat{x}}-\frac{1}{4}a\,\mathbf{\hat{y}}+c\left(z_4+\frac{1}{4}\right)\,\mathbf{\hat{z}}$	(16h)	Bi II
$\mathbf{B_{28}}$	=	$z_4\,\mathbf{a}_1+\left(y_4+z_4\right)\,\mathbf{a}_2+\left(y_4+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(y_4+\frac{1}{4}\right)\,\mathbf{\hat{x}}+\frac{1}{4}a\,\mathbf{\hat{y}}+c\left(z_4-\frac{1}{4}\right)\,\mathbf{\hat{z}}$	(16h)	Bi II
$\mathbf{B_{29}}$	=	$\left(y_4-z_4+\frac{1}{2}\right)\,\mathbf{a}_1-z_4\,\mathbf{a}_2+\left(y_4+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(y_4+\frac{1}{2}\right)\,\mathbf{\hat{y}}-cz_4\,\mathbf{\hat{z}}$	(16h)	Bi II
$\mathbf{B_{30}}$	=	$-\left(y_4+z_4\right)\,\mathbf{a}_1-z_4\,\mathbf{a}_2-y_4\,\mathbf{a}_3$	=	$-ay_4\,\mathbf{\hat{y}}-cz_4\,\mathbf{\hat{z}}$	(16h)	Bi II
$\mathbf{B_{31}}$	=	$-z_4\,\mathbf{a}_1+\left(y_4-z_4+\frac{1}{2}\right)\,\mathbf{a}_2+y_4\,\mathbf{a}_3$	=	$a\left(y_4+\frac{1}{4}\right)\,\mathbf{\hat{x}}-\frac{1}{4}a\,\mathbf{\hat{y}}-c\left(z_4-\frac{1}{4}\right)\,\mathbf{\hat{z}}$	(16h)	Bi II
$\mathbf{B_{32}}$	=	$-z_4\,\mathbf{a}_1-\left(y_4+z_4\right)\,\mathbf{a}_2-\left(y_4-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(y_4-\frac{1}{4}\right)\,\mathbf{\hat{x}}+\frac{1}{4}a\,\mathbf{\hat{y}}-c\left(z_4+\frac{1}{4}\right)\,\mathbf{\hat{z}}$	(16h)	Bi II
$\mathbf{B_{33}}$	=	$\left(y_5+z_5\right)\,\mathbf{a}_1+z_5\,\mathbf{a}_2+y_5\,\mathbf{a}_3$	=	$ay_5\,\mathbf{\hat{y}}+cz_5\,\mathbf{\hat{z}}$	(16h)	O II
$\mathbf{B_{34}}$	=	$\left(-y_5+z_5+\frac{1}{2}\right)\,\mathbf{a}_1+z_5\,\mathbf{a}_2-\left(y_5-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(y_5-\frac{1}{2}\right)\,\mathbf{\hat{y}}+cz_5\,\mathbf{\hat{z}}$	(16h)	O II
$\mathbf{B_{35}}$	=	$z_5\,\mathbf{a}_1+\left(-y_5+z_5+\frac{1}{2}\right)\,\mathbf{a}_2-y_5\,\mathbf{a}_3$	=	$-a\left(y_5-\frac{1}{4}\right)\,\mathbf{\hat{x}}-\frac{1}{4}a\,\mathbf{\hat{y}}+c\left(z_5+\frac{1}{4}\right)\,\mathbf{\hat{z}}$	(16h)	O II
$\mathbf{B_{36}}$	=	$z_5\,\mathbf{a}_1+\left(y_5+z_5\right)\,\mathbf{a}_2+\left(y_5+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(y_5+\frac{1}{4}\right)\,\mathbf{\hat{x}}+\frac{1}{4}a\,\mathbf{\hat{y}}+c\left(z_5-\frac{1}{4}\right)\,\mathbf{\hat{z}}$	(16h)	O II
$\mathbf{B_{37}}$	=	$\left(y_5-z_5+\frac{1}{2}\right)\,\mathbf{a}_1-z_5\,\mathbf{a}_2+\left(y_5+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(y_5+\frac{1}{2}\right)\,\mathbf{\hat{y}}-cz_5\,\mathbf{\hat{z}}$	(16h)	O II
$\mathbf{B_{38}}$	=	$-\left(y_5+z_5\right)\,\mathbf{a}_1-z_5\,\mathbf{a}_2-y_5\,\mathbf{a}_3$	=	$-ay_5\,\mathbf{\hat{y}}-cz_5\,\mathbf{\hat{z}}$	(16h)	O II
$\mathbf{B_{39}}$	=	$-z_5\,\mathbf{a}_1+\left(y_5-z_5+\frac{1}{2}\right)\,\mathbf{a}_2+y_5\,\mathbf{a}_3$	=	$a\left(y_5+\frac{1}{4}\right)\,\mathbf{\hat{x}}-\frac{1}{4}a\,\mathbf{\hat{y}}-c\left(z_5-\frac{1}{4}\right)\,\mathbf{\hat{z}}$	(16h)	O II
$\mathbf{B_{40}}$	=	$-z_5\,\mathbf{a}_1-\left(y_5+z_5\right)\,\mathbf{a}_2-\left(y_5-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(y_5-\frac{1}{4}\right)\,\mathbf{\hat{x}}+\frac{1}{4}a\,\mathbf{\hat{y}}-c\left(z_5+\frac{1}{4}\right)\,\mathbf{\hat{z}}$	(16h)	O II
$\mathbf{B_{41}}$	=	$\left(y_6+z_6\right)\,\mathbf{a}_1+\left(x_6+z_6\right)\,\mathbf{a}_2+\left(x_6+y_6\right)\,\mathbf{a}_3$	=	$ax_6\,\mathbf{\hat{x}}+ay_6\,\mathbf{\hat{y}}+cz_6\,\mathbf{\hat{z}}$	(32i)	O III
$\mathbf{B_{42}}$	=	$\left(-y_6+z_6+\frac{1}{2}\right)\,\mathbf{a}_1-\left(x_6-z_6\right)\,\mathbf{a}_2-\left(x_6+y_6-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_6\,\mathbf{\hat{x}}-a\left(y_6-\frac{1}{2}\right)\,\mathbf{\hat{y}}+cz_6\,\mathbf{\hat{z}}$	(32i)	O III
$\mathbf{B_{43}}$	=	$\left(x_6+z_6\right)\,\mathbf{a}_1+\left(-y_6+z_6+\frac{1}{2}\right)\,\mathbf{a}_2+\left(x_6-y_6\right)\,\mathbf{a}_3$	=	$-a\left(y_6-\frac{1}{4}\right)\,\mathbf{\hat{x}}+a\left(x_6-\frac{1}{4}\right)\,\mathbf{\hat{y}}+c\left(z_6+\frac{1}{4}\right)\,\mathbf{\hat{z}}$	(32i)	O III
$\mathbf{B_{44}}$	=	$-\left(x_6-z_6\right)\,\mathbf{a}_1+\left(y_6+z_6\right)\,\mathbf{a}_2+\left(-x_6+y_6+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(y_6+\frac{1}{4}\right)\,\mathbf{\hat{x}}-a\left(x_6-\frac{1}{4}\right)\,\mathbf{\hat{y}}+c\left(z_6-\frac{1}{4}\right)\,\mathbf{\hat{z}}$	(32i)	O III

$\mathbf{B_{45}}$	$=$	$\left(y_6 - z_6 + \frac{1}{2}\right)\,\mathbf{a}_1 - (x_6 + z_6)\,\mathbf{a}_2 + \left(-x_6 + y_6 + \frac{1}{2}\right)\,\mathbf{a}_3$	$=$	$-ax_6\,\hat{\mathbf{x}} + a\left(y_6 + \frac{1}{2}\right)\,\hat{\mathbf{y}} - cz_6\,\hat{\mathbf{z}}$	(32i)	O III
$\mathbf{B_{46}}$	$=$	$-(y_6 + z_6)\,\mathbf{a}_1 + (x_6 - z_6)\,\mathbf{a}_2 + (x_6 - y_6)\,\mathbf{a}_3$	$=$	$ax_6\,\hat{\mathbf{x}} - ay_6\,\hat{\mathbf{y}} - cz_6\,\hat{\mathbf{z}}$	(32i)	O III
$\mathbf{B_{47}}$	$=$	$(x_6 - z_6)\,\mathbf{a}_1 + \left(y_6 - z_6 + \frac{1}{2}\right)\,\mathbf{a}_2 + (x_6 + y_6)\,\mathbf{a}_3$	$=$	$a\left(y_6 + \frac{1}{4}\right)\,\hat{\mathbf{x}} + a\left(x_6 - \frac{1}{4}\right)\,\hat{\mathbf{y}} - c\left(z_6 - \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(32i)	O III
$\mathbf{B_{48}}$	$=$	$-(x_6 + z_6)\,\mathbf{a}_1 - (y_6 + z_6)\,\mathbf{a}_2 - \left(x_6 + y_6 - \frac{1}{2}\right)\,\mathbf{a}_3$	$=$	$-a\left(y_6 - \frac{1}{4}\right)\,\hat{\mathbf{x}} - a\left(x_6 - \frac{1}{4}\right)\,\hat{\mathbf{y}} - c\left(z_6 + \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(32i)	O III
$\mathbf{B_{49}}$	$=$	$-(y_6 + z_6)\,\mathbf{a}_1 - (x_6 + z_6)\,\mathbf{a}_2 - (x_6 + y_6)\,\mathbf{a}_3$	$=$	$-ax_6\,\hat{\mathbf{x}} - ay_6\,\hat{\mathbf{y}} - cz_6\,\hat{\mathbf{z}}$	(32i)	O III
$\mathbf{B_{50}}$	$=$	$\left(y_6 - z_6 + \frac{1}{2}\right)\,\mathbf{a}_1 + (x_6 - z_6)\,\mathbf{a}_2 + \left(x_6 + y_6 + \frac{1}{2}\right)\,\mathbf{a}_3$	$=$	$ax_6\,\hat{\mathbf{x}} + a\left(y_6 + \frac{1}{2}\right)\,\hat{\mathbf{y}} - cz_6\,\hat{\mathbf{z}}$	(32i)	O III
$\mathbf{B_{51}}$	$=$	$-(x_6 + z_6)\,\mathbf{a}_1 + \left(y_6 - z_6 + \frac{1}{2}\right)\,\mathbf{a}_2 - (x_6 - y_6)\,\mathbf{a}_3$	$=$	$a\left(y_6 + \frac{1}{4}\right)\,\hat{\mathbf{x}} - a\left(x_6 + \frac{1}{4}\right)\,\hat{\mathbf{y}} - c\left(z_6 - \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(32i)	O III
$\mathbf{B_{52}}$	$=$	$(x_6 - z_6)\,\mathbf{a}_1 - (y_6 + z_6)\,\mathbf{a}_2 + \left(x_6 - y_6 + \frac{1}{2}\right)\,\mathbf{a}_3$	$=$	$-a\left(y_6 - \frac{1}{4}\right)\,\hat{\mathbf{x}} + a\left(x_6 + \frac{1}{4}\right)\,\hat{\mathbf{y}} - c\left(z_6 + \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(32i)	O III
$\mathbf{B_{53}}$	$=$	$\left(-y_6 + z_6 + \frac{1}{2}\right)\,\mathbf{a}_1 + (x_6 + z_6)\,\mathbf{a}_2 + \left(x_6 - y_6 + \frac{1}{2}\right)\,\mathbf{a}_3$	$=$	$ax_6\,\hat{\mathbf{x}} - a\left(y_6 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(32i)	O III
$\mathbf{B_{54}}$	$=$	$(y_6 + z_6)\,\mathbf{a}_1 - (x_6 - z_6)\,\mathbf{a}_2 - (x_6 - y_6)\,\mathbf{a}_3$	$=$	$-ax_6\,\hat{\mathbf{x}} + ay_6\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(32i)	O III
$\mathbf{B_{55}}$	$=$	$-(x_6 - z_6)\,\mathbf{a}_1 + \left(-y_6 + z_6 + \frac{1}{2}\right)\,\mathbf{a}_2 - (x_6 + y_6)\,\mathbf{a}_3$	$=$	$-a\left(y_6 - \frac{1}{4}\right)\,\hat{\mathbf{x}} - a\left(x_6 + \frac{1}{4}\right)\,\hat{\mathbf{y}} + c\left(z_6 + \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(32i)	O III
$\mathbf{B_{56}}$	$=$	$(x_6 + z_6)\,\mathbf{a}_1 + (y_6 + z_6)\,\mathbf{a}_2 + \left(x_6 + y_6 + \frac{1}{2}\right)\,\mathbf{a}_3$	$=$	$a\left(y_6 + \frac{1}{4}\right)\,\hat{\mathbf{x}} + a\left(x_6 + \frac{1}{4}\right)\,\hat{\mathbf{y}} + c\left(z_6 - \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(32i)	O III

References

[1] S. D. Kirik, A. F. Shimanskiy, and T. I. Koryagina, *Crystal structure investigation and conductivity of binary bismuth–cadmium oxide Bi_2CdO_4*, Solid State Ion. **122**, 249–254 (1999), doi:10.1016/S0167-2738(98)00444-5.

First cited in

N. Anderson, M. J. Mehl, H. Eckert, S. Divilov, X. Campilongo, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 5.* Submitted to Computational Materials Science (2026).