$Bi_2Sr_2Ca_2Cu_3O_{10+x}$ (Bi-2223) Structure: A2B2C3D10E2_oC76_37_d_d_cd_5d_d-001

https://aflow.org/p/ZBUL

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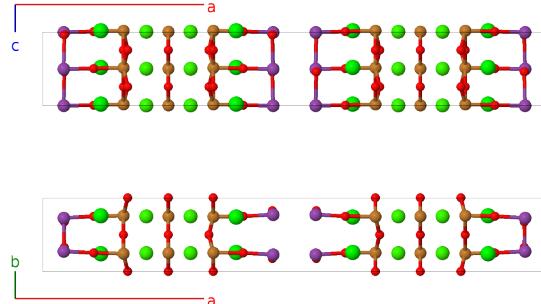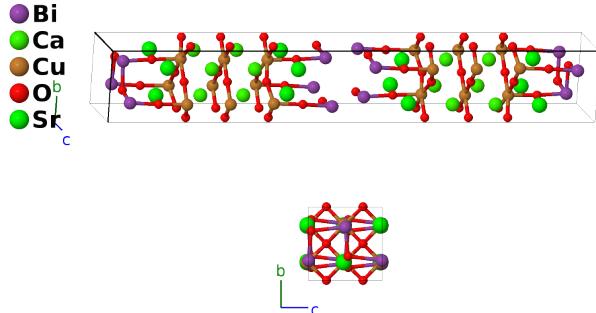
Prototype	$Bi_2Ca_2Cu_3O_{10}Sr_2$
AFLOW prototype label	A2B2C3D10E2_oC76_37_d_d_cd_5d_d-001
ICSD	174012
Pearson symbol	oC76
Space group number	37
Space group symbol	$Ccc2$
AFLOW prototype command	aflow --proto=A2B2C3D10E2_oC76_37_d_d_cd_5d_d-001
	--params=$a, b/a, c/a, z_1, x_2, y_2, z_2, x_3, y_3, z_3, x_4, y_4, z_4, x_5, y_5, z_5, x_6, y_6, z_6, x_7, y_7, z_7, x_8,$ $y_8, z_8, x_9, y_9, z_9, x_{10}, y_{10}, z_{10}$

- (Shamray, 2009) found some disorder in this crystal: the Bi (8d) site has 6% vacancies, the Cu (8d) site is actually 90% copper and 9% bismuth, and the Sr (8d) site has 3% vacancies. It is not clear where the extra oxygens needed to control the superconducting behavior are added to the crystal.

- (Shamray, 2009) give the structure in the $A2aa$ setting of space group #37. We used FINDSYM to transform this to the standard $Ccc2$ setting.

- Space group $Ccc2$ #37 does not fix the origin of the z-coordinate. We do this by setting $z_1 = 0$ for the Cu (4c) site.

Base-centered Orthorhombic primitive vectors

$$\mathbf{a_1} = \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{1}{2}b\,\hat{\mathbf{y}}$$

$$\mathbf{a_2} = \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}b\,\hat{\mathbf{y}}$$

$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$
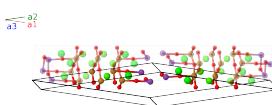
Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	$=$	$\frac{1}{2}\,\mathbf{a}_2 + z_1\,\mathbf{a}_3$	$=$	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} + cz_1\,\hat{\mathbf{z}}$	(4c)	Cu I
$\mathbf{B_2}$	$=$	$\frac{1}{2}\,\mathbf{a}_1 + \left(z_1 + \frac{1}{2}\right)\,\mathbf{a}_3$	$=$	$\frac{1}{4}a\,\hat{\mathbf{x}} - \frac{1}{4}b\,\hat{\mathbf{y}} + c\left(z_1 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4c)	Cu I
$\mathbf{B_3}$	$=$	$(x_2 - y_2)\,\mathbf{a}_1 + (x_2 + y_2)\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	$=$	$ax_2\,\hat{\mathbf{x}} + by_2\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(8d)	Bi I
$\mathbf{B_4}$	$=$	$-(x_2 - y_2)\,\mathbf{a}_1 - (x_2 + y_2)\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	$=$	$-ax_2\,\hat{\mathbf{x}} - by_2\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(8d)	Bi I
$\mathbf{B_5}$	$=$	$(x_2 + y_2)\,\mathbf{a}_1 + (x_2 - y_2)\,\mathbf{a}_2 + \left(z_2 + \frac{1}{2}\right)\,\mathbf{a}_3$	$=$	$ax_2\,\hat{\mathbf{x}} - by_2\,\hat{\mathbf{y}} + c\left(z_2 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8d)	Bi I
$\mathbf{B_6}$	$=$	$-(x_2 + y_2)\,\mathbf{a}_1 - (x_2 - y_2)\,\mathbf{a}_2 + \left(z_2 + \frac{1}{2}\right)\,\mathbf{a}_3$	$=$	$-ax_2\,\hat{\mathbf{x}} + by_2\,\hat{\mathbf{y}} + c\left(z_2 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8d)	Bi I
$\mathbf{B_7}$	$=$	$(x_3 - y_3)\,\mathbf{a}_1 + (x_3 + y_3)\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	$=$	$ax_3\,\hat{\mathbf{x}} + by_3\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(8d)	Ca I
$\mathbf{B_8}$	$=$	$-(x_3 - y_3)\,\mathbf{a}_1 - (x_3 + y_3)\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	$=$	$-ax_3\,\hat{\mathbf{x}} - by_3\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(8d)	Ca I
$\mathbf{B_9}$	$=$	$(x_3 + y_3)\,\mathbf{a}_1 + (x_3 - y_3)\,\mathbf{a}_2 + \left(z_3 + \frac{1}{2}\right)\,\mathbf{a}_3$	$=$	$ax_3\,\hat{\mathbf{x}} - by_3\,\hat{\mathbf{y}} + c\left(z_3 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8d)	Ca I
$\mathbf{B_{10}}$	$=$	$-(x_3 + y_3)\,\mathbf{a}_1 - (x_3 - y_3)\,\mathbf{a}_2 + \left(z_3 + \frac{1}{2}\right)\,\mathbf{a}_3$	$=$	$-ax_3\,\hat{\mathbf{x}} + by_3\,\hat{\mathbf{y}} + c\left(z_3 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8d)	Ca I
$\mathbf{B_{11}}$	$=$	$(x_4 - y_4)\,\mathbf{a}_1 + (x_4 + y_4)\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	$=$	$ax_4\,\hat{\mathbf{x}} + by_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(8d)	Cu II
$\mathbf{B_{12}}$	$=$	$-(x_4 - y_4)\,\mathbf{a}_1 - (x_4 + y_4)\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	$=$	$-ax_4\,\hat{\mathbf{x}} - by_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(8d)	Cu II
$\mathbf{B_{13}}$	$=$	$(x_4 + y_4)\,\mathbf{a}_1 + (x_4 - y_4)\,\mathbf{a}_2 + \left(z_4 + \frac{1}{2}\right)\,\mathbf{a}_3$	$=$	$ax_4\,\hat{\mathbf{x}} - by_4\,\hat{\mathbf{y}} + c\left(z_4 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8d)	Cu II
$\mathbf{B_{14}}$	$=$	$-(x_4 + y_4)\,\mathbf{a}_1 - (x_4 - y_4)\,\mathbf{a}_2 + \left(z_4 + \frac{1}{2}\right)\,\mathbf{a}_3$	$=$	$-ax_4\,\hat{\mathbf{x}} + by_4\,\hat{\mathbf{y}} + c\left(z_4 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8d)	Cu II
$\mathbf{B_{15}}$	$=$	$(x_5 - y_5)\,\mathbf{a}_1 + (x_5 + y_5)\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	$=$	$ax_5\,\hat{\mathbf{x}} + by_5\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(8d)	O I
$\mathbf{B_{16}}$	$=$	$-(x_5 - y_5)\,\mathbf{a}_1 - (x_5 + y_5)\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	$=$	$-ax_5\,\hat{\mathbf{x}} - by_5\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(8d)	O I
$\mathbf{B_{17}}$	$=$	$(x_5 + y_5)\,\mathbf{a}_1 + (x_5 - y_5)\,\mathbf{a}_2 + \left(z_5 + \frac{1}{2}\right)\,\mathbf{a}_3$	$=$	$ax_5\,\hat{\mathbf{x}} - by_5\,\hat{\mathbf{y}} + c\left(z_5 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8d)	O I
$\mathbf{B_{18}}$	$=$	$-(x_5 + y_5)\,\mathbf{a}_1 - (x_5 - y_5)\,\mathbf{a}_2 + \left(z_5 + \frac{1}{2}\right)\,\mathbf{a}_3$	$=$	$-ax_5\,\hat{\mathbf{x}} + by_5\,\hat{\mathbf{y}} + c\left(z_5 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8d)	O I
$\mathbf{B_{19}}$	$=$	$(x_6 - y_6)\,\mathbf{a}_1 + (x_6 + y_6)\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	$=$	$ax_6\,\hat{\mathbf{x}} + by_6\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(8d)	O II
$\mathbf{B_{20}}$	$=$	$-(x_6 - y_6)\,\mathbf{a}_1 - (x_6 + y_6)\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	$=$	$-ax_6\,\hat{\mathbf{x}} - by_6\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(8d)	O II
$\mathbf{B_{21}}$	$=$	$(x_6 + y_6)\,\mathbf{a}_1 + (x_6 - y_6)\,\mathbf{a}_2 + \left(z_6 + \frac{1}{2}\right)\,\mathbf{a}_3$	$=$	$ax_6\,\hat{\mathbf{x}} - by_6\,\hat{\mathbf{y}} + c\left(z_6 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8d)	O II
$\mathbf{B_{22}}$	$=$	$-(x_6 + y_6)\,\mathbf{a}_1 - (x_6 - y_6)\,\mathbf{a}_2 + \left(z_6 + \frac{1}{2}\right)\,\mathbf{a}_3$	$=$	$-ax_6\,\hat{\mathbf{x}} + by_6\,\hat{\mathbf{y}} + c\left(z_6 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8d)	O II
$\mathbf{B_{23}}$	$=$	$(x_7 - y_7)\,\mathbf{a}_1 + (x_7 + y_7)\,\mathbf{a}_2 + z_7\,\mathbf{a}_3$	$=$	$ax_7\,\hat{\mathbf{x}} + by_7\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}}$	(8d)	O III
$\mathbf{B_{24}}$	$=$	$-(x_7 - y_7)\,\mathbf{a}_1 - (x_7 + y_7)\,\mathbf{a}_2 + z_7\,\mathbf{a}_3$	$=$	$-ax_7\,\hat{\mathbf{x}} - by_7\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}}$	(8d)	O III

$$\mathbf{B_{25}} = \begin{array}{c}(x_7 + y_7)\,\mathbf{a}_1 + (x_7 - y_7)\,\mathbf{a}_2 + \\ \left(z_7 + \tfrac{1}{2}\right)\mathbf{a}_3\end{array} \quad = \quad ax_7\,\hat{\mathbf{x}} - by_7\,\hat{\mathbf{y}} + c\left(z_7 + \tfrac{1}{2}\right)\hat{\mathbf{z}} \qquad (8d) \qquad \text{O III}$$

$$\mathbf{B_{26}} = \begin{array}{c}-(x_7 + y_7)\,\mathbf{a}_1 - (x_7 - y_7)\,\mathbf{a}_2 + \\ \left(z_7 + \tfrac{1}{2}\right)\mathbf{a}_3\end{array} \quad = \quad -ax_7\,\hat{\mathbf{x}} + by_7\,\hat{\mathbf{y}} + c\left(z_7 + \tfrac{1}{2}\right)\hat{\mathbf{z}} \qquad (8d) \qquad \text{O III}$$

$$\mathbf{B_{27}} = \begin{array}{c}(x_8 - y_8)\,\mathbf{a}_1 + (x_8 + y_8)\,\mathbf{a}_2 + \\ z_8\,\mathbf{a}_3\end{array} \quad = \quad ax_8\,\hat{\mathbf{x}} + by_8\,\hat{\mathbf{y}} + cz_8\,\hat{\mathbf{z}} \qquad (8d) \qquad \text{O IV}$$

$$\mathbf{B_{28}} = \begin{array}{c}-(x_8 - y_8)\,\mathbf{a}_1 - (x_8 + y_8)\,\mathbf{a}_2 + \\ z_8\,\mathbf{a}_3\end{array} \quad = \quad -ax_8\,\hat{\mathbf{x}} - by_8\,\hat{\mathbf{y}} + cz_8\,\hat{\mathbf{z}} \qquad (8d) \qquad \text{O IV}$$

$$\mathbf{B_{29}} = \begin{array}{c}(x_8 + y_8)\,\mathbf{a}_1 + (x_8 - y_8)\,\mathbf{a}_2 + \\ \left(z_8 + \tfrac{1}{2}\right)\mathbf{a}_3\end{array} \quad = \quad ax_8\,\hat{\mathbf{x}} - by_8\,\hat{\mathbf{y}} + c\left(z_8 + \tfrac{1}{2}\right)\hat{\mathbf{z}} \qquad (8d) \qquad \text{O IV}$$

$$\mathbf{B_{30}} = \begin{array}{c}-(x_8 + y_8)\,\mathbf{a}_1 - (x_8 - y_8)\,\mathbf{a}_2 + \\ \left(z_8 + \tfrac{1}{2}\right)\mathbf{a}_3\end{array} \quad = \quad -ax_8\,\hat{\mathbf{x}} + by_8\,\hat{\mathbf{y}} + c\left(z_8 + \tfrac{1}{2}\right)\hat{\mathbf{z}} \qquad (8d) \qquad \text{O IV}$$

$$\mathbf{B_{31}} = \begin{array}{c}(x_9 - y_9)\,\mathbf{a}_1 + (x_9 + y_9)\,\mathbf{a}_2 + \\ z_9\,\mathbf{a}_3\end{array} \quad = \quad ax_9\,\hat{\mathbf{x}} + by_9\,\hat{\mathbf{y}} + cz_9\,\hat{\mathbf{z}} \qquad (8d) \qquad \text{O V}$$

$$\mathbf{B_{32}} = \begin{array}{c}-(x_9 - y_9)\,\mathbf{a}_1 - (x_9 + y_9)\,\mathbf{a}_2 + \\ z_9\,\mathbf{a}_3\end{array} \quad = \quad -ax_9\,\hat{\mathbf{x}} - by_9\,\hat{\mathbf{y}} + cz_9\,\hat{\mathbf{z}} \qquad (8d) \qquad \text{O V}$$

$$\mathbf{B_{33}} = \begin{array}{c}(x_9 + y_9)\,\mathbf{a}_1 + (x_9 - y_9)\,\mathbf{a}_2 + \\ \left(z_9 + \tfrac{1}{2}\right)\mathbf{a}_3\end{array} \quad = \quad ax_9\,\hat{\mathbf{x}} - by_9\,\hat{\mathbf{y}} + c\left(z_9 + \tfrac{1}{2}\right)\hat{\mathbf{z}} \qquad (8d) \qquad \text{O V}$$

$$\mathbf{B_{34}} = \begin{array}{c}-(x_9 + y_9)\,\mathbf{a}_1 - (x_9 - y_9)\,\mathbf{a}_2 + \\ \left(z_9 + \tfrac{1}{2}\right)\mathbf{a}_3\end{array} \quad = \quad -ax_9\,\hat{\mathbf{x}} + by_9\,\hat{\mathbf{y}} + c\left(z_9 + \tfrac{1}{2}\right)\hat{\mathbf{z}} \qquad (8d) \qquad \text{O V}$$

$$\mathbf{B_{35}} = \begin{array}{c}(x_{10} - y_{10})\,\mathbf{a}_1 + \\ (x_{10} + y_{10})\,\mathbf{a}_2 + z_{10}\,\mathbf{a}_3\end{array} \quad = \quad ax_{10}\,\hat{\mathbf{x}} + by_{10}\,\hat{\mathbf{y}} + cz_{10}\,\hat{\mathbf{z}} \qquad (8d) \qquad \text{Sr I}$$

$$\mathbf{B_{36}} = \begin{array}{c}-(x_{10} - y_{10})\,\mathbf{a}_1 - \\ (x_{10} + y_{10})\,\mathbf{a}_2 + z_{10}\,\mathbf{a}_3\end{array} \quad = \quad -ax_{10}\,\hat{\mathbf{x}} - by_{10}\,\hat{\mathbf{y}} + cz_{10}\,\hat{\mathbf{z}} \qquad (8d) \qquad \text{Sr I}$$

$$\mathbf{B_{37}} = \begin{array}{c}(x_{10} + y_{10})\,\mathbf{a}_1 + \\ (x_{10} - y_{10})\,\mathbf{a}_2 + \left(z_{10} + \tfrac{1}{2}\right)\mathbf{a}_3\end{array} \quad = \quad ax_{10}\,\hat{\mathbf{x}} - by_{10}\,\hat{\mathbf{y}} + c\left(z_{10} + \tfrac{1}{2}\right)\hat{\mathbf{z}} \qquad (8d) \qquad \text{Sr I}$$

$$\mathbf{B_{38}} = \begin{array}{c}-(x_{10} + y_{10})\,\mathbf{a}_1 - \\ (x_{10} - y_{10})\,\mathbf{a}_2 + \left(z_{10} + \tfrac{1}{2}\right)\mathbf{a}_3\end{array} \quad = \quad -ax_{10}\,\hat{\mathbf{x}} + by_{10}\,\hat{\mathbf{y}} + c\left(z_{10} + \tfrac{1}{2}\right)\hat{\mathbf{z}} \qquad (8d) \qquad \text{Sr I}$$

References

[1] V. F. Shamray, A. B. Mikhailova, and A. V. Mitin, *Crystal structure and superconductivity of Bi-2223*, Crystallogr. Rep. **54**, 584–590 (2009), doi:10.1134/S1063774509040075.