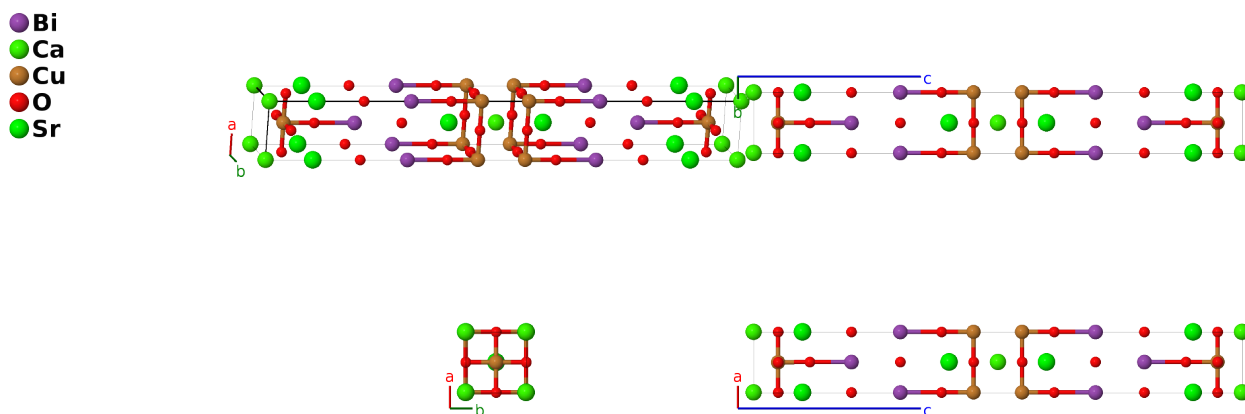


Bi₂Sr₂CaCu₂O₈ (BSCCO) Structure: A2BC2D8E2_tI30_139_e_a_e_2eg_e-001

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<https://aflow.org/p/BZRA>

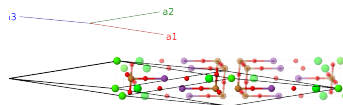
https://aflow.org/p/A2BC2D8E2_tI30_139_e_a_e_2eg_e-001



Prototype	Ba ₂ CaCu ₂ O ₈ Sr ₂
AFLOW prototype label	A2BC2D8E2_tI30_139_e_a_e_2eg_e-001
ICSD	68188
Pearson symbol	tI30
Space group number	139
Space group symbol	<i>I4/mmm</i>
AFLOW prototype command	<code>aflow --proto=A2BC2D8E2_tI30_139_e_a_e_2eg_e-001 --params=a, c/a, z₂, z₃, z₄, z₅, z₆, z₇</code>

Body-centered Tetragonal primitive vectors

$$\begin{aligned} \mathbf{a}_1 &= -\frac{1}{2}a \hat{x} + \frac{1}{2}a \hat{y} + \frac{1}{2}c \hat{z} \\ \mathbf{a}_2 &= \frac{1}{2}a \hat{x} - \frac{1}{2}a \hat{y} + \frac{1}{2}c \hat{z} \\ \mathbf{a}_3 &= \frac{1}{2}a \hat{x} + \frac{1}{2}a \hat{y} - \frac{1}{2}c \hat{z} \end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
\mathbf{B}_1	=	0	=	0	(2a) Ca I
\mathbf{B}_2	=	$z_2 \mathbf{a}_1 + z_2 \mathbf{a}_2$	=	$cz_2 \hat{z}$	(4e) Bi I
\mathbf{B}_3	=	$-z_2 \mathbf{a}_1 - z_2 \mathbf{a}_2$	=	$-cz_2 \hat{z}$	(4e) Bi I
\mathbf{B}_4	=	$z_3 \mathbf{a}_1 + z_3 \mathbf{a}_2$	=	$cz_3 \hat{z}$	(4e) Cu I

\mathbf{B}_5	$=$	$-z_3 \mathbf{a}_1 - z_3 \mathbf{a}_2$	$=$	$-cz_3 \hat{\mathbf{z}}$	(4e)	Cu I
\mathbf{B}_6	$=$	$z_4 \mathbf{a}_1 + z_4 \mathbf{a}_2$	$=$	$cz_4 \hat{\mathbf{z}}$	(4e)	O I
\mathbf{B}_7	$=$	$-z_4 \mathbf{a}_1 - z_4 \mathbf{a}_2$	$=$	$-cz_4 \hat{\mathbf{z}}$	(4e)	O I
\mathbf{B}_8	$=$	$z_5 \mathbf{a}_1 + z_5 \mathbf{a}_2$	$=$	$cz_5 \hat{\mathbf{z}}$	(4e)	O II
\mathbf{B}_9	$=$	$-z_5 \mathbf{a}_1 - z_5 \mathbf{a}_2$	$=$	$-cz_5 \hat{\mathbf{z}}$	(4e)	O II
\mathbf{B}_{10}	$=$	$z_6 \mathbf{a}_1 + z_6 \mathbf{a}_2$	$=$	$cz_6 \hat{\mathbf{z}}$	(4e)	Sr I
\mathbf{B}_{11}	$=$	$-z_6 \mathbf{a}_1 - z_6 \mathbf{a}_2$	$=$	$-cz_6 \hat{\mathbf{z}}$	(4e)	Sr I
\mathbf{B}_{12}	$=$	$(z_7 + \frac{1}{2}) \mathbf{a}_1 + z_7 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{y}} + cz_7 \hat{\mathbf{z}}$	(8g)	O III
\mathbf{B}_{13}	$=$	$z_7 \mathbf{a}_1 + (z_7 + \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + cz_7 \hat{\mathbf{z}}$	(8g)	O III
\mathbf{B}_{14}	$=$	$-(z_7 - \frac{1}{2}) \mathbf{a}_1 - z_7 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{y}} - cz_7 \hat{\mathbf{z}}$	(8g)	O III
\mathbf{B}_{15}	$=$	$-z_7 \mathbf{a}_1 - (z_7 - \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} - cz_7 \hat{\mathbf{z}}$	(8g)	O III

References

- [1] J. K. Liang, S. S. Xie, G. C. Che, J. Q. Huang, Y. L. Zhang, and Z. X. Zhao, *Crystal Structure and Superconductivity of $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_8$ Compound*, Mod. Phys. Lett. B **2**, 483–489 (1988), doi:10.1142/S0217984988000059.