$SrCu_2(BO_3)_2$ Structure: A2B2C6D_tI44_121_i_i_ij_c-001

This structure originally had the label `A2B2C6D_tI44_121_i_i_ij_c`. Calls to that address will be redirected here.

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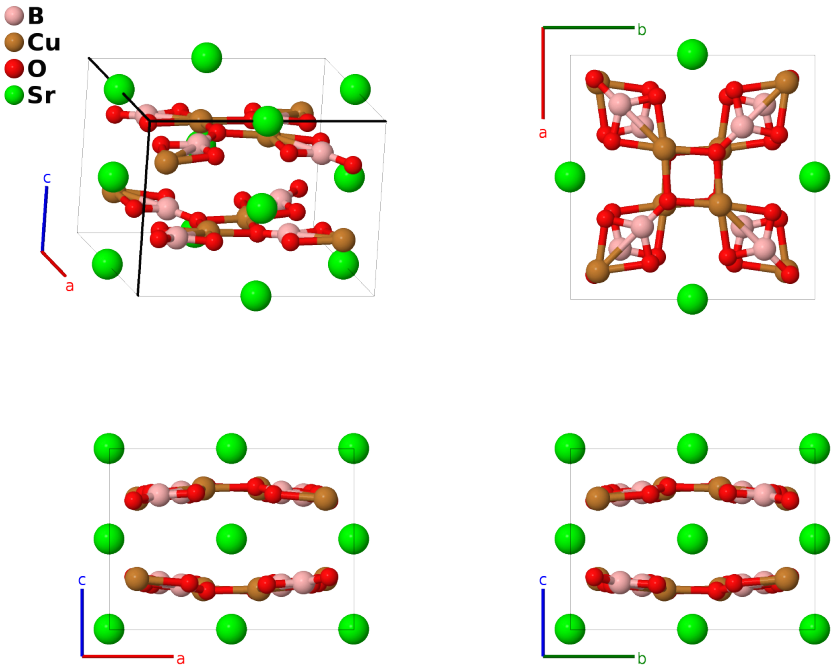
https://aflow.org/p/USSD

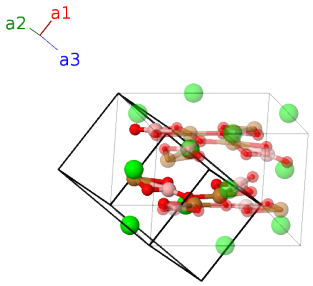
https://aflow.org/p/A2B2C6D_tI44_121_i_i_ij_c-001



Prototype	$B_2Cu_2O_6Sr$
AFLOW prototype label	A2B2C6D_tI44_121_i_i_ij_c-001
ICSD	80592
Pearson symbol	tI44
Space group number	121
Space group symbol	$I\bar{4}2m$
AFLOW prototype command	`aflow --proto=A2B2C6D_tI44_121_i_i_ij_c-001 --params=`$a, c/a, x_2, z_2, x_3, z_3, x_4, z_4, x_5, y_5, z_5$

Body-centered Tetragonal primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{y}}$	(4c)	Sr I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}}$	(4c)	Sr I
$\mathbf{B_3}$	=	$(x_2 + z_2)\,\mathbf{a}_1 + (x_2 + z_2)\,\mathbf{a}_2 + 2x_2\,\mathbf{a}_3$	=	$ax_2\,\hat{\mathbf{x}} + ax_2\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(8i)	B I
$\mathbf{B_4}$	=	$-(x_2 - z_2)\,\mathbf{a}_1 - (x_2 - z_2)\,\mathbf{a}_2 - 2x_2\,\mathbf{a}_3$	=	$-ax_2\,\hat{\mathbf{x}} - ax_2\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(8i)	B I
$\mathbf{B_5}$	=	$-(x_2 + z_2)\,\mathbf{a}_1 + (x_2 - z_2)\,\mathbf{a}_2$	=	$ax_2\,\hat{\mathbf{x}} - ax_2\,\hat{\mathbf{y}} - cz_2\,\hat{\mathbf{z}}$	(8i)	B I
$\mathbf{B_6}$	=	$(x_2 - z_2)\,\mathbf{a}_1 - (x_2 + z_2)\,\mathbf{a}_2$	=	$-ax_2\,\hat{\mathbf{x}} + ax_2\,\hat{\mathbf{y}} - cz_2\,\hat{\mathbf{z}}$	(8i)	B I
$\mathbf{B_7}$	=	$(x_3 + z_3)\,\mathbf{a}_1 + (x_3 + z_3)\,\mathbf{a}_2 + 2x_3\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} + ax_3\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(8i)	Cu I
$\mathbf{B_8}$	=	$-(x_3 - z_3)\,\mathbf{a}_1 - (x_3 - z_3)\,\mathbf{a}_2 - 2x_3\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} - ax_3\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(8i)	Cu I
$\mathbf{B_9}$	=	$-(x_3 + z_3)\,\mathbf{a}_1 + (x_3 - z_3)\,\mathbf{a}_2$	=	$ax_3\,\hat{\mathbf{x}} - ax_3\,\hat{\mathbf{y}} - cz_3\,\hat{\mathbf{z}}$	(8i)	Cu I
$\mathbf{B_{10}}$	=	$(x_3 - z_3)\,\mathbf{a}_1 - (x_3 + z_3)\,\mathbf{a}_2$	=	$-ax_3\,\hat{\mathbf{x}} + ax_3\,\hat{\mathbf{y}} - cz_3\,\hat{\mathbf{z}}$	(8i)	Cu I
$\mathbf{B_{11}}$	=	$(x_4 + z_4)\,\mathbf{a}_1 + (x_4 + z_4)\,\mathbf{a}_2 + 2x_4\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}} + ax_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(8i)	O I
$\mathbf{B_{12}}$	=	$-(x_4 - z_4)\,\mathbf{a}_1 - (x_4 - z_4)\,\mathbf{a}_2 - 2x_4\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}} - ax_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(8i)	O I
$\mathbf{B_{13}}$	=	$-(x_4 + z_4)\,\mathbf{a}_1 + (x_4 - z_4)\,\mathbf{a}_2$	=	$ax_4\,\hat{\mathbf{x}} - ax_4\,\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$	(8i)	O I
$\mathbf{B_{14}}$	=	$(x_4 - z_4)\,\mathbf{a}_1 - (x_4 + z_4)\,\mathbf{a}_2$	=	$-ax_4\,\hat{\mathbf{x}} + ax_4\,\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$	(8i)	O I
$\mathbf{B_{15}}$	=	$(y_5 + z_5)\,\mathbf{a}_1 + (x_5 + z_5)\,\mathbf{a}_2 + (x_5 + y_5)\,\mathbf{a}_3$	=	$ax_5\,\hat{\mathbf{x}} + ay_5\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(16j)	O II
$\mathbf{B_{16}}$	=	$-(y_5 - z_5)\,\mathbf{a}_1 - (x_5 - z_5)\,\mathbf{a}_2 - (x_5 + y_5)\,\mathbf{a}_3$	=	$-ax_5\,\hat{\mathbf{x}} - ay_5\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(16j)	O II
$\mathbf{B_{17}}$	=	$-(x_5 + z_5)\,\mathbf{a}_1 + (y_5 - z_5)\,\mathbf{a}_2 - (x_5 - y_5)\,\mathbf{a}_3$	=	$ay_5\,\hat{\mathbf{x}} - ax_5\,\hat{\mathbf{y}} - cz_5\,\hat{\mathbf{z}}$	(16j)	O II
$\mathbf{B_{18}}$	=	$(x_5 - z_5)\,\mathbf{a}_1 - (y_5 + z_5)\,\mathbf{a}_2 + (x_5 - y_5)\,\mathbf{a}_3$	=	$-ay_5\,\hat{\mathbf{x}} + ax_5\,\hat{\mathbf{y}} - cz_5\,\hat{\mathbf{z}}$	(16j)	O II
$\mathbf{B_{19}}$	=	$(y_5 - z_5)\,\mathbf{a}_1 - (x_5 + z_5)\,\mathbf{a}_2 - (x_5 - y_5)\,\mathbf{a}_3$	=	$-ax_5\,\hat{\mathbf{x}} + ay_5\,\hat{\mathbf{y}} - cz_5\,\hat{\mathbf{z}}$	(16j)	O II
$\mathbf{B_{20}}$	=	$-(y_5 + z_5)\,\mathbf{a}_1 + (x_5 - z_5)\,\mathbf{a}_2 + (x_5 - y_5)\,\mathbf{a}_3$	=	$ax_5\,\hat{\mathbf{x}} - ay_5\,\hat{\mathbf{y}} - cz_5\,\hat{\mathbf{z}}$	(16j)	O II
$\mathbf{B_{21}}$	=	$-(x_5 - z_5)\,\mathbf{a}_1 - (y_5 - z_5)\,\mathbf{a}_2 - (x_5 + y_5)\,\mathbf{a}_3$	=	$-ay_5\,\hat{\mathbf{x}} - ax_5\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(16j)	O II

$$\mathbf{B_{22}} = (x_5 + z_5)\,\mathbf{a}_1 + (y_5 + z_5)\,\mathbf{a}_2 + (x_5 + y_5)\,\mathbf{a}_3 = a y_5\,\hat{\mathbf{x}} + a x_5\,\hat{\mathbf{y}} + c z_5\,\hat{\mathbf{z}} \quad \text{(16j)} \quad \text{O II}$$

References

[1] R. W. Smith and D. A. Keszler, *Synthesis, structure, and properties of the orthoborate $SrCu_2(BO_3)_2$*, J. Solid State Chem. **93**, 430–435 (1991), doi:10.1016/0022-4596(91)90316-A.

Found in

[1] H. Kageyama, K. Yoshimura, R. Stern, N. V. Mushnikov, K. Onizuka, M. Kato, K. Kosuge, C. P. Slichter, T. Goto, and Y. Ueda, *Exact Dimer Ground State and Quantized Magnetization Plateaus in the Two-Dimensional Spin System $SrCu_2(BO_3)_2$*, Phys. Rev. Lett. **82**, 3168–3171 (1999), doi:10.1103/PhysRevLett.82.3168.