"124 Superconductor" ($YBa_2Cu_4O_8$) Structure: A2B4C8D_oC30_65_h_2g_3gh_c-001

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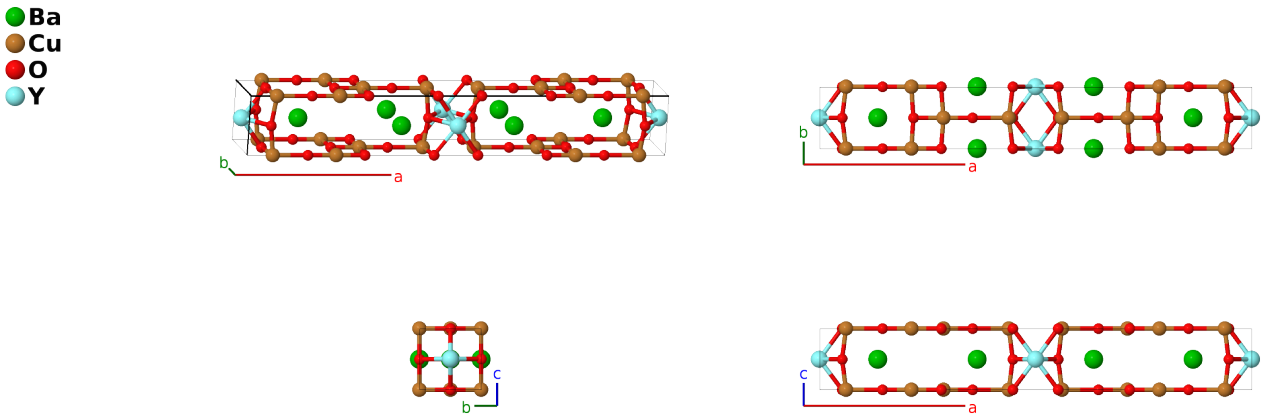
https://aflow.org/p/2EBJ

https://aflow.org/p/A2B4C8D_oC30_65_h_2g_3gh_c-001

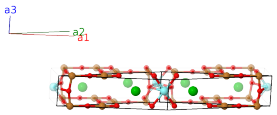


Prototype	$Ba_2Cu_4O_8Y$
AFLOW prototype label	A2B4C8D_oC30_65_h_2g_3gh_c-001
ICSD	none
Pearson symbol	oC30
Space group number	65
Space group symbol	$Cmmm$
AFLOW prototype command	`aflow --proto=A2B4C8D_oC30_65_h_2g_3gh_c-001 --params=`$a, b/a, c/a, x_2, x_3, x_4, x_5, x_6, x_7, x_8$

- Unlike most BCO-type superconductors, the stoichiometry of $YBa_2Cu_4O_8$ is fixed.
- We use the ambient pressure data from (Bordet, 1989) taken at room temperature.
- Although it is never explicitly stated by (Bordet, 1989), (Nelmes, 1990) notes that this data is given in the $Ammm$ setting of space group #65, making the long axis in the z-direction. The standard orientation is $Cmmm$, and we use FINDSYM to rotate the structure, putting the long axis in the x-direction.

Base-centered Orthorhombic primitive vectors

$$\mathbf{a_1} = \frac{1}{2}a\,\hat{\mathbf{x}} - \frac{1}{2}b\,\hat{\mathbf{y}}$$
$$\mathbf{a_2} = \frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}b\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(2c)	Y I
$\mathbf{B_2}$	=	$x_2\,\mathbf{a}_1 + x_2\,\mathbf{a}_2$	=	$ax_2\,\hat{\mathbf{x}}$	(4g)	Cu I
$\mathbf{B_3}$	=	$-x_2\,\mathbf{a}_1 - x_2\,\mathbf{a}_2$	=	$-ax_2\,\hat{\mathbf{x}}$	(4g)	Cu I
$\mathbf{B_4}$	=	$x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2$	=	$ax_3\,\hat{\mathbf{x}}$	(4g)	Cu II
$\mathbf{B_5}$	=	$-x_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2$	=	$-ax_3\,\hat{\mathbf{x}}$	(4g)	Cu II
$\mathbf{B_6}$	=	$x_4\,\mathbf{a}_1 + x_4\,\mathbf{a}_2$	=	$ax_4\,\hat{\mathbf{x}}$	(4g)	O I
$\mathbf{B_7}$	=	$-x_4\,\mathbf{a}_1 - x_4\,\mathbf{a}_2$	=	$-ax_4\,\hat{\mathbf{x}}$	(4g)	O I
$\mathbf{B_8}$	=	$x_5\,\mathbf{a}_1 + x_5\,\mathbf{a}_2$	=	$ax_5\,\hat{\mathbf{x}}$	(4g)	O II
$\mathbf{B_9}$	=	$-x_5\,\mathbf{a}_1 - x_5\,\mathbf{a}_2$	=	$-ax_5\,\hat{\mathbf{x}}$	(4g)	O II
$\mathbf{B_{10}}$	=	$x_6\,\mathbf{a}_1 + x_6\,\mathbf{a}_2$	=	$ax_6\,\hat{\mathbf{x}}$	(4g)	O III
$\mathbf{B_{11}}$	=	$-x_6\,\mathbf{a}_1 - x_6\,\mathbf{a}_2$	=	$-ax_6\,\hat{\mathbf{x}}$	(4g)	O III
$\mathbf{B_{12}}$	=	$x_7\,\mathbf{a}_1 + x_7\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$ax_7\,\hat{\mathbf{x}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4h)	Ba I
$\mathbf{B_{13}}$	=	$-x_7\,\mathbf{a}_1 - x_7\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-ax_7\,\hat{\mathbf{x}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4h)	Ba I
$\mathbf{B_{14}}$	=	$x_8\,\mathbf{a}_1 + x_8\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$ax_8\,\hat{\mathbf{x}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4h)	O IV
$\mathbf{B_{15}}$	=	$-x_8\,\mathbf{a}_1 - x_8\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-ax_8\,\hat{\mathbf{x}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4h)	O IV

References

[1] P. Bordet, J. L. Hodeau, R. Argoud, J. Muller, M. Marezio, , J. C. Martinez, J. J. Prejean, J. Karpinski, E. Kaldis, S. Rusiecki, and B. Bucher, *Single crystal study of the 80K superconductor $YBa_2Cu_4O_8$*, Prog. Solid State Chem. **162-164**, 524–525 (1989), doi:10.1016/0921-4534(89)91137-4.

Found in

[1] R. J. Nelmes, J. S. Loveday, E. Kaldis, and J. Karpinski, *The crystal structure of $YBa_2Cu_4O_8$ as a function of pressure up to 5 GPa*, Prog. Solid State Chem. **172**, 311–324 (1990), doi:10.1016/0921-4534(90)90622-L.