# "247 Superconductor" ($Y_2Ba_4Cu_7O_{15}$) Structure: A4B7C16D2_oC58_65_2h_b3g_ac5g2h_h-001

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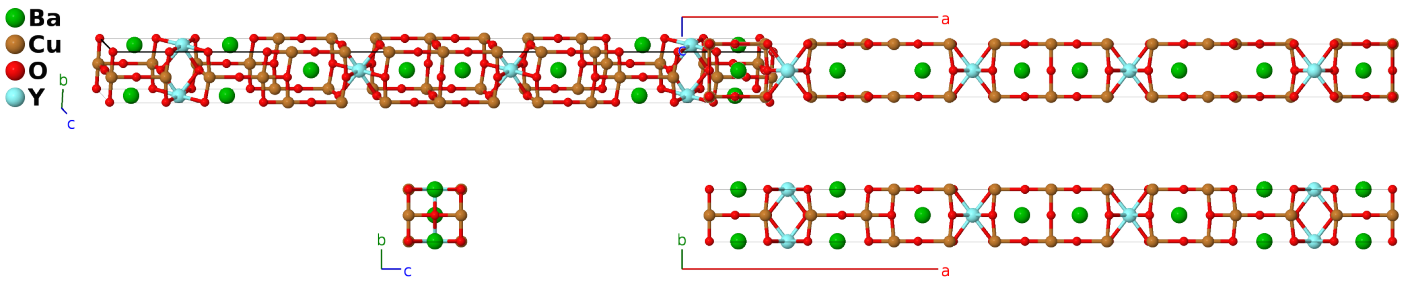
https://aflow.org/p/A4B7C16D2_oC58_65_2h_b3g_ac5g2h_h-001




| | |
|---|---|
| **Prototype** | $Ba_4Cu_7O_{15}Y_2$ |
| **AFLOW prototype label** | A4B7C16D2_oC58_65_2h_b3g_ac5g2h_h-001 |
| **ICSD** | 69254 |
| **Pearson symbol** | oC58 |
| **Space group number** | 65 |
| **Space group symbol** | $Cmmm$ |
| **AFLOW prototype command** | `aflow --proto=A4B7C16D2_oC58_65_2h_b3g_ac5g2h_h-001 --params=`$a, b/a, c/a, x_4, x_5, x_6, x_7, x_8, x_9, x_{10}, x_{11}, x_{12}, x_{13}, x_{14}, x_{15}, x_{16}$ |

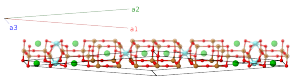
**Other compounds with this structure**

$Pr_2Ba_4Cu_7O_{15}$

- We use the ambient pressure data from (Hewat, 1990) taken at 22K. The stoichiometry of this system is $Y_2Ba_4Cu_7O_{15+\delta}$, and here the O-I (2a) site is only occupied 84% of the time, while the O-II (2c) occupation is 24%.
- Traditionally this structure is shown in the $Ammm$ setting of space group #65 so that the long axis in the $z$-direction. The standard orientation is $Cmmm$, and we use FINDSYM and AFLOW 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 |
|---|---|---|---|---|---|
| $\mathbf{B_1}$ = | 0 | = | 0 | (2a) | O I |

| | | | | | | |
|---|---|---|---|---|---|---|
| $\mathbf{B_2}$ | = | $\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2$ | = | $\frac{1}{2}a\,\hat{\mathbf{x}}$ | (2b) | Cu I |
| $\mathbf{B_3}$ | = | $\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$ | = | $\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}c\,\hat{\mathbf{z}}$ | (2c) | O II |
| $\mathbf{B_4}$ | = | $x_4\,\mathbf{a}_1 + x_4\,\mathbf{a}_2$ | = | $ax_4\,\hat{\mathbf{x}}$ | (4g) | Cu II |
| $\mathbf{B_5}$ | = | $-x_4\,\mathbf{a}_1 - x_4\,\mathbf{a}_2$ | = | $-ax_4\,\hat{\mathbf{x}}$ | (4g) | Cu II |
| $\mathbf{B_6}$ | = | $x_5\,\mathbf{a}_1 + x_5\,\mathbf{a}_2$ | = | $ax_5\,\hat{\mathbf{x}}$ | (4g) | Cu III |
| $\mathbf{B_7}$ | = | $-x_5\,\mathbf{a}_1 - x_5\,\mathbf{a}_2$ | = | $-ax_5\,\hat{\mathbf{x}}$ | (4g) | Cu III |
| $\mathbf{B_8}$ | = | $x_6\,\mathbf{a}_1 + x_6\,\mathbf{a}_2$ | = | $ax_6\,\hat{\mathbf{x}}$ | (4g) | Cu IV |
| $\mathbf{B_9}$ | = | $-x_6\,\mathbf{a}_1 - x_6\,\mathbf{a}_2$ | = | $-ax_6\,\hat{\mathbf{x}}$ | (4g) | Cu IV |
| $\mathbf{B_{10}}$ | = | $x_7\,\mathbf{a}_1 + x_7\,\mathbf{a}_2$ | = | $ax_7\,\hat{\mathbf{x}}$ | (4g) | O III |
| $\mathbf{B_{11}}$ | = | $-x_7\,\mathbf{a}_1 - x_7\,\mathbf{a}_2$ | = | $-ax_7\,\hat{\mathbf{x}}$ | (4g) | O III |
| $\mathbf{B_{12}}$ | = | $x_8\,\mathbf{a}_1 + x_8\,\mathbf{a}_2$ | = | $ax_8\,\hat{\mathbf{x}}$ | (4g) | O IV |
| $\mathbf{B_{13}}$ | = | $-x_8\,\mathbf{a}_1 - x_8\,\mathbf{a}_2$ | = | $-ax_8\,\hat{\mathbf{x}}$ | (4g) | O IV |
| $\mathbf{B_{14}}$ | = | $x_9\,\mathbf{a}_1 + x_9\,\mathbf{a}_2$ | = | $ax_9\,\hat{\mathbf{x}}$ | (4g) | O V |
| $\mathbf{B_{15}}$ | = | $-x_9\,\mathbf{a}_1 - x_9\,\mathbf{a}_2$ | = | $-ax_9\,\hat{\mathbf{x}}$ | (4g) | O V |
| $\mathbf{B_{16}}$ | = | $x_{10}\,\mathbf{a}_1 + x_{10}\,\mathbf{a}_2$ | = | $ax_{10}\,\hat{\mathbf{x}}$ | (4g) | O VI |
| $\mathbf{B_{17}}$ | = | $-x_{10}\,\mathbf{a}_1 - x_{10}\,\mathbf{a}_2$ | = | $-ax_{10}\,\hat{\mathbf{x}}$ | (4g) | O VI |
| $\mathbf{B_{18}}$ | = | $x_{11}\,\mathbf{a}_1 + x_{11}\,\mathbf{a}_2$ | = | $ax_{11}\,\hat{\mathbf{x}}$ | (4g) | O VII |
| $\mathbf{B_{19}}$ | = | $-x_{11}\,\mathbf{a}_1 - x_{11}\,\mathbf{a}_2$ | = | $-ax_{11}\,\hat{\mathbf{x}}$ | (4g) | O VII |
| $\mathbf{B_{20}}$ | = | $x_{12}\,\mathbf{a}_1 + x_{12}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$ | = | $ax_{12}\,\hat{\mathbf{x}} + \frac{1}{2}c\,\hat{\mathbf{z}}$ | (4h) | Ba I |
| $\mathbf{B_{21}}$ | = | $-x_{12}\,\mathbf{a}_1 - x_{12}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$ | = | $-ax_{12}\,\hat{\mathbf{x}} + \frac{1}{2}c\,\hat{\mathbf{z}}$ | (4h) | Ba I |
| $\mathbf{B_{22}}$ | = | $x_{13}\,\mathbf{a}_1 + x_{13}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$ | = | $ax_{13}\,\hat{\mathbf{x}} + \frac{1}{2}c\,\hat{\mathbf{z}}$ | (4h) | Ba II |
| $\mathbf{B_{23}}$ | = | $-x_{13}\,\mathbf{a}_1 - x_{13}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$ | = | $-ax_{13}\,\hat{\mathbf{x}} + \frac{1}{2}c\,\hat{\mathbf{z}}$ | (4h) | Ba II |
| $\mathbf{B_{24}}$ | = | $x_{14}\,\mathbf{a}_1 + x_{14}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$ | = | $ax_{14}\,\hat{\mathbf{x}} + \frac{1}{2}c\,\hat{\mathbf{z}}$ | (4h) | O VIII |
| $\mathbf{B_{25}}$ | = | $-x_{14}\,\mathbf{a}_1 - x_{14}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$ | = | $-ax_{14}\,\hat{\mathbf{x}} + \frac{1}{2}c\,\hat{\mathbf{z}}$ | (4h) | O VIII |
| $\mathbf{B_{26}}$ | = | $x_{15}\,\mathbf{a}_1 + x_{15}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$ | = | $ax_{15}\,\hat{\mathbf{x}} + \frac{1}{2}c\,\hat{\mathbf{z}}$ | (4h) | O IX |
| $\mathbf{B_{27}}$ | = | $-x_{15}\,\mathbf{a}_1 - x_{15}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$ | = | $-ax_{15}\,\hat{\mathbf{x}} + \frac{1}{2}c\,\hat{\mathbf{z}}$ | (4h) | O IX |
| $\mathbf{B_{28}}$ | = | $x_{16}\,\mathbf{a}_1 + x_{16}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$ | = | $ax_{16}\,\hat{\mathbf{x}} + \frac{1}{2}c\,\hat{\mathbf{z}}$ | (4h) | Y I |
| $\mathbf{B_{29}}$ | = | $-x_{16}\,\mathbf{a}_1 - x_{16}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$ | = | $-ax_{16}\,\hat{\mathbf{x}} + \frac{1}{2}c\,\hat{\mathbf{z}}$ | (4h) | Y I |

## References


[1] A. W. Hewat, P. Fischer, E. Kaldis, J. Karpinski, S. Rusiecki, and E. Jilek, *High resolution neutron powder diffraction investigation of temperature and pressure effects on the structure of the high-$T_c$ superconductor $Y_2Ba_4Cu_7O_{15}$*, Physica C **167**, 579–590 (1990), doi:10.1016/0921-4534(90)90677-7.