1212C [$YBa_2Cu_3O_{7-x}$] High-T_c Structure: A2B3C7D_oP13_47_k_cj_aijl_f-001

This structure originally had the label `A2B3C7D_oP13_47_t_aq_eqrs_h`. Calls to that address will be redirected here.

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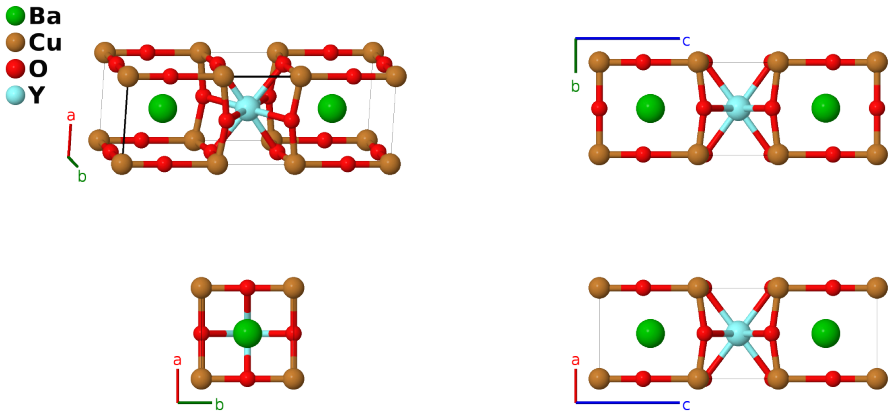
https://aflow.org/p/MZYC

https://aflow.org/p/A2B3C7D_oP13_47_k_cj_aijl_f-001



Prototype	$Ba_2Cu_3O_{7-x}Y$
AFLOW prototype label	A2B3C7D_oP13_47_k_cj_aijl_f-001
ICSD	62943
Pearson symbol	oP13
Space group number	47
Space group symbol	$Pmmm$
AFLOW prototype command	`aflow --proto=A2B3C7D_oP13_47_k_cj_aijl_f-001 --params=`$a, b/a, c/a, x_4, x_5, x_6, x_7, x_8$

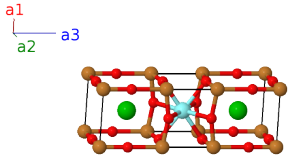
Other compounds with this structure

$GaSr_2(Y, Ca)Cu_2O_7$, $DyBa_2Cu_3O_{7-x}$

- The designation 1212C is from (Shaked, 1994). We will assume that the oxygen concentration is exactly 7. In experiment the O (2s) site is 92% occupied.

Simple Orthorhombic primitive vectors

$$\mathbf{a_1} = a\,\hat{\mathbf{x}}$$
$$\mathbf{a_2} = b\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(1a)	O I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}c\,\hat{\mathbf{z}}$	(1c)	Cu I
$\mathbf{B_3}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}b\,\hat{\mathbf{y}}$	(1f)	Y I
$\mathbf{B_4}$	=	$x_4\,\mathbf{a}_1$	=	$ax_4\,\hat{\mathbf{x}}$	(2i)	O II
$\mathbf{B_5}$	=	$-x_4\,\mathbf{a}_1$	=	$-ax_4\,\hat{\mathbf{x}}$	(2i)	O II
$\mathbf{B_6}$	=	$x_5\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_3$	=	$ax_5\,\hat{\mathbf{x}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(2j)	Cu II
$\mathbf{B_7}$	=	$-x_5\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_3$	=	$-ax_5\,\hat{\mathbf{x}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(2j)	Cu II
$\mathbf{B_8}$	=	$x_6\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_3$	=	$ax_6\,\hat{\mathbf{x}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(2j)	O III
$\mathbf{B_9}$	=	$-x_6\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_3$	=	$-ax_6\,\hat{\mathbf{x}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(2j)	O III
$\mathbf{B_{10}}$	=	$x_7\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2$	=	$ax_7\,\hat{\mathbf{x}} + \frac{1}{2}b\,\hat{\mathbf{y}}$	(2k)	Ba I
$\mathbf{B_{11}}$	=	$-x_7\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2$	=	$-ax_7\,\hat{\mathbf{x}} + \frac{1}{2}b\,\hat{\mathbf{y}}$	(2k)	Ba I
$\mathbf{B_{12}}$	=	$x_8\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$ax_8\,\hat{\mathbf{x}} + \frac{1}{2}b\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(2l)	O IV
$\mathbf{B_{13}}$	=	$-x_8\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-ax_8\,\hat{\mathbf{x}} + \frac{1}{2}b\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(2l)	O IV

References

[1] W. I. F. David, W. T. A. Harrison, J. M. F. Gunn, A. K. S. O. Moze, P. Day, J. D. Jorgensen, D. G. Hinks, M. A. Beno, L. Soderholm, D. W. C. Ii, I. K. Schuller, C. U. Segre, K. Zhang, and J. D. Grace, *Structure and crystal chemistry of the high-Tc superconductor $YBa_2Cu_3O_{7-x}$*, Nature **327**, 310–312 (1987), doi:10.1038/327310a0.

[2] H. Shaked, P. M. Keane, J. C. Rodrigues, F. F. Owen, R. L. Hitterman, and J. D. Jorgensen, *Crystal Structures of the High-T_c Superconducting Copper Oxides*, Elsevier Science B. V., Amsterdam (1994).