$HgBa_2CaCu_2O_{6+\delta}$ Structure: A2BC2DE7_tP13_123_g_b_h_c_ahi-001

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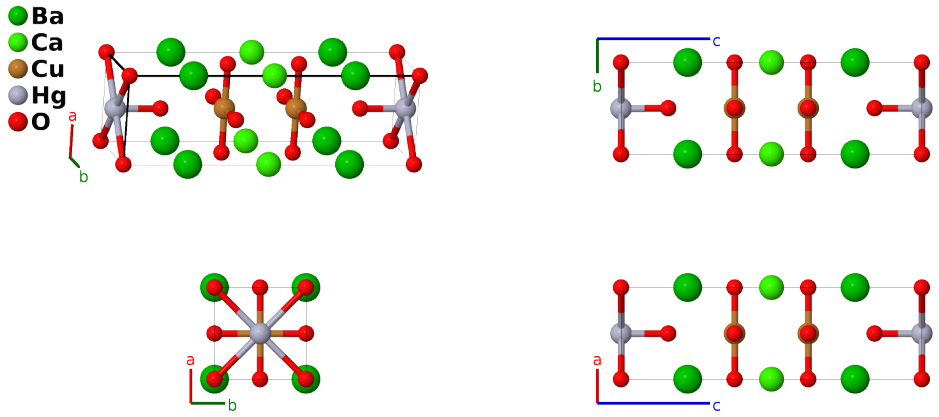
https://aflow.org/p/BESE

https://aflow.org/p/A2BC2DE7_tP13_123_g_b_h_c_ahi-001



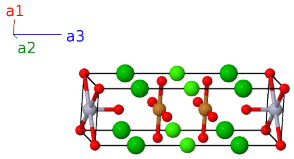
Prototype	$Ba_2CaCu_2HgO_7$
AFLOW prototype label	A2BC2DE7_tP13_123_g_b_h_c_ahi-001
ICSD	74142
Pearson symbol	tP13
Space group number	123
Space group symbol	$P4/mmm$
AFLOW prototype command	`aflow --proto=A2BC2DE7_tP13_123_g_b_h_c_ahi-001 --params=`$a, c/a, z_4, z_5, z_6, z_7$

Other compounds with this structure
$TlBa_2CaCu_2O_{6+\delta}$

- We use the data of (Huang, 1993) taken at 10K.
- The O-I (1c) site, in the layer with the mercury atoms, is fractionally occupied, with $\delta = 0.219$ for the present sample.
- (Huang, 1993) refer to the (2i) Wyckoff position for the O-III site, but this should be (4i).
- (Villars, 2016) give $TlBa_2CaCu_2O_{6+\delta}$ as the prototype for this system, but we can find no information for that structure, even in that reference.

Simple Tetragonal primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(1a)	O I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}c\,\hat{\mathbf{z}}$	(1b)	Ca I
$\mathbf{B_3}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}}$	(1c)	Hg I
$\mathbf{B_4}$	=	$z_4\,\mathbf{a}_3$	=	$cz_4\,\hat{\mathbf{z}}$	(2g)	Ba I
$\mathbf{B_5}$	=	$-z_4\,\mathbf{a}_3$	=	$-cz_4\,\hat{\mathbf{z}}$	(2g)	Ba I
$\mathbf{B_6}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(2h)	Cu I
$\mathbf{B_7}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 - z_5\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}} - cz_5\,\hat{\mathbf{z}}$	(2h)	Cu I
$\mathbf{B_8}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(2h)	O II
$\mathbf{B_9}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 - z_6\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}} - cz_6\,\hat{\mathbf{z}}$	(2h)	O II
$\mathbf{B_{10}}$	=	$\frac{1}{2}\,\mathbf{a}_2 + z_7\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}}$	(4i)	O III
$\mathbf{B_{11}}$	=	$\frac{1}{2}\,\mathbf{a}_1 + z_7\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + cz_7\,\hat{\mathbf{z}}$	(4i)	O III
$\mathbf{B_{12}}$	=	$\frac{1}{2}\,\mathbf{a}_2 - z_7\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{y}} - cz_7\,\hat{\mathbf{z}}$	(4i)	O III
$\mathbf{B_{13}}$	=	$\frac{1}{2}\,\mathbf{a}_1 - z_7\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - cz_7\,\hat{\mathbf{z}}$	(4i)	O III

References

[1] Q. Huang, J. W. Lynn, R. L. Meng, and C. W. Chu, *Crystal structure of annealed and as-prepared $HgBa_2CaCu_2O_{6+\delta}$ superconductors*, Physica C **218**, 356–364 (1993), doi:10.1016/0921-4534(93)90036-P.

[2] *Ba2CaCu2HgO6.2 Crystal Structure: Datasheet from "PAULING FILE Multinaries Edition – 2012" in SpringerMaterials.* Copyright 2016 Springer-Verlag Berlin Heidelberg and Material Phases Data System (MPDS), Switzerland, and National Institute for Materials Science (NIMS), Japan.