$HgBa_2Ca_2Cu_3O_8$ (Hg-1223) Structure: A2B2C3DE8_tP16_123_h_h_bg_a_egi-001

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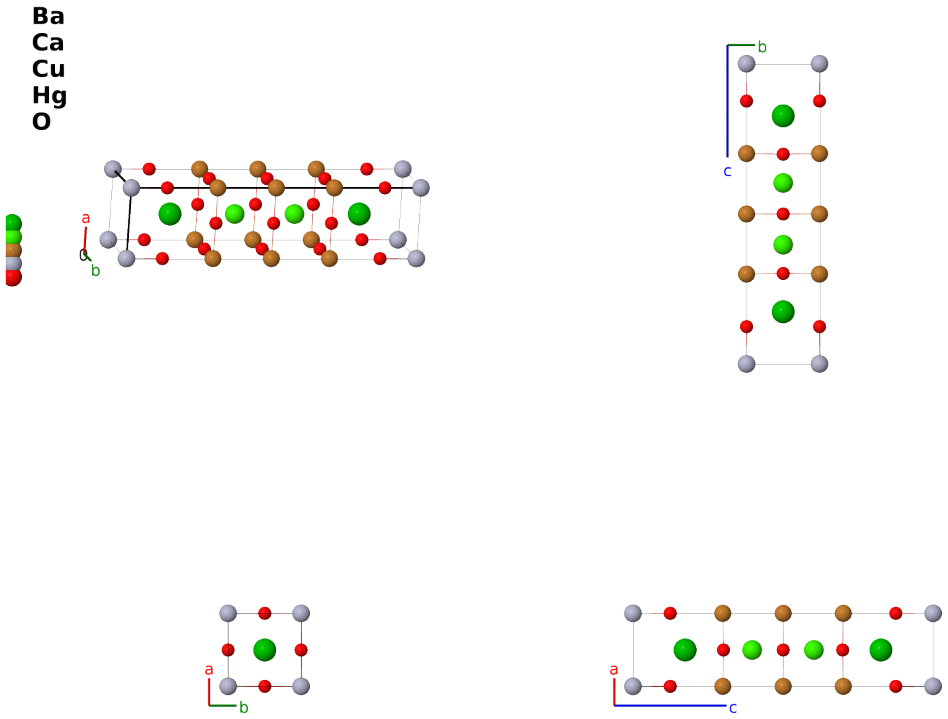
https://aflow.org/prototype-encyclopedia/Y6VW

https://aflow.org/prototype-encyclopedia/A2B2C3DE8_tP16_123_h_h_bg_a_egi-001

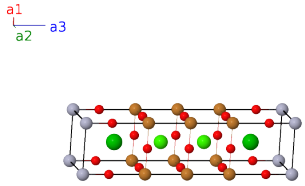


Prototype	$Ba_2Ca_2Cu_3HgO_6$
AFLOW prototype label	A2B2C3DE8_tP16_123_h_h_bg_a_egi-001
ICSD	75730
CCDC	1636374
Pearson symbol	tP16
Space group number	123
Space group symbol	$P4/mmm$
AFLOW prototype command	`aflow --proto=A2B2C3DE8_tP16_123_h_h_bg_a_egi-001 --params=`$a, c/a, z_4, z_5, z_6, z_7, z_8$

- The Hg-12$(n-1)n$, or nHBCCO in the notation of (Bacq-Labreuil, 2025), cuprates have the general formula $HgBa_2Ca_{n-1}Cu_nO_{2n+2+\delta}$. These are tetragonally-stacked perovskite-like compounds similar to tetragonal $YBa_2Cu_3O_7 - x$, and all are superconducting at temperatures near or above 100K. Although compounds have been structured for $n \leq 16$ (Bacq-Labreuil, 2025) we will limit ourselves to tabluating the first three. In addition, we will only list the zero-pressure structures and assume perfect stoiciometry. In practice the can be additional oxygen ($\delta > 0$) and a deficit of barium.
- We include the structures
  - Hg1201/1HBCCO: $HgBa_2CuO_4$,
  - Hg1212/2HBCCO: $HgBa_2CaCu_2O_6$, and
  - Hg1223/3HBCCO: $HgBa_2Ca_2Cu_3O_8$. (this structure)

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)	Hg I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}c\,\hat{\mathbf{z}}$	(1b)	Cu I
$\mathbf{B_3}$	=	$\frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(2e)	O I
$\mathbf{B_4}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(2e)	O I
$\mathbf{B_5}$	=	$z_4\,\mathbf{a}_3$	=	$cz_4\,\hat{\mathbf{z}}$	(2g)	Cu II
$\mathbf{B_6}$	=	$-z_4\,\mathbf{a}_3$	=	$-cz_4\,\hat{\mathbf{z}}$	(2g)	Cu II
$\mathbf{B_7}$	=	$z_5\,\mathbf{a}_3$	=	$cz_5\,\hat{\mathbf{z}}$	(2g)	O II
$\mathbf{B_8}$	=	$-z_5\,\mathbf{a}_3$	=	$-cz_5\,\hat{\mathbf{z}}$	(2g)	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)	Ba I
$\mathbf{B_{10}}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 - z_6\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}} - cz_6\,\hat{\mathbf{z}}$	(2h)	Ba I
$\mathbf{B_{11}}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + z_7\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}}$	(2h)	Ca I
$\mathbf{B_{12}}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 - z_7\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}} - cz_7\,\hat{\mathbf{z}}$	(2h)	Ca I
$\mathbf{B_{13}}$	=	$\frac{1}{2}\,\mathbf{a}_2 + z_8\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{y}} + cz_8\,\hat{\mathbf{z}}$	(4i)	O III
$\mathbf{B_{14}}$	=	$\frac{1}{2}\,\mathbf{a}_1 + z_8\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + cz_8\,\hat{\mathbf{z}}$	(4i)	O III
$\mathbf{B_{15}}$	=	$\frac{1}{2}\,\mathbf{a}_2 - z_8\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{y}} - cz_8\,\hat{\mathbf{z}}$	(4i)	O III
$\mathbf{B_{16}}$	=	$\frac{1}{2}\,\mathbf{a}_1 - z_8\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - cz_8\,\hat{\mathbf{z}}$	(4i)	O III

References

[1] B. A. Hunter, J. D. Jorgensen, J. L. Wagner, P. G. Radaelli, D. G. Hinks, H. Shaked, R. L. Hitterman, and R. B. V. Dreele, *Pressure-induced structural changes in superconducting* $HgBa_2Ca_{n-1}CunO_{2n+2+\delta}$ *(n = 1, 2, 3) compounds*, Physica C **221**, 1–10 (1994), doi:10.1016/0921-4534(94)90659-9.

Found in

[1] B. Bacq-Labreuil, B. Lacasse, A.-M. S. Tremblay, D. Sénéchal, and K. Haule, *Towards an* ab initio *theory of high-temperature superconductors: a study of multilayer cuprates*, Phys. Rev. X **15**, 021071 (2025), doi:10.1103/PhysRevX.15.021071.

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