$HoCuP_2$ Structure: ABC2_oC16_67_a_g_bg-001

This structure originally had the label `ABC2_oC16_67_b_g_ag`. Calls to that address will be redirected here.

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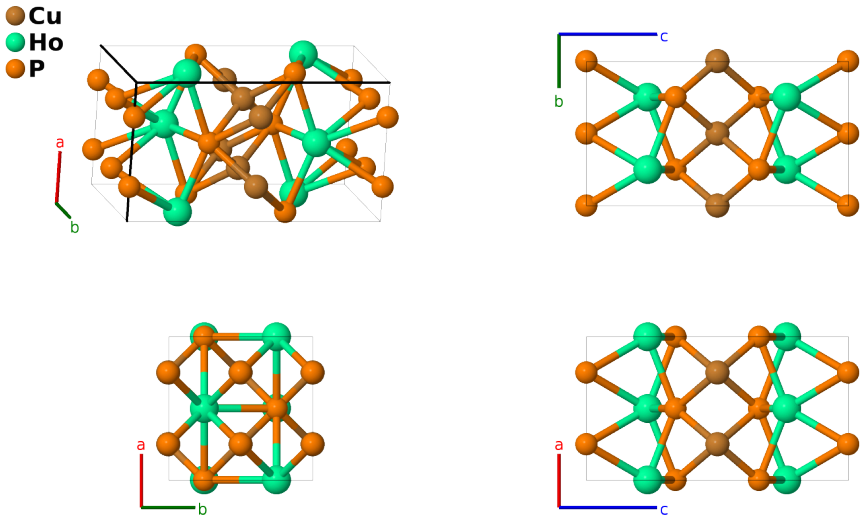
https://aflow.org/p/BX6K

https://aflow.org/p/ABC2_oC16_67_a_g_bg-001

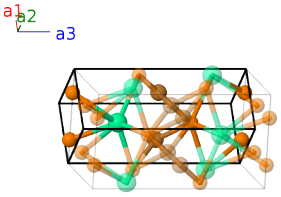


Prototype	$CuHoP_2$
AFLOW prototype label	ABC2_oC16_67_a_g_bg-001
ICSD	94443
Pearson symbol	oC16
Space group number	67
Space group symbol	*Cmme*
AFLOW prototype command	`aflow --proto=ABC2_oC16_67_a_g_bg-001 --params=`$a, b/a, c/a, z_3, z_4$

- Al_2CuIr (A2BC_oC16_67_ag_b_g) and $CuHoP_2$ (ABC2_oC16_67_b_g_ag) have similar AFLOW prototype labels (i.e., same symmetry and set of Wyckoff positions with different stoichiometry labels due to alphabetic ordering of atomic species). They are generated by the same symmetry operations with different sets of parameters (`--params`) specified in their corresponding CIF files.

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
$\mathbf{B_1}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2$	=	$\frac{1}{4}a\,\hat{\mathbf{x}}$	(4a)	Cu I
$\mathbf{B_2}$	=	$\frac{3}{4}\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2$	=	$\frac{3}{4}a\,\hat{\mathbf{x}}$	(4a)	Cu I
$\mathbf{B_3}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4b)	P I
$\mathbf{B_4}$	=	$\frac{3}{4}\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{3}{4}a\,\hat{\mathbf{x}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4b)	P I
$\mathbf{B_5}$	=	$\frac{3}{4}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{1}{4}b\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(4g)	Ho I
$\mathbf{B_6}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} - cz_3\,\hat{\mathbf{z}}$	(4g)	Ho I
$\mathbf{B_7}$	=	$\frac{3}{4}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{1}{4}b\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(4g)	P II
$\mathbf{B_8}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 - z_4\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$	(4g)	P II

References

[1] Y. Mozharivsky, D. Kaczorowski, and H. F. Franzen, *Symmetry-Breaking Transitions in $HoCuAs_{2-x}P_x$ and $ErCuAs_{2-x}P_x$ (x=0-2): Crystal Structure, Application of Landau Theory, Magnetic and Electrical Properties*, Z. Anorganische und Allgemeine Chemie **627**, 2163–2172 (2001), doi:10.1002/1521-3749(200109)627:9<2163::AID-ZAAC2163>3.0.CO;2-N.

Found in

[1] P. Villars and K. Cenzual, *Pearson's Crystal Data – Crystal Structure Database for Inorganic Compounds* (2013). ASM International.