BaCuSm$_2$O$_5$ Structure: ABC5D2_oP36_62_c_c_c2d_2c-001

https://aflow.org/p/W9F8

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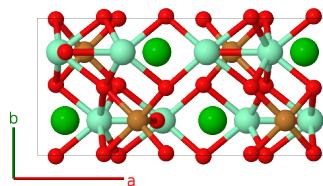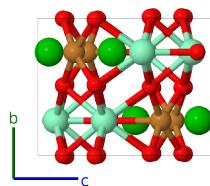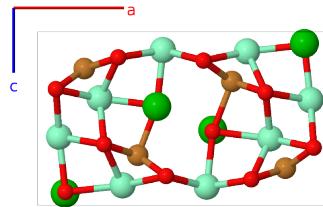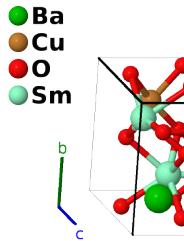
Prototype	BaCuO$_5$Sm$_2$
AFLOW prototype label	ABC5D2_oP36_62_c_c_c2d_2c-001
ICSD	49812
Pearson symbol	oP36
Space group number	62
Space group symbol	$Pnma$
AFLOW prototype command	aflow --proto=ABC5D2_oP36_62_c_c_c2d_2c-001
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Other compounds with this structure

BaCoHo$_2$O$_5$, BaCoTb$_2$O$_5$, BaCoY$_2$O$_5$, BaCoYb$_2$O$_5$, BaCuDy$_2$O$_5$, BaCuEr$_2$O$_5$, BaCuEu$_2$O$_5$, BaCuGd$_2$O$_5$, BaCuHo$_2$O$_5$, BaCuLu$_2$O$_5$, BaCuTb$_2$O$_5$, BaCuTm$_2$O$_5$, BaCuY$_2$O$_5$, BaCuYb$_2$O$_5$, BaNiLu$_2$O$_5$, BaNiTm$_2$O$_5$, BaNiYb$_2$O$_5$, BaZnDy$_2$O$_5$, BaZnEr$_2$O$_5$, BaZnEu$_2$O$_5$, BaZnGd$_2$O$_5$, BaZnHo$_2$O$_5$, BaZnSm$_2$O$_5$, BaZnTm$_2$O$_5$

- Some authors designate BaCuY$_2$O$_5$ as the prototype for this structure.

Simple Orthorhombic primitive vectors

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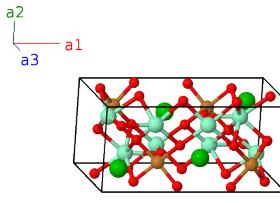
Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$x_1\,\mathbf{a_1} + \frac{1}{4}\,\mathbf{a_2} + z_1\,\mathbf{a_3}$	=	$ax_1\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} + cz_1\,\hat{\mathbf{z}}$	(4c)	Ba I
$\mathbf{B_2}$	=	$-\left(x_1 - \frac{1}{2}\right)\mathbf{a_1} + \frac{3}{4}\,\mathbf{a_2} + \left(z_1 + \frac{1}{2}\right)\mathbf{a_3}$	=	$-a\left(x_1 - \frac{1}{2}\right)\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} + c\left(z_1 + \frac{1}{2}\right)\hat{\mathbf{z}}$	(4c)	Ba I
$\mathbf{B_3}$	=	$-x_1\,\mathbf{a_1} + \frac{3}{4}\,\mathbf{a_2} - z_1\,\mathbf{a_3}$	=	$-ax_1\,\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} - cz_1\,\hat{\mathbf{z}}$	(4c)	Ba I
$\mathbf{B_4}$	=	$\left(x_1 + \frac{1}{2}\right)\mathbf{a_1} + \frac{1}{4}\,\mathbf{a_2} - \left(z_1 - \frac{1}{2}\right)\mathbf{a_3}$	=	$a\left(x_1 + \frac{1}{2}\right)\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} - c\left(z_1 - \frac{1}{2}\right)\hat{\mathbf{z}}$	(4c)	Ba I
$\mathbf{B_5}$	=	$x_2\,\mathbf{a_1} + \frac{1}{4}\,\mathbf{a_2} + z_2\,\mathbf{a_3}$	=	$ax_2\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(4c)	Cu I
$\mathbf{B_6}$	=	$-\left(x_2 - \frac{1}{2}\right)\mathbf{a_1} + \frac{3}{4}\,\mathbf{a_2} + \left(z_2 + \frac{1}{2}\right)\mathbf{a_3}$	=	$-a\left(x_2 - \frac{1}{2}\right)\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} + c\left(z_2 + \frac{1}{2}\right)\hat{\mathbf{z}}$	(4c)	Cu I
$\mathbf{B_7}$	=	$-x_2\,\mathbf{a_1} + \frac{3}{4}\,\mathbf{a_2} - z_2\,\mathbf{a_3}$	=	$-ax_2\,\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} - cz_2\,\hat{\mathbf{z}}$	(4c)	Cu I
$\mathbf{B_8}$	=	$\left(x_2 + \frac{1}{2}\right)\mathbf{a_1} + \frac{1}{4}\,\mathbf{a_2} - \left(z_2 - \frac{1}{2}\right)\mathbf{a_3}$	=	$a\left(x_2 + \frac{1}{2}\right)\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} - c\left(z_2 - \frac{1}{2}\right)\hat{\mathbf{z}}$	(4c)	Cu I
$\mathbf{B_9}$	=	$x_3\,\mathbf{a_1} + \frac{1}{4}\,\mathbf{a_2} + z_3\,\mathbf{a_3}$	=	$ax_3\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(4c)	O I
$\mathbf{B_{10}}$	=	$-\left(x_3 - \frac{1}{2}\right)\mathbf{a_1} + \frac{3}{4}\,\mathbf{a_2} + \left(z_3 + \frac{1}{2}\right)\mathbf{a_3}$	=	$-a\left(x_3 - \frac{1}{2}\right)\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} + c\left(z_3 + \frac{1}{2}\right)\hat{\mathbf{z}}$	(4c)	O I
$\mathbf{B_{11}}$	=	$-x_3\,\mathbf{a_1} + \frac{3}{4}\,\mathbf{a_2} - z_3\,\mathbf{a_3}$	=	$-ax_3\,\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} - cz_3\,\hat{\mathbf{z}}$	(4c)	O I
$\mathbf{B_{12}}$	=	$\left(x_3 + \frac{1}{2}\right)\mathbf{a_1} + \frac{1}{4}\,\mathbf{a_2} - \left(z_3 - \frac{1}{2}\right)\mathbf{a_3}$	=	$a\left(x_3 + \frac{1}{2}\right)\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} - c\left(z_3 - \frac{1}{2}\right)\hat{\mathbf{z}}$	(4c)	O I
$\mathbf{B_{13}}$	=	$x_4\,\mathbf{a_1} + \frac{1}{4}\,\mathbf{a_2} + z_4\,\mathbf{a_3}$	=	$ax_4\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(4c)	Sm I
$\mathbf{B_{14}}$	=	$-\left(x_4 - \frac{1}{2}\right)\mathbf{a_1} + \frac{3}{4}\,\mathbf{a_2} + \left(z_4 + \frac{1}{2}\right)\mathbf{a_3}$	=	$-a\left(x_4 - \frac{1}{2}\right)\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} + c\left(z_4 + \frac{1}{2}\right)\hat{\mathbf{z}}$	(4c)	Sm I
$\mathbf{B_{15}}$	=	$-x_4\,\mathbf{a_1} + \frac{3}{4}\,\mathbf{a_2} - z_4\,\mathbf{a_3}$	=	$-ax_4\,\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$	(4c)	Sm I
$\mathbf{B_{16}}$	=	$\left(x_4 + \frac{1}{2}\right)\mathbf{a_1} + \frac{1}{4}\,\mathbf{a_2} - \left(z_4 - \frac{1}{2}\right)\mathbf{a_3}$	=	$a\left(x_4 + \frac{1}{2}\right)\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} - c\left(z_4 - \frac{1}{2}\right)\hat{\mathbf{z}}$	(4c)	Sm I
$\mathbf{B_{17}}$	=	$x_5\,\mathbf{a_1} + \frac{1}{4}\,\mathbf{a_2} + z_5\,\mathbf{a_3}$	=	$ax_5\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(4c)	Sm II
$\mathbf{B_{18}}$	=	$-\left(x_5 - \frac{1}{2}\right)\mathbf{a_1} + \frac{3}{4}\,\mathbf{a_2} + \left(z_5 + \frac{1}{2}\right)\mathbf{a_3}$	=	$-a\left(x_5 - \frac{1}{2}\right)\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} + c\left(z_5 + \frac{1}{2}\right)\hat{\mathbf{z}}$	(4c)	Sm II
$\mathbf{B_{19}}$	=	$-x_5\,\mathbf{a_1} + \frac{3}{4}\,\mathbf{a_2} - z_5\,\mathbf{a_3}$	=	$-ax_5\,\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} - cz_5\,\hat{\mathbf{z}}$	(4c)	Sm II
$\mathbf{B_{20}}$	=	$\left(x_5 + \frac{1}{2}\right)\mathbf{a_1} + \frac{1}{4}\,\mathbf{a_2} - \left(z_5 - \frac{1}{2}\right)\mathbf{a_3}$	=	$a\left(x_5 + \frac{1}{2}\right)\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} - c\left(z_5 - \frac{1}{2}\right)\hat{\mathbf{z}}$	(4c)	Sm II
$\mathbf{B_{21}}$	=	$x_6\,\mathbf{a_1} + y_6\,\mathbf{a_2} + z_6\,\mathbf{a_3}$	=	$ax_6\,\hat{\mathbf{x}} + by_6\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(8d)	O II
$\mathbf{B_{22}}$	=	$-\left(x_6 - \frac{1}{2}\right)\mathbf{a_1} - y_6\,\mathbf{a_2} + \left(z_6 + \frac{1}{2}\right)\mathbf{a_3}$	=	$-a\left(x_6 - \frac{1}{2}\right)\hat{\mathbf{x}} - by_6\,\hat{\mathbf{y}} + c\left(z_6 + \frac{1}{2}\right)\hat{\mathbf{z}}$	(8d)	O II
$\mathbf{B_{23}}$	=	$-x_6\,\mathbf{a_1} + \left(y_6 + \frac{1}{2}\right)\mathbf{a_2} - z_6\,\mathbf{a_3}$	=	$-ax_6\,\hat{\mathbf{x}} + b\left(y_6 + \frac{1}{2}\right)\hat{\mathbf{y}} - cz_6\,\hat{\mathbf{z}}$	(8d)	O II
$\mathbf{B_{24}}$	=	$\left(x_6 + \frac{1}{2}\right)\mathbf{a_1} - \left(y_6 - \frac{1}{2}\right)\mathbf{a_2} - \left(z_6 - \frac{1}{2}\right)\mathbf{a_3}$	=	$a\left(x_6 + \frac{1}{2}\right)\hat{\mathbf{x}} - b\left(y_6 - \frac{1}{2}\right)\hat{\mathbf{y}} - c\left(z_6 - \frac{1}{2}\right)\hat{\mathbf{z}}$	(8d)	O II
$\mathbf{B_{25}}$	=	$-x_6\,\mathbf{a_1} - y_6\,\mathbf{a_2} - z_6\,\mathbf{a_3}$	=	$-ax_6\,\hat{\mathbf{x}} - by_6\,\hat{\mathbf{y}} - cz_6\,\hat{\mathbf{z}}$	(8d)	O II
$\mathbf{B_{26}}$	=	$\left(x_6 + \frac{1}{2}\right)\mathbf{a_1} + y_6\,\mathbf{a_2} - \left(z_6 - \frac{1}{2}\right)\mathbf{a_3}$	=	$a\left(x_6 + \frac{1}{2}\right)\hat{\mathbf{x}} + by_6\,\hat{\mathbf{y}} - c\left(z_6 - \frac{1}{2}\right)\hat{\mathbf{z}}$	(8d)	O II

$$\mathbf{B_{27}} = x_6\,\mathbf{a}_1 - \left(y_6 - \tfrac{1}{2}\right)\mathbf{a}_2 + z_6\,\mathbf{a}_3 \qquad = \qquad ax_6\,\hat{\mathbf{x}} - b\left(y_6 - \tfrac{1}{2}\right)\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}} \qquad \text{(8d)} \qquad \text{O II}$$

$$\mathbf{B_{28}} = -\left(x_6 - \tfrac{1}{2}\right)\mathbf{a}_1 + \left(y_6 + \tfrac{1}{2}\right)\mathbf{a}_2 + \left(z_6 + \tfrac{1}{2}\right)\mathbf{a}_3 \qquad = \qquad -a\left(x_6 - \tfrac{1}{2}\right)\hat{\mathbf{x}} + b\left(y_6 + \tfrac{1}{2}\right)\hat{\mathbf{y}} + c\left(z_6 + \tfrac{1}{2}\right)\hat{\mathbf{z}} \qquad \text{(8d)} \qquad \text{O II}$$

$$\mathbf{B_{29}} = x_7\,\mathbf{a}_1 + y_7\,\mathbf{a}_2 + z_7\,\mathbf{a}_3 \qquad = \qquad ax_7\,\hat{\mathbf{x}} + by_7\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}} \qquad \text{(8d)} \qquad \text{O III}$$

$$\mathbf{B_{30}} = -\left(x_7 - \tfrac{1}{2}\right)\mathbf{a}_1 - y_7\,\mathbf{a}_2 + \left(z_7 + \tfrac{1}{2}\right)\mathbf{a}_3 \qquad = \qquad -a\left(x_7 - \tfrac{1}{2}\right)\hat{\mathbf{x}} - by_7\,\hat{\mathbf{y}} + c\left(z_7 + \tfrac{1}{2}\right)\hat{\mathbf{z}} \qquad \text{(8d)} \qquad \text{O III}$$

$$\mathbf{B_{31}} = -x_7\,\mathbf{a}_1 + \left(y_7 + \tfrac{1}{2}\right)\mathbf{a}_2 - z_7\,\mathbf{a}_3 \qquad = \qquad -ax_7\,\hat{\mathbf{x}} + b\left(y_7 + \tfrac{1}{2}\right)\hat{\mathbf{y}} - cz_7\,\hat{\mathbf{z}} \qquad \text{(8d)} \qquad \text{O III}$$

$$\mathbf{B_{32}} = \left(x_7 + \tfrac{1}{2}\right)\mathbf{a}_1 - \left(y_7 - \tfrac{1}{2}\right)\mathbf{a}_2 - \left(z_7 - \tfrac{1}{2}\right)\mathbf{a}_3 \qquad = \qquad a\left(x_7 + \tfrac{1}{2}\right)\hat{\mathbf{x}} - b\left(y_7 - \tfrac{1}{2}\right)\hat{\mathbf{y}} - c\left(z_7 - \tfrac{1}{2}\right)\hat{\mathbf{z}} \qquad \text{(8d)} \qquad \text{O III}$$

$$\mathbf{B_{33}} = -x_7\,\mathbf{a}_1 - y_7\,\mathbf{a}_2 - z_7\,\mathbf{a}_3 \qquad = \qquad -ax_7\,\hat{\mathbf{x}} - by_7\,\hat{\mathbf{y}} - cz_7\,\hat{\mathbf{z}} \qquad \text{(8d)} \qquad \text{O III}$$

$$\mathbf{B_{34}} = \left(x_7 + \tfrac{1}{2}\right)\mathbf{a}_1 + y_7\,\mathbf{a}_2 - \left(z_7 - \tfrac{1}{2}\right)\mathbf{a}_3 \qquad = \qquad a\left(x_7 + \tfrac{1}{2}\right)\hat{\mathbf{x}} + by_7\,\hat{\mathbf{y}} - c\left(z_7 - \tfrac{1}{2}\right)\hat{\mathbf{z}} \qquad \text{(8d)} \qquad \text{O III}$$

$$\mathbf{B_{35}} = x_7\,\mathbf{a}_1 - \left(y_7 - \tfrac{1}{2}\right)\mathbf{a}_2 + z_7\,\mathbf{a}_3 \qquad = \qquad ax_7\,\hat{\mathbf{x}} - b\left(y_7 - \tfrac{1}{2}\right)\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}} \qquad \text{(8d)} \qquad \text{O III}$$

$$\mathbf{B_{36}} = -\left(x_7 - \tfrac{1}{2}\right)\mathbf{a}_1 + \left(y_7 + \tfrac{1}{2}\right)\mathbf{a}_2 + \left(z_7 + \tfrac{1}{2}\right)\mathbf{a}_3 \qquad = \qquad -a\left(x_7 - \tfrac{1}{2}\right)\hat{\mathbf{x}} + b\left(y_7 + \tfrac{1}{2}\right)\hat{\mathbf{y}} + c\left(z_7 + \tfrac{1}{2}\right)\hat{\mathbf{z}} \qquad \text{(8d)} \qquad \text{O III}$$

References

[1] S. Schiffler and H. Müller-Buschbaum, *BaNiYb$_2$O$_5$ - eine Verbindung, die nicht im BaNiLn$_2$O$_5$-Typ kristallisiert Mit einem Beitrag über BaCuSm$_2$O$_5$*, Z. Anorganische und Allgemeine Chemie **540**, 243–250 (1986), doi:10.1002/zaac.19865400927.

Found in

[1] J. Hernández-Velasco and R. Sáez-Puche, *Synthesis, polymorphism and magnetic properties of novel Tb$_2$BaMoO$_5$ (M=Co, or Ni) oxides*, J. Alloys Compd. **225**, 147–151 (1995), doi:10.1016/0925-8388(94)07094-6.