$BaLa_2ZnO_5$ Structure: AB2C5D_tI36_140_a_h_cl_b-001

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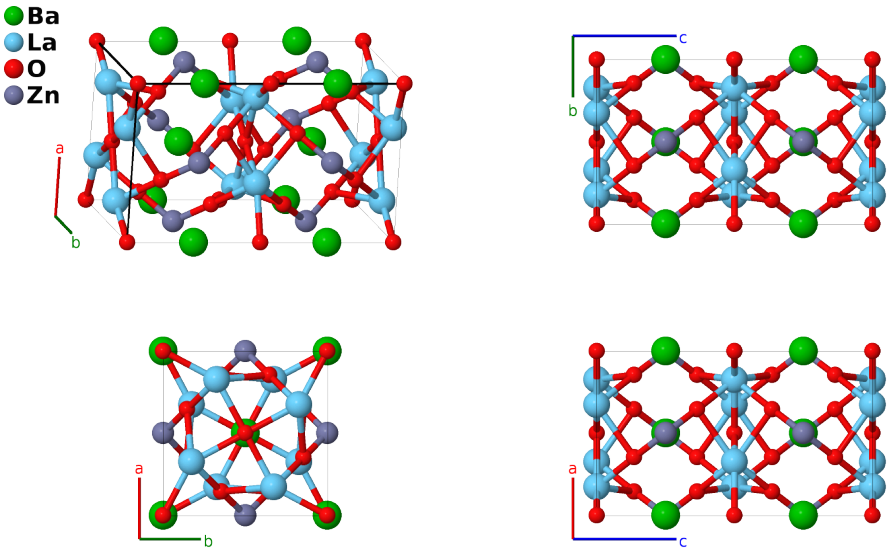


Prototype	$BaLa_2O_5Zn$
AFLOW prototype label	AB2C5D_tI36_140_a_h_cl_b-001
ICSD	88598
Pearson symbol	tI36
Space group number	140
Space group symbol	$I4/mcm$
AFLOW prototype command	`aflow --proto=AB2C5D_tI36_140_a_h_cl_b-001 --params=`$a, c/a, x_4, x_5, z_5$

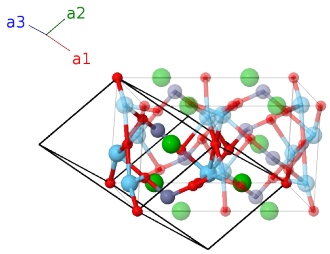
Other compounds with this structure

$BaNd_2MnS_5$, $BaNd_2ZnO_5$, $BaNd_2ZnS_5$, $BaPr_2FeS_5$, $BaPr_2ZnS_5$, $BaSm_2FeS_5$, Ba_3SnS_5, Ba_3TiS_5, Eu_3AlO_5, Sr_3AlO_5, Sr_3GaO_4F, Tl_3CoCl_5, Tl_3FeCl_5, $Sr(Sr_{0.5}Gd_{0.5})_2GaO_5$

- Some authors designate $Sr(Sr_{0.5}Gd_{0.5})_2GaO_5$ as the prototype for this structure, with the (8h) site randomly occupied by strontium and gadolinium atoms. We prefer a structure with ordered atoms on this site.
- Removing the O-I atoms from the (4c) site reduces this to the $NH_4Pb_2Br_5$ ($K3_4$) structure.
- This is the quaternary form of the Cs_3CoCl_5 ($K3_1$) structure.

Body-centered Tetragonal primitive vectors

$$\begin{aligned}\mathbf{a_1} &= -\tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}a\,\hat{\mathbf{y}} + \tfrac{1}{2}c\,\hat{\mathbf{z}}\\ \mathbf{a_2} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{1}{2}a\,\hat{\mathbf{y}} + \tfrac{1}{2}c\,\hat{\mathbf{z}}\\ \mathbf{a_3} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}a\,\hat{\mathbf{y}} - \tfrac{1}{2}c\,\hat{\mathbf{z}}\end{aligned}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2$	=	$\frac{1}{4}c\,\hat{\mathbf{z}}$	(4a)	Ba I
$\mathbf{B_2}$	=	$\frac{3}{4}\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2$	=	$\frac{3}{4}c\,\hat{\mathbf{z}}$	(4a)	Ba I
$\mathbf{B_3}$	=	$\frac{3}{4}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(4b)	Zn I
$\mathbf{B_4}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(4b)	Zn I
$\mathbf{B_5}$	=	0	=	0	(4c)	O I
$\mathbf{B_6}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2$	=	$\frac{1}{2}c\,\hat{\mathbf{z}}$	(4c)	O I
$\mathbf{B_7}$	=	$\left(x_4 + \frac{1}{2}\right)\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 + \left(2x_4 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}} + a\left(x_4 + \frac{1}{2}\right)\,\hat{\mathbf{y}}$	(8h)	La I
$\mathbf{B_8}$	=	$-\left(x_4 - \frac{1}{2}\right)\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 - \left(2x_4 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}} - a\left(x_4 - \frac{1}{2}\right)\,\hat{\mathbf{y}}$	(8h)	La I
$\mathbf{B_9}$	=	$x_4\,\mathbf{a}_1 - \left(x_4 - \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-a\left(x_4 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + ax_4\,\hat{\mathbf{y}}$	(8h)	La I
$\mathbf{B_{10}}$	=	$-x_4\,\mathbf{a}_1 + \left(x_4 + \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$a\left(x_4 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - ax_4\,\hat{\mathbf{y}}$	(8h)	La I
$\mathbf{B_{11}}$	=	$\left(x_5 + z_5 + \frac{1}{2}\right)\,\mathbf{a}_1 + (x_5 + z_5)\,\mathbf{a}_2 + \left(2x_5 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$ax_5\,\hat{\mathbf{x}} + a\left(x_5 + \frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(16l)	O II
$\mathbf{B_{12}}$	=	$\left(-x_5 + z_5 + \frac{1}{2}\right)\,\mathbf{a}_1 - (x_5 - z_5)\,\mathbf{a}_2 - \left(2x_5 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_5\,\hat{\mathbf{x}} - a\left(x_5 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(16l)	O II
$\mathbf{B_{13}}$	=	$(x_5 + z_5)\,\mathbf{a}_1 + \left(-x_5 + z_5 + \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-a\left(x_5 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + ax_5\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(16l)	O II
$\mathbf{B_{14}}$	=	$-(x_5 - z_5)\,\mathbf{a}_1 + \left(x_5 + z_5 + \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$a\left(x_5 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - ax_5\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(16l)	O II
$\mathbf{B_{15}}$	=	$(x_5 - z_5)\,\mathbf{a}_1 - \left(x_5 + z_5 - \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-a\left(x_5 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + ax_5\,\hat{\mathbf{y}} - cz_5\,\hat{\mathbf{z}}$	(16l)	O II
$\mathbf{B_{16}}$	=	$-(x_5 + z_5)\,\mathbf{a}_1 + \left(x_5 - z_5 + \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$a\left(x_5 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - ax_5\,\hat{\mathbf{y}} - cz_5\,\hat{\mathbf{z}}$	(16l)	O II
$\mathbf{B_{17}}$	=	$\left(x_5 - z_5 + \frac{1}{2}\right)\,\mathbf{a}_1 + (x_5 - z_5)\,\mathbf{a}_2 + \left(2x_5 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$ax_5\,\hat{\mathbf{x}} + a\left(x_5 + \frac{1}{2}\right)\,\hat{\mathbf{y}} - cz_5\,\hat{\mathbf{z}}$	(16l)	O II
$\mathbf{B_{18}}$	=	$-\left(x_5 + z_5 - \frac{1}{2}\right)\,\mathbf{a}_1 - (x_5 + z_5)\,\mathbf{a}_2 - \left(2x_5 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_5\,\hat{\mathbf{x}} - a\left(x_5 - \frac{1}{2}\right)\,\hat{\mathbf{y}} - cz_5\,\hat{\mathbf{z}}$	(16l)	O II

References

[1] J. A. Kaduk, W. Wong-Ng, W. Greenwood, J. Dillingham, and B. H. Troy, *Crystal Structures and Reference PowderPatterns of BaR_2ZnO_5 (R = La, Nd, Sm,Eu, Gd, Dy, Ho, Y, Er, and Tm)*, J. Res. NIST **104**, 147–171 (1999), doi:10.6028/jres.104.011.