$BaZnF_4$ Structure: AB4C_oC24_36_a_4a_a-002

Cite this page as: H. Eckert, S. Divilov, A. Zettel, M. J. Mehl, D. Hicks, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*. In preparation.

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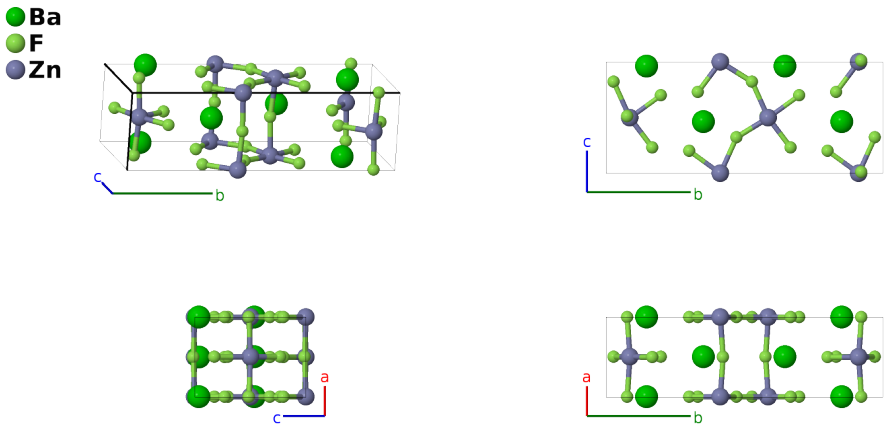
https://aflow.org/p/AB4C_oC24_36_a_4a_a-002



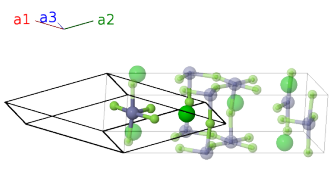
Prototype	BaF_4Zn
AFLOW prototype label	AB4C_oC24_36_a_4a_a-002
ICSD	402925
Pearson symbol	oC24
Space group number	36
Space group symbol	$Cmc2_1$
AFLOW prototype command	`aflow --proto=AB4C_oC24_36_a_4a_a-002 --params=`$a, b/a, c/a, y_1, z_1, y_2, z_2, y_3, z_3, y_4, z_4, y_5, z_5, y_6, z_6$

Other compounds with this structure
$BaCoF_4$, $BaFeF_4$, $BaMgF_4$, $BaNiF_4$, $LaTaO_4$, $NaOsO_4$

- We use the data from (Lapasset, 1996) taken at 295K.
- Space group $Cmc2_1$ #36 allows an arbitrary choice of the origin of the z-axis. Here we set $z_6 = 0$ for the zinc (2a) site.

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
$\mathbf{B_1}$	=	$-y_1\,\mathbf{a}_1 + y_1\,\mathbf{a}_2 + z_1\,\mathbf{a}_3$	=	$by_1\,\hat{\mathbf{y}} + cz_1\,\hat{\mathbf{z}}$	(4a)	Ba I
$\mathbf{B_2}$	=	$y_1\,\mathbf{a}_1 - y_1\,\mathbf{a}_2 + \left(z_1 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-by_1\,\hat{\mathbf{y}} + c\left(z_1 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4a)	Ba I
$\mathbf{B_3}$	=	$-y_2\,\mathbf{a}_1 + y_2\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$by_2\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(4a)	F I
$\mathbf{B_4}$	=	$y_2\,\mathbf{a}_1 - y_2\,\mathbf{a}_2 + \left(z_2 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-by_2\,\hat{\mathbf{y}} + c\left(z_2 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4a)	F I
$\mathbf{B_5}$	=	$-y_3\,\mathbf{a}_1 + y_3\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$by_3\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(4a)	F II
$\mathbf{B_6}$	=	$y_3\,\mathbf{a}_1 - y_3\,\mathbf{a}_2 + \left(z_3 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-by_3\,\hat{\mathbf{y}} + c\left(z_3 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4a)	F II
$\mathbf{B_7}$	=	$-y_4\,\mathbf{a}_1 + y_4\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$by_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(4a)	F III
$\mathbf{B_8}$	=	$y_4\,\mathbf{a}_1 - y_4\,\mathbf{a}_2 + \left(z_4 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-by_4\,\hat{\mathbf{y}} + c\left(z_4 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4a)	F III
$\mathbf{B_9}$	=	$-y_5\,\mathbf{a}_1 + y_5\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$by_5\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(4a)	F IV
$\mathbf{B_{10}}$	=	$y_5\,\mathbf{a}_1 - y_5\,\mathbf{a}_2 + \left(z_5 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-by_5\,\hat{\mathbf{y}} + c\left(z_5 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4a)	F IV
$\mathbf{B_{11}}$	=	$-y_6\,\mathbf{a}_1 + y_6\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	=	$by_6\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(4a)	Zn I
$\mathbf{B_{12}}$	=	$y_6\,\mathbf{a}_1 - y_6\,\mathbf{a}_2 + \left(z_6 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-by_6\,\hat{\mathbf{y}} + c\left(z_6 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4a)	Zn I

References

[1] J. Lapasset, H. N. Bordallo, R. Almairac, and J. Nouet, *Redetermination of the crystal structure of barium tetrafluorozincate, $BaZnF_4$, at 295 K and 113 K*, Z. Krystallogr. **211**, 934–935 (1996), doi:10.1524/zkri.1996.211.12.934.

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[1] E. G. Víllora, K. Shimamura, F. Jing, A. Medvedev, S. Takekawa, and K. Kitamura, *Ferroelectric and optical properties of single crystal $BaZnF_4$*, Appl. Phys. Lett. **90**, 192909 (2007), doi:10.1063/1.2737365.