$BaZnSb_2$ Structure: AB2C_tI16_139_e_ce_d-003

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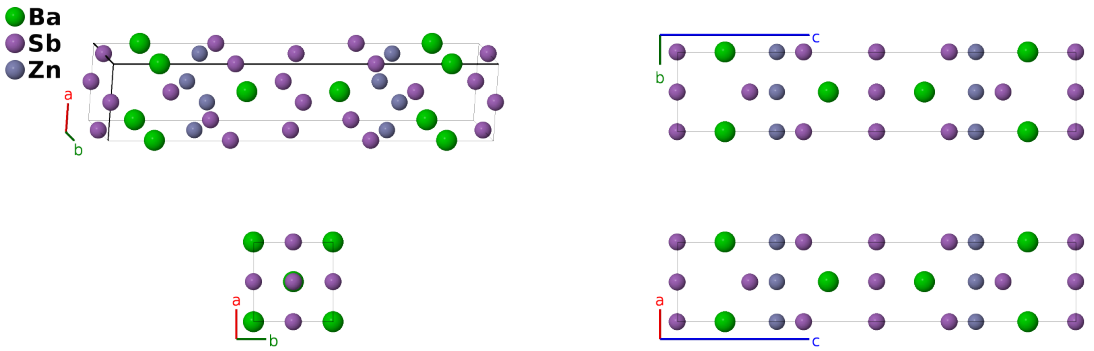
https://aflow.org/p/00JM

https://aflow.org/p/AB2C_tI16_139_e_ce_d-003



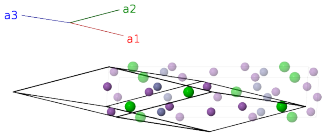
Prototype	$BaSb_2Zn$
AFLOW prototype label	AB2C_tI16_139_e_ce_d-003
ICSD	52694
Pearson symbol	tI16
Space group number	139
Space group symbol	$I4/mmm$
AFLOW prototype command	`aflow --proto=AB2C_tI16_139_e_ce_d-003 --params=`$a, c/a, z_3, z_4$

Other compounds with this structure
$BaCdBi_2$, $BaCdSb_2$, $BaMnSb_2$, $BaZnBi_2$, $SrCdBi_2$, $SrZnBi_2$

- Many authorities designate $SrZnBi_2$ as the prototype for this structure.

Body-centered Tetragonal primitive vectors

$$\mathbf{a_1} = -\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$$
$$\mathbf{a_2} = \frac{1}{2}a\,\hat{\mathbf{x}} - \frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$$
$$\mathbf{a_3} = \frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}} - \frac{1}{2}c\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{y}}$	(4c)	Sb I

$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}}$	(4c)	Sb I
$\mathbf{B_3}$	=	$\frac{3}{4}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(4d)	Zn I
$\mathbf{B_4}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(4d)	Zn I
$\mathbf{B_5}$	=	$z_3\,\mathbf{a}_1 + z_3\,\mathbf{a}_2$	=	$cz_3\,\hat{\mathbf{z}}$	(4e)	Ba I
$\mathbf{B_6}$	=	$-z_3\,\mathbf{a}_1 - z_3\,\mathbf{a}_2$	=	$-cz_3\,\hat{\mathbf{z}}$	(4e)	Ba I
$\mathbf{B_7}$	=	$z_4\,\mathbf{a}_1 + z_4\,\mathbf{a}_2$	=	$cz_4\,\hat{\mathbf{z}}$	(4e)	Sb II
$\mathbf{B_8}$	=	$-z_4\,\mathbf{a}_1 - z_4\,\mathbf{a}_2$	=	$-cz_4\,\hat{\mathbf{z}}$	(4e)	Sb II

References

[1] E. Brechtel, G. Cordier, and H. Schäfer, *Neue ternäre erdalkali-übergangselement-pnictide*, J. Less-Common Met. **79**, 131–138 (1981), doi:10.1016/0022-5088(81)90057-6.

Found in

[1] C. Yi, S. Yang, M. Yang, L. Wang, Y. Matsushita, S. Miao, Y. Jiao, J. Cheng, Y. Li, K. Yamaura, Y. Shi, and J. Luo, *Large negative magnetoresistance of a nearly Dirac material: Layered antimonide $EuMnSb_2$*, Phys. Rev. B **96**, 205103 (2017), doi:10.1103/PhysRevB.96.205103.