BaS_3 ($D0_{17}$) Structure: AB3_tP8_113_a_ce-001

This structure originally had the label `AB3_tP8_113_a_ce`. Calls to that address will be redirected here.

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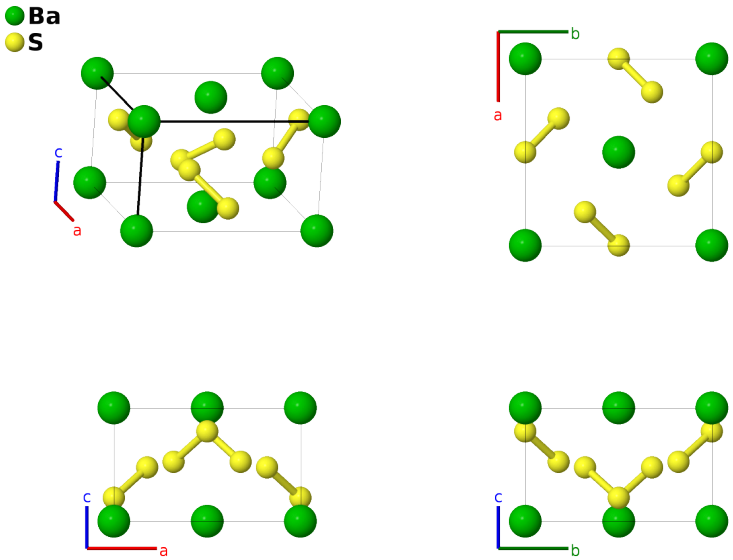
https://aflow.org/p/0A77

https://aflow.org/p/AB3_tP8_113_a_ce-001



Prototype	BaS_3
AFLOW prototype label	AB3_tP8_113_a_ce-001
***Strukturbericht* designation**	$D0_{17}$
ICSD	70059
Pearson symbol	tP8
Space group number	113
Space group symbol	$P\bar{4}2_1m$
AFLOW prototype command	`aflow --proto=AB3_tP8_113_a_ce-001 --params=`$a, c/a, z_2, x_3, z_3$

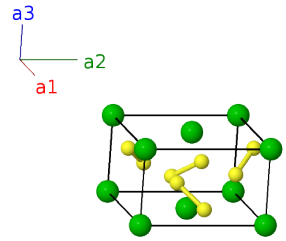
Other compounds with this structure

$AgDyTe_2$, $AgHgTe_2$, $AgErTe_2$, $AgTe_2Tm$, $AgGdTe_2$, $AgTe_2Y$, $BaSe_3$, $BaTe_3$

- (Gottfried, 1938) originally gave the $D0_{17}$ label to the $P2_12_12$ #94 BaS_3 structure, however we follow (Partheé, 1993), who uses the current structure as the $D0_{17}$ prototype.

Simple Tetragonal primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(2a)	Ba I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}}$	(2a)	Ba I
$\mathbf{B_3}$	=	$\frac{1}{2}\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(2c)	S I
$\mathbf{B_4}$	=	$\frac{1}{2}\,\mathbf{a}_1 - z_2\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - cz_2\,\hat{\mathbf{z}}$	(2c)	S I
$\mathbf{B_5}$	=	$x_3\,\mathbf{a}_1 + \left(x_3 + \frac{1}{2}\right)\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} + a\left(x_3 + \frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(4e)	S II
$\mathbf{B_6}$	=	$-x_3\,\mathbf{a}_1 - \left(x_3 - \frac{1}{2}\right)\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} - a\left(x_3 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(4e)	S II
$\mathbf{B_7}$	=	$\left(x_3 + \frac{1}{2}\right)\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$	=	$a\left(x_3 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - ax_3\,\hat{\mathbf{y}} - cz_3\,\hat{\mathbf{z}}$	(4e)	S II
$\mathbf{B_8}$	=	$-\left(x_3 - \frac{1}{2}\right)\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$	=	$-a\left(x_3 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + ax_3\,\hat{\mathbf{y}} - cz_3\,\hat{\mathbf{z}}$	(4e)	S II

References

[1] S. Yamaoka, J. T. Lemley, J. M. Jenks, and H. Steinfink, *Structural chemistry of the polysulfides dibarium trisulfide and monobarium trisulfide*, Inorg. Chem. **14**, 129–131 (1975), doi:10.1021/ic50143a027.

[2] E. Parthé, L. Gelato, B. Chabot, M. Penso, K. Cenzula, and R. Gladyshevskii, *Standardized Data and Crystal Chemical Characterization of Inorganic Structure Types*, *Gmelin Handbook of Inorganic and Organometallic Chemistry*, vol. 2 (Springer-Verlag, Berlin, Heidelberg, 1993), 8 edn., doi:10.1007/978-3-662-02909-1_3.

[3] C. Gottfried, ed., *Strukturbericht Band IV 1936* (Akademische Verlagsgesellschaft M. B. H., Leipzig, 1938).

Found in

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