$BaSi_4O_9$ ($S3_2$) Structure: AB9C4_hP28_188_a_kl_ck-001

This structure originally had the label `AB9C4_hP28_188_e_kl_ak`. Calls to that address will be redirected here.

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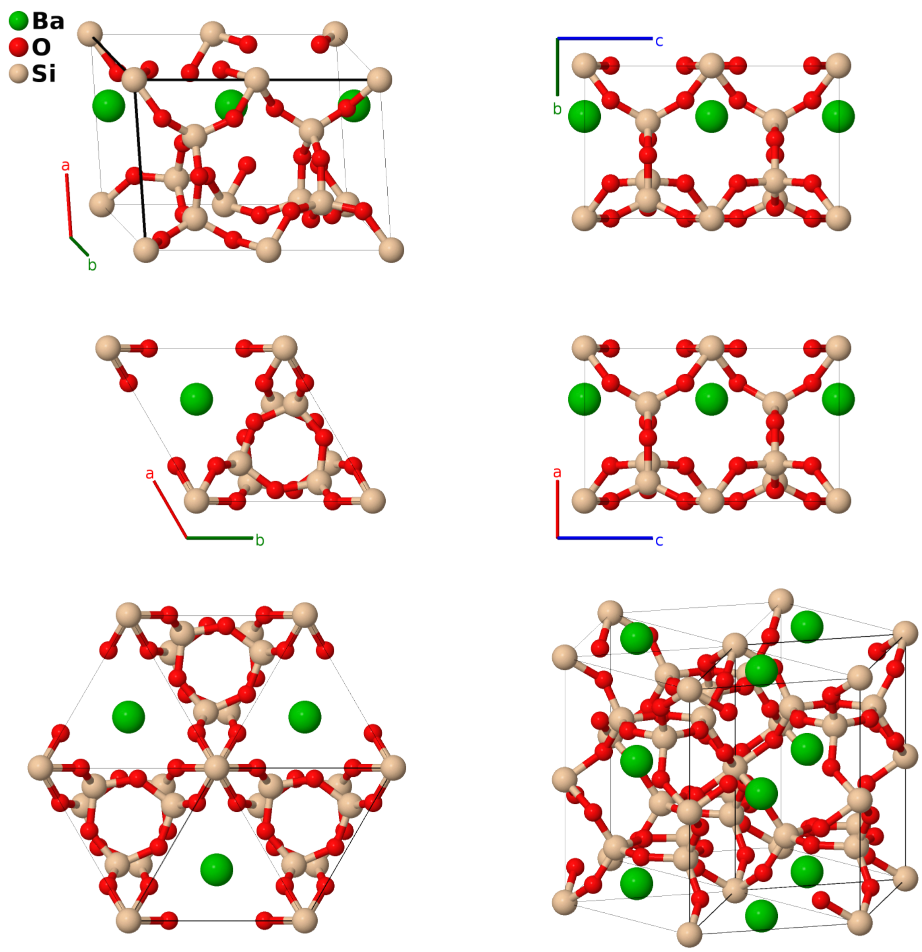
https://aflow.org/p/2DJ4

https://aflow.org/p/AB9C4_hP28_188_a_kl_ck-001



Prototype	$BaSi_4O_9$
AFLOW prototype label	AB9C4_hP28_188_a_kl_ck-001
***Strukturbericht* designation**	$S3_2$
ICSD	80067
Pearson symbol	hP28
Space group number	188
Space group symbol	$P\bar{6}c2$

AFLOW prototype command `aflow --proto=AB9C4_hP28_188_a_kl_ck-001`
`--params=`$a, c/a, x_3, y_3, x_4, y_4, x_5, y_5, z_5$

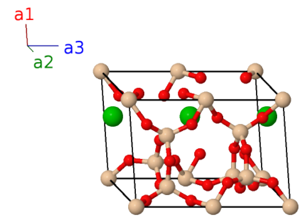
Other compounds with this structure

$Ba(Si_xTi_{1-x})Si_3O_9$ (pabstite), $BaSnGe_3O_9$, $BaTiSi_3O_9$ (benitoite), $BaZrSi_3O_9$ (bazrite), $CaKP_3O_9$, $MgKP_3O_9$, $TaKGe_3O_9$, $TaRbGe_3O_9$, $TaTlGe_3O_9$

- (Hermann, 1937) applied the *Strukturbericht* label $S3_2$ to benitoite, $BaTiSi_3O_9$. The only difference between $BaSi_4O_9$ and benitoite is that titanium replaces silicon at the $(2a)$ Wyckoff position.

Hexagonal primitive vectors

$$\mathbf{a_1} = \frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,\hat{\mathbf{y}}$$
$$\mathbf{a_2} = \frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(2a)	Ba I
$\mathbf{B_2}$	=	$\frac{1}{2}\mathbf{a}_3$	=	$\frac{1}{2}c\,\hat{\mathbf{z}}$	(2a)	Ba I
$\mathbf{B_3}$	=	$\frac{1}{3}\mathbf{a}_1 + \frac{2}{3}\mathbf{a}_2$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}}$	(2c)	Si I
$\mathbf{B_4}$	=	$\frac{1}{3}\mathbf{a}_1 + \frac{2}{3}\mathbf{a}_2 + \frac{1}{2}\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(2c)	Si I
$\mathbf{B_5}$	=	$x_3\,\mathbf{a}_1 + y_3\,\mathbf{a}_2 + \frac{1}{4}\mathbf{a}_3$	=	$\frac{1}{2}a\left(x_3+y_3\right)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\left(x_3-y_3\right)\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(6k)	O I
$\mathbf{B_6}$	=	$-y_3\,\mathbf{a}_1 + \left(x_3-y_3\right)\,\mathbf{a}_2 + \frac{1}{4}\mathbf{a}_3$	=	$\frac{1}{2}a\left(x_3-2y_3\right)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_3\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(6k)	O I
$\mathbf{B_7}$	=	$-\left(x_3-y_3\right)\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 + \frac{1}{4}\mathbf{a}_3$	=	$-\frac{1}{2}a\left(2x_3-y_3\right)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_3\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(6k)	O I
$\mathbf{B_8}$	=	$-y_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 + \frac{3}{4}\mathbf{a}_3$	=	$-\frac{1}{2}a\left(x_3+y_3\right)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\left(x_3-y_3\right)\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(6k)	O I
$\mathbf{B_9}$	=	$-\left(x_3-y_3\right)\,\mathbf{a}_1 + y_3\,\mathbf{a}_2 + \frac{3}{4}\mathbf{a}_3$	=	$\frac{1}{2}a\left(-x_3+2y_3\right)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_3\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(6k)	O I
$\mathbf{B_{10}}$	=	$x_3\,\mathbf{a}_1 + \left(x_3-y_3\right)\,\mathbf{a}_2 + \frac{3}{4}\mathbf{a}_3$	=	$\frac{1}{2}a\left(2x_3-y_3\right)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_3\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(6k)	O I
$\mathbf{B_{11}}$	=	$x_4\,\mathbf{a}_1 + y_4\,\mathbf{a}_2 + \frac{1}{4}\mathbf{a}_3$	=	$\frac{1}{2}a\left(x_4+y_4\right)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\left(x_4-y_4\right)\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(6k)	Si II
$\mathbf{B_{12}}$	=	$-y_4\,\mathbf{a}_1 + \left(x_4-y_4\right)\,\mathbf{a}_2 + \frac{1}{4}\mathbf{a}_3$	=	$\frac{1}{2}a\left(x_4-2y_4\right)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_4\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(6k)	Si II
$\mathbf{B_{13}}$	=	$-\left(x_4-y_4\right)\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 + \frac{1}{4}\mathbf{a}_3$	=	$-\frac{1}{2}a\left(2x_4-y_4\right)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_4\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(6k)	Si II
$\mathbf{B_{14}}$	=	$-y_4\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 + \frac{3}{4}\mathbf{a}_3$	=	$-\frac{1}{2}a\left(x_4+y_4\right)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\left(x_4-y_4\right)\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(6k)	Si II
$\mathbf{B_{15}}$	=	$-\left(x_4-y_4\right)\,\mathbf{a}_1 + y_4\,\mathbf{a}_2 + \frac{3}{4}\mathbf{a}_3$	=	$\frac{1}{2}a\left(-x_4+2y_4\right)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_4\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(6k)	Si II
$\mathbf{B_{16}}$	=	$x_4\,\mathbf{a}_1 + \left(x_4-y_4\right)\,\mathbf{a}_2 + \frac{3}{4}\mathbf{a}_3$	=	$\frac{1}{2}a\left(2x_4-y_4\right)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_4\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(6k)	Si II
$\mathbf{B_{17}}$	=	$x_5\,\mathbf{a}_1 + y_5\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$\frac{1}{2}a\left(x_5+y_5\right)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\left(x_5-y_5\right)\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(12l)	O II
$\mathbf{B_{18}}$	=	$-y_5\,\mathbf{a}_1 + \left(x_5-y_5\right)\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$\frac{1}{2}a\left(x_5-2y_5\right)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_5\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(12l)	O II
$\mathbf{B_{19}}$	=	$-\left(x_5-y_5\right)\,\mathbf{a}_1 - x_5\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$-\frac{1}{2}a\left(2x_5-y_5\right)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_5\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(12l)	O II
$\mathbf{B_{20}}$	=	$x_5\,\mathbf{a}_1 + y_5\,\mathbf{a}_2 - \left(z_5-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\left(x_5+y_5\right)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\left(x_5-y_5\right)\,\hat{\mathbf{y}} - c\left(z_5-\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(12l)	O II
$\mathbf{B_{21}}$	=	$-y_5\,\mathbf{a}_1 + \left(x_5-y_5\right)\,\mathbf{a}_2 - \left(z_5-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\left(x_5-2y_5\right)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_5\,\hat{\mathbf{y}} - c\left(z_5-\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(12l)	O II

$\mathbf{B_{22}}$	$=$	$-\left(x_5 - y_5\right)\,\mathbf{a}_1 - x_5\,\mathbf{a}_2 - \left(z_5 - \frac{1}{2}\right)\,\mathbf{a}_3$	$=$	$-\frac{1}{2}a\left(2x_5 - y_5\right)\,\mathbf{\hat{x}} - \frac{\sqrt{3}}{2}ay_5\,\mathbf{\hat{y}} - c\left(z_5 - \frac{1}{2}\right)\,\mathbf{\hat{z}}$	(12l)	O II
$\mathbf{B_{23}}$	$=$	$-y_5\,\mathbf{a}_1 - x_5\,\mathbf{a}_2 + \left(z_5 + \frac{1}{2}\right)\,\mathbf{a}_3$	$=$	$-\frac{1}{2}a\left(x_5 + y_5\right)\,\mathbf{\hat{x}} - \frac{\sqrt{3}}{2}a\left(x_5 - y_5\right)\,\mathbf{\hat{y}} + c\left(z_5 + \frac{1}{2}\right)\,\mathbf{\hat{z}}$	(12l)	O II
$\mathbf{B_{24}}$	$=$	$-\left(x_5 - y_5\right)\,\mathbf{a}_1 + y_5\,\mathbf{a}_2 + \left(z_5 + \frac{1}{2}\right)\,\mathbf{a}_3$	$=$	$\frac{1}{2}a\left(-x_5 + 2y_5\right)\,\mathbf{\hat{x}} + \frac{\sqrt{3}}{2}ax_5\,\mathbf{\hat{y}} + c\left(z_5 + \frac{1}{2}\right)\,\mathbf{\hat{z}}$	(12l)	O II
$\mathbf{B_{25}}$	$=$	$x_5\,\mathbf{a}_1 + \left(x_5 - y_5\right)\,\mathbf{a}_2 + \left(z_5 + \frac{1}{2}\right)\,\mathbf{a}_3$	$=$	$\frac{1}{2}a\left(2x_5 - y_5\right)\,\mathbf{\hat{x}} - \frac{\sqrt{3}}{2}ay_5\,\mathbf{\hat{y}} + c\left(z_5 + \frac{1}{2}\right)\,\mathbf{\hat{z}}$	(12l)	O II
$\mathbf{B_{26}}$	$=$	$-y_5\,\mathbf{a}_1 - x_5\,\mathbf{a}_2 - z_5\,\mathbf{a}_3$	$=$	$-\frac{1}{2}a\left(x_5 + y_5\right)\,\mathbf{\hat{x}} - \frac{\sqrt{3}}{2}a\left(x_5 - y_5\right)\,\mathbf{\hat{y}} - cz_5\,\mathbf{\hat{z}}$	(12l)	O II
$\mathbf{B_{27}}$	$=$	$-\left(x_5 - y_5\right)\,\mathbf{a}_1 + y_5\,\mathbf{a}_2 - z_5\,\mathbf{a}_3$	$=$	$\frac{1}{2}a\left(-x_5 + 2y_5\right)\,\mathbf{\hat{x}} + \frac{\sqrt{3}}{2}ax_5\,\mathbf{\hat{y}} - cz_5\,\mathbf{\hat{z}}$	(12l)	O II
$\mathbf{B_{28}}$	$=$	$x_5\,\mathbf{a}_1 + \left(x_5 - y_5\right)\,\mathbf{a}_2 - z_5\,\mathbf{a}_3$	$=$	$\frac{1}{2}a\left(2x_5 - y_5\right)\,\mathbf{\hat{x}} - \frac{\sqrt{3}}{2}ay_5\,\mathbf{\hat{y}} - cz_5\,\mathbf{\hat{z}}$	(12l)	O II

References

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[2] C. Hermann, O. Lohrmann, and H. Philipp, eds., *Strukturbericht Band II 1928-1932* (Akademische Verlagsgesellschaft M. B. H., Leipzig, 1937).