

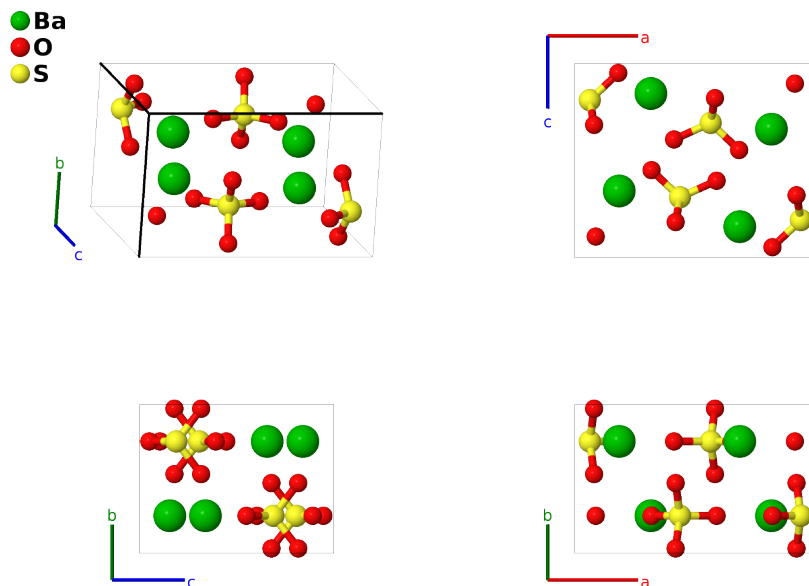
Barite (BaSO_4 , $H0_2$) Structure: AB4C_oP24_62_c_2cd_c-001

This structure originally had the label AB4C_oP24_62_c_2cd_c. Calls to that address will be redirected here.

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<https://aflow.org/p/CXQX>

https://aflow.org/p/AB4C_oP24_62_c_2cd_c-001



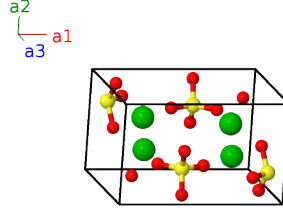
Prototype	BaO_4S
AFLOW prototype label	AB4C_oP24_62_c_2cd_c-001
<i>Strukturbericht</i> designation	$H0_2$
Mineral name	barite
ICSD	16904
Pearson symbol	oP24
Space group number	62
Space group symbol	$Pnma$
AFLOW prototype command	<code>aflow --proto=AB4C_oP24_62_c_2cd_c-001 --params=a, b/a, c/a, x1, z1, x2, z2, x3, z3, x4, z4, x5, y5, z5</code>

Other compounds with this structure

BaBeF_4 , InBF_4 , KBF_4 , KGaH_4 , KClO_4 (LT), NaBH_4 , PbSO_4 (anglesite), RbBF_4 , RbMnO_4 , SrSO_4 (celestite), TlBF_4

Simple Orthorhombic primitive vectors

$$\begin{aligned}\mathbf{a}_1 &= a \hat{\mathbf{x}} \\ \mathbf{a}_2 &= b \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}}\end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
\mathbf{B}_1	$= x_1 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_1 \mathbf{a}_3$	$=$	$ax_1 \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} + cz_1 \hat{\mathbf{z}}$	(4c)	Ba I
\mathbf{B}_2	$= -\left(x_1 - \frac{1}{2}\right) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \left(z_1 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a \left(x_1 - \frac{1}{2}\right) \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} + c \left(z_1 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(4c)	Ba I
\mathbf{B}_3	$= -x_1 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_1 \mathbf{a}_3$	$=$	$-ax_1 \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} - cz_1 \hat{\mathbf{z}}$	(4c)	Ba I
\mathbf{B}_4	$= \left(x_1 + \frac{1}{2}\right) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 - \left(z_1 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$a \left(x_1 + \frac{1}{2}\right) \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} - c \left(z_1 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(4c)	Ba I
\mathbf{B}_5	$= x_2 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$ax_2 \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$	(4c)	O I
\mathbf{B}_6	$= -\left(x_2 - \frac{1}{2}\right) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \left(z_2 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a \left(x_2 - \frac{1}{2}\right) \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} + c \left(z_2 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(4c)	O I
\mathbf{B}_7	$= -x_2 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_2 \mathbf{a}_3$	$=$	$-ax_2 \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} - cz_2 \hat{\mathbf{z}}$	(4c)	O I
\mathbf{B}_8	$= \left(x_2 + \frac{1}{2}\right) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 - \left(z_2 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$a \left(x_2 + \frac{1}{2}\right) \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} - c \left(z_2 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(4c)	O I
\mathbf{B}_9	$= x_3 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$ax_3 \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(4c)	O II
\mathbf{B}_{10}	$= -\left(x_3 - \frac{1}{2}\right) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \left(z_3 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a \left(x_3 - \frac{1}{2}\right) \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} + c \left(z_3 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(4c)	O II
\mathbf{B}_{11}	$= -x_3 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$-ax_3 \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} - cz_3 \hat{\mathbf{z}}$	(4c)	O II
\mathbf{B}_{12}	$= \left(x_3 + \frac{1}{2}\right) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 - \left(z_3 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$a \left(x_3 + \frac{1}{2}\right) \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} - c \left(z_3 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(4c)	O II
\mathbf{B}_{13}	$= x_4 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$ax_4 \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(4c)	S I
\mathbf{B}_{14}	$= -\left(x_4 - \frac{1}{2}\right) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \left(z_4 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a \left(x_4 - \frac{1}{2}\right) \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} + c \left(z_4 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(4c)	S I
\mathbf{B}_{15}	$= -x_4 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$-ax_4 \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}}$	(4c)	S I
\mathbf{B}_{16}	$= \left(x_4 + \frac{1}{2}\right) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 - \left(z_4 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$a \left(x_4 + \frac{1}{2}\right) \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} - c \left(z_4 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(4c)	S I
\mathbf{B}_{17}	$= x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$ax_5 \hat{\mathbf{x}} + by_5 \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(8d)	O III
\mathbf{B}_{18}	$= -\left(x_5 - \frac{1}{2}\right) \mathbf{a}_1 - y_5 \mathbf{a}_2 + \left(z_5 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a \left(x_5 - \frac{1}{2}\right) \hat{\mathbf{x}} - by_5 \hat{\mathbf{y}} + c \left(z_5 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(8d)	O III
\mathbf{B}_{19}	$= -x_5 \mathbf{a}_1 + \left(y_5 + \frac{1}{2}\right) \mathbf{a}_2 - z_5 \mathbf{a}_3$	$=$	$-ax_5 \hat{\mathbf{x}} + b \left(y_5 + \frac{1}{2}\right) \hat{\mathbf{y}} - cz_5 \hat{\mathbf{z}}$	(8d)	O III
\mathbf{B}_{20}	$= \left(x_5 + \frac{1}{2}\right) \mathbf{a}_1 - \left(y_5 - \frac{1}{2}\right) \mathbf{a}_2 - \left(z_5 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$a \left(x_5 + \frac{1}{2}\right) \hat{\mathbf{x}} - b \left(y_5 - \frac{1}{2}\right) \hat{\mathbf{y}} - c \left(z_5 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(8d)	O III
\mathbf{B}_{21}	$= -x_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 - z_5 \mathbf{a}_3$	$=$	$-ax_5 \hat{\mathbf{x}} - by_5 \hat{\mathbf{y}} - cz_5 \hat{\mathbf{z}}$	(8d)	O III
\mathbf{B}_{22}	$= \left(x_5 + \frac{1}{2}\right) \mathbf{a}_1 + y_5 \mathbf{a}_2 - \left(z_5 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$a \left(x_5 + \frac{1}{2}\right) \hat{\mathbf{x}} + by_5 \hat{\mathbf{y}} - c \left(z_5 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(8d)	O III
\mathbf{B}_{23}	$= x_5 \mathbf{a}_1 - \left(y_5 - \frac{1}{2}\right) \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$ax_5 \hat{\mathbf{x}} - b \left(y_5 - \frac{1}{2}\right) \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(8d)	O III
\mathbf{B}_{24}	$= -\left(x_5 - \frac{1}{2}\right) \mathbf{a}_1 + \left(y_5 + \frac{1}{2}\right) \mathbf{a}_2 + \left(z_5 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a \left(x_5 - \frac{1}{2}\right) \hat{\mathbf{x}} + b \left(y_5 + \frac{1}{2}\right) \hat{\mathbf{y}} + c \left(z_5 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(8d)	O III

References

- [1] A. A. Colville and K. Staudhammer, *A refinement of the structure of barite*, Am. Mineral. **52**, 1877–1880 (1967).

Found in

- [1] D. Barthelmy, *Mineralogy Database* (2012). Barite.