

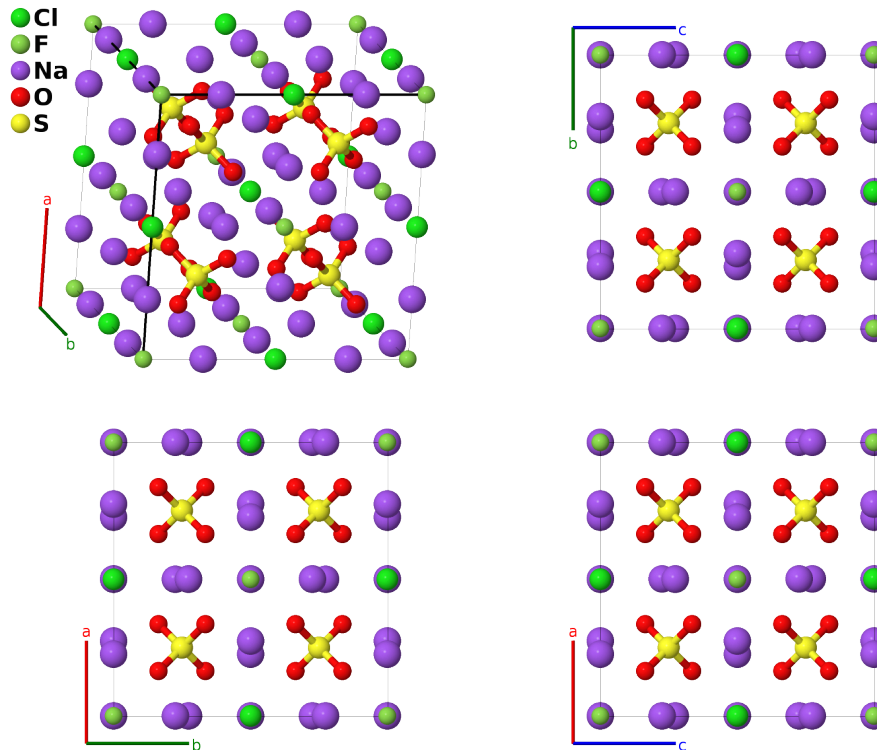
Sulphohalite $[\text{Na}_6\text{ClF}(\text{SO}_4)_2, H5_8]$ Structure: ABC6D8E2_cF72_225_a_b_e_f_c-001

This structure originally had the label ABC6D8E2_cF72_225_b_a_e_f_c. Calls to that address will be redirected here.

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<https://aflow.org/p/8Y3K>

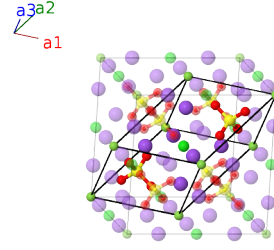
https://aflow.org/p/ABC6D8E2_cF72_225_a_b_e_f_c-001



Prototype	$\text{ClFNa}_6\text{O}_8\text{S}_2$
AFLOW prototype label	ABC6D8E2_cF72_225_a_b_e_f_c-001
<i>Strukturbericht</i> designation	$H5_8$
Mineral name	sulphohalite
ICSD	52291
Pearson symbol	cF72
Space group number	225
Space group symbol	$Fm\bar{3}m$
AFLOW prototype command	<code>aflow --proto=ABC6D8E2_cF72_225_a_b_e_f_c-001 --params=a, x4, x5</code>

Face-centered Cubic primitive vectors

$$\begin{aligned}\mathbf{a}_1 &= \frac{1}{2}a \hat{\mathbf{y}} + \frac{1}{2}a \hat{\mathbf{z}} \\ \mathbf{a}_2 &= \frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{2}a \hat{\mathbf{z}} \\ \mathbf{a}_3 &= \frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{2}a \hat{\mathbf{y}}\end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
\mathbf{B}_1	$=$	0	$=$	0	(4a) Cl I
\mathbf{B}_2	$=$	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{2}a \hat{\mathbf{y}} + \frac{1}{2}a \hat{\mathbf{z}}$	(4b) F I
\mathbf{B}_3	$=$	$\frac{1}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} + \frac{1}{4}a \hat{\mathbf{y}} + \frac{1}{4}a \hat{\mathbf{z}}$	(8c) S I
\mathbf{B}_4	$=$	$\frac{3}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{3}{4}a \hat{\mathbf{x}} + \frac{3}{4}a \hat{\mathbf{y}} + \frac{3}{4}a \hat{\mathbf{z}}$	(8c) S I
\mathbf{B}_5	$=$	$-x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + x_4 \mathbf{a}_3$	$=$	$ax_4 \hat{\mathbf{x}}$	(24e) Na I
\mathbf{B}_6	$=$	$x_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 - x_4 \mathbf{a}_3$	$=$	$-ax_4 \hat{\mathbf{x}}$	(24e) Na I
\mathbf{B}_7	$=$	$x_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 + x_4 \mathbf{a}_3$	$=$	$ax_4 \hat{\mathbf{y}}$	(24e) Na I
\mathbf{B}_8	$=$	$-x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 - x_4 \mathbf{a}_3$	$=$	$-ax_4 \hat{\mathbf{y}}$	(24e) Na I
\mathbf{B}_9	$=$	$x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 - x_4 \mathbf{a}_3$	$=$	$ax_4 \hat{\mathbf{z}}$	(24e) Na I
\mathbf{B}_{10}	$=$	$-x_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 + x_4 \mathbf{a}_3$	$=$	$-ax_4 \hat{\mathbf{z}}$	(24e) Na I
\mathbf{B}_{11}	$=$	$x_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 + x_5 \mathbf{a}_3$	$=$	$ax_5 \hat{\mathbf{x}} + ax_5 \hat{\mathbf{y}} + ax_5 \hat{\mathbf{z}}$	(32f) O I
\mathbf{B}_{12}	$=$	$x_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 - 3x_5 \mathbf{a}_3$	$=$	$-ax_5 \hat{\mathbf{x}} - ax_5 \hat{\mathbf{y}} + ax_5 \hat{\mathbf{z}}$	(32f) O I
\mathbf{B}_{13}	$=$	$x_5 \mathbf{a}_1 - 3x_5 \mathbf{a}_2 + x_5 \mathbf{a}_3$	$=$	$-ax_5 \hat{\mathbf{x}} + ax_5 \hat{\mathbf{y}} - ax_5 \hat{\mathbf{z}}$	(32f) O I
\mathbf{B}_{14}	$=$	$-3x_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 + x_5 \mathbf{a}_3$	$=$	$ax_5 \hat{\mathbf{x}} - ax_5 \hat{\mathbf{y}} - ax_5 \hat{\mathbf{z}}$	(32f) O I
\mathbf{B}_{15}	$=$	$-x_5 \mathbf{a}_1 - x_5 \mathbf{a}_2 + 3x_5 \mathbf{a}_3$	$=$	$ax_5 \hat{\mathbf{x}} + ax_5 \hat{\mathbf{y}} - ax_5 \hat{\mathbf{z}}$	(32f) O I
\mathbf{B}_{16}	$=$	$-x_5 \mathbf{a}_1 - x_5 \mathbf{a}_2 - x_5 \mathbf{a}_3$	$=$	$-ax_5 \hat{\mathbf{x}} - ax_5 \hat{\mathbf{y}} - ax_5 \hat{\mathbf{z}}$	(32f) O I
\mathbf{B}_{17}	$=$	$-x_5 \mathbf{a}_1 + 3x_5 \mathbf{a}_2 - x_5 \mathbf{a}_3$	$=$	$ax_5 \hat{\mathbf{x}} - ax_5 \hat{\mathbf{y}} + ax_5 \hat{\mathbf{z}}$	(32f) O I
\mathbf{B}_{18}	$=$	$3x_5 \mathbf{a}_1 - x_5 \mathbf{a}_2 - x_5 \mathbf{a}_3$	$=$	$-ax_5 \hat{\mathbf{x}} + ax_5 \hat{\mathbf{y}} + ax_5 \hat{\mathbf{z}}$	(32f) O I

References

- [1] A. Pabst, *The Crystal Structure of Sulphohalite*, Z. Kristallogr. **89**, 514–517 (1934), doi:10.1524/zkri.1934.89.1.514.

Found in

- [1] C. Gottfried and F. Schosberger, eds., *Strukturbericht Band III 1933-1935* (Akademische Verlagsgesellschaft M. B. H., Leipzig, 1937).