

NaSbF₆ Structure:

A6BC_cP32_205_d_a_b-001

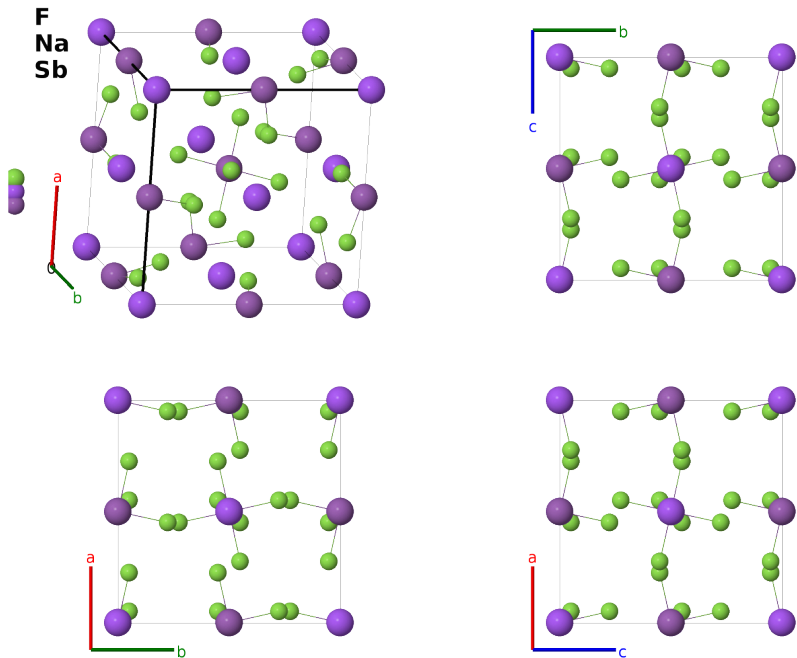
This structure previously used the label(s) **A6BC_cP32_205_d_b_a**. Calls to these addresses will be redirected here.

Cite this page as:

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<https://aflow.org/prototype-encyclopedia/N7XD>

https://aflow.org/prototype-encyclopedia/A6BC_cP32_205_d_a_b-001



Prototype	F ₆ NaSb
AFLOW prototype label	A6BC_cP32_205_d_a_b-001
ICSD	25538
CCDC	1601192
Pearson symbol	cP32
Space group number	205
Space group symbol	$Pa\bar{3}$
AFLOW prototype command	<code>aflow --proto=A6BC_cP32_205_d_a_b-001</code> <code>--params=a, x_3, y_3, z_3</code>

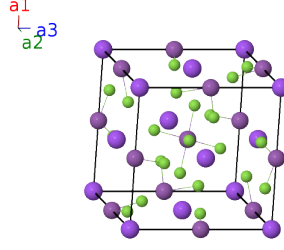
- This is the pure fluorine end-point of the NaSbF_{6-x}(OH)_x compounds. Although the replacement of fluorine by OH does not affect the shape of the Sb(F,OH)₆ ions, it has a profound effect on the structure, as can be seen by looking at NaSb(OH)₆ (*J*₁₁₁) and NaSbF₄(OH)₂ (*J*₁₁₂).

Simple Cubic primitive vectors

$$\mathbf{a}_1 = a \hat{\mathbf{x}}$$

$$\mathbf{a}_2 = a \hat{\mathbf{y}}$$

$$\mathbf{a}_3 = a \hat{\mathbf{z}}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$=$	0	$=$	0	(4a) Na I
$\mathbf{B}_2$	$=$	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{z}}$	(4a) Na I
$\mathbf{B}_3$	$=$	$\frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{y}} + \frac{1}{2} a \hat{\mathbf{z}}$	(4a) Na I
$\mathbf{B}_4$	$=$	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}}$	(4a) Na I
$\mathbf{B}_5$	$=$	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} + \frac{1}{2} a \hat{\mathbf{z}}$	(4b) Sb I
$\mathbf{B}_6$	$=$	$\frac{1}{2} \mathbf{a}_2$	$=$	$\frac{1}{2} a \hat{\mathbf{y}}$	(4b) Sb I
$\mathbf{B}_7$	$=$	$\frac{1}{2} \mathbf{a}_1$	$=$	$\frac{1}{2} a \hat{\mathbf{x}}$	(4b) Sb I
$\mathbf{B}_8$	$=$	$\frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{z}}$	(4b) Sb I
$\mathbf{B}_9$	$=$	$x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$ax_3 \hat{\mathbf{x}} + ay_3 \hat{\mathbf{y}} + az_3 \hat{\mathbf{z}}$	(24d) F I
$\mathbf{B}_{10}$	$=$	$-(x_3 - \frac{1}{2}) \mathbf{a}_1 - y_3 \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_3 - \frac{1}{2}) \hat{\mathbf{x}} - ay_3 \hat{\mathbf{y}} + a(z_3 + \frac{1}{2}) \hat{\mathbf{z}}$	(24d) F I
$\mathbf{B}_{11}$	$=$	$-x_3 \mathbf{a}_1 + (y_3 + \frac{1}{2}) \mathbf{a}_2 - (z_3 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_3 \hat{\mathbf{x}} + a(y_3 + \frac{1}{2}) \hat{\mathbf{y}} - a(z_3 - \frac{1}{2}) \hat{\mathbf{z}}$	(24d) F I
$\mathbf{B}_{12}$	$=$	$(x_3 + \frac{1}{2}) \mathbf{a}_1 - (y_3 - \frac{1}{2}) \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$a(x_3 + \frac{1}{2}) \hat{\mathbf{x}} - a(y_3 - \frac{1}{2}) \hat{\mathbf{y}} - az_3 \hat{\mathbf{z}}$	(24d) F I
$\mathbf{B}_{13}$	$=$	$z_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + y_3 \mathbf{a}_3$	$=$	$az_3 \hat{\mathbf{x}} + ax_3 \hat{\mathbf{y}} + ay_3 \hat{\mathbf{z}}$	(24d) F I
$\mathbf{B}_{14}$	$=$	$(z_3 + \frac{1}{2}) \mathbf{a}_1 - (x_3 - \frac{1}{2}) \mathbf{a}_2 - y_3 \mathbf{a}_3$	$=$	$a(z_3 + \frac{1}{2}) \hat{\mathbf{x}} - a(x_3 - \frac{1}{2}) \hat{\mathbf{y}} - ay_3 \hat{\mathbf{z}}$	(24d) F I
$\mathbf{B}_{15}$	$=$	$-(z_3 - \frac{1}{2}) \mathbf{a}_1 - x_3 \mathbf{a}_2 + (y_3 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(z_3 - \frac{1}{2}) \hat{\mathbf{x}} - ax_3 \hat{\mathbf{y}} + a(y_3 + \frac{1}{2}) \hat{\mathbf{z}}$	(24d) F I
$\mathbf{B}_{16}$	$=$	$-z_3 \mathbf{a}_1 + (x_3 + \frac{1}{2}) \mathbf{a}_2 - (y_3 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-az_3 \hat{\mathbf{x}} + a(x_3 + \frac{1}{2}) \hat{\mathbf{y}} - a(y_3 - \frac{1}{2}) \hat{\mathbf{z}}$	(24d) F I
$\mathbf{B}_{17}$	$=$	$y_3 \mathbf{a}_1 + z_3 \mathbf{a}_2 + x_3 \mathbf{a}_3$	$=$	$ay_3 \hat{\mathbf{x}} + az_3 \hat{\mathbf{y}} + ax_3 \hat{\mathbf{z}}$	(24d) F I
$\mathbf{B}_{18}$	$=$	$-y_3 \mathbf{a}_1 + (z_3 + \frac{1}{2}) \mathbf{a}_2 - (x_3 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-ay_3 \hat{\mathbf{x}} + a(z_3 + \frac{1}{2}) \hat{\mathbf{y}} - a(x_3 - \frac{1}{2}) \hat{\mathbf{z}}$	(24d) F I
$\mathbf{B}_{19}$	$=$	$(y_3 + \frac{1}{2}) \mathbf{a}_1 - (z_3 - \frac{1}{2}) \mathbf{a}_2 - x_3 \mathbf{a}_3$	$=$	$a(y_3 + \frac{1}{2}) \hat{\mathbf{x}} - a(z_3 - \frac{1}{2}) \hat{\mathbf{y}} - ax_3 \hat{\mathbf{z}}$	(24d) F I
$\mathbf{B}_{20}$	$=$	$-(y_3 - \frac{1}{2}) \mathbf{a}_1 - z_3 \mathbf{a}_2 + (x_3 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(y_3 - \frac{1}{2}) \hat{\mathbf{x}} - az_3 \hat{\mathbf{y}} + a(x_3 + \frac{1}{2}) \hat{\mathbf{z}}$	(24d) F I
$\mathbf{B}_{21}$	$=$	$-x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$-ax_3 \hat{\mathbf{x}} - ay_3 \hat{\mathbf{y}} - az_3 \hat{\mathbf{z}}$	(24d) F I
$\mathbf{B}_{22}$	$=$	$(x_3 + \frac{1}{2}) \mathbf{a}_1 + y_3 \mathbf{a}_2 - (z_3 - \frac{1}{2}) \mathbf{a}_3$	$=$	$a(x_3 + \frac{1}{2}) \hat{\mathbf{x}} + ay_3 \hat{\mathbf{y}} - a(z_3 - \frac{1}{2}) \hat{\mathbf{z}}$	(24d) F I
$\mathbf{B}_{23}$	$=$	$x_3 \mathbf{a}_1 - (y_3 - \frac{1}{2}) \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$	$=$	$ax_3 \hat{\mathbf{x}} - a(y_3 - \frac{1}{2}) \hat{\mathbf{y}} + a(z_3 + \frac{1}{2}) \hat{\mathbf{z}}$	(24d) F I

$$\begin{aligned}
\mathbf{B}_{24} &= -\left(x_3 - \frac{1}{2}\right) \mathbf{a}_1 + \left(y_3 + \frac{1}{2}\right) \mathbf{a}_2 + z_3 \mathbf{a}_3 = -a\left(x_3 - \frac{1}{2}\right) \hat{\mathbf{x}} + a\left(y_3 + \frac{1}{2}\right) \hat{\mathbf{y}} + az_3 \hat{\mathbf{z}} & (24d) & \text{F I} \\
\mathbf{B}_{25} &= -z_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 - y_3 \mathbf{a}_3 = -az_3 \hat{\mathbf{x}} - ax_3 \hat{\mathbf{y}} - ay_3 \hat{\mathbf{z}} & (24d) & \text{F I} \\
\mathbf{B}_{26} &= -\left(z_3 - \frac{1}{2}\right) \mathbf{a}_1 + \left(x_3 + \frac{1}{2}\right) \mathbf{a}_2 + y_3 \mathbf{a}_3 = -a\left(z_3 - \frac{1}{2}\right) \hat{\mathbf{x}} + a\left(x_3 + \frac{1}{2}\right) \hat{\mathbf{y}} + ay_3 \hat{\mathbf{z}} & (24d) & \text{F I} \\
\mathbf{B}_{27} &= \left(z_3 + \frac{1}{2}\right) \mathbf{a}_1 + x_3 \mathbf{a}_2 - \left(y_3 - \frac{1}{2}\right) \mathbf{a}_3 = a\left(z_3 + \frac{1}{2}\right) \hat{\mathbf{x}} + ax_3 \hat{\mathbf{y}} - a\left(y_3 - \frac{1}{2}\right) \hat{\mathbf{z}} & (24d) & \text{F I} \\
\mathbf{B}_{28} &= z_3 \mathbf{a}_1 - \left(x_3 - \frac{1}{2}\right) \mathbf{a}_2 + \left(y_3 + \frac{1}{2}\right) \mathbf{a}_3 = az_3 \hat{\mathbf{x}} - a\left(x_3 - \frac{1}{2}\right) \hat{\mathbf{y}} + a\left(y_3 + \frac{1}{2}\right) \hat{\mathbf{z}} & (24d) & \text{F I} \\
\mathbf{B}_{29} &= -y_3 \mathbf{a}_1 - z_3 \mathbf{a}_2 - x_3 \mathbf{a}_3 = -ay_3 \hat{\mathbf{x}} - az_3 \hat{\mathbf{y}} - ax_3 \hat{\mathbf{z}} & (24d) & \text{F I} \\
\mathbf{B}_{30} &= y_3 \mathbf{a}_1 - \left(z_3 - \frac{1}{2}\right) \mathbf{a}_2 + \left(x_3 + \frac{1}{2}\right) \mathbf{a}_3 = ay_3 \hat{\mathbf{x}} - a\left(z_3 - \frac{1}{2}\right) \hat{\mathbf{y}} + a\left(x_3 + \frac{1}{2}\right) \hat{\mathbf{z}} & (24d) & \text{F I} \\
\mathbf{B}_{31} &= -\left(y_3 - \frac{1}{2}\right) \mathbf{a}_1 + \left(z_3 + \frac{1}{2}\right) \mathbf{a}_2 + x_3 \mathbf{a}_3 = -a\left(y_3 - \frac{1}{2}\right) \hat{\mathbf{x}} + a\left(z_3 + \frac{1}{2}\right) \hat{\mathbf{y}} + ax_3 \hat{\mathbf{z}} & (24d) & \text{F I} \\
\mathbf{B}_{32} &= \left(y_3 + \frac{1}{2}\right) \mathbf{a}_1 + z_3 \mathbf{a}_2 - \left(x_3 - \frac{1}{2}\right) \mathbf{a}_3 = a\left(y_3 + \frac{1}{2}\right) \hat{\mathbf{x}} + az_3 \hat{\mathbf{y}} - a\left(x_3 - \frac{1}{2}\right) \hat{\mathbf{z}} & (24d) & \text{F I}
\end{aligned}$$

References

- [1] N. Schrewelius, *Röntgenuntersuchung der Verbindungen NaSb(OH)₆, NaSbF₆, NaSbO₃ und gleichartiger Stoffe*, Z. Anorganische und Allgemeine Chemie **238**, 241–254 (1938), doi:10.1002/zaac.19382380209.

Found in

- [1] R. T. Downs and M. Hall-Wallace, *The American Mineralogist Crystal Structure Database*, Am. Mineral. **88**, 247–250 (2003).

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