# $NaSbF_4(OH)_2$ ($J1_{12}$) Structure: A6BC_hP16_163_i_b_c-001

This structure originally had the label `A6BC_hP16_163_i_b_c`. Calls to that address will be redirected here.

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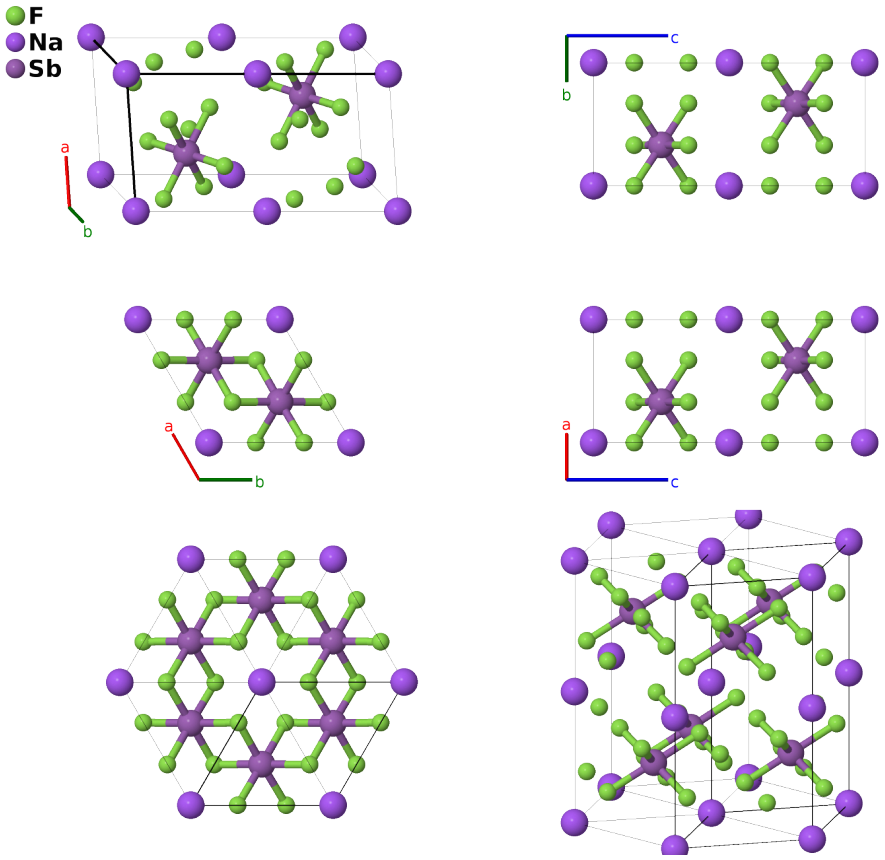
https://aflow.org/p/KLNT

https://aflow.org/p/A6BC_hP16_163_i_b_c-001




| | |
|---|---|
| **Prototype** | $F_6NaSb$ |
| **AFLOW prototype label** | A6BC_hP16_163_i_b_c-001 |
| ***Strukturbericht* designation** | $J1_{12}$ |
| **ICSD** | 25539 |
| **Pearson symbol** | hP16 |
| **Space group number** | 163 |
| **Space group symbol** | $P\bar{3}1c$ |
| **AFLOW prototype command** | `aflow --proto=A6BC_hP16_163_i_b_c-001 --params=`$a, c/a, x_3, y_3, z_3$ |

- The (2i) site, which we show as occupied by fluorine, is actually occupied by a random mixture of fluorine atoms (67%) and OH radicals (33%).
- 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 $NaSbF_6$ and $NaSb(OH)_6$ ($J1_{11}$).

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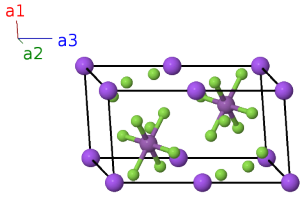
**Trigonal (Hexagonal) primitive vectors**

$$\begin{aligned}\mathbf{a_1} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}a\,\hat{\mathbf{y}} \\ \mathbf{a_2} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}a\,\hat{\mathbf{y}} \\ \mathbf{a_3} &= c\,\hat{\mathbf{z}}\end{aligned}$$

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**Basis vectors**

| | | Lattice coordinates | | Cartesian coordinates | Wyckoff position | Atom type |
|---|---|---|---|---|---|---|
| $\mathbf{B_1}$ | = | $0$ | = | $0$ | (2b) | Na I |
| $\mathbf{B_2}$ | = | $\frac{1}{2}\,\mathbf{a}_3$ | = | $\frac{1}{2}c\,\hat{\mathbf{z}}$ | (2b) | Na I |
| $\mathbf{B_3}$ | = | $\frac{1}{3}\,\mathbf{a}_1 + \frac{2}{3}\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$ | = | $\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$ | (2c) | Sb I |
| $\mathbf{B_4}$ | = | $\frac{2}{3}\,\mathbf{a}_1 + \frac{1}{3}\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$ | = | $\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$ | (2c) | Sb I |
| $\mathbf{B_5}$ | = | $x_3\,\mathbf{a}_1 + y_3\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$ | = | $\frac{1}{2}a\,(x_3 + y_3)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,(x_3 - y_3)\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$ | (12i) | F I |
| $\mathbf{B_6}$ | = | $-y_3\,\mathbf{a}_1 + (x_3 - y_3)\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$ | = | $\frac{1}{2}a\,(x_3 - 2y_3)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_3\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$ | (12i) | F I |
| $\mathbf{B_7}$ | = | $-(x_3 - y_3)\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$ | = | $-\frac{1}{2}a\,(2x_3 - y_3)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_3\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$ | (12i) | F I |
| $\mathbf{B_8}$ | = | $-y_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 - \left(z_3 - \frac{1}{2}\right)\,\mathbf{a}_3$ | = | $-\frac{1}{2}a\,(x_3 + y_3)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,(x_3 - y_3)\,\hat{\mathbf{y}} - c\left(z_3 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$ | (12i) | F I |
| $\mathbf{B_9}$ | = | $-(x_3 - y_3)\,\mathbf{a}_1 + y_3\,\mathbf{a}_2 - \left(z_3 - \frac{1}{2}\right)\,\mathbf{a}_3$ | = | $\frac{1}{2}a\,(-x_3 + 2y_3)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_3\,\hat{\mathbf{y}} - c\left(z_3 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$ | (12i) | F I |
| $\mathbf{B_{10}}$ | = | $x_3\,\mathbf{a}_1 + (x_3 - y_3)\,\mathbf{a}_2 - \left(z_3 - \frac{1}{2}\right)\,\mathbf{a}_3$ | = | $\frac{1}{2}a\,(2x_3 - y_3)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_3\,\hat{\mathbf{y}} - c\left(z_3 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$ | (12i) | F I |
| $\mathbf{B_{11}}$ | = | $-x_3\,\mathbf{a}_1 - y_3\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$ | = | $-\frac{1}{2}a\,(x_3 + y_3)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\,(x_3 - y_3)\,\hat{\mathbf{y}} - cz_3\,\hat{\mathbf{z}}$ | (12i) | F I |
| $\mathbf{B_{12}}$ | = | $y_3\,\mathbf{a}_1 - (x_3 - y_3)\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$ | = | $\frac{1}{2}a\,(-x_3 + 2y_3)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_3\,\hat{\mathbf{y}} - cz_3\,\hat{\mathbf{z}}$ | (12i) | F I |
| $\mathbf{B_{13}}$ | = | $(x_3 - y_3)\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$ | = | $\frac{1}{2}a\,(2x_3 - y_3)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_3\,\hat{\mathbf{y}} - cz_3\,\hat{\mathbf{z}}$ | (12i) | F I |
| $\mathbf{B_{14}}$ | = | $y_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + \left(z_3 + \frac{1}{2}\right)\,\mathbf{a}_3$ | = | $\frac{1}{2}a\,(x_3 + y_3)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\,(x_3 - y_3)\,\hat{\mathbf{y}} + c\left(z_3 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$ | (12i) | F I |
| $\mathbf{B_{15}}$ | = | $(x_3 - y_3)\,\mathbf{a}_1 - y_3\,\mathbf{a}_2 + \left(z_3 + \frac{1}{2}\right)\,\mathbf{a}_3$ | = | $\frac{1}{2}a\,(x_3 - 2y_3)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_3\,\hat{\mathbf{y}} + c\left(z_3 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$ | (12i) | F I |
| $\mathbf{B_{16}}$ | = | $-x_3\,\mathbf{a}_1 - (x_3 - y_3)\,\mathbf{a}_2 + \left(z_3 + \frac{1}{2}\right)\,\mathbf{a}_3$ | = | $-\frac{1}{2}a\,(2x_3 - y_3)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_3\,\hat{\mathbf{y}} + c\left(z_3 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$ | (12i) | F I |

**References**


[1] N. Schrewelius, *Röntgenuntersuchung der Verbindungen $NaSb(OH)_6$, $NaSbF_6$, $NaSbO_3$ 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).