Bararite [Trigonal $(NH_4)_2SiF_6$, $J1_6$] Structure: A6B2C_hP9_164_i_d_a-001

This structure originally had the label `A6B2C_hP9_164_i_d_a`. Calls to that address will be redirected here.

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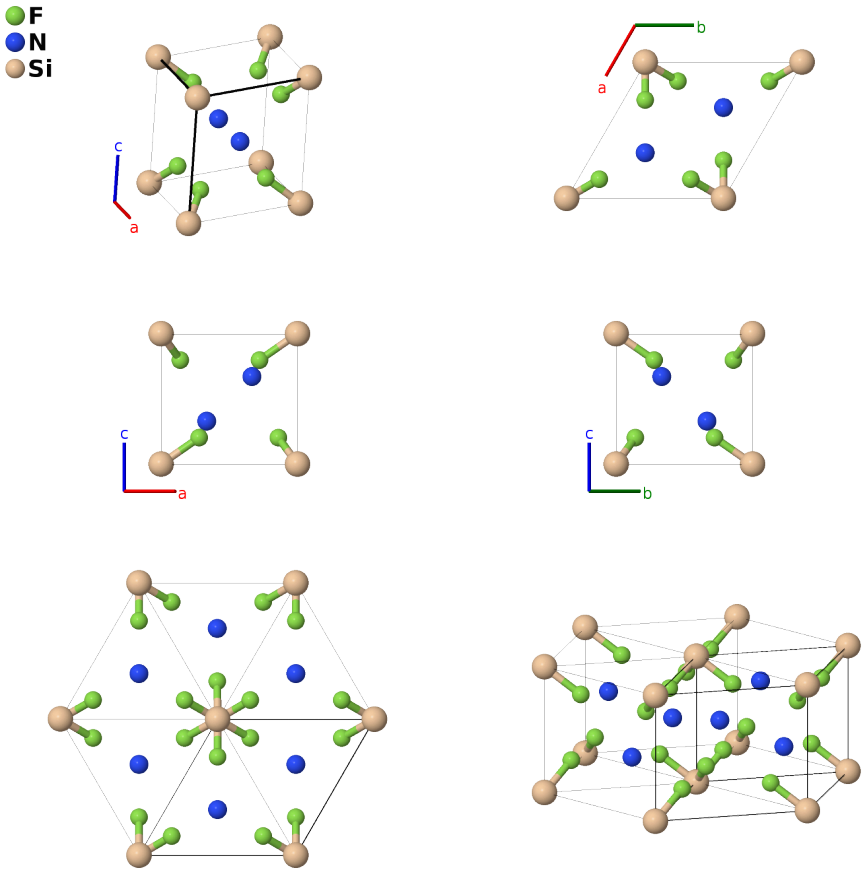
https://aflow.org/p/4BR9

https://aflow.org/p/A6B2C_hP9_164_i_d_a-001

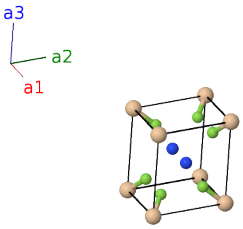


Prototype	$Fe_6(NH_4)_2Si$
AFLOW prototype label	A6B2C_hP9_164_i_d_a-001
***Strukturbericht* designation**	$J1_6$
Mineral name	bararite
ICSD	18027
Pearson symbol	hP9
Space group number	164
Space group symbol	$P\bar{3}m1$
AFLOW prototype command	`aflow --proto=A6B2C_hP9_164_i_d_a-001 --params=`$a, c/a, z_2, x_3, z_3$

- Bararite is a trigonal form of $(NH_4)_2SiF_6$, metastable at room temperature. The room temperature stable form is cubic cryptohalite, which takes on the $J1_1$ structure. Except for the hydrogen atoms, this structure is very similar to $J1_{13}$, K_2GeF_6. (Schlemper, 1966) state that the hydrogen atoms are on (2d) and (6i) sites, but were not able to determine the coordinates because of large thermal fluctuations. They were to study the system at 77K, but we have not found any evidence that this work was ever published.
- Originally (Hicks, 2021) we had the wrong sign for z_3. This has been corrected.

Trigonal (Hexagonal) primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(1a)	Si I
$\mathbf{B_2}$	=	$\frac{1}{3}\,\mathbf{a}_1 + \frac{2}{3}\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(2d)	N I
$\mathbf{B_3}$	=	$\frac{2}{3}\,\mathbf{a}_1 + \frac{1}{3}\,\mathbf{a}_2 - z_2\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} - cz_2\,\hat{\mathbf{z}}$	(2d)	N I
$\mathbf{B_4}$	=	$x_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$-\sqrt{3}ax_3\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(6i)	F I
$\mathbf{B_5}$	=	$x_3\,\mathbf{a}_1 + 2x_3\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$\frac{3}{2}ax_3\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_3\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(6i)	F I
$\mathbf{B_6}$	=	$-2x_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$-\frac{3}{2}ax_3\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_3\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(6i)	F I
$\mathbf{B_7}$	=	$-x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$	=	$\sqrt{3}ax_3\,\hat{\mathbf{y}} - cz_3\,\hat{\mathbf{z}}$	(6i)	F I
$\mathbf{B_8}$	=	$2x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$	=	$\frac{3}{2}ax_3\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_3\,\hat{\mathbf{y}} - cz_3\,\hat{\mathbf{z}}$	(6i)	F I
$\mathbf{B_9}$	=	$-x_3\,\mathbf{a}_1 - 2x_3\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$	=	$-\frac{3}{2}ax_3\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_3\,\hat{\mathbf{y}} - cz_3\,\hat{\mathbf{z}}$	(6i)	F I

References

[1] E. O. Schlemper and W. C. Hamilton, *On the Structure of Trigonal Ammonium Flourosilicate*, J. Chem. Phys. **45**, 408–409 (1966), doi:10.1063/1.2716548.

[2] D. Hicks, M. J.Mehl, M. Esters, C. Oses, O. Levy, G. L. W. Hart, C. Toher, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 3*, Comput. Mater. Sci. **199**, 110450 (2021), doi:10.1016/j.commatsci.2021.110450.

Found in

[1] J. Fábry, J. Chval, and V. Petrícek, *A new modification of diammonium hexafluorosilicate, $(NH_4)_2SiF_6$*, Acta Crystallogr. Sect. E **57**, i90–i91 (2001), doi:10.1107/S160053680101501X.