Crancrinite ($Na_6Ca_2Al_6Si_6O_{24}(CO_3)_2$, $S3_3$(I)) Structure: A3BCD3E15F3_hP52_173_c_b_b_c_5c_c-001

This structure previously used the label(s) `A3BCD3E15F3_hP52_173_c_b_b_c_5c_c`. Calls to these addresses will be redirected here.

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- 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.

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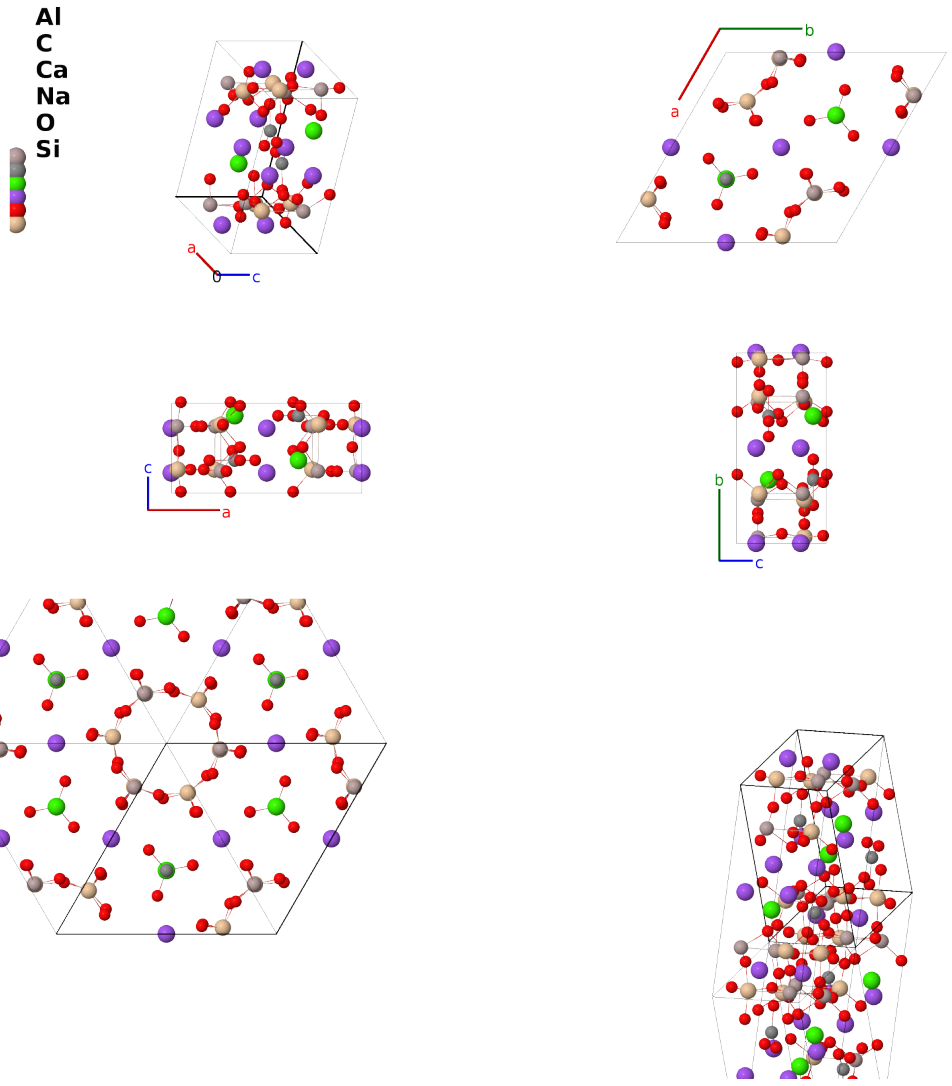
https://aflow.org/prototype-encyclopedia/7U5Z

https://aflow.org/prototype-encyclopedia/A3BCD3E15F3_hP52_173_c_b_b_c_5c_c-001



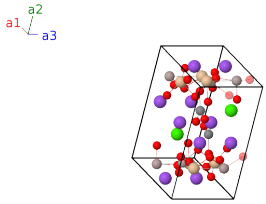
Prototype	$Al_3CCaNa_3O_{15}Si_3$
AFLOW prototype label	A3BCD3E15F3_hP52_173_c_b_b_c_5c_c-001
***Strukturbericht* designation**	$S3_3$(I)
Mineral name	crancrinite

ICSD	151383
CCDC	1668218
Pearson symbol	hP52
Space group number	173
Space group symbol	$P6_3$
AFLOW prototype command	`aflow --proto=A3BCD3E15F3_hP52_173_c_b_b_c_5c_c-001 --params=`$a, c/a, z_1, z_2, x_3, y_3, z_3, x_4, y_4, z_4, x_5, y_5, z_5, x_6, y_6, z_6, x_7, y_7, z_7, x_8, y_8, z_8, x_9, y_9, z_9, x_{10}, y_{10}, z_{10}$

- The term "crancrinite" covers a wide range of mineral compositions, some of which may include OH radicals and H_2O molecules. We use this early determination of the structure as the base.
- There are two major inconsistencies between (Kozu, 1933) and (Gottfried, 1937):
  - (Gottfried, 1937) interchanges the z coordinates of the carbon and calcium ions compared to (Kozu, 1933). Kozu's coordinates are consistent with CO_3 radicals, so we use their version.
  - (Kozu, 1933) and the ICSD entry give $x_{10} = 0.33$ for the x coordinate of silicon. This puts the silicon atoms very close to carbon atoms. We follow (Gottfried, 1937) and take $x_{10} = 0.033$, which gives a reasonable distance.
- (Gottfried, 1937) gave this structure the label $S3_3$, but later (Gottfried, 1938) gave the same label to parawollastonite, $CaSiO_3$. We will refer to crancrinite as $S3_3$(I) and parawollastonite as $S3_3$(II).

Hexagonal primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$\frac{1}{3}\,\mathbf{a}_1 + \frac{2}{3}\,\mathbf{a}_2 + z_1\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + cz_1\,\hat{\mathbf{z}}$	(2b)	C I
$\mathbf{B_2}$	=	$\frac{2}{3}\,\mathbf{a}_1 + \frac{1}{3}\,\mathbf{a}_2 + \left(z_1 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + c\left(z_1 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(2b)	C I
$\mathbf{B_3}$	=	$\frac{1}{3}\,\mathbf{a}_1 + \frac{2}{3}\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(2b)	Ca I
$\mathbf{B_4}$	=	$\frac{2}{3}\,\mathbf{a}_1 + \frac{1}{3}\,\mathbf{a}_2 + \left(z_2 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + c\left(z_2 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(2b)	Ca I
$\mathbf{B_5}$	=	$x_3\,\mathbf{a}_1 + y_3\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_3 + y_3)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,(x_3 - y_3)\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(6c)	Al I
$\mathbf{B_6}$	=	$-y_3\,\mathbf{a}_1 + (x_3 - y_3)\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_3 - 2y_3)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_3\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(6c)	Al I
$\mathbf{B_7}$	=	$-(x_3 - y_3)\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(2x_3 - y_3)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_3\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(6c)	Al I
$\mathbf{B_8}$	=	$-x_3\,\mathbf{a}_1 - y_3\,\mathbf{a}_2 + \left(z_3 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(x_3 + y_3)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\,(x_3 - y_3)\,\hat{\mathbf{y}} + c\left(z_3 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(6c)	Al I
$\mathbf{B_9}$	=	$y_3\,\mathbf{a}_1 - (x_3 - y_3)\,\mathbf{a}_2 + \left(z_3 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(-x_3 + 2y_3)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_3\,\hat{\mathbf{y}} + c\left(z_3 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(6c)	Al I
$\mathbf{B_{10}}$	=	$(x_3 - y_3)\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + \left(z_3 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(2x_3 - y_3)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_3\,\hat{\mathbf{y}} + c\left(z_3 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(6c)	Al I
$\mathbf{B_{11}}$	=	$x_4\,\mathbf{a}_1 + y_4\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_4 + y_4)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,(x_4 - y_4)\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(6c)	Na I

$$
\begin{array}{lcccccl}
\mathbf{B_{12}} & = & -y_4\,\mathbf{a}_1+(x_4-y_4)\,\mathbf{a}_2+z_4\,\mathbf{a}_3 & = & \frac{1}{2}a\,(x_4-2y_4)\,\hat{\mathbf{x}}+\frac{\sqrt{3}}{2}ax_4\,\hat{\mathbf{y}}+cz_4\,\hat{\mathbf{z}} & \text{(6c)} & \text{Na I}\\
\mathbf{B_{13}} & = & -(x_4-y_4)\,\mathbf{a}_1-x_4\,\mathbf{a}_2+z_4\,\mathbf{a}_3 & = & -\frac{1}{2}a\,(2x_4-y_4)\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{2}ay_4\,\hat{\mathbf{y}}+cz_4\,\hat{\mathbf{z}} & \text{(6c)} & \text{Na I}\\
\mathbf{B_{14}} & = & -x_4\,\mathbf{a}_1-y_4\,\mathbf{a}_2+\left(z_4+\frac{1}{2}\right)\,\mathbf{a}_3 & = & -\frac{1}{2}a\,(x_4+y_4)\,\hat{\mathbf{x}}+\frac{\sqrt{3}}{2}a\,(x_4-y_4)\,\hat{\mathbf{y}}+c\left(z_4+\frac{1}{2}\right)\,\hat{\mathbf{z}} & \text{(6c)} & \text{Na I}\\
\mathbf{B_{15}} & = & y_4\,\mathbf{a}_1-(x_4-y_4)\,\mathbf{a}_2+\left(z_4+\frac{1}{2}\right)\,\mathbf{a}_3 & = & \frac{1}{2}a\,(-x_4+2y_4)\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{2}ax_4\,\hat{\mathbf{y}}+c\left(z_4+\frac{1}{2}\right)\,\hat{\mathbf{z}} & \text{(6c)} & \text{Na I}\\
\mathbf{B_{16}} & = & (x_4-y_4)\,\mathbf{a}_1+x_4\,\mathbf{a}_2+\left(z_4+\frac{1}{2}\right)\,\mathbf{a}_3 & = & \frac{1}{2}a\,(2x_4-y_4)\,\hat{\mathbf{x}}+\frac{\sqrt{3}}{2}ay_4\,\hat{\mathbf{y}}+c\left(z_4+\frac{1}{2}\right)\,\hat{\mathbf{z}} & \text{(6c)} & \text{Na I}\\
\mathbf{B_{17}} & = & x_5\,\mathbf{a}_1+y_5\,\mathbf{a}_2+z_5\,\mathbf{a}_3 & = & \frac{1}{2}a\,(x_5+y_5)\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{2}a\,(x_5-y_5)\,\hat{\mathbf{y}}+cz_5\,\hat{\mathbf{z}} & \text{(6c)} & \text{O I}\\
\mathbf{B_{18}} & = & -y_5\,\mathbf{a}_1+(x_5-y_5)\,\mathbf{a}_2+z_5\,\mathbf{a}_3 & = & \frac{1}{2}a\,(x_5-2y_5)\,\hat{\mathbf{x}}+\frac{\sqrt{3}}{2}ax_5\,\hat{\mathbf{y}}+cz_5\,\hat{\mathbf{z}} & \text{(6c)} & \text{O I}\\
\mathbf{B_{19}} & = & -(x_5-y_5)\,\mathbf{a}_1-x_5\,\mathbf{a}_2+z_5\,\mathbf{a}_3 & = & -\frac{1}{2}a\,(2x_5-y_5)\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{2}ay_5\,\hat{\mathbf{y}}+cz_5\,\hat{\mathbf{z}} & \text{(6c)} & \text{O I}\\
\mathbf{B_{20}} & = & -x_5\,\mathbf{a}_1-y_5\,\mathbf{a}_2+\left(z_5+\frac{1}{2}\right)\,\mathbf{a}_3 & = & -\frac{1}{2}a\,(x_5+y_5)\,\hat{\mathbf{x}}+\frac{\sqrt{3}}{2}a\,(x_5-y_5)\,\hat{\mathbf{y}}+c\left(z_5+\frac{1}{2}\right)\,\hat{\mathbf{z}} & \text{(6c)} & \text{O I}\\
\mathbf{B_{21}} & = & y_5\,\mathbf{a}_1-(x_5-y_5)\,\mathbf{a}_2+\left(z_5+\frac{1}{2}\right)\,\mathbf{a}_3 & = & \frac{1}{2}a\,(-x_5+2y_5)\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{2}ax_5\,\hat{\mathbf{y}}+c\left(z_5+\frac{1}{2}\right)\,\hat{\mathbf{z}} & \text{(6c)} & \text{O I}\\
\mathbf{B_{22}} & = & (x_5-y_5)\,\mathbf{a}_1+x_5\,\mathbf{a}_2+\left(z_5+\frac{1}{2}\right)\,\mathbf{a}_3 & = & \frac{1}{2}a\,(2x_5-y_5)\,\hat{\mathbf{x}}+\frac{\sqrt{3}}{2}ay_5\,\hat{\mathbf{y}}+c\left(z_5+\frac{1}{2}\right)\,\hat{\mathbf{z}} & \text{(6c)} & \text{O I}\\
\mathbf{B_{23}} & = & x_6\,\mathbf{a}_1+y_6\,\mathbf{a}_2+z_6\,\mathbf{a}_3 & = & \frac{1}{2}a\,(x_6+y_6)\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{2}a\,(x_6-y_6)\,\hat{\mathbf{y}}+cz_6\,\hat{\mathbf{z}} & \text{(6c)} & \text{O II}\\
\mathbf{B_{24}} & = & -y_6\,\mathbf{a}_1+(x_6-y_6)\,\mathbf{a}_2+z_6\,\mathbf{a}_3 & = & \frac{1}{2}a\,(x_6-2y_6)\,\hat{\mathbf{x}}+\frac{\sqrt{3}}{2}ax_6\,\hat{\mathbf{y}}+cz_6\,\hat{\mathbf{z}} & \text{(6c)} & \text{O II}\\
\mathbf{B_{25}} & = & -(x_6-y_6)\,\mathbf{a}_1-x_6\,\mathbf{a}_2+z_6\,\mathbf{a}_3 & = & -\frac{1}{2}a\,(2x_6-y_6)\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{2}ay_6\,\hat{\mathbf{y}}+cz_6\,\hat{\mathbf{z}} & \text{(6c)} & \text{O II}\\
\mathbf{B_{26}} & = & -x_6\,\mathbf{a}_1-y_6\,\mathbf{a}_2+\left(z_6+\frac{1}{2}\right)\,\mathbf{a}_3 & = & -\frac{1}{2}a\,(x_6+y_6)\,\hat{\mathbf{x}}+\frac{\sqrt{3}}{2}a\,(x_6-y_6)\,\hat{\mathbf{y}}+c\left(z_6+\frac{1}{2}\right)\,\hat{\mathbf{z}} & \text{(6c)} & \text{O II}\\
\mathbf{B_{27}} & = & y_6\,\mathbf{a}_1-(x_6-y_6)\,\mathbf{a}_2+\left(z_6+\frac{1}{2}\right)\,\mathbf{a}_3 & = & \frac{1}{2}a\,(-x_6+2y_6)\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{2}ax_6\,\hat{\mathbf{y}}+c\left(z_6+\frac{1}{2}\right)\,\hat{\mathbf{z}} & \text{(6c)} & \text{O II}\\
\mathbf{B_{28}} & = & (x_6-y_6)\,\mathbf{a}_1+x_6\,\mathbf{a}_2+\left(z_6+\frac{1}{2}\right)\,\mathbf{a}_3 & = & \frac{1}{2}a\,(2x_6-y_6)\,\hat{\mathbf{x}}+\frac{\sqrt{3}}{2}ay_6\,\hat{\mathbf{y}}+c\left(z_6+\frac{1}{2}\right)\,\hat{\mathbf{z}} & \text{(6c)} & \text{O II}\\
\mathbf{B_{29}} & = & x_7\,\mathbf{a}_1+y_7\,\mathbf{a}_2+z_7\,\mathbf{a}_3 & = & \frac{1}{2}a\,(x_7+y_7)\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{2}a\,(x_7-y_7)\,\hat{\mathbf{y}}+cz_7\,\hat{\mathbf{z}} & \text{(6c)} & \text{O III}\\
\mathbf{B_{30}} & = & -y_7\,\mathbf{a}_1+(x_7-y_7)\,\mathbf{a}_2+z_7\,\mathbf{a}_3 & = & \frac{1}{2}a\,(x_7-2y_7)\,\hat{\mathbf{x}}+\frac{\sqrt{3}}{2}ax_7\,\hat{\mathbf{y}}+cz_7\,\hat{\mathbf{z}} & \text{(6c)} & \text{O III}\\
\mathbf{B_{31}} & = & -(x_7-y_7)\,\mathbf{a}_1-x_7\,\mathbf{a}_2+z_7\,\mathbf{a}_3 & = & -\frac{1}{2}a\,(2x_7-y_7)\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{2}ay_7\,\hat{\mathbf{y}}+cz_7\,\hat{\mathbf{z}} & \text{(6c)} & \text{O III}\\
\mathbf{B_{32}} & = & -x_7\,\mathbf{a}_1-y_7\,\mathbf{a}_2+\left(z_7+\frac{1}{2}\right)\,\mathbf{a}_3 & = & -\frac{1}{2}a\,(x_7+y_7)\,\hat{\mathbf{x}}+\frac{\sqrt{3}}{2}a\,(x_7-y_7)\,\hat{\mathbf{y}}+c\left(z_7+\frac{1}{2}\right)\,\hat{\mathbf{z}} & \text{(6c)} & \text{O III}\\
\mathbf{B_{33}} & = & y_7\,\mathbf{a}_1-(x_7-y_7)\,\mathbf{a}_2+\left(z_7+\frac{1}{2}\right)\,\mathbf{a}_3 & = & \frac{1}{2}a\,(-x_7+2y_7)\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{2}ax_7\,\hat{\mathbf{y}}+c\left(z_7+\frac{1}{2}\right)\,\hat{\mathbf{z}} & \text{(6c)} & \text{O III}\\
\mathbf{B_{34}} & = & (x_7-y_7)\,\mathbf{a}_1+x_7\,\mathbf{a}_2+\left(z_7+\frac{1}{2}\right)\,\mathbf{a}_3 & = & \frac{1}{2}a\,(2x_7-y_7)\,\hat{\mathbf{x}}+\frac{\sqrt{3}}{2}ay_7\,\hat{\mathbf{y}}+c\left(z_7+\frac{1}{2}\right)\,\hat{\mathbf{z}} & \text{(6c)} & \text{O III}\\
\mathbf{B_{35}} & = & x_8\,\mathbf{a}_1+y_8\,\mathbf{a}_2+z_8\,\mathbf{a}_3 & = & \frac{1}{2}a\,(x_8+y_8)\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{2}a\,(x_8-y_8)\,\hat{\mathbf{y}}+cz_8\,\hat{\mathbf{z}} & \text{(6c)} & \text{O IV}\\
\mathbf{B_{36}} & = & -y_8\,\mathbf{a}_1+(x_8-y_8)\,\mathbf{a}_2+z_8\,\mathbf{a}_3 & = & \frac{1}{2}a\,(x_8-2y_8)\,\hat{\mathbf{x}}+\frac{\sqrt{3}}{2}ax_8\,\hat{\mathbf{y}}+cz_8\,\hat{\mathbf{z}} & \text{(6c)} & \text{O IV}\\
\mathbf{B_{37}} & = & -(x_8-y_8)\,\mathbf{a}_1-x_8\,\mathbf{a}_2+z_8\,\mathbf{a}_3 & = & -\frac{1}{2}a\,(2x_8-y_8)\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{2}ay_8\,\hat{\mathbf{y}}+cz_8\,\hat{\mathbf{z}} & \text{(6c)} & \text{O IV}\\
\mathbf{B_{38}} & = & -x_8\,\mathbf{a}_1-y_8\,\mathbf{a}_2+\left(z_8+\frac{1}{2}\right)\,\mathbf{a}_3 & = & -\frac{1}{2}a\,(x_8+y_8)\,\hat{\mathbf{x}}+\frac{\sqrt{3}}{2}a\,(x_8-y_8)\,\hat{\mathbf{y}}+c\left(z_8+\frac{1}{2}\right)\,\hat{\mathbf{z}} & \text{(6c)} & \text{O IV}\\
\mathbf{B_{39}} & = & y_8\,\mathbf{a}_1-(x_8-y_8)\,\mathbf{a}_2+\left(z_8+\frac{1}{2}\right)\,\mathbf{a}_3 & = & \frac{1}{2}a\,(-x_8+2y_8)\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{2}ax_8\,\hat{\mathbf{y}}+c\left(z_8+\frac{1}{2}\right)\,\hat{\mathbf{z}} & \text{(6c)} & \text{O IV}\\
\mathbf{B_{40}} & = & (x_8-y_8)\,\mathbf{a}_1+x_8\,\mathbf{a}_2+\left(z_8+\frac{1}{2}\right)\,\mathbf{a}_3 & = & \frac{1}{2}a\,(2x_8-y_8)\,\hat{\mathbf{x}}+\frac{\sqrt{3}}{2}ay_8\,\hat{\mathbf{y}}+c\left(z_8+\frac{1}{2}\right)\,\hat{\mathbf{z}} & \text{(6c)} & \text{O IV}\\
\mathbf{B_{41}} & = & x_9\,\mathbf{a}_1+y_9\,\mathbf{a}_2+z_9\,\mathbf{a}_3 & = & \frac{1}{2}a\,(x_9+y_9)\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{2}a\,(x_9-y_9)\,\hat{\mathbf{y}}+cz_9\,\hat{\mathbf{z}} & \text{(6c)} & \text{O V}\\
\mathbf{B_{42}} & = & -y_9\,\mathbf{a}_1+(x_9-y_9)\,\mathbf{a}_2+z_9\,\mathbf{a}_3 & = & \frac{1}{2}a\,(x_9-2y_9)\,\hat{\mathbf{x}}+\frac{\sqrt{3}}{2}ax_9\,\hat{\mathbf{y}}+cz_9\,\hat{\mathbf{z}} & \text{(6c)} & \text{O V}\\
\mathbf{B_{43}} & = & -(x_9-y_9)\,\mathbf{a}_1-x_9\,\mathbf{a}_2+z_9\,\mathbf{a}_3 & = & -\frac{1}{2}a\,(2x_9-y_9)\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{2}ay_9\,\hat{\mathbf{y}}+cz_9\,\hat{\mathbf{z}} & \text{(6c)} & \text{O V}\\
\mathbf{B_{44}} & = & -x_9\,\mathbf{a}_1-y_9\,\mathbf{a}_2+\left(z_9+\frac{1}{2}\right)\,\mathbf{a}_3 & = & -\frac{1}{2}a\,(x_9+y_9)\,\hat{\mathbf{x}}+\frac{\sqrt{3}}{2}a\,(x_9-y_9)\,\hat{\mathbf{y}}+c\left(z_9+\frac{1}{2}\right)\,\hat{\mathbf{z}} & \text{(6c)} & \text{O V}\\
\mathbf{B_{45}} & = & y_9\,\mathbf{a}_1-(x_9-y_9)\,\mathbf{a}_2+\left(z_9+\frac{1}{2}\right)\,\mathbf{a}_3 & = & \frac{1}{2}a\,(-x_9+2y_9)\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{2}ax_9\,\hat{\mathbf{y}}+c\left(z_9+\frac{1}{2}\right)\,\hat{\mathbf{z}} & \text{(6c)} & \text{O V}\\
\mathbf{B_{46}} & = & (x_9-y_9)\,\mathbf{a}_1+x_9\,\mathbf{a}_2+\left(z_9+\frac{1}{2}\right)\,\mathbf{a}_3 & = & \frac{1}{2}a\,(2x_9-y_9)\,\hat{\mathbf{x}}+\frac{\sqrt{3}}{2}ay_9\,\hat{\mathbf{y}}+c\left(z_9+\frac{1}{2}\right)\,\hat{\mathbf{z}} & \text{(6c)} & \text{O V}\\
\mathbf{B_{47}} & = & x_{10}\,\mathbf{a}_1+y_{10}\,\mathbf{a}_2+z_{10}\,\mathbf{a}_3 & = & \frac{1}{2}a\,(x_{10}+y_{10})\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{2}a\,(x_{10}-y_{10})\,\hat{\mathbf{y}}+cz_{10}\,\hat{\mathbf{z}} & \text{(6c)} & \text{Si I}
\end{array}
$$

$$\mathbf{B_{48}} = -y_{10}\,\mathbf{a}_1 + (x_{10} - y_{10})\,\mathbf{a}_2 + z_{10}\,\mathbf{a}_3 = \tfrac{1}{2}a\,(x_{10} - 2y_{10})\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}ax_{10}\,\hat{\mathbf{y}} + cz_{10}\,\hat{\mathbf{z}} \quad \text{(6c)} \quad \text{Si I}$$

$$\mathbf{B_{49}} = -(x_{10} - y_{10})\,\mathbf{a}_1 - x_{10}\,\mathbf{a}_2 + z_{10}\,\mathbf{a}_3 = -\tfrac{1}{2}a\,(2x_{10} - y_{10})\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}ay_{10}\,\hat{\mathbf{y}} + cz_{10}\,\hat{\mathbf{z}} \quad \text{(6c)} \quad \text{Si I}$$

$$\mathbf{B_{50}} = -x_{10}\,\mathbf{a}_1 - y_{10}\,\mathbf{a}_2 + \left(z_{10} + \tfrac{1}{2}\right)\,\mathbf{a}_3 = -\tfrac{1}{2}a\,(x_{10} + y_{10})\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}a\,(x_{10} - y_{10})\,\hat{\mathbf{y}} + c\left(z_{10} + \tfrac{1}{2}\right)\,\hat{\mathbf{z}} \quad \text{(6c)} \quad \text{Si I}$$

$$\mathbf{B_{51}} = y_{10}\,\mathbf{a}_1 - (x_{10} - y_{10})\,\mathbf{a}_2 + \left(z_{10} + \tfrac{1}{2}\right)\,\mathbf{a}_3 = \tfrac{1}{2}a\,(-x_{10} + 2y_{10})\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}ax_{10}\,\hat{\mathbf{y}} + c\left(z_{10} + \tfrac{1}{2}\right)\,\hat{\mathbf{z}} \quad \text{(6c)} \quad \text{Si I}$$

$$\mathbf{B_{52}} = (x_{10} - y_{10})\,\mathbf{a}_1 + x_{10}\,\mathbf{a}_2 + \left(z_{10} + \tfrac{1}{2}\right)\,\mathbf{a}_3 = \tfrac{1}{2}a\,(2x_{10} - y_{10})\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}ay_{10}\,\hat{\mathbf{y}} + c\left(z_{10} + \tfrac{1}{2}\right)\,\hat{\mathbf{z}} \quad \text{(6c)} \quad \text{Si I}$$

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[2] S. Kôzu and K. Takané, *Crystal Structure of Cancrinite from Dôdô, Korea (Parts II)*, Proceedings of the Imperial Academy (Japan) **9**, 105–108 (1933).

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