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 originally had the label `A3BCD3E15F3_hP52_173_c_b_b_c_5c_c`. Calls to that address will be redirected here.

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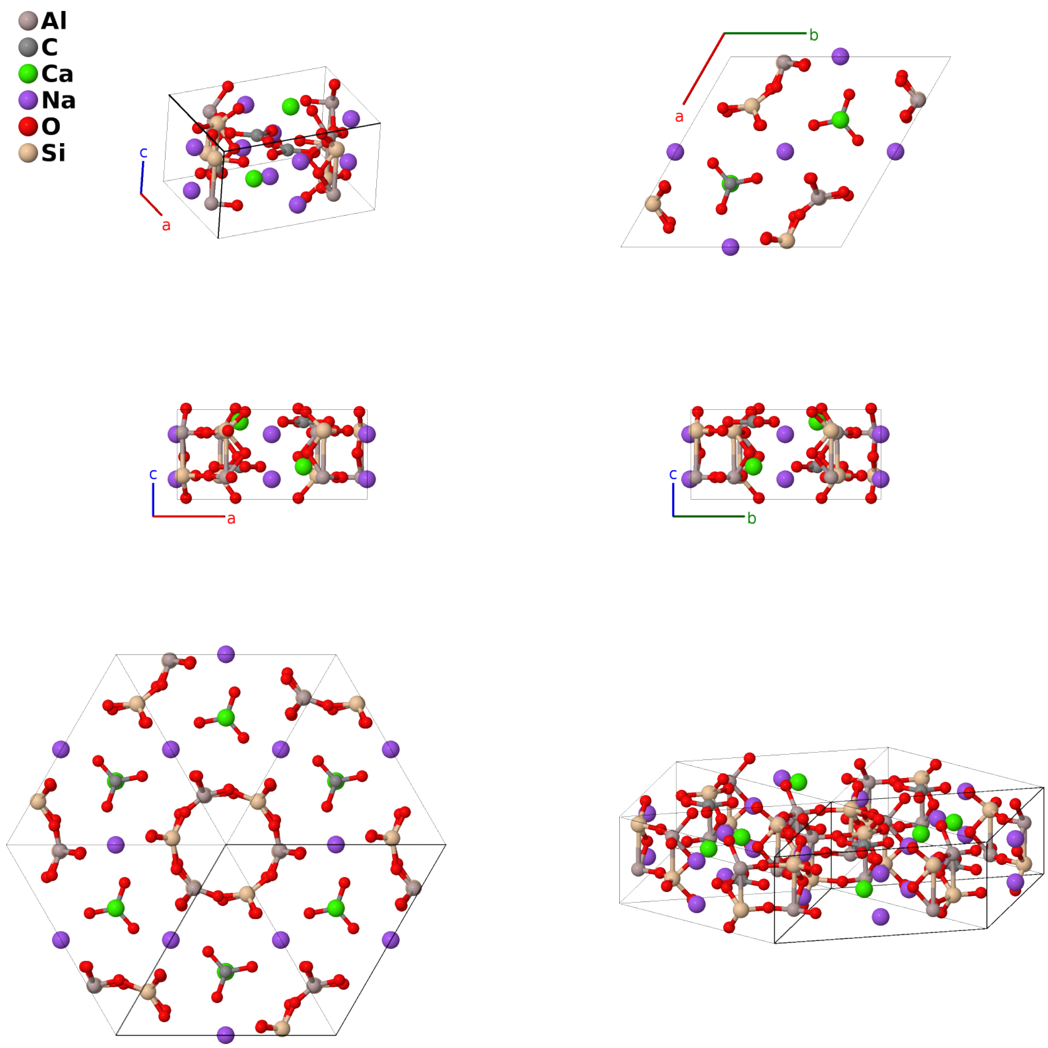
https://aflow.org/p/7U5Z

https://aflow.org/p/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

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`
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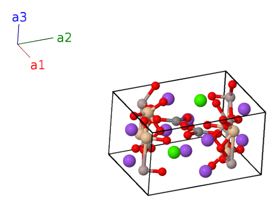
- The term "crancrinite" covers a wide range of mineral compositions, some of which may include OH radicals and H_2O molecules. We use this early determination of the structure as the base.
- There are two major inconsistencies between (Kozu, 1933) and (Gottfried, 1937):
  - (Gottfried, 1937) interchanges 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
$\mathbf{B_5}$ =	$x_3\,\mathbf{a}_1 + y_3\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$\frac{1}{2}a\left(x_3 + y_3\right)\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\left(x_3 - y_3\right)\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(6c)	Al I
$\mathbf{B_6}$ =	$-y_3\,\mathbf{a}_1 + \left(x_3 - y_3\right)\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$\frac{1}{2}a\left(x_3 - 2y_3\right)\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_3\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(6c)	Al I
$\mathbf{B_7}$ =	$-\left(x_3 - y_3\right)\mathbf{a}_1 - x_3\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$-\frac{1}{2}a\left(2x_3 - y_3\right)\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_3\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(6c)	Al I
$\mathbf{B_8}$ =	$-x_3\,\mathbf{a}_1 - y_3\,\mathbf{a}_2 + \left(z_3 + \frac{1}{2}\right)\mathbf{a}_3$	=	$-\frac{1}{2}a\left(x_3 + y_3\right)\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\left(x_3 - y_3\right)\hat{\mathbf{y}} + c\left(z_3 + \frac{1}{2}\right)\hat{\mathbf{z}}$	(6c)	Al I
$\mathbf{B_9}$ =	$y_3\,\mathbf{a}_1 - \left(x_3 - y_3\right)\mathbf{a}_2 + \left(z_3 + \frac{1}{2}\right)\mathbf{a}_3$	=	$\frac{1}{2}a\left(-x_3 + 2y_3\right)\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_3\,\hat{\mathbf{y}} + c\left(z_3 + \frac{1}{2}\right)\hat{\mathbf{z}}$	(6c)	Al I
$\mathbf{B_{10}}$ =	$\left(x_3 - y_3\right)\mathbf{a}_1 + x_3\,\mathbf{a}_2 + \left(z_3 + \frac{1}{2}\right)\mathbf{a}_3$	=	$\frac{1}{2}a\left(2x_3 - y_3\right)\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_3\,\hat{\mathbf{y}} + c\left(z_3 + \frac{1}{2}\right)\hat{\mathbf{z}}$	(6c)	Al I
$\mathbf{B_{11}}$ =	$x_4\,\mathbf{a}_1 + y_4\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$\frac{1}{2}a\left(x_4 + y_4\right)\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\left(x_4 - y_4\right)\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(6c)	Na I
$\mathbf{B_{12}}$ =	$-y_4\,\mathbf{a}_1 + \left(x_4 - y_4\right)\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$\frac{1}{2}a\left(x_4 - 2y_4\right)\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(6c)	Na I
$\mathbf{B_{13}}$ =	$-\left(x_4 - y_4\right)\mathbf{a}_1 - x_4\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$-\frac{1}{2}a\left(2x_4 - y_4\right)\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(6c)	Na I
$\mathbf{B_{14}}$ =	$-x_4\,\mathbf{a}_1 - y_4\,\mathbf{a}_2 + \left(z_4 + \frac{1}{2}\right)\mathbf{a}_3$	=	$-\frac{1}{2}a\left(x_4 + y_4\right)\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\left(x_4 - y_4\right)\hat{\mathbf{y}} + c\left(z_4 + \frac{1}{2}\right)\hat{\mathbf{z}}$	(6c)	Na I

$\mathbf{B_{15}}$	=	$y_4\,\mathbf{a}_1 - (x_4 - y_4)\,\mathbf{a}_2 + \left(z_4 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(-x_4 + 2y_4)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_4\,\hat{\mathbf{y}} + c\left(z_4 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(6c)	Na I
$\mathbf{B_{16}}$	=	$(x_4 - y_4)\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 + \left(z_4 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(2x_4 - y_4)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_4\,\hat{\mathbf{y}} + c\left(z_4 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(6c)	Na I
$\mathbf{B_{17}}$	=	$x_5\,\mathbf{a}_1 + y_5\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_5 + y_5)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,(x_5 - y_5)\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(6c)	O I
$\mathbf{B_{18}}$	=	$-y_5\,\mathbf{a}_1 + (x_5 - y_5)\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_5 - 2y_5)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_5\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(6c)	O I
$\mathbf{B_{19}}$	=	$-(x_5 - y_5)\,\mathbf{a}_1 - x_5\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(2x_5 - y_5)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_5\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(6c)	O I
$\mathbf{B_{20}}$	=	$-x_5\,\mathbf{a}_1 - y_5\,\mathbf{a}_2 + \left(z_5 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(x_5 + y_5)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\,(x_5 - y_5)\,\hat{\mathbf{y}} + c\left(z_5 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(6c)	O I
$\mathbf{B_{21}}$	=	$y_5\,\mathbf{a}_1 - (x_5 - y_5)\,\mathbf{a}_2 + \left(z_5 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(-x_5 + 2y_5)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_5\,\hat{\mathbf{y}} + c\left(z_5 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(6c)	O I
$\mathbf{B_{22}}$	=	$(x_5 - y_5)\,\mathbf{a}_1 + x_5\,\mathbf{a}_2 + \left(z_5 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(2x_5 - y_5)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_5\,\hat{\mathbf{y}} + c\left(z_5 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(6c)	O I
$\mathbf{B_{23}}$	=	$x_6\,\mathbf{a}_1 + y_6\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_6 + y_6)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,(x_6 - y_6)\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(6c)	O II
$\mathbf{B_{24}}$	=	$-y_6\,\mathbf{a}_1 + (x_6 - y_6)\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_6 - 2y_6)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_6\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(6c)	O II
$\mathbf{B_{25}}$	=	$-(x_6 - y_6)\,\mathbf{a}_1 - x_6\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(2x_6 - y_6)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_6\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(6c)	O II
$\mathbf{B_{26}}$	=	$-x_6\,\mathbf{a}_1 - y_6\,\mathbf{a}_2 + \left(z_6 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(x_6 + y_6)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\,(x_6 - y_6)\,\hat{\mathbf{y}} + c\left(z_6 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(6c)	O II
$\mathbf{B_{27}}$	=	$y_6\,\mathbf{a}_1 - (x_6 - y_6)\,\mathbf{a}_2 + \left(z_6 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(-x_6 + 2y_6)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_6\,\hat{\mathbf{y}} + c\left(z_6 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(6c)	O II
$\mathbf{B_{28}}$	=	$(x_6 - y_6)\,\mathbf{a}_1 + x_6\,\mathbf{a}_2 + \left(z_6 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(2x_6 - y_6)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_6\,\hat{\mathbf{y}} + c\left(z_6 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(6c)	O II
$\mathbf{B_{29}}$	=	$x_7\,\mathbf{a}_1 + y_7\,\mathbf{a}_2 + z_7\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_7 + y_7)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,(x_7 - y_7)\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}}$	(6c)	O III
$\mathbf{B_{30}}$	=	$-y_7\,\mathbf{a}_1 + (x_7 - y_7)\,\mathbf{a}_2 + z_7\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_7 - 2y_7)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_7\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}}$	(6c)	O III
$\mathbf{B_{31}}$	=	$-(x_7 - y_7)\,\mathbf{a}_1 - x_7\,\mathbf{a}_2 + z_7\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(2x_7 - y_7)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_7\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}}$	(6c)	O III
$\mathbf{B_{32}}$	=	$-x_7\,\mathbf{a}_1 - y_7\,\mathbf{a}_2 + \left(z_7 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(x_7 + y_7)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\,(x_7 - y_7)\,\hat{\mathbf{y}} + c\left(z_7 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(6c)	O III
$\mathbf{B_{33}}$	=	$y_7\,\mathbf{a}_1 - (x_7 - y_7)\,\mathbf{a}_2 + \left(z_7 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(-x_7 + 2y_7)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_7\,\hat{\mathbf{y}} + c\left(z_7 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(6c)	O III
$\mathbf{B_{34}}$	=	$(x_7 - y_7)\,\mathbf{a}_1 + x_7\,\mathbf{a}_2 + \left(z_7 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(2x_7 - y_7)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_7\,\hat{\mathbf{y}} + c\left(z_7 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(6c)	O III
$\mathbf{B_{35}}$	=	$x_8\,\mathbf{a}_1 + y_8\,\mathbf{a}_2 + z_8\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_8 + y_8)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,(x_8 - y_8)\,\hat{\mathbf{y}} + cz_8\,\hat{\mathbf{z}}$	(6c)	O IV
$\mathbf{B_{36}}$	=	$-y_8\,\mathbf{a}_1 + (x_8 - y_8)\,\mathbf{a}_2 + z_8\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_8 - 2y_8)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_8\,\hat{\mathbf{y}} + cz_8\,\hat{\mathbf{z}}$	(6c)	O IV
$\mathbf{B_{37}}$	=	$-(x_8 - y_8)\,\mathbf{a}_1 - x_8\,\mathbf{a}_2 + z_8\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(2x_8 - y_8)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_8\,\hat{\mathbf{y}} + cz_8\,\hat{\mathbf{z}}$	(6c)	O IV
$\mathbf{B_{38}}$	=	$-x_8\,\mathbf{a}_1 - y_8\,\mathbf{a}_2 + \left(z_8 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(x_8 + y_8)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\,(x_8 - y_8)\,\hat{\mathbf{y}} + c\left(z_8 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(6c)	O IV
$\mathbf{B_{39}}$	=	$y_8\,\mathbf{a}_1 - (x_8 - y_8)\,\mathbf{a}_2 + \left(z_8 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(-x_8 + 2y_8)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_8\,\hat{\mathbf{y}} + c\left(z_8 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(6c)	O IV
$\mathbf{B_{40}}$	=	$(x_8 - y_8)\,\mathbf{a}_1 + x_8\,\mathbf{a}_2 + \left(z_8 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(2x_8 - y_8)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_8\,\hat{\mathbf{y}} + c\left(z_8 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(6c)	O IV
$\mathbf{B_{41}}$	=	$x_9\,\mathbf{a}_1 + y_9\,\mathbf{a}_2 + z_9\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_9 + y_9)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,(x_9 - y_9)\,\hat{\mathbf{y}} + cz_9\,\hat{\mathbf{z}}$	(6c)	O V
$\mathbf{B_{42}}$	=	$-y_9\,\mathbf{a}_1 + (x_9 - y_9)\,\mathbf{a}_2 + z_9\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_9 - 2y_9)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_9\,\hat{\mathbf{y}} + cz_9\,\hat{\mathbf{z}}$	(6c)	O V
$\mathbf{B_{43}}$	=	$-(x_9 - y_9)\,\mathbf{a}_1 - x_9\,\mathbf{a}_2 + z_9\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(2x_9 - y_9)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_9\,\hat{\mathbf{y}} + cz_9\,\hat{\mathbf{z}}$	(6c)	O V
$\mathbf{B_{44}}$	=	$-x_9\,\mathbf{a}_1 - y_9\,\mathbf{a}_2 + \left(z_9 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(x_9 + y_9)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\,(x_9 - y_9)\,\hat{\mathbf{y}} + c\left(z_9 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(6c)	O V
$\mathbf{B_{45}}$	=	$y_9\,\mathbf{a}_1 - (x_9 - y_9)\,\mathbf{a}_2 + \left(z_9 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(-x_9 + 2y_9)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_9\,\hat{\mathbf{y}} + c\left(z_9 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(6c)	O V
$\mathbf{B_{46}}$	=	$(x_9 - y_9)\,\mathbf{a}_1 + x_9\,\mathbf{a}_2 + \left(z_9 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(2x_9 - y_9)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_9\,\hat{\mathbf{y}} + c\left(z_9 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(6c)	O V
$\mathbf{B_{47}}$	=	$x_{10}\,\mathbf{a}_1 + y_{10}\,\mathbf{a}_2 + z_{10}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_{10} + y_{10})\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,(x_{10} - y_{10})\,\hat{\mathbf{y}} + cz_{10}\,\hat{\mathbf{z}}$	(6c)	Si I
$\mathbf{B_{48}}$	=	$-y_{10}\,\mathbf{a}_1 + (x_{10} - y_{10})\,\mathbf{a}_2 + z_{10}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_{10} - 2y_{10})\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_{10}\,\hat{\mathbf{y}} + cz_{10}\,\hat{\mathbf{z}}$	(6c)	Si I
$\mathbf{B_{49}}$	=	$-(x_{10} - y_{10})\,\mathbf{a}_1 - x_{10}\,\mathbf{a}_2 + z_{10}\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(2x_{10} - y_{10})\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_{10}\,\hat{\mathbf{y}} + cz_{10}\,\hat{\mathbf{z}}$	(6c)	Si I
$\mathbf{B_{50}}$	=	$-x_{10}\,\mathbf{a}_1 - y_{10}\,\mathbf{a}_2 + \left(z_{10} + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(x_{10} + y_{10})\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\,(x_{10} - y_{10})\,\hat{\mathbf{y}} + c\left(z_{10} + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(6c)	Si I

$\mathbf{B_{51}}$	=	$y_{10}\,\mathbf{a}_1 - (x_{10} - y_{10})\,\mathbf{a}_2 + \left(z_{10} + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(-x_{10} + 2y_{10})\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_{10}\,\hat{\mathbf{y}} + c\left(z_{10} + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(6c)	Si I
$\mathbf{B_{52}}$	=	$(x_{10} - y_{10})\,\mathbf{a}_1 + x_{10}\,\mathbf{a}_2 + \left(z_{10} + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(2x_{10} - y_{10})\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_{10}\,\hat{\mathbf{y}} + c\left(z_{10} + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(6c)	Si I

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[1] S. Kôzu and K. Takané, *Crystal Structure of Cancrinite from Dôdô, Korea (Part I)*, Proceedings of the Imperial Academy (Japan) **9**, 56–59 (1933).

[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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