Rinneite ($K_3NaFeCl_6$) Structure: A6BC3D_hR22_167_f_b_e_a-001

This structure originally had the label `A6BC3D_hR22_167_f_b_e_a`. Calls to that address will be redirected here.

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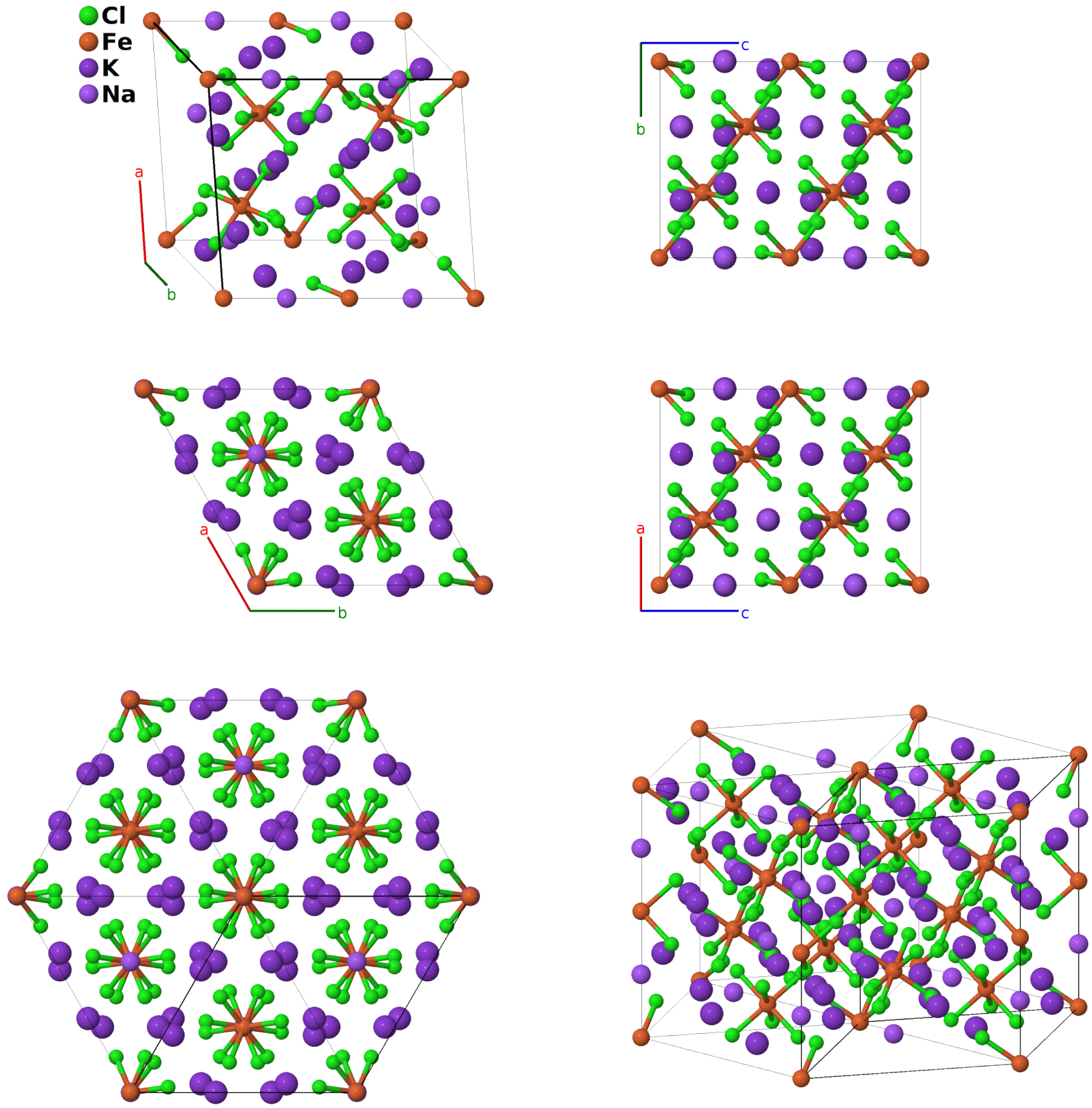
https://aflow.org/p/PYAM

https://aflow.org/p/A6BC3D_hR22_167_f_b_e_a-001



Prototype Cl_6FeK_3Na

AFLOW prototype label A6BC3D_hR22_167_f_b_e_a-001

Mineral name rinneite

ICSD 170745

Pearson symbol hR22

Space group number 167

Space group symbol $R\bar{3}c$

AFLOW prototype command `aflow --proto=A6BC3D_hR22_167_f_b_e_a-001`
`--params=`$a, c/a, x_3, x_4, y_4, z_4$

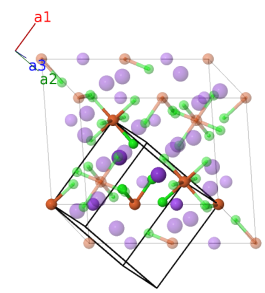
Other compounds with this structure

Ca_3LiOsO_6, Ca_3LiRuO_6, Sr_3NiIrO_6, K_4CdCl_6

- We use the data taken at 293K.

Rhombohedral primitive vectors

$$\mathbf{a_1} = \frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{1}{3}c\,\hat{\mathbf{z}}$$
$$\mathbf{a_2} = \frac{1}{\sqrt{3}}a\,\hat{\mathbf{y}} + \frac{1}{3}c\,\hat{\mathbf{z}}$$
$$\mathbf{a_3} = -\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{1}{3}c\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{4}c\,\hat{\mathbf{z}}$	(2a)	Na I
$\mathbf{B_2}$	=	$\frac{3}{4}\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{3}{4}c\,\hat{\mathbf{z}}$	(2a)	Na I
$\mathbf{B_3}$	=	0	=	0	(2b)	Fe I
$\mathbf{B_4}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}c\,\hat{\mathbf{z}}$	(2b)	Fe I
$\mathbf{B_5}$	=	$x_3\,\mathbf{a}_1 - \left(x_3 - \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{8}a\left(4x_3 - 1\right)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{8}a\left(4x_3 - 1\right)\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(6e)	K I
$\mathbf{B_6}$	=	$\frac{1}{4}\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 - \left(x_3 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{8}a\left(4x_3 - 1\right)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{8}a\left(4x_3 - 1\right)\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(6e)	K I
$\mathbf{B_7}$	=	$-\left(x_3 - \frac{1}{2}\right)\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + x_3\,\mathbf{a}_3$	=	$-a\left(x_3 - \frac{1}{4}\right)\,\hat{\mathbf{x}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(6e)	K I
$\mathbf{B_8}$	=	$-x_3\,\mathbf{a}_1 + \left(x_3 + \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$-\frac{1}{8}a\left(4x_3 + 3\right)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{24}a\left(12x_3 + 1\right)\,\hat{\mathbf{y}} + \frac{5}{12}c\,\hat{\mathbf{z}}$	(6e)	K I
$\mathbf{B_9}$	=	$\frac{3}{4}\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 + \left(x_3 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\frac{1}{8}a\left(4x_3 - 1\right)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{24}a\left(12x_3 + 5\right)\,\hat{\mathbf{y}} + \frac{5}{12}c\,\hat{\mathbf{z}}$	(6e)	K I
$\mathbf{B_{10}}$	=	$\left(x_3 + \frac{1}{2}\right)\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 - x_3\,\mathbf{a}_3$	=	$a\left(x_3 + \frac{1}{4}\right)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{5}{12}c\,\hat{\mathbf{z}}$	(6e)	K I
$\mathbf{B_{11}}$	=	$x_4\,\mathbf{a}_1 + y_4\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$\frac{1}{2}a\left(x_4 - z_4\right)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\left(x_4 - 2y_4 + z_4\right)\,\hat{\mathbf{y}} + \frac{1}{3}c\left(x_4 + y_4 + z_4\right)\,\hat{\mathbf{z}}$	(12f)	Cl I
$\mathbf{B_{12}}$	=	$z_4\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 + y_4\,\mathbf{a}_3$	=	$-\frac{1}{2}a\left(y_4 - z_4\right)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\left(2x_4 - y_4 - z_4\right)\,\hat{\mathbf{y}} + \frac{1}{3}c\left(x_4 + y_4 + z_4\right)\,\hat{\mathbf{z}}$	(12f)	Cl I
$\mathbf{B_{13}}$	=	$y_4\,\mathbf{a}_1 + z_4\,\mathbf{a}_2 + x_4\,\mathbf{a}_3$	=	$-\frac{1}{2}a\left(x_4 - y_4\right)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\left(x_4 + y_4 - 2z_4\right)\,\hat{\mathbf{y}} + \frac{1}{3}c\left(x_4 + y_4 + z_4\right)\,\hat{\mathbf{z}}$	(12f)	Cl I
$\mathbf{B_{14}}$	=	$-\left(z_4 - \frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_4 - \frac{1}{2}\right)\,\mathbf{a}_2 - \left(x_4 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\left(x_4 - z_4\right)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\left(x_4 - 2y_4 + z_4\right)\,\hat{\mathbf{y}} - \frac{1}{6}c\left(2x_4 + 2y_4 + 2z_4 - 3\right)\,\hat{\mathbf{z}}$	(12f)	Cl I
$\mathbf{B_{15}}$	=	$-\left(y_4 - \frac{1}{2}\right)\,\mathbf{a}_1 - \left(x_4 - \frac{1}{2}\right)\,\mathbf{a}_2 - \left(z_4 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\frac{1}{2}a\left(y_4 - z_4\right)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\left(2x_4 - y_4 - z_4\right)\,\hat{\mathbf{y}} - \frac{1}{6}c\left(2x_4 + 2y_4 + 2z_4 - 3\right)\,\hat{\mathbf{z}}$	(12f)	Cl I

$$\mathbf{B_{16}} = -\left(x_4 - \frac{1}{2}\right)\,\mathbf{a}_1 - \left(z_4 - \frac{1}{2}\right)\,\mathbf{a}_2 - \left(y_4 - \frac{1}{2}\right)\,\mathbf{a}_3 = -\frac{1}{2}a\,(x_4 - y_4)\,\mathbf{\hat{x}} + \frac{\sqrt{3}}{6}a\,(x_4 + y_4 - 2z_4)\,\mathbf{\hat{y}} - \frac{1}{6}c\,(2x_4 + 2y_4 + 2z_4 - 3)\,\mathbf{\hat{z}} \quad \text{(12f)} \quad \text{Cl I}$$

$$\mathbf{B_{17}} = -x_4\,\mathbf{a}_1 - y_4\,\mathbf{a}_2 - z_4\,\mathbf{a}_3 = -\frac{1}{2}a\,(x_4 - z_4)\,\mathbf{\hat{x}} + \frac{\sqrt{3}}{6}a\,(x_4 - 2y_4 + z_4)\,\mathbf{\hat{y}} - \frac{1}{3}c\,(x_4 + y_4 + z_4)\,\mathbf{\hat{z}} \quad \text{(12f)} \quad \text{Cl I}$$

$$\mathbf{B_{18}} = -z_4\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 - y_4\,\mathbf{a}_3 = \frac{1}{2}a\,(y_4 - z_4)\,\mathbf{\hat{x}} - \frac{\sqrt{3}}{6}a\,(2x_4 - y_4 - z_4)\,\mathbf{\hat{y}} - \frac{1}{3}c\,(x_4 + y_4 + z_4)\,\mathbf{\hat{z}} \quad \text{(12f)} \quad \text{Cl I}$$

$$\mathbf{B_{19}} = -y_4\,\mathbf{a}_1 - z_4\,\mathbf{a}_2 - x_4\,\mathbf{a}_3 = \frac{1}{2}a\,(x_4 - y_4)\,\mathbf{\hat{x}} + \frac{\sqrt{3}}{6}a\,(x_4 + y_4 - 2z_4)\,\mathbf{\hat{y}} - \frac{1}{3}c\,(x_4 + y_4 + z_4)\,\mathbf{\hat{z}} \quad \text{(12f)} \quad \text{Cl I}$$

$$\mathbf{B_{20}} = \left(z_4 + \frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_4 + \frac{1}{2}\right)\,\mathbf{a}_2 + \left(x_4 + \frac{1}{2}\right)\,\mathbf{a}_3 = -\frac{1}{2}a\,(x_4 - z_4)\,\mathbf{\hat{x}} - \frac{\sqrt{3}}{6}a\,(x_4 - 2y_4 + z_4)\,\mathbf{\hat{y}} + \frac{1}{6}c\,(2x_4 + 2y_4 + 2z_4 + 3)\,\mathbf{\hat{z}} \quad \text{(12f)} \quad \text{Cl I}$$

$$\mathbf{B_{21}} = \left(y_4 + \frac{1}{2}\right)\,\mathbf{a}_1 + \left(x_4 + \frac{1}{2}\right)\,\mathbf{a}_2 + \left(z_4 + \frac{1}{2}\right)\,\mathbf{a}_3 = \frac{1}{2}a\,(y_4 - z_4)\,\mathbf{\hat{x}} + \frac{\sqrt{3}}{6}a\,(2x_4 - y_4 - z_4)\,\mathbf{\hat{y}} + \frac{1}{6}c\,(2x_4 + 2y_4 + 2z_4 + 3)\,\mathbf{\hat{z}} \quad \text{(12f)} \quad \text{Cl I}$$

$$\mathbf{B_{22}} = \left(x_4 + \frac{1}{2}\right)\,\mathbf{a}_1 + \left(z_4 + \frac{1}{2}\right)\,\mathbf{a}_2 + \left(y_4 + \frac{1}{2}\right)\,\mathbf{a}_3 = \frac{1}{2}a\,(x_4 - y_4)\,\mathbf{\hat{x}} - \frac{\sqrt{3}}{6}a\,(x_4 + y_4 - 2z_4)\,\mathbf{\hat{y}} + \frac{1}{6}c\,(2x_4 + 2y_4 + 2z_4 + 3)\,\mathbf{\hat{z}} \quad \text{(12f)} \quad \text{Cl I}$$

References

[1] B. N. Figgis, A. N. Sobolev, E. S. Kucharski, and V. Broughton, *Rinneite, $K_3Na[FeCl_6]$, at 293, 84 and 9.5K*, Acta Crystallogr. Sect. C **56**, e228–e229 (2000), doi:10.1107/S0108270100006053.