$NaGdCu_2F_8$ Structure: A2B8CD_tI24_97_d_k_a_b-001

This structure originally had the label `A2B8CD_tI24_97_d_k_a_b`. Calls to that address will be redirected here.

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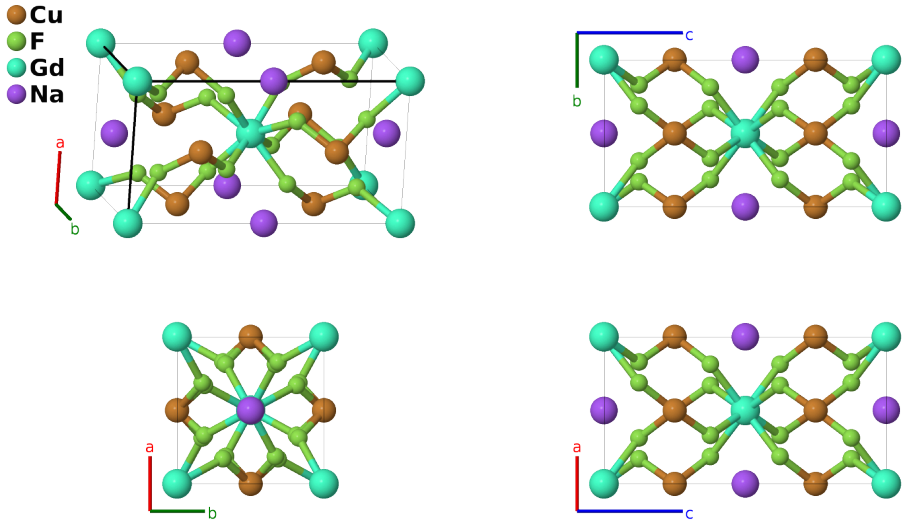
https://aflow.org/p/FH59

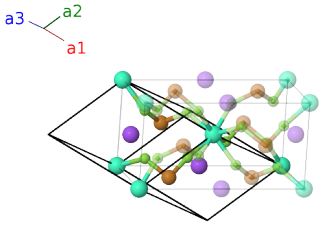
https://aflow.org/p/A2B8CD_tI24_97_d_k_a_b-001



Prototype	Cu_2F_8GdNa
AFLOW prototype label	A2B8CD_tI24_97_d_k_a_b-001
ICSD	none
Pearson symbol	tI24
Space group number	97
Space group symbol	$I422$
AFLOW prototype command	`aflow --proto=A2B8CD_tI24_97_d_k_a_b-001 --params=`$a, c/a, x_4, y_4, z_4$

Body-centered Tetragonal primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(2a)	Gd I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2$	=	$\frac{1}{2}c\,\hat{\mathbf{z}}$	(2b)	Na I
$\mathbf{B_3}$	=	$\frac{3}{4}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(4d)	Cu I
$\mathbf{B_4}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(4d)	Cu I
$\mathbf{B_5}$	=	$(y_4 + z_4)\,\mathbf{a}_1 + (x_4 + z_4)\,\mathbf{a}_2 + (x_4 + y_4)\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}} + ay_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(16k)	F I
$\mathbf{B_6}$	=	$-(y_4 - z_4)\,\mathbf{a}_1 - (x_4 - z_4)\,\mathbf{a}_2 - (x_4 + y_4)\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}} - ay_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(16k)	F I
$\mathbf{B_7}$	=	$(x_4 + z_4)\,\mathbf{a}_1 - (y_4 - z_4)\,\mathbf{a}_2 + (x_4 - y_4)\,\mathbf{a}_3$	=	$-ay_4\,\hat{\mathbf{x}} + ax_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(16k)	F I
$\mathbf{B_8}$	=	$-(x_4 - z_4)\,\mathbf{a}_1 + (y_4 + z_4)\,\mathbf{a}_2 - (x_4 - y_4)\,\mathbf{a}_3$	=	$ay_4\,\hat{\mathbf{x}} - ax_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(16k)	F I
$\mathbf{B_9}$	=	$(y_4 - z_4)\,\mathbf{a}_1 - (x_4 + z_4)\,\mathbf{a}_2 - (x_4 - y_4)\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}} + ay_4\,\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$	(16k)	F I
$\mathbf{B_{10}}$	=	$-(y_4 + z_4)\,\mathbf{a}_1 + (x_4 - z_4)\,\mathbf{a}_2 + (x_4 - y_4)\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}} - ay_4\,\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$	(16k)	F I
$\mathbf{B_{11}}$	=	$(x_4 - z_4)\,\mathbf{a}_1 + (y_4 - z_4)\,\mathbf{a}_2 + (x_4 + y_4)\,\mathbf{a}_3$	=	$ay_4\,\hat{\mathbf{x}} + ax_4\,\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$	(16k)	F I
$\mathbf{B_{12}}$	=	$-(x_4 + z_4)\,\mathbf{a}_1 - (y_4 + z_4)\,\mathbf{a}_2 - (x_4 + y_4)\,\mathbf{a}_3$	=	$-ay_4\,\hat{\mathbf{x}} - ax_4\,\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$	(16k)	F I

References

[1] C. D. Nadaï, A. Demourgues, L. Lozano, P. Gravereau, and J. Grannec, *Structural investigations of new copper fluorides $NaRECu_2F_8$ ($RE^{3+} = Sm^{3+}$, Eu^{3+}, Gd^{3+}, Y^{3+}, Er^{3+}, Yb^{3+})*, J. Mater. Chem. **8**, 2487–2491 (1998), doi:10.1039/A803015D.

Found in

[1] P. Villars and K. Cenzual, *Pearson's Crystal Data – Crystal Structure Database for Inorganic Compounds* (2013). ASM International.