

K₂NiF₄ Structure:

A4B2C_tI14_139_ce_e_a-001

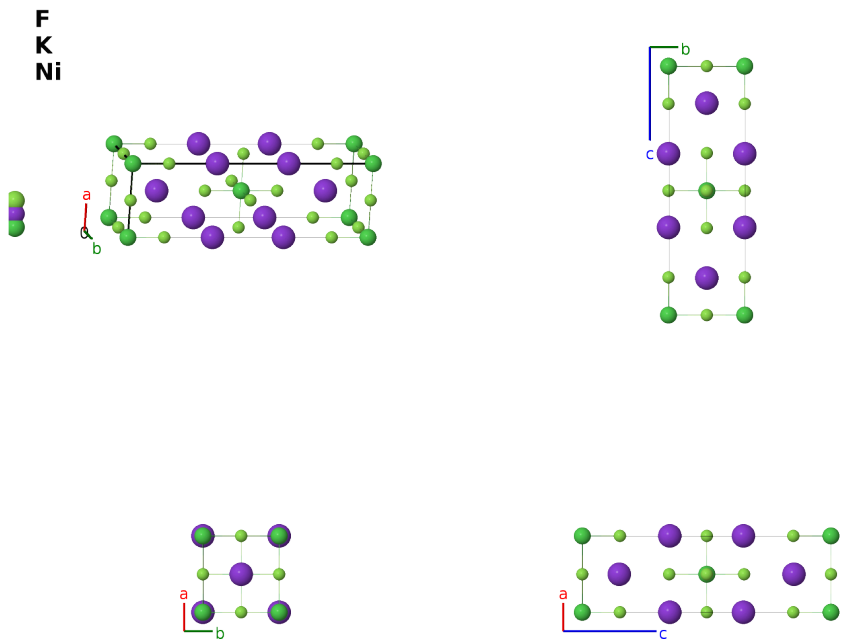
This structure previously used the label(s) **A4B2C_tI14_139_ce_e_a**. Calls to these addresses will be redirected here.

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<https://aflow.org/prototype-encyclopedia/SENW>

https://aflow.org/prototype-encyclopedia/A4B2C_tI14_139_ce_e_a-001



Prototype	F ₄ K ₂ Ni
AFLOW prototype label	A4B2C_tI14_139_ce_e_a-001
ICSD	15576
CCDC	1596315
Pearson symbol	tI14
Space group number	139
Space group symbol	I4/mmm
AFLOW prototype command	<code>aflow --proto=A4B2C_tI14_139_ce_e_a-001</code> <code>--params=a, c/a, z₃, z₄</code>

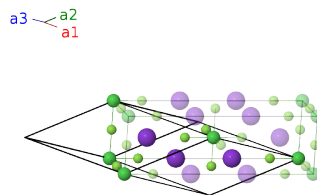
Other compounds with this structure

Ba₂SnO₄, Ba₂ZrS₄, Ca₂MnO₄, Cs₂CrCl₄, Cs₂CrF₄, Cs₂CuCl₄, Cs₂CuF₄, K₂CrCl₄, K₂CrF₄, K₂CuCl₄, K₂CuF₄, La₂NiO₄, La₂PdO₄, Nd₂CuO₄, Sr₂IrO₄, Sr₂MnO₄, Sr₂RuO₄, Sr₂SnO₄, Sr₂TiO₄, Sr₂VO₄, (Fe, La)₂SrO₄, (Sr, La)₂AlO₄, (Sr, La)₂CoO₄

- This is the parent compound of the simplest layered-perovskite Ruddlesden-Popper series (Wikipedia). The series also includes the parent of the high- T_c cuprates, (La,Ba)₂CuO₄, but we keep that separate as it represents a new class of materials.
 - Sr₂CuO₂Cl₂ is the quaternary form of this structure.
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Body-centered Tetragonal primitive vectors

$$\begin{aligned}\mathbf{a}_1 &= -\frac{1}{2}a\hat{\mathbf{x}} + \frac{1}{2}a\hat{\mathbf{y}} + \frac{1}{2}c\hat{\mathbf{z}} \\ \mathbf{a}_2 &= \frac{1}{2}a\hat{\mathbf{x}} - \frac{1}{2}a\hat{\mathbf{y}} + \frac{1}{2}c\hat{\mathbf{z}} \\ \mathbf{a}_3 &= \frac{1}{2}a\hat{\mathbf{x}} + \frac{1}{2}a\hat{\mathbf{y}} - \frac{1}{2}c\hat{\mathbf{z}}\end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	=	0	=	0	(2a) Ni I
$\mathbf{B}_2$	=	$\frac{1}{2}\mathbf{a}_1 + \frac{1}{2}\mathbf{a}_3$	=	$\frac{1}{2}a\hat{\mathbf{y}}$	(4c) F I
$\mathbf{B}_3$	=	$\frac{1}{2}\mathbf{a}_2 + \frac{1}{2}\mathbf{a}_3$	=	$\frac{1}{2}a\hat{\mathbf{x}}$	(4c) F I
$\mathbf{B}_4$	=	$z_3\mathbf{a}_1 + z_3\mathbf{a}_2$	=	$cz_3\hat{\mathbf{z}}$	(4e) F II
$\mathbf{B}_5$	=	$-z_3\mathbf{a}_1 - z_3\mathbf{a}_2$	=	$-cz_3\hat{\mathbf{z}}$	(4e) F II
$\mathbf{B}_6$	=	$z_4\mathbf{a}_1 + z_4\mathbf{a}_2$	=	$cz_4\hat{\mathbf{z}}$	(4e) K I
$\mathbf{B}_7$	=	$-z_4\mathbf{a}_1 - z_4\mathbf{a}_2$	=	$-cz_4\hat{\mathbf{z}}$	(4e) K I

References

- [1] D. Balz and K. Pleith, *Die Struktur des Kaliumnickelfluorids*, K_2NiF_4 , Z. Elektrochemie **59**, 545–551 (1955).

Found in

- [1] S. N. Ruddlesden and P. Popper, *New compounds of the K_2NiF_4 type*, Acta Cryst. **10**, 538–539 (1957), doi:10.1107/S0365110X57001929.

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