Sr_2NiWO_6 Structure: AB6C2D_tI20_87_a_eh_d_b-001

This structure originally had the label `AB6C2D_tI20_87_a_eh_d_b`. Calls to that address will be redirected here.

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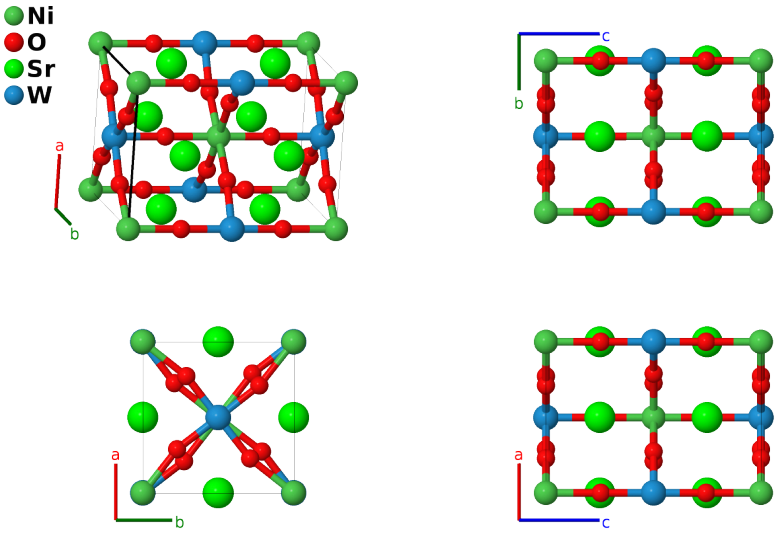
https://aflow.org/p/QP36

https://aflow.org/p/AB6C2D_tI20_87_a_eh_d_b-001



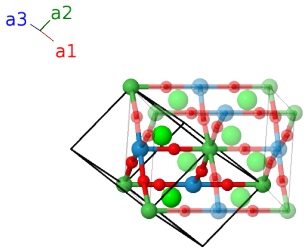
Prototype	NiO_6Sr_2W
AFLOW prototype label	AB6C2D_tI20_87_a_eh_d_b-001
ICSD	91791
Pearson symbol	tI20
Space group number	87
Space group symbol	$I4/m$
AFLOW prototype command	`aflow --proto=AB6C2D_tI20_87_a_eh_d_b-001 --params=`$a, c/a, z_4, x_5, y_5$

Other compounds with this structure
Sr_2MgWO_6

- This double perovskite crystal is the ground state structure of Sr_2NiWO_6. Above 300°C it transforms into the cubic perovskite $E2_1$ structure.
- (Iwanga, 2000) places the strontium atoms on the (4c) Wyckoff position, but gives the coordinates for the (4d) site. The interatomic distances they give with this structure are consistent with the (4d) site.

Body-centered Tetragonal primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(2a)	Ni I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2$	=	$\frac{1}{2}c\,\hat{\mathbf{z}}$	(2b)	W 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)	Sr 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)	Sr I
$\mathbf{B_5}$	=	$z_4\,\mathbf{a}_1 + z_4\,\mathbf{a}_2$	=	$cz_4\,\hat{\mathbf{z}}$	(4e)	O I
$\mathbf{B_6}$	=	$-z_4\,\mathbf{a}_1 - z_4\,\mathbf{a}_2$	=	$-cz_4\,\hat{\mathbf{z}}$	(4e)	O I
$\mathbf{B_7}$	=	$y_5\,\mathbf{a}_1 + x_5\,\mathbf{a}_2 + (x_5+y_5)\,\mathbf{a}_3$	=	$ax_5\,\hat{\mathbf{x}} + ay_5\,\hat{\mathbf{y}}$	(8h)	O II
$\mathbf{B_8}$	=	$-y_5\,\mathbf{a}_1 - x_5\,\mathbf{a}_2 - (x_5+y_5)\,\mathbf{a}_3$	=	$-ax_5\,\hat{\mathbf{x}} - ay_5\,\hat{\mathbf{y}}$	(8h)	O II
$\mathbf{B_9}$	=	$x_5\,\mathbf{a}_1 - y_5\,\mathbf{a}_2 + (x_5-y_5)\,\mathbf{a}_3$	=	$-ay_5\,\hat{\mathbf{x}} + ax_5\,\hat{\mathbf{y}}$	(8h)	O II
$\mathbf{B_{10}}$	=	$-x_5\,\mathbf{a}_1 + y_5\,\mathbf{a}_2 - (x_5-y_5)\,\mathbf{a}_3$	=	$ay_5\,\hat{\mathbf{x}} - ax_5\,\hat{\mathbf{y}}$	(8h)	O II

References

[1] D. Iwanaga, Y. Inaguma, and M. Itoh, *Structure and Magnetic Properties of Sr_2NiAO_6 (A = W, Te)*, Mater. Res. Bull. **35**, 449–457 (2000), doi:10.1016/S0025-5408(00)00222-1.