Hazelwoodite (Ni_3S_2, $D5_e$) Structure: A3B2_hR5_155_e_c-001

This structure originally had the label `A3B2_hR5_155_e_c`. Calls to that address will be redirected here.

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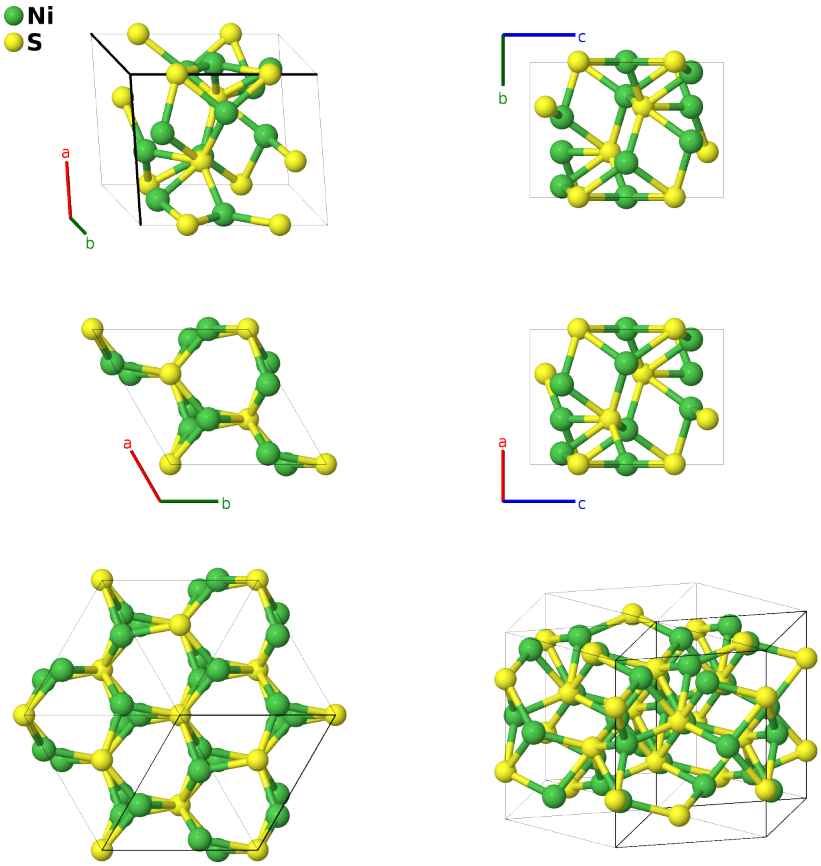
https://aflow.org/p/WQGS

https://aflow.org/p/A3B2_hR5_155_e_c-001



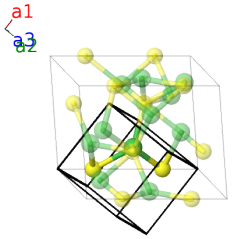
Prototype	Ni_3S_2
AFLOW prototype label	A3B2_hR5_155_e_c-001
***Strukturbericht* designation**	$D5_3$
Mineral name	hazelwoodite
ICSD	23114
Pearson symbol	hR5
Space group number	155
Space group symbol	$R32$
AFLOW prototype command	`aflow --proto=A3B2_hR5_155_e_c-001 --params=`$a, c/a, x_1, y_2$

Other compounds with this structure
Ni_3Se_2

- This can be considered as a prototype for a high concentration of ordered vacancies in the hcp structure. We get the ideal hcp atomic positions when z_1=1/3 and y_2=1/6, leaving a vacancy at the origin.
- Hexagonal settings of this structure can be obtained with the option `--hex`.

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
$\mathbf{B_1}$	=	$x_1\,\mathbf{a}_1 + x_1\,\mathbf{a}_2 + x_1\,\mathbf{a}_3$	=	$cx_1\,\hat{\mathbf{z}}$	(2c)	S I
$\mathbf{B_2}$	=	$-x_1\,\mathbf{a}_1 - x_1\,\mathbf{a}_2 - x_1\,\mathbf{a}_3$	=	$-cx_1\,\hat{\mathbf{z}}$	(2c)	S I
$\mathbf{B_3}$	=	$\frac{1}{2}\,\mathbf{a}_1 + y_2\,\mathbf{a}_2 - y_2\,\mathbf{a}_3$	=	$\frac{1}{4}a\,(2y_2+1)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{12}a\,(6y_2-1)\,\hat{\mathbf{y}} + \frac{1}{6}c\,\hat{\mathbf{z}}$	(3e)	Ni I
$\mathbf{B_4}$	=	$-y_2\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + y_2\,\mathbf{a}_3$	=	$-ay_2\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{1}{6}c\,\hat{\mathbf{z}}$	(3e)	Ni I
$\mathbf{B_5}$	=	$y_2\,\mathbf{a}_1 - y_2\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,(2y_2-1)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{12}a\,(6y_2+1)\,\hat{\mathbf{y}} + \frac{1}{6}c\,\hat{\mathbf{z}}$	(3e)	Ni I

References

[1] J. B. Parise, *Structure of Hazelwoodite (Ni_3S_2*, Acta Cryst. **B36**, 1179–1180 (1980), doi:10.1107/S0567740880005523.