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

This structure previously used the label(s) `A3B2_hR5_155_e_c`. Calls to these addresses will be redirected here.

Cite this page as:

- H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettel, M. Esters, X. Campilongo, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*, Comput. Mater. Sci. **240**, 112988 (2024), doi: 10.1016/j.commatsci.2024.112988.
- D. Hicks, M. J. Mehl, M. Esters, C. Oses, O. Levy, G. L. W. Hart, C. Toher, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 3*, Comput. Mater. Sci. **199**, 110450 (2021), doi: 10.1016/j.commatsci.2021.110450.

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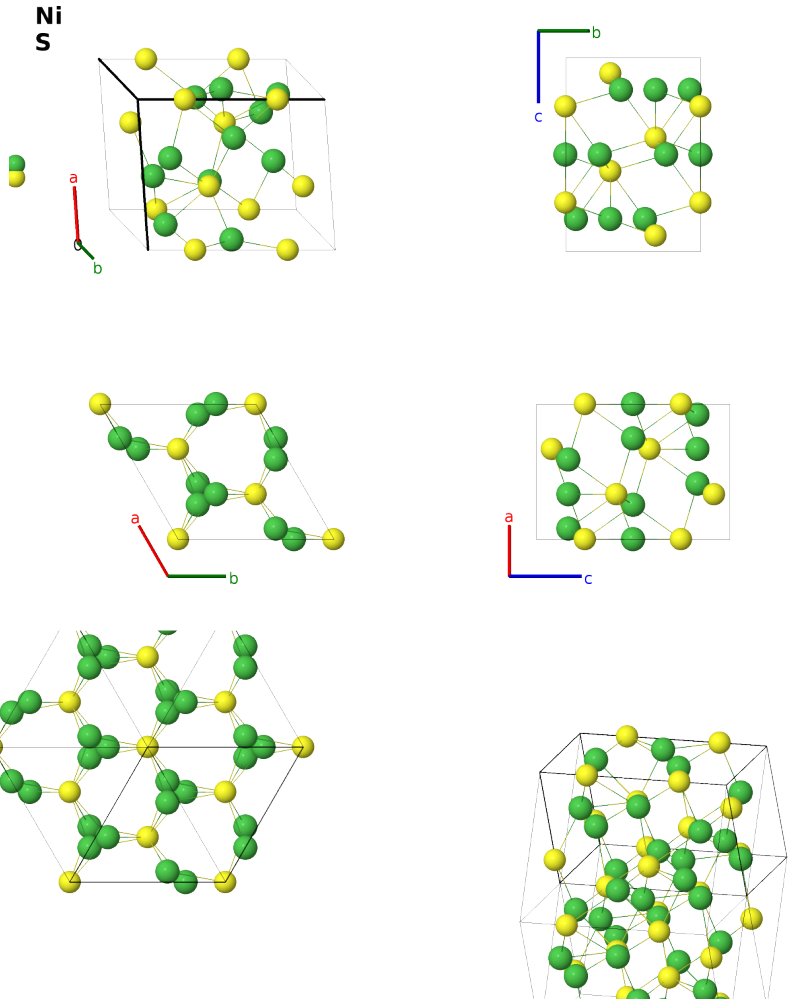
https://aflow.org/prototype-encyclopedia/WQGS

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

CCDC	1599267
Pearson symbol	hR5
Space group number	155
Space group symbol	$R32$
AFLOW prototype command	`aflow --proto=A3B2_hR5_155_e_c-001 --params=`$a, c/a, x_1, y_2$

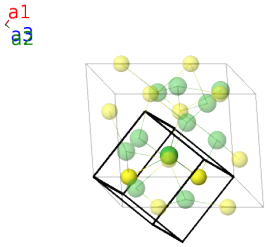
Other compounds with this structure

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.

First cited in

M. J. Mehl, D. Hicks, C. Toher, O. Levy, R. M. Hanson, G. L. W. Hart, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 1*, Comput. Mater. Sci. **136**, S1-828 (2017). doi: 10.1016/j.commatsci.2017.01.017