Millerite (NiS, $B13$) Structure: AB_hR6_160_b_b-001

This structure previously used the label(s) `AB_hR6_160_b_b`. Calls to these addresses will be redirected here.

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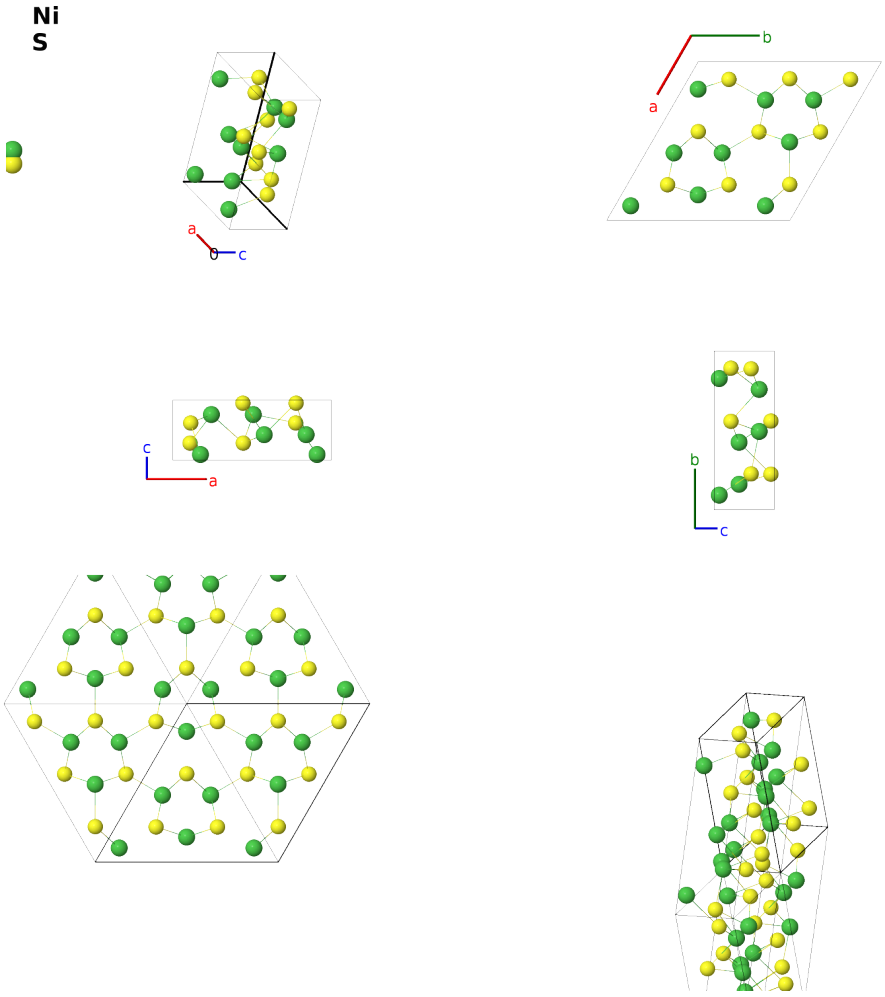
https://aflow.org/prototype-encyclopedia/MV4U

https://aflow.org/prototype-encyclopedia/AB_hR6_160_b_b-001



Prototype	NiS
AFLOW prototype label	AB_hR6_160_b_b-001
***Strukturbericht* designation**	$B13$
Mineral name	millerite
ICSD	40054

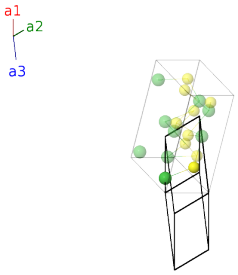
CCDC	1609971
Pearson symbol	hR6
Space group number	160
Space group symbol	$R3m$
AFLOW prototype command	`aflow --proto=AB_hR6_160_b_b-001 --params=`$a, c/a, x_1, z_1, x_2, z_2$

Other compounds with this structure
β-FeS, NiSe

- 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
$\mathbf{B_1}$	=	$x_1\,\mathbf{a}_1 + x_1\,\mathbf{a}_2 + z_1\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_1 - z_1)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(x_1 - z_1)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(2x_1 + z_1)\,\hat{\mathbf{z}}$	(3b)	Ni I
$\mathbf{B_2}$	=	$z_1\,\mathbf{a}_1 + x_1\,\mathbf{a}_2 + x_1\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(x_1 - z_1)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(x_1 - z_1)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(2x_1 + z_1)\,\hat{\mathbf{z}}$	(3b)	Ni I
$\mathbf{B_3}$	=	$x_1\,\mathbf{a}_1 + z_1\,\mathbf{a}_2 + x_1\,\mathbf{a}_3$	=	$-\frac{1}{\sqrt{3}}a\,(x_1 - z_1)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(2x_1 + z_1)\,\hat{\mathbf{z}}$	(3b)	Ni I
$\mathbf{B_4}$	=	$x_2\,\mathbf{a}_1 + x_2\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_2 - z_2)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(x_2 - z_2)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(2x_2 + z_2)\,\hat{\mathbf{z}}$	(3b)	S I
$\mathbf{B_5}$	=	$z_2\,\mathbf{a}_1 + x_2\,\mathbf{a}_2 + x_2\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(x_2 - z_2)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(x_2 - z_2)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(2x_2 + z_2)\,\hat{\mathbf{z}}$	(3b)	S I
$\mathbf{B_6}$	=	$x_2\,\mathbf{a}_1 + z_2\,\mathbf{a}_2 + x_2\,\mathbf{a}_3$	=	$-\frac{1}{\sqrt{3}}a\,(x_2 - z_2)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(2x_2 + z_2)\,\hat{\mathbf{z}}$	(3b)	S I

References

[1] V. Rajamani and C. T. Prewitt, *The Crystal Structure of Millerite*, Can. Mineral. **12**, 253–257 (1974).

Found in

[1] R. T. Downs and M. Hall-Wallace, *The American Mineralogist Crystal Structure Database*, Am. Mineral. **88**, 247–250 (2003).

First cited in

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