Shandite ($Ni_3Pb_2S_2$) Structure: A3B2C2_hR7_166_d_ab_c-001

This structure originally had the label `A3B2C2_hR7_166_d_ab_c`. Calls to that address will be redirected here.

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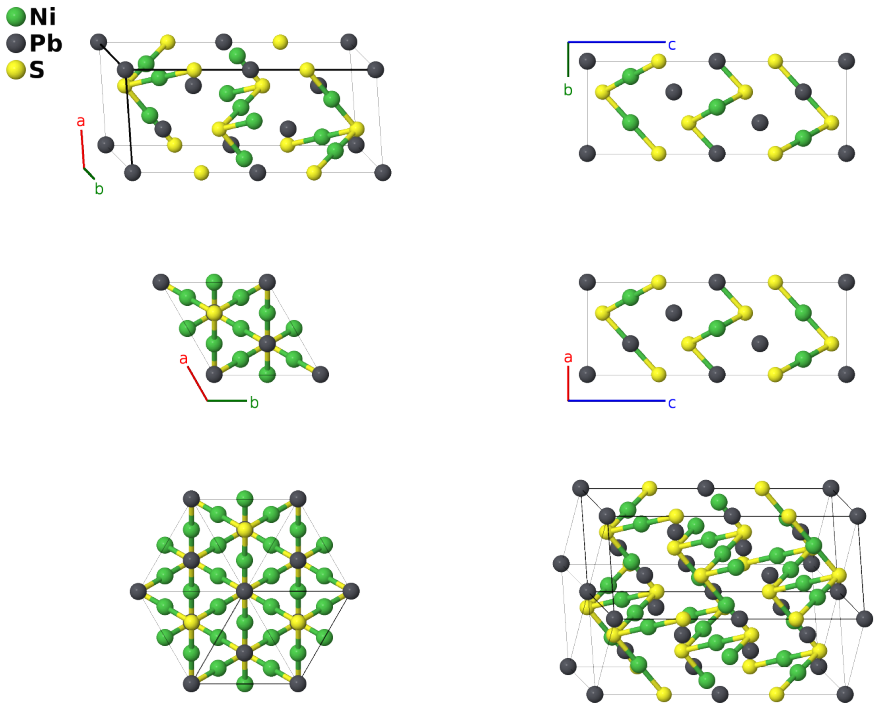
https://aflow.org/p/SD1B

https://aflow.org/p/A3B2C2_hR7_166_d_ab_c-001



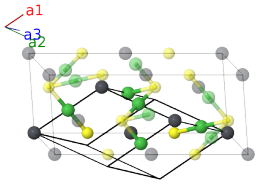
Prototype	$Ni_3Pb_2S_2$
AFLOW prototype label	A3B2C2_hR7_166_d_ab_c-001
Mineral name	shandite
ICSD	417632
Pearson symbol	hR7
Space group number	166
Space group symbol	$R\bar{3}m$
AFLOW prototype command	`aflow --proto=A3B2C2_hR7_166_d_ab_c-001 --params=`$a, c/a, x_3$

Other compounds with this structure

$Co_3In_2S_2$, $Co_3Sn_2S_2$, $Ni_3In_2S_2$, $Ni_3Sn_2S_2$, $O_3K_2Sn_2$, $Pd_3Bi_2S_2$

Rhombohedral primitive vectors

$$
\begin{aligned}
\mathbf{a_1} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \tfrac{1}{3}c\,\hat{\mathbf{z}} \\
\mathbf{a_2} &= \tfrac{1}{\sqrt{3}}a\,\hat{\mathbf{y}} + \tfrac{1}{3}c\,\hat{\mathbf{z}} \\
\mathbf{a_3} &= -\tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \tfrac{1}{3}c\,\hat{\mathbf{z}}
\end{aligned}
$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(1a)	Pb I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}c\,\hat{\mathbf{z}}$	(1b)	Pb II
$\mathbf{B_3}$	=	$x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + x_3\,\mathbf{a}_3$	=	$cx_3\,\hat{\mathbf{z}}$	(2c)	S I
$\mathbf{B_4}$	=	$-x_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 - x_3\,\mathbf{a}_3$	=	$-cx_3\,\hat{\mathbf{z}}$	(2c)	S I
$\mathbf{B_5}$	=	$\frac{1}{2}\,\mathbf{a}_1$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{12}a\,\hat{\mathbf{y}} + \frac{1}{6}c\,\hat{\mathbf{z}}$	(3d)	Ni I
$\mathbf{B_6}$	=	$\frac{1}{2}\,\mathbf{a}_2$	=	$\frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{1}{6}c\,\hat{\mathbf{z}}$	(3d)	Ni I
$\mathbf{B_7}$	=	$\frac{1}{2}\,\mathbf{a}_3$	=	$-\frac{1}{4}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{12}a\,\hat{\mathbf{y}} + \frac{1}{6}c\,\hat{\mathbf{z}}$	(3d)	Ni I

References

[1] R. Weihrich, S. F. Matar, V. Eyert, F. Rau, M. Zabel, M. Andratschke, I. Anusca, and T. Bernert, *Structure, ordering, and bonding of half antiperovskites: $PbNi_{3/2}S$ and $BiPd_{3/2}S$*, Prog. Solid State Chem. **35**, 309–322 (2007), doi:10.1016/j.progsolidstchem.2007.01.011.