

Parkerite ($\text{Ni}_3\text{Bi}_2\text{S}_4$) Structure:

AB2C_oP8_51_e_be_f-001

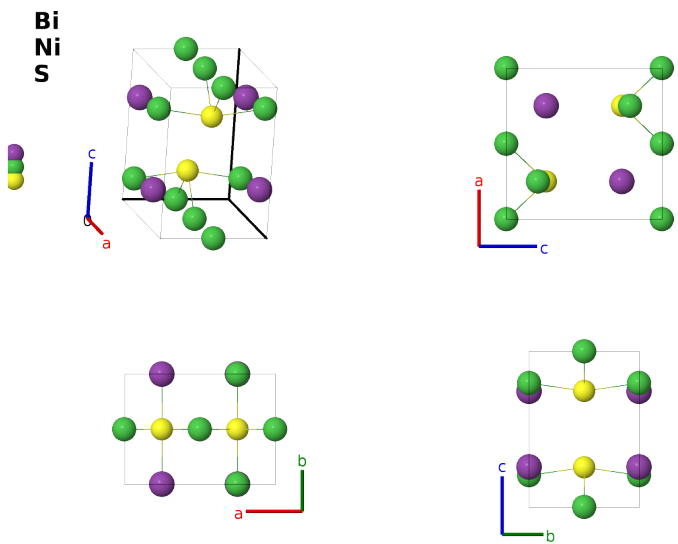
This structure previously used the label(s) **AB2C_oP8_51_e_be_f**. Calls to these addresses will be redirected here.

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<https://aflow.org/prototype-encyclopedia/LY1V>

https://aflow.org/prototype-encyclopedia/AB2C_oP8_51_e_be_f-001



Prototype	$\text{Bi}_2\text{Ni}_3\text{S}_2$
AFLOW prototype label	AB2C_oP8_51_e_be_f-001
Mineral name	parkerite
ICSD	70052
CCDC	1631876
Pearson symbol	oP8
Space group number	51
Space group symbol	$Pmma$
AFLOW prototype command	<code>aflow --proto=AB2C_oP8_51_e_be_f-001</code> <code>--params=$a, b/a, c/a, z_2, z_3, z_4$</code>

Other compounds with this structure

$\text{Ni}_3(\text{Bi}, \text{Pb})_2\text{S}_4$

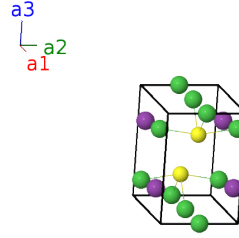
- (Fleet, 1973) states that parkerite is a derivative of the shandite ($\text{Ni}_3\text{Pb}_2\text{S}_2$) structure, and changes to shandite if more than 4% of the bismuth is replaced by lead.
- The Ni-II (2e) site is occupied 50% of the time, given the observed stoichiometry.
- Earlier sources give parkerite a monoclinic structure. This may be due to an ordering of the nickel atoms at lower temperature. We follow (Downs, 2003) and use the orthorhombic structure.
- (Fleet, 1973) describes the structure in the $Pmam$ setting of space group #51. We used FINDSYM to transform it to the standard $Pmma$ setting.

Simple Orthorhombic primitive vectors

$$\mathbf{a}_1 = a \hat{\mathbf{x}}$$

$$\mathbf{a}_2 = b \hat{\mathbf{y}}$$

$$\mathbf{a}_3 = c \hat{\mathbf{z}}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= \frac{1}{2} \mathbf{a}_2$	$=$	$\frac{1}{2} b \hat{\mathbf{y}}$	(2b)	Ni I
$\mathbf{B}_2$	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} b \hat{\mathbf{y}}$	(2b)	Ni I
$\mathbf{B}_3$	$= \frac{1}{4} \mathbf{a}_1 + z_2 \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} + cz_2 \hat{\mathbf{z}}$	(2e)	Bi I
$\mathbf{B}_4$	$= \frac{3}{4} \mathbf{a}_1 - z_2 \mathbf{a}_3$	$=$	$\frac{3}{4} a \hat{\mathbf{x}} - cz_2 \hat{\mathbf{z}}$	(2e)	Bi I
$\mathbf{B}_5$	$= \frac{1}{4} \mathbf{a}_1 + z_3 \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} + cz_3 \hat{\mathbf{z}}$	(2e)	Ni II
$\mathbf{B}_6$	$= \frac{3}{4} \mathbf{a}_1 - z_3 \mathbf{a}_3$	$=$	$\frac{3}{4} a \hat{\mathbf{x}} - cz_3 \hat{\mathbf{z}}$	(2e)	Ni II
$\mathbf{B}_7$	$= \frac{1}{4} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} + \frac{1}{2} b \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(2f)	S I
$\mathbf{B}_8$	$= \frac{3}{4} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$\frac{3}{4} a \hat{\mathbf{x}} + \frac{1}{2} b \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}}$	(2f)	S I

References

- [1] M. E. Fleet, *The Crystal Structure of Parkerite ($\text{Ni}_3\text{Bi}_2\text{S}_4$)*, Am. Mineral. **58**, 435–439 (1973).
- [2] 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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