Parkerite ($Ni_3Bi_2S_4$) Structure: AB2C_oP8_51_e_be_f-001

This structure originally had the label `AB2C_oP8_51_e_be_f`. Calls to that address will be redirected here.

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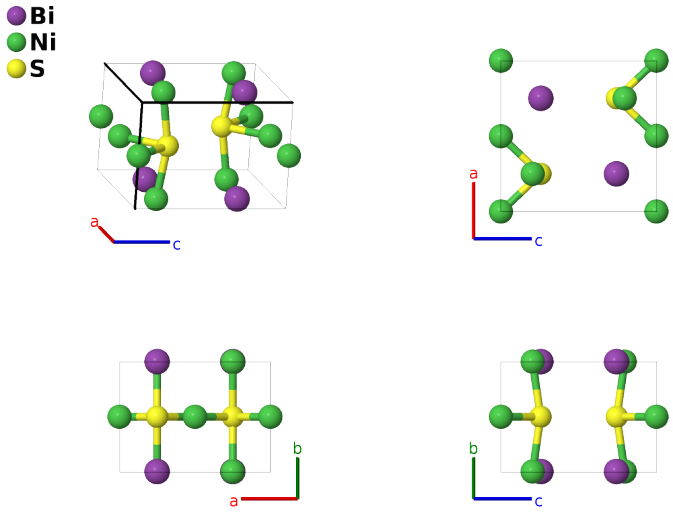
https://aflow.org/p/LY1V

https://aflow.org/p/AB2C_oP8_51_e_be_f-001



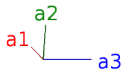
Prototype	$Bi_2Ni_3S_2$
AFLOW prototype label	AB2C_oP8_51_e_be_f-001
Mineral name	parkerite
ICSD	70052
Pearson symbol	oP8
Space group number	51
Space group symbol	*Pmma*
AFLOW prototype command	`aflow --proto=AB2C_oP8_51_e_be_f-001 --params=`$a, b/a, c/a, z_2, z_3, z_4$

Other compounds with this structure
$Ni_3(Bi, Pb)_2S_4$

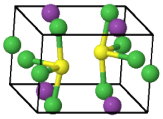
- (Fleet, 1973) states that parkerite is a derivative of the shandite ($Ni_3Pb_2S_2$) structure, and changes to shandite if more than 4% of the bismuth is replaced by lead.
- The Ni-II (2e) site is occupied 50% of the time, given the observed stoichiometry.
- Earlier sources give parkerite a monoclinic 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 ($Ni_3Bi_2S_4$)*, 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).