Rosiaite ($PbSb_2O_6$) Structure: A6BC2_hP9_162_k_a_d-001

This structure originally had the label `A6BC2_hP9_162_k_a_d`. Calls to that address will be redirected here.

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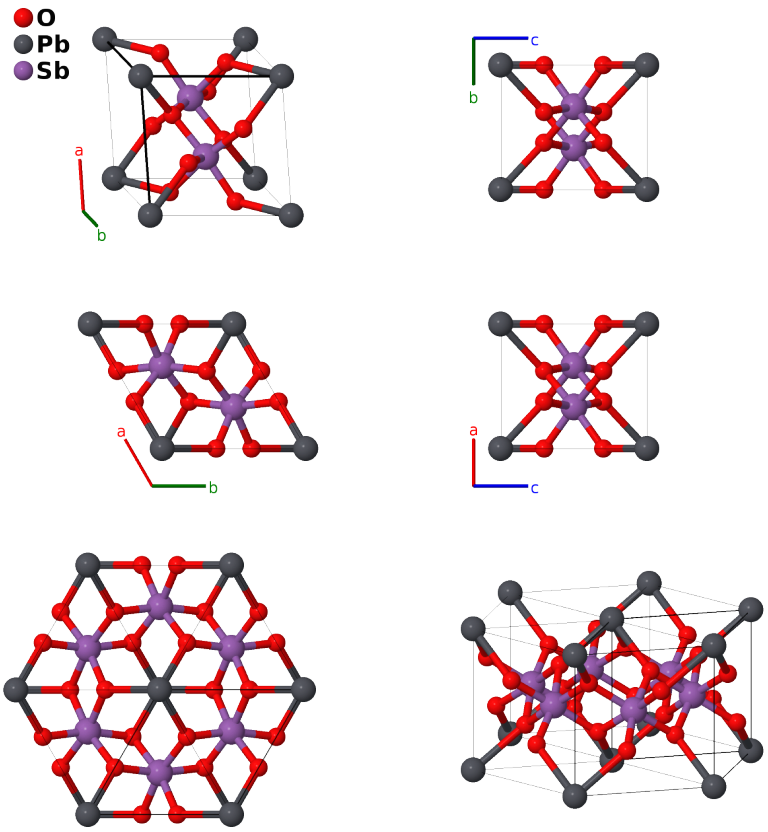
https://aflow.org/p/80KE

https://aflow.org/p/A6BC2_hP9_162_k_a_d-001



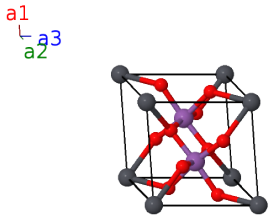
Prototype	O_6PbSb_2
AFLOW prototype label	A6BC2_hP9_162_k_a_d-001
Mineral name	rosiaite
ICSD	81387
Pearson symbol	hP9
Space group number	162
Space group symbol	$P\bar{3}1m$
AFLOW prototype command	`aflow --proto=A6BC2_hP9_162_k_a_d-001 --params=`$a, c/a, x_3, z_3$

Other compounds with this structure
$MnSeTeO_6$, $MnSnTeO_6$, $PbTeGeO_6$, $SrIr_2O_6$

- This is the ternary form of the $L'3_2$ (β-V_2N) structure.

Trigonal (Hexagonal) primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(1a)	Pb I
$\mathbf{B_2}$	=	$\frac{1}{3}\,\mathbf{a}_1 + \frac{2}{3}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(2d)	Sb I
$\mathbf{B_3}$	=	$\frac{2}{3}\,\mathbf{a}_1 + \frac{1}{3}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(2d)	Sb I
$\mathbf{B_4}$	=	$x_3\,\mathbf{a}_1 + z_3\,\mathbf{a}_3$	=	$\frac{1}{2}ax_3\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_3\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(6k)	O I
$\mathbf{B_5}$	=	$x_3\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$\frac{1}{2}ax_3\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_3\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(6k)	O I
$\mathbf{B_6}$	=	$-x_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} + cz_3\,\hat{\mathbf{z}}$	(6k)	O I
$\mathbf{B_7}$	=	$-x_3\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$	=	$-\frac{1}{2}ax_3\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_3\,\hat{\mathbf{y}} - cz_3\,\hat{\mathbf{z}}$	(6k)	O I
$\mathbf{B_8}$	=	$-x_3\,\mathbf{a}_1 - z_3\,\mathbf{a}_3$	=	$-\frac{1}{2}ax_3\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_3\,\hat{\mathbf{y}} - cz_3\,\hat{\mathbf{z}}$	(6k)	O I
$\mathbf{B_9}$	=	$x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} - cz_3\,\hat{\mathbf{z}}$	(6k)	O I

References

[1] R. Basso, G. Lucchetti, L. Zefiro, and A. Palenzona, *Rosiaite, $PbSb_2O_6$, a new mineral from the Cetine mine, Siena, Italy*, Eur. J. of Mineral. **8**, 487–492 (1996).