Luberoite (Pt$_5$Se$_4$) Structure: A5B4_mP18_14_a2e_2e-001

https://aflow.org/p/1FWE

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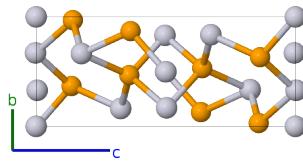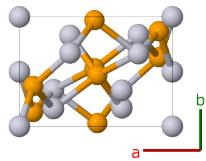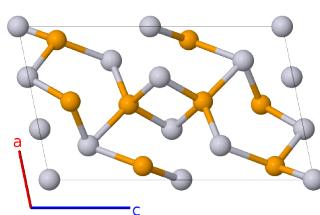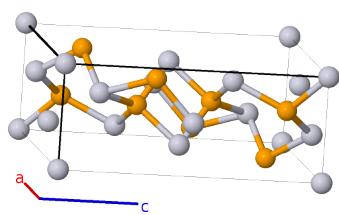
Prototype	Pt$_5$Se$_4$
AFLOW prototype label	A5B4_mP18_14_a2e_2e-001
Mineral name	luberoite
ICSD	87926
Pearson symbol	mP18
Space group number	14
Space group symbol	$P2_1/c$
AFLOW prototype command	aflow --proto=A5B4_mP18_14_a2e_2e-001 --params=$a, b/a, c/a, \beta, x_2, y_2, z_2, x_3, y_3, z_3, x_4, y_4, z_4, x_5, y_5, z_5$

Simple Monoclinic primitive vectors

$$\mathbf{a_1} = a\,\hat{\mathbf{x}}$$

$$\mathbf{a_2} = b\,\hat{\mathbf{y}}$$

$$\mathbf{a_3} = c\cos\beta\,\hat{\mathbf{x}} + c\sin\beta\,\hat{\mathbf{z}}$$
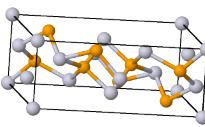
Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	$=$	0	$=$	0	(2a)	Pt I
$\mathbf{B_2}$	$=$	$\frac{1}{2}\mathbf{a}_2 + \frac{1}{2}\mathbf{a}_3$	$=$	$\frac{1}{2}c\cos\beta\,\hat{\mathbf{x}} + \frac{1}{2}b\,\hat{\mathbf{y}} + \frac{1}{2}c\sin\beta\,\hat{\mathbf{z}}$	(2a)	Pt I
$\mathbf{B_3}$	$=$	$x_2\mathbf{a}_1 + y_2\mathbf{a}_2 + z_2\mathbf{a}_3$	$=$	$(ax_2 + cz_2\cos\beta)\,\hat{\mathbf{x}} + by_2\,\hat{\mathbf{y}} + cz_2\sin\beta\,\hat{\mathbf{z}}$	(4e)	Pt II
$\mathbf{B_4}$	$=$	$-x_2\mathbf{a}_1 + \left(y_2 + \frac{1}{2}\right)\mathbf{a}_2 - \left(z_2 - \frac{1}{2}\right)\mathbf{a}_3$	$=$	$-\left(ax_2 + c\left(z_2 - \frac{1}{2}\right)\cos\beta\right)\hat{\mathbf{x}} + b\left(y_2 + \frac{1}{2}\right)\hat{\mathbf{y}} - c\left(z_2 - \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4e)	Pt II
$\mathbf{B_5}$	$=$	$-x_2\mathbf{a}_1 - y_2\mathbf{a}_2 - z_2\mathbf{a}_3$	$=$	$-(ax_2 + cz_2\cos\beta)\,\hat{\mathbf{x}} - by_2\,\hat{\mathbf{y}} - cz_2\sin\beta\,\hat{\mathbf{z}}$	(4e)	Pt II
$\mathbf{B_6}$	$=$	$x_2\mathbf{a}_1 - \left(y_2 - \frac{1}{2}\right)\mathbf{a}_2 + \left(z_2 + \frac{1}{2}\right)\mathbf{a}_3$	$=$	$\left(ax_2 + c\left(z_2 + \frac{1}{2}\right)\cos\beta\right)\hat{\mathbf{x}} - b\left(y_2 - \frac{1}{2}\right)\hat{\mathbf{y}} + c\left(z_2 + \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4e)	Pt II
$\mathbf{B_7}$	$=$	$x_3\mathbf{a}_1 + y_3\mathbf{a}_2 + z_3\mathbf{a}_3$	$=$	$(ax_3 + cz_3\cos\beta)\,\hat{\mathbf{x}} + by_3\,\hat{\mathbf{y}} + cz_3\sin\beta\,\hat{\mathbf{z}}$	(4e)	Pt III
$\mathbf{B_8}$	$=$	$-x_3\mathbf{a}_1 + \left(y_3 + \frac{1}{2}\right)\mathbf{a}_2 - \left(z_3 - \frac{1}{2}\right)\mathbf{a}_3$	$=$	$-\left(ax_3 + c\left(z_3 - \frac{1}{2}\right)\cos\beta\right)\hat{\mathbf{x}} + b\left(y_3 + \frac{1}{2}\right)\hat{\mathbf{y}} - c\left(z_3 - \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4e)	Pt III
$\mathbf{B_9}$	$=$	$-x_3\mathbf{a}_1 - y_3\mathbf{a}_2 - z_3\mathbf{a}_3$	$=$	$-(ax_3 + cz_3\cos\beta)\,\hat{\mathbf{x}} - by_3\,\hat{\mathbf{y}} - cz_3\sin\beta\,\hat{\mathbf{z}}$	(4e)	Pt III
$\mathbf{B_{10}}$	$=$	$x_3\mathbf{a}_1 - \left(y_3 - \frac{1}{2}\right)\mathbf{a}_2 + \left(z_3 + \frac{1}{2}\right)\mathbf{a}_3$	$=$	$\left(ax_3 + c\left(z_3 + \frac{1}{2}\right)\cos\beta\right)\hat{\mathbf{x}} - b\left(y_3 - \frac{1}{2}\right)\hat{\mathbf{y}} + c\left(z_3 + \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4e)	Pt III
$\mathbf{B_{11}}$	$=$	$x_4\mathbf{a}_1 + y_4\mathbf{a}_2 + z_4\mathbf{a}_3$	$=$	$(ax_4 + cz_4\cos\beta)\,\hat{\mathbf{x}} + by_4\,\hat{\mathbf{y}} + cz_4\sin\beta\,\hat{\mathbf{z}}$	(4e)	Se I
$\mathbf{B_{12}}$	$=$	$-x_4\mathbf{a}_1 + \left(y_4 + \frac{1}{2}\right)\mathbf{a}_2 - \left(z_4 - \frac{1}{2}\right)\mathbf{a}_3$	$=$	$-\left(ax_4 + c\left(z_4 - \frac{1}{2}\right)\cos\beta\right)\hat{\mathbf{x}} + b\left(y_4 + \frac{1}{2}\right)\hat{\mathbf{y}} - c\left(z_4 - \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4e)	Se I
$\mathbf{B_{13}}$	$=$	$-x_4\mathbf{a}_1 - y_4\mathbf{a}_2 - z_4\mathbf{a}_3$	$=$	$-(ax_4 + cz_4\cos\beta)\,\hat{\mathbf{x}} - by_4\,\hat{\mathbf{y}} - cz_4\sin\beta\,\hat{\mathbf{z}}$	(4e)	Se I
$\mathbf{B_{14}}$	$=$	$x_4\mathbf{a}_1 - \left(y_4 - \frac{1}{2}\right)\mathbf{a}_2 + \left(z_4 + \frac{1}{2}\right)\mathbf{a}_3$	$=$	$\left(ax_4 + c\left(z_4 + \frac{1}{2}\right)\cos\beta\right)\hat{\mathbf{x}} - b\left(y_4 - \frac{1}{2}\right)\hat{\mathbf{y}} + c\left(z_4 + \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4e)	Se I
$\mathbf{B_{15}}$	$=$	$x_5\mathbf{a}_1 + y_5\mathbf{a}_2 + z_5\mathbf{a}_3$	$=$	$(ax_5 + cz_5\cos\beta)\,\hat{\mathbf{x}} + by_5\,\hat{\mathbf{y}} + cz_5\sin\beta\,\hat{\mathbf{z}}$	(4e)	Se II
$\mathbf{B_{16}}$	$=$	$-x_5\mathbf{a}_1 + \left(y_5 + \frac{1}{2}\right)\mathbf{a}_2 - \left(z_5 - \frac{1}{2}\right)\mathbf{a}_3$	$=$	$-\left(ax_5 + c\left(z_5 - \frac{1}{2}\right)\cos\beta\right)\hat{\mathbf{x}} + b\left(y_5 + \frac{1}{2}\right)\hat{\mathbf{y}} - c\left(z_5 - \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4e)	Se II
$\mathbf{B_{17}}$	$=$	$-x_5\mathbf{a}_1 - y_5\mathbf{a}_2 - z_5\mathbf{a}_3$	$=$	$-(ax_5 + cz_5\cos\beta)\,\hat{\mathbf{x}} - by_5\,\hat{\mathbf{y}} - cz_5\sin\beta\,\hat{\mathbf{z}}$	(4e)	Se II
$\mathbf{B_{18}}$	$=$	$x_5\mathbf{a}_1 - \left(y_5 - \frac{1}{2}\right)\mathbf{a}_2 + \left(z_5 + \frac{1}{2}\right)\mathbf{a}_3$	$=$	$\left(ax_5 + c\left(z_5 + \frac{1}{2}\right)\cos\beta\right)\hat{\mathbf{x}} - b\left(y_5 - \frac{1}{2}\right)\hat{\mathbf{y}} + c\left(z_5 + \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4e)	Se II

References

[1] P. Matković and K. Schubert, *Kristallstruktur von Pt$_5$Se$_4$*, J. Less-Common Met. **55**, 185–190 (1977), doi:10.1016/0022-5088(77)90191-6.