Pt_2Ge_3 Structure: A3B2_oP20_62_3c_2c-002
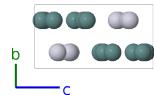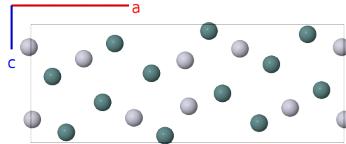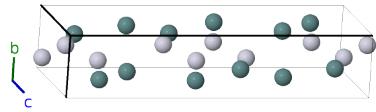
Prototype	Ge_3Pt_2
AFLOW prototype label	A3B2_oP20_62_3c_2c-002
ICSD	42912
Pearson symbol	oP20
Space group number	62
Space group symbol	$Pnma$
AFLOW prototype command	aflow --proto=A3B2_oP20_62_3c_2c-002 --params=$a, b/a, c/a, x_1, z_1, x_2, z_2, x_3, z_3, x_4, z_4, x_5, z_5$

Other compounds with this structure

Pt_2Si_3

- This structure has the same AFLOW label, A3B2_oP20_62_3c_2c, as stibnite (Sb_2S_3, $D5_8$) and ottemannite (Sn_2S_3). The structures are generated by the same symmetry operations with different sets of parameters (--params) specified in their corresponding CIF files.

Simple Orthorhombic primitive vectors

$$\mathbf{a_1} = a\,\hat{\mathbf{x}}$$
$$\mathbf{a_2} = b\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$
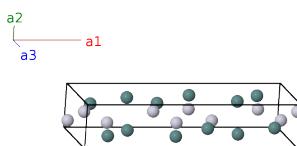
Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	$=$	$x_1\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + z_1\,\mathbf{a}_3$	$=$	$ax_1\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} + cz_1\,\hat{\mathbf{z}}$	(4c)	Ge I
$\mathbf{B_2}$	$=$	$-\left(x_1 - \frac{1}{2}\right)\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 + \left(z_1 + \frac{1}{2}\right)\mathbf{a}_3$	$=$	$-a\left(x_1 - \frac{1}{2}\right)\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} + c\left(z_1 + \frac{1}{2}\right)\hat{\mathbf{z}}$	(4c)	Ge I
$\mathbf{B_3}$	$=$	$-x_1\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 - z_1\,\mathbf{a}_3$	$=$	$-ax_1\,\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} - cz_1\,\hat{\mathbf{z}}$	(4c)	Ge I
$\mathbf{B_4}$	$=$	$\left(x_1 + \frac{1}{2}\right)\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 - \left(z_1 - \frac{1}{2}\right)\mathbf{a}_3$	$=$	$a\left(x_1 + \frac{1}{2}\right)\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} - c\left(z_1 - \frac{1}{2}\right)\hat{\mathbf{z}}$	(4c)	Ge I
$\mathbf{B_5}$	$=$	$x_2\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	$=$	$ax_2\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(4c)	Ge II
$\mathbf{B_6}$	$=$	$-\left(x_2 - \frac{1}{2}\right)\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 + \left(z_2 + \frac{1}{2}\right)\mathbf{a}_3$	$=$	$-a\left(x_2 - \frac{1}{2}\right)\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} + c\left(z_2 + \frac{1}{2}\right)\hat{\mathbf{z}}$	(4c)	Ge II
$\mathbf{B_7}$	$=$	$-x_2\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 - z_2\,\mathbf{a}_3$	$=$	$-ax_2\,\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} - cz_2\,\hat{\mathbf{z}}$	(4c)	Ge II
$\mathbf{B_8}$	$=$	$\left(x_2 + \frac{1}{2}\right)\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 - \left(z_2 - \frac{1}{2}\right)\mathbf{a}_3$	$=$	$a\left(x_2 + \frac{1}{2}\right)\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} - c\left(z_2 - \frac{1}{2}\right)\hat{\mathbf{z}}$	(4c)	Ge II
$\mathbf{B_9}$	$=$	$x_3\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	$=$	$ax_3\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(4c)	Ge III
$\mathbf{B_{10}}$	$=$	$-\left(x_3 - \frac{1}{2}\right)\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 + \left(z_3 + \frac{1}{2}\right)\mathbf{a}_3$	$=$	$-a\left(x_3 - \frac{1}{2}\right)\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} + c\left(z_3 + \frac{1}{2}\right)\hat{\mathbf{z}}$	(4c)	Ge III
$\mathbf{B_{11}}$	$=$	$-x_3\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$	$=$	$-ax_3\,\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} - cz_3\,\hat{\mathbf{z}}$	(4c)	Ge III
$\mathbf{B_{12}}$	$=$	$\left(x_3 + \frac{1}{2}\right)\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 - \left(z_3 - \frac{1}{2}\right)\mathbf{a}_3$	$=$	$a\left(x_3 + \frac{1}{2}\right)\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} - c\left(z_3 - \frac{1}{2}\right)\hat{\mathbf{z}}$	(4c)	Ge III
$\mathbf{B_{13}}$	$=$	$x_4\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	$=$	$ax_4\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(4c)	Pt I
$\mathbf{B_{14}}$	$=$	$-\left(x_4 - \frac{1}{2}\right)\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 + \left(z_4 + \frac{1}{2}\right)\mathbf{a}_3$	$=$	$-a\left(x_4 - \frac{1}{2}\right)\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} + c\left(z_4 + \frac{1}{2}\right)\hat{\mathbf{z}}$	(4c)	Pt I
$\mathbf{B_{15}}$	$=$	$-x_4\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 - z_4\,\mathbf{a}_3$	$=$	$-ax_4\,\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$	(4c)	Pt I
$\mathbf{B_{16}}$	$=$	$\left(x_4 + \frac{1}{2}\right)\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 - \left(z_4 - \frac{1}{2}\right)\mathbf{a}_3$	$=$	$a\left(x_4 + \frac{1}{2}\right)\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} - c\left(z_4 - \frac{1}{2}\right)\hat{\mathbf{z}}$	(4c)	Pt I
$\mathbf{B_{17}}$	$=$	$x_5\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	$=$	$ax_5\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(4c)	Pt II
$\mathbf{B_{18}}$	$=$	$-\left(x_5 - \frac{1}{2}\right)\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 + \left(z_5 + \frac{1}{2}\right)\mathbf{a}_3$	$=$	$-a\left(x_5 - \frac{1}{2}\right)\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} + c\left(z_5 + \frac{1}{2}\right)\hat{\mathbf{z}}$	(4c)	Pt II
$\mathbf{B_{19}}$	$=$	$-x_5\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 - z_5\,\mathbf{a}_3$	$=$	$-ax_5\,\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} - cz_5\,\hat{\mathbf{z}}$	(4c)	Pt II
$\mathbf{B_{20}}$	$=$	$\left(x_5 + \frac{1}{2}\right)\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 - \left(z_5 - \frac{1}{2}\right)\mathbf{a}_3$	$=$	$a\left(x_5 + \frac{1}{2}\right)\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} - c\left(z_5 - \frac{1}{2}\right)\hat{\mathbf{z}}$	(4c)	Pt II

References

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