Na$_2$FeSbO$_5$ Structure: AB2C5D_oP72_60_d_2cd_5d_2c-001

https://aflow.org/p/2H6S

https://aflow.org/p/AB2C5D_oP72_60_d_2cd_5d_2c-001
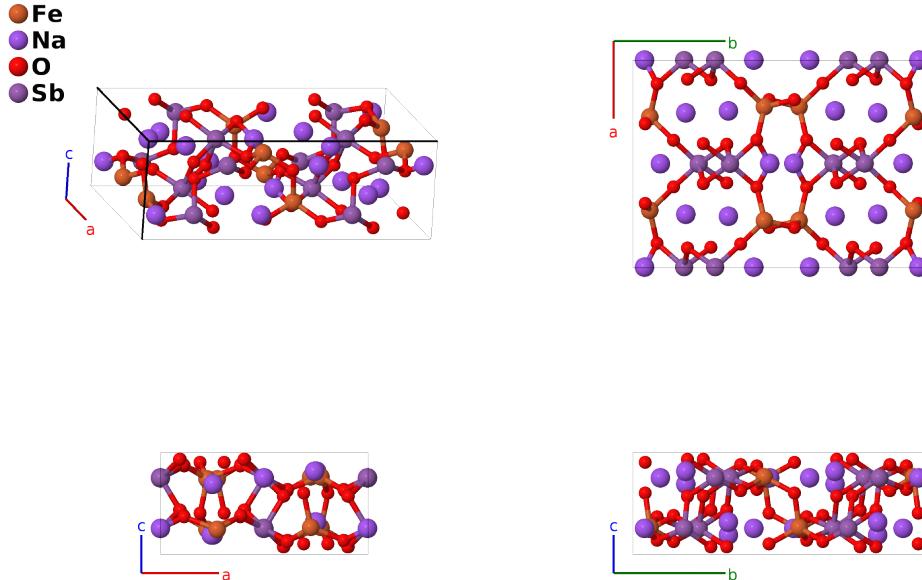
Prototype	FeNa$_2$O$_5$Sb
AFLOW prototype label	AB2C5D_oP72_60_d_2cd_5d_2c-001
ICSD	102575
Pearson symbol	oP72
Space group number	60
Space group symbol	*Pbcn*
AFLOW prototype command	aflow --proto=AB2C5D_oP72_60_d_2cd_5d_2c-001

$$\texttt{--params=}a, b/a, c/a, y_1, y_2, y_3, y_4, x_5, y_5, z_5, x_6, y_6, z_6, x_7, y_7, z_7, x_8, y_8, z_8, x_9, y_9, z_9, x_{10},$$
$$y_{10}, z_{10}, x_{11}, y_{11}, z_{11}$$

Simple Orthorhombic primitive vectors

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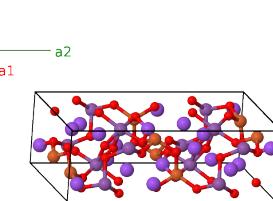
Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$y_1\,\mathbf{a_2} + \frac{1}{4}\,\mathbf{a_3}$	=	$by_1\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(4c)	Na I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a_1} - \left(y_1 - \frac{1}{2}\right)\mathbf{a_2} + \frac{3}{4}\,\mathbf{a_3}$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - b\left(y_1 - \frac{1}{2}\right)\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(4c)	Na I
$\mathbf{B_3}$	=	$-y_1\,\mathbf{a_2} + \frac{3}{4}\,\mathbf{a_3}$	=	$-by_1\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(4c)	Na I
$\mathbf{B_4}$	=	$\frac{1}{2}\,\mathbf{a_1} + \left(y_1 + \frac{1}{2}\right)\mathbf{a_2} + \frac{1}{4}\,\mathbf{a_3}$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + b\left(y_1 + \frac{1}{2}\right)\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(4c)	Na I
$\mathbf{B_5}$	=	$y_2\,\mathbf{a_2} + \frac{1}{4}\,\mathbf{a_3}$	=	$by_2\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(4c)	Na II
$\mathbf{B_6}$	=	$\frac{1}{2}\,\mathbf{a_1} - \left(y_2 - \frac{1}{2}\right)\mathbf{a_2} + \frac{3}{4}\,\mathbf{a_3}$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - b\left(y_2 - \frac{1}{2}\right)\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(4c)	Na II
$\mathbf{B_7}$	=	$-y_2\,\mathbf{a_2} + \frac{3}{4}\,\mathbf{a_3}$	=	$-by_2\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(4c)	Na II
$\mathbf{B_8}$	=	$\frac{1}{2}\,\mathbf{a_1} + \left(y_2 + \frac{1}{2}\right)\mathbf{a_2} + \frac{1}{4}\,\mathbf{a_3}$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + b\left(y_2 + \frac{1}{2}\right)\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(4c)	Na II
$\mathbf{B_9}$	=	$y_3\,\mathbf{a_2} + \frac{1}{4}\,\mathbf{a_3}$	=	$by_3\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(4c)	Sb I
$\mathbf{B_{10}}$	=	$\frac{1}{2}\,\mathbf{a_1} - \left(y_3 - \frac{1}{2}\right)\mathbf{a_2} + \frac{3}{4}\,\mathbf{a_3}$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - b\left(y_3 - \frac{1}{2}\right)\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(4c)	Sb I
$\mathbf{B_{11}}$	=	$-y_3\,\mathbf{a_2} + \frac{3}{4}\,\mathbf{a_3}$	=	$-by_3\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(4c)	Sb I
$\mathbf{B_{12}}$	=	$\frac{1}{2}\,\mathbf{a_1} + \left(y_3 + \frac{1}{2}\right)\mathbf{a_2} + \frac{1}{4}\,\mathbf{a_3}$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + b\left(y_3 + \frac{1}{2}\right)\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(4c)	Sb I
$\mathbf{B_{13}}$	=	$y_4\,\mathbf{a_2} + \frac{1}{4}\,\mathbf{a_3}$	=	$by_4\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(4c)	Sb II
$\mathbf{B_{14}}$	=	$\frac{1}{2}\,\mathbf{a_1} - \left(y_4 - \frac{1}{2}\right)\mathbf{a_2} + \frac{3}{4}\,\mathbf{a_3}$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - b\left(y_4 - \frac{1}{2}\right)\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(4c)	Sb II
$\mathbf{B_{15}}$	=	$-y_4\,\mathbf{a_2} + \frac{3}{4}\,\mathbf{a_3}$	=	$-by_4\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(4c)	Sb II
$\mathbf{B_{16}}$	=	$\frac{1}{2}\,\mathbf{a_1} + \left(y_4 + \frac{1}{2}\right)\mathbf{a_2} + \frac{1}{4}\,\mathbf{a_3}$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + b\left(y_4 + \frac{1}{2}\right)\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(4c)	Sb II
$\mathbf{B_{17}}$	=	$x_5\,\mathbf{a_1} + y_5\,\mathbf{a_2} + z_5\,\mathbf{a_3}$	=	$ax_5\,\hat{\mathbf{x}} + by_5\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(8d)	Fe I
$\mathbf{B_{18}}$	=	$-\left(x_5 - \frac{1}{2}\right)\mathbf{a_1} - \left(y_5 - \frac{1}{2}\right)\mathbf{a_2} + \left(z_5 + \frac{1}{2}\right)\mathbf{a_3}$	=	$-a\left(x_5 - \frac{1}{2}\right)\hat{\mathbf{x}} - b\left(y_5 - \frac{1}{2}\right)\hat{\mathbf{y}} + c\left(z_5 + \frac{1}{2}\right)\hat{\mathbf{z}}$	(8d)	Fe I
$\mathbf{B_{19}}$	=	$-x_5\,\mathbf{a_1} + y_5\,\mathbf{a_2} - \left(z_5 - \frac{1}{2}\right)\mathbf{a_3}$	=	$-ax_5\,\hat{\mathbf{x}} + by_5\,\hat{\mathbf{y}} - c\left(z_5 - \frac{1}{2}\right)\hat{\mathbf{z}}$	(8d)	Fe I
$\mathbf{B_{20}}$	=	$\left(x_5 + \frac{1}{2}\right)\mathbf{a_1} - \left(y_5 - \frac{1}{2}\right)\mathbf{a_2} - z_5\,\mathbf{a_3}$	=	$a\left(x_5 + \frac{1}{2}\right)\hat{\mathbf{x}} - b\left(y_5 - \frac{1}{2}\right)\hat{\mathbf{y}} - cz_5\,\hat{\mathbf{z}}$	(8d)	Fe I
$\mathbf{B_{21}}$	=	$-x_5\,\mathbf{a_1} - y_5\,\mathbf{a_2} - z_5\,\mathbf{a_3}$	=	$-ax_5\,\hat{\mathbf{x}} - by_5\,\hat{\mathbf{y}} - cz_5\,\hat{\mathbf{z}}$	(8d)	Fe I
$\mathbf{B_{22}}$	=	$\left(x_5 + \frac{1}{2}\right)\mathbf{a_1} + \left(y_5 + \frac{1}{2}\right)\mathbf{a_2} - \left(z_5 - \frac{1}{2}\right)\mathbf{a_3}$	=	$a\left(x_5 + \frac{1}{2}\right)\hat{\mathbf{x}} + b\left(y_5 + \frac{1}{2}\right)\hat{\mathbf{y}} - c\left(z_5 - \frac{1}{2}\right)\hat{\mathbf{z}}$	(8d)	Fe I
$\mathbf{B_{23}}$	=	$x_5\,\mathbf{a_1} - y_5\,\mathbf{a_2} + \left(z_5 + \frac{1}{2}\right)\mathbf{a_3}$	=	$ax_5\,\hat{\mathbf{x}} - by_5\,\hat{\mathbf{y}} + c\left(z_5 + \frac{1}{2}\right)\hat{\mathbf{z}}$	(8d)	Fe I
$\mathbf{B_{24}}$	=	$-\left(x_5 - \frac{1}{2}\right)\mathbf{a_1} + \left(y_5 + \frac{1}{2}\right)\mathbf{a_2} + z_5\,\mathbf{a_3}$	=	$-a\left(x_5 - \frac{1}{2}\right)\hat{\mathbf{x}} + b\left(y_5 + \frac{1}{2}\right)\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(8d)	Fe I
$\mathbf{B_{25}}$	=	$x_6\,\mathbf{a_1} + y_6\,\mathbf{a_2} + z_6\,\mathbf{a_3}$	=	$ax_6\,\hat{\mathbf{x}} + by_6\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(8d)	Na III
$\mathbf{B_{26}}$	=	$-\left(x_6 - \frac{1}{2}\right)\mathbf{a_1} - \left(y_6 - \frac{1}{2}\right)\mathbf{a_2} + \left(z_6 + \frac{1}{2}\right)\mathbf{a_3}$	=	$-a\left(x_6 - \frac{1}{2}\right)\hat{\mathbf{x}} - b\left(y_6 - \frac{1}{2}\right)\hat{\mathbf{y}} + c\left(z_6 + \frac{1}{2}\right)\hat{\mathbf{z}}$	(8d)	Na III
$\mathbf{B_{27}}$	=	$-x_6\,\mathbf{a_1} + y_6\,\mathbf{a_2} - \left(z_6 - \frac{1}{2}\right)\mathbf{a_3}$	=	$-ax_6\,\hat{\mathbf{x}} + by_6\,\hat{\mathbf{y}} - c\left(z_6 - \frac{1}{2}\right)\hat{\mathbf{z}}$	(8d)	Na III
$\mathbf{B_{28}}$	=	$\left(x_6 + \frac{1}{2}\right)\mathbf{a_1} - \left(y_6 - \frac{1}{2}\right)\mathbf{a_2} - z_6\,\mathbf{a_3}$	=	$a\left(x_6 + \frac{1}{2}\right)\hat{\mathbf{x}} - b\left(y_6 - \frac{1}{2}\right)\hat{\mathbf{y}} - cz_6\,\hat{\mathbf{z}}$	(8d)	Na III
$\mathbf{B_{29}}$	=	$-x_6\,\mathbf{a_1} - y_6\,\mathbf{a_2} - z_6\,\mathbf{a_3}$	=	$-ax_6\,\hat{\mathbf{x}} - by_6\,\hat{\mathbf{y}} - cz_6\,\hat{\mathbf{z}}$	(8d)	Na III
$\mathbf{B_{30}}$	=	$\left(x_6 + \frac{1}{2}\right)\mathbf{a_1} + \left(y_6 + \frac{1}{2}\right)\mathbf{a_2} - \left(z_6 - \frac{1}{2}\right)\mathbf{a_3}$	=	$a\left(x_6 + \frac{1}{2}\right)\hat{\mathbf{x}} + b\left(y_6 + \frac{1}{2}\right)\hat{\mathbf{y}} - c\left(z_6 - \frac{1}{2}\right)\hat{\mathbf{z}}$	(8d)	Na III
$\mathbf{B_{31}}$	=	$x_6\,\mathbf{a_1} - y_6\,\mathbf{a_2} + \left(z_6 + \frac{1}{2}\right)\mathbf{a_3}$	=	$ax_6\,\hat{\mathbf{x}} - by_6\,\hat{\mathbf{y}} + c\left(z_6 + \frac{1}{2}\right)\hat{\mathbf{z}}$	(8d)	Na III
$\mathbf{B_{32}}$	=	$-\left(x_6 - \frac{1}{2}\right)\mathbf{a_1} + \left(y_6 + \frac{1}{2}\right)\mathbf{a_2} + z_6\,\mathbf{a_3}$	=	$-a\left(x_6 - \frac{1}{2}\right)\hat{\mathbf{x}} + b\left(y_6 + \frac{1}{2}\right)\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(8d)	Na III
$\mathbf{B_{33}}$	=	$x_7\,\mathbf{a_1} + y_7\,\mathbf{a_2} + z_7\,\mathbf{a_3}$	=	$ax_7\,\hat{\mathbf{x}} + by_7\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}}$	(8d)	O I

$$\mathbf{B_{34}} = \quad -\left(x_7 - \tfrac{1}{2}\right)\mathbf{a}_1 - \left(y_7 - \tfrac{1}{2}\right)\mathbf{a}_2 + \left(z_7 + \tfrac{1}{2}\right)\mathbf{a}_3 \quad = \quad -a\left(x_7 - \tfrac{1}{2}\right)\hat{\mathbf{x}} - b\left(y_7 - \tfrac{1}{2}\right)\hat{\mathbf{y}} + c\left(z_7 + \tfrac{1}{2}\right)\hat{\mathbf{z}} \qquad (8d) \qquad \text{O I}$$

$$\mathbf{B_{35}} = \quad -x_7\,\mathbf{a}_1 + y_7\,\mathbf{a}_2 - \left(z_7 - \tfrac{1}{2}\right)\mathbf{a}_3 \quad = \quad -ax_7\,\hat{\mathbf{x}} + by_7\,\hat{\mathbf{y}} - c\left(z_7 - \tfrac{1}{2}\right)\hat{\mathbf{z}} \qquad (8d) \qquad \text{O I}$$

$$\mathbf{B_{36}} = \quad \left(x_7 + \tfrac{1}{2}\right)\mathbf{a}_1 - \left(y_7 - \tfrac{1}{2}\right)\mathbf{a}_2 - z_7\,\mathbf{a}_3 \quad = \quad a\left(x_7 + \tfrac{1}{2}\right)\hat{\mathbf{x}} - b\left(y_7 - \tfrac{1}{2}\right)\hat{\mathbf{y}} - cz_7\,\hat{\mathbf{z}} \qquad (8d) \qquad \text{O I}$$

$$\mathbf{B_{37}} = \quad -x_7\,\mathbf{a}_1 - y_7\,\mathbf{a}_2 - z_7\,\mathbf{a}_3 \quad = \quad -ax_7\,\hat{\mathbf{x}} - by_7\,\hat{\mathbf{y}} - cz_7\,\hat{\mathbf{z}} \qquad (8d) \qquad \text{O I}$$

$$\mathbf{B_{38}} = \quad \left(x_7 + \tfrac{1}{2}\right)\mathbf{a}_1 + \left(y_7 + \tfrac{1}{2}\right)\mathbf{a}_2 - \left(z_7 - \tfrac{1}{2}\right)\mathbf{a}_3 \quad = \quad a\left(x_7 + \tfrac{1}{2}\right)\hat{\mathbf{x}} + b\left(y_7 + \tfrac{1}{2}\right)\hat{\mathbf{y}} - c\left(z_7 - \tfrac{1}{2}\right)\hat{\mathbf{z}} \qquad (8d) \qquad \text{O I}$$

$$\mathbf{B_{39}} = \quad x_7\,\mathbf{a}_1 - y_7\,\mathbf{a}_2 + \left(z_7 + \tfrac{1}{2}\right)\mathbf{a}_3 \quad = \quad ax_7\,\hat{\mathbf{x}} - by_7\,\hat{\mathbf{y}} + c\left(z_7 + \tfrac{1}{2}\right)\hat{\mathbf{z}} \qquad (8d) \qquad \text{O I}$$

$$\mathbf{B_{40}} = \quad -\left(x_7 - \tfrac{1}{2}\right)\mathbf{a}_1 + \left(y_7 + \tfrac{1}{2}\right)\mathbf{a}_2 + z_7\,\mathbf{a}_3 \quad = \quad -a\left(x_7 - \tfrac{1}{2}\right)\hat{\mathbf{x}} + b\left(y_7 + \tfrac{1}{2}\right)\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}} \qquad (8d) \qquad \text{O I}$$

$$\mathbf{B_{41}} = \quad x_8\,\mathbf{a}_1 + y_8\,\mathbf{a}_2 + z_8\,\mathbf{a}_3 \quad = \quad ax_8\,\hat{\mathbf{x}} + by_8\,\hat{\mathbf{y}} + cz_8\,\hat{\mathbf{z}} \qquad (8d) \qquad \text{O II}$$

$$\mathbf{B_{42}} = \quad -\left(x_8 - \tfrac{1}{2}\right)\mathbf{a}_1 - \left(y_8 - \tfrac{1}{2}\right)\mathbf{a}_2 + \left(z_8 + \tfrac{1}{2}\right)\mathbf{a}_3 \quad = \quad -a\left(x_8 - \tfrac{1}{2}\right)\hat{\mathbf{x}} - b\left(y_8 - \tfrac{1}{2}\right)\hat{\mathbf{y}} + c\left(z_8 + \tfrac{1}{2}\right)\hat{\mathbf{z}} \qquad (8d) \qquad \text{O II}$$

$$\mathbf{B_{43}} = \quad -x_8\,\mathbf{a}_1 + y_8\,\mathbf{a}_2 - \left(z_8 - \tfrac{1}{2}\right)\mathbf{a}_3 \quad = \quad -ax_8\,\hat{\mathbf{x}} + by_8\,\hat{\mathbf{y}} - c\left(z_8 - \tfrac{1}{2}\right)\hat{\mathbf{z}} \qquad (8d) \qquad \text{O II}$$

$$\mathbf{B_{44}} = \quad \left(x_8 + \tfrac{1}{2}\right)\mathbf{a}_1 - \left(y_8 - \tfrac{1}{2}\right)\mathbf{a}_2 - z_8\,\mathbf{a}_3 \quad = \quad a\left(x_8 + \tfrac{1}{2}\right)\hat{\mathbf{x}} - b\left(y_8 - \tfrac{1}{2}\right)\hat{\mathbf{y}} - cz_8\,\hat{\mathbf{z}} \qquad (8d) \qquad \text{O II}$$

$$\mathbf{B_{45}} = \quad -x_8\,\mathbf{a}_1 - y_8\,\mathbf{a}_2 - z_8\,\mathbf{a}_3 \quad = \quad -ax_8\,\hat{\mathbf{x}} - by_8\,\hat{\mathbf{y}} - cz_8\,\hat{\mathbf{z}} \qquad (8d) \qquad \text{O II}$$

$$\mathbf{B_{46}} = \quad \left(x_8 + \tfrac{1}{2}\right)\mathbf{a}_1 + \left(y_8 + \tfrac{1}{2}\right)\mathbf{a}_2 - \left(z_8 - \tfrac{1}{2}\right)\mathbf{a}_3 \quad = \quad a\left(x_8 + \tfrac{1}{2}\right)\hat{\mathbf{x}} + b\left(y_8 + \tfrac{1}{2}\right)\hat{\mathbf{y}} - c\left(z_8 - \tfrac{1}{2}\right)\hat{\mathbf{z}} \qquad (8d) \qquad \text{O II}$$

$$\mathbf{B_{47}} = \quad x_8\,\mathbf{a}_1 - y_8\,\mathbf{a}_2 + \left(z_8 + \tfrac{1}{2}\right)\mathbf{a}_3 \quad = \quad ax_8\,\hat{\mathbf{x}} - by_8\,\hat{\mathbf{y}} + c\left(z_8 + \tfrac{1}{2}\right)\hat{\mathbf{z}} \qquad (8d) \qquad \text{O II}$$

$$\mathbf{B_{48}} = \quad -\left(x_8 - \tfrac{1}{2}\right)\mathbf{a}_1 + \left(y_8 + \tfrac{1}{2}\right)\mathbf{a}_2 + z_8\,\mathbf{a}_3 \quad = \quad -a\left(x_8 - \tfrac{1}{2}\right)\hat{\mathbf{x}} + b\left(y_8 + \tfrac{1}{2}\right)\hat{\mathbf{y}} + cz_8\,\hat{\mathbf{z}} \qquad (8d) \qquad \text{O II}$$

$$\mathbf{B_{49}} = \quad x_9\,\mathbf{a}_1 + y_9\,\mathbf{a}_2 + z_9\,\mathbf{a}_3 \quad = \quad ax_9\,\hat{\mathbf{x}} + by_9\,\hat{\mathbf{y}} + cz_9\,\hat{\mathbf{z}} \qquad (8d) \qquad \text{O III}$$

$$\mathbf{B_{50}} = \quad -\left(x_9 - \tfrac{1}{2}\right)\mathbf{a}_1 - \left(y_9 - \tfrac{1}{2}\right)\mathbf{a}_2 + \left(z_9 + \tfrac{1}{2}\right)\mathbf{a}_3 \quad = \quad -a\left(x_9 - \tfrac{1}{2}\right)\hat{\mathbf{x}} - b\left(y_9 - \tfrac{1}{2}\right)\hat{\mathbf{y}} + c\left(z_9 + \tfrac{1}{2}\right)\hat{\mathbf{z}} \qquad (8d) \qquad \text{O III}$$

$$\mathbf{B_{51}} = \quad -x_9\,\mathbf{a}_1 + y_9\,\mathbf{a}_2 - \left(z_9 - \tfrac{1}{2}\right)\mathbf{a}_3 \quad = \quad -ax_9\,\hat{\mathbf{x}} + by_9\,\hat{\mathbf{y}} - c\left(z_9 - \tfrac{1}{2}\right)\hat{\mathbf{z}} \qquad (8d) \qquad \text{O III}$$

$$\mathbf{B_{52}} = \quad \left(x_9 + \tfrac{1}{2}\right)\mathbf{a}_1 - \left(y_9 - \tfrac{1}{2}\right)\mathbf{a}_2 - z_9\,\mathbf{a}_3 \quad = \quad a\left(x_9 + \tfrac{1}{2}\right)\hat{\mathbf{x}} - b\left(y_9 - \tfrac{1}{2}\right)\hat{\mathbf{y}} - cz_9\,\hat{\mathbf{z}} \qquad (8d) \qquad \text{O III}$$

$$\mathbf{B_{53}} = \quad -x_9\,\mathbf{a}_1 - y_9\,\mathbf{a}_2 - z_9\,\mathbf{a}_3 \quad = \quad -ax_9\,\hat{\mathbf{x}} - by_9\,\hat{\mathbf{y}} - cz_9\,\hat{\mathbf{z}} \qquad (8d) \qquad \text{O III}$$

$$\mathbf{B_{54}} = \quad \left(x_9 + \tfrac{1}{2}\right)\mathbf{a}_1 + \left(y_9 + \tfrac{1}{2}\right)\mathbf{a}_2 - \left(z_9 - \tfrac{1}{2}\right)\mathbf{a}_3 \quad = \quad a\left(x_9 + \tfrac{1}{2}\right)\hat{\mathbf{x}} + b\left(y_9 + \tfrac{1}{2}\right)\hat{\mathbf{y}} - c\left(z_9 - \tfrac{1}{2}\right)\hat{\mathbf{z}} \qquad (8d) \qquad \text{O III}$$

$$\mathbf{B_{55}} = \quad x_9\,\mathbf{a}_1 - y_9\,\mathbf{a}_2 + \left(z_9 + \tfrac{1}{2}\right)\mathbf{a}_3 \quad = \quad ax_9\,\hat{\mathbf{x}} - by_9\,\hat{\mathbf{y}} + c\left(z_9 + \tfrac{1}{2}\right)\hat{\mathbf{z}} \qquad (8d) \qquad \text{O III}$$

$$\mathbf{B_{56}} = \quad -\left(x_9 - \tfrac{1}{2}\right)\mathbf{a}_1 + \left(y_9 + \tfrac{1}{2}\right)\mathbf{a}_2 + z_9\,\mathbf{a}_3 \quad = \quad -a\left(x_9 - \tfrac{1}{2}\right)\hat{\mathbf{x}} + b\left(y_9 + \tfrac{1}{2}\right)\hat{\mathbf{y}} + cz_9\,\hat{\mathbf{z}} \qquad (8d) \qquad \text{O III}$$

$$\mathbf{B_{57}} = \quad x_{10}\,\mathbf{a}_1 + y_{10}\,\mathbf{a}_2 + z_{10}\,\mathbf{a}_3 \quad = \quad ax_{10}\,\hat{\mathbf{x}} + by_{10}\,\hat{\mathbf{y}} + cz_{10}\,\hat{\mathbf{z}} \qquad (8d) \qquad \text{O IV}$$

$$\mathbf{B_{58}} = \quad -\left(x_{10} - \tfrac{1}{2}\right)\mathbf{a}_1 - \left(y_{10} - \tfrac{1}{2}\right)\mathbf{a}_2 + \left(z_{10} + \tfrac{1}{2}\right)\mathbf{a}_3 \quad = \quad -a\left(x_{10} - \tfrac{1}{2}\right)\hat{\mathbf{x}} - b\left(y_{10} - \tfrac{1}{2}\right)\hat{\mathbf{y}} + c\left(z_{10} + \tfrac{1}{2}\right)\hat{\mathbf{z}} \qquad (8d) \qquad \text{O IV}$$

$$\mathbf{B_{59}} = \quad -x_{10}\,\mathbf{a}_1 + y_{10}\,\mathbf{a}_2 - \left(z_{10} - \tfrac{1}{2}\right)\mathbf{a}_3 \quad = \quad -ax_{10}\,\hat{\mathbf{x}} + by_{10}\,\hat{\mathbf{y}} - c\left(z_{10} - \tfrac{1}{2}\right)\hat{\mathbf{z}} \qquad (8d) \qquad \text{O IV}$$

$$\mathbf{B_{60}} = \quad \left(x_{10} + \tfrac{1}{2}\right)\mathbf{a}_1 - \left(y_{10} - \tfrac{1}{2}\right)\mathbf{a}_2 - z_{10}\,\mathbf{a}_3 \quad = \quad a\left(x_{10} + \tfrac{1}{2}\right)\hat{\mathbf{x}} - b\left(y_{10} - \tfrac{1}{2}\right)\hat{\mathbf{y}} - cz_{10}\,\hat{\mathbf{z}} \qquad (8d) \qquad \text{O IV}$$

$$\mathbf{B_{61}} = \quad -x_{10}\,\mathbf{a}_1 - y_{10}\,\mathbf{a}_2 - z_{10}\,\mathbf{a}_3 \quad = \quad -ax_{10}\,\hat{\mathbf{x}} - by_{10}\,\hat{\mathbf{y}} - cz_{10}\,\hat{\mathbf{z}} \qquad (8d) \qquad \text{O IV}$$

$$\mathbf{B_{62}} = \quad \left(x_{10} + \tfrac{1}{2}\right)\mathbf{a}_1 + \left(y_{10} + \tfrac{1}{2}\right)\mathbf{a}_2 - \left(z_{10} - \tfrac{1}{2}\right)\mathbf{a}_3 \quad = \quad a\left(x_{10} + \tfrac{1}{2}\right)\hat{\mathbf{x}} + b\left(y_{10} + \tfrac{1}{2}\right)\hat{\mathbf{y}} - c\left(z_{10} - \tfrac{1}{2}\right)\hat{\mathbf{z}} \qquad (8d) \qquad \text{O IV}$$

$$\mathbf{B_{63}} = \quad x_{10}\,\mathbf{a}_1 - y_{10}\,\mathbf{a}_2 + \left(z_{10} + \tfrac{1}{2}\right)\mathbf{a}_3 \quad = \quad ax_{10}\,\hat{\mathbf{x}} - by_{10}\,\hat{\mathbf{y}} + c\left(z_{10} + \tfrac{1}{2}\right)\hat{\mathbf{z}} \qquad (8d) \qquad \text{O IV}$$

$$\mathbf{B_{64}} = \quad -\left(x_{10} - \tfrac{1}{2}\right)\mathbf{a}_1 + \left(y_{10} + \tfrac{1}{2}\right)\mathbf{a}_2 + z_{10}\,\mathbf{a}_3 \quad = \quad -a\left(x_{10} - \tfrac{1}{2}\right)\hat{\mathbf{x}} + b\left(y_{10} + \tfrac{1}{2}\right)\hat{\mathbf{y}} + cz_{10}\,\hat{\mathbf{z}} \qquad (8d) \qquad \text{O IV}$$

$$\mathbf{B_{65}} = x_{11}\,\mathbf{a}_1 + y_{11}\,\mathbf{a}_2 + z_{11}\,\mathbf{a}_3 = ax_{11}\,\hat{\mathbf{x}} + by_{11}\,\hat{\mathbf{y}} + cz_{11}\,\hat{\mathbf{z}} \qquad (8d) \qquad \text{O V}$$

$$\mathbf{B_{66}} = -\left(x_{11}-\tfrac{1}{2}\right)\mathbf{a}_1 - \left(y_{11}-\tfrac{1}{2}\right)\mathbf{a}_2 + \left(z_{11}+\tfrac{1}{2}\right)\mathbf{a}_3 = -a\left(x_{11}-\tfrac{1}{2}\right)\hat{\mathbf{x}} - b\left(y_{11}-\tfrac{1}{2}\right)\hat{\mathbf{y}} + c\left(z_{11}+\tfrac{1}{2}\right)\hat{\mathbf{z}} \qquad (8d) \qquad \text{O V}$$

$$\mathbf{B_{67}} = -x_{11}\,\mathbf{a}_1 + y_{11}\,\mathbf{a}_2 - \left(z_{11}-\tfrac{1}{2}\right)\mathbf{a}_3 = -ax_{11}\,\hat{\mathbf{x}} + by_{11}\,\hat{\mathbf{y}} - c\left(z_{11}-\tfrac{1}{2}\right)\hat{\mathbf{z}} \qquad (8d) \qquad \text{O V}$$

$$\mathbf{B_{68}} = \left(x_{11}+\tfrac{1}{2}\right)\mathbf{a}_1 - \left(y_{11}-\tfrac{1}{2}\right)\mathbf{a}_2 - z_{11}\,\mathbf{a}_3 = a\left(x_{11}+\tfrac{1}{2}\right)\hat{\mathbf{x}} - b\left(y_{11}-\tfrac{1}{2}\right)\hat{\mathbf{y}} - cz_{11}\,\hat{\mathbf{z}} \qquad (8d) \qquad \text{O V}$$

$$\mathbf{B_{69}} = -x_{11}\,\mathbf{a}_1 - y_{11}\,\mathbf{a}_2 - z_{11}\,\mathbf{a}_3 = -ax_{11}\,\hat{\mathbf{x}} - by_{11}\,\hat{\mathbf{y}} - cz_{11}\,\hat{\mathbf{z}} \qquad (8d) \qquad \text{O V}$$

$$\mathbf{B_{70}} = \left(x_{11}+\tfrac{1}{2}\right)\mathbf{a}_1 + \left(y_{11}+\tfrac{1}{2}\right)\mathbf{a}_2 - \left(z_{11}-\tfrac{1}{2}\right)\mathbf{a}_3 = a\left(x_{11}+\tfrac{1}{2}\right)\hat{\mathbf{x}} + b\left(y_{11}+\tfrac{1}{2}\right)\hat{\mathbf{y}} - c\left(z_{11}-\tfrac{1}{2}\right)\hat{\mathbf{z}} \qquad (8d) \qquad \text{O V}$$

$$\mathbf{B_{71}} = x_{11}\,\mathbf{a}_1 - y_{11}\,\mathbf{a}_2 + \left(z_{11}+\tfrac{1}{2}\right)\mathbf{a}_3 = ax_{11}\,\hat{\mathbf{x}} - by_{11}\,\hat{\mathbf{y}} + c\left(z_{11}+\tfrac{1}{2}\right)\hat{\mathbf{z}} \qquad (8d) \qquad \text{O V}$$

$$\mathbf{B_{72}} = -\left(x_{11}-\tfrac{1}{2}\right)\mathbf{a}_1 + \left(y_{11}+\tfrac{1}{2}\right)\mathbf{a}_2 + z_{11}\,\mathbf{a}_3 = -a\left(x_{11}-\tfrac{1}{2}\right)\hat{\mathbf{x}} + b\left(y_{11}+\tfrac{1}{2}\right)\hat{\mathbf{y}} + cz_{11}\,\hat{\mathbf{z}} \qquad (8d) \qquad \text{O V}$$

References

[1] S. Uma, T. Vasilchikova, A. Sobolev, G. Raganyan, A. Sethi, H.-J. Koo, M.-H. Whangbo, I. Presniakov, I. Glazkova, A. Vasiliev, S. Streltsov, and E. Zvereva, *Synthesis and Characterization of Sodium–Iron Antimonate Na_2FeSbO_5: One-Dimensional Antiferromagnetic Chain Compound with a Spin-Glass Ground State*, Inorg. Chem. **58**, 11333–11350 (2019), doi:10.1021/acs.inorgchem.9b00212.