SbI_3S_{24} Structure: A3B24C_hR28_160_b_2b3c_a-001

This structure originally had the label `A3B24C_hR28_160_b_2b3c_a`. Calls to that address will be redirected here.

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https://aflow.org/p/8TMQ

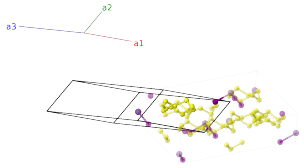
https://aflow.org/p/A3B24C_hR28_160_b_2b3c_a-001

Prototype	$I_3S_{24}Sb$
AFLOW prototype label	A3B24C_hR28_160_b_2b3c_a-001
ICSD	14200
Pearson symbol	hR28
Space group number	160
Space group symbol	$R3m$
AFLOW prototype command	`aflow --proto=A3B24C_hR28_160_b_2b3c_a-001 --params=`$a, c/a, x_1, x_2, z_2, x_3, z_3, x_4, z_4, x_5, y_5, z_5, x_6, y_6, z_6, x_7, y_7, z_7$

- Since there are three S_8 molecules in this structure, (Bjorvatten, 1963) refer to it as SbI_3:$3S_8$.
- Space group $R3m$ #160 does not fix the zero of the z-axis. Here it is set to coincide with the plane of the iodine atoms.

Rhombohedral primitive vectors

$$\mathbf{a_1} = \frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{1}{3}c\,\hat{\mathbf{z}}$$
$$\mathbf{a_2} = \frac{1}{\sqrt{3}}a\,\hat{\mathbf{y}} + \frac{1}{3}c\,\hat{\mathbf{z}}$$
$$\mathbf{a_3} = -\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{1}{3}c\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$x_1\,\mathbf{a}_1 + x_1\,\mathbf{a}_2 + x_1\,\mathbf{a}_3$	=	$cx_1\,\hat{\mathbf{z}}$	(1a)	Sb I
$\mathbf{B_2}$	=	$x_2\,\mathbf{a}_1 + x_2\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_2 - z_2)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(x_2 - z_2)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(2x_2 + z_2)\,\hat{\mathbf{z}}$	(3b)	I I
$\mathbf{B_3}$	=	$z_2\,\mathbf{a}_1 + x_2\,\mathbf{a}_2 + x_2\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(x_2 - z_2)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(x_2 - z_2)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(2x_2 + z_2)\,\hat{\mathbf{z}}$	(3b)	I I
$\mathbf{B_4}$	=	$x_2\,\mathbf{a}_1 + z_2\,\mathbf{a}_2 + x_2\,\mathbf{a}_3$	=	$-\frac{1}{\sqrt{3}}a\,(x_2 - z_2)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(2x_2 + z_2)\,\hat{\mathbf{z}}$	(3b)	I I
$\mathbf{B_5}$	=	$x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_3 - z_3)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(x_3 - z_3)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(2x_3 + z_3)\,\hat{\mathbf{z}}$	(3b)	S I

$$\mathbf{B_6} = z_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + x_3\,\mathbf{a}_3 = -\tfrac{1}{2}a\,(x_3 - z_3)\;\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{6}a\,(x_3 - z_3)\;\hat{\mathbf{y}} + \tfrac{1}{3}c\,(2x_3 + z_3)\;\hat{\mathbf{z}} \quad (3b) \quad \text{S I}$$

$$\mathbf{B_7} = x_3\,\mathbf{a}_1 + z_3\,\mathbf{a}_2 + x_3\,\mathbf{a}_3 = -\tfrac{1}{\sqrt{3}}a\,(x_3 - z_3)\;\hat{\mathbf{y}} + \tfrac{1}{3}c\,(2x_3 + z_3)\;\hat{\mathbf{z}} \quad (3b) \quad \text{S I}$$

$$\mathbf{B_8} = x_4\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 + z_4\,\mathbf{a}_3 = \tfrac{1}{2}a\,(x_4 - z_4)\;\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{6}a\,(x_4 - z_4)\;\hat{\mathbf{y}} + \tfrac{1}{3}c\,(2x_4 + z_4)\;\hat{\mathbf{z}} \quad (3b) \quad \text{S II}$$

$$\mathbf{B_9} = z_4\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 + x_4\,\mathbf{a}_3 = -\tfrac{1}{2}a\,(x_4 - z_4)\;\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{6}a\,(x_4 - z_4)\;\hat{\mathbf{y}} + \tfrac{1}{3}c\,(2x_4 + z_4)\;\hat{\mathbf{z}} \quad (3b) \quad \text{S II}$$

$$\mathbf{B_{10}} = x_4\,\mathbf{a}_1 + z_4\,\mathbf{a}_2 + x_4\,\mathbf{a}_3 = -\tfrac{1}{\sqrt{3}}a\,(x_4 - z_4)\;\hat{\mathbf{y}} + \tfrac{1}{3}c\,(2x_4 + z_4)\;\hat{\mathbf{z}} \quad (3b) \quad \text{S II}$$

$$\mathbf{B_{11}} = x_5\,\mathbf{a}_1 + y_5\,\mathbf{a}_2 + z_5\,\mathbf{a}_3 = \tfrac{1}{2}a\,(x_5 - z_5)\;\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\,(x_5 - 2y_5 + z_5)\;\hat{\mathbf{y}} + \tfrac{1}{3}c\,(x_5 + y_5 + z_5)\;\hat{\mathbf{z}} \quad (6c) \quad \text{S III}$$

$$\mathbf{B_{12}} = z_5\,\mathbf{a}_1 + x_5\,\mathbf{a}_2 + y_5\,\mathbf{a}_3 = -\tfrac{1}{2}a\,(y_5 - z_5)\;\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{6}a\,(2x_5 - y_5 - z_5)\;\hat{\mathbf{y}} + \tfrac{1}{3}c\,(x_5 + y_5 + z_5)\;\hat{\mathbf{z}} \quad (6c) \quad \text{S III}$$

$$\mathbf{B_{13}} = y_5\,\mathbf{a}_1 + z_5\,\mathbf{a}_2 + x_5\,\mathbf{a}_3 = -\tfrac{1}{2}a\,(x_5 - y_5)\;\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\,(x_5 + y_5 - 2z_5)\;\hat{\mathbf{y}} + \tfrac{1}{3}c\,(x_5 + y_5 + z_5)\;\hat{\mathbf{z}} \quad (6c) \quad \text{S III}$$

$$\mathbf{B_{14}} = z_5\,\mathbf{a}_1 + y_5\,\mathbf{a}_2 + x_5\,\mathbf{a}_3 = -\tfrac{1}{2}a\,(x_5 - z_5)\;\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\,(x_5 - 2y_5 + z_5)\;\hat{\mathbf{y}} + \tfrac{1}{3}c\,(x_5 + y_5 + z_5)\;\hat{\mathbf{z}} \quad (6c) \quad \text{S III}$$

$$\mathbf{B_{15}} = y_5\,\mathbf{a}_1 + x_5\,\mathbf{a}_2 + z_5\,\mathbf{a}_3 = \tfrac{1}{2}a\,(y_5 - z_5)\;\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{6}a\,(2x_5 - y_5 - z_5)\;\hat{\mathbf{y}} + \tfrac{1}{3}c\,(x_5 + y_5 + z_5)\;\hat{\mathbf{z}} \quad (6c) \quad \text{S III}$$

$$\mathbf{B_{16}} = x_5\,\mathbf{a}_1 + z_5\,\mathbf{a}_2 + y_5\,\mathbf{a}_3 = \tfrac{1}{2}a\,(x_5 - y_5)\;\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\,(x_5 + y_5 - 2z_5)\;\hat{\mathbf{y}} + \tfrac{1}{3}c\,(x_5 + y_5 + z_5)\;\hat{\mathbf{z}} \quad (6c) \quad \text{S III}$$

$$\mathbf{B_{17}} = x_6\,\mathbf{a}_1 + y_6\,\mathbf{a}_2 + z_6\,\mathbf{a}_3 = \tfrac{1}{2}a\,(x_6 - z_6)\;\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\,(x_6 - 2y_6 + z_6)\;\hat{\mathbf{y}} + \tfrac{1}{3}c\,(x_6 + y_6 + z_6)\;\hat{\mathbf{z}} \quad (6c) \quad \text{S IV}$$

$$\mathbf{B_{18}} = z_6\,\mathbf{a}_1 + x_6\,\mathbf{a}_2 + y_6\,\mathbf{a}_3 = -\tfrac{1}{2}a\,(y_6 - z_6)\;\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{6}a\,(2x_6 - y_6 - z_6)\;\hat{\mathbf{y}} + \tfrac{1}{3}c\,(x_6 + y_6 + z_6)\;\hat{\mathbf{z}} \quad (6c) \quad \text{S IV}$$

$$\mathbf{B_{19}} = y_6\,\mathbf{a}_1 + z_6\,\mathbf{a}_2 + x_6\,\mathbf{a}_3 = -\tfrac{1}{2}a\,(x_6 - y_6)\;\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\,(x_6 + y_6 - 2z_6)\;\hat{\mathbf{y}} + \tfrac{1}{3}c\,(x_6 + y_6 + z_6)\;\hat{\mathbf{z}} \quad (6c) \quad \text{S IV}$$

$$\mathbf{B_{20}} = z_6\,\mathbf{a}_1 + y_6\,\mathbf{a}_2 + x_6\,\mathbf{a}_3 = -\tfrac{1}{2}a\,(x_6 - z_6)\;\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\,(x_6 - 2y_6 + z_6)\;\hat{\mathbf{y}} + \tfrac{1}{3}c\,(x_6 + y_6 + z_6)\;\hat{\mathbf{z}} \quad (6c) \quad \text{S IV}$$

$$\mathbf{B_{21}} = y_6\,\mathbf{a}_1 + x_6\,\mathbf{a}_2 + z_6\,\mathbf{a}_3 = \tfrac{1}{2}a\,(y_6 - z_6)\;\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{6}a\,(2x_6 - y_6 - z_6)\;\hat{\mathbf{y}} + \tfrac{1}{3}c\,(x_6 + y_6 + z_6)\;\hat{\mathbf{z}} \quad (6c) \quad \text{S IV}$$

$$\mathbf{B_{22}} = x_6\,\mathbf{a}_1 + z_6\,\mathbf{a}_2 + y_6\,\mathbf{a}_3 = \tfrac{1}{2}a\,(x_6 - y_6)\;\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\,(x_6 + y_6 - 2z_6)\;\hat{\mathbf{y}} + \tfrac{1}{3}c\,(x_6 + y_6 + z_6)\;\hat{\mathbf{z}} \quad (6c) \quad \text{S IV}$$

$$\mathbf{B_{23}} = x_7\,\mathbf{a}_1 + y_7\,\mathbf{a}_2 + z_7\,\mathbf{a}_3 = \tfrac{1}{2}a\,(x_7 - z_7)\;\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\,(x_7 - 2y_7 + z_7)\;\hat{\mathbf{y}} + \tfrac{1}{3}c\,(x_7 + y_7 + z_7)\;\hat{\mathbf{z}} \quad (6c) \quad \text{S V}$$

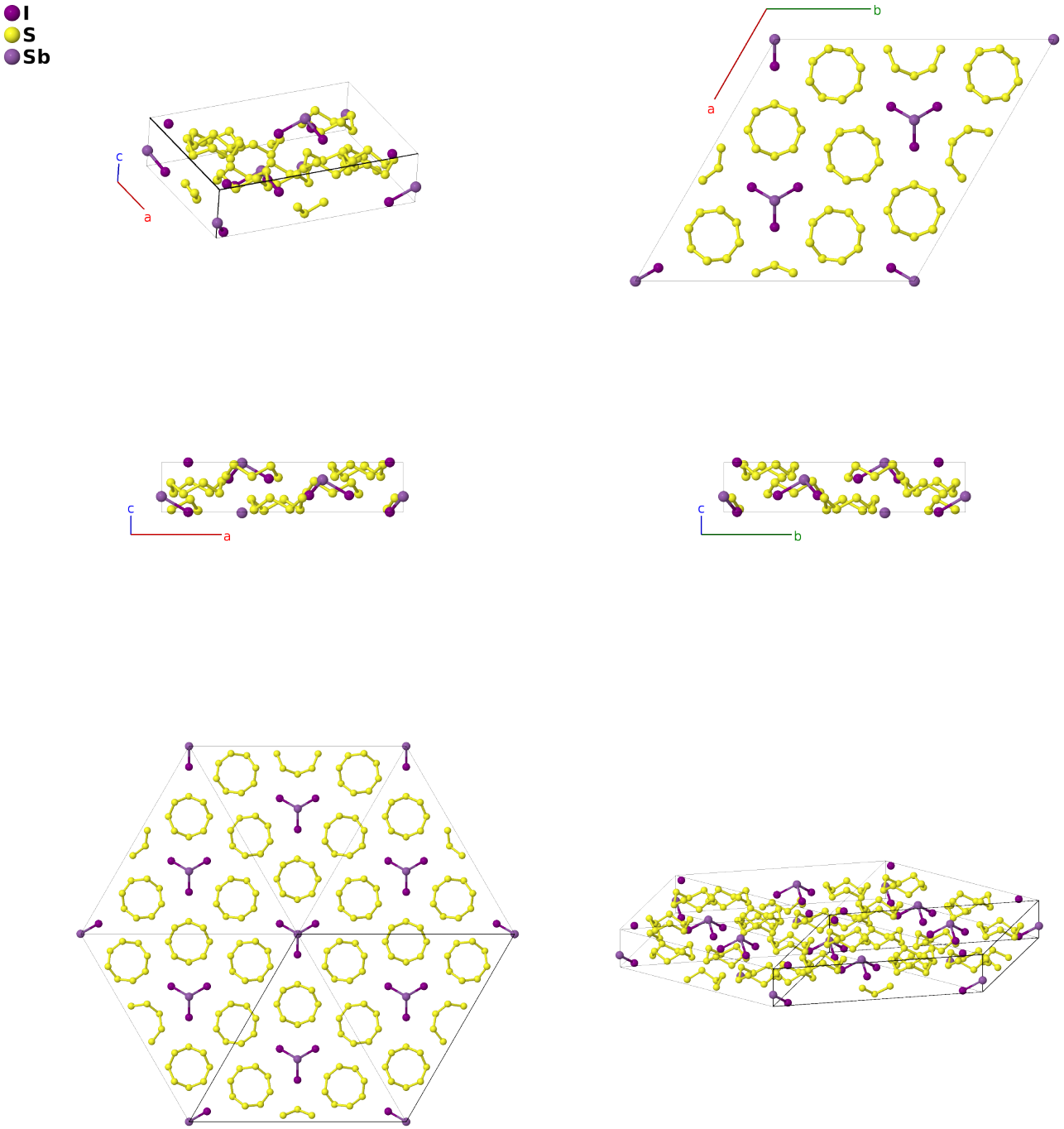
$$\mathbf{B_{24}} = z_7\,\mathbf{a}_1 + x_7\,\mathbf{a}_2 + y_7\,\mathbf{a}_3 = -\tfrac{1}{2}a\,(y_7 - z_7)\;\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{6}a\,(2x_7 - y_7 - z_7)\;\hat{\mathbf{y}} + \tfrac{1}{3}c\,(x_7 + y_7 + z_7)\;\hat{\mathbf{z}} \quad (6c) \quad \text{S V}$$

$$\mathbf{B_{25}} = y_7\,\mathbf{a}_1 + z_7\,\mathbf{a}_2 + x_7\,\mathbf{a}_3 = -\tfrac{1}{2}a\,(x_7 - y_7)\;\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\,(x_7 + y_7 - 2z_7)\;\hat{\mathbf{y}} + \tfrac{1}{3}c\,(x_7 + y_7 + z_7)\;\hat{\mathbf{z}} \quad (6c) \quad \text{S V}$$

$$\mathbf{B_{26}} = z_7\,\mathbf{a}_1 + y_7\,\mathbf{a}_2 + x_7\,\mathbf{a}_3 = -\tfrac{1}{2}a\,(x_7 - z_7)\;\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\,(x_7 - 2y_7 + z_7)\;\hat{\mathbf{y}} + \tfrac{1}{3}c\,(x_7 + y_7 + z_7)\;\hat{\mathbf{z}} \quad (6c) \quad \text{S V}$$

$$\mathbf{B_{27}} = y_7\,\mathbf{a}_1 + x_7\,\mathbf{a}_2 + z_7\,\mathbf{a}_3 = \tfrac{1}{2}a\,(y_7 - z_7)\;\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{6}a\,(2x_7 - y_7 - z_7)\;\hat{\mathbf{y}} + \tfrac{1}{3}c\,(x_7 + y_7 + z_7)\;\hat{\mathbf{z}} \quad (6c) \quad \text{S V}$$

$$\mathbf{B_{28}} = x_7\,\mathbf{a}_1 + z_7\,\mathbf{a}_2 + y_7\,\mathbf{a}_3 = \tfrac{1}{2}a\,(x_7 - y_7)\;\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\,(x_7 + y_7 - 2z_7)\;\hat{\mathbf{y}} + \tfrac{1}{3}c\,(x_7 + y_7 + z_7)\;\hat{\mathbf{z}} \quad (6c) \quad \text{S V}$$


I
S
Sb
c
a
b
a
c
a
c
b

References

[1] T. Bjorvatten, O. Hassel, and A. Lindheim, *Crystal Structure of the Addition Compound SbI_3:3S_8*, Acta Chem. Scand. **17**, 689–702 (1963), doi:10.3891/acta.chem.scand.17-0689.