Room Temperature $SmBaMn_2O_6$ Structure: AB2C6D_oP80_62_2c_2d_2c5d_d-001

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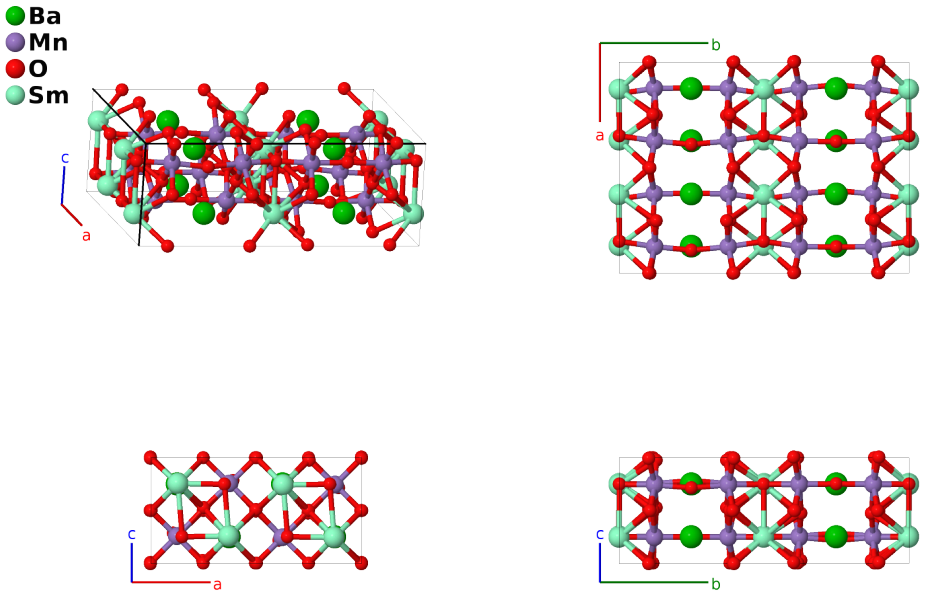
https://aflow.org/p/8TUC

https://aflow.org/p/AB2C6D_oP80_62_2c_2d_2c5d_d-001



Prototype	$BaMn_2O_6Sm$
AFLOW prototype label	AB2C6D_oP80_62_2c_2d_2c5d_d-001
ICSD	none
Pearson symbol	oP80
Space group number	62
Space group symbol	*Pnma*
AFLOW prototype command	`aflow --proto=AB2C6D_oP80_62_2c_2d_2c5d_d-001 --params=`$a, b/a, c/a, x_1, z_1, x_2, z_2, x_3, z_3, x_4, z_4, x_5, y_5, z_5, x_6, y_6, z_6, x_7, y_7, z_7, x_8, y_8, z_8, x_9, y_9, z_9, x_{10}, y_{10}, z_{10}, x_{11}, y_{11}, z_{11}, x_{12}, y_{12}, z_{12}$

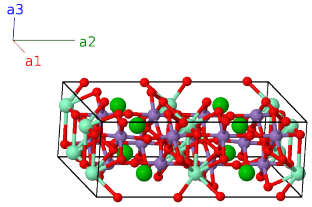
- $SmBaMn_2O_6$ undergoes several structural and magnetic phase transitions with changing temperature (Sagayama, 2014; Chen, 2019):
  - Below 190K the structure is in a polar orthorhombic phase with space group $Pmc2_1$ #26.
  - Between 190K and 362 K the structure is in a non-polar orthorhombic phase with space group *Pnma* #62 (this structure).
  - Above 362 K the structure is in quadrupled perovskite orthorhombic phase with space group *Cmmm* #65.

– In the high temperature phase the samarium and barium sites may be disordered, in which case the system is in the cubic perovskite ($E2_1$) structure.

- Here we use the structural information from (Sagayama, 2019) at 300K. They give two possible structures: The first has the samarium atoms on the (4c) sites and barium atoms on an (8d) site. The second, shown here, has barium atoms on the (4c) sites and samarium on an (8d) site.
- (Sagayama, 2019) give the structure of this phase in the *Pnam* setting of space group #62. We used FINDSYM to transform this into the standard *Pnma* setting.

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)	Ba 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)	Ba 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)	Ba 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)	Ba 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)	Ba 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)	Ba 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)	Ba 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)	Ba 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)	O I
$\mathbf{B_{10}}$	=	$-\left(x_3 - \frac{1}{2}\right)\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 + \left(z_3 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_3 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} + c\left(z_3 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4c)	O I
$\mathbf{B_{11}}$	=	$-x_3\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} - cz_3\,\hat{\mathbf{z}}$	(4c)	O I
$\mathbf{B_{12}}$	=	$\left(x_3 + \frac{1}{2}\right)\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 - \left(z_3 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(x_3 + \frac{1}{2}\right)\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} - c\left(z_3 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4c)	O I
$\mathbf{B_{13}}$	=	$x_4\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(4c)	O II
$\mathbf{B_{14}}$	=	$-\left(x_4 - \frac{1}{2}\right)\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 + \left(z_4 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_4 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} + c\left(z_4 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4c)	O II
$\mathbf{B_{15}}$	=	$-x_4\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 - z_4\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$	(4c)	O II
$\mathbf{B_{16}}$	=	$\left(x_4 + \frac{1}{2}\right)\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 - \left(z_4 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(x_4 + \frac{1}{2}\right)\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} - c\left(z_4 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4c)	O 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)	Mn I
$\mathbf{B_{18}}$	=	$-\left(x_5 - \frac{1}{2}\right)\,\mathbf{a}_1 - y_5\,\mathbf{a}_2 + \left(z_5 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_5 - \frac{1}{2}\right)\,\hat{\mathbf{x}} - by_5\,\hat{\mathbf{y}} + c\left(z_5 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8d)	Mn I
$\mathbf{B_{19}}$	=	$-x_5\,\mathbf{a}_1 + \left(y_5 + \frac{1}{2}\right)\,\mathbf{a}_2 - z_5\,\mathbf{a}_3$	=	$-ax_5\,\hat{\mathbf{x}} + b\left(y_5 + \frac{1}{2}\right)\,\hat{\mathbf{y}} - cz_5\,\hat{\mathbf{z}}$	(8d)	Mn I

$$\mathbf{B_{20}} = \left(x_5+\tfrac{1}{2}\right)\mathbf{a}_1 - \left(y_5-\tfrac{1}{2}\right)\mathbf{a}_2 - \left(z_5-\tfrac{1}{2}\right)\mathbf{a}_3 = a\left(x_5+\tfrac{1}{2}\right)\hat{\mathbf{x}} - b\left(y_5-\tfrac{1}{2}\right)\hat{\mathbf{y}} - c\left(z_5-\tfrac{1}{2}\right)\hat{\mathbf{z}} \quad (8d) \quad \text{Mn I}$$

$$\mathbf{B_{21}} = -x_5\,\mathbf{a}_1 - y_5\,\mathbf{a}_2 - z_5\,\mathbf{a}_3 = -ax_5\,\hat{\mathbf{x}} - by_5\,\hat{\mathbf{y}} - cz_5\,\hat{\mathbf{z}} \quad (8d) \quad \text{Mn I}$$

$$\mathbf{B_{22}} = \left(x_5+\tfrac{1}{2}\right)\mathbf{a}_1 + y_5\,\mathbf{a}_2 - \left(z_5-\tfrac{1}{2}\right)\mathbf{a}_3 = a\left(x_5+\tfrac{1}{2}\right)\hat{\mathbf{x}} + by_5\,\hat{\mathbf{y}} - c\left(z_5-\tfrac{1}{2}\right)\hat{\mathbf{z}} \quad (8d) \quad \text{Mn I}$$

$$\mathbf{B_{23}} = x_5\,\mathbf{a}_1 - \left(y_5-\tfrac{1}{2}\right)\mathbf{a}_2 + z_5\,\mathbf{a}_3 = ax_5\,\hat{\mathbf{x}} - b\left(y_5-\tfrac{1}{2}\right)\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}} \quad (8d) \quad \text{Mn I}$$

$$\mathbf{B_{24}} = -\left(x_5-\tfrac{1}{2}\right)\mathbf{a}_1 + \left(y_5+\tfrac{1}{2}\right)\mathbf{a}_2 + \left(z_5+\tfrac{1}{2}\right)\mathbf{a}_3 = -a\left(x_5-\tfrac{1}{2}\right)\hat{\mathbf{x}} + b\left(y_5+\tfrac{1}{2}\right)\hat{\mathbf{y}} + c\left(z_5+\tfrac{1}{2}\right)\hat{\mathbf{z}} \quad (8d) \quad \text{Mn I}$$

$$\mathbf{B_{25}} = x_6\,\mathbf{a}_1 + y_6\,\mathbf{a}_2 + z_6\,\mathbf{a}_3 = ax_6\,\hat{\mathbf{x}} + by_6\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}} \quad (8d) \quad \text{Mn II}$$

$$\mathbf{B_{26}} = -\left(x_6-\tfrac{1}{2}\right)\mathbf{a}_1 - y_6\,\mathbf{a}_2 + \left(z_6+\tfrac{1}{2}\right)\mathbf{a}_3 = -a\left(x_6-\tfrac{1}{2}\right)\hat{\mathbf{x}} - by_6\,\hat{\mathbf{y}} + c\left(z_6+\tfrac{1}{2}\right)\hat{\mathbf{z}} \quad (8d) \quad \text{Mn II}$$

$$\mathbf{B_{27}} = -x_6\,\mathbf{a}_1 + \left(y_6+\tfrac{1}{2}\right)\mathbf{a}_2 - z_6\,\mathbf{a}_3 = -ax_6\,\hat{\mathbf{x}} + b\left(y_6+\tfrac{1}{2}\right)\hat{\mathbf{y}} - cz_6\,\hat{\mathbf{z}} \quad (8d) \quad \text{Mn II}$$

$$\mathbf{B_{28}} = \left(x_6+\tfrac{1}{2}\right)\mathbf{a}_1 - \left(y_6-\tfrac{1}{2}\right)\mathbf{a}_2 - \left(z_6-\tfrac{1}{2}\right)\mathbf{a}_3 = a\left(x_6+\tfrac{1}{2}\right)\hat{\mathbf{x}} - b\left(y_6-\tfrac{1}{2}\right)\hat{\mathbf{y}} - c\left(z_6-\tfrac{1}{2}\right)\hat{\mathbf{z}} \quad (8d) \quad \text{Mn II}$$

$$\mathbf{B_{29}} = -x_6\,\mathbf{a}_1 - y_6\,\mathbf{a}_2 - z_6\,\mathbf{a}_3 = -ax_6\,\hat{\mathbf{x}} - by_6\,\hat{\mathbf{y}} - cz_6\,\hat{\mathbf{z}} \quad (8d) \quad \text{Mn II}$$

$$\mathbf{B_{30}} = \left(x_6+\tfrac{1}{2}\right)\mathbf{a}_1 + y_6\,\mathbf{a}_2 - \left(z_6-\tfrac{1}{2}\right)\mathbf{a}_3 = a\left(x_6+\tfrac{1}{2}\right)\hat{\mathbf{x}} + by_6\,\hat{\mathbf{y}} - c\left(z_6-\tfrac{1}{2}\right)\hat{\mathbf{z}} \quad (8d) \quad \text{Mn II}$$

$$\mathbf{B_{31}} = x_6\,\mathbf{a}_1 - \left(y_6-\tfrac{1}{2}\right)\mathbf{a}_2 + z_6\,\mathbf{a}_3 = ax_6\,\hat{\mathbf{x}} - b\left(y_6-\tfrac{1}{2}\right)\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}} \quad (8d) \quad \text{Mn II}$$

$$\mathbf{B_{32}} = -\left(x_6-\tfrac{1}{2}\right)\mathbf{a}_1 + \left(y_6+\tfrac{1}{2}\right)\mathbf{a}_2 + \left(z_6+\tfrac{1}{2}\right)\mathbf{a}_3 = -a\left(x_6-\tfrac{1}{2}\right)\hat{\mathbf{x}} + b\left(y_6+\tfrac{1}{2}\right)\hat{\mathbf{y}} + c\left(z_6+\tfrac{1}{2}\right)\hat{\mathbf{z}} \quad (8d) \quad \text{Mn II}$$

$$\mathbf{B_{33}} = x_7\,\mathbf{a}_1 + y_7\,\mathbf{a}_2 + z_7\,\mathbf{a}_3 = ax_7\,\hat{\mathbf{x}} + by_7\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}} \quad (8d) \quad \text{O III}$$

$$\mathbf{B_{34}} = -\left(x_7-\tfrac{1}{2}\right)\mathbf{a}_1 - y_7\,\mathbf{a}_2 + \left(z_7+\tfrac{1}{2}\right)\mathbf{a}_3 = -a\left(x_7-\tfrac{1}{2}\right)\hat{\mathbf{x}} - by_7\,\hat{\mathbf{y}} + c\left(z_7+\tfrac{1}{2}\right)\hat{\mathbf{z}} \quad (8d) \quad \text{O III}$$

$$\mathbf{B_{35}} = -x_7\,\mathbf{a}_1 + \left(y_7+\tfrac{1}{2}\right)\mathbf{a}_2 - z_7\,\mathbf{a}_3 = -ax_7\,\hat{\mathbf{x}} + b\left(y_7+\tfrac{1}{2}\right)\hat{\mathbf{y}} - cz_7\,\hat{\mathbf{z}} \quad (8d) \quad \text{O III}$$

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

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

$$\mathbf{B_{38}} = \left(x_7+\tfrac{1}{2}\right)\mathbf{a}_1 + y_7\,\mathbf{a}_2 - \left(z_7-\tfrac{1}{2}\right)\mathbf{a}_3 = a\left(x_7+\tfrac{1}{2}\right)\hat{\mathbf{x}} + by_7\,\hat{\mathbf{y}} - c\left(z_7-\tfrac{1}{2}\right)\hat{\mathbf{z}} \quad (8d) \quad \text{O III}$$

$$\mathbf{B_{39}} = x_7\,\mathbf{a}_1 - \left(y_7-\tfrac{1}{2}\right)\mathbf{a}_2 + z_7\,\mathbf{a}_3 = ax_7\,\hat{\mathbf{x}} - b\left(y_7-\tfrac{1}{2}\right)\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}} \quad (8d) \quad \text{O III}$$

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

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

$$\mathbf{B_{42}} = -\left(x_8-\tfrac{1}{2}\right)\mathbf{a}_1 - y_8\,\mathbf{a}_2 + \left(z_8+\tfrac{1}{2}\right)\mathbf{a}_3 = -a\left(x_8-\tfrac{1}{2}\right)\hat{\mathbf{x}} - by_8\,\hat{\mathbf{y}} + c\left(z_8+\tfrac{1}{2}\right)\hat{\mathbf{z}} \quad (8d) \quad \text{O IV}$$

$$\mathbf{B_{43}} = -x_8\,\mathbf{a}_1 + \left(y_8+\tfrac{1}{2}\right)\mathbf{a}_2 - z_8\,\mathbf{a}_3 = -ax_8\,\hat{\mathbf{x}} + b\left(y_8+\tfrac{1}{2}\right)\hat{\mathbf{y}} - cz_8\,\hat{\mathbf{z}} \quad (8d) \quad \text{O IV}$$

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

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

$$\mathbf{B_{46}} = \left(x_8+\tfrac{1}{2}\right)\mathbf{a}_1 + y_8\,\mathbf{a}_2 - \left(z_8-\tfrac{1}{2}\right)\mathbf{a}_3 = a\left(x_8+\tfrac{1}{2}\right)\hat{\mathbf{x}} + by_8\,\hat{\mathbf{y}} - c\left(z_8-\tfrac{1}{2}\right)\hat{\mathbf{z}} \quad (8d) \quad \text{O IV}$$

$$\mathbf{B_{47}} = x_8\,\mathbf{a}_1 - \left(y_8-\tfrac{1}{2}\right)\mathbf{a}_2 + z_8\,\mathbf{a}_3 = ax_8\,\hat{\mathbf{x}} - b\left(y_8-\tfrac{1}{2}\right)\hat{\mathbf{y}} + cz_8\,\hat{\mathbf{z}} \quad (8d) \quad \text{O IV}$$

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

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

$$\mathbf{B_{50}} = -\left(x_9-\tfrac{1}{2}\right)\mathbf{a}_1 - y_9\,\mathbf{a}_2 + \left(z_9+\tfrac{1}{2}\right)\mathbf{a}_3 = -a\left(x_9-\tfrac{1}{2}\right)\hat{\mathbf{x}} - by_9\,\hat{\mathbf{y}} + c\left(z_9+\tfrac{1}{2}\right)\hat{\mathbf{z}} \quad (8d) \quad \text{O V}$$

$$\mathbf{B_{51}} = -x_9\,\mathbf{a}_1 + \left(y_9+\tfrac{1}{2}\right)\mathbf{a}_2 - z_9\,\mathbf{a}_3 = -ax_9\,\hat{\mathbf{x}} + b\left(y_9+\tfrac{1}{2}\right)\hat{\mathbf{y}} - cz_9\,\hat{\mathbf{z}} \quad (8d) \quad \text{O V}$$

$\mathbf{B_{52}}$	=	$\left(x_9+\frac{1}{2}\right)\mathbf{a}_1-\left(y_9-\frac{1}{2}\right)\mathbf{a}_2-\left(z_9-\frac{1}{2}\right)\mathbf{a}_3$	=	$a\left(x_9+\frac{1}{2}\right)\hat{\mathbf{x}}-b\left(y_9-\frac{1}{2}\right)\hat{\mathbf{y}}-c\left(z_9-\frac{1}{2}\right)\hat{\mathbf{z}}$	(8d)	O V
$\mathbf{B_{53}}$	=	$-x_9\,\mathbf{a}_1-y_9\,\mathbf{a}_2-z_9\,\mathbf{a}_3$	=	$-ax_9\,\hat{\mathbf{x}}-by_9\,\hat{\mathbf{y}}-cz_9\,\hat{\mathbf{z}}$	(8d)	O V
$\mathbf{B_{54}}$	=	$\left(x_9+\frac{1}{2}\right)\mathbf{a}_1+y_9\,\mathbf{a}_2-\left(z_9-\frac{1}{2}\right)\mathbf{a}_3$	=	$a\left(x_9+\frac{1}{2}\right)\hat{\mathbf{x}}+by_9\,\hat{\mathbf{y}}-c\left(z_9-\frac{1}{2}\right)\hat{\mathbf{z}}$	(8d)	O V
$\mathbf{B_{55}}$	=	$x_9\,\mathbf{a}_1-\left(y_9-\frac{1}{2}\right)\mathbf{a}_2+z_9\,\mathbf{a}_3$	=	$ax_9\,\hat{\mathbf{x}}-b\left(y_9-\frac{1}{2}\right)\hat{\mathbf{y}}+cz_9\,\hat{\mathbf{z}}$	(8d)	O V
$\mathbf{B_{56}}$	=	$-\left(x_9-\frac{1}{2}\right)\mathbf{a}_1+\left(y_9+\frac{1}{2}\right)\mathbf{a}_2+\left(z_9+\frac{1}{2}\right)\mathbf{a}_3$	=	$-a\left(x_9-\frac{1}{2}\right)\hat{\mathbf{x}}+b\left(y_9+\frac{1}{2}\right)\hat{\mathbf{y}}+c\left(z_9+\frac{1}{2}\right)\hat{\mathbf{z}}$	(8d)	O V
$\mathbf{B_{57}}$	=	$x_{10}\,\mathbf{a}_1+y_{10}\,\mathbf{a}_2+z_{10}\,\mathbf{a}_3$	=	$ax_{10}\,\hat{\mathbf{x}}+by_{10}\,\hat{\mathbf{y}}+cz_{10}\,\hat{\mathbf{z}}$	(8d)	O VI
$\mathbf{B_{58}}$	=	$-\left(x_{10}-\frac{1}{2}\right)\mathbf{a}_1-y_{10}\,\mathbf{a}_2+\left(z_{10}+\frac{1}{2}\right)\mathbf{a}_3$	=	$-a\left(x_{10}-\frac{1}{2}\right)\hat{\mathbf{x}}-by_{10}\,\hat{\mathbf{y}}+c\left(z_{10}+\frac{1}{2}\right)\hat{\mathbf{z}}$	(8d)	O VI
$\mathbf{B_{59}}$	=	$-x_{10}\,\mathbf{a}_1+\left(y_{10}+\frac{1}{2}\right)\mathbf{a}_2-z_{10}\,\mathbf{a}_3$	=	$-ax_{10}\,\hat{\mathbf{x}}+b\left(y_{10}+\frac{1}{2}\right)\hat{\mathbf{y}}-cz_{10}\,\hat{\mathbf{z}}$	(8d)	O VI
$\mathbf{B_{60}}$	=	$\left(x_{10}+\frac{1}{2}\right)\mathbf{a}_1-\left(y_{10}-\frac{1}{2}\right)\mathbf{a}_2-\left(z_{10}-\frac{1}{2}\right)\mathbf{a}_3$	=	$a\left(x_{10}+\frac{1}{2}\right)\hat{\mathbf{x}}-b\left(y_{10}-\frac{1}{2}\right)\hat{\mathbf{y}}-c\left(z_{10}-\frac{1}{2}\right)\hat{\mathbf{z}}$	(8d)	O VI
$\mathbf{B_{61}}$	=	$-x_{10}\,\mathbf{a}_1-y_{10}\,\mathbf{a}_2-z_{10}\,\mathbf{a}_3$	=	$-ax_{10}\,\hat{\mathbf{x}}-by_{10}\,\hat{\mathbf{y}}-cz_{10}\,\hat{\mathbf{z}}$	(8d)	O VI
$\mathbf{B_{62}}$	=	$\left(x_{10}+\frac{1}{2}\right)\mathbf{a}_1+y_{10}\,\mathbf{a}_2-\left(z_{10}-\frac{1}{2}\right)\mathbf{a}_3$	=	$a\left(x_{10}+\frac{1}{2}\right)\hat{\mathbf{x}}+by_{10}\,\hat{\mathbf{y}}-c\left(z_{10}-\frac{1}{2}\right)\hat{\mathbf{z}}$	(8d)	O VI
$\mathbf{B_{63}}$	=	$x_{10}\,\mathbf{a}_1-\left(y_{10}-\frac{1}{2}\right)\mathbf{a}_2+z_{10}\,\mathbf{a}_3$	=	$ax_{10}\,\hat{\mathbf{x}}-b\left(y_{10}-\frac{1}{2}\right)\hat{\mathbf{y}}+cz_{10}\,\hat{\mathbf{z}}$	(8d)	O VI
$\mathbf{B_{64}}$	=	$-\left(x_{10}-\frac{1}{2}\right)\mathbf{a}_1+\left(y_{10}+\frac{1}{2}\right)\mathbf{a}_2+\left(z_{10}+\frac{1}{2}\right)\mathbf{a}_3$	=	$-a\left(x_{10}-\frac{1}{2}\right)\hat{\mathbf{x}}+b\left(y_{10}+\frac{1}{2}\right)\hat{\mathbf{y}}+c\left(z_{10}+\frac{1}{2}\right)\hat{\mathbf{z}}$	(8d)	O VI
$\mathbf{B_{65}}$	=	$x_{11}\,\mathbf{a}_1+y_{11}\,\mathbf{a}_2+z_{11}\,\mathbf{a}_3$	=	$ax_{11}\,\hat{\mathbf{x}}+by_{11}\,\hat{\mathbf{y}}+cz_{11}\,\hat{\mathbf{z}}$	(8d)	O VII
$\mathbf{B_{66}}$	=	$-\left(x_{11}-\frac{1}{2}\right)\mathbf{a}_1-y_{11}\,\mathbf{a}_2+\left(z_{11}+\frac{1}{2}\right)\mathbf{a}_3$	=	$-a\left(x_{11}-\frac{1}{2}\right)\hat{\mathbf{x}}-by_{11}\,\hat{\mathbf{y}}+c\left(z_{11}+\frac{1}{2}\right)\hat{\mathbf{z}}$	(8d)	O VII
$\mathbf{B_{67}}$	=	$-x_{11}\,\mathbf{a}_1+\left(y_{11}+\frac{1}{2}\right)\mathbf{a}_2-z_{11}\,\mathbf{a}_3$	=	$-ax_{11}\,\hat{\mathbf{x}}+b\left(y_{11}+\frac{1}{2}\right)\hat{\mathbf{y}}-cz_{11}\,\hat{\mathbf{z}}$	(8d)	O VII
$\mathbf{B_{68}}$	=	$\left(x_{11}+\frac{1}{2}\right)\mathbf{a}_1-\left(y_{11}-\frac{1}{2}\right)\mathbf{a}_2-\left(z_{11}-\frac{1}{2}\right)\mathbf{a}_3$	=	$a\left(x_{11}+\frac{1}{2}\right)\hat{\mathbf{x}}-b\left(y_{11}-\frac{1}{2}\right)\hat{\mathbf{y}}-c\left(z_{11}-\frac{1}{2}\right)\hat{\mathbf{z}}$	(8d)	O VII
$\mathbf{B_{69}}$	=	$-x_{11}\,\mathbf{a}_1-y_{11}\,\mathbf{a}_2-z_{11}\,\mathbf{a}_3$	=	$-ax_{11}\,\hat{\mathbf{x}}-by_{11}\,\hat{\mathbf{y}}-cz_{11}\,\hat{\mathbf{z}}$	(8d)	O VII
$\mathbf{B_{70}}$	=	$\left(x_{11}+\frac{1}{2}\right)\mathbf{a}_1+y_{11}\,\mathbf{a}_2-\left(z_{11}-\frac{1}{2}\right)\mathbf{a}_3$	=	$a\left(x_{11}+\frac{1}{2}\right)\hat{\mathbf{x}}+by_{11}\,\hat{\mathbf{y}}-c\left(z_{11}-\frac{1}{2}\right)\hat{\mathbf{z}}$	(8d)	O VII
$\mathbf{B_{71}}$	=	$x_{11}\,\mathbf{a}_1-\left(y_{11}-\frac{1}{2}\right)\mathbf{a}_2+z_{11}\,\mathbf{a}_3$	=	$ax_{11}\,\hat{\mathbf{x}}-b\left(y_{11}-\frac{1}{2}\right)\hat{\mathbf{y}}+cz_{11}\,\hat{\mathbf{z}}$	(8d)	O VII
$\mathbf{B_{72}}$	=	$-\left(x_{11}-\frac{1}{2}\right)\mathbf{a}_1+\left(y_{11}+\frac{1}{2}\right)\mathbf{a}_2+\left(z_{11}+\frac{1}{2}\right)\mathbf{a}_3$	=	$-a\left(x_{11}-\frac{1}{2}\right)\hat{\mathbf{x}}+b\left(y_{11}+\frac{1}{2}\right)\hat{\mathbf{y}}+c\left(z_{11}+\frac{1}{2}\right)\hat{\mathbf{z}}$	(8d)	O VII
$\mathbf{B_{73}}$	=	$x_{12}\,\mathbf{a}_1+y_{12}\,\mathbf{a}_2+z_{12}\,\mathbf{a}_3$	=	$ax_{12}\,\hat{\mathbf{x}}+by_{12}\,\hat{\mathbf{y}}+cz_{12}\,\hat{\mathbf{z}}$	(8d)	Sm I
$\mathbf{B_{74}}$	=	$-\left(x_{12}-\frac{1}{2}\right)\mathbf{a}_1-y_{12}\,\mathbf{a}_2+\left(z_{12}+\frac{1}{2}\right)\mathbf{a}_3$	=	$-a\left(x_{12}-\frac{1}{2}\right)\hat{\mathbf{x}}-by_{12}\,\hat{\mathbf{y}}+c\left(z_{12}+\frac{1}{2}\right)\hat{\mathbf{z}}$	(8d)	Sm I
$\mathbf{B_{75}}$	=	$-x_{12}\,\mathbf{a}_1+\left(y_{12}+\frac{1}{2}\right)\mathbf{a}_2-z_{12}\,\mathbf{a}_3$	=	$-ax_{12}\,\hat{\mathbf{x}}+b\left(y_{12}+\frac{1}{2}\right)\hat{\mathbf{y}}-cz_{12}\,\hat{\mathbf{z}}$	(8d)	Sm I
$\mathbf{B_{76}}$	=	$\left(x_{12}+\frac{1}{2}\right)\mathbf{a}_1-\left(y_{12}-\frac{1}{2}\right)\mathbf{a}_2-\left(z_{12}-\frac{1}{2}\right)\mathbf{a}_3$	=	$a\left(x_{12}+\frac{1}{2}\right)\hat{\mathbf{x}}-b\left(y_{12}-\frac{1}{2}\right)\hat{\mathbf{y}}-c\left(z_{12}-\frac{1}{2}\right)\hat{\mathbf{z}}$	(8d)	Sm I
$\mathbf{B_{77}}$	=	$-x_{12}\,\mathbf{a}_1-y_{12}\,\mathbf{a}_2-z_{12}\,\mathbf{a}_3$	=	$-ax_{12}\,\hat{\mathbf{x}}-by_{12}\,\hat{\mathbf{y}}-cz_{12}\,\hat{\mathbf{z}}$	(8d)	Sm I
$\mathbf{B_{78}}$	=	$\left(x_{12}+\frac{1}{2}\right)\mathbf{a}_1+y_{12}\,\mathbf{a}_2-\left(z_{12}-\frac{1}{2}\right)\mathbf{a}_3$	=	$a\left(x_{12}+\frac{1}{2}\right)\hat{\mathbf{x}}+by_{12}\,\hat{\mathbf{y}}-c\left(z_{12}-\frac{1}{2}\right)\hat{\mathbf{z}}$	(8d)	Sm I
$\mathbf{B_{79}}$	=	$x_{12}\,\mathbf{a}_1-\left(y_{12}-\frac{1}{2}\right)\mathbf{a}_2+z_{12}\,\mathbf{a}_3$	=	$ax_{12}\,\hat{\mathbf{x}}-b\left(y_{12}-\frac{1}{2}\right)\hat{\mathbf{y}}+cz_{12}\,\hat{\mathbf{z}}$	(8d)	Sm I
$\mathbf{B_{80}}$	=	$-\left(x_{12}-\frac{1}{2}\right)\mathbf{a}_1+\left(y_{12}+\frac{1}{2}\right)\mathbf{a}_2+\left(z_{12}+\frac{1}{2}\right)\mathbf{a}_3$	=	$-a\left(x_{12}-\frac{1}{2}\right)\hat{\mathbf{x}}+b\left(y_{12}+\frac{1}{2}\right)\hat{\mathbf{y}}+c\left(z_{12}+\frac{1}{2}\right)\hat{\mathbf{z}}$	(8d)	Sm I

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