MoP_3SiO_{11} (Rhombohedral Model) Structure: AB11C3D_hR64_167_c_be3f_f_c-001

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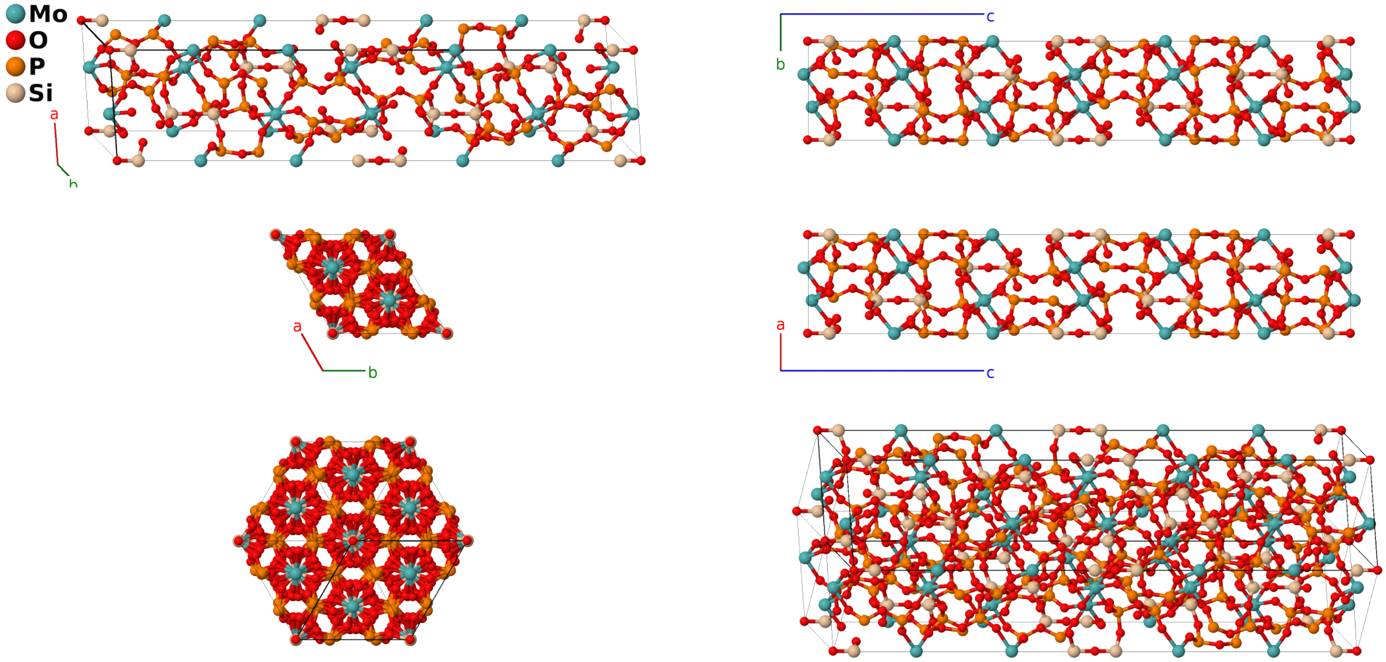
https://aflow.org/p/A76C

https://aflow.org/p/AB11C3D_hR64_167_c_be3f_f_c-001



Prototype	$MoO_{11}P_3Si$
AFLOW prototype label	AB11C3D_hR64_167_c_be3f_f_c-001
ICSD	45564
Pearson symbol	hR64
Space group number	167
Space group symbol	$R\bar{3}c$
AFLOW prototype command	`aflow --proto=AB11C3D_hR64_167_c_be3f_f_c-001` `--params=`$a, c/a, x_2, x_3, x_4, x_5, y_5, z_5, x_6, y_6, z_6, x_7, y_7, z_7, x_8, y_8, z_8$

- (Leclaire, 1987) originally proposed that MoP_3SiO_{11} was in a monoclinic structure. Later, (Badrtdinov, 2021) placed the compound in the rhombohedral $R\bar{3}c$ #167 space group as shown here. When we allow a 0.1Å uncertainty in the atomic positions the monoclinic structure reduces to the rhombohedral structure. Given this ambiguity we retain both structures in the library.

- (Badrtdinov, 2021) place the O-I atom in this structure at the (2a) Wyckoff position, however the coordinates they give are for the (2b) site. This makes the oxygen part of two PO_4 tetrahedra, rather than leaving it isolated, so we prefer the (2b) site. The (2b) site can also be derived from the monoclinic structure.

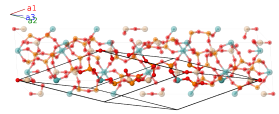
- Hexagonal settings of this structure can be obtained with the option `--hex`.

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
$\mathbf{B_1}$	=	0	=	0	(2b)	O I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}c\,\hat{\mathbf{z}}$	(2b)	O I
$\mathbf{B_3}$	=	$x_2\,\mathbf{a}_1 + x_2\,\mathbf{a}_2 + x_2\,\mathbf{a}_3$	=	$cx_2\,\hat{\mathbf{z}}$	(4c)	Mo I
$\mathbf{B_4}$	=	$-\left(x_2 - \frac{1}{2}\right)\,\mathbf{a}_1 - \left(x_2 - \frac{1}{2}\right)\,\mathbf{a}_2 - \left(x_2 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-c\left(x_2 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4c)	Mo I
$\mathbf{B_5}$	=	$-x_2\,\mathbf{a}_1 - x_2\,\mathbf{a}_2 - x_2\,\mathbf{a}_3$	=	$-cx_2\,\hat{\mathbf{z}}$	(4c)	Mo I
$\mathbf{B_6}$	=	$\left(x_2 + \frac{1}{2}\right)\,\mathbf{a}_1 + \left(x_2 + \frac{1}{2}\right)\,\mathbf{a}_2 + \left(x_2 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$c\left(x_2 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4c)	Mo I
$\mathbf{B_7}$	=	$x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + x_3\,\mathbf{a}_3$	=	$cx_3\,\hat{\mathbf{z}}$	(4c)	Si I
$\mathbf{B_8}$	=	$-\left(x_3 - \frac{1}{2}\right)\,\mathbf{a}_1 - \left(x_3 - \frac{1}{2}\right)\,\mathbf{a}_2 - \left(x_3 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-c\left(x_3 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4c)	Si I
$\mathbf{B_9}$	=	$-x_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 - x_3\,\mathbf{a}_3$	=	$-cx_3\,\hat{\mathbf{z}}$	(4c)	Si I
$\mathbf{B_{10}}$	=	$\left(x_3 + \frac{1}{2}\right)\,\mathbf{a}_1 + \left(x_3 + \frac{1}{2}\right)\,\mathbf{a}_2 + \left(x_3 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$c\left(x_3 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4c)	Si I
$\mathbf{B_{11}}$	=	$x_4\,\mathbf{a}_1 - \left(x_4 - \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{8}a\left(4x_4 - 1\right)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{8}a\left(4x_4 - 1\right)\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(6e)	O II
$\mathbf{B_{12}}$	=	$\frac{1}{4}\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 - \left(x_4 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{8}a\left(4x_4 - 1\right)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{8}a\left(4x_4 - 1\right)\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(6e)	O II
$\mathbf{B_{13}}$	=	$-\left(x_4 - \frac{1}{2}\right)\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + x_4\,\mathbf{a}_3$	=	$-a\left(x_4 - \frac{1}{4}\right)\,\hat{\mathbf{x}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(6e)	O II
$\mathbf{B_{14}}$	=	$-x_4\,\mathbf{a}_1 + \left(x_4 + \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$-\frac{1}{8}a\left(4x_4 + 3\right)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{24}a\left(12x_4 + 1\right)\,\hat{\mathbf{y}} + \frac{5}{12}c\,\hat{\mathbf{z}}$	(6e)	O II
$\mathbf{B_{15}}$	=	$\frac{3}{4}\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 + \left(x_4 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\frac{1}{8}a\left(4x_4 - 1\right)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{24}a\left(12x_4 + 5\right)\,\hat{\mathbf{y}} + \frac{5}{12}c\,\hat{\mathbf{z}}$	(6e)	O II
$\mathbf{B_{16}}$	=	$\left(x_4 + \frac{1}{2}\right)\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 - x_4\,\mathbf{a}_3$	=	$a\left(x_4 + \frac{1}{4}\right)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{5}{12}c\,\hat{\mathbf{z}}$	(6e)	O II
$\mathbf{B_{17}}$	=	$x_5\,\mathbf{a}_1 + y_5\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$\frac{1}{2}a\left(x_5 - z_5\right)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\left(x_5 - 2y_5 + z_5\right)\,\hat{\mathbf{y}} + \frac{1}{3}c\left(x_5 + y_5 + z_5\right)\,\hat{\mathbf{z}}$	(12f)	O III
$\mathbf{B_{18}}$	=	$z_5\,\mathbf{a}_1 + x_5\,\mathbf{a}_2 + y_5\,\mathbf{a}_3$	=	$-\frac{1}{2}a\left(y_5 - z_5\right)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\left(2x_5 - y_5 - z_5\right)\,\hat{\mathbf{y}} + \frac{1}{3}c\left(x_5 + y_5 + z_5\right)\,\hat{\mathbf{z}}$	(12f)	O III
$\mathbf{B_{19}}$	=	$y_5\,\mathbf{a}_1 + z_5\,\mathbf{a}_2 + x_5\,\mathbf{a}_3$	=	$-\frac{1}{2}a\left(x_5 - y_5\right)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\left(x_5 + y_5 - 2z_5\right)\,\hat{\mathbf{y}} + \frac{1}{3}c\left(x_5 + y_5 + z_5\right)\,\hat{\mathbf{z}}$	(12f)	O III
$\mathbf{B_{20}}$	=	$-\left(z_5 - \frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_5 - \frac{1}{2}\right)\,\mathbf{a}_2 - \left(x_5 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\left(x_5 - z_5\right)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\left(x_5 - 2y_5 + z_5\right)\,\hat{\mathbf{y}} - \frac{1}{6}c\left(2x_5 + 2y_5 + 2z_5 - 3\right)\,\hat{\mathbf{z}}$	(12f)	O III
$\mathbf{B_{21}}$	=	$-\left(y_5 - \frac{1}{2}\right)\,\mathbf{a}_1 - \left(x_5 - \frac{1}{2}\right)\,\mathbf{a}_2 - \left(z_5 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\frac{1}{2}a\left(y_5 - z_5\right)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\left(2x_5 - y_5 - z_5\right)\,\hat{\mathbf{y}} - \frac{1}{6}c\left(2x_5 + 2y_5 + 2z_5 - 3\right)\,\hat{\mathbf{z}}$	(12f)	O III
$\mathbf{B_{22}}$	=	$-\left(x_5 - \frac{1}{2}\right)\,\mathbf{a}_1 - \left(z_5 - \frac{1}{2}\right)\,\mathbf{a}_2 - \left(y_5 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\frac{1}{2}a\left(x_5 - y_5\right)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\left(x_5 + y_5 - 2z_5\right)\,\hat{\mathbf{y}} - \frac{1}{6}c\left(2x_5 + 2y_5 + 2z_5 - 3\right)\,\hat{\mathbf{z}}$	(12f)	O III
$\mathbf{B_{23}}$	=	$-x_5\,\mathbf{a}_1 - y_5\,\mathbf{a}_2 - z_5\,\mathbf{a}_3$	=	$-\frac{1}{2}a\left(x_5 - z_5\right)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\left(x_5 - 2y_5 + z_5\right)\,\hat{\mathbf{y}} - \frac{1}{3}c\left(x_5 + y_5 + z_5\right)\,\hat{\mathbf{z}}$	(12f)	O III

$\mathbf{B_{24}}$	=	$-z_5\,\mathbf{a}_1 - x_5\,\mathbf{a}_2 - y_5\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(y_5 - z_5)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,(2x_5 - y_5 - z_5)\,\hat{\mathbf{y}} - \frac{1}{3}c\,(x_5 + y_5 + z_5)\,\hat{\mathbf{z}}$	(12f)	O III
$\mathbf{B_{25}}$	=	$-y_5\,\mathbf{a}_1 - z_5\,\mathbf{a}_2 - x_5\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_5 - y_5)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(x_5 + y_5 - 2z_5)\,\hat{\mathbf{y}} - \frac{1}{3}c\,(x_5 + y_5 + z_5)\,\hat{\mathbf{z}}$	(12f)	O III
$\mathbf{B_{26}}$	=	$\left(z_5 + \frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_5 + \frac{1}{2}\right)\,\mathbf{a}_2 + \left(x_5 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(x_5 - z_5)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,(x_5 - 2y_5 + z_5)\,\hat{\mathbf{y}} + \frac{1}{6}c\,(2x_5 + 2y_5 + 2z_5 + 3)\,\hat{\mathbf{z}}$	(12f)	O III
$\mathbf{B_{27}}$	=	$\left(y_5 + \frac{1}{2}\right)\,\mathbf{a}_1 + \left(x_5 + \frac{1}{2}\right)\,\mathbf{a}_2 + \left(z_5 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(y_5 - z_5)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(2x_5 - y_5 - z_5)\,\hat{\mathbf{y}} + \frac{1}{6}c\,(2x_5 + 2y_5 + 2z_5 + 3)\,\hat{\mathbf{z}}$	(12f)	O III
$\mathbf{B_{28}}$	=	$\left(x_5 + \frac{1}{2}\right)\,\mathbf{a}_1 + \left(z_5 + \frac{1}{2}\right)\,\mathbf{a}_2 + \left(y_5 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_5 - y_5)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,(x_5 + y_5 - 2z_5)\,\hat{\mathbf{y}} + \frac{1}{6}c\,(2x_5 + 2y_5 + 2z_5 + 3)\,\hat{\mathbf{z}}$	(12f)	O III
$\mathbf{B_{29}}$	=	$x_6\,\mathbf{a}_1 + y_6\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_6 - z_6)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,(x_6 - 2y_6 + z_6)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(x_6 + y_6 + z_6)\,\hat{\mathbf{z}}$	(12f)	O IV
$\mathbf{B_{30}}$	=	$z_6\,\mathbf{a}_1 + x_6\,\mathbf{a}_2 + y_6\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(y_6 - z_6)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(2x_6 - y_6 - z_6)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(x_6 + y_6 + z_6)\,\hat{\mathbf{z}}$	(12f)	O IV
$\mathbf{B_{31}}$	=	$y_6\,\mathbf{a}_1 + z_6\,\mathbf{a}_2 + x_6\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(x_6 - y_6)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,(x_6 + y_6 - 2z_6)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(x_6 + y_6 + z_6)\,\hat{\mathbf{z}}$	(12f)	O IV
$\mathbf{B_{32}}$	=	$-\left(z_6 - \frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_6 - \frac{1}{2}\right)\,\mathbf{a}_2 - \left(x_6 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_6 - z_6)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(x_6 - 2y_6 + z_6)\,\hat{\mathbf{y}} - \frac{1}{6}c\,(2x_6 + 2y_6 + 2z_6 - 3)\,\hat{\mathbf{z}}$	(12f)	O IV
$\mathbf{B_{33}}$	=	$-\left(y_6 - \frac{1}{2}\right)\,\mathbf{a}_1 - \left(x_6 - \frac{1}{2}\right)\,\mathbf{a}_2 - \left(z_6 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(y_6 - z_6)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,(2x_6 - y_6 - z_6)\,\hat{\mathbf{y}} - \frac{1}{6}c\,(2x_6 + 2y_6 + 2z_6 - 3)\,\hat{\mathbf{z}}$	(12f)	O IV
$\mathbf{B_{34}}$	=	$-\left(x_6 - \frac{1}{2}\right)\,\mathbf{a}_1 - \left(z_6 - \frac{1}{2}\right)\,\mathbf{a}_2 - \left(y_6 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(x_6 - y_6)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(x_6 + y_6 - 2z_6)\,\hat{\mathbf{y}} - \frac{1}{6}c\,(2x_6 + 2y_6 + 2z_6 - 3)\,\hat{\mathbf{z}}$	(12f)	O IV
$\mathbf{B_{35}}$	=	$-x_6\,\mathbf{a}_1 - y_6\,\mathbf{a}_2 - z_6\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(x_6 - z_6)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(x_6 - 2y_6 + z_6)\,\hat{\mathbf{y}} - \frac{1}{3}c\,(x_6 + y_6 + z_6)\,\hat{\mathbf{z}}$	(12f)	O IV
$\mathbf{B_{36}}$	=	$-z_6\,\mathbf{a}_1 - x_6\,\mathbf{a}_2 - y_6\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(y_6 - z_6)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,(2x_6 - y_6 - z_6)\,\hat{\mathbf{y}} - \frac{1}{3}c\,(x_6 + y_6 + z_6)\,\hat{\mathbf{z}}$	(12f)	O IV
$\mathbf{B_{37}}$	=	$-y_6\,\mathbf{a}_1 - z_6\,\mathbf{a}_2 - x_6\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_6 - y_6)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(x_6 + y_6 - 2z_6)\,\hat{\mathbf{y}} - \frac{1}{3}c\,(x_6 + y_6 + z_6)\,\hat{\mathbf{z}}$	(12f)	O IV
$\mathbf{B_{38}}$	=	$\left(z_6 + \frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_6 + \frac{1}{2}\right)\,\mathbf{a}_2 + \left(x_6 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(x_6 - z_6)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,(x_6 - 2y_6 + z_6)\,\hat{\mathbf{y}} + \frac{1}{6}c\,(2x_6 + 2y_6 + 2z_6 + 3)\,\hat{\mathbf{z}}$	(12f)	O IV
$\mathbf{B_{39}}$	=	$\left(y_6 + \frac{1}{2}\right)\,\mathbf{a}_1 + \left(x_6 + \frac{1}{2}\right)\,\mathbf{a}_2 + \left(z_6 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(y_6 - z_6)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(2x_6 - y_6 - z_6)\,\hat{\mathbf{y}} + \frac{1}{6}c\,(2x_6 + 2y_6 + 2z_6 + 3)\,\hat{\mathbf{z}}$	(12f)	O IV
$\mathbf{B_{40}}$	=	$\left(x_6 + \frac{1}{2}\right)\,\mathbf{a}_1 + \left(z_6 + \frac{1}{2}\right)\,\mathbf{a}_2 + \left(y_6 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_6 - y_6)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,(x_6 + y_6 - 2z_6)\,\hat{\mathbf{y}} + \frac{1}{6}c\,(2x_6 + 2y_6 + 2z_6 + 3)\,\hat{\mathbf{z}}$	(12f)	O IV
$\mathbf{B_{41}}$	=	$x_7\,\mathbf{a}_1 + y_7\,\mathbf{a}_2 + z_7\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_7 - z_7)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,(x_7 - 2y_7 + z_7)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(x_7 + y_7 + z_7)\,\hat{\mathbf{z}}$	(12f)	O V
$\mathbf{B_{42}}$	=	$z_7\,\mathbf{a}_1 + x_7\,\mathbf{a}_2 + y_7\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(y_7 - z_7)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(2x_7 - y_7 - z_7)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(x_7 + y_7 + z_7)\,\hat{\mathbf{z}}$	(12f)	O V
$\mathbf{B_{43}}$	=	$y_7\,\mathbf{a}_1 + z_7\,\mathbf{a}_2 + x_7\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(x_7 - y_7)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,(x_7 + y_7 - 2z_7)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(x_7 + y_7 + z_7)\,\hat{\mathbf{z}}$	(12f)	O V
$\mathbf{B_{44}}$	=	$-\left(z_7 - \frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_7 - \frac{1}{2}\right)\,\mathbf{a}_2 - \left(x_7 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_7 - z_7)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(x_7 - 2y_7 + z_7)\,\hat{\mathbf{y}} - \frac{1}{6}c\,(2x_7 + 2y_7 + 2z_7 - 3)\,\hat{\mathbf{z}}$	(12f)	O V
$\mathbf{B_{45}}$	=	$-\left(y_7 - \frac{1}{2}\right)\,\mathbf{a}_1 - \left(x_7 - \frac{1}{2}\right)\,\mathbf{a}_2 - \left(z_7 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(y_7 - z_7)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,(2x_7 - y_7 - z_7)\,\hat{\mathbf{y}} - \frac{1}{6}c\,(2x_7 + 2y_7 + 2z_7 - 3)\,\hat{\mathbf{z}}$	(12f)	O V
$\mathbf{B_{46}}$	=	$-\left(x_7 - \frac{1}{2}\right)\,\mathbf{a}_1 - \left(z_7 - \frac{1}{2}\right)\,\mathbf{a}_2 - \left(y_7 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(x_7 - y_7)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(x_7 + y_7 - 2z_7)\,\hat{\mathbf{y}} - \frac{1}{6}c\,(2x_7 + 2y_7 + 2z_7 - 3)\,\hat{\mathbf{z}}$	(12f)	O V

$\mathbf{B_{47}}$	=	$-x_7\,\mathbf{a}_1 - y_7\,\mathbf{a}_2 - z_7\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(x_7 - z_7)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(x_7 - 2y_7 + z_7)\,\hat{\mathbf{y}} - \frac{1}{3}c\,(x_7 + y_7 + z_7)\,\hat{\mathbf{z}}$	(12f)	O V
$\mathbf{B_{48}}$	=	$-z_7\,\mathbf{a}_1 - x_7\,\mathbf{a}_2 - y_7\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(y_7 - z_7)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,(2x_7 - y_7 - z_7)\,\hat{\mathbf{y}} - \frac{1}{3}c\,(x_7 + y_7 + z_7)\,\hat{\mathbf{z}}$	(12f)	O V
$\mathbf{B_{49}}$	=	$-y_7\,\mathbf{a}_1 - z_7\,\mathbf{a}_2 - x_7\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_7 - y_7)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(x_7 + y_7 - 2z_7)\,\hat{\mathbf{y}} - \frac{1}{3}c\,(x_7 + y_7 + z_7)\,\hat{\mathbf{z}}$	(12f)	O V
$\mathbf{B_{50}}$	=	$\left(z_7 + \frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_7 + \frac{1}{2}\right)\,\mathbf{a}_2 + \left(x_7 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(x_7 - z_7)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,(x_7 - 2y_7 + z_7)\,\hat{\mathbf{y}} + \frac{1}{6}c\,(2x_7 + 2y_7 + 2z_7 + 3)\,\hat{\mathbf{z}}$	(12f)	O V
$\mathbf{B_{51}}$	=	$\left(y_7 + \frac{1}{2}\right)\,\mathbf{a}_1 + \left(x_7 + \frac{1}{2}\right)\,\mathbf{a}_2 + \left(z_7 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(y_7 - z_7)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(2x_7 - y_7 - z_7)\,\hat{\mathbf{y}} + \frac{1}{6}c\,(2x_7 + 2y_7 + 2z_7 + 3)\,\hat{\mathbf{z}}$	(12f)	O V
$\mathbf{B_{52}}$	=	$\left(x_7 + \frac{1}{2}\right)\,\mathbf{a}_1 + \left(z_7 + \frac{1}{2}\right)\,\mathbf{a}_2 + \left(y_7 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_7 - y_7)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,(x_7 + y_7 - 2z_7)\,\hat{\mathbf{y}} + \frac{1}{6}c\,(2x_7 + 2y_7 + 2z_7 + 3)\,\hat{\mathbf{z}}$	(12f)	O V
$\mathbf{B_{53}}$	=	$x_8\,\mathbf{a}_1 + y_8\,\mathbf{a}_2 + z_8\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_8 - z_8)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,(x_8 - 2y_8 + z_8)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(x_8 + y_8 + z_8)\,\hat{\mathbf{z}}$	(12f)	P I
$\mathbf{B_{54}}$	=	$z_8\,\mathbf{a}_1 + x_8\,\mathbf{a}_2 + y_8\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(y_8 - z_8)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(2x_8 - y_8 - z_8)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(x_8 + y_8 + z_8)\,\hat{\mathbf{z}}$	(12f)	P I
$\mathbf{B_{55}}$	=	$y_8\,\mathbf{a}_1 + z_8\,\mathbf{a}_2 + x_8\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(x_8 - y_8)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,(x_8 + y_8 - 2z_8)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(x_8 + y_8 + z_8)\,\hat{\mathbf{z}}$	(12f)	P I
$\mathbf{B_{56}}$	=	$-\left(z_8 - \frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_8 - \frac{1}{2}\right)\,\mathbf{a}_2 - \left(x_8 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_8 - z_8)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(x_8 - 2y_8 + z_8)\,\hat{\mathbf{y}} - \frac{1}{6}c\,(2x_8 + 2y_8 + 2z_8 - 3)\,\hat{\mathbf{z}}$	(12f)	P I
$\mathbf{B_{57}}$	=	$-\left(y_8 - \frac{1}{2}\right)\,\mathbf{a}_1 - \left(x_8 - \frac{1}{2}\right)\,\mathbf{a}_2 - \left(z_8 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(y_8 - z_8)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,(2x_8 - y_8 - z_8)\,\hat{\mathbf{y}} - \frac{1}{6}c\,(2x_8 + 2y_8 + 2z_8 - 3)\,\hat{\mathbf{z}}$	(12f)	P I
$\mathbf{B_{58}}$	=	$-\left(x_8 - \frac{1}{2}\right)\,\mathbf{a}_1 - \left(z_8 - \frac{1}{2}\right)\,\mathbf{a}_2 - \left(y_8 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(x_8 - y_8)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(x_8 + y_8 - 2z_8)\,\hat{\mathbf{y}} - \frac{1}{6}c\,(2x_8 + 2y_8 + 2z_8 - 3)\,\hat{\mathbf{z}}$	(12f)	P I
$\mathbf{B_{59}}$	=	$-x_8\,\mathbf{a}_1 - y_8\,\mathbf{a}_2 - z_8\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(x_8 - z_8)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(x_8 - 2y_8 + z_8)\,\hat{\mathbf{y}} - \frac{1}{3}c\,(x_8 + y_8 + z_8)\,\hat{\mathbf{z}}$	(12f)	P I
$\mathbf{B_{60}}$	=	$-z_8\,\mathbf{a}_1 - x_8\,\mathbf{a}_2 - y_8\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(y_8 - z_8)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,(2x_8 - y_8 - z_8)\,\hat{\mathbf{y}} - \frac{1}{3}c\,(x_8 + y_8 + z_8)\,\hat{\mathbf{z}}$	(12f)	P I
$\mathbf{B_{61}}$	=	$-y_8\,\mathbf{a}_1 - z_8\,\mathbf{a}_2 - x_8\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_8 - y_8)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(x_8 + y_8 - 2z_8)\,\hat{\mathbf{y}} - \frac{1}{3}c\,(x_8 + y_8 + z_8)\,\hat{\mathbf{z}}$	(12f)	P I
$\mathbf{B_{62}}$	=	$\left(z_8 + \frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_8 + \frac{1}{2}\right)\,\mathbf{a}_2 + \left(x_8 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(x_8 - z_8)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,(x_8 - 2y_8 + z_8)\,\hat{\mathbf{y}} + \frac{1}{6}c\,(2x_8 + 2y_8 + 2z_8 + 3)\,\hat{\mathbf{z}}$	(12f)	P I
$\mathbf{B_{63}}$	=	$\left(y_8 + \frac{1}{2}\right)\,\mathbf{a}_1 + \left(x_8 + \frac{1}{2}\right)\,\mathbf{a}_2 + \left(z_8 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(y_8 - z_8)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(2x_8 - y_8 - z_8)\,\hat{\mathbf{y}} + \frac{1}{6}c\,(2x_8 + 2y_8 + 2z_8 + 3)\,\hat{\mathbf{z}}$	(12f)	P I
$\mathbf{B_{64}}$	=	$\left(x_8 + \frac{1}{2}\right)\,\mathbf{a}_1 + \left(z_8 + \frac{1}{2}\right)\,\mathbf{a}_2 + \left(y_8 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_8 - y_8)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,(x_8 + y_8 - 2z_8)\,\hat{\mathbf{y}} + \frac{1}{6}c\,(2x_8 + 2y_8 + 2z_8 + 3)\,\hat{\mathbf{z}}$	(12f)	P I

References

[1] D. I. Badrtdinov, L. Ding, C. Ritter, J. Hembacher, N. Ahmed, Y. Skourski, and A. A. Tsirlin, *MoP_3SiO_{11}: A 4d^3 honeycomb antiferromagnet with disconnected octahedra*, Phys. Rev. B **104**, 094428 (2021), doi:10.1103/PhysRevB.104.094428.

[2] A. Leclaire and B. Raveau, *MoP_3SiO_{11}: A silicophosphate of molybdenum(III)*, J. Solid State Chem. **71**, 283–290 (1987), doi:10.1016/0022-4596(87)90235-0.