Muscovite ($KH_2Al_3Si_3O_{12}$, $S5_1$) Structure: A2BC10D2E4_mC76_15_f_e_5f_f_2f-001

This structure previously used the label(s) `A2BC10D2E4_mC76_15_f_e_5f_f_2f`. Calls to these addresses will be redirected here.

Cite this page as:

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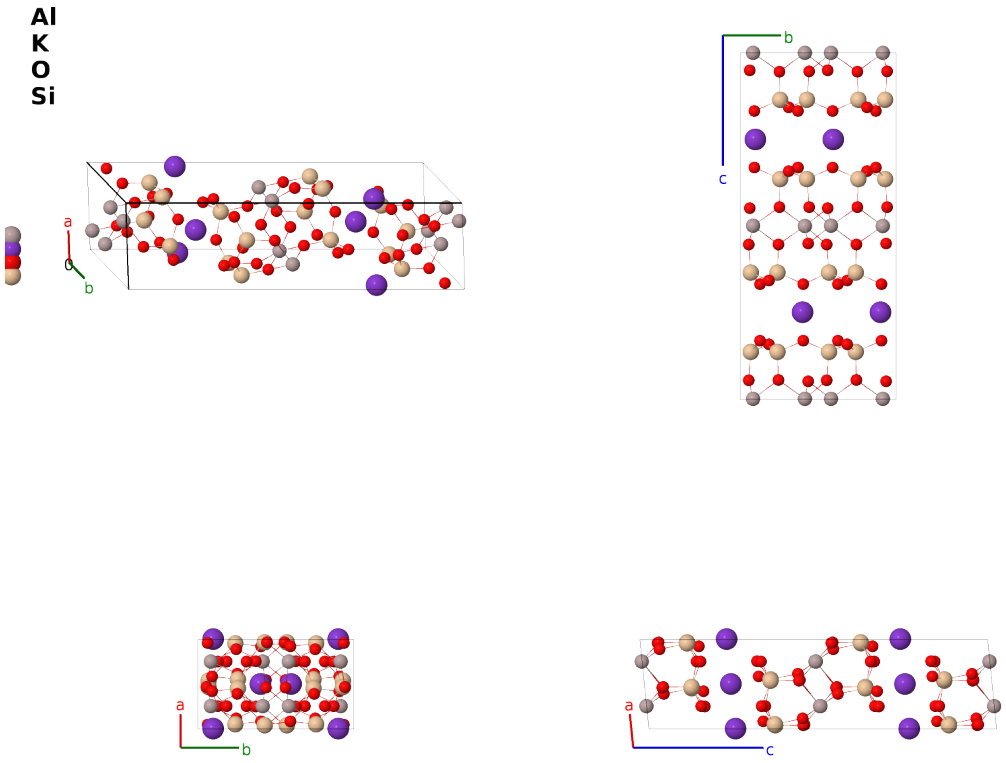
https://aflow.org/prototype-encyclopedia/8J4A

https://aflow.org/prototype-encyclopedia/A2BC10D2E4_mC76_15_f_e_5f_f_2f-001



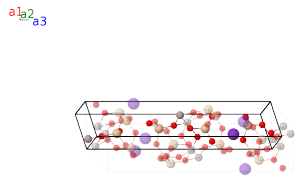
Prototype	$Al_3H_2KO_{12}Si_3$
AFLOW prototype label	A2BC10D2E4_mC76_15_f_e_5f_f_2f-001
***Strukturbericht* designation**	$S5_1$
Mineral name	muscovite
ICSD	17049
CCDC	1597544
Pearson symbol	mC76

Space group number	15
Space group symbol	$C2/c$
AFLOW prototype command	`aflow --proto=A2BC10D2E4_mC76_15_f_e_5f_f_2f-001 --params=`$a, b/a, c/a, \beta, y_1, x_2, y_2, z_2, x_3, y_3, z_3, x_4, y_4, z_4, x_5, y_5, z_5, x_6, y_6, z_6, x_7, y_7, z_7, x_8, y_8, z_8, x_9, y_9, z_9, x_{10}, y_{10}, z_{10}$

- The sites we label Si-I and Si-II are actually approximately 75% silicon and 25% aluminum, but trace elements such as manganese can appear on both sites. In addition, the potassium site (K) can be alloyed with small amounts of sodium, and the aluminum site (Al) with iron. These trace elements give muscovite a variety of colors. The sample studied by (Richardson, 1982) was pink.

Base-centered Monoclinic primitive vectors

$$\mathbf{a_1} = \frac{1}{2}a\,\hat{\mathbf{x}} - \frac{1}{2}b\,\hat{\mathbf{y}}$$
$$\mathbf{a_2} = \frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}b\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\cos\beta\,\hat{\mathbf{x}} + c\sin\beta\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$-y_1\,\mathbf{a}_1 + y_1\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{4}c\cos\beta\,\hat{\mathbf{x}} + by_1\,\hat{\mathbf{y}} + \frac{1}{4}c\sin\beta\,\hat{\mathbf{z}}$	(4e)	K I
$\mathbf{B_2}$	=	$y_1\,\mathbf{a}_1 - y_1\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{3}{4}c\cos\beta\,\hat{\mathbf{x}} - by_1\,\hat{\mathbf{y}} + \frac{3}{4}c\sin\beta\,\hat{\mathbf{z}}$	(4e)	K I
$\mathbf{B_3}$	=	$(x_2 - y_2)\,\mathbf{a}_1 + (x_2 + y_2)\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$(ax_2 + cz_2\cos\beta)\,\hat{\mathbf{x}} + by_2\,\hat{\mathbf{y}} + cz_2\sin\beta\,\hat{\mathbf{z}}$	(8f)	Al I
$\mathbf{B_4}$	=	$-(x_2 + y_2)\,\mathbf{a}_1 - (x_2 - y_2)\,\mathbf{a}_2 - \left(z_2 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\left(ax_2 + c\left(z_2 - \frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} + by_2\,\hat{\mathbf{y}} - c\left(z_2 - \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(8f)	Al I
$\mathbf{B_5}$	=	$-(x_2 - y_2)\,\mathbf{a}_1 - (x_2 + y_2)\,\mathbf{a}_2 - z_2\,\mathbf{a}_3$	=	$-(ax_2 + cz_2\cos\beta)\,\hat{\mathbf{x}} - by_2\,\hat{\mathbf{y}} - cz_2\sin\beta\,\hat{\mathbf{z}}$	(8f)	Al I
$\mathbf{B_6}$	=	$(x_2 + y_2)\,\mathbf{a}_1 + (x_2 - y_2)\,\mathbf{a}_2 + \left(z_2 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\left(ax_2 + c\left(z_2 + \frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} - by_2\,\hat{\mathbf{y}} + c\left(z_2 + \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(8f)	Al I
$\mathbf{B_7}$	=	$(x_3 - y_3)\,\mathbf{a}_1 + (x_3 + y_3)\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$(ax_3 + cz_3\cos\beta)\,\hat{\mathbf{x}} + by_3\,\hat{\mathbf{y}} + cz_3\sin\beta\,\hat{\mathbf{z}}$	(8f)	O I
$\mathbf{B_8}$	=	$-(x_3 + y_3)\,\mathbf{a}_1 - (x_3 - y_3)\,\mathbf{a}_2 - \left(z_3 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\left(ax_3 + c\left(z_3 - \frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} + by_3\,\hat{\mathbf{y}} - c\left(z_3 - \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(8f)	O I
$\mathbf{B_9}$	=	$-(x_3 - y_3)\,\mathbf{a}_1 - (x_3 + y_3)\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$	=	$-(ax_3 + cz_3\cos\beta)\,\hat{\mathbf{x}} - by_3\,\hat{\mathbf{y}} - cz_3\sin\beta\,\hat{\mathbf{z}}$	(8f)	O I
$\mathbf{B_{10}}$	=	$(x_3 + y_3)\,\mathbf{a}_1 + (x_3 - y_3)\,\mathbf{a}_2 + \left(z_3 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\left(ax_3 + c\left(z_3 + \frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} - by_3\,\hat{\mathbf{y}} + c\left(z_3 + \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(8f)	O I
$\mathbf{B_{11}}$	=	$(x_4 - y_4)\,\mathbf{a}_1 + (x_4 + y_4)\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$(ax_4 + cz_4\cos\beta)\,\hat{\mathbf{x}} + by_4\,\hat{\mathbf{y}} + cz_4\sin\beta\,\hat{\mathbf{z}}$	(8f)	O II

$$\mathbf{B_{12}} = -(x_4+y_4)\,\mathbf{a}_1-(x_4-y_4)\,\mathbf{a}_2-\left(z_4-\tfrac{1}{2}\right)\mathbf{a}_3 = -\left(ax_4+c\left(z_4-\tfrac{1}{2}\right)\cos\beta\right)\hat{\mathbf{x}}+by_4\,\hat{\mathbf{y}}-c\left(z_4-\tfrac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}} \quad (8f) \quad \text{O II}$$

$$\mathbf{B_{13}} = -(x_4-y_4)\,\mathbf{a}_1-(x_4+y_4)\,\mathbf{a}_2-z_4\,\mathbf{a}_3 = -(ax_4+cz_4\cos\beta)\,\hat{\mathbf{x}}-by_4\,\hat{\mathbf{y}}-cz_4\sin\beta\,\hat{\mathbf{z}} \quad (8f) \quad \text{O II}$$

$$\mathbf{B_{14}} = (x_4+y_4)\,\mathbf{a}_1+(x_4-y_4)\,\mathbf{a}_2+\left(z_4+\tfrac{1}{2}\right)\mathbf{a}_3 = \left(ax_4+c\left(z_4+\tfrac{1}{2}\right)\cos\beta\right)\hat{\mathbf{x}}-by_4\,\hat{\mathbf{y}}+c\left(z_4+\tfrac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}} \quad (8f) \quad \text{O II}$$

$$\mathbf{B_{15}} = (x_5-y_5)\,\mathbf{a}_1+(x_5+y_5)\,\mathbf{a}_2+z_5\,\mathbf{a}_3 = (ax_5+cz_5\cos\beta)\,\hat{\mathbf{x}}+by_5\,\hat{\mathbf{y}}+cz_5\sin\beta\,\hat{\mathbf{z}} \quad (8f) \quad \text{O III}$$

$$\mathbf{B_{16}} = -(x_5+y_5)\,\mathbf{a}_1-(x_5-y_5)\,\mathbf{a}_2-\left(z_5-\tfrac{1}{2}\right)\mathbf{a}_3 = -\left(ax_5+c\left(z_5-\tfrac{1}{2}\right)\cos\beta\right)\hat{\mathbf{x}}+by_5\,\hat{\mathbf{y}}-c\left(z_5-\tfrac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}} \quad (8f) \quad \text{O III}$$

$$\mathbf{B_{17}} = -(x_5-y_5)\,\mathbf{a}_1-(x_5+y_5)\,\mathbf{a}_2-z_5\,\mathbf{a}_3 = -(ax_5+cz_5\cos\beta)\,\hat{\mathbf{x}}-by_5\,\hat{\mathbf{y}}-cz_5\sin\beta\,\hat{\mathbf{z}} \quad (8f) \quad \text{O III}$$

$$\mathbf{B_{18}} = (x_5+y_5)\,\mathbf{a}_1+(x_5-y_5)\,\mathbf{a}_2+\left(z_5+\tfrac{1}{2}\right)\mathbf{a}_3 = \left(ax_5+c\left(z_5+\tfrac{1}{2}\right)\cos\beta\right)\hat{\mathbf{x}}-by_5\,\hat{\mathbf{y}}+c\left(z_5+\tfrac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}} \quad (8f) \quad \text{O III}$$

$$\mathbf{B_{19}} = (x_6-y_6)\,\mathbf{a}_1+(x_6+y_6)\,\mathbf{a}_2+z_6\,\mathbf{a}_3 = (ax_6+cz_6\cos\beta)\,\hat{\mathbf{x}}+by_6\,\hat{\mathbf{y}}+cz_6\sin\beta\,\hat{\mathbf{z}} \quad (8f) \quad \text{O IV}$$

$$\mathbf{B_{20}} = -(x_6+y_6)\,\mathbf{a}_1-(x_6-y_6)\,\mathbf{a}_2-\left(z_6-\tfrac{1}{2}\right)\mathbf{a}_3 = -\left(ax_6+c\left(z_6-\tfrac{1}{2}\right)\cos\beta\right)\hat{\mathbf{x}}+by_6\,\hat{\mathbf{y}}-c\left(z_6-\tfrac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}} \quad (8f) \quad \text{O IV}$$

$$\mathbf{B_{21}} = -(x_6-y_6)\,\mathbf{a}_1-(x_6+y_6)\,\mathbf{a}_2-z_6\,\mathbf{a}_3 = -(ax_6+cz_6\cos\beta)\,\hat{\mathbf{x}}-by_6\,\hat{\mathbf{y}}-cz_6\sin\beta\,\hat{\mathbf{z}} \quad (8f) \quad \text{O IV}$$

$$\mathbf{B_{22}} = (x_6+y_6)\,\mathbf{a}_1+(x_6-y_6)\,\mathbf{a}_2+\left(z_6+\tfrac{1}{2}\right)\mathbf{a}_3 = \left(ax_6+c\left(z_6+\tfrac{1}{2}\right)\cos\beta\right)\hat{\mathbf{x}}-by_6\,\hat{\mathbf{y}}+c\left(z_6+\tfrac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}} \quad (8f) \quad \text{O IV}$$

$$\mathbf{B_{23}} = (x_7-y_7)\,\mathbf{a}_1+(x_7+y_7)\,\mathbf{a}_2+z_7\,\mathbf{a}_3 = (ax_7+cz_7\cos\beta)\,\hat{\mathbf{x}}+by_7\,\hat{\mathbf{y}}+cz_7\sin\beta\,\hat{\mathbf{z}} \quad (8f) \quad \text{O V}$$

$$\mathbf{B_{24}} = -(x_7+y_7)\,\mathbf{a}_1-(x_7-y_7)\,\mathbf{a}_2-\left(z_7-\tfrac{1}{2}\right)\mathbf{a}_3 = -\left(ax_7+c\left(z_7-\tfrac{1}{2}\right)\cos\beta\right)\hat{\mathbf{x}}+by_7\,\hat{\mathbf{y}}-c\left(z_7-\tfrac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}} \quad (8f) \quad \text{O V}$$

$$\mathbf{B_{25}} = -(x_7-y_7)\,\mathbf{a}_1-(x_7+y_7)\,\mathbf{a}_2-z_7\,\mathbf{a}_3 = -(ax_7+cz_7\cos\beta)\,\hat{\mathbf{x}}-by_7\,\hat{\mathbf{y}}-cz_7\sin\beta\,\hat{\mathbf{z}} \quad (8f) \quad \text{O V}$$

$$\mathbf{B_{26}} = (x_7+y_7)\,\mathbf{a}_1+(x_7-y_7)\,\mathbf{a}_2+\left(z_7+\tfrac{1}{2}\right)\mathbf{a}_3 = \left(ax_7+c\left(z_7+\tfrac{1}{2}\right)\cos\beta\right)\hat{\mathbf{x}}-by_7\,\hat{\mathbf{y}}+c\left(z_7+\tfrac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}} \quad (8f) \quad \text{O V}$$

$$\mathbf{B_{27}} = (x_8-y_8)\,\mathbf{a}_1+(x_8+y_8)\,\mathbf{a}_2+z_8\,\mathbf{a}_3 = (ax_8+cz_8\cos\beta)\,\hat{\mathbf{x}}+by_8\,\hat{\mathbf{y}}+cz_8\sin\beta\,\hat{\mathbf{z}} \quad (8f) \quad \text{OH I}$$

$$\mathbf{B_{28}} = -(x_8+y_8)\,\mathbf{a}_1-(x_8-y_8)\,\mathbf{a}_2-\left(z_8-\tfrac{1}{2}\right)\mathbf{a}_3 = -\left(ax_8+c\left(z_8-\tfrac{1}{2}\right)\cos\beta\right)\hat{\mathbf{x}}+by_8\,\hat{\mathbf{y}}-c\left(z_8-\tfrac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}} \quad (8f) \quad \text{OH I}$$

$$\mathbf{B_{29}} = -(x_8-y_8)\,\mathbf{a}_1-(x_8+y_8)\,\mathbf{a}_2-z_8\,\mathbf{a}_3 = -(ax_8+cz_8\cos\beta)\,\hat{\mathbf{x}}-by_8\,\hat{\mathbf{y}}-cz_8\sin\beta\,\hat{\mathbf{z}} \quad (8f) \quad \text{OH I}$$

$$\mathbf{B_{30}} = (x_8+y_8)\,\mathbf{a}_1+(x_8-y_8)\,\mathbf{a}_2+\left(z_8+\tfrac{1}{2}\right)\mathbf{a}_3 = \left(ax_8+c\left(z_8+\tfrac{1}{2}\right)\cos\beta\right)\hat{\mathbf{x}}-by_8\,\hat{\mathbf{y}}+c\left(z_8+\tfrac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}} \quad (8f) \quad \text{OH I}$$

$$\mathbf{B_{31}} = (x_9-y_9)\,\mathbf{a}_1+(x_9+y_9)\,\mathbf{a}_2+z_9\,\mathbf{a}_3 = (ax_9+cz_9\cos\beta)\,\hat{\mathbf{x}}+by_9\,\hat{\mathbf{y}}+cz_9\sin\beta\,\hat{\mathbf{z}} \quad (8f) \quad \text{Si I}$$

$$\mathbf{B_{32}} = -(x_9+y_9)\,\mathbf{a}_1-(x_9-y_9)\,\mathbf{a}_2-\left(z_9-\tfrac{1}{2}\right)\mathbf{a}_3 = -\left(ax_9+c\left(z_9-\tfrac{1}{2}\right)\cos\beta\right)\hat{\mathbf{x}}+by_9\,\hat{\mathbf{y}}-c\left(z_9-\tfrac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}} \quad (8f) \quad \text{Si I}$$

$$\mathbf{B_{33}} = -(x_9-y_9)\,\mathbf{a}_1-(x_9+y_9)\,\mathbf{a}_2-z_9\,\mathbf{a}_3 = -(ax_9+cz_9\cos\beta)\,\hat{\mathbf{x}}-by_9\,\hat{\mathbf{y}}-cz_9\sin\beta\,\hat{\mathbf{z}} \quad (8f) \quad \text{Si I}$$

$$\mathbf{B_{34}} = (x_9+y_9)\,\mathbf{a}_1+(x_9-y_9)\,\mathbf{a}_2+\left(z_9+\tfrac{1}{2}\right)\mathbf{a}_3 = \left(ax_9+c\left(z_9+\tfrac{1}{2}\right)\cos\beta\right)\hat{\mathbf{x}}-by_9\,\hat{\mathbf{y}}+c\left(z_9+\tfrac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}} \quad (8f) \quad \text{Si I}$$

$\mathbf{B_{35}}$	=	$(x_{10} - y_{10})\ \mathbf{a}_1 + (x_{10} + y_{10})\ \mathbf{a}_2 + z_{10}\,\mathbf{a}_3$	=	$(ax_{10} + cz_{10}\cos\beta)\ \hat{\mathbf{x}} + by_{10}\,\hat{\mathbf{y}} + cz_{10}\sin\beta\,\hat{\mathbf{z}}$	(8f)	Si II
$\mathbf{B_{36}}$	=	$-(x_{10} + y_{10})\ \mathbf{a}_1 - (x_{10} - y_{10})\ \mathbf{a}_2 - \left(z_{10} - \frac{1}{2}\right)\ \mathbf{a}_3$	=	$-\left(ax_{10} + c\left(z_{10} - \frac{1}{2}\right)\cos\beta\right)\ \hat{\mathbf{x}} + by_{10}\,\hat{\mathbf{y}} - c\left(z_{10} - \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(8f)	Si II
$\mathbf{B_{37}}$	=	$-(x_{10} - y_{10})\ \mathbf{a}_1 - (x_{10} + y_{10})\ \mathbf{a}_2 - z_{10}\,\mathbf{a}_3$	=	$-(ax_{10} + cz_{10}\cos\beta)\ \hat{\mathbf{x}} - by_{10}\,\hat{\mathbf{y}} - cz_{10}\sin\beta\,\hat{\mathbf{z}}$	(8f)	Si II
$\mathbf{B_{38}}$	=	$(x_{10} + y_{10})\ \mathbf{a}_1 + (x_{10} - y_{10})\ \mathbf{a}_2 + \left(z_{10} + \frac{1}{2}\right)\ \mathbf{a}_3$	=	$\left(ax_{10} + c\left(z_{10} + \frac{1}{2}\right)\cos\beta\right)\ \hat{\mathbf{x}} - by_{10}\,\hat{\mathbf{y}} + c\left(z_{10} + \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(8f)	Si II

References

[1] S. M. Richardson and J. J. W. Richardson, *Crystal structure of a pink muscovite from Archer's Post, Kenya: Implications for reverse pleochroism in dioctahedral micas*, Am. Mineral. **67**, 69–75 (1982).

Found in

[1] R. T. Downs and M. Hall-Wallace, *The American Mineralogist Crystal Structure Database*, Am. Mineral. **88**, 247–250 (2003).

First cited in

D. Hicks, M. J. Mehl, M. Esters, C. Oses, O. Levy, G. L. W. Hart, C. Toher, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 3*, Comput. Mater. Sci. **199**, 110450 (2021), doi: 10.1016/j.commatsci.2021.110450.