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

This structure originally had the label `A2BC10D2E4_mC76_15_f_e_5f_f_2f`. Calls to that address will be redirected here.

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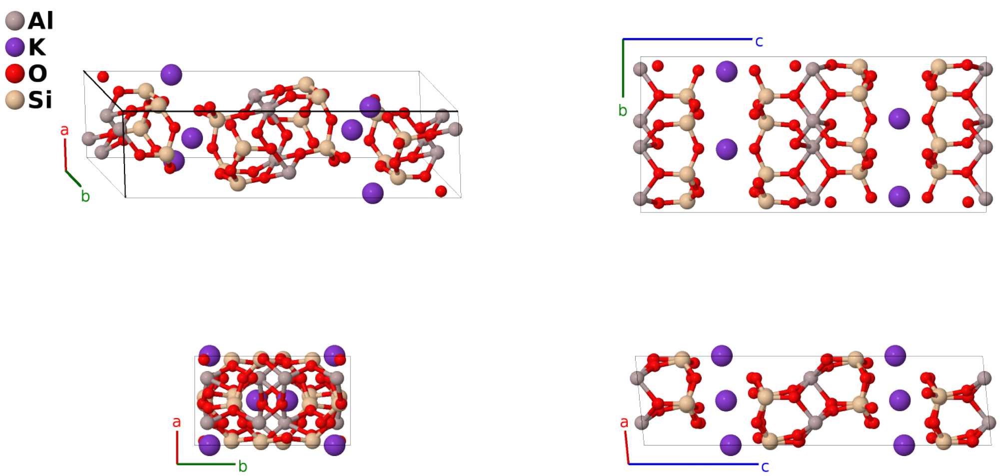
https://aflow.org/p/8J4A

https://aflow.org/p/A2BC10D2E4_mC76_15_f_e_5f_f_2f-001

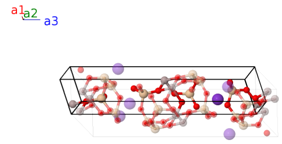


Prototype	$Al_3H_2KO_{12}Si_3$
AFLOW prototype label	A2BC10D2E4_mC76_15_f_e_5f_f_2f-001
***Strukturbericht* designation**	$S5_1$
Mineral name	muscovite
ICSD	17049
Pearson symbol	mC76
Space group number	15
Space group symbol	$C2/c$
AFLOW prototype command	`aflow --proto=A2BC10D2E4_mC76_15_f_e_5f_f_2f-001` `--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

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



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$ =	$-y_1\,\mathbf{a}_1 + y_1\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{4}c\cos\beta\,\mathbf{\hat{x}} + by_1\,\mathbf{\hat{y}} + \frac{1}{4}c\sin\beta\,\mathbf{\hat{z}}$	(4e)	K I
$\mathbf{B_2}$ =	$y_1\,\mathbf{a}_1 - y_1\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{3}{4}c\cos\beta\,\mathbf{\hat{x}} - by_1\,\mathbf{\hat{y}} + \frac{3}{4}c\sin\beta\,\mathbf{\hat{z}}$	(4e)	K I
$\mathbf{B_3}$ =	$(x_2 - y_2)\,\mathbf{a}_1 + (x_2 + y_2)\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$(ax_2 + cz_2\cos\beta)\,\mathbf{\hat{x}} + by_2\,\mathbf{\hat{y}} + cz_2\sin\beta\,\mathbf{\hat{z}}$	(8f)	Al I
$\mathbf{B_4}$ =	$-(x_2 + y_2)\,\mathbf{a}_1 - (x_2 - y_2)\,\mathbf{a}_2 - \left(z_2 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\left(ax_2 + c\left(z_2 - \frac{1}{2}\right)\cos\beta\right)\,\mathbf{\hat{x}} + by_2\,\mathbf{\hat{y}} - c\left(z_2 - \frac{1}{2}\right)\sin\beta\,\mathbf{\hat{z}}$	(8f)	Al I
$\mathbf{B_5}$ =	$-(x_2 - y_2)\,\mathbf{a}_1 - (x_2 + y_2)\,\mathbf{a}_2 - z_2\,\mathbf{a}_3$	=	$-(ax_2 + cz_2\cos\beta)\,\mathbf{\hat{x}} - by_2\,\mathbf{\hat{y}} - cz_2\sin\beta\,\mathbf{\hat{z}}$	(8f)	Al I
$\mathbf{B_6}$ =	$(x_2 + y_2)\,\mathbf{a}_1 + (x_2 - y_2)\,\mathbf{a}_2 + \left(z_2 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\left(ax_2 + c\left(z_2 + \frac{1}{2}\right)\cos\beta\right)\,\mathbf{\hat{x}} - by_2\,\mathbf{\hat{y}} + c\left(z_2 + \frac{1}{2}\right)\sin\beta\,\mathbf{\hat{z}}$	(8f)	Al I
$\mathbf{B_7}$ =	$(x_3 - y_3)\,\mathbf{a}_1 + (x_3 + y_3)\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$(ax_3 + cz_3\cos\beta)\,\mathbf{\hat{x}} + by_3\,\mathbf{\hat{y}} + cz_3\sin\beta\,\mathbf{\hat{z}}$	(8f)	O I
$\mathbf{B_8}$ =	$-(x_3 + y_3)\,\mathbf{a}_1 - (x_3 - y_3)\,\mathbf{a}_2 - \left(z_3 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\left(ax_3 + c\left(z_3 - \frac{1}{2}\right)\cos\beta\right)\,\mathbf{\hat{x}} + by_3\,\mathbf{\hat{y}} - c\left(z_3 - \frac{1}{2}\right)\sin\beta\,\mathbf{\hat{z}}$	(8f)	O I
$\mathbf{B_9}$ =	$-(x_3 - y_3)\,\mathbf{a}_1 - (x_3 + y_3)\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$	=	$-(ax_3 + cz_3\cos\beta)\,\mathbf{\hat{x}} - by_3\,\mathbf{\hat{y}} - cz_3\sin\beta\,\mathbf{\hat{z}}$	(8f)	O I
$\mathbf{B_{10}}$ =	$(x_3 + y_3)\,\mathbf{a}_1 + (x_3 - y_3)\,\mathbf{a}_2 + \left(z_3 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\left(ax_3 + c\left(z_3 + \frac{1}{2}\right)\cos\beta\right)\,\mathbf{\hat{x}} - by_3\,\mathbf{\hat{y}} + c\left(z_3 + \frac{1}{2}\right)\sin\beta\,\mathbf{\hat{z}}$	(8f)	O I
$\mathbf{B_{11}}$ =	$(x_4 - y_4)\,\mathbf{a}_1 + (x_4 + y_4)\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$(ax_4 + cz_4\cos\beta)\,\mathbf{\hat{x}} + by_4\,\mathbf{\hat{y}} + cz_4\sin\beta\,\mathbf{\hat{z}}$	(8f)	O II
$\mathbf{B_{12}}$ =	$-(x_4 + y_4)\,\mathbf{a}_1 - (x_4 - y_4)\,\mathbf{a}_2 - \left(z_4 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\left(ax_4 + c\left(z_4 - \frac{1}{2}\right)\cos\beta\right)\,\mathbf{\hat{x}} + by_4\,\mathbf{\hat{y}} - c\left(z_4 - \frac{1}{2}\right)\sin\beta\,\mathbf{\hat{z}}$	(8f)	O II
$\mathbf{B_{13}}$ =	$-(x_4 - y_4)\,\mathbf{a}_1 - (x_4 + y_4)\,\mathbf{a}_2 - z_4\,\mathbf{a}_3$	=	$-(ax_4 + cz_4\cos\beta)\,\mathbf{\hat{x}} - by_4\,\mathbf{\hat{y}} - cz_4\sin\beta\,\mathbf{\hat{z}}$	(8f)	O II
$\mathbf{B_{14}}$ =	$(x_4 + y_4)\,\mathbf{a}_1 + (x_4 - y_4)\,\mathbf{a}_2 + \left(z_4 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\left(ax_4 + c\left(z_4 + \frac{1}{2}\right)\cos\beta\right)\,\mathbf{\hat{x}} - by_4\,\mathbf{\hat{y}} + c\left(z_4 + \frac{1}{2}\right)\sin\beta\,\mathbf{\hat{z}}$	(8f)	O II
$\mathbf{B_{15}}$ =	$(x_5 - y_5)\,\mathbf{a}_1 + (x_5 + y_5)\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$(ax_5 + cz_5\cos\beta)\,\mathbf{\hat{x}} + by_5\,\mathbf{\hat{y}} + cz_5\sin\beta\,\mathbf{\hat{z}}$	(8f)	O III
$\mathbf{B_{16}}$ =	$-(x_5 + y_5)\,\mathbf{a}_1 - (x_5 - y_5)\,\mathbf{a}_2 - \left(z_5 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\left(ax_5 + c\left(z_5 - \frac{1}{2}\right)\cos\beta\right)\,\mathbf{\hat{x}} + by_5\,\mathbf{\hat{y}} - c\left(z_5 - \frac{1}{2}\right)\sin\beta\,\mathbf{\hat{z}}$	(8f)	O III
$\mathbf{B_{17}}$ =	$-(x_5 - y_5)\,\mathbf{a}_1 - (x_5 + y_5)\,\mathbf{a}_2 - z_5\,\mathbf{a}_3$	=	$-(ax_5 + cz_5\cos\beta)\,\mathbf{\hat{x}} - by_5\,\mathbf{\hat{y}} - cz_5\sin\beta\,\mathbf{\hat{z}}$	(8f)	O III
$\mathbf{B_{18}}$ =	$(x_5 + y_5)\,\mathbf{a}_1 + (x_5 - y_5)\,\mathbf{a}_2 + \left(z_5 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\left(ax_5 + c\left(z_5 + \frac{1}{2}\right)\cos\beta\right)\,\mathbf{\hat{x}} - by_5\,\mathbf{\hat{y}} + c\left(z_5 + \frac{1}{2}\right)\sin\beta\,\mathbf{\hat{z}}$	(8f)	O III

$\mathbf{B_{19}}$	=	$(x_6 - y_6)\,\mathbf{a}_1 + (x_6 + y_6)\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	=	$(ax_6 + cz_6\cos\beta)\,\hat{\mathbf{x}} + by_6\,\hat{\mathbf{y}} + cz_6\sin\beta\,\hat{\mathbf{z}}$	(8f)	O IV
$\mathbf{B_{20}}$	=	$-(x_6 + y_6)\,\mathbf{a}_1 - (x_6 - y_6)\,\mathbf{a}_2 - \left(z_6 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\left(ax_6 + c\left(z_6 - \frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} + by_6\,\hat{\mathbf{y}} - c\left(z_6 - \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(8f)	O IV
$\mathbf{B_{21}}$	=	$-(x_6 - y_6)\,\mathbf{a}_1 - (x_6 + y_6)\,\mathbf{a}_2 - z_6\,\mathbf{a}_3$	=	$-(ax_6 + cz_6\cos\beta)\,\hat{\mathbf{x}} - by_6\,\hat{\mathbf{y}} - cz_6\sin\beta\,\hat{\mathbf{z}}$	(8f)	O IV
$\mathbf{B_{22}}$	=	$(x_6 + y_6)\,\mathbf{a}_1 + (x_6 - y_6)\,\mathbf{a}_2 + \left(z_6 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\left(ax_6 + c\left(z_6 + \frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} - by_6\,\hat{\mathbf{y}} + c\left(z_6 + \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(8f)	O IV
$\mathbf{B_{23}}$	=	$(x_7 - y_7)\,\mathbf{a}_1 + (x_7 + y_7)\,\mathbf{a}_2 + z_7\,\mathbf{a}_3$	=	$(ax_7 + cz_7\cos\beta)\,\hat{\mathbf{x}} + by_7\,\hat{\mathbf{y}} + cz_7\sin\beta\,\hat{\mathbf{z}}$	(8f)	O V
$\mathbf{B_{24}}$	=	$-(x_7 + y_7)\,\mathbf{a}_1 - (x_7 - y_7)\,\mathbf{a}_2 - \left(z_7 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\left(ax_7 + c\left(z_7 - \frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} + by_7\,\hat{\mathbf{y}} - c\left(z_7 - \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(8f)	O V
$\mathbf{B_{25}}$	=	$-(x_7 - y_7)\,\mathbf{a}_1 - (x_7 + y_7)\,\mathbf{a}_2 - z_7\,\mathbf{a}_3$	=	$-(ax_7 + cz_7\cos\beta)\,\hat{\mathbf{x}} - by_7\,\hat{\mathbf{y}} - cz_7\sin\beta\,\hat{\mathbf{z}}$	(8f)	O V
$\mathbf{B_{26}}$	=	$(x_7 + y_7)\,\mathbf{a}_1 + (x_7 - y_7)\,\mathbf{a}_2 + \left(z_7 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\left(ax_7 + c\left(z_7 + \frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} - by_7\,\hat{\mathbf{y}} + c\left(z_7 + \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(8f)	O V
$\mathbf{B_{27}}$	=	$(x_8 - y_8)\,\mathbf{a}_1 + (x_8 + y_8)\,\mathbf{a}_2 + z_8\,\mathbf{a}_3$	=	$(ax_8 + cz_8\cos\beta)\,\hat{\mathbf{x}} + by_8\,\hat{\mathbf{y}} + cz_8\sin\beta\,\hat{\mathbf{z}}$	(8f)	OH I
$\mathbf{B_{28}}$	=	$-(x_8 + y_8)\,\mathbf{a}_1 - (x_8 - y_8)\,\mathbf{a}_2 - \left(z_8 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\left(ax_8 + c\left(z_8 - \frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} + by_8\,\hat{\mathbf{y}} - c\left(z_8 - \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(8f)	OH I
$\mathbf{B_{29}}$	=	$-(x_8 - y_8)\,\mathbf{a}_1 - (x_8 + y_8)\,\mathbf{a}_2 - z_8\,\mathbf{a}_3$	=	$-(ax_8 + cz_8\cos\beta)\,\hat{\mathbf{x}} - by_8\,\hat{\mathbf{y}} - cz_8\sin\beta\,\hat{\mathbf{z}}$	(8f)	OH I
$\mathbf{B_{30}}$	=	$(x_8 + y_8)\,\mathbf{a}_1 + (x_8 - y_8)\,\mathbf{a}_2 + \left(z_8 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\left(ax_8 + c\left(z_8 + \frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} - by_8\,\hat{\mathbf{y}} + c\left(z_8 + \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(8f)	OH I
$\mathbf{B_{31}}$	=	$(x_9 - y_9)\,\mathbf{a}_1 + (x_9 + y_9)\,\mathbf{a}_2 + z_9\,\mathbf{a}_3$	=	$(ax_9 + cz_9\cos\beta)\,\hat{\mathbf{x}} + by_9\,\hat{\mathbf{y}} + cz_9\sin\beta\,\hat{\mathbf{z}}$	(8f)	Si I
$\mathbf{B_{32}}$	=	$-(x_9 + y_9)\,\mathbf{a}_1 - (x_9 - y_9)\,\mathbf{a}_2 - \left(z_9 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\left(ax_9 + c\left(z_9 - \frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} + by_9\,\hat{\mathbf{y}} - c\left(z_9 - \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(8f)	Si I
$\mathbf{B_{33}}$	=	$-(x_9 - y_9)\,\mathbf{a}_1 - (x_9 + y_9)\,\mathbf{a}_2 - z_9\,\mathbf{a}_3$	=	$-(ax_9 + cz_9\cos\beta)\,\hat{\mathbf{x}} - by_9\,\hat{\mathbf{y}} - cz_9\sin\beta\,\hat{\mathbf{z}}$	(8f)	Si I
$\mathbf{B_{34}}$	=	$(x_9 + y_9)\,\mathbf{a}_1 + (x_9 - y_9)\,\mathbf{a}_2 + \left(z_9 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\left(ax_9 + c\left(z_9 + \frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} - by_9\,\hat{\mathbf{y}} + c\left(z_9 + \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(8f)	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).