Moskvinite ($Na_2KYSi_6O_{15}$) Structure: AB2C15D6E_oI100_74_e_g_e2hi2j_hj_a-001

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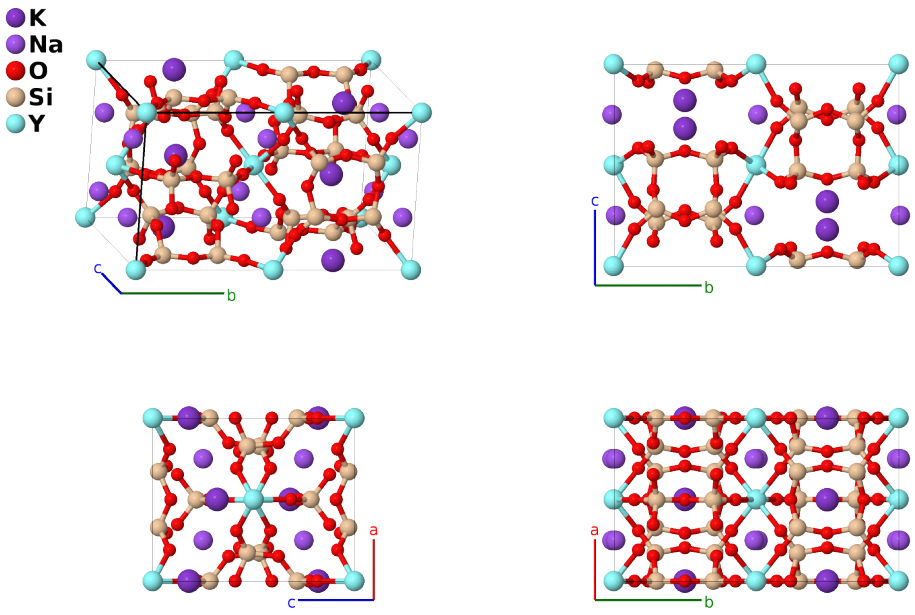
https://aflow.org/p/F0JR

https://aflow.org/p/AB2C15D6E_oI100_74_e_g_e2hi2j_hj_a-001

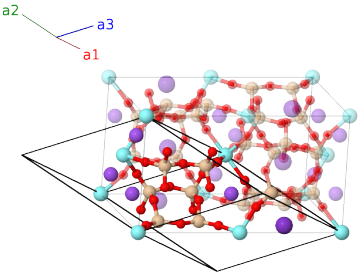


Prototype	$KNa_2O_{15}Si_6Y$
AFLOW prototype label	AB2C15D6E_oI100_74_e_g_e2hi2j_hj_a-001
Mineral name	moskvinite
ICSD	97289
Pearson symbol	oI100
Space group number	74
Space group symbol	*Imma*
AFLOW prototype command	`aflow --proto=AB2C15D6E_oI100_74_e_g_e2hi2j_hj_a-001 --params=`$a, b/a, c/a, z_2, z_3, y_4, y_5, z_5, y_6, z_6, y_7, z_7, x_8, z_8, x_9, y_9, z_9, x_{10}, y_{10}, z_{10}, x_{11}, y_{11}, z_{11}$

- This is technically named moskvinite-(Y). The yttrium on the (4a) site can be replaced rare-earth elements. The composition of this sample is actually $Na_{2.06}K_{0.95}(Y_{0.77}Dy_{0.09}Gd_{0.04}Er_{0.04}Ho_{0.02}Sm_{0.02}Nd_{0.01}Tb_{0.01})_{\Sigma 1.00}Si_6O_{15}$.
- (Sokolova, 2003) give the data for this structure in the *Ibmm* setting of space group #74. We used FINDSYM to shift this to the standard *Imma* setting. This involved rotation of the axes and shifting the Y-I atom from (1/4 1/4 1/4) to the origin.

Body-centered Orthorhombic primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(4a)	Y I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}b\,\hat{\mathbf{y}}$	(4a)	Y I
$\mathbf{B_3}$	=	$\left(z_2 + \frac{1}{4}\right)\,\mathbf{a}_1 + z_2\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{4}b\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(4e)	K I
$\mathbf{B_4}$	=	$-\left(z_2 - \frac{3}{4}\right)\,\mathbf{a}_1 - z_2\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{3}{4}b\,\hat{\mathbf{y}} - cz_2\,\hat{\mathbf{z}}$	(4e)	K I
$\mathbf{B_5}$	=	$\left(z_3 + \frac{1}{4}\right)\,\mathbf{a}_1 + z_3\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{4}b\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(4e)	O I
$\mathbf{B_6}$	=	$-\left(z_3 - \frac{3}{4}\right)\,\mathbf{a}_1 - z_3\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{3}{4}b\,\hat{\mathbf{y}} - cz_3\,\hat{\mathbf{z}}$	(4e)	O I
$\mathbf{B_7}$	=	$\left(y_4 + \frac{1}{4}\right)\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + \left(y_4 + \frac{1}{4}\right)\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + by_4\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(8g)	Na I
$\mathbf{B_8}$	=	$-\left(y_4 - \frac{3}{4}\right)\,\mathbf{a}_1 - \left(y_4 - \frac{1}{4}\right)\,\mathbf{a}_3$	=	$-\frac{1}{4}a\,\hat{\mathbf{x}} - b\left(y_4 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(8g)	Na I
$\mathbf{B_9}$	=	$-\left(y_4 - \frac{3}{4}\right)\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 - \left(y_4 - \frac{3}{4}\right)\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} - b\left(y_4 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(8g)	Na I
$\mathbf{B_{10}}$	=	$\left(y_4 + \frac{1}{4}\right)\,\mathbf{a}_1 + \left(y_4 + \frac{3}{4}\right)\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + b\left(y_4 + \frac{1}{2}\right)\,\hat{\mathbf{y}} - \frac{1}{4}c\,\hat{\mathbf{z}}$	(8g)	Na I
$\mathbf{B_{11}}$	=	$(y_5 + z_5)\,\mathbf{a}_1 + z_5\,\mathbf{a}_2 + y_5\,\mathbf{a}_3$	=	$by_5\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(8h)	O II
$\mathbf{B_{12}}$	=	$\left(-y_5 + z_5 + \frac{1}{2}\right)\,\mathbf{a}_1 + z_5\,\mathbf{a}_2 - \left(y_5 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-b\left(y_5 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(8h)	O II
$\mathbf{B_{13}}$	=	$\left(y_5 - z_5 + \frac{1}{2}\right)\,\mathbf{a}_1 - z_5\,\mathbf{a}_2 + \left(y_5 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$b\left(y_5 + \frac{1}{2}\right)\,\hat{\mathbf{y}} - cz_5\,\hat{\mathbf{z}}$	(8h)	O II
$\mathbf{B_{14}}$	=	$-\left(y_5 + z_5\right)\,\mathbf{a}_1 - z_5\,\mathbf{a}_2 - y_5\,\mathbf{a}_3$	=	$-by_5\,\hat{\mathbf{y}} - cz_5\,\hat{\mathbf{z}}$	(8h)	O II
$\mathbf{B_{15}}$	=	$(y_6 + z_6)\,\mathbf{a}_1 + z_6\,\mathbf{a}_2 + y_6\,\mathbf{a}_3$	=	$by_6\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(8h)	O III
$\mathbf{B_{16}}$	=	$\left(-y_6 + z_6 + \frac{1}{2}\right)\,\mathbf{a}_1 + z_6\,\mathbf{a}_2 - \left(y_6 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-b\left(y_6 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(8h)	O III
$\mathbf{B_{17}}$	=	$\left(y_6 - z_6 + \frac{1}{2}\right)\,\mathbf{a}_1 - z_6\,\mathbf{a}_2 + \left(y_6 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$b\left(y_6 + \frac{1}{2}\right)\,\hat{\mathbf{y}} - cz_6\,\hat{\mathbf{z}}$	(8h)	O III
$\mathbf{B_{18}}$	=	$-\left(y_6 + z_6\right)\,\mathbf{a}_1 - z_6\,\mathbf{a}_2 - y_6\,\mathbf{a}_3$	=	$-by_6\,\hat{\mathbf{y}} - cz_6\,\hat{\mathbf{z}}$	(8h)	O III
$\mathbf{B_{19}}$	=	$(y_7 + z_7)\,\mathbf{a}_1 + z_7\,\mathbf{a}_2 + y_7\,\mathbf{a}_3$	=	$by_7\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}}$	(8h)	Si I
$\mathbf{B_{20}}$	=	$\left(-y_7 + z_7 + \frac{1}{2}\right)\,\mathbf{a}_1 + z_7\,\mathbf{a}_2 - \left(y_7 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-b\left(y_7 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}}$	(8h)	Si I
$\mathbf{B_{21}}$	=	$\left(y_7 - z_7 + \frac{1}{2}\right)\,\mathbf{a}_1 - z_7\,\mathbf{a}_2 + \left(y_7 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$b\left(y_7 + \frac{1}{2}\right)\,\hat{\mathbf{y}} - cz_7\,\hat{\mathbf{z}}$	(8h)	Si I
$\mathbf{B_{22}}$	=	$-\left(y_7 + z_7\right)\,\mathbf{a}_1 - z_7\,\mathbf{a}_2 - y_7\,\mathbf{a}_3$	=	$-by_7\,\hat{\mathbf{y}} - cz_7\,\hat{\mathbf{z}}$	(8h)	Si I
$\mathbf{B_{23}}$	=	$\left(z_8 + \frac{1}{4}\right)\,\mathbf{a}_1 + (x_8 + z_8)\,\mathbf{a}_2 + \left(x_8 + \frac{1}{4}\right)\,\mathbf{a}_3$	=	$ax_8\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} + cz_8\,\hat{\mathbf{z}}$	(8i)	O IV

$\mathbf{B_{24}}$	=	$\left(z_8+\frac{1}{4}\right)\,\mathbf{a}_1-(x_8-z_8)\,\mathbf{a}_2-\left(x_8-\frac{1}{4}\right)\,\mathbf{a}_3$	=	$-ax_8\,\hat{\mathbf{x}}+\frac{1}{4}b\,\hat{\mathbf{y}}+cz_8\,\hat{\mathbf{z}}$	(8i)	O IV
$\mathbf{B_{25}}$	=	$-\left(z_8-\frac{3}{4}\right)\,\mathbf{a}_1-(x_8+z_8)\,\mathbf{a}_2-\left(x_8-\frac{3}{4}\right)\,\mathbf{a}_3$	=	$-ax_8\,\hat{\mathbf{x}}+\frac{3}{4}b\,\hat{\mathbf{y}}-cz_8\,\hat{\mathbf{z}}$	(8i)	O IV
$\mathbf{B_{26}}$	=	$-\left(z_8-\frac{3}{4}\right)\,\mathbf{a}_1+(x_8-z_8)\,\mathbf{a}_2+\left(x_8+\frac{3}{4}\right)\,\mathbf{a}_3$	=	$ax_8\,\hat{\mathbf{x}}+\frac{3}{4}b\,\hat{\mathbf{y}}-cz_8\,\hat{\mathbf{z}}$	(8i)	O IV
$\mathbf{B_{27}}$	=	$(y_9+z_9)\,\mathbf{a}_1+(x_9+z_9)\,\mathbf{a}_2+(x_9+y_9)\,\mathbf{a}_3$	=	$ax_9\,\hat{\mathbf{x}}+by_9\,\hat{\mathbf{y}}+cz_9\,\hat{\mathbf{z}}$	(16j)	O V
$\mathbf{B_{28}}$	=	$\left(-y_9+z_9+\frac{1}{2}\right)\,\mathbf{a}_1-(x_9-z_9)\,\mathbf{a}_2-\left(x_9+y_9-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_9\,\hat{\mathbf{x}}-b\left(y_9-\frac{1}{2}\right)\,\hat{\mathbf{y}}+cz_9\,\hat{\mathbf{z}}$	(16j)	O V
$\mathbf{B_{29}}$	=	$\left(y_9-z_9+\frac{1}{2}\right)\,\mathbf{a}_1-(x_9+z_9)\,\mathbf{a}_2+\left(-x_9+y_9+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_9\,\hat{\mathbf{x}}+b\left(y_9+\frac{1}{2}\right)\,\hat{\mathbf{y}}-cz_9\,\hat{\mathbf{z}}$	(16j)	O V
$\mathbf{B_{30}}$	=	$-(y_9+z_9)\,\mathbf{a}_1+(x_9-z_9)\,\mathbf{a}_2+(x_9-y_9)\,\mathbf{a}_3$	=	$ax_9\,\hat{\mathbf{x}}-by_9\,\hat{\mathbf{y}}-cz_9\,\hat{\mathbf{z}}$	(16j)	O V
$\mathbf{B_{31}}$	=	$-(y_9+z_9)\,\mathbf{a}_1-(x_9+z_9)\,\mathbf{a}_2-(x_9+y_9)\,\mathbf{a}_3$	=	$-ax_9\,\hat{\mathbf{x}}-by_9\,\hat{\mathbf{y}}-cz_9\,\hat{\mathbf{z}}$	(16j)	O V
$\mathbf{B_{32}}$	=	$\left(y_9-z_9+\frac{1}{2}\right)\,\mathbf{a}_1+(x_9-z_9)\,\mathbf{a}_2+\left(x_9+y_9+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$ax_9\,\hat{\mathbf{x}}+b\left(y_9+\frac{1}{2}\right)\,\hat{\mathbf{y}}-cz_9\,\hat{\mathbf{z}}$	(16j)	O V
$\mathbf{B_{33}}$	=	$\left(-y_9+z_9+\frac{1}{2}\right)\,\mathbf{a}_1+(x_9+z_9)\,\mathbf{a}_2+\left(x_9-y_9+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$ax_9\,\hat{\mathbf{x}}-b\left(y_9-\frac{1}{2}\right)\,\hat{\mathbf{y}}+cz_9\,\hat{\mathbf{z}}$	(16j)	O V
$\mathbf{B_{34}}$	=	$(y_9+z_9)\,\mathbf{a}_1-(x_9-z_9)\,\mathbf{a}_2-(x_9-y_9)\,\mathbf{a}_3$	=	$-ax_9\,\hat{\mathbf{x}}+by_9\,\hat{\mathbf{y}}+cz_9\,\hat{\mathbf{z}}$	(16j)	O V
$\mathbf{B_{35}}$	=	$(y_{10}+z_{10})\,\mathbf{a}_1+(x_{10}+z_{10})\,\mathbf{a}_2+(x_{10}+y_{10})\,\mathbf{a}_3$	=	$ax_{10}\,\hat{\mathbf{x}}+by_{10}\,\hat{\mathbf{y}}+cz_{10}\,\hat{\mathbf{z}}$	(16j)	O VI
$\mathbf{B_{36}}$	=	$\left(-y_{10}+z_{10}+\frac{1}{2}\right)\,\mathbf{a}_1-(x_{10}-z_{10})\,\mathbf{a}_2-\left(x_{10}+y_{10}-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_{10}\,\hat{\mathbf{x}}-b\left(y_{10}-\frac{1}{2}\right)\,\hat{\mathbf{y}}+cz_{10}\,\hat{\mathbf{z}}$	(16j)	O VI
$\mathbf{B_{37}}$	=	$\left(y_{10}-z_{10}+\frac{1}{2}\right)\,\mathbf{a}_1-(x_{10}+z_{10})\,\mathbf{a}_2+\left(-x_{10}+y_{10}+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_{10}\,\hat{\mathbf{x}}+b\left(y_{10}+\frac{1}{2}\right)\,\hat{\mathbf{y}}-cz_{10}\,\hat{\mathbf{z}}$	(16j)	O VI
$\mathbf{B_{38}}$	=	$-(y_{10}+z_{10})\,\mathbf{a}_1+(x_{10}-z_{10})\,\mathbf{a}_2+(x_{10}-y_{10})\,\mathbf{a}_3$	=	$ax_{10}\,\hat{\mathbf{x}}-by_{10}\,\hat{\mathbf{y}}-cz_{10}\,\hat{\mathbf{z}}$	(16j)	O VI
$\mathbf{B_{39}}$	=	$-(y_{10}+z_{10})\,\mathbf{a}_1-(x_{10}+z_{10})\,\mathbf{a}_2-(x_{10}+y_{10})\,\mathbf{a}_3$	=	$-ax_{10}\,\hat{\mathbf{x}}-by_{10}\,\hat{\mathbf{y}}-cz_{10}\,\hat{\mathbf{z}}$	(16j)	O VI
$\mathbf{B_{40}}$	=	$\left(y_{10}-z_{10}+\frac{1}{2}\right)\,\mathbf{a}_1+(x_{10}-z_{10})\,\mathbf{a}_2+\left(x_{10}+y_{10}+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$ax_{10}\,\hat{\mathbf{x}}+b\left(y_{10}+\frac{1}{2}\right)\,\hat{\mathbf{y}}-cz_{10}\,\hat{\mathbf{z}}$	(16j)	O VI
$\mathbf{B_{41}}$	=	$\left(-y_{10}+z_{10}+\frac{1}{2}\right)\,\mathbf{a}_1+(x_{10}+z_{10})\,\mathbf{a}_2+\left(x_{10}-y_{10}+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$ax_{10}\,\hat{\mathbf{x}}-b\left(y_{10}-\frac{1}{2}\right)\,\hat{\mathbf{y}}+cz_{10}\,\hat{\mathbf{z}}$	(16j)	O VI
$\mathbf{B_{42}}$	=	$(y_{10}+z_{10})\,\mathbf{a}_1-(x_{10}-z_{10})\,\mathbf{a}_2-(x_{10}-y_{10})\,\mathbf{a}_3$	=	$-ax_{10}\,\hat{\mathbf{x}}+by_{10}\,\hat{\mathbf{y}}+cz_{10}\,\hat{\mathbf{z}}$	(16j)	O VI
$\mathbf{B_{43}}$	=	$(y_{11}+z_{11})\,\mathbf{a}_1+(x_{11}+z_{11})\,\mathbf{a}_2+(x_{11}+y_{11})\,\mathbf{a}_3$	=	$ax_{11}\,\hat{\mathbf{x}}+by_{11}\,\hat{\mathbf{y}}+cz_{11}\,\hat{\mathbf{z}}$	(16j)	Si II
$\mathbf{B_{44}}$	=	$\left(-y_{11}+z_{11}+\frac{1}{2}\right)\,\mathbf{a}_1-(x_{11}-z_{11})\,\mathbf{a}_2-\left(x_{11}+y_{11}-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_{11}\,\hat{\mathbf{x}}-b\left(y_{11}-\frac{1}{2}\right)\,\hat{\mathbf{y}}+cz_{11}\,\hat{\mathbf{z}}$	(16j)	Si II

$\mathbf{B_{45}}$	=	$\left(y_{11} - z_{11} + \frac{1}{2}\right)\,\mathbf{a}_1 - (x_{11} + z_{11})\,\mathbf{a}_2 + \left(-x_{11} + y_{11} + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_{11}\,\hat{\mathbf{x}} + b\left(y_{11} + \frac{1}{2}\right)\,\hat{\mathbf{y}} - cz_{11}\,\hat{\mathbf{z}}$	(16j)	Si II
$\mathbf{B_{46}}$	=	$-\left(y_{11} + z_{11}\right)\,\mathbf{a}_1 + (x_{11} - z_{11})\,\mathbf{a}_2 + (x_{11} - y_{11})\,\mathbf{a}_3$	=	$ax_{11}\,\hat{\mathbf{x}} - by_{11}\,\hat{\mathbf{y}} - cz_{11}\,\hat{\mathbf{z}}$	(16j)	Si II
$\mathbf{B_{47}}$	=	$-\left(y_{11} + z_{11}\right)\,\mathbf{a}_1 - (x_{11} + z_{11})\,\mathbf{a}_2 - (x_{11} + y_{11})\,\mathbf{a}_3$	=	$-ax_{11}\,\hat{\mathbf{x}} - by_{11}\,\hat{\mathbf{y}} - cz_{11}\,\hat{\mathbf{z}}$	(16j)	Si II
$\mathbf{B_{48}}$	=	$\left(y_{11} - z_{11} + \frac{1}{2}\right)\,\mathbf{a}_1 + (x_{11} - z_{11})\,\mathbf{a}_2 + \left(x_{11} + y_{11} + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$ax_{11}\,\hat{\mathbf{x}} + b\left(y_{11} + \frac{1}{2}\right)\,\hat{\mathbf{y}} - cz_{11}\,\hat{\mathbf{z}}$	(16j)	Si II
$\mathbf{B_{49}}$	=	$\left(-y_{11} + z_{11} + \frac{1}{2}\right)\,\mathbf{a}_1 + (x_{11} + z_{11})\,\mathbf{a}_2 + \left(x_{11} - y_{11} + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$ax_{11}\,\hat{\mathbf{x}} - b\left(y_{11} - \frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_{11}\,\hat{\mathbf{z}}$	(16j)	Si II
$\mathbf{B_{50}}$	=	$(y_{11} + z_{11})\,\mathbf{a}_1 - (x_{11} - z_{11})\,\mathbf{a}_2 - (x_{11} - y_{11})\,\mathbf{a}_3$	=	$-ax_{11}\,\hat{\mathbf{x}} + by_{11}\,\hat{\mathbf{y}} + cz_{11}\,\hat{\mathbf{z}}$	(16j)	Si II

References

[1] E. Sokolova, F. C. Hawthorne, A. A. Agakhanov, and L. A. Pautov, *The crystal structure of Moskvinite-(Y), $Na_2K(Y,REE)[Si_6O_{15}]$, a new silicate mineral with $[Si_6O_{15}]$ three-membered double rings from the Dara-I-Pioz Moraine, Tien-Shan Mountains, Tajikistan*, Can. Mineral. **41**, 513–520 (2003), doi:10.2113/gscanmin.41.2.513.