# Murataite $[(Y,Na)_6(Zn,Fe)_5Ti_{12}O_{29}(O,F)_{10}F_4]$ Structure: A16B40C12D6E5_cF316_216_eh_e2g2h_h_f_ae-001

This structure originally had the label `A16B40C12D6E5_cF316_216_eh_e2g2h_h_f_be`. Calls to that address will be redirected here.

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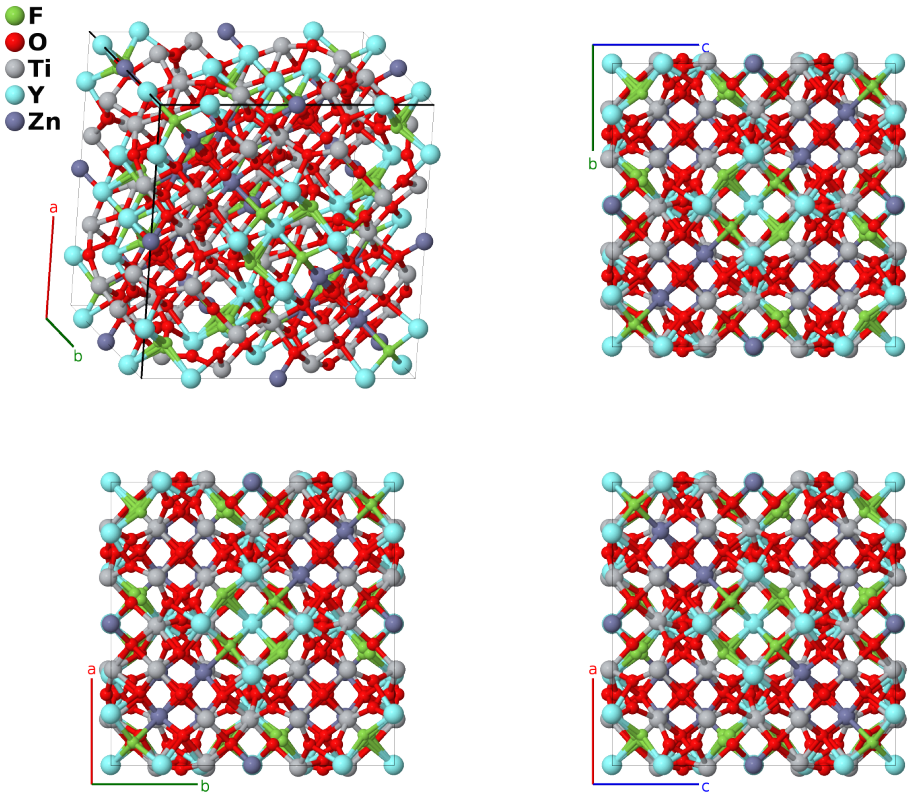
https://aflow.org/p/ZX49

https://aflow.org/p/A16B40C12D6E5_cF316_216_eh_e2g2h_h_f_ae-001




| | |
|---|---|
| **Prototype** | $F_{16}O_{40}Ti_{12}Y_6Zn_5$ |
| **AFLOW prototype label** | A16B40C12D6E5_cF316_216_eh_e2g2h_h_f_ae-001 |
| **Mineral name** | murataite |
| **ICSD** | 81595 |
| **Pearson symbol** | cF316 |
| **Space group number** | 216 |
| **Space group symbol** | $F\bar{4}3m$ |
| **AFLOW prototype command** | `aflow --proto=A16B40C12D6E5_cF316_216_eh_e2g2h_h_f_ae-001 --params=`$a, x_2, x_3, x_4, x_5, x_6, x_7, x_8, z_8, x_9, z_9, x_{10}, z_{10}, x_{11}, z_{11}$ |

- Most of the sites in this structure are somewhat disordered. The "nominal" composition is given as $F_{16}O_{40}Ti_{12}Y_6Zn_5$ by (Ercit, 1995), but as the CIF in (Downs, 2003) shows, even these labels are not quite correct. In our listing we label each Wyckoff position by the type of atom that has the largest concentration on that site. Following (Downs, 2003):
  - Site Zn-I has the composition $Zn_{0.89}Si_{0.11}$.
  - Site F-I has the composition $F_{0.55}O_{0.45}$.
  - Site O-I is pure oxygen.
  - Site Zn-II has the composition $Zn_{0.48}Fe_{0.25}Na_{0.16}Ti_{0.11}$.
  - Site Y has the composition $Y_{0.37}Na_{0.35}Mn_{0.03}HREE_{0.25}$, where "HREE" is a mixture of heavy Rare Earth elements.
  - Site O-II is pure oxygen, but only 8.3333% of the sites are occupied.
  - Site O-III has the composition $O_{0.7}F_{0.3}$.
  - Site O-IV is pure oxygen.
  - Site O-V is pure oxygen, but only 87% of the sites are occupied.
  - Site F-II is pure fluorine, but only 33.333% of the sites are occupied.
  - Site Ti has the composition $Ti_{0.76}Nb_{0.13}Na_{0.11}$.

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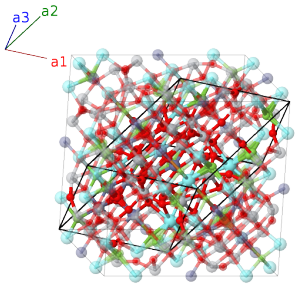
**Face-centered Cubic primitive vectors**

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

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**Basis vectors**

| | | Lattice coordinates | | Cartesian coordinates | Wyckoff position | Atom type |
|---|---|---|---|---|---|---|
| $\mathbf{B_1}$ | = | $0$ | = | $0$ | (4a) | Zn I |
| $\mathbf{B_2}$ | = | $x_2\,\mathbf{a}_1 + x_2\,\mathbf{a}_2 + x_2\,\mathbf{a}_3$ | = | $ax_2\,\hat{\mathbf{x}} + ax_2\,\hat{\mathbf{y}} + ax_2\,\hat{\mathbf{z}}$ | (16e) | F I |
| $\mathbf{B_3}$ | = | $x_2\,\mathbf{a}_1 + x_2\,\mathbf{a}_2 - 3x_2\,\mathbf{a}_3$ | = | $-ax_2\,\hat{\mathbf{x}} - ax_2\,\hat{\mathbf{y}} + ax_2\,\hat{\mathbf{z}}$ | (16e) | F I |
| $\mathbf{B_4}$ | = | $x_2\,\mathbf{a}_1 - 3x_2\,\mathbf{a}_2 + x_2\,\mathbf{a}_3$ | = | $-ax_2\,\hat{\mathbf{x}} + ax_2\,\hat{\mathbf{y}} - ax_2\,\hat{\mathbf{z}}$ | (16e) | F I |
| $\mathbf{B_5}$ | = | $-3x_2\,\mathbf{a}_1 + x_2\,\mathbf{a}_2 + x_2\,\mathbf{a}_3$ | = | $ax_2\,\hat{\mathbf{x}} - ax_2\,\hat{\mathbf{y}} - ax_2\,\hat{\mathbf{z}}$ | (16e) | F I |
| $\mathbf{B_6}$ | = | $x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + x_3\,\mathbf{a}_3$ | = | $ax_3\,\hat{\mathbf{x}} + ax_3\,\hat{\mathbf{y}} + ax_3\,\hat{\mathbf{z}}$ | (16e) | O I |
| $\mathbf{B_7}$ | = | $x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 - 3x_3\,\mathbf{a}_3$ | = | $-ax_3\,\hat{\mathbf{x}} - ax_3\,\hat{\mathbf{y}} + ax_3\,\hat{\mathbf{z}}$ | (16e) | O I |
| $\mathbf{B_8}$ | = | $x_3\,\mathbf{a}_1 - 3x_3\,\mathbf{a}_2 + x_3\,\mathbf{a}_3$ | = | $-ax_3\,\hat{\mathbf{x}} + ax_3\,\hat{\mathbf{y}} - ax_3\,\hat{\mathbf{z}}$ | (16e) | O I |
| $\mathbf{B_9}$ | = | $-3x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + x_3\,\mathbf{a}_3$ | = | $ax_3\,\hat{\mathbf{x}} - ax_3\,\hat{\mathbf{y}} - ax_3\,\hat{\mathbf{z}}$ | (16e) | O I |
| $\mathbf{B_{10}}$ | = | $x_4\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 + x_4\,\mathbf{a}_3$ | = | $ax_4\,\hat{\mathbf{x}} + ax_4\,\hat{\mathbf{y}} + ax_4\,\hat{\mathbf{z}}$ | (16e) | Zn II |
| $\mathbf{B_{11}}$ | = | $x_4\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 - 3x_4\,\mathbf{a}_3$ | = | $-ax_4\,\hat{\mathbf{x}} - ax_4\,\hat{\mathbf{y}} + ax_4\,\hat{\mathbf{z}}$ | (16e) | Zn II |
| $\mathbf{B_{12}}$ | = | $x_4\,\mathbf{a}_1 - 3x_4\,\mathbf{a}_2 + x_4\,\mathbf{a}_3$ | = | $-ax_4\,\hat{\mathbf{x}} + ax_4\,\hat{\mathbf{y}} - ax_4\,\hat{\mathbf{z}}$ | (16e) | Zn II |
| $\mathbf{B_{13}}$ | = | $-3x_4\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 + x_4\,\mathbf{a}_3$ | = | $ax_4\,\hat{\mathbf{x}} - ax_4\,\hat{\mathbf{y}} - ax_4\,\hat{\mathbf{z}}$ | (16e) | Zn II |
| $\mathbf{B_{14}}$ | = | $-x_5\,\mathbf{a}_1 + x_5\,\mathbf{a}_2 + x_5\,\mathbf{a}_3$ | = | $ax_5\,\hat{\mathbf{x}}$ | (24f) | Y I |
| $\mathbf{B_{15}}$ | = | $x_5\,\mathbf{a}_1 - x_5\,\mathbf{a}_2 - x_5\,\mathbf{a}_3$ | = | $-ax_5\,\hat{\mathbf{x}}$ | (24f) | Y I |

| | | | | | | |
|---|---|---|---|---|---|---|
| $\mathbf{B_{16}}$ | = | $x_5\,\mathbf{a}_1 - x_5\,\mathbf{a}_2 + x_5\,\mathbf{a}_3$ | = | $ax_5\,\hat{\mathbf{y}}$ | (24f) | Y I |
| $\mathbf{B_{17}}$ | = | $-x_5\,\mathbf{a}_1 + x_5\,\mathbf{a}_2 - x_5\,\mathbf{a}_3$ | = | $-ax_5\,\hat{\mathbf{y}}$ | (24f) | Y I |
| $\mathbf{B_{18}}$ | = | $x_5\,\mathbf{a}_1 + x_5\,\mathbf{a}_2 - x_5\,\mathbf{a}_3$ | = | $ax_5\,\hat{\mathbf{z}}$ | (24f) | Y I |
| $\mathbf{B_{19}}$ | = | $-x_5\,\mathbf{a}_1 - x_5\,\mathbf{a}_2 + x_5\,\mathbf{a}_3$ | = | $-ax_5\,\hat{\mathbf{z}}$ | (24f) | Y I |
| $\mathbf{B_{20}}$ | = | $-\left(x_6 - \frac{1}{2}\right)\,\mathbf{a}_1 + x_6\,\mathbf{a}_2 + x_6\,\mathbf{a}_3$ | = | $ax_6\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} + \frac{1}{4}a\,\hat{\mathbf{z}}$ | (24g) | O II |
| $\mathbf{B_{21}}$ | = | $x_6\,\mathbf{a}_1 - \left(x_6 - \frac{1}{2}\right)\,\mathbf{a}_2 - \left(x_6 - \frac{1}{2}\right)\,\mathbf{a}_3$ | = | $-a\left(x_6 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} + \frac{1}{4}a\,\hat{\mathbf{z}}$ | (24g) | O II |
| $\mathbf{B_{22}}$ | = | $x_6\,\mathbf{a}_1 - \left(x_6 - \frac{1}{2}\right)\,\mathbf{a}_2 + x_6\,\mathbf{a}_3$ | = | $\frac{1}{4}a\,\hat{\mathbf{x}} + ax_6\,\hat{\mathbf{y}} + \frac{1}{4}a\,\hat{\mathbf{z}}$ | (24g) | O II |
| $\mathbf{B_{23}}$ | = | $-\left(x_6 - \frac{1}{2}\right)\,\mathbf{a}_1 + x_6\,\mathbf{a}_2 - \left(x_6 - \frac{1}{2}\right)\,\mathbf{a}_3$ | = | $\frac{1}{4}a\,\hat{\mathbf{x}} - a\left(x_6 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + \frac{1}{4}a\,\hat{\mathbf{z}}$ | (24g) | O II |
| $\mathbf{B_{24}}$ | = | $x_6\,\mathbf{a}_1 + x_6\,\mathbf{a}_2 - \left(x_6 - \frac{1}{2}\right)\,\mathbf{a}_3$ | = | $\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} + ax_6\,\hat{\mathbf{z}}$ | (24g) | O II |
| $\mathbf{B_{25}}$ | = | $-\left(x_6 - \frac{1}{2}\right)\,\mathbf{a}_1 - \left(x_6 - \frac{1}{2}\right)\,\mathbf{a}_2 + x_6\,\mathbf{a}_3$ | = | $\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} - a\left(x_6 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$ | (24g) | O II |
| $\mathbf{B_{26}}$ | = | $-\left(x_7 - \frac{1}{2}\right)\,\mathbf{a}_1 + x_7\,\mathbf{a}_2 + x_7\,\mathbf{a}_3$ | = | $ax_7\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} + \frac{1}{4}a\,\hat{\mathbf{z}}$ | (24g) | O III |
| $\mathbf{B_{27}}$ | = | $x_7\,\mathbf{a}_1 - \left(x_7 - \frac{1}{2}\right)\,\mathbf{a}_2 - \left(x_7 - \frac{1}{2}\right)\,\mathbf{a}_3$ | = | $-a\left(x_7 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} + \frac{1}{4}a\,\hat{\mathbf{z}}$ | (24g) | O III |
| $\mathbf{B_{28}}$ | = | $x_7\,\mathbf{a}_1 - \left(x_7 - \frac{1}{2}\right)\,\mathbf{a}_2 + x_7\,\mathbf{a}_3$ | = | $\frac{1}{4}a\,\hat{\mathbf{x}} + ax_7\,\hat{\mathbf{y}} + \frac{1}{4}a\,\hat{\mathbf{z}}$ | (24g) | O III |
| $\mathbf{B_{29}}$ | = | $-\left(x_7 - \frac{1}{2}\right)\,\mathbf{a}_1 + x_7\,\mathbf{a}_2 - \left(x_7 - \frac{1}{2}\right)\,\mathbf{a}_3$ | = | $\frac{1}{4}a\,\hat{\mathbf{x}} - a\left(x_7 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + \frac{1}{4}a\,\hat{\mathbf{z}}$ | (24g) | O III |
| $\mathbf{B_{30}}$ | = | $x_7\,\mathbf{a}_1 + x_7\,\mathbf{a}_2 - \left(x_7 - \frac{1}{2}\right)\,\mathbf{a}_3$ | = | $\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} + ax_7\,\hat{\mathbf{z}}$ | (24g) | O III |
| $\mathbf{B_{31}}$ | = | $-\left(x_7 - \frac{1}{2}\right)\,\mathbf{a}_1 - \left(x_7 - \frac{1}{2}\right)\,\mathbf{a}_2 + x_7\,\mathbf{a}_3$ | = | $\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} - a\left(x_7 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$ | (24g) | O III |
| $\mathbf{B_{32}}$ | = | $z_8\,\mathbf{a}_1 + z_8\,\mathbf{a}_2 + (2x_8 - z_8)\,\mathbf{a}_3$ | = | $ax_8\,\hat{\mathbf{x}} + ax_8\,\hat{\mathbf{y}} + az_8\,\hat{\mathbf{z}}$ | (48h) | F II |
| $\mathbf{B_{33}}$ | = | $z_8\,\mathbf{a}_1 + z_8\,\mathbf{a}_2 - (2x_8 + z_8)\,\mathbf{a}_3$ | = | $-ax_8\,\hat{\mathbf{x}} - ax_8\,\hat{\mathbf{y}} + az_8\,\hat{\mathbf{z}}$ | (48h) | F II |
| $\mathbf{B_{34}}$ | = | $(2x_8 - z_8)\,\mathbf{a}_1 - (2x_8 + z_8)\,\mathbf{a}_2 + z_8\,\mathbf{a}_3$ | = | $-ax_8\,\hat{\mathbf{x}} + ax_8\,\hat{\mathbf{y}} - az_8\,\hat{\mathbf{z}}$ | (48h) | F II |
| $\mathbf{B_{35}}$ | = | $-(2x_8 + z_8)\,\mathbf{a}_1 + (2x_8 - z_8)\,\mathbf{a}_2 + z_8\,\mathbf{a}_3$ | = | $ax_8\,\hat{\mathbf{x}} - ax_8\,\hat{\mathbf{y}} - az_8\,\hat{\mathbf{z}}$ | (48h) | F II |
| $\mathbf{B_{36}}$ | = | $(2x_8 - z_8)\,\mathbf{a}_1 + z_8\,\mathbf{a}_2 + z_8\,\mathbf{a}_3$ | = | $az_8\,\hat{\mathbf{x}} + ax_8\,\hat{\mathbf{y}} + ax_8\,\hat{\mathbf{z}}$ | (48h) | F II |
| $\mathbf{B_{37}}$ | = | $-(2x_8 + z_8)\,\mathbf{a}_1 + z_8\,\mathbf{a}_2 + z_8\,\mathbf{a}_3$ | = | $az_8\,\hat{\mathbf{x}} - ax_8\,\hat{\mathbf{y}} - ax_8\,\hat{\mathbf{z}}$ | (48h) | F II |
| $\mathbf{B_{38}}$ | = | $z_8\,\mathbf{a}_1 + (2x_8 - z_8)\,\mathbf{a}_2 - (2x_8 + z_8)\,\mathbf{a}_3$ | = | $-az_8\,\hat{\mathbf{x}} - ax_8\,\hat{\mathbf{y}} + ax_8\,\hat{\mathbf{z}}$ | (48h) | F II |
| $\mathbf{B_{39}}$ | = | $z_8\,\mathbf{a}_1 - (2x_8 + z_8)\,\mathbf{a}_2 + (2x_8 - z_8)\,\mathbf{a}_3$ | = | $-az_8\,\hat{\mathbf{x}} + ax_8\,\hat{\mathbf{y}} - ax_8\,\hat{\mathbf{z}}$ | (48h) | F II |
| $\mathbf{B_{40}}$ | = | $z_8\,\mathbf{a}_1 + (2x_8 - z_8)\,\mathbf{a}_2 + z_8\,\mathbf{a}_3$ | = | $ax_8\,\hat{\mathbf{x}} + az_8\,\hat{\mathbf{y}} + ax_8\,\hat{\mathbf{z}}$ | (48h) | F II |
| $\mathbf{B_{41}}$ | = | $z_8\,\mathbf{a}_1 - (2x_8 + z_8)\,\mathbf{a}_2 + z_8\,\mathbf{a}_3$ | = | $-ax_8\,\hat{\mathbf{x}} + az_8\,\hat{\mathbf{y}} - ax_8\,\hat{\mathbf{z}}$ | (48h) | F II |
| $\mathbf{B_{42}}$ | = | $-(2x_8 + z_8)\,\mathbf{a}_1 + z_8\,\mathbf{a}_2 + (2x_8 - z_8)\,\mathbf{a}_3$ | = | $ax_8\,\hat{\mathbf{x}} - az_8\,\hat{\mathbf{y}} - ax_8\,\hat{\mathbf{z}}$ | (48h) | F II |
| $\mathbf{B_{43}}$ | = | $(2x_8 - z_8)\,\mathbf{a}_1 + z_8\,\mathbf{a}_2 - (2x_8 + z_8)\,\mathbf{a}_3$ | = | $-ax_8\,\hat{\mathbf{x}} - az_8\,\hat{\mathbf{y}} + ax_8\,\hat{\mathbf{z}}$ | (48h) | F II |
| $\mathbf{B_{44}}$ | = | $z_9\,\mathbf{a}_1 + z_9\,\mathbf{a}_2 + (2x_9 - z_9)\,\mathbf{a}_3$ | = | $ax_9\,\hat{\mathbf{x}} + ax_9\,\hat{\mathbf{y}} + az_9\,\hat{\mathbf{z}}$ | (48h) | O IV |
| $\mathbf{B_{45}}$ | = | $z_9\,\mathbf{a}_1 + z_9\,\mathbf{a}_2 - (2x_9 + z_9)\,\mathbf{a}_3$ | = | $-ax_9\,\hat{\mathbf{x}} - ax_9\,\hat{\mathbf{y}} + az_9\,\hat{\mathbf{z}}$ | (48h) | O IV |
| $\mathbf{B_{46}}$ | = | $(2x_9 - z_9)\,\mathbf{a}_1 - (2x_9 + z_9)\,\mathbf{a}_2 + z_9\,\mathbf{a}_3$ | = | $-ax_9\,\hat{\mathbf{x}} + ax_9\,\hat{\mathbf{y}} - az_9\,\hat{\mathbf{z}}$ | (48h) | O IV |
| $\mathbf{B_{47}}$ | = | $-(2x_9 + z_9)\,\mathbf{a}_1 + (2x_9 - z_9)\,\mathbf{a}_2 + z_9\,\mathbf{a}_3$ | = | $ax_9\,\hat{\mathbf{x}} - ax_9\,\hat{\mathbf{y}} - az_9\,\hat{\mathbf{z}}$ | (48h) | O IV |

$$
\begin{array}{lcccccc}
\mathbf{B_{48}} & = & (2x_9 - z_9)\,\mathbf{a}_1 + z_9\,\mathbf{a}_2 + z_9\,\mathbf{a}_3 & = & az_9\,\hat{\mathbf{x}} + ax_9\,\hat{\mathbf{y}} + ax_9\,\hat{\mathbf{z}} & \text{(48h)} & \text{O IV} \\
\mathbf{B_{49}} & = & -(2x_9 + z_9)\,\mathbf{a}_1 + z_9\,\mathbf{a}_2 + z_9\,\mathbf{a}_3 & = & az_9\,\hat{\mathbf{x}} - ax_9\,\hat{\mathbf{y}} - ax_9\,\hat{\mathbf{z}} & \text{(48h)} & \text{O IV} \\
\mathbf{B_{50}} & = & z_9\,\mathbf{a}_1 + (2x_9 - z_9)\,\mathbf{a}_2 - (2x_9 + z_9)\,\mathbf{a}_3 & = & -az_9\,\hat{\mathbf{x}} - ax_9\,\hat{\mathbf{y}} + ax_9\,\hat{\mathbf{z}} & \text{(48h)} & \text{O IV} \\
\mathbf{B_{51}} & = & z_9\,\mathbf{a}_1 - (2x_9 + z_9)\,\mathbf{a}_2 + (2x_9 - z_9)\,\mathbf{a}_3 & = & -az_9\,\hat{\mathbf{x}} + ax_9\,\hat{\mathbf{y}} - ax_9\,\hat{\mathbf{z}} & \text{(48h)} & \text{O IV} \\
\mathbf{B_{52}} & = & z_9\,\mathbf{a}_1 + (2x_9 - z_9)\,\mathbf{a}_2 + z_9\,\mathbf{a}_3 & = & ax_9\,\hat{\mathbf{x}} + az_9\,\hat{\mathbf{y}} + ax_9\,\hat{\mathbf{z}} & \text{(48h)} & \text{O IV} \\
\mathbf{B_{53}} & = & z_9\,\mathbf{a}_1 - (2x_9 + z_9)\,\mathbf{a}_2 + z_9\,\mathbf{a}_3 & = & -ax_9\,\hat{\mathbf{x}} + az_9\,\hat{\mathbf{y}} - ax_9\,\hat{\mathbf{z}} & \text{(48h)} & \text{O IV} \\
\mathbf{B_{54}} & = & -(2x_9 + z_9)\,\mathbf{a}_1 + z_9\,\mathbf{a}_2 + (2x_9 - z_9)\,\mathbf{a}_3 & = & ax_9\,\hat{\mathbf{x}} - az_9\,\hat{\mathbf{y}} - ax_9\,\hat{\mathbf{z}} & \text{(48h)} & \text{O IV} \\
\mathbf{B_{55}} & = & (2x_9 - z_9)\,\mathbf{a}_1 + z_9\,\mathbf{a}_2 - (2x_9 + z_9)\,\mathbf{a}_3 & = & -ax_9\,\hat{\mathbf{x}} - az_9\,\hat{\mathbf{y}} + ax_9\,\hat{\mathbf{z}} & \text{(48h)} & \text{O IV} \\
\mathbf{B_{56}} & = & z_{10}\,\mathbf{a}_1 + z_{10}\,\mathbf{a}_2 + (2x_{10} - z_{10})\,\mathbf{a}_3 & = & ax_{10}\,\hat{\mathbf{x}} + ax_{10}\,\hat{\mathbf{y}} + az_{10}\,\hat{\mathbf{z}} & \text{(48h)} & \text{O V} \\
\mathbf{B_{57}} & = & z_{10}\,\mathbf{a}_1 + z_{10}\,\mathbf{a}_2 - (2x_{10} + z_{10})\,\mathbf{a}_3 & = & -ax_{10}\,\hat{\mathbf{x}} - ax_{10}\,\hat{\mathbf{y}} + az_{10}\,\hat{\mathbf{z}} & \text{(48h)} & \text{O V} \\
\mathbf{B_{58}} & = & (2x_{10} - z_{10})\,\mathbf{a}_1 - (2x_{10} + z_{10})\,\mathbf{a}_2 + z_{10}\,\mathbf{a}_3 & = & -ax_{10}\,\hat{\mathbf{x}} + ax_{10}\,\hat{\mathbf{y}} - az_{10}\,\hat{\mathbf{z}} & \text{(48h)} & \text{O V} \\
\mathbf{B_{59}} & = & -(2x_{10} + z_{10})\,\mathbf{a}_1 + (2x_{10} - z_{10})\,\mathbf{a}_2 + z_{10}\,\mathbf{a}_3 & = & ax_{10}\,\hat{\mathbf{x}} - ax_{10}\,\hat{\mathbf{y}} - az_{10}\,\hat{\mathbf{z}} & \text{(48h)} & \text{O V} \\
\mathbf{B_{60}} & = & (2x_{10} - z_{10})\,\mathbf{a}_1 + z_{10}\,\mathbf{a}_2 + z_{10}\,\mathbf{a}_3 & = & az_{10}\,\hat{\mathbf{x}} + ax_{10}\,\hat{\mathbf{y}} + ax_{10}\,\hat{\mathbf{z}} & \text{(48h)} & \text{O V} \\
\mathbf{B_{61}} & = & -(2x_{10} + z_{10})\,\mathbf{a}_1 + z_{10}\,\mathbf{a}_2 + z_{10}\,\mathbf{a}_3 & = & az_{10}\,\hat{\mathbf{x}} - ax_{10}\,\hat{\mathbf{y}} - ax_{10}\,\hat{\mathbf{z}} & \text{(48h)} & \text{O V} \\
\mathbf{B_{62}} & = & z_{10}\,\mathbf{a}_1 + (2x_{10} - z_{10})\,\mathbf{a}_2 - (2x_{10} + z_{10})\,\mathbf{a}_3 & = & -az_{10}\,\hat{\mathbf{x}} - ax_{10}\,\hat{\mathbf{y}} + ax_{10}\,\hat{\mathbf{z}} & \text{(48h)} & \text{O V} \\
\mathbf{B_{63}} & = & z_{10}\,\mathbf{a}_1 - (2x_{10} + z_{10})\,\mathbf{a}_2 + (2x_{10} - z_{10})\,\mathbf{a}_3 & = & -az_{10}\,\hat{\mathbf{x}} + ax_{10}\,\hat{\mathbf{y}} - ax_{10}\,\hat{\mathbf{z}} & \text{(48h)} & \text{O V} \\
\mathbf{B_{64}} & = & z_{10}\,\mathbf{a}_1 + (2x_{10} - z_{10})\,\mathbf{a}_2 + z_{10}\,\mathbf{a}_3 & = & ax_{10}\,\hat{\mathbf{x}} + az_{10}\,\hat{\mathbf{y}} + ax_{10}\,\hat{\mathbf{z}} & \text{(48h)} & \text{O V} \\
\mathbf{B_{65}} & = & z_{10}\,\mathbf{a}_1 - (2x_{10} + z_{10})\,\mathbf{a}_2 + z_{10}\,\mathbf{a}_3 & = & -ax_{10}\,\hat{\mathbf{x}} + az_{10}\,\hat{\mathbf{y}} - ax_{10}\,\hat{\mathbf{z}} & \text{(48h)} & \text{O V} \\
\mathbf{B_{66}} & = & -(2x_{10} + z_{10})\,\mathbf{a}_1 + z_{10}\,\mathbf{a}_2 + (2x_{10} - z_{10})\,\mathbf{a}_3 & = & ax_{10}\,\hat{\mathbf{x}} - az_{10}\,\hat{\mathbf{y}} - ax_{10}\,\hat{\mathbf{z}} & \text{(48h)} & \text{O V} \\
\mathbf{B_{67}} & = & (2x_{10} - z_{10})\,\mathbf{a}_1 + z_{10}\,\mathbf{a}_2 - (2x_{10} + z_{10})\,\mathbf{a}_3 & = & -ax_{10}\,\hat{\mathbf{x}} - az_{10}\,\hat{\mathbf{y}} + ax_{10}\,\hat{\mathbf{z}} & \text{(48h)} & \text{O V} \\
\mathbf{B_{68}} & = & z_{11}\,\mathbf{a}_1 + z_{11}\,\mathbf{a}_2 + (2x_{11} - z_{11})\,\mathbf{a}_3 & = & ax_{11}\,\hat{\mathbf{x}} + ax_{11}\,\hat{\mathbf{y}} + az_{11}\,\hat{\mathbf{z}} & \text{(48h)} & \text{Ti I} \\
\mathbf{B_{69}} & = & z_{11}\,\mathbf{a}_1 + z_{11}\,\mathbf{a}_2 - (2x_{11} + z_{11})\,\mathbf{a}_3 & = & -ax_{11}\,\hat{\mathbf{x}} - ax_{11}\,\hat{\mathbf{y}} + az_{11}\,\hat{\mathbf{z}} & \text{(48h)} & \text{Ti I} \\
\mathbf{B_{70}} & = & (2x_{11} - z_{11})\,\mathbf{a}_1 - (2x_{11} + z_{11})\,\mathbf{a}_2 + z_{11}\,\mathbf{a}_3 & = & -ax_{11}\,\hat{\mathbf{x}} + ax_{11}\,\hat{\mathbf{y}} - az_{11}\,\hat{\mathbf{z}} & \text{(48h)} & \text{Ti I} \\
\mathbf{B_{71}} & = & -(2x_{11} + z_{11})\,\mathbf{a}_1 + (2x_{11} - z_{11})\,\mathbf{a}_2 + z_{11}\,\mathbf{a}_3 & = & ax_{11}\,\hat{\mathbf{x}} - ax_{11}\,\hat{\mathbf{y}} - az_{11}\,\hat{\mathbf{z}} & \text{(48h)} & \text{Ti I} \\
\mathbf{B_{72}} & = & (2x_{11} - z_{11})\,\mathbf{a}_1 + z_{11}\,\mathbf{a}_2 + z_{11}\,\mathbf{a}_3 & = & az_{11}\,\hat{\mathbf{x}} + ax_{11}\,\hat{\mathbf{y}} + ax_{11}\,\hat{\mathbf{z}} & \text{(48h)} & \text{Ti I} \\
\mathbf{B_{73}} & = & -(2x_{11} + z_{11})\,\mathbf{a}_1 + z_{11}\,\mathbf{a}_2 + z_{11}\,\mathbf{a}_3 & = & az_{11}\,\hat{\mathbf{x}} - ax_{11}\,\hat{\mathbf{y}} - ax_{11}\,\hat{\mathbf{z}} & \text{(48h)} & \text{Ti I} \\
\mathbf{B_{74}} & = & z_{11}\,\mathbf{a}_1 + (2x_{11} - z_{11})\,\mathbf{a}_2 - (2x_{11} + z_{11})\,\mathbf{a}_3 & = & -az_{11}\,\hat{\mathbf{x}} - ax_{11}\,\hat{\mathbf{y}} + ax_{11}\,\hat{\mathbf{z}} & \text{(48h)} & \text{Ti I} \\
\mathbf{B_{75}} & = & z_{11}\,\mathbf{a}_1 - (2x_{11} + z_{11})\,\mathbf{a}_2 + (2x_{11} - z_{11})\,\mathbf{a}_3 & = & -az_{11}\,\hat{\mathbf{x}} + ax_{11}\,\hat{\mathbf{y}} - ax_{11}\,\hat{\mathbf{z}} & \text{(48h)} & \text{Ti I} \\
\mathbf{B_{76}} & = & z_{11}\,\mathbf{a}_1 + (2x_{11} - z_{11})\,\mathbf{a}_2 + z_{11}\,\mathbf{a}_3 & = & ax_{11}\,\hat{\mathbf{x}} + az_{11}\,\hat{\mathbf{y}} + ax_{11}\,\hat{\mathbf{z}} & \text{(48h)} & \text{Ti I} \\
\mathbf{B_{77}} & = & z_{11}\,\mathbf{a}_1 - (2x_{11} + z_{11})\,\mathbf{a}_2 + z_{11}\,\mathbf{a}_3 & = & -ax_{11}\,\hat{\mathbf{x}} + az_{11}\,\hat{\mathbf{y}} - ax_{11}\,\hat{\mathbf{z}} & \text{(48h)} & \text{Ti I}
\end{array}
$$

| | | | | | | |
|---|---|---|---|---|---|---|
| $\mathbf{B_{78}}$ | = | $-(2x_{11}+z_{11})\,\mathbf{a}_1+z_{11}\,\mathbf{a}_2+(2x_{11}-z_{11})\,\mathbf{a}_3$ | = | $ax_{11}\,\hat{\mathbf{x}}-az_{11}\,\hat{\mathbf{y}}-ax_{11}\,\hat{\mathbf{z}}$ | (48h) | Ti I |
| $\mathbf{B_{79}}$ | = | $(2x_{11}-z_{11})\,\mathbf{a}_1+z_{11}\,\mathbf{a}_2-(2x_{11}+z_{11})\,\mathbf{a}_3$ | = | $-ax_{11}\,\hat{\mathbf{x}}-az_{11}\,\hat{\mathbf{y}}+ax_{11}\,\hat{\mathbf{z}}$ | (48h) | Ti I |

## References


[1] T. S. Ercit and F. C. Hawthorne, *Murataite, A $UB_{12}$ derivative structure with condensed Keggin molecules*, Can. Mineral. **33**, 1233–1229 (1995).

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