

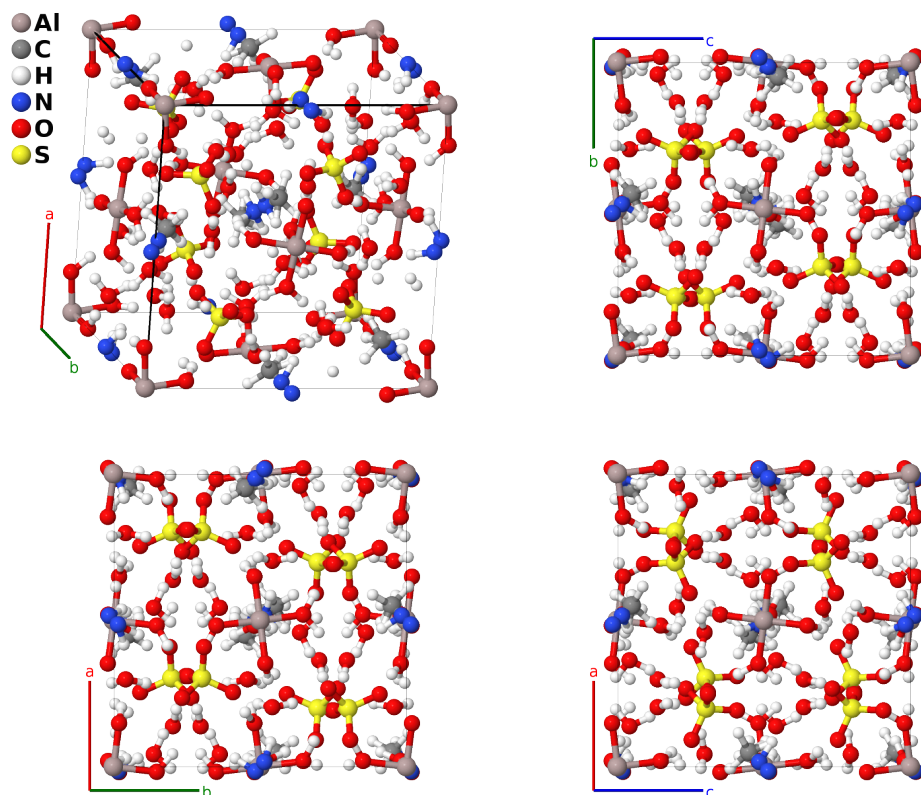
β -Alum $[\text{Al}(\text{NH}_3\text{CH}_3)_2(\text{SO}_4)_2 \cdot 12\text{H}_2\text{O}, H_{414}]$ Structure: AB2C36D2E20F2_cP252_205_a_c_6d_c_c3d_c-001

This structure originally had the label AB2C36D2E20F2_cP252_205_a_c_6d_c_c3d_c. Calls to that address will be redirected here.

Cite this page as: 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.

<https://afLOW.org/p/SFC7>

https://afLOW.org/p/AB2C36D2E20F2_cP252_205_a_c_6d_c_c3d_c-001



Prototype	$\text{AlC}_2\text{H}_{36}\text{N}_2\text{O}_{20}\text{S}_2$
AFLOW prototype label	AB2C36D2E20F2_cP252_205_a_c_6d_c_c3d_c-001
<i>Strukturbericht</i> designation	H_{414}
Mineral name	β -alum
ICSD	77599
Pearson symbol	cP252
Space group number	205
Space group symbol	$P\bar{a}3$
AFLOW prototype command	<pre>afLOW --proto=AB2C36D2E20F2_cP252_205_a_c_6d_c_c3d_c-001 --params=a, x2, x3, x4, x5, x6, y6, z6, x7, y7, z7, x8, y8, z8, x9, y9, z9, x10, y10, z10, x11, y11, z11, x12, y12, z12, x13, y13, z13, x14, y14, z14</pre>

Other compounds with this structure

$\text{AlCs}(\text{SO}_4)_2 \cdot 12\text{H}_2\text{O}$

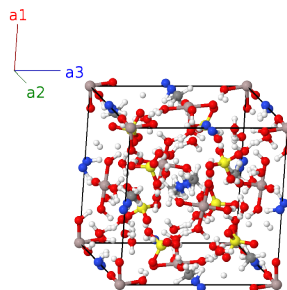
- The alums have the general formula $\text{AB}(\text{XO}_4)_2 \cdot 12\text{H}_2\text{O}$, where A is a monovalent ion, B is a trivalent ion, and X is a chalcogen. In most cases atom B is aluminum and atom X is sulfur, leading to the name alum.
- All alums have their room-temperature form in space group $Pa\bar{3}$ #205, but the bonding between the A and B ions and the XO_4 complex can be quite different.
- (Lipson, 1935ab) described three general forms of alum based on the sizes of the monovalent ions. Each of these forms was given a *Strukturbericht* designation by (Gottfried, 1937):
 - α -alum, with intermediate sized ions, prototype $\text{KAl}(\text{SO}_4)_2 \cdot 12\text{H}_2\text{O}$, $H4_{13}$,
 - β -alum, with large ions, prototype $(\text{NH}_3\text{CH}_3)\text{Al}(\text{SO}_4)_2 \cdot 12\text{H}_2\text{O}$, $H4_{14}$ (this structure), and
 - γ -alum, with small ions, prototype $\text{NaAl}(\text{SO}_4)_2 \cdot 12\text{H}_2\text{O}$, $H4_{15}$.
- This classification scheme is not complete, *e.g.*, (Ledsham, 1968) points out that $\text{NaCr}(\text{SO}_4)_2 \cdot 12\text{H}_2\text{O}$ does not fit into any of these categories, and that the actual structure depends on the combination of monovalent and trivalent ions.
- As noted above, the $Pa\bar{3}$ structures of alum are the room temperature form. As the temperature decreases the alum structure may transform. For example, in the temperature range 150-170K the β -alum $(\text{NH}_3\text{CH}_3)\text{Al}(\text{SO}_4)_2 \cdot 12\text{H}_2\text{O}$ transforms into an orthorhombic structure with fully ordered NH_3CH_3 ions.
- This structure was originally determined by (Lipson, 1935c), could only determine that the NH_3CH_3 ion occupied the (4b) Wyckoff position. (Abdeen, 1981) showed that the ion was statistically distributed at two possible sites. The C-N bond distance is 1.4\AA , slightly smaller than the 1.51\AA distance observed in the low temperature structure. At any site, one of the two nitrogen positions is occupied, along with the carbon position 1.4\AA away. Six hydrogen positions from the (H-I) and (H-II) sites are then occupied.

Simple Cubic primitive vectors

$$\mathbf{a}_1 = a \hat{\mathbf{x}}$$

$$\mathbf{a}_2 = a \hat{\mathbf{y}}$$

$$\mathbf{a}_3 = a \hat{\mathbf{z}}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
\mathbf{B}_1	=	0	=	0	(4a) Al I
\mathbf{B}_2	=	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_3$	=	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{z}}$	(4a) Al I
\mathbf{B}_3	=	$\frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	=	$\frac{1}{2} a \hat{\mathbf{y}} + \frac{1}{2} a \hat{\mathbf{z}}$	(4a) Al I
\mathbf{B}_4	=	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2$	=	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}}$	(4a) Al I
\mathbf{B}_5	=	$x_2 \mathbf{a}_1 + x_2 \mathbf{a}_2 + x_2 \mathbf{a}_3$	=	$a x_2 \hat{\mathbf{x}} + a x_2 \hat{\mathbf{y}} + a x_2 \hat{\mathbf{z}}$	(8c) C I
\mathbf{B}_6	=	$-(x_2 - \frac{1}{2}) \mathbf{a}_1 - x_2 \mathbf{a}_2 + (x_2 + \frac{1}{2}) \mathbf{a}_3$	=	$-a (x_2 - \frac{1}{2}) \hat{\mathbf{x}} - a x_2 \hat{\mathbf{y}} + a (x_2 + \frac{1}{2}) \hat{\mathbf{z}}$	(8c) C I

$$\begin{aligned}
\mathbf{B}_{186} &= (z_{12} + \frac{1}{2}) \mathbf{a}_1 - (x_{12} - \frac{1}{2}) \mathbf{a}_2 - y_{12} \mathbf{a}_3 &= a(z_{12} + \frac{1}{2}) \hat{\mathbf{x}} - a(x_{12} - \frac{1}{2}) \hat{\mathbf{y}} - ay_{12} \hat{\mathbf{z}} &(24d) & \text{O II} \\
\mathbf{B}_{187} &= -(z_{12} - \frac{1}{2}) \mathbf{a}_1 - x_{12} \mathbf{a}_2 + (y_{12} + \frac{1}{2}) \mathbf{a}_3 &= -a(z_{12} - \frac{1}{2}) \hat{\mathbf{x}} - ax_{12} \hat{\mathbf{y}} + a(y_{12} + \frac{1}{2}) \hat{\mathbf{z}} &(24d) & \text{O II} \\
\mathbf{B}_{188} &= -z_{12} \mathbf{a}_1 + (x_{12} + \frac{1}{2}) \mathbf{a}_2 - (y_{12} - \frac{1}{2}) \mathbf{a}_3 &= -az_{12} \hat{\mathbf{x}} + a(x_{12} + \frac{1}{2}) \hat{\mathbf{y}} - a(y_{12} - \frac{1}{2}) \hat{\mathbf{z}} &(24d) & \text{O II} \\
\mathbf{B}_{189} &= y_{12} \mathbf{a}_1 + z_{12} \mathbf{a}_2 + x_{12} \mathbf{a}_3 &= ay_{12} \hat{\mathbf{x}} + az_{12} \hat{\mathbf{y}} + ax_{12} \hat{\mathbf{z}} &(24d) & \text{O II} \\
\mathbf{B}_{190} &= -y_{12} \mathbf{a}_1 + (z_{12} + \frac{1}{2}) \mathbf{a}_2 - (x_{12} - \frac{1}{2}) \mathbf{a}_3 &= -ay_{12} \hat{\mathbf{x}} + a(z_{12} + \frac{1}{2}) \hat{\mathbf{y}} - a(x_{12} - \frac{1}{2}) \hat{\mathbf{z}} &(24d) & \text{O II} \\
\mathbf{B}_{191} &= (y_{12} + \frac{1}{2}) \mathbf{a}_1 - (z_{12} - \frac{1}{2}) \mathbf{a}_2 - x_{12} \mathbf{a}_3 &= a(y_{12} + \frac{1}{2}) \hat{\mathbf{x}} - a(z_{12} - \frac{1}{2}) \hat{\mathbf{y}} - ax_{12} \hat{\mathbf{z}} &(24d) & \text{O II} \\
\mathbf{B}_{192} &= -(y_{12} - \frac{1}{2}) \mathbf{a}_1 - z_{12} \mathbf{a}_2 + (x_{12} + \frac{1}{2}) \mathbf{a}_3 &= -a(y_{12} - \frac{1}{2}) \hat{\mathbf{x}} - az_{12} \hat{\mathbf{y}} + a(x_{12} + \frac{1}{2}) \hat{\mathbf{z}} &(24d) & \text{O II} \\
\mathbf{B}_{193} &= -x_{12} \mathbf{a}_1 - y_{12} \mathbf{a}_2 - z_{12} \mathbf{a}_3 &= -ax_{12} \hat{\mathbf{x}} - ay_{12} \hat{\mathbf{y}} - az_{12} \hat{\mathbf{z}} &(24d) & \text{O II} \\
\mathbf{B}_{194} &= (x_{12} + \frac{1}{2}) \mathbf{a}_1 + y_{12} \mathbf{a}_2 - (z_{12} - \frac{1}{2}) \mathbf{a}_3 &= a(x_{12} + \frac{1}{2}) \hat{\mathbf{x}} + ay_{12} \hat{\mathbf{y}} - a(z_{12} - \frac{1}{2}) \hat{\mathbf{z}} &(24d) & \text{O II} \\
\mathbf{B}_{195} &= x_{12} \mathbf{a}_1 - (y_{12} - \frac{1}{2}) \mathbf{a}_2 + (z_{12} + \frac{1}{2}) \mathbf{a}_3 &= ax_{12} \hat{\mathbf{x}} - a(y_{12} - \frac{1}{2}) \hat{\mathbf{y}} + a(z_{12} + \frac{1}{2}) \hat{\mathbf{z}} &(24d) & \text{O II} \\
\mathbf{B}_{196} &= -(x_{12} - \frac{1}{2}) \mathbf{a}_1 + (y_{12} + \frac{1}{2}) \mathbf{a}_2 + z_{12} \mathbf{a}_3 &= -a(x_{12} - \frac{1}{2}) \hat{\mathbf{x}} + a(y_{12} + \frac{1}{2}) \hat{\mathbf{y}} + az_{12} \hat{\mathbf{z}} &(24d) & \text{O II} \\
\mathbf{B}_{197} &= -z_{12} \mathbf{a}_1 - x_{12} \mathbf{a}_2 - y_{12} \mathbf{a}_3 &= -az_{12} \hat{\mathbf{x}} - ax_{12} \hat{\mathbf{y}} - ay_{12} \hat{\mathbf{z}} &(24d) & \text{O II} \\
\mathbf{B}_{198} &= -(z_{12} - \frac{1}{2}) \mathbf{a}_1 + (x_{12} + \frac{1}{2}) \mathbf{a}_2 + y_{12} \mathbf{a}_3 &= -a(z_{12} - \frac{1}{2}) \hat{\mathbf{x}} + a(x_{12} + \frac{1}{2}) \hat{\mathbf{y}} + ay_{12} \hat{\mathbf{z}} &(24d) & \text{O II} \\
\mathbf{B}_{199} &= (z_{12} + \frac{1}{2}) \mathbf{a}_1 + x_{12} \mathbf{a}_2 - (y_{12} - \frac{1}{2}) \mathbf{a}_3 &= a(z_{12} + \frac{1}{2}) \hat{\mathbf{x}} + ax_{12} \hat{\mathbf{y}} - a(y_{12} - \frac{1}{2}) \hat{\mathbf{z}} &(24d) & \text{O II} \\
\mathbf{B}_{200} &= z_{12} \mathbf{a}_1 - (x_{12} - \frac{1}{2}) \mathbf{a}_2 + (y_{12} + \frac{1}{2}) \mathbf{a}_3 &= az_{12} \hat{\mathbf{x}} - a(x_{12} - \frac{1}{2}) \hat{\mathbf{y}} + a(y_{12} + \frac{1}{2}) \hat{\mathbf{z}} &(24d) & \text{O II} \\
\mathbf{B}_{201} &= -y_{12} \mathbf{a}_1 - z_{12} \mathbf{a}_2 - x_{12} \mathbf{a}_3 &= -ay_{12} \hat{\mathbf{x}} - az_{12} \hat{\mathbf{y}} - ax_{12} \hat{\mathbf{z}} &(24d) & \text{O II} \\
\mathbf{B}_{202} &= y_{12} \mathbf{a}_1 - (z_{12} - \frac{1}{2}) \mathbf{a}_2 + (x_{12} + \frac{1}{2}) \mathbf{a}_3 &= ay_{12} \hat{\mathbf{x}} - a(z_{12} - \frac{1}{2}) \hat{\mathbf{y}} + a(x_{12} + \frac{1}{2}) \hat{\mathbf{z}} &(24d) & \text{O II} \\
\mathbf{B}_{203} &= -(y_{12} - \frac{1}{2}) \mathbf{a}_1 + (z_{12} + \frac{1}{2}) \mathbf{a}_2 + x_{12} \mathbf{a}_3 &= -a(y_{12} - \frac{1}{2}) \hat{\mathbf{x}} + a(z_{12} + \frac{1}{2}) \hat{\mathbf{y}} + ax_{12} \hat{\mathbf{z}} &(24d) & \text{O II} \\
\mathbf{B}_{204} &= (y_{12} + \frac{1}{2}) \mathbf{a}_1 + z_{12} \mathbf{a}_2 - (x_{12} - \frac{1}{2}) \mathbf{a}_3 &= a(y_{12} + \frac{1}{2}) \hat{\mathbf{x}} + az_{12} \hat{\mathbf{y}} - a(x_{12} - \frac{1}{2}) \hat{\mathbf{z}} &(24d) & \text{O II} \\
\mathbf{B}_{205} &= x_{13} \mathbf{a}_1 + y_{13} \mathbf{a}_2 + z_{13} \mathbf{a}_3 &= ax_{13} \hat{\mathbf{x}} + ay_{13} \hat{\mathbf{y}} + az_{13} \hat{\mathbf{z}} &(24d) & \text{O III} \\
\mathbf{B}_{206} &= -(x_{13} - \frac{1}{2}) \mathbf{a}_1 - y_{13} \mathbf{a}_2 + (z_{13} + \frac{1}{2}) \mathbf{a}_3 &= -a(x_{13} - \frac{1}{2}) \hat{\mathbf{x}} - ay_{13} \hat{\mathbf{y}} + a(z_{13} + \frac{1}{2}) \hat{\mathbf{z}} &(24d) & \text{O III} \\
\mathbf{B}_{207} &= -x_{13} \mathbf{a}_1 + (y_{13} + \frac{1}{2}) \mathbf{a}_2 - (z_{13} - \frac{1}{2}) \mathbf{a}_3 &= -ax_{13} \hat{\mathbf{x}} + a(y_{13} + \frac{1}{2}) \hat{\mathbf{y}} - a(z_{13} - \frac{1}{2}) \hat{\mathbf{z}} &(24d) & \text{O III} \\
\mathbf{B}_{208} &= (x_{13} + \frac{1}{2}) \mathbf{a}_1 - (y_{13} - \frac{1}{2}) \mathbf{a}_2 - z_{13} \mathbf{a}_3 &= a(x_{13} + \frac{1}{2}) \hat{\mathbf{x}} - a(y_{13} - \frac{1}{2}) \hat{\mathbf{y}} - az_{13} \hat{\mathbf{z}} &(24d) & \text{O III} \\
\mathbf{B}_{209} &= z_{13} \mathbf{a}_1 + x_{13} \mathbf{a}_2 + y_{13} \mathbf{a}_3 &= az_{13} \hat{\mathbf{x}} + ax_{13} \hat{\mathbf{y}} + ay_{13} \hat{\mathbf{z}} &(24d) & \text{O III} \\
\mathbf{B}_{210} &= (z_{13} + \frac{1}{2}) \mathbf{a}_1 - (x_{13} - \frac{1}{2}) \mathbf{a}_2 - y_{13} \mathbf{a}_3 &= a(z_{13} + \frac{1}{2}) \hat{\mathbf{x}} - a(x_{13} - \frac{1}{2}) \hat{\mathbf{y}} - ay_{13} \hat{\mathbf{z}} &(24d) & \text{O III} \\
\mathbf{B}_{211} &= -(z_{13} - \frac{1}{2}) \mathbf{a}_1 - x_{13} \mathbf{a}_2 + (y_{13} + \frac{1}{2}) \mathbf{a}_3 &= -a(z_{13} - \frac{1}{2}) \hat{\mathbf{x}} - ax_{13} \hat{\mathbf{y}} + a(y_{13} + \frac{1}{2}) \hat{\mathbf{z}} &(24d) & \text{O III}
\end{aligned}$$

$$\begin{aligned}
\mathbf{B}_{238} &= \begin{matrix} -y_{14} \mathbf{a}_1 + (z_{14} + \frac{1}{2}) \mathbf{a}_2 - \\ (x_{14} - \frac{1}{2}) \mathbf{a}_3 \end{matrix} = -ay_{14} \hat{\mathbf{x}} + a(z_{14} + \frac{1}{2}) \hat{\mathbf{y}} - a(x_{14} - \frac{1}{2}) \hat{\mathbf{z}} & (24d) & \text{O IV} \\
\mathbf{B}_{239} &= \begin{matrix} (y_{14} + \frac{1}{2}) \mathbf{a}_1 - (z_{14} - \frac{1}{2}) \mathbf{a}_2 - \\ x_{14} \mathbf{a}_3 \end{matrix} = a(y_{14} + \frac{1}{2}) \hat{\mathbf{x}} - a(z_{14} - \frac{1}{2}) \hat{\mathbf{y}} - ax_{14} \hat{\mathbf{z}} & (24d) & \text{O IV} \\
\mathbf{B}_{240} &= \begin{matrix} -(y_{14} - \frac{1}{2}) \mathbf{a}_1 - z_{14} \mathbf{a}_2 + \\ (x_{14} + \frac{1}{2}) \mathbf{a}_3 \end{matrix} = -a(y_{14} - \frac{1}{2}) \hat{\mathbf{x}} - az_{14} \hat{\mathbf{y}} + a(x_{14} + \frac{1}{2}) \hat{\mathbf{z}} & (24d) & \text{O IV} \\
\mathbf{B}_{241} &= -x_{14} \mathbf{a}_1 - y_{14} \mathbf{a}_2 - z_{14} \mathbf{a}_3 = -ax_{14} \hat{\mathbf{x}} - ay_{14} \hat{\mathbf{y}} - az_{14} \hat{\mathbf{z}} & (24d) & \text{O IV} \\
\mathbf{B}_{242} &= \begin{matrix} (x_{14} + \frac{1}{2}) \mathbf{a}_1 + y_{14} \mathbf{a}_2 - \\ (z_{14} - \frac{1}{2}) \mathbf{a}_3 \end{matrix} = a(x_{14} + \frac{1}{2}) \hat{\mathbf{x}} + ay_{14} \hat{\mathbf{y}} - a(z_{14} - \frac{1}{2}) \hat{\mathbf{z}} & (24d) & \text{O IV} \\
\mathbf{B}_{243} &= \begin{matrix} x_{14} \mathbf{a}_1 - (y_{14} - \frac{1}{2}) \mathbf{a}_2 + \\ (z_{14} + \frac{1}{2}) \mathbf{a}_3 \end{matrix} = ax_{14} \hat{\mathbf{x}} - a(y_{14} - \frac{1}{2}) \hat{\mathbf{y}} + a(z_{14} + \frac{1}{2}) \hat{\mathbf{z}} & (24d) & \text{O IV} \\
\mathbf{B}_{244} &= \begin{matrix} -(x_{14} - \frac{1}{2}) \mathbf{a}_1 + (y_{14} + \frac{1}{2}) \mathbf{a}_2 + \\ z_{14} \mathbf{a}_3 \end{matrix} = -a(x_{14} - \frac{1}{2}) \hat{\mathbf{x}} + a(y_{14} + \frac{1}{2}) \hat{\mathbf{y}} + az_{14} \hat{\mathbf{z}} & (24d) & \text{O IV} \\
\mathbf{B}_{245} &= -z_{14} \mathbf{a}_1 - x_{14} \mathbf{a}_2 - y_{14} \mathbf{a}_3 = -az_{14} \hat{\mathbf{x}} - ax_{14} \hat{\mathbf{y}} - ay_{14} \hat{\mathbf{z}} & (24d) & \text{O IV} \\
\mathbf{B}_{246} &= \begin{matrix} -(z_{14} - \frac{1}{2}) \mathbf{a}_1 + (x_{14} + \frac{1}{2}) \mathbf{a}_2 + \\ y_{14} \mathbf{a}_3 \end{matrix} = -a(z_{14} - \frac{1}{2}) \hat{\mathbf{x}} + a(x_{14} + \frac{1}{2}) \hat{\mathbf{y}} + ay_{14} \hat{\mathbf{z}} & (24d) & \text{O IV} \\
\mathbf{B}_{247} &= \begin{matrix} (z_{14} + \frac{1}{2}) \mathbf{a}_1 + x_{14} \mathbf{a}_2 - \\ (y_{14} - \frac{1}{2}) \mathbf{a}_3 \end{matrix} = a(z_{14} + \frac{1}{2}) \hat{\mathbf{x}} + ax_{14} \hat{\mathbf{y}} - a(y_{14} - \frac{1}{2}) \hat{\mathbf{z}} & (24d) & \text{O IV} \\
\mathbf{B}_{248} &= \begin{matrix} z_{14} \mathbf{a}_1 - (x_{14} - \frac{1}{2}) \mathbf{a}_2 + \\ (y_{14} + \frac{1}{2}) \mathbf{a}_3 \end{matrix} = az_{14} \hat{\mathbf{x}} - a(x_{14} - \frac{1}{2}) \hat{\mathbf{y}} + a(y_{14} + \frac{1}{2}) \hat{\mathbf{z}} & (24d) & \text{O IV} \\
\mathbf{B}_{249} &= -y_{14} \mathbf{a}_1 - z_{14} \mathbf{a}_2 - x_{14} \mathbf{a}_3 = -ay_{14} \hat{\mathbf{x}} - az_{14} \hat{\mathbf{y}} - ax_{14} \hat{\mathbf{z}} & (24d) & \text{O IV} \\
\mathbf{B}_{250} &= \begin{matrix} y_{14} \mathbf{a}_1 - (z_{14} - \frac{1}{2}) \mathbf{a}_2 + \\ (x_{14} + \frac{1}{2}) \mathbf{a}_3 \end{matrix} = ay_{14} \hat{\mathbf{x}} - a(z_{14} - \frac{1}{2}) \hat{\mathbf{y}} + a(x_{14} + \frac{1}{2}) \hat{\mathbf{z}} & (24d) & \text{O IV} \\
\mathbf{B}_{251} &= \begin{matrix} -(y_{14} - \frac{1}{2}) \mathbf{a}_1 + (z_{14} + \frac{1}{2}) \mathbf{a}_2 + \\ x_{14} \mathbf{a}_3 \end{matrix} = -a(y_{14} - \frac{1}{2}) \hat{\mathbf{x}} + a(z_{14} + \frac{1}{2}) \hat{\mathbf{y}} + ax_{14} \hat{\mathbf{z}} & (24d) & \text{O IV} \\
\mathbf{B}_{252} &= \begin{matrix} (y_{14} + \frac{1}{2}) \mathbf{a}_1 + z_{14} \mathbf{a}_2 - \\ (x_{14} - \frac{1}{2}) \mathbf{a}_3 \end{matrix} = a(y_{14} + \frac{1}{2}) \hat{\mathbf{x}} + az_{14} \hat{\mathbf{y}} - a(x_{14} - \frac{1}{2}) \hat{\mathbf{z}} & (24d) & \text{O IV}
\end{aligned}$$

References

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