Zunyite [$Al_{13}(OH,F)_{18}Si_5O_{20}Cl$ ($S0_8$)] Structure: A13BC18D20E5_cF228_216_ah_c_gh_2eh_be-001

This structure originally had the label `A13BC18D20E5_cF228_216_dh_b_fh_2eh_ce`. Calls to that address will be redirected here.

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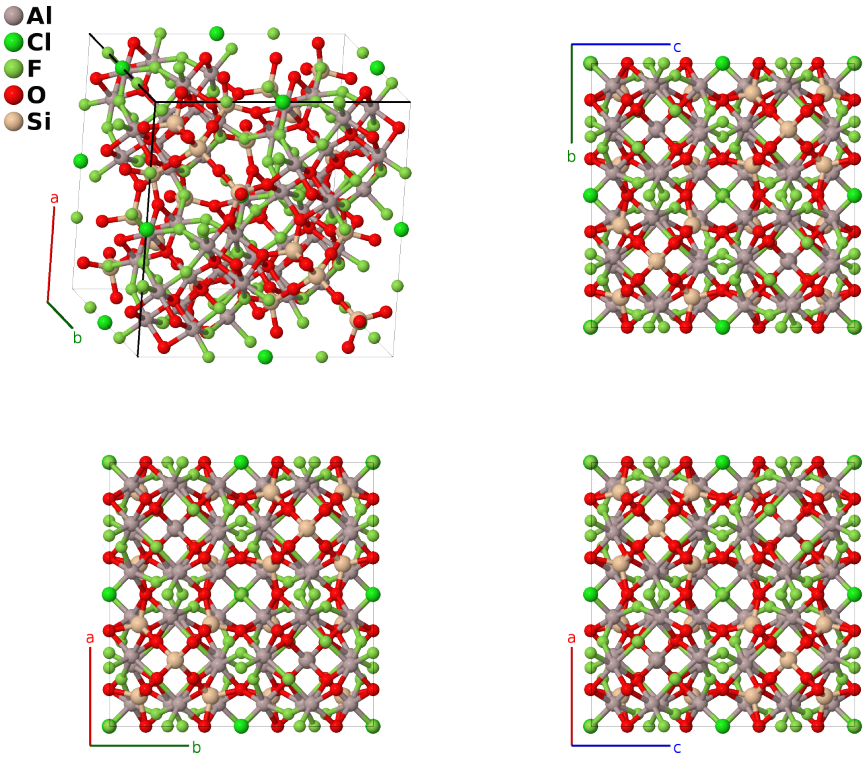
https://aflow.org/p/R5TJ

https://aflow.org/p/A13BC18D20E5_cF228_216_ah_c_gh_2eh_be-001

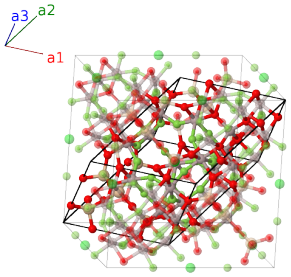


Prototype	$Al_{13}ClF_{18}O_{20}Si_5$
AFLOW prototype label	A13BC18D20E5_cF228_216_ah_c_gh_2eh_be-001
***Strukturbericht* designation**	$S0_8$
Mineral name	zunyite
ICSD	15745
Pearson symbol	cF228
Space group number	216
Space group symbol	$F\bar{4}3m$
AFLOW prototype command	`aflow --proto=A13BC18D20E5_cF228_216_ah_c_gh_2eh_be-001 --params=`$a, x_4, x_5, x_6, x_7, x_8, z_8, x_9, z_9, x_{10}, z_{10}$

- We use the structure proposed by (Kamb, 1960), a refinement of the original (Pauling, 1933) $S0_8$ structure. The only major difference is the y coordinate of the OH/F-I site, which is now at a more reasonable distance from the chlorine atom.
- For easy of visualization, we have used fluorine atoms to represent all of the $(OH,F)_{18}$ positions, but in reality the system is dominated by OH, not F. Kamb argues that the physics of hydrogen bonding makes it likely that the actual structure has composition $(OH)_{16}F_2$, with the fluorine atoms substituting for OH on the second (48h) site.

Face-centered Cubic primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(4a)	Al I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{2}a\,\hat{\mathbf{z}}$	(4b)	Si I
$\mathbf{B_3}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} + \frac{1}{4}a\,\hat{\mathbf{z}}$	(4c)	Cl I
$\mathbf{B_4}$	=	$x_4\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 + x_4\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}} + ax_4\,\hat{\mathbf{y}} + ax_4\,\hat{\mathbf{z}}$	(16e)	O I
$\mathbf{B_5}$	=	$x_4\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 - 3x_4\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}} - ax_4\,\hat{\mathbf{y}} + ax_4\,\hat{\mathbf{z}}$	(16e)	O I
$\mathbf{B_6}$	=	$x_4\,\mathbf{a}_1 - 3x_4\,\mathbf{a}_2 + x_4\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}} + ax_4\,\hat{\mathbf{y}} - ax_4\,\hat{\mathbf{z}}$	(16e)	O I
$\mathbf{B_7}$	=	$-3x_4\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 + x_4\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}} - ax_4\,\hat{\mathbf{y}} - ax_4\,\hat{\mathbf{z}}$	(16e)	O I
$\mathbf{B_8}$	=	$x_5\,\mathbf{a}_1 + x_5\,\mathbf{a}_2 + x_5\,\mathbf{a}_3$	=	$ax_5\,\hat{\mathbf{x}} + ax_5\,\hat{\mathbf{y}} + ax_5\,\hat{\mathbf{z}}$	(16e)	O II
$\mathbf{B_9}$	=	$x_5\,\mathbf{a}_1 + x_5\,\mathbf{a}_2 - 3x_5\,\mathbf{a}_3$	=	$-ax_5\,\hat{\mathbf{x}} - ax_5\,\hat{\mathbf{y}} + ax_5\,\hat{\mathbf{z}}$	(16e)	O II
$\mathbf{B_{10}}$	=	$x_5\,\mathbf{a}_1 - 3x_5\,\mathbf{a}_2 + x_5\,\mathbf{a}_3$	=	$-ax_5\,\hat{\mathbf{x}} + ax_5\,\hat{\mathbf{y}} - ax_5\,\hat{\mathbf{z}}$	(16e)	O II
$\mathbf{B_{11}}$	=	$-3x_5\,\mathbf{a}_1 + x_5\,\mathbf{a}_2 + x_5\,\mathbf{a}_3$	=	$ax_5\,\hat{\mathbf{x}} - ax_5\,\hat{\mathbf{y}} - ax_5\,\hat{\mathbf{z}}$	(16e)	O II
$\mathbf{B_{12}}$	=	$x_6\,\mathbf{a}_1 + x_6\,\mathbf{a}_2 + x_6\,\mathbf{a}_3$	=	$ax_6\,\hat{\mathbf{x}} + ax_6\,\hat{\mathbf{y}} + ax_6\,\hat{\mathbf{z}}$	(16e)	Si II
$\mathbf{B_{13}}$	=	$x_6\,\mathbf{a}_1 + x_6\,\mathbf{a}_2 - 3x_6\,\mathbf{a}_3$	=	$-ax_6\,\hat{\mathbf{x}} - ax_6\,\hat{\mathbf{y}} + ax_6\,\hat{\mathbf{z}}$	(16e)	Si II
$\mathbf{B_{14}}$	=	$x_6\,\mathbf{a}_1 - 3x_6\,\mathbf{a}_2 + x_6\,\mathbf{a}_3$	=	$-ax_6\,\hat{\mathbf{x}} + ax_6\,\hat{\mathbf{y}} - ax_6\,\hat{\mathbf{z}}$	(16e)	Si II
$\mathbf{B_{15}}$	=	$-3x_6\,\mathbf{a}_1 + x_6\,\mathbf{a}_2 + x_6\,\mathbf{a}_3$	=	$ax_6\,\hat{\mathbf{x}} - ax_6\,\hat{\mathbf{y}} - ax_6\,\hat{\mathbf{z}}$	(16e)	Si II
$\mathbf{B_{16}}$	=	$-\left(x_7 - \frac{1}{2}\right)\,\mathbf{a}_1 + x_7\,\mathbf{a}_2 + x_7\,\mathbf{a}_3$	=	$ax_7\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} + \frac{1}{4}a\,\hat{\mathbf{z}}$	(24g)	F I
$\mathbf{B_{17}}$	=	$x_7\,\mathbf{a}_1 - \left(x_7 - \frac{1}{2}\right)\,\mathbf{a}_2 - \left(x_7 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_7 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} + \frac{1}{4}a\,\hat{\mathbf{z}}$	(24g)	F I
$\mathbf{B_{18}}$	=	$x_7\,\mathbf{a}_1 - \left(x_7 - \frac{1}{2}\right)\,\mathbf{a}_2 + x_7\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + ax_7\,\hat{\mathbf{y}} + \frac{1}{4}a\,\hat{\mathbf{z}}$	(24g)	F I
$\mathbf{B_{19}}$	=	$-\left(x_7 - \frac{1}{2}\right)\,\mathbf{a}_1 + x_7\,\mathbf{a}_2 - \left(x_7 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} - a\left(x_7 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + \frac{1}{4}a\,\hat{\mathbf{z}}$	(24g)	F I
$\mathbf{B_{20}}$	=	$x_7\,\mathbf{a}_1 + x_7\,\mathbf{a}_2 - \left(x_7 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} + ax_7\,\hat{\mathbf{z}}$	(24g)	F I
$\mathbf{B_{21}}$	=	$-\left(x_7 - \frac{1}{2}\right)\,\mathbf{a}_1 - \left(x_7 - \frac{1}{2}\right)\,\mathbf{a}_2 + x_7\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} - a\left(x_7 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(24g)	F I
$\mathbf{B_{22}}$	=	$z_8\,\mathbf{a}_1 + z_8\,\mathbf{a}_2 + (2x_8 - z_8)\,\mathbf{a}_3$	=	$ax_8\,\hat{\mathbf{x}} + ax_8\,\hat{\mathbf{y}} + az_8\,\hat{\mathbf{z}}$	(48h)	Al II

$\mathbf{B_{23}}$	=	$z_8\,\mathbf{a}_1 + z_8\,\mathbf{a}_2 - (2x_8 + z_8)\,\mathbf{a}_3$	=	$-ax_8\,\hat{\mathbf{x}} - ax_8\,\hat{\mathbf{y}} + az_8\,\hat{\mathbf{z}}$	(48h)	Al II
$\mathbf{B_{24}}$	=	$(2x_8 - z_8)\,\mathbf{a}_1 - (2x_8 + z_8)\,\mathbf{a}_2 + z_8\,\mathbf{a}_3$	=	$-ax_8\,\hat{\mathbf{x}} + ax_8\,\hat{\mathbf{y}} - az_8\,\hat{\mathbf{z}}$	(48h)	Al II
$\mathbf{B_{25}}$	=	$-(2x_8 + z_8)\,\mathbf{a}_1 + (2x_8 - z_8)\,\mathbf{a}_2 + z_8\,\mathbf{a}_3$	=	$ax_8\,\hat{\mathbf{x}} - ax_8\,\hat{\mathbf{y}} - az_8\,\hat{\mathbf{z}}$	(48h)	Al II
$\mathbf{B_{26}}$	=	$(2x_8 - z_8)\,\mathbf{a}_1 + z_8\,\mathbf{a}_2 + z_8\,\mathbf{a}_3$	=	$az_8\,\hat{\mathbf{x}} + ax_8\,\hat{\mathbf{y}} + ax_8\,\hat{\mathbf{z}}$	(48h)	Al II
$\mathbf{B_{27}}$	=	$-(2x_8 + z_8)\,\mathbf{a}_1 + z_8\,\mathbf{a}_2 + z_8\,\mathbf{a}_3$	=	$az_8\,\hat{\mathbf{x}} - ax_8\,\hat{\mathbf{y}} - ax_8\,\hat{\mathbf{z}}$	(48h)	Al II
$\mathbf{B_{28}}$	=	$z_8\,\mathbf{a}_1 + (2x_8 - z_8)\,\mathbf{a}_2 - (2x_8 + z_8)\,\mathbf{a}_3$	=	$-az_8\,\hat{\mathbf{x}} - ax_8\,\hat{\mathbf{y}} + ax_8\,\hat{\mathbf{z}}$	(48h)	Al II
$\mathbf{B_{29}}$	=	$z_8\,\mathbf{a}_1 - (2x_8 + z_8)\,\mathbf{a}_2 + (2x_8 - z_8)\,\mathbf{a}_3$	=	$-az_8\,\hat{\mathbf{x}} + ax_8\,\hat{\mathbf{y}} - ax_8\,\hat{\mathbf{z}}$	(48h)	Al II
$\mathbf{B_{30}}$	=	$z_8\,\mathbf{a}_1 + (2x_8 - z_8)\,\mathbf{a}_2 + z_8\,\mathbf{a}_3$	=	$ax_8\,\hat{\mathbf{x}} + az_8\,\hat{\mathbf{y}} + ax_8\,\hat{\mathbf{z}}$	(48h)	Al II
$\mathbf{B_{31}}$	=	$z_8\,\mathbf{a}_1 - (2x_8 + z_8)\,\mathbf{a}_2 + z_8\,\mathbf{a}_3$	=	$-ax_8\,\hat{\mathbf{x}} + az_8\,\hat{\mathbf{y}} - ax_8\,\hat{\mathbf{z}}$	(48h)	Al II
$\mathbf{B_{32}}$	=	$-(2x_8 + z_8)\,\mathbf{a}_1 + z_8\,\mathbf{a}_2 + (2x_8 - z_8)\,\mathbf{a}_3$	=	$ax_8\,\hat{\mathbf{x}} - az_8\,\hat{\mathbf{y}} - ax_8\,\hat{\mathbf{z}}$	(48h)	Al II
$\mathbf{B_{33}}$	=	$(2x_8 - z_8)\,\mathbf{a}_1 + z_8\,\mathbf{a}_2 - (2x_8 + z_8)\,\mathbf{a}_3$	=	$-ax_8\,\hat{\mathbf{x}} - az_8\,\hat{\mathbf{y}} + ax_8\,\hat{\mathbf{z}}$	(48h)	Al II
$\mathbf{B_{34}}$	=	$z_9\,\mathbf{a}_1 + z_9\,\mathbf{a}_2 + (2x_9 - z_9)\,\mathbf{a}_3$	=	$ax_9\,\hat{\mathbf{x}} + ax_9\,\hat{\mathbf{y}} + az_9\,\hat{\mathbf{z}}$	(48h)	F II
$\mathbf{B_{35}}$	=	$z_9\,\mathbf{a}_1 + z_9\,\mathbf{a}_2 - (2x_9 + z_9)\,\mathbf{a}_3$	=	$-ax_9\,\hat{\mathbf{x}} - ax_9\,\hat{\mathbf{y}} + az_9\,\hat{\mathbf{z}}$	(48h)	F II
$\mathbf{B_{36}}$	=	$(2x_9 - z_9)\,\mathbf{a}_1 - (2x_9 + z_9)\,\mathbf{a}_2 + z_9\,\mathbf{a}_3$	=	$-ax_9\,\hat{\mathbf{x}} + ax_9\,\hat{\mathbf{y}} - az_9\,\hat{\mathbf{z}}$	(48h)	F II
$\mathbf{B_{37}}$	=	$-(2x_9 + z_9)\,\mathbf{a}_1 + (2x_9 - z_9)\,\mathbf{a}_2 + z_9\,\mathbf{a}_3$	=	$ax_9\,\hat{\mathbf{x}} - ax_9\,\hat{\mathbf{y}} - az_9\,\hat{\mathbf{z}}$	(48h)	F II
$\mathbf{B_{38}}$	=	$(2x_9 - z_9)\,\mathbf{a}_1 + z_9\,\mathbf{a}_2 + z_9\,\mathbf{a}_3$	=	$az_9\,\hat{\mathbf{x}} + ax_9\,\hat{\mathbf{y}} + ax_9\,\hat{\mathbf{z}}$	(48h)	F II
$\mathbf{B_{39}}$	=	$-(2x_9 + z_9)\,\mathbf{a}_1 + z_9\,\mathbf{a}_2 + z_9\,\mathbf{a}_3$	=	$az_9\,\hat{\mathbf{x}} - ax_9\,\hat{\mathbf{y}} - ax_9\,\hat{\mathbf{z}}$	(48h)	F II
$\mathbf{B_{40}}$	=	$z_9\,\mathbf{a}_1 + (2x_9 - z_9)\,\mathbf{a}_2 - (2x_9 + z_9)\,\mathbf{a}_3$	=	$-az_9\,\hat{\mathbf{x}} - ax_9\,\hat{\mathbf{y}} + ax_9\,\hat{\mathbf{z}}$	(48h)	F II
$\mathbf{B_{41}}$	=	$z_9\,\mathbf{a}_1 - (2x_9 + z_9)\,\mathbf{a}_2 + (2x_9 - z_9)\,\mathbf{a}_3$	=	$-az_9\,\hat{\mathbf{x}} + ax_9\,\hat{\mathbf{y}} - ax_9\,\hat{\mathbf{z}}$	(48h)	F II
$\mathbf{B_{42}}$	=	$z_9\,\mathbf{a}_1 + (2x_9 - z_9)\,\mathbf{a}_2 + z_9\,\mathbf{a}_3$	=	$ax_9\,\hat{\mathbf{x}} + az_9\,\hat{\mathbf{y}} + ax_9\,\hat{\mathbf{z}}$	(48h)	F II
$\mathbf{B_{43}}$	=	$z_9\,\mathbf{a}_1 - (2x_9 + z_9)\,\mathbf{a}_2 + z_9\,\mathbf{a}_3$	=	$-ax_9\,\hat{\mathbf{x}} + az_9\,\hat{\mathbf{y}} - ax_9\,\hat{\mathbf{z}}$	(48h)	F II
$\mathbf{B_{44}}$	=	$-(2x_9 + z_9)\,\mathbf{a}_1 + z_9\,\mathbf{a}_2 + (2x_9 - z_9)\,\mathbf{a}_3$	=	$ax_9\,\hat{\mathbf{x}} - az_9\,\hat{\mathbf{y}} - ax_9\,\hat{\mathbf{z}}$	(48h)	F II
$\mathbf{B_{45}}$	=	$(2x_9 - z_9)\,\mathbf{a}_1 + z_9\,\mathbf{a}_2 - (2x_9 + z_9)\,\mathbf{a}_3$	=	$-ax_9\,\hat{\mathbf{x}} - az_9\,\hat{\mathbf{y}} + ax_9\,\hat{\mathbf{z}}$	(48h)	F II
$\mathbf{B_{46}}$	=	$z_{10}\,\mathbf{a}_1 + z_{10}\,\mathbf{a}_2 + (2x_{10} - z_{10})\,\mathbf{a}_3$	=	$ax_{10}\,\hat{\mathbf{x}} + ax_{10}\,\hat{\mathbf{y}} + az_{10}\,\hat{\mathbf{z}}$	(48h)	O III
$\mathbf{B_{47}}$	=	$z_{10}\,\mathbf{a}_1 + z_{10}\,\mathbf{a}_2 - (2x_{10} + z_{10})\,\mathbf{a}_3$	=	$-ax_{10}\,\hat{\mathbf{x}} - ax_{10}\,\hat{\mathbf{y}} + az_{10}\,\hat{\mathbf{z}}$	(48h)	O III
$\mathbf{B_{48}}$	=	$(2x_{10} - z_{10})\,\mathbf{a}_1 - (2x_{10} + z_{10})\,\mathbf{a}_2 + z_{10}\,\mathbf{a}_3$	=	$-ax_{10}\,\hat{\mathbf{x}} + ax_{10}\,\hat{\mathbf{y}} - az_{10}\,\hat{\mathbf{z}}$	(48h)	O III
$\mathbf{B_{49}}$	=	$-(2x_{10} + z_{10})\,\mathbf{a}_1 + (2x_{10} - z_{10})\,\mathbf{a}_2 + z_{10}\,\mathbf{a}_3$	=	$ax_{10}\,\hat{\mathbf{x}} - ax_{10}\,\hat{\mathbf{y}} - az_{10}\,\hat{\mathbf{z}}$	(48h)	O III
$\mathbf{B_{50}}$	=	$(2x_{10} - z_{10})\,\mathbf{a}_1 + z_{10}\,\mathbf{a}_2 + z_{10}\,\mathbf{a}_3$	=	$az_{10}\,\hat{\mathbf{x}} + ax_{10}\,\hat{\mathbf{y}} + ax_{10}\,\hat{\mathbf{z}}$	(48h)	O III
$\mathbf{B_{51}}$	=	$-(2x_{10} + z_{10})\,\mathbf{a}_1 + z_{10}\,\mathbf{a}_2 + z_{10}\,\mathbf{a}_3$	=	$az_{10}\,\hat{\mathbf{x}} - ax_{10}\,\hat{\mathbf{y}} - ax_{10}\,\hat{\mathbf{z}}$	(48h)	O III
$\mathbf{B_{52}}$	=	$z_{10}\,\mathbf{a}_1 + (2x_{10} - z_{10})\,\mathbf{a}_2 - (2x_{10} + z_{10})\,\mathbf{a}_3$	=	$-az_{10}\,\hat{\mathbf{x}} - ax_{10}\,\hat{\mathbf{y}} + ax_{10}\,\hat{\mathbf{z}}$	(48h)	O III

$\mathbf{B_{53}}$	=	$z_{10}\,\mathbf{a}_1 - (2x_{10} + z_{10})\,\mathbf{a}_2 + (2x_{10} - z_{10})\,\mathbf{a}_3$	=	$-az_{10}\,\hat{\mathbf{x}} + ax_{10}\,\hat{\mathbf{y}} - ax_{10}\,\hat{\mathbf{z}}$	(48h)	O III
$\mathbf{B_{54}}$	=	$z_{10}\,\mathbf{a}_1 + (2x_{10} - z_{10})\,\mathbf{a}_2 + z_{10}\,\mathbf{a}_3$	=	$ax_{10}\,\hat{\mathbf{x}} + az_{10}\,\hat{\mathbf{y}} + ax_{10}\,\hat{\mathbf{z}}$	(48h)	O III
$\mathbf{B_{55}}$	=	$z_{10}\,\mathbf{a}_1 - (2x_{10} + z_{10})\,\mathbf{a}_2 + z_{10}\,\mathbf{a}_3$	=	$-ax_{10}\,\hat{\mathbf{x}} + az_{10}\,\hat{\mathbf{y}} - ax_{10}\,\hat{\mathbf{z}}$	(48h)	O III
$\mathbf{B_{56}}$	=	$-(2x_{10} + z_{10})\,\mathbf{a}_1 + z_{10}\,\mathbf{a}_2 + (2x_{10} - z_{10})\,\mathbf{a}_3$	=	$ax_{10}\,\hat{\mathbf{x}} - az_{10}\,\hat{\mathbf{y}} - ax_{10}\,\hat{\mathbf{z}}$	(48h)	O III
$\mathbf{B_{57}}$	=	$(2x_{10} - z_{10})\,\mathbf{a}_1 + z_{10}\,\mathbf{a}_2 - (2x_{10} + z_{10})\,\mathbf{a}_3$	=	$-ax_{10}\,\hat{\mathbf{x}} - az_{10}\,\hat{\mathbf{y}} + ax_{10}\,\hat{\mathbf{z}}$	(48h)	O III

References

[1] W. B. Kamb, *The Crystal Structure of Zunyite*, Acta Cryst. **13**, 15–24 (1960), doi:10.1107/S0365110X60000030.

[2] L. Pauling, *The Crystal Structure of Zunyite*, Z. Kristallogr. **84**, 442–452 (1933), doi:10.1524/zkri.1933.84.1.442.