

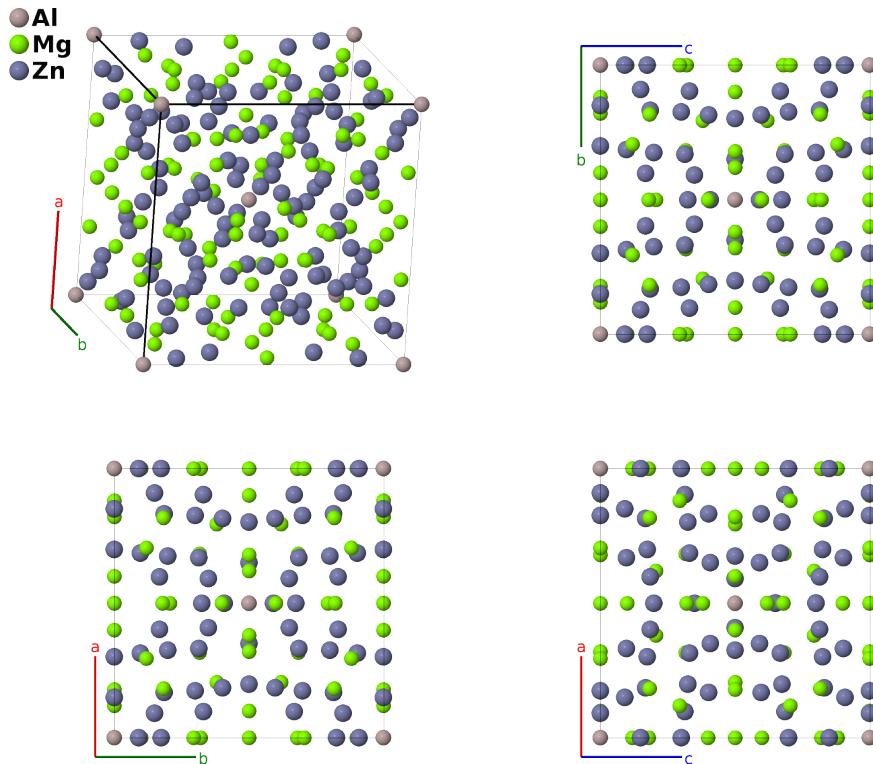
Bergman [Mg₃₂(Al,Zn)₄₉] Structure: AB32C48_cI162_204_a_2efg_2gh-001

This structure originally had the label AB32C48_cI162_204_a_2efg_2gh. Calls to that address will be redirected here.

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<https://aflow.org/p/9AQF>

https://aflow.org/p/AB32C48_cI162_204_a_2efg_2gh-001



Prototype	AlMg ₃₂ Zn ₄₈
AFLOW prototype label	AB32C48_cI162_204_a_2efg_2gh-001
Strukturbericht designation	D8 _e
Mineral name	bergman structure
ICSD	57968
Pearson symbol	cI162
Space group number	204
Space group symbol	$Im\bar{3}$
AFLOW prototype command	<code>aflow --proto=AB32C48_cI162_204_a_2efg_2gh-001 --params=a,x₂,x₃,x₄,y₅,z₅,y₆,z₆,y₇,z₇,x₈,y₈,z₈</code>

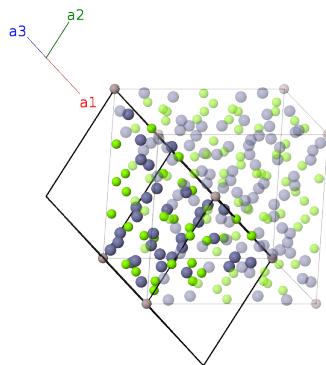
Other compounds with this structure

$\text{Li}_{20}\text{Mg}_6\text{Cu}_{13}\text{Al}_{42}$, Al_5CuLi_3

- Most of the sites in this lattice have random occupancy. In particular, according to (Bergman, 1957): The Al-I (2a) site is only occupied 80% of the time, the Zn-I (24g) site is occupied by Al 19% of the time, the Zn-II (24g) site is occupied by Al 43% of the time, and the Zn-III (48h) site is occupied by Al 36% of the time.
- The $\text{Li}_{20}\text{Mg}_6\text{Cu}_{13}\text{Al}_{42}$ structure found by (Pavlyuk, 2019) has all sites fully occupied.

Body-centered Cubic primitive vectors

$$\begin{aligned}\mathbf{a}_1 &= -\frac{1}{2}a\hat{\mathbf{x}} + \frac{1}{2}a\hat{\mathbf{y}} + \frac{1}{2}a\hat{\mathbf{z}} \\ \mathbf{a}_2 &= \frac{1}{2}a\hat{\mathbf{x}} - \frac{1}{2}a\hat{\mathbf{y}} + \frac{1}{2}a\hat{\mathbf{z}} \\ \mathbf{a}_3 &= \frac{1}{2}a\hat{\mathbf{x}} + \frac{1}{2}a\hat{\mathbf{y}} - \frac{1}{2}a\hat{\mathbf{z}}\end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
\mathbf{B}_1	= 0	=	0	(2a)	Al I
\mathbf{B}_2	= $\frac{1}{2}\mathbf{a}_1 + (x_2 + \frac{1}{2})\mathbf{a}_2 + x_2\mathbf{a}_3$	=	$ax_2\hat{\mathbf{x}} + \frac{1}{2}a\hat{\mathbf{z}}$	(12e)	Mg I
\mathbf{B}_3	= $\frac{1}{2}\mathbf{a}_1 - (x_2 - \frac{1}{2})\mathbf{a}_2 - x_2\mathbf{a}_3$	=	$-ax_2\hat{\mathbf{x}} + \frac{1}{2}a\hat{\mathbf{z}}$	(12e)	Mg I
\mathbf{B}_4	= $x_2\mathbf{a}_1 + \frac{1}{2}\mathbf{a}_2 + (x_2 + \frac{1}{2})\mathbf{a}_3$	=	$\frac{1}{2}a\hat{\mathbf{x}} + ax_2\hat{\mathbf{y}}$	(12e)	Mg I
\mathbf{B}_5	= $-x_2\mathbf{a}_1 + \frac{1}{2}\mathbf{a}_2 - (x_2 - \frac{1}{2})\mathbf{a}_3$	=	$\frac{1}{2}a\hat{\mathbf{x}} - ax_2\hat{\mathbf{y}}$	(12e)	Mg I
\mathbf{B}_6	= $(x_2 + \frac{1}{2})\mathbf{a}_1 + x_2\mathbf{a}_2 + \frac{1}{2}\mathbf{a}_3$	=	$\frac{1}{2}a\hat{\mathbf{y}} + ax_2\hat{\mathbf{z}}$	(12e)	Mg I
\mathbf{B}_7	= $-(x_2 - \frac{1}{2})\mathbf{a}_1 - x_2\mathbf{a}_2 + \frac{1}{2}\mathbf{a}_3$	=	$\frac{1}{2}a\hat{\mathbf{y}} - ax_2\hat{\mathbf{z}}$	(12e)	Mg I
\mathbf{B}_8	= $\frac{1}{2}\mathbf{a}_1 + (x_3 + \frac{1}{2})\mathbf{a}_2 + x_3\mathbf{a}_3$	=	$ax_3\hat{\mathbf{x}} + \frac{1}{2}a\hat{\mathbf{z}}$	(12e)	Mg II
\mathbf{B}_9	= $\frac{1}{2}\mathbf{a}_1 - (x_3 - \frac{1}{2})\mathbf{a}_2 - x_3\mathbf{a}_3$	=	$-ax_3\hat{\mathbf{x}} + \frac{1}{2}a\hat{\mathbf{z}}$	(12e)	Mg II
\mathbf{B}_{10}	= $x_3\mathbf{a}_1 + \frac{1}{2}\mathbf{a}_2 + (x_3 + \frac{1}{2})\mathbf{a}_3$	=	$\frac{1}{2}a\hat{\mathbf{x}} + ax_3\hat{\mathbf{y}}$	(12e)	Mg II
\mathbf{B}_{11}	= $-x_3\mathbf{a}_1 + \frac{1}{2}\mathbf{a}_2 - (x_3 - \frac{1}{2})\mathbf{a}_3$	=	$\frac{1}{2}a\hat{\mathbf{x}} - ax_3\hat{\mathbf{y}}$	(12e)	Mg II
\mathbf{B}_{12}	= $(x_3 + \frac{1}{2})\mathbf{a}_1 + x_3\mathbf{a}_2 + \frac{1}{2}\mathbf{a}_3$	=	$\frac{1}{2}a\hat{\mathbf{y}} + ax_3\hat{\mathbf{z}}$	(12e)	Mg II
\mathbf{B}_{13}	= $-(x_3 - \frac{1}{2})\mathbf{a}_1 - x_3\mathbf{a}_2 + \frac{1}{2}\mathbf{a}_3$	=	$\frac{1}{2}a\hat{\mathbf{y}} - ax_3\hat{\mathbf{z}}$	(12e)	Mg II
\mathbf{B}_{14}	= $2x_4\mathbf{a}_1 + 2x_4\mathbf{a}_2 + 2x_4\mathbf{a}_3$	=	$ax_4\hat{\mathbf{x}} + ax_4\hat{\mathbf{y}} + ax_4\hat{\mathbf{z}}$	(16f)	Mg III
\mathbf{B}_{15}	= $-2x_4\mathbf{a}_3$	=	$-ax_4\hat{\mathbf{x}} - ax_4\hat{\mathbf{y}} + ax_4\hat{\mathbf{z}}$	(16f)	Mg III
\mathbf{B}_{16}	= $-2x_4\mathbf{a}_2$	=	$-ax_4\hat{\mathbf{x}} + ax_4\hat{\mathbf{y}} - ax_4\hat{\mathbf{z}}$	(16f)	Mg III
\mathbf{B}_{17}	= $-2x_4\mathbf{a}_1$	=	$ax_4\hat{\mathbf{x}} - ax_4\hat{\mathbf{y}} - ax_4\hat{\mathbf{z}}$	(16f)	Mg III
\mathbf{B}_{18}	= $-2x_4\mathbf{a}_1 - 2x_4\mathbf{a}_2 - 2x_4\mathbf{a}_3$	=	$-ax_4\hat{\mathbf{x}} - ax_4\hat{\mathbf{y}} - ax_4\hat{\mathbf{z}}$	(16f)	Mg III
\mathbf{B}_{19}	= $2x_4\mathbf{a}_3$	=	$ax_4\hat{\mathbf{x}} + ax_4\hat{\mathbf{y}} - ax_4\hat{\mathbf{z}}$	(16f)	Mg III
\mathbf{B}_{20}	= $2x_4\mathbf{a}_2$	=	$ax_4\hat{\mathbf{x}} - ax_4\hat{\mathbf{y}} + ax_4\hat{\mathbf{z}}$	(16f)	Mg III
\mathbf{B}_{21}	= $2x_4\mathbf{a}_1$	=	$-ax_4\hat{\mathbf{x}} + ax_4\hat{\mathbf{y}} + ax_4\hat{\mathbf{z}}$	(16f)	Mg III

\mathbf{B}_{22}	$(y_5 + z_5) \mathbf{a}_1 + z_5 \mathbf{a}_2 + y_5 \mathbf{a}_3$	$=$	$ay_5 \hat{\mathbf{y}} + az_5 \hat{\mathbf{z}}$	(24g)	Mg IV
\mathbf{B}_{23}	$-(y_5 - z_5) \mathbf{a}_1 + z_5 \mathbf{a}_2 - y_5 \mathbf{a}_3$	$=$	$-ay_5 \hat{\mathbf{y}} + az_5 \hat{\mathbf{z}}$	(24g)	Mg IV
\mathbf{B}_{24}	$(y_5 - z_5) \mathbf{a}_1 - z_5 \mathbf{a}_2 + y_5 \mathbf{a}_3$	$=$	$ay_5 \hat{\mathbf{y}} - az_5 \hat{\mathbf{z}}$	(24g)	Mg IV
\mathbf{B}_{25}	$-(y_5 + z_5) \mathbf{a}_1 - z_5 \mathbf{a}_2 - y_5 \mathbf{a}_3$	$=$	$-ay_5 \hat{\mathbf{y}} - az_5 \hat{\mathbf{z}}$	(24g)	Mg IV
\mathbf{B}_{26}	$y_5 \mathbf{a}_1 + (y_5 + z_5) \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$az_5 \hat{\mathbf{x}} + ay_5 \hat{\mathbf{z}}$	(24g)	Mg IV
\mathbf{B}_{27}	$-y_5 \mathbf{a}_1 - (y_5 - z_5) \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$az_5 \hat{\mathbf{x}} - ay_5 \hat{\mathbf{z}}$	(24g)	Mg IV
\mathbf{B}_{28}	$y_5 \mathbf{a}_1 + (y_5 - z_5) \mathbf{a}_2 - z_5 \mathbf{a}_3$	$=$	$-az_5 \hat{\mathbf{x}} + ay_5 \hat{\mathbf{z}}$	(24g)	Mg IV
\mathbf{B}_{29}	$-y_5 \mathbf{a}_1 - (y_5 + z_5) \mathbf{a}_2 - z_5 \mathbf{a}_3$	$=$	$-az_5 \hat{\mathbf{x}} - ay_5 \hat{\mathbf{z}}$	(24g)	Mg IV
\mathbf{B}_{30}	$z_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + (y_5 + z_5) \mathbf{a}_3$	$=$	$ay_5 \hat{\mathbf{x}} + az_5 \hat{\mathbf{y}}$	(24g)	Mg IV
\mathbf{B}_{31}	$z_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 - (y_5 - z_5) \mathbf{a}_3$	$=$	$-ay_5 \hat{\mathbf{x}} + az_5 \hat{\mathbf{y}}$	(24g)	Mg IV
\mathbf{B}_{32}	$-z_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + (y_5 - z_5) \mathbf{a}_3$	$=$	$ay_5 \hat{\mathbf{x}} - az_5 \hat{\mathbf{y}}$	(24g)	Mg IV
\mathbf{B}_{33}	$-z_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 - (y_5 + z_5) \mathbf{a}_3$	$=$	$-ay_5 \hat{\mathbf{x}} - az_5 \hat{\mathbf{y}}$	(24g)	Mg IV
\mathbf{B}_{34}	$(y_6 + z_6) \mathbf{a}_1 + z_6 \mathbf{a}_2 + y_6 \mathbf{a}_3$	$=$	$ay_6 \hat{\mathbf{y}} + az_6 \hat{\mathbf{z}}$	(24g)	Zn I
\mathbf{B}_{35}	$-(y_6 - z_6) \mathbf{a}_1 + z_6 \mathbf{a}_2 - y_6 \mathbf{a}_3$	$=$	$-ay_6 \hat{\mathbf{y}} + az_6 \hat{\mathbf{z}}$	(24g)	Zn I
\mathbf{B}_{36}	$(y_6 - z_6) \mathbf{a}_1 - z_6 \mathbf{a}_2 + y_6 \mathbf{a}_3$	$=$	$ay_6 \hat{\mathbf{y}} - az_6 \hat{\mathbf{z}}$	(24g)	Zn I
\mathbf{B}_{37}	$-(y_6 + z_6) \mathbf{a}_1 - z_6 \mathbf{a}_2 - y_6 \mathbf{a}_3$	$=$	$-ay_6 \hat{\mathbf{y}} - az_6 \hat{\mathbf{z}}$	(24g)	Zn I
\mathbf{B}_{38}	$y_6 \mathbf{a}_1 + (y_6 + z_6) \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$az_6 \hat{\mathbf{x}} + ay_6 \hat{\mathbf{z}}$	(24g)	Zn I
\mathbf{B}_{39}	$-y_6 \mathbf{a}_1 - (y_6 - z_6) \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$az_6 \hat{\mathbf{x}} - ay_6 \hat{\mathbf{z}}$	(24g)	Zn I
\mathbf{B}_{40}	$y_6 \mathbf{a}_1 + (y_6 - z_6) \mathbf{a}_2 - z_6 \mathbf{a}_3$	$=$	$-az_6 \hat{\mathbf{x}} + ay_6 \hat{\mathbf{z}}$	(24g)	Zn I
\mathbf{B}_{41}	$-y_6 \mathbf{a}_1 - (y_6 + z_6) \mathbf{a}_2 - z_6 \mathbf{a}_3$	$=$	$-az_6 \hat{\mathbf{x}} - ay_6 \hat{\mathbf{z}}$	(24g)	Zn I
\mathbf{B}_{42}	$z_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 + (y_6 + z_6) \mathbf{a}_3$	$=$	$ay_6 \hat{\mathbf{x}} + az_6 \hat{\mathbf{y}}$	(24g)	Zn I
\mathbf{B}_{43}	$z_6 \mathbf{a}_1 - y_6 \mathbf{a}_2 - (y_6 - z_6) \mathbf{a}_3$	$=$	$-ay_6 \hat{\mathbf{x}} + az_6 \hat{\mathbf{y}}$	(24g)	Zn I
\mathbf{B}_{44}	$-z_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 + (y_6 - z_6) \mathbf{a}_3$	$=$	$ay_6 \hat{\mathbf{x}} - az_6 \hat{\mathbf{y}}$	(24g)	Zn I
\mathbf{B}_{45}	$-z_6 \mathbf{a}_1 - y_6 \mathbf{a}_2 - (y_6 + z_6) \mathbf{a}_3$	$=$	$-ay_6 \hat{\mathbf{x}} - az_6 \hat{\mathbf{y}}$	(24g)	Zn I
\mathbf{B}_{46}	$(y_7 + z_7) \mathbf{a}_1 + z_7 \mathbf{a}_2 + y_7 \mathbf{a}_3$	$=$	$ay_7 \hat{\mathbf{y}} + az_7 \hat{\mathbf{z}}$	(24g)	Zn II
\mathbf{B}_{47}	$-(y_7 - z_7) \mathbf{a}_1 + z_7 \mathbf{a}_2 - y_7 \mathbf{a}_3$	$=$	$-ay_7 \hat{\mathbf{y}} + az_7 \hat{\mathbf{z}}$	(24g)	Zn II
\mathbf{B}_{48}	$(y_7 - z_7) \mathbf{a}_1 - z_7 \mathbf{a}_2 + y_7 \mathbf{a}_3$	$=$	$ay_7 \hat{\mathbf{y}} - az_7 \hat{\mathbf{z}}$	(24g)	Zn II
\mathbf{B}_{49}	$-(y_7 + z_7) \mathbf{a}_1 - z_7 \mathbf{a}_2 - y_7 \mathbf{a}_3$	$=$	$-ay_7 \hat{\mathbf{y}} - az_7 \hat{\mathbf{z}}$	(24g)	Zn II
\mathbf{B}_{50}	$y_7 \mathbf{a}_1 + (y_7 + z_7) \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$az_7 \hat{\mathbf{x}} + ay_7 \hat{\mathbf{z}}$	(24g)	Zn II
\mathbf{B}_{51}	$-y_7 \mathbf{a}_1 - (y_7 - z_7) \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$az_7 \hat{\mathbf{x}} - ay_7 \hat{\mathbf{z}}$	(24g)	Zn II
\mathbf{B}_{52}	$y_7 \mathbf{a}_1 + (y_7 - z_7) \mathbf{a}_2 - z_7 \mathbf{a}_3$	$=$	$-az_7 \hat{\mathbf{x}} + ay_7 \hat{\mathbf{z}}$	(24g)	Zn II
\mathbf{B}_{53}	$-y_7 \mathbf{a}_1 - (y_7 + z_7) \mathbf{a}_2 - z_7 \mathbf{a}_3$	$=$	$-az_7 \hat{\mathbf{x}} - ay_7 \hat{\mathbf{z}}$	(24g)	Zn II
\mathbf{B}_{54}	$z_7 \mathbf{a}_1 + y_7 \mathbf{a}_2 + (y_7 + z_7) \mathbf{a}_3$	$=$	$ay_7 \hat{\mathbf{x}} + az_7 \hat{\mathbf{y}}$	(24g)	Zn II
\mathbf{B}_{55}	$z_7 \mathbf{a}_1 - y_7 \mathbf{a}_2 - (y_7 - z_7) \mathbf{a}_3$	$=$	$-ay_7 \hat{\mathbf{x}} + az_7 \hat{\mathbf{y}}$	(24g)	Zn II
\mathbf{B}_{56}	$-z_7 \mathbf{a}_1 + y_7 \mathbf{a}_2 + (y_7 - z_7) \mathbf{a}_3$	$=$	$ay_7 \hat{\mathbf{x}} - az_7 \hat{\mathbf{y}}$	(24g)	Zn II
\mathbf{B}_{57}	$-z_7 \mathbf{a}_1 - y_7 \mathbf{a}_2 - (y_7 + z_7) \mathbf{a}_3$	$=$	$-ay_7 \hat{\mathbf{x}} - az_7 \hat{\mathbf{y}}$	(24g)	Zn II
\mathbf{B}_{58}	$(y_8 + z_8) \mathbf{a}_1 + (x_8 + z_8) \mathbf{a}_2 + (x_8 + y_8) \mathbf{a}_3$	$=$	$ax_8 \hat{\mathbf{x}} + ay_8 \hat{\mathbf{y}} + az_8 \hat{\mathbf{z}}$	(48h)	Zn III
\mathbf{B}_{59}	$-(y_8 - z_8) \mathbf{a}_1 - (x_8 - z_8) \mathbf{a}_2 - (x_8 + y_8) \mathbf{a}_3$	$=$	$-ax_8 \hat{\mathbf{x}} - ay_8 \hat{\mathbf{y}} + az_8 \hat{\mathbf{z}}$	(48h)	Zn III
\mathbf{B}_{60}	$(y_8 - z_8) \mathbf{a}_1 - (x_8 + z_8) \mathbf{a}_2 - (x_8 - y_8) \mathbf{a}_3$	$=$	$-ax_8 \hat{\mathbf{x}} + ays_8 \hat{\mathbf{y}} - az_8 \hat{\mathbf{z}}$	(48h)	Zn III

\mathbf{B}_{61}	$= -(y_8 + z_8) \mathbf{a}_1 + (x_8 - z_8) \mathbf{a}_2 + (x_8 - y_8) \mathbf{a}_3$	$=$	$ax_8 \hat{\mathbf{x}} - ay_8 \hat{\mathbf{y}} - az_8 \hat{\mathbf{z}}$	(48h)	Zn III
\mathbf{B}_{62}	$= (x_8 + y_8) \mathbf{a}_1 + (y_8 + z_8) \mathbf{a}_2 + (x_8 + z_8) \mathbf{a}_3$	$=$	$az_8 \hat{\mathbf{x}} + ax_8 \hat{\mathbf{y}} + ay_8 \hat{\mathbf{z}}$	(48h)	Zn III
\mathbf{B}_{63}	$= -(x_8 + y_8) \mathbf{a}_1 - (y_8 - z_8) \mathbf{a}_2 - (x_8 - z_8) \mathbf{a}_3$	$=$	$az_8 \hat{\mathbf{x}} - ax_8 \hat{\mathbf{y}} - ay_8 \hat{\mathbf{z}}$	(48h)	Zn III
\mathbf{B}_{64}	$= -(x_8 - y_8) \mathbf{a}_1 + (y_8 - z_8) \mathbf{a}_2 - (x_8 + z_8) \mathbf{a}_3$	$=$	$-az_8 \hat{\mathbf{x}} - ax_8 \hat{\mathbf{y}} + ay_8 \hat{\mathbf{z}}$	(48h)	Zn III
\mathbf{B}_{65}	$= (x_8 - y_8) \mathbf{a}_1 - (y_8 + z_8) \mathbf{a}_2 + (x_8 - z_8) \mathbf{a}_3$	$=$	$-az_8 \hat{\mathbf{x}} + ax_8 \hat{\mathbf{y}} - ay_8 \hat{\mathbf{z}}$	(48h)	Zn III
\mathbf{B}_{66}	$= (x_8 + z_8) \mathbf{a}_1 + (x_8 + y_8) \mathbf{a}_2 + (y_8 + z_8) \mathbf{a}_3$	$=$	$ay_8 \hat{\mathbf{x}} + az_8 \hat{\mathbf{y}} + ax_8 \hat{\mathbf{z}}$	(48h)	Zn III
\mathbf{B}_{67}	$= -(x_8 - z_8) \mathbf{a}_1 - (x_8 + y_8) \mathbf{a}_2 - (y_8 - z_8) \mathbf{a}_3$	$=$	$-ay_8 \hat{\mathbf{x}} + az_8 \hat{\mathbf{y}} - ax_8 \hat{\mathbf{z}}$	(48h)	Zn III
\mathbf{B}_{68}	$= -(x_8 + z_8) \mathbf{a}_1 - (x_8 - y_8) \mathbf{a}_2 + (y_8 - z_8) \mathbf{a}_3$	$=$	$ay_8 \hat{\mathbf{x}} - az_8 \hat{\mathbf{y}} - ax_8 \hat{\mathbf{z}}$	(48h)	Zn III
\mathbf{B}_{69}	$= (x_8 - z_8) \mathbf{a}_1 + (x_8 - y_8) \mathbf{a}_2 - (y_8 + z_8) \mathbf{a}_3$	$=$	$-ay_8 \hat{\mathbf{x}} - az_8 \hat{\mathbf{y}} + ax_8 \hat{\mathbf{z}}$	(48h)	Zn III
\mathbf{B}_{70}	$= -(y_8 + z_8) \mathbf{a}_1 - (x_8 + z_8) \mathbf{a}_2 - (x_8 + y_8) \mathbf{a}_3$	$=$	$-ax_8 \hat{\mathbf{x}} - ay_8 \hat{\mathbf{y}} - az_8 \hat{\mathbf{z}}$	(48h)	Zn III
\mathbf{B}_{71}	$= (y_8 - z_8) \mathbf{a}_1 + (x_8 - z_8) \mathbf{a}_2 + (x_8 + y_8) \mathbf{a}_3$	$=$	$ax_8 \hat{\mathbf{x}} + ay_8 \hat{\mathbf{y}} - az_8 \hat{\mathbf{z}}$	(48h)	Zn III
\mathbf{B}_{72}	$= -(y_8 - z_8) \mathbf{a}_1 + (x_8 + z_8) \mathbf{a}_2 + (x_8 - y_8) \mathbf{a}_3$	$=$	$ax_8 \hat{\mathbf{x}} - ay_8 \hat{\mathbf{y}} + az_8 \hat{\mathbf{z}}$	(48h)	Zn III
\mathbf{B}_{73}	$= (y_8 + z_8) \mathbf{a}_1 - (x_8 - z_8) \mathbf{a}_2 - (x_8 - y_8) \mathbf{a}_3$	$=$	$-ax_8 \hat{\mathbf{x}} + ay_8 \hat{\mathbf{y}} + az_8 \hat{\mathbf{z}}$	(48h)	Zn III
\mathbf{B}_{74}	$= -(x_8 + y_8) \mathbf{a}_1 - (y_8 + z_8) \mathbf{a}_2 - (x_8 + z_8) \mathbf{a}_3$	$=$	$-az_8 \hat{\mathbf{x}} - ax_8 \hat{\mathbf{y}} - ay_8 \hat{\mathbf{z}}$	(48h)	Zn III
\mathbf{B}_{75}	$= (x_8 + y_8) \mathbf{a}_1 + (y_8 - z_8) \mathbf{a}_2 + (x_8 - z_8) \mathbf{a}_3$	$=$	$-az_8 \hat{\mathbf{x}} + ax_8 \hat{\mathbf{y}} + ay_8 \hat{\mathbf{z}}$	(48h)	Zn III
\mathbf{B}_{76}	$= (x_8 - y_8) \mathbf{a}_1 - (y_8 - z_8) \mathbf{a}_2 + (x_8 + z_8) \mathbf{a}_3$	$=$	$az_8 \hat{\mathbf{x}} + ax_8 \hat{\mathbf{y}} - ay_8 \hat{\mathbf{z}}$	(48h)	Zn III
\mathbf{B}_{77}	$= -(x_8 - y_8) \mathbf{a}_1 + (y_8 + z_8) \mathbf{a}_2 - (x_8 - z_8) \mathbf{a}_3$	$=$	$az_8 \hat{\mathbf{x}} - ax_8 \hat{\mathbf{y}} + ay_8 \hat{\mathbf{z}}$	(48h)	Zn III
\mathbf{B}_{78}	$= -(x_8 + z_8) \mathbf{a}_1 - (x_8 + y_8) \mathbf{a}_2 - (y_8 + z_8) \mathbf{a}_3$	$=$	$-ay_8 \hat{\mathbf{x}} - az_8 \hat{\mathbf{y}} - ax_8 \hat{\mathbf{z}}$	(48h)	Zn III
\mathbf{B}_{79}	$= (x_8 - z_8) \mathbf{a}_1 + (x_8 + y_8) \mathbf{a}_2 + (y_8 - z_8) \mathbf{a}_3$	$=$	$ay_8 \hat{\mathbf{x}} - az_8 \hat{\mathbf{y}} + ax_8 \hat{\mathbf{z}}$	(48h)	Zn III
\mathbf{B}_{80}	$= (x_8 + z_8) \mathbf{a}_1 + (x_8 - y_8) \mathbf{a}_2 - (y_8 - z_8) \mathbf{a}_3$	$=$	$-ay_8 \hat{\mathbf{x}} + az_8 \hat{\mathbf{y}} + ax_8 \hat{\mathbf{z}}$	(48h)	Zn III
\mathbf{B}_{81}	$= -(x_8 - z_8) \mathbf{a}_1 - (x_8 - y_8) \mathbf{a}_2 + (y_8 + z_8) \mathbf{a}_3$	$=$	$ay_8 \hat{\mathbf{x}} + az_8 \hat{\mathbf{y}} - ax_8 \hat{\mathbf{z}}$	(48h)	Zn III

References

- [1] G. Bergman, J. L. T. Waugh, and L. Pauling, *The crystal structure of the metallic phase Mg₃₂(Al,Zn)₄₉* **10**, 254–9 (1957), doi:10.1107/S0365110X57000808.
- [2] N. Pavlyuk, G. Dmytriv, V. Pavlyuk, and H. Ehrenberg, *Li₂₀Mg₆Cu₁₃Al₄₂: a new ordered quaternary superstructure to the icosahedral T-Mg₃₂(Zn,Al)₄₉ phase with fullerene-like Al₆₀ cluster*, *Acta Crystallogr. Sect. B* **75**, 168–174 (2019),

