

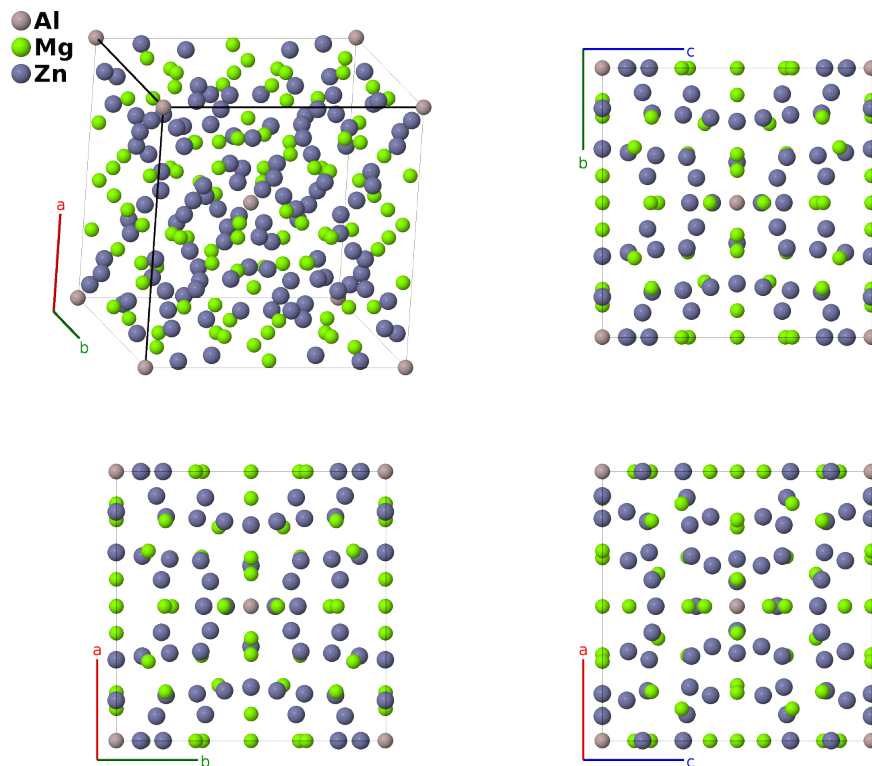
# Bergman $[\text{Mg}_{32}(\text{Al},\text{Zn})_{49}]$ Structure: AB32C48\_cI162\_204\_a\_2efg\_2gh-001

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](https://aflow.org/p/AB32C48_cI162_204_a_2efg_2gh-001)



Prototype	$\text{AlMg}_{32}\text{Zn}_{48}$
AFLOW prototype label	AB32C48_cI162_204_a_2efg_2gh-001
<i>Strukturbericht</i> 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>

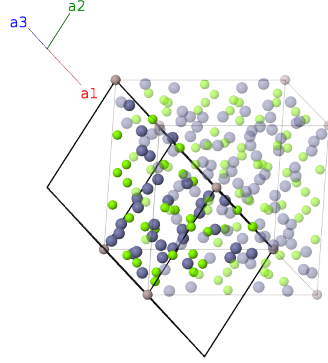
## Other compounds with this structure

$\text{Li}_{20}\text{Mg}_6\text{Cu}_{13}\text{Al}_{42}$ ,  $\text{Al}_5\text{CuLi}_3$

- 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



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

## References

- [1] G. Bergman, J. L. T. Waugh, and L. Pauling, *The crystal structure of the metallic phase Mg<sub>32</sub>(Al,Zn)<sub>49</sub>* **10**, 254–9 (1957), doi:10.1107/S0365110X57000808.
- [2] N. Pavlyuk, G. Dmytriv, V. Pavlyuk, and H. Ehrenberg, *Li<sub>20</sub>Mg<sub>6</sub>Cu<sub>13</sub>Al<sub>42</sub>: a new ordered quaternary superstructure to the icosahedral T-Mg<sub>32</sub>(Zn,Al)<sub>49</sub> phase with fullerene-like Al<sub>60</sub> cluster*, *Acta Crystallogr. Sect. B* **75**, 168–174 (2019),

doi:10.1107/S2052520619000349.