

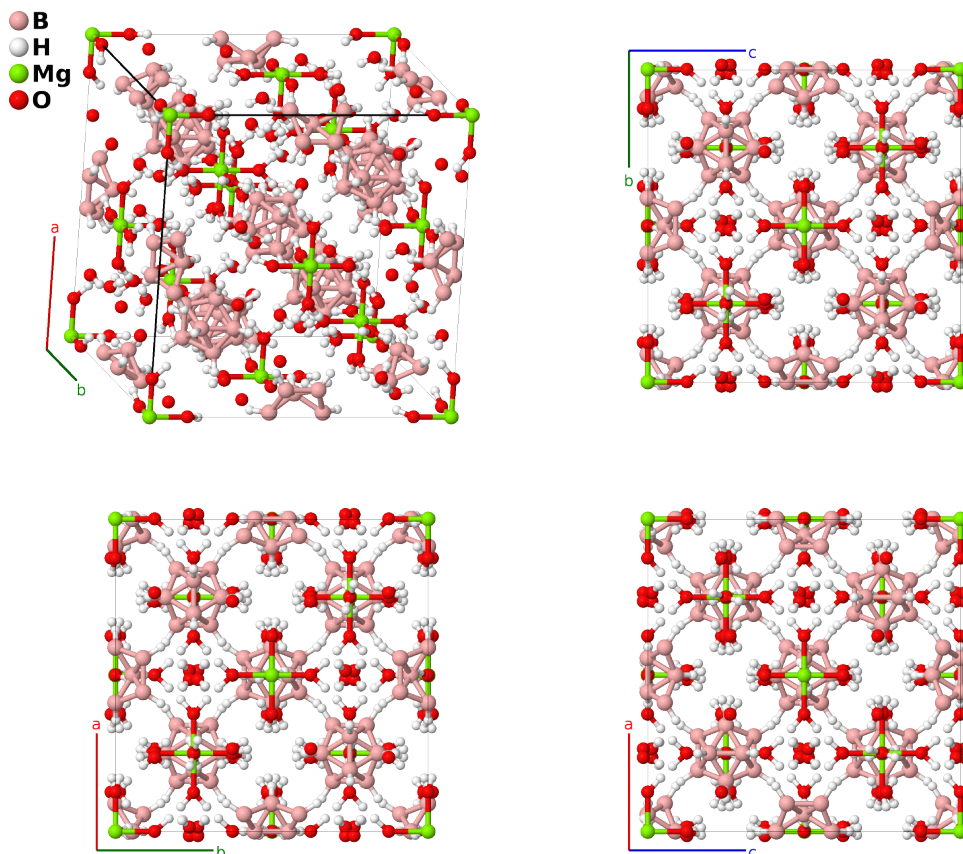
# MgB<sub>12</sub>H<sub>12</sub>[H<sub>2</sub>O]<sub>12</sub> Structure: A12B36CD12\_cF488\_210\_h\_3h\_a\_fg-001

This structure originally had the label A12B36CD12\_cF488\_210\_h\_3h\_a\_fg. Calls to that address will be redirected here.

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<https://aflow.org/p/X29X>

[https://aflow.org/p/A12B36CD12\\_cF488\\_210\\_h\\_3h\\_a\\_fg-001](https://aflow.org/p/A12B36CD12_cF488_210_h_3h_a_fg-001)



Prototype	B <sub>12</sub> H <sub>36</sub> MgO <sub>12</sub>
AFLOW prototype label	A12B36CD12_cF488_210_h_3h_a_fg-001
ICSD	413594
Pearson symbol	cF488
Space group number	210
Space group symbol	F <sub>4</sub> 132
AFLOW prototype command	aflow --proto=A12B36CD12_cF488_210_h_3h_a_fg-001 --params=a, x <sub>2</sub> , y <sub>3</sub> , x <sub>4</sub> , y <sub>4</sub> , z <sub>4</sub> , x <sub>5</sub> , y <sub>5</sub> , z <sub>5</sub> , x <sub>6</sub> , y <sub>6</sub> , z <sub>6</sub> , x <sub>7</sub> , y <sub>7</sub> , z <sub>7</sub>

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## Other compounds with this structure

NiB<sub>12</sub>H<sub>12</sub>[H<sub>2</sub>O]<sub>12</sub>

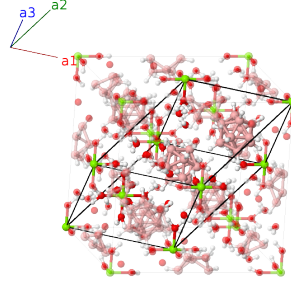
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### Face-centered Cubic primitive vectors

$$\mathbf{a}_1 = \frac{1}{2}a \hat{\mathbf{y}} + \frac{1}{2}a \hat{\mathbf{z}}$$

$$\mathbf{a}_2 = \frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{2}a \hat{\mathbf{z}}$$

$$\mathbf{a}_3 = \frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{2}a \hat{\mathbf{y}}$$




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### Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	=	0	=	0	(8a) Mg I
$\mathbf{B}_2$	=	$\frac{1}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	=	$\frac{1}{4}a \hat{\mathbf{x}} + \frac{1}{4}a \hat{\mathbf{y}} + \frac{1}{4}a \hat{\mathbf{z}}$	(8a) Mg I
$\mathbf{B}_3$	=	$-x_2 \mathbf{a}_1 + x_2 \mathbf{a}_2 + x_2 \mathbf{a}_3$	=	$ax_2 \hat{\mathbf{x}}$	(48f) O I
$\mathbf{B}_4$	=	$x_2 \mathbf{a}_1 - x_2 \mathbf{a}_2 - x_2 \mathbf{a}_3$	=	$-ax_2 \hat{\mathbf{x}}$	(48f) O I
$\mathbf{B}_5$	=	$x_2 \mathbf{a}_1 - x_2 \mathbf{a}_2 + x_2 \mathbf{a}_3$	=	$ax_2 \hat{\mathbf{y}}$	(48f) O I
$\mathbf{B}_6$	=	$-x_2 \mathbf{a}_1 + x_2 \mathbf{a}_2 - x_2 \mathbf{a}_3$	=	$-ax_2 \hat{\mathbf{y}}$	(48f) O I
$\mathbf{B}_7$	=	$x_2 \mathbf{a}_1 + x_2 \mathbf{a}_2 - x_2 \mathbf{a}_3$	=	$ax_2 \hat{\mathbf{z}}$	(48f) O I
$\mathbf{B}_8$	=	$-x_2 \mathbf{a}_1 - x_2 \mathbf{a}_2 + x_2 \mathbf{a}_3$	=	$-ax_2 \hat{\mathbf{z}}$	(48f) O I
$\mathbf{B}_9$	=	$(x_2 + \frac{1}{4}) \mathbf{a}_1 - (x_2 - \frac{1}{4}) \mathbf{a}_2 + (x_2 + \frac{1}{4}) \mathbf{a}_3$	=	$\frac{1}{4}a \hat{\mathbf{x}} + a(x_2 + \frac{1}{4}) \hat{\mathbf{y}} + \frac{1}{4}a \hat{\mathbf{z}}$	(48f) O I
$\mathbf{B}_{10}$	=	$-(x_2 - \frac{1}{4}) \mathbf{a}_1 + (x_2 + \frac{1}{4}) \mathbf{a}_2 - (x_2 - \frac{1}{4}) \mathbf{a}_3$	=	$\frac{1}{4}a \hat{\mathbf{x}} - a(x_2 - \frac{1}{4}) \hat{\mathbf{y}} + \frac{1}{4}a \hat{\mathbf{z}}$	(48f) O I
$\mathbf{B}_{11}$	=	$-(x_2 - \frac{1}{4}) \mathbf{a}_1 + (x_2 + \frac{1}{4}) \mathbf{a}_2 + (x_2 + \frac{1}{4}) \mathbf{a}_3$	=	$a(x_2 + \frac{1}{4}) \hat{\mathbf{x}} + \frac{1}{4}a \hat{\mathbf{y}} + \frac{1}{4}a \hat{\mathbf{z}}$	(48f) O I
$\mathbf{B}_{12}$	=	$(x_2 + \frac{1}{4}) \mathbf{a}_1 - (x_2 - \frac{1}{4}) \mathbf{a}_2 - (x_2 - \frac{1}{4}) \mathbf{a}_3$	=	$-a(x_2 - \frac{1}{4}) \hat{\mathbf{x}} + \frac{1}{4}a \hat{\mathbf{y}} + \frac{1}{4}a \hat{\mathbf{z}}$	(48f) O I
$\mathbf{B}_{13}$	=	$-(x_2 - \frac{1}{4}) \mathbf{a}_1 - (x_2 - \frac{1}{4}) \mathbf{a}_2 + (x_2 + \frac{1}{4}) \mathbf{a}_3$	=	$\frac{1}{4}a \hat{\mathbf{x}} + \frac{1}{4}a \hat{\mathbf{y}} - a(x_2 - \frac{1}{4}) \hat{\mathbf{z}}$	(48f) O I
$\mathbf{B}_{14}$	=	$(x_2 + \frac{1}{4}) \mathbf{a}_1 + (x_2 + \frac{1}{4}) \mathbf{a}_2 - (x_2 - \frac{1}{4}) \mathbf{a}_3$	=	$\frac{1}{4}a \hat{\mathbf{x}} + \frac{1}{4}a \hat{\mathbf{y}} + a(x_2 + \frac{1}{4}) \hat{\mathbf{z}}$	(48f) O I
$\mathbf{B}_{15}$	=	$\frac{1}{8} \mathbf{a}_1 - (2y_3 - \frac{3}{8}) \mathbf{a}_2 + (2y_3 + \frac{7}{8}) \mathbf{a}_3$	=	$\frac{5}{8}a \hat{\mathbf{x}} + a(y_3 + \frac{1}{2}) \hat{\mathbf{y}} - a(y_3 - \frac{1}{4}) \hat{\mathbf{z}}$	(48g) O II
$\mathbf{B}_{16}$	=	$-(2y_3 - \frac{3}{8}) \mathbf{a}_1 + \frac{1}{8} \mathbf{a}_2 + \frac{5}{8} \mathbf{a}_3$	=	$\frac{3}{8}a \hat{\mathbf{x}} - a(y_3 - \frac{1}{2}) \hat{\mathbf{y}} - a(y_3 - \frac{1}{4}) \hat{\mathbf{z}}$	(48g) O II
$\mathbf{B}_{17}$	=	$(2y_3 + \frac{7}{8}) \mathbf{a}_1 + \frac{5}{8} \mathbf{a}_2 + \frac{1}{8} \mathbf{a}_3$	=	$\frac{3}{8}a \hat{\mathbf{x}} + a(y_3 + \frac{1}{2}) \hat{\mathbf{y}} + a(y_3 + \frac{3}{4}) \hat{\mathbf{z}}$	(48g) O II
$\mathbf{B}_{18}$	=	$\frac{5}{8} \mathbf{a}_1 + (2y_3 + \frac{7}{8}) \mathbf{a}_2 - (2y_3 - \frac{3}{8}) \mathbf{a}_3$	=	$\frac{5}{8}a \hat{\mathbf{x}} - a(y_3 - \frac{1}{2}) \hat{\mathbf{y}} + a(y_3 + \frac{3}{4}) \hat{\mathbf{z}}$	(48g) O II
$\mathbf{B}_{19}$	=	$(2y_3 + \frac{7}{8}) \mathbf{a}_1 + \frac{1}{8} \mathbf{a}_2 - (2y_3 - \frac{3}{8}) \mathbf{a}_3$	=	$-a(y_3 - \frac{1}{4}) \hat{\mathbf{x}} + \frac{5}{8}a \hat{\mathbf{y}} + a(y_3 + \frac{1}{2}) \hat{\mathbf{z}}$	(48g) O II

$$\begin{aligned}
\mathbf{B}_{20} &= \frac{5}{8} \mathbf{a}_1 - (2y_3 - \frac{3}{8}) \mathbf{a}_2 + \frac{1}{8} \mathbf{a}_3 &= & -a(y_3 - \frac{1}{4}) \hat{\mathbf{x}} + \frac{3}{8}a \hat{\mathbf{y}} - a(y_3 - \frac{1}{2}) \hat{\mathbf{z}} & (48g) & \text{O II} \\
\mathbf{B}_{21} &= \frac{1}{8} \mathbf{a}_1 + (2y_3 + \frac{7}{8}) \mathbf{a}_2 + \frac{5}{8} \mathbf{a}_3 &= & a(y_3 + \frac{3}{4}) \hat{\mathbf{x}} + \frac{3}{8}a \hat{\mathbf{y}} + a(y_3 + \frac{1}{2}) \hat{\mathbf{z}} & (48g) & \text{O II} \\
\mathbf{B}_{22} &= -(2y_3 - \frac{3}{8}) \mathbf{a}_1 + \frac{5}{8} \mathbf{a}_2 + &= & a(y_3 + \frac{3}{4}) \hat{\mathbf{x}} + \frac{5}{8}a \hat{\mathbf{y}} - a(y_3 - \frac{1}{2}) \hat{\mathbf{z}} & (48g) & \text{O II} \\
&\quad (2y_3 + \frac{7}{8}) \mathbf{a}_3 \\
\mathbf{B}_{23} &= -(2y_3 - \frac{3}{8}) \mathbf{a}_1 + (2y_3 + \frac{7}{8}) \mathbf{a}_2 + &= & a(y_3 + \frac{1}{2}) \hat{\mathbf{x}} - a(y_3 - \frac{1}{4}) \hat{\mathbf{y}} + \frac{5}{8}a \hat{\mathbf{z}} & (48g) & \text{O II} \\
&\quad \frac{1}{8} \mathbf{a}_3 \\
\mathbf{B}_{24} &= \frac{1}{8} \mathbf{a}_1 + \frac{5}{8} \mathbf{a}_2 - (2y_3 - \frac{3}{8}) \mathbf{a}_3 &= & -a(y_3 - \frac{1}{2}) \hat{\mathbf{x}} - a(y_3 - \frac{1}{4}) \hat{\mathbf{y}} + \frac{3}{8}a \hat{\mathbf{z}} & (48g) & \text{O II} \\
\mathbf{B}_{25} &= \frac{5}{8} \mathbf{a}_1 + \frac{1}{8} \mathbf{a}_2 + (2y_3 + \frac{7}{8}) \mathbf{a}_3 &= & a(y_3 + \frac{1}{2}) \hat{\mathbf{x}} + a(y_3 + \frac{3}{4}) \hat{\mathbf{y}} + \frac{3}{8}a \hat{\mathbf{z}} & (48g) & \text{O II} \\
\mathbf{B}_{26} &= (2y_3 + \frac{7}{8}) \mathbf{a}_1 - (2y_3 - \frac{3}{8}) \mathbf{a}_2 + &= & -a(y_3 - \frac{1}{2}) \hat{\mathbf{x}} + a(y_3 + \frac{3}{4}) \hat{\mathbf{y}} + \frac{5}{8}a \hat{\mathbf{z}} & (48g) & \text{O II} \\
&\quad \frac{5}{8} \mathbf{a}_3 \\
\mathbf{B}_{27} &= (-x_4 + y_4 + z_4) \mathbf{a}_1 + &= & ax_4 \hat{\mathbf{x}} + ay_4 \hat{\mathbf{y}} + az_4 \hat{\mathbf{z}} & (96h) & \text{B I} \\
&\quad (x_4 - y_4 + z_4) \mathbf{a}_2 + \\
&\quad (x_4 + y_4 - z_4) \mathbf{a}_3 \\
\mathbf{B}_{28} &= (x_4 - y_4 + z_4) \mathbf{a}_1 + &= & -ax_4 \hat{\mathbf{x}} - ay_4 \hat{\mathbf{y}} + az_4 \hat{\mathbf{z}} & (96h) & \text{B I} \\
&\quad (-x_4 + y_4 + z_4) \mathbf{a}_2 - \\
&\quad (x_4 + y_4 + z_4) \mathbf{a}_3 \\
\mathbf{B}_{29} &= (x_4 + y_4 - z_4) \mathbf{a}_1 - &= & -ax_4 \hat{\mathbf{x}} + ay_4 \hat{\mathbf{y}} - az_4 \hat{\mathbf{z}} & (96h) & \text{B I} \\
&\quad (x_4 + y_4 + z_4) \mathbf{a}_2 + \\
&\quad (-x_4 + y_4 + z_4) \mathbf{a}_3 \\
\mathbf{B}_{30} &= -(x_4 + y_4 + z_4) \mathbf{a}_1 + &= & ax_4 \hat{\mathbf{x}} - ay_4 \hat{\mathbf{y}} - az_4 \hat{\mathbf{z}} & (96h) & \text{B I} \\
&\quad (x_4 + y_4 - z_4) \mathbf{a}_2 + \\
&\quad (x_4 - y_4 + z_4) \mathbf{a}_3 \\
\mathbf{B}_{31} &= (x_4 + y_4 - z_4) \mathbf{a}_1 + &= & az_4 \hat{\mathbf{x}} + ax_4 \hat{\mathbf{y}} + ay_4 \hat{\mathbf{z}} & (96h) & \text{B I} \\
&\quad (-x_4 + y_4 + z_4) \mathbf{a}_2 + \\
&\quad (x_4 - y_4 + z_4) \mathbf{a}_3 \\
\mathbf{B}_{32} &= -(x_4 + y_4 + z_4) \mathbf{a}_1 + &= & az_4 \hat{\mathbf{x}} - ax_4 \hat{\mathbf{y}} - ay_4 \hat{\mathbf{z}} & (96h) & \text{B I} \\
&\quad (x_4 - y_4 + z_4) \mathbf{a}_2 + \\
&\quad (-x_4 + y_4 + z_4) \mathbf{a}_3 \\
\mathbf{B}_{33} &= (-x_4 + y_4 + z_4) \mathbf{a}_1 + &= & -az_4 \hat{\mathbf{x}} - ax_4 \hat{\mathbf{y}} + ay_4 \hat{\mathbf{z}} & (96h) & \text{B I} \\
&\quad (x_4 + y_4 - z_4) \mathbf{a}_2 - \\
&\quad (x_4 + y_4 + z_4) \mathbf{a}_3 \\
\mathbf{B}_{34} &= (x_4 - y_4 + z_4) \mathbf{a}_1 - &= & -az_4 \hat{\mathbf{x}} + ax_4 \hat{\mathbf{y}} - ay_4 \hat{\mathbf{z}} & (96h) & \text{B I} \\
&\quad (x_4 + y_4 + z_4) \mathbf{a}_2 + \\
&\quad (x_4 + y_4 - z_4) \mathbf{a}_3 \\
\mathbf{B}_{35} &= (x_4 - y_4 + z_4) \mathbf{a}_1 + &= & ay_4 \hat{\mathbf{x}} + az_4 \hat{\mathbf{y}} + ax_4 \hat{\mathbf{z}} & (96h) & \text{B I} \\
&\quad (x_4 + y_4 - z_4) \mathbf{a}_2 + \\
&\quad (-x_4 + y_4 + z_4) \mathbf{a}_3 \\
\mathbf{B}_{36} &= (-x_4 + y_4 + z_4) \mathbf{a}_1 - &= & -ay_4 \hat{\mathbf{x}} + az_4 \hat{\mathbf{y}} - ax_4 \hat{\mathbf{z}} & (96h) & \text{B I} \\
&\quad (x_4 + y_4 + z_4) \mathbf{a}_2 + \\
&\quad (x_4 - y_4 + z_4) \mathbf{a}_3 \\
\mathbf{B}_{37} &= -(x_4 + y_4 + z_4) \mathbf{a}_1 + &= & ay_4 \hat{\mathbf{x}} - az_4 \hat{\mathbf{y}} - ax_4 \hat{\mathbf{z}} & (96h) & \text{B I} \\
&\quad (-x_4 + y_4 + z_4) \mathbf{a}_2 + \\
&\quad (x_4 + y_4 - z_4) \mathbf{a}_3 \\
\mathbf{B}_{38} &= (x_4 + y_4 - z_4) \mathbf{a}_1 + &= & -ay_4 \hat{\mathbf{x}} - az_4 \hat{\mathbf{y}} + ax_4 \hat{\mathbf{z}} & (96h) & \text{B I} \\
&\quad (x_4 - y_4 + z_4) \mathbf{a}_2 - \\
&\quad (x_4 + y_4 + z_4) \mathbf{a}_3 \\
\mathbf{B}_{39} &= (x_4 - y_4 - z_4 + \frac{1}{4}) \mathbf{a}_1 - &= & a(y_4 + \frac{1}{4}) \hat{\mathbf{x}} + a(x_4 + \frac{1}{4}) \hat{\mathbf{y}} - a(z_4 - \frac{1}{4}) \hat{\mathbf{z}} & (96h) & \text{B I} \\
&\quad (x_4 - y_4 + z_4 - \frac{1}{4}) \mathbf{a}_2 + \\
&\quad (x_4 + y_4 + z_4 + \frac{1}{4}) \mathbf{a}_3
\end{aligned}$$













$$\mathbf{B}_{120} = \begin{pmatrix} x_7 - y_7 - z_7 + \frac{1}{4} \\ x_7 + y_7 + z_7 + \frac{1}{4} \\ x_7 + y_7 - z_7 - \frac{1}{4} \end{pmatrix} \mathbf{a}_1 + \begin{pmatrix} x_7 + y_7 + z_7 + \frac{1}{4} \\ x_7 - y_7 - z_7 + \frac{1}{4} \\ x_7 + y_7 - z_7 - \frac{1}{4} \end{pmatrix} \mathbf{a}_2 - \begin{pmatrix} x_7 + y_7 - z_7 - \frac{1}{4} \\ x_7 - y_7 + z_7 - \frac{1}{4} \\ x_7 - y_7 - z_7 + \frac{1}{4} \end{pmatrix} \mathbf{a}_3 = a \left( z_7 + \frac{1}{4} \right) \hat{\mathbf{x}} - a \left( y_7 - \frac{1}{4} \right) \hat{\mathbf{y}} + a \left( x_7 + \frac{1}{4} \right) \hat{\mathbf{z}} \quad (96h) \quad \text{H III}$$

$$\mathbf{B}_{121} = \begin{pmatrix} x_7 + y_7 + z_7 + \frac{1}{4} \\ x_7 - y_7 - z_7 + \frac{1}{4} \\ x_7 - y_7 + z_7 - \frac{1}{4} \end{pmatrix} \mathbf{a}_1 + \begin{pmatrix} x_7 + y_7 + z_7 + \frac{1}{4} \\ x_7 - y_7 - z_7 + \frac{1}{4} \\ x_7 - y_7 + z_7 - \frac{1}{4} \end{pmatrix} \mathbf{a}_2 - \begin{pmatrix} x_7 + y_7 - z_7 - \frac{1}{4} \\ x_7 - y_7 + z_7 - \frac{1}{4} \\ x_7 - y_7 - z_7 + \frac{1}{4} \end{pmatrix} \mathbf{a}_3 = -a \left( z_7 - \frac{1}{4} \right) \hat{\mathbf{x}} + a \left( y_7 + \frac{1}{4} \right) \hat{\mathbf{y}} + a \left( x_7 + \frac{1}{4} \right) \hat{\mathbf{z}} \quad (96h) \quad \text{H III}$$

$$\mathbf{B}_{122} = -\begin{pmatrix} x_7 + y_7 - z_7 - \frac{1}{4} \\ x_7 - y_7 + z_7 - \frac{1}{4} \\ x_7 - y_7 - z_7 + \frac{1}{4} \end{pmatrix} \mathbf{a}_1 - \begin{pmatrix} x_7 + y_7 - z_7 - \frac{1}{4} \\ x_7 - y_7 + z_7 - \frac{1}{4} \\ x_7 - y_7 - z_7 + \frac{1}{4} \end{pmatrix} \mathbf{a}_2 + \begin{pmatrix} x_7 + y_7 - z_7 - \frac{1}{4} \\ x_7 - y_7 + z_7 - \frac{1}{4} \\ x_7 - y_7 - z_7 + \frac{1}{4} \end{pmatrix} \mathbf{a}_3 = -a \left( z_7 - \frac{1}{4} \right) \hat{\mathbf{x}} - a \left( y_7 - \frac{1}{4} \right) \hat{\mathbf{y}} - a \left( x_7 - \frac{1}{4} \right) \hat{\mathbf{z}} \quad (96h) \quad \text{H III}$$

## References

- [1] I. Tiritiris and T. Schleid, *Synthese, Kristallstruktur und thermischer Abbau von  $Mg(H_2O)_6[B_{12}H_{12}] \cdot 6H_2O$* , Zeitschrift für anorganische und allgemeine Chemie **630**, 541–546 (2004).

## Found in

- [1] I. Tiritiris and T. Schleid, *Synthesis, Crystal Structure, and Thermal Decomposition of  $Mg(H_2O)_6[B_{12}H_{12}] \times 6H_2O$* , ChemInform (2004), doi:10.1002/chin.200425008.
- [2] P. Villars and K. Cenzual, *Pearson's Crystal Data – Crystal Structure Database for Inorganic Compounds* (2013). ASM International.