$Mg(ClO_4)_2{\cdot}6H_2O$ ($H4_{11}$) Structure: A2B6CD8_oP34_31_2a_2a2b_a_4a2b-001

This structure originally had the label `A2B6CD8_oP34_31_2a_2a2b_a_4a2b`. Calls to that address will be redirected here.

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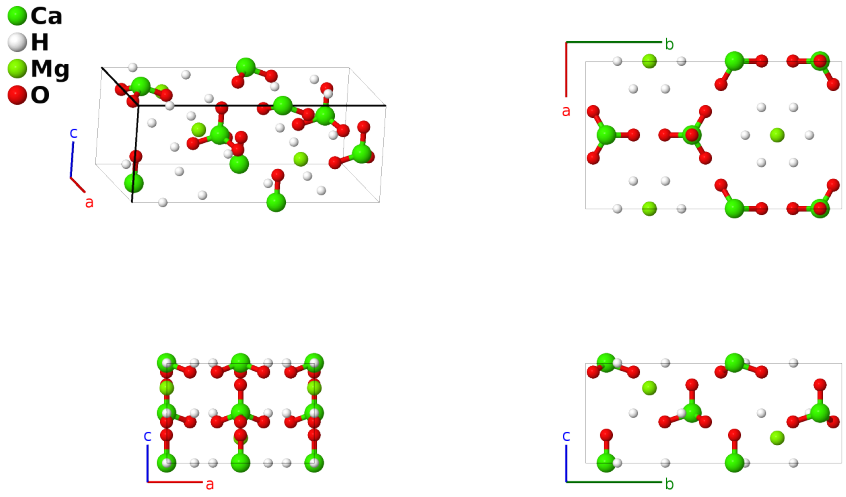
https://aflow.org/p/ZN0T

https://aflow.org/p/A2B6CD8_oP34_31_2a_2a2b_a_4a2b-001



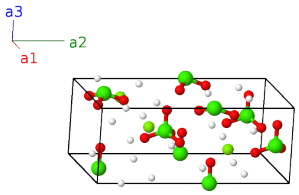
Prototype	$Ca_2(H_2O)_6MgO_8$
AFLOW prototype label	A2B6CD8_oP34_31_2a_2a2b_a_4a2b-001
***Strukturbericht* designation**	$H4_{11}$
ICSD	24250
Pearson symbol	oP34
Space group number	31
Space group symbol	$Pmn2_1$
AFLOW prototype command	`aflow --proto=A2B6CD8_oP34_31_2a_2a2b_a_4a2b-001 --params=`$a, b/a, c/a, y_1, z_1, y_2, z_2, y_3, z_3, y_4, z_4, y_5, z_5, y_6, z_6, y_7, z_7, y_8, z_8, y_9, z_9, x_{10}, y_{10}, z_{10}, x_{11}, y_{11}, z_{11}, x_{12}, y_{12}, z_{12}, x_{13}, y_{13}, z_{13}$

Other compounds with this structure
$Co(ClO_4)_2{\cdot}6H_2O$, $Fe(ClO_4)_2{\cdot}6H_2O$, $Mn(ClO_4)_2{\cdot}6H_2O$, $Ni(ClO_4)_2{\cdot}6H_2O$, $Zn(ClO_4)_2{\cdot}6H_2O$, $Mg(BF_4)_2{\cdot}6H_2O$, $Co(BF_4)_2{\cdot}6H_2O$, $Fe(BF_4)_2{\cdot}6H_2O$, $Mn(BF_4)_2{\cdot}6H_2O$, $Ni(BF_4)_2{\cdot}6H_2O$, $Zn(BF_4)_2{\cdot}6H_2O$

- (Gottfried, 1937) writes $z_{13} = 0.408$ for the coordinate of the (H_2O-II) molecule, but the value given by West is $z_{13} = 0$, which gives a symmetric arrangement of water molecules around the chlorine atom.

Simple Orthorhombic primitive vectors

$$\begin{aligned}\mathbf{a_1} &= a\,\hat{\mathbf{x}}\\ \mathbf{a_2} &= b\,\hat{\mathbf{y}}\\ \mathbf{a_3} &= c\,\hat{\mathbf{z}}\end{aligned}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$y_1\,\mathbf{a}_2 + z_1\,\mathbf{a}_3$	=	$by_1\,\hat{\mathbf{y}} + cz_1\,\hat{\mathbf{z}}$	(2a)	Ca I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_1 - y_1\,\mathbf{a}_2 + \left(z_1 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - by_1\,\hat{\mathbf{y}} + c\left(z_1 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(2a)	Ca I
$\mathbf{B_3}$	=	$y_2\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$by_2\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(2a)	Ca II
$\mathbf{B_4}$	=	$\frac{1}{2}\,\mathbf{a}_1 - y_2\,\mathbf{a}_2 + \left(z_2 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - by_2\,\hat{\mathbf{y}} + c\left(z_2 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(2a)	Ca II
$\mathbf{B_5}$	=	$y_3\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$by_3\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(2a)	H I
$\mathbf{B_6}$	=	$\frac{1}{2}\,\mathbf{a}_1 - y_3\,\mathbf{a}_2 + \left(z_3 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - by_3\,\hat{\mathbf{y}} + c\left(z_3 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(2a)	H I
$\mathbf{B_7}$	=	$y_4\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$by_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(2a)	H II
$\mathbf{B_8}$	=	$\frac{1}{2}\,\mathbf{a}_1 - y_4\,\mathbf{a}_2 + \left(z_4 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - by_4\,\hat{\mathbf{y}} + c\left(z_4 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(2a)	H II
$\mathbf{B_9}$	=	$y_5\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$by_5\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(2a)	Mg I
$\mathbf{B_{10}}$	=	$\frac{1}{2}\,\mathbf{a}_1 - y_5\,\mathbf{a}_2 + \left(z_5 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - by_5\,\hat{\mathbf{y}} + c\left(z_5 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(2a)	Mg I
$\mathbf{B_{11}}$	=	$y_6\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	=	$by_6\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(2a)	O I
$\mathbf{B_{12}}$	=	$\frac{1}{2}\,\mathbf{a}_1 - y_6\,\mathbf{a}_2 + \left(z_6 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - by_6\,\hat{\mathbf{y}} + c\left(z_6 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(2a)	O I
$\mathbf{B_{13}}$	=	$y_7\,\mathbf{a}_2 + z_7\,\mathbf{a}_3$	=	$by_7\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}}$	(2a)	O II
$\mathbf{B_{14}}$	=	$\frac{1}{2}\,\mathbf{a}_1 - y_7\,\mathbf{a}_2 + \left(z_7 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - by_7\,\hat{\mathbf{y}} + c\left(z_7 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(2a)	O II
$\mathbf{B_{15}}$	=	$y_8\,\mathbf{a}_2 + z_8\,\mathbf{a}_3$	=	$by_8\,\hat{\mathbf{y}} + cz_8\,\hat{\mathbf{z}}$	(2a)	O III
$\mathbf{B_{16}}$	=	$\frac{1}{2}\,\mathbf{a}_1 - y_8\,\mathbf{a}_2 + \left(z_8 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - by_8\,\hat{\mathbf{y}} + c\left(z_8 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(2a)	O III
$\mathbf{B_{17}}$	=	$y_9\,\mathbf{a}_2 + z_9\,\mathbf{a}_3$	=	$by_9\,\hat{\mathbf{y}} + cz_9\,\hat{\mathbf{z}}$	(2a)	O IV
$\mathbf{B_{18}}$	=	$\frac{1}{2}\,\mathbf{a}_1 - y_9\,\mathbf{a}_2 + \left(z_9 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - by_9\,\hat{\mathbf{y}} + c\left(z_9 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(2a)	O IV
$\mathbf{B_{19}}$	=	$x_{10}\,\mathbf{a}_1 + y_{10}\,\mathbf{a}_2 + z_{10}\,\mathbf{a}_3$	=	$ax_{10}\,\hat{\mathbf{x}} + by_{10}\,\hat{\mathbf{y}} + cz_{10}\,\hat{\mathbf{z}}$	(4b)	H III
$\mathbf{B_{20}}$	=	$-\left(x_{10} - \frac{1}{2}\right)\,\mathbf{a}_1 - y_{10}\,\mathbf{a}_2 + \left(z_{10} + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_{10} - \frac{1}{2}\right)\,\hat{\mathbf{x}} - by_{10}\,\hat{\mathbf{y}} + c\left(z_{10} + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4b)	H III
$\mathbf{B_{21}}$	=	$\left(x_{10} + \frac{1}{2}\right)\,\mathbf{a}_1 - y_{10}\,\mathbf{a}_2 + \left(z_{10} + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(x_{10} + \frac{1}{2}\right)\,\hat{\mathbf{x}} - by_{10}\,\hat{\mathbf{y}} + c\left(z_{10} + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4b)	H III
$\mathbf{B_{22}}$	=	$-x_{10}\,\mathbf{a}_1 + y_{10}\,\mathbf{a}_2 + z_{10}\,\mathbf{a}_3$	=	$-ax_{10}\,\hat{\mathbf{x}} + by_{10}\,\hat{\mathbf{y}} + cz_{10}\,\hat{\mathbf{z}}$	(4b)	H III
$\mathbf{B_{23}}$	=	$x_{11}\,\mathbf{a}_1 + y_{11}\,\mathbf{a}_2 + z_{11}\,\mathbf{a}_3$	=	$ax_{11}\,\hat{\mathbf{x}} + by_{11}\,\hat{\mathbf{y}} + cz_{11}\,\hat{\mathbf{z}}$	(4b)	H IV
$\mathbf{B_{24}}$	=	$-\left(x_{11} - \frac{1}{2}\right)\,\mathbf{a}_1 - y_{11}\,\mathbf{a}_2 + \left(z_{11} + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_{11} - \frac{1}{2}\right)\,\hat{\mathbf{x}} - by_{11}\,\hat{\mathbf{y}} + c\left(z_{11} + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4b)	H IV
$\mathbf{B_{25}}$	=	$\left(x_{11} + \frac{1}{2}\right)\,\mathbf{a}_1 - y_{11}\,\mathbf{a}_2 + \left(z_{11} + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(x_{11} + \frac{1}{2}\right)\,\hat{\mathbf{x}} - by_{11}\,\hat{\mathbf{y}} + c\left(z_{11} + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4b)	H IV
$\mathbf{B_{26}}$	=	$-x_{11}\,\mathbf{a}_1 + y_{11}\,\mathbf{a}_2 + z_{11}\,\mathbf{a}_3$	=	$-ax_{11}\,\hat{\mathbf{x}} + by_{11}\,\hat{\mathbf{y}} + cz_{11}\,\hat{\mathbf{z}}$	(4b)	H IV
$\mathbf{B_{27}}$	=	$x_{12}\,\mathbf{a}_1 + y_{12}\,\mathbf{a}_2 + z_{12}\,\mathbf{a}_3$	=	$ax_{12}\,\hat{\mathbf{x}} + by_{12}\,\hat{\mathbf{y}} + cz_{12}\,\hat{\mathbf{z}}$	(4b)	O V

$\mathbf{B_{28}}$	=	$-\left(x_{12}-\frac{1}{2}\right)\mathbf{a}_1 - y_{12}\,\mathbf{a}_2 + \left(z_{12}+\frac{1}{2}\right)\mathbf{a}_3$	=	$-a\left(x_{12}-\frac{1}{2}\right)\hat{\mathbf{x}} - by_{12}\,\hat{\mathbf{y}} + c\left(z_{12}+\frac{1}{2}\right)\hat{\mathbf{z}}$	(4b)	O V
$\mathbf{B_{29}}$	=	$\left(x_{12}+\frac{1}{2}\right)\mathbf{a}_1 - y_{12}\,\mathbf{a}_2 + \left(z_{12}+\frac{1}{2}\right)\mathbf{a}_3$	=	$a\left(x_{12}+\frac{1}{2}\right)\hat{\mathbf{x}} - by_{12}\,\hat{\mathbf{y}} + c\left(z_{12}+\frac{1}{2}\right)\hat{\mathbf{z}}$	(4b)	O V
$\mathbf{B_{30}}$	=	$-x_{12}\,\mathbf{a}_1 + y_{12}\,\mathbf{a}_2 + z_{12}\,\mathbf{a}_3$	=	$-ax_{12}\,\hat{\mathbf{x}} + by_{12}\,\hat{\mathbf{y}} + cz_{12}\,\hat{\mathbf{z}}$	(4b)	O V
$\mathbf{B_{31}}$	=	$x_{13}\,\mathbf{a}_1 + y_{13}\,\mathbf{a}_2 + z_{13}\,\mathbf{a}_3$	=	$ax_{13}\,\hat{\mathbf{x}} + by_{13}\,\hat{\mathbf{y}} + cz_{13}\,\hat{\mathbf{z}}$	(4b)	O VI
$\mathbf{B_{32}}$	=	$-\left(x_{13}-\frac{1}{2}\right)\mathbf{a}_1 - y_{13}\,\mathbf{a}_2 + \left(z_{13}+\frac{1}{2}\right)\mathbf{a}_3$	=	$-a\left(x_{13}-\frac{1}{2}\right)\hat{\mathbf{x}} - by_{13}\,\hat{\mathbf{y}} + c\left(z_{13}+\frac{1}{2}\right)\hat{\mathbf{z}}$	(4b)	O VI
$\mathbf{B_{33}}$	=	$\left(x_{13}+\frac{1}{2}\right)\mathbf{a}_1 - y_{13}\,\mathbf{a}_2 + \left(z_{13}+\frac{1}{2}\right)\mathbf{a}_3$	=	$a\left(x_{13}+\frac{1}{2}\right)\hat{\mathbf{x}} - by_{13}\,\hat{\mathbf{y}} + c\left(z_{13}+\frac{1}{2}\right)\hat{\mathbf{z}}$	(4b)	O VI
$\mathbf{B_{34}}$	=	$-x_{13}\,\mathbf{a}_1 + y_{13}\,\mathbf{a}_2 + z_{13}\,\mathbf{a}_3$	=	$-ax_{13}\,\hat{\mathbf{x}} + by_{13}\,\hat{\mathbf{y}} + cz_{13}\,\hat{\mathbf{z}}$	(4b)	O VI

References

[1] C. D. West, *Crystal Structures of Hydrated Compounds II. Structure Type $Mg(ClO_4)_2{\cdot}6H_2O$*, Z. Krystallogr. **91**, 480–493 (1935), doi:10.1524/zkri.1935.91.1.480.

[2] C. Gottfried and F. Schossberger, eds., *Strukturbericht Band III 1933-1935* (Akademische Verlagsgesellschaft M. B. H., Leipzig, 1937).

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[1] K. Robertson and D. Bish, *Stability of phases in the $Mg(ClO_4)_2{\cdot}nH_2O$ system and implications for perchlorate occurrences on Mars*, J. Geophys. Res. **116**, E07006 (2011), doi:10.1029/2010JE003754.