Bischofite (MgCl$_2$·6H$_2$O, $J1_7$) Structure: A2B12CD6_mC42_12_i_2i2j_a_ij-001
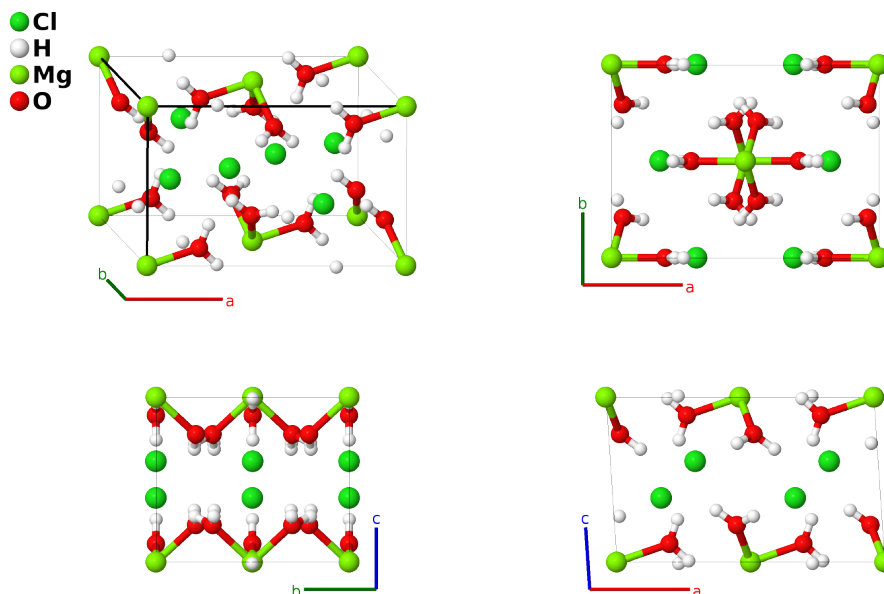
This structure originally had the label `A2B12CD6_mC42_12_i_2i2j_a_ij`. Calls to that address will be redirected here.

https://aflow.org/p/3SX5

https://aflow.org/p/A2B12CD6_mC42_12_i_2i2j_a_ij-001

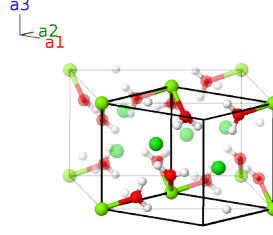|	
Prototype	Cl$_2$H$_{12}$MgO$_6$
AFLOW prototype label	A2B12CD6_mC42_12_i_2i2j_a_ij-001
***Strukturbericht* designation**	$J1_7$
Mineral name	bischofite
ICSD	47161
Pearson symbol	mC42
Space group number	12
Space group symbol	$C2/m$
AFLOW prototype command	aflow --proto=A2B12CD6_mC42_12_i_2i2j_a_ij-001 --params=$a, b/a, c/a, \beta, x_2, z_2, x_3, z_3, x_4, z_4, x_5, z_5, x_6, y_6, z_6, x_7, y_7, z_7, x_8, y_8, z_8$

Other compounds with this structure
MgBr$_2$·6H$_2$O

- This structure is nearly identical to the one presented in (Gottfried, 1937) as $J1_7$, but now includes the positions of the hydrogen atoms.

Base-centered Monoclinic primitive vectors

$$\mathbf{a_1} = \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{1}{2}b\,\hat{\mathbf{y}}$$

$$\mathbf{a_2} = \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}b\,\hat{\mathbf{y}}$$

$$\mathbf{a_3} = c\cos\beta\,\hat{\mathbf{x}} + c\sin\beta\,\hat{\mathbf{z}}$$

Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	$=$	0	$=$	0	(2a)	Mg I
$\mathbf{B_2}$	$=$	$x_2\,\mathbf{a_1} + x_2\,\mathbf{a_2} + z_2\,\mathbf{a_3}$	$=$	$(ax_2 + cz_2\cos\beta)\,\hat{\mathbf{x}} + cz_2\sin\beta\,\hat{\mathbf{z}}$	(4i)	Cl I
$\mathbf{B_3}$	$=$	$-x_2\,\mathbf{a_1} - x_2\,\mathbf{a_2} - z_2\,\mathbf{a_3}$	$=$	$-(ax_2 + cz_2\cos\beta)\,\hat{\mathbf{x}} - cz_2\sin\beta\,\hat{\mathbf{z}}$	(4i)	Cl I
$\mathbf{B_4}$	$=$	$x_3\,\mathbf{a_1} + x_3\,\mathbf{a_2} + z_3\,\mathbf{a_3}$	$=$	$(ax_3 + cz_3\cos\beta)\,\hat{\mathbf{x}} + cz_3\sin\beta\,\hat{\mathbf{z}}$	(4i)	H I
$\mathbf{B_5}$	$=$	$-x_3\,\mathbf{a_1} - x_3\,\mathbf{a_2} - z_3\,\mathbf{a_3}$	$=$	$-(ax_3 + cz_3\cos\beta)\,\hat{\mathbf{x}} - cz_3\sin\beta\,\hat{\mathbf{z}}$	(4i)	H I
$\mathbf{B_6}$	$=$	$x_4\,\mathbf{a_1} + x_4\,\mathbf{a_2} + z_4\,\mathbf{a_3}$	$=$	$(ax_4 + cz_4\cos\beta)\,\hat{\mathbf{x}} + cz_4\sin\beta\,\hat{\mathbf{z}}$	(4i)	H II
$\mathbf{B_7}$	$=$	$-x_4\,\mathbf{a_1} - x_4\,\mathbf{a_2} - z_4\,\mathbf{a_3}$	$=$	$-(ax_4 + cz_4\cos\beta)\,\hat{\mathbf{x}} - cz_4\sin\beta\,\hat{\mathbf{z}}$	(4i)	H II
$\mathbf{B_8}$	$=$	$x_5\,\mathbf{a_1} + x_5\,\mathbf{a_2} + z_5\,\mathbf{a_3}$	$=$	$(ax_5 + cz_5\cos\beta)\,\hat{\mathbf{x}} + cz_5\sin\beta\,\hat{\mathbf{z}}$	(4i)	O I
$\mathbf{B_9}$	$=$	$-x_5\,\mathbf{a_1} - x_5\,\mathbf{a_2} - z_5\,\mathbf{a_3}$	$=$	$-(ax_5 + cz_5\cos\beta)\,\hat{\mathbf{x}} - cz_5\sin\beta\,\hat{\mathbf{z}}$	(4i)	O I
$\mathbf{B_{10}}$	$=$	$(x_6 - y_6)\,\mathbf{a_1} + (x_6 + y_6)\,\mathbf{a_2} + z_6\,\mathbf{a_3}$	$=$	$(ax_6 + cz_6\cos\beta)\,\hat{\mathbf{x}} + by_6\,\hat{\mathbf{y}} + cz_6\sin\beta\,\hat{\mathbf{z}}$	(8j)	H III
$\mathbf{B_{11}}$	$=$	$-(x_6 + y_6)\,\mathbf{a_1} - (x_6 - y_6)\,\mathbf{a_2} - z_6\,\mathbf{a_3}$	$=$	$-(ax_6 + cz_6\cos\beta)\,\hat{\mathbf{x}} + by_6\,\hat{\mathbf{y}} - cz_6\sin\beta\,\hat{\mathbf{z}}$	(8j)	H III
$\mathbf{B_{12}}$	$=$	$-(x_6 - y_6)\,\mathbf{a_1} - (x_6 + y_6)\,\mathbf{a_2} - z_6\,\mathbf{a_3}$	$=$	$-(ax_6 + cz_6\cos\beta)\,\hat{\mathbf{x}} - by_6\,\hat{\mathbf{y}} - cz_6\sin\beta\,\hat{\mathbf{z}}$	(8j)	H III
$\mathbf{B_{13}}$	$=$	$(x_6 + y_6)\,\mathbf{a_1} + (x_6 - y_6)\,\mathbf{a_2} + z_6\,\mathbf{a_3}$	$=$	$(ax_6 + cz_6\cos\beta)\,\hat{\mathbf{x}} - by_6\,\hat{\mathbf{y}} + cz_6\sin\beta\,\hat{\mathbf{z}}$	(8j)	H III
$\mathbf{B_{14}}$	$=$	$(x_7 - y_7)\,\mathbf{a_1} + (x_7 + y_7)\,\mathbf{a_2} + z_7\,\mathbf{a_3}$	$=$	$(ax_7 + cz_7\cos\beta)\,\hat{\mathbf{x}} + by_7\,\hat{\mathbf{y}} + cz_7\sin\beta\,\hat{\mathbf{z}}$	(8j)	H IV
$\mathbf{B_{15}}$	$=$	$-(x_7 + y_7)\,\mathbf{a_1} - (x_7 - y_7)\,\mathbf{a_2} - z_7\,\mathbf{a_3}$	$=$	$-(ax_7 + cz_7\cos\beta)\,\hat{\mathbf{x}} + by_7\,\hat{\mathbf{y}} - cz_7\sin\beta\,\hat{\mathbf{z}}$	(8j)	H IV
$\mathbf{B_{16}}$	$=$	$-(x_7 - y_7)\,\mathbf{a_1} - (x_7 + y_7)\,\mathbf{a_2} - z_7\,\mathbf{a_3}$	$=$	$-(ax_7 + cz_7\cos\beta)\,\hat{\mathbf{x}} - by_7\,\hat{\mathbf{y}} - cz_7\sin\beta\,\hat{\mathbf{z}}$	(8j)	H IV
$\mathbf{B_{17}}$	$=$	$(x_7 + y_7)\,\mathbf{a_1} + (x_7 - y_7)\,\mathbf{a_2} + z_7\,\mathbf{a_3}$	$=$	$(ax_7 + cz_7\cos\beta)\,\hat{\mathbf{x}} - by_7\,\hat{\mathbf{y}} + cz_7\sin\beta\,\hat{\mathbf{z}}$	(8j)	H IV
$\mathbf{B_{18}}$	$=$	$(x_8 - y_8)\,\mathbf{a_1} + (x_8 + y_8)\,\mathbf{a_2} + z_8\,\mathbf{a_3}$	$=$	$(ax_8 + cz_8\cos\beta)\,\hat{\mathbf{x}} + by_8\,\hat{\mathbf{y}} + cz_8\sin\beta\,\hat{\mathbf{z}}$	(8j)	O II
$\mathbf{B_{19}}$	$=$	$-(x_8 + y_8)\,\mathbf{a_1} - (x_8 - y_8)\,\mathbf{a_2} - z_8\,\mathbf{a_3}$	$=$	$-(ax_8 + cz_8\cos\beta)\,\hat{\mathbf{x}} + by_8\,\hat{\mathbf{y}} - cz_8\sin\beta\,\hat{\mathbf{z}}$	(8j)	O II
$\mathbf{B_{20}}$	$=$	$-(x_8 - y_8)\,\mathbf{a_1} - (x_8 + y_8)\,\mathbf{a_2} - z_8\,\mathbf{a_3}$	$=$	$-(ax_8 + cz_8\cos\beta)\,\hat{\mathbf{x}} - by_8\,\hat{\mathbf{y}} - cz_8\sin\beta\,\hat{\mathbf{z}}$	(8j)	O II
$\mathbf{B_{21}}$	$=$	$(x_8 + y_8)\,\mathbf{a_1} + (x_8 - y_8)\,\mathbf{a_2} + z_8\,\mathbf{a_3}$	$=$	$(ax_8 + cz_8\cos\beta)\,\hat{\mathbf{x}} - by_8\,\hat{\mathbf{y}} + cz_8\sin\beta\,\hat{\mathbf{z}}$	(8j)	O II

References

[1] P. A. Agron and W. R. Busing, *Magnesium dichloride hexahydrate, MgCl$_2$·6H$_2$O, by neutron diffraction*, Acta Crystallogr. Sect. C **41**, 8–10 (1985), doi:10.1107/S0108270185002591.

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