Brucite [$Mg(OH)_2$] Structure: A2BC2_hP5_164_d_a_d-001

This structure originally had the label `A2BC2_hP5_164_d_a_d`. Calls to that address will be redirected here.

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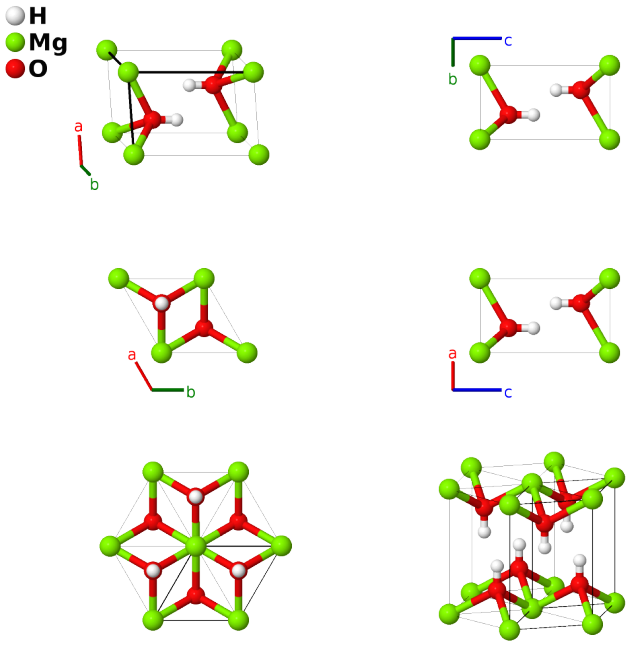
https://aflow.org/p/N2MR

https://aflow.org/p/A2BC2_hP5_164_d_a_d-001



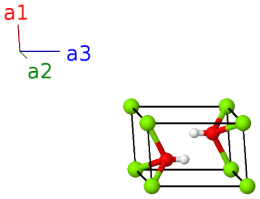
Prototype	H_2MgO_2
AFLOW prototype label	A2BC2_hP5_164_d_a_d-001
Mineral name	brucite
ICSD	79031
Pearson symbol	hP5
Space group number	164
Space group symbol	$P\bar{3}m1$
AFLOW prototype command	`aflow --proto=A2BC2_hP5_164_d_a_d-001 --params=`$a, c/a, z_2, z_3$

Other compounds with this structure
$Ca(OH)_2$ (Portlandite), $Fe(OH)_2$, $Mn(OH)_2$ (Pyrochroite), $Ni(OH)_2$ (Theophrastite), β-$Co(OH)_2$

- We used the data from (Catti, 1995) at ambient pressure. In some Brucite-like materials the hydrogen atoms are displaced to the (6i) Wyckoff positions $(x, -x, z)$ of space group $P3m1$ #164, and these sites are 1/3 occupied.

Trigonal (Hexagonal) primitive vectors

$$\mathbf{a_1} = \frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,\hat{\mathbf{y}}$$
$$\mathbf{a_2} = \frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(1a)	Mg I
$\mathbf{B_2}$	=	$\frac{1}{3}\,\mathbf{a}_1 + \frac{2}{3}\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(2d)	H I
$\mathbf{B_3}$	=	$\frac{2}{3}\,\mathbf{a}_1 + \frac{1}{3}\,\mathbf{a}_2 - z_2\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} - cz_2\,\hat{\mathbf{z}}$	(2d)	H I
$\mathbf{B_4}$	=	$\frac{1}{3}\,\mathbf{a}_1 + \frac{2}{3}\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(2d)	O I
$\mathbf{B_5}$	=	$\frac{2}{3}\,\mathbf{a}_1 + \frac{1}{3}\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} - cz_3\,\hat{\mathbf{z}}$	(2d)	O I

References

[1] M. Catti, G. Ferraris, S. Hull, and A. Pavese, *Static compression and H disorder in brucite, Mg(OH)$_2$, to 11 GPa: a powder neutron diffraction study*, Phys. Chem. Min. **22**, 200–206 (1995), doi:10.1007/BF00202300.