Hexagonal Close Packed (Mg, $A3$, hcp) Structure: A_hP2_194_c-001

This structure originally had the label `A_hP2_194_c`. Calls to that address will be redirected here.

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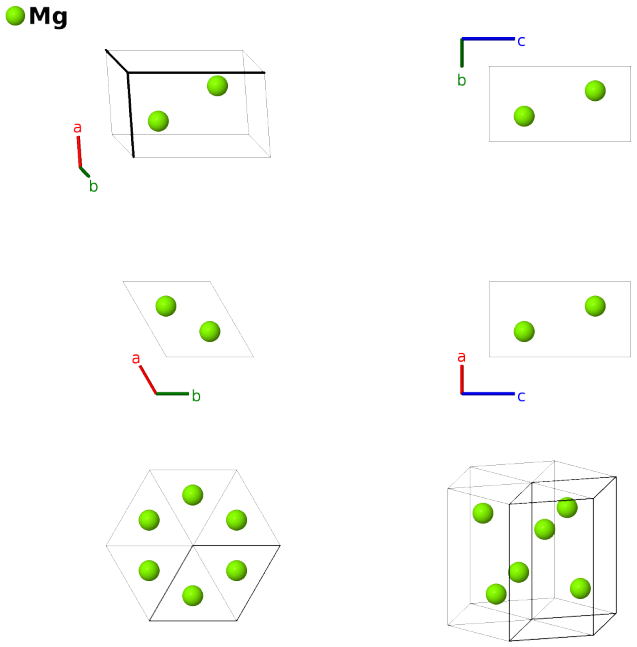
https://aflow.org/p/LZW5

https://aflow.org/p/A_hP2_194_c-001



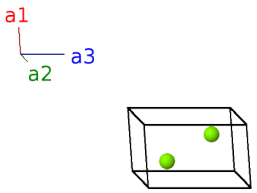
Prototype	Mg
AFLOW prototype label	A_hP2_194_c-001
***Strukturbericht* designation**	$A3$
ICSD	608404
Pearson symbol	hP2
Space group number	194
Space group symbol	$P6_3/mmc$
AFLOW prototype command	`aflow --proto=A_hP2_194_c-001 --params=`$a, c/a$

Other compounds with this structure
Be, Cd, Co, Dy, Er, ϵ-Fe, Gd, Hf, Ho, Lu, Os, Re, Ru, Sc, Tb, Tc, Ti, Tl, Tm, Y, Zn, Zr

- We use the 'pure magnesium' lattice constants from (Batchelder, 1957), but the ICSD entry uses the data for $Mg_{0.976}Al_{0.024}$.

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
$\mathbf{B_1}$	=	$\frac{1}{3}\,\mathbf{a}_1 + \frac{2}{3}\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(2c)	Mg I
$\mathbf{B_2}$	=	$\frac{2}{3}\,\mathbf{a}_1 + \frac{1}{3}\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(2c)	Mg I

References

[1] F. W. von Batchelder and R. F. Raeuchle, *Lattice Constants and Brillouin Zone Overlap in Dilute Magnesium Alloys*, Phys. Rev. **105**, 59–61 (1957), doi:10.1103/PhysRev.105.59.

Found in

[1] R. T. Downs and M. Hall-Wallace, *The American Mineralogist Crystal Structure Database*, Am. Mineral. **88**, 247–250 (2003).