

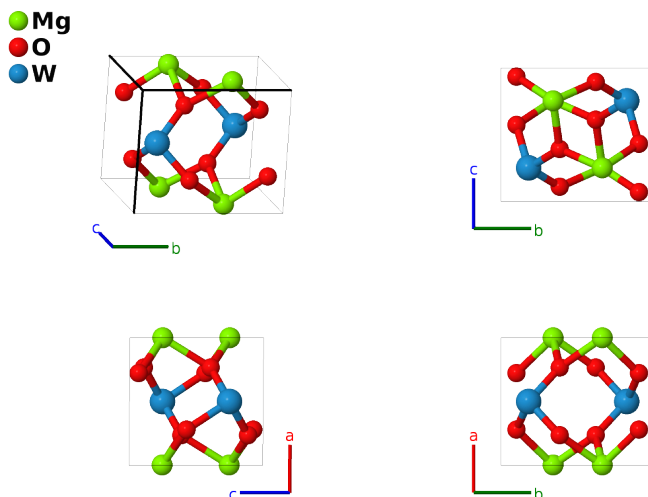
# Huanzalaite ( $\text{MgWO}_4$ , $H0_6$ ) Structure: AB4C\_mP12\_13\_e\_2g\_f-003

This structure originally had the label AB4C\_mP12\_13\_f\_2g\_e. Calls to that address will be redirected here.

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<https://afLOW.org/p/2SHQ>

[https://afLOW.org/p/AB4C\\_mP12\\_13\\_e\\_2g\\_f-003](https://afLOW.org/p/AB4C_mP12_13_e_2g_f-003)



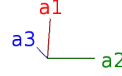
Prototype	$\text{MgO}_4\text{W}$
AFLOW prototype label	AB4C_mP12_13_e_2g_f-003
<i>Strukturbericht</i> designation	$H0_6$
Mineral name	huanzalaite
ICSD	20470
Pearson symbol	mP12
Space group number	13
Space group symbol	$P2/c$
AFLOW prototype command	<code>afLOW --proto=AB4C_mP12_13_e_2g_f-003 --params=a, b/a, c/a, <math>\beta</math>, <math>y_1</math>, <math>y_2</math>, <math>x_3</math>, <math>y_3</math>, <math>z_3</math>, <math>x_4</math>, <math>y_4</math>, <math>z_4</math></code>

## Other compounds with this structure

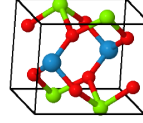
$\text{CoWO}_4$ ,  $\text{FeWO}_4$  (ferberite),  $\text{MnWO}_4$  (hüberrite),  $\text{NiWO}_4$ ,  $\text{ZnWO}_4$

- Most authors refer to this as the wolframite structure, but that name properly belongs to the solid solution  $(\text{Mn,Fe})\text{WO}_4$ . (Herman, 1937) chose this “magnesium wolframite” compound to represent the  $H0_6$  structures.

## Simple Monoclinic primitive vectors



$$\begin{aligned} \mathbf{a}_1 &= a \hat{\mathbf{x}} \\ \mathbf{a}_2 &= b \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \cos \beta \hat{\mathbf{x}} + c \sin \beta \hat{\mathbf{z}} \end{aligned}$$



## Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= y_1 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{4} c \cos \beta \hat{\mathbf{x}} + by_1 \hat{\mathbf{y}} + \frac{1}{4} c \sin \beta \hat{\mathbf{z}}$	(2e)	Mg I
$\mathbf{B}_2$	$= -y_1 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{3}{4} c \cos \beta \hat{\mathbf{x}} - by_1 \hat{\mathbf{y}} + \frac{3}{4} c \sin \beta \hat{\mathbf{z}}$	(2e)	Mg I
$\mathbf{B}_3$	$= \frac{1}{2} \mathbf{a}_1 + y_2 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\left(\frac{a}{2} + \frac{c \cos \beta}{4}\right) \hat{\mathbf{x}} + by_2 \hat{\mathbf{y}} + \frac{1}{4} c \sin \beta \hat{\mathbf{z}}$	(2f)	W I
$\mathbf{B}_4$	$= \frac{1}{2} \mathbf{a}_1 - y_2 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\left(\frac{a}{2} + \frac{3c \cos \beta}{4}\right) \hat{\mathbf{x}} - by_2 \hat{\mathbf{y}} + \frac{3}{4} c \sin \beta \hat{\mathbf{z}}$	(2f)	W I
$\mathbf{B}_5$	$= x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$(ax_3 + cz_3 \cos \beta) \hat{\mathbf{x}} + by_3 \hat{\mathbf{y}} + cz_3 \sin \beta \hat{\mathbf{z}}$	(4g)	O I
$\mathbf{B}_6$	$= -x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 - \left(z_3 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-(ax_3 + c(z_3 - \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} + by_3 \hat{\mathbf{y}} - c(z_3 - \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(4g)	O I
$\mathbf{B}_7$	$= -x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$-(ax_3 + cz_3 \cos \beta) \hat{\mathbf{x}} - by_3 \hat{\mathbf{y}} - cz_3 \sin \beta \hat{\mathbf{z}}$	(4g)	O I
$\mathbf{B}_8$	$= x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 + \left(z_3 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$(ax_3 + c(z_3 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_3 \hat{\mathbf{y}} + c(z_3 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(4g)	O I
$\mathbf{B}_9$	$= x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$(ax_4 + cz_4 \cos \beta) \hat{\mathbf{x}} + by_4 \hat{\mathbf{y}} + cz_4 \sin \beta \hat{\mathbf{z}}$	(4g)	O II
$\mathbf{B}_{10}$	$= -x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 - \left(z_4 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-(ax_4 + c(z_4 - \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} + by_4 \hat{\mathbf{y}} - c(z_4 - \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(4g)	O II
$\mathbf{B}_{11}$	$= -x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$-(ax_4 + cz_4 \cos \beta) \hat{\mathbf{x}} - by_4 \hat{\mathbf{y}} - cz_4 \sin \beta \hat{\mathbf{z}}$	(4g)	O II
$\mathbf{B}_{12}$	$= x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 + \left(z_4 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$(ax_4 + c(z_4 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_4 \hat{\mathbf{y}} + c(z_4 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(4g)	O II

## References

- [1] V. B. Kravchenko, *Crystal structure of the monoclinic form of magnesium tungstate  $MgWO_4$* , J. Struct. Chem. **10**, 139–140 (1969), doi:10.1007/BF00751974.
- [2] C. Hermann, O. Lohrmann, and H. Philipp, eds., *Strukturbericht Band II 1928-1932* (Akademische Verlagsgesellschaft M. B. H., Leipzig, 1937).