Huanzalaite ($MgWO_4$, $H0_6$) Structure: AB4C_mP12_13_e_2g_f-003

This structure previously used the label(s) `AB4C_mP12_13_f_2g_e`. Calls to these addresses will be redirected here.

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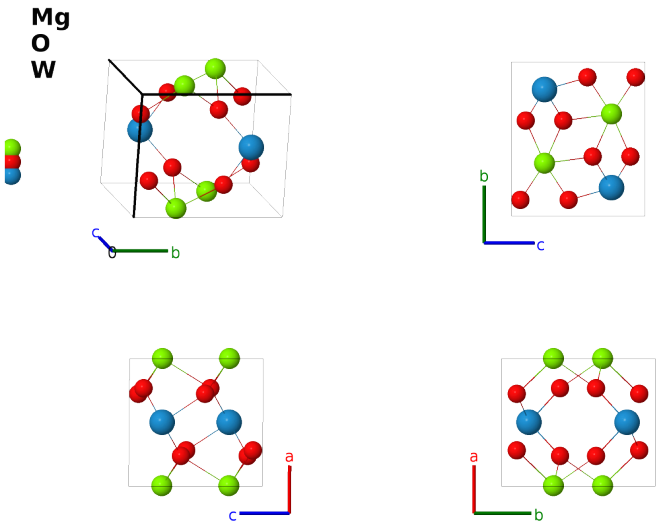
https://aflow.org/prototype-encyclopedia/2SHQ

https://aflow.org/prototype-encyclopedia/AB4C_mP12_13_e_2g_f-003



Prototype	MgO_4W
AFLOW prototype label	AB4C_mP12_13_e_2g_f-003
***Strukturbericht* designation**	$H0_6$
Mineral name	huanzalaite
ICSD	20470
CCDC	1598269
Pearson symbol	mP12
Space group number	13
Space group symbol	$P2/c$
AFLOW prototype command	`aflow --proto=AB4C_mP12_13_e_2g_f-003 --params=`$a, b/a, c/a, \beta, y_1, y_2, x_3, y_3, z_3, x_4, y_4, z_4$

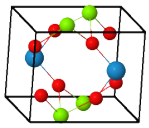
Other compounds with this structure

$ErTaO_4$, $EuTaO_4$, $FeNbO_4$, $FeVO_4$, $GdTaO_4$, $HoTaO_4$, $InNbO_4$, $InTaO_4$, $LuTaO_4$, $NaErCl_4$, $NbGaO_4$, $ScTaO_4$, $YbTaO_4$, $CoWO_4$, $FeWO_4$ (ferberite), $MnReO_4$, $MnWO_4$ (hübernite), $NiMoO_4$, $NiWO_4$, $ZnMoO_4$, $ZnWO_4$

- Most authors refer to this as the wolframite structure, but that name properly belongs to the solid solution (Mn,Fe)WO_4. (Herman, 1937) chose this "magnesium wolframite" compound to represent the $H0_6$ structures.
- the ICSD designates names this structure type $NiWO_3$, but we use $MnWO_3$ to maintain compatibility with the *Strukturbericht* label.

Simple Monoclinic primitive vectors

$$\mathbf{a_1} = a\,\hat{\mathbf{x}}$$
$$\mathbf{a_2} = b\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\cos\beta\,\hat{\mathbf{x}} + c\sin\beta\,\hat{\mathbf{z}}$$



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
$\mathbf{B_6}$	=	$-x_3\,\mathbf{a}_1 + y_3\,\mathbf{a}_2 - \left(z_3 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\left(ax_3 + c\left(z_3 - \frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} + by_3\,\hat{\mathbf{y}} - c\left(z_3 - \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4g)	O I
$\mathbf{B_7}$	=	$-x_3\,\mathbf{a}_1 - y_3\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$	=	$-\left(ax_3 + cz_3\cos\beta\right)\,\hat{\mathbf{x}} - by_3\,\hat{\mathbf{y}} - cz_3\sin\beta\,\hat{\mathbf{z}}$	(4g)	O I
$\mathbf{B_8}$	=	$x_3\,\mathbf{a}_1 - y_3\,\mathbf{a}_2 + \left(z_3 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\left(ax_3 + c\left(z_3 + \frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} - by_3\,\hat{\mathbf{y}} + c\left(z_3 + \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(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
$\mathbf{B_{10}}$	=	$-x_4\,\mathbf{a}_1 + y_4\,\mathbf{a}_2 - \left(z_4 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\left(ax_4 + c\left(z_4 - \frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} + by_4\,\hat{\mathbf{y}} - c\left(z_4 - \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4g)	O II
$\mathbf{B_{11}}$	=	$-x_4\,\mathbf{a}_1 - y_4\,\mathbf{a}_2 - z_4\,\mathbf{a}_3$	=	$-\left(ax_4 + cz_4\cos\beta\right)\,\hat{\mathbf{x}} - by_4\,\hat{\mathbf{y}} - cz_4\sin\beta\,\hat{\mathbf{z}}$	(4g)	O II
$\mathbf{B_{12}}$	=	$x_4\,\mathbf{a}_1 - y_4\,\mathbf{a}_2 + \left(z_4 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\left(ax_4 + c\left(z_4 + \frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} - by_4\,\hat{\mathbf{y}} + c\left(z_4 + \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(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).

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