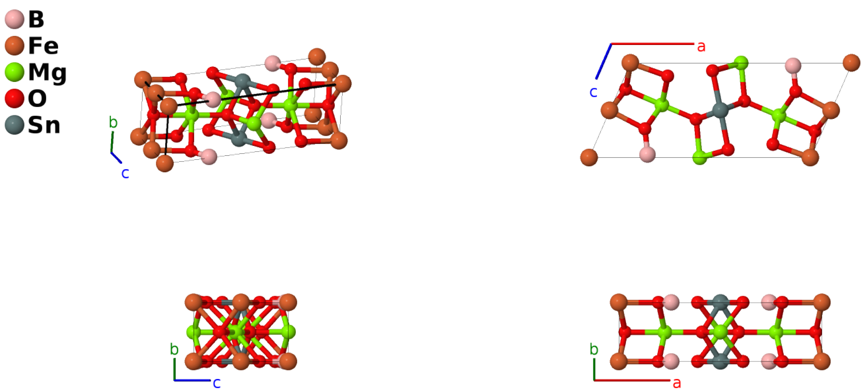
Hulsite [$(Fe_{1.315}Mg_{0.56}Sn_{0.1})BO_5$] Structure: A2B2C3D10E_mP18_10_m_ac_en_3m2n_g-001

Cite this page as: H. Eckert, S. Divilov, A. Zettel, M. J. Mehl, D. Hicks, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*. In preparation.

https://aflow.org/p/8URQ

https://aflow.org/p/A2B2C3D10E_mP18_10_m_ac_en_3m2n_g-001



Prototype $BFe_{1.315}Mg_{0.56}O_5Sn_{0.1}$

AFLOW prototype label A2B2C3D10E_mP18_10_m_ac_en_3m2n_g-001

Mineral name hulsite

ICSD 12133

Pearson symbol mP18

Space group number 10

Space group symbol $P2/m$

AFLOW prototype command `aflow --proto=A2B2C3D10E_mP18_10_m_ac_en_3m2n_g-001 --params=`$a, b/a, c/a, \beta, x_5, z_5, x_6, z_6, x_7, z_7, x_8, z_8, x_9, z_9, x_{10}, z_{10}, x_{11}, z_{11}$

Other compounds with this structure

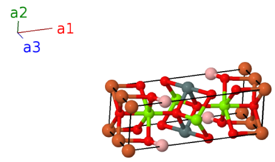
$Na_{2.57}Sn_{0.43}BO_5$

- As can be seen from the composition, the metallic atoms in this mineral are on mixed sites with many vacancies. The labels we have assigned to each site are purely for convenience.
- According to (Konnert, 1976), the composition of each site is:
  - (1a) 50% Fe
  - (1c) 50% Fe
  - (1e) 36% Fe, 16% Mg (labeled Mg)
  - (1g) 20% Sn, 27% Fe (labeled Sn here)
  - Metallic (2n) 50% Fe, 48% Mg (labeled Mg).
  - The boron and oxygen sites are fully occupied.

- We have switched the a and c axis from that defined by (Konnert, 1976). This swaps the (1a) and (1g) Wyckoff positions, while the (1d) Wyckoff postion becomes (1c) and (1f) becomes (1e).

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
$\mathbf{B_1}$	=	0	=	0	(1a)	Fe I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}c\cos\beta\,\hat{\mathbf{x}} + \frac{1}{2}c\sin\beta\,\hat{\mathbf{z}}$	(1c)	Fe II
$\mathbf{B_3}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}b\,\hat{\mathbf{y}}$	(1e)	Mg I
$\mathbf{B_4}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}\left(a + c\cos\beta\right)\,\hat{\mathbf{x}} + \frac{1}{2}c\sin\beta\,\hat{\mathbf{z}}$	(1g)	Sn I
$\mathbf{B_5}$	=	$x_5\,\mathbf{a}_1 + z_5\,\mathbf{a}_3$	=	$\left(ax_5 + cz_5\cos\beta\right)\,\hat{\mathbf{x}} + cz_5\sin\beta\,\hat{\mathbf{z}}$	(2m)	B I
$\mathbf{B_6}$	=	$-x_5\,\mathbf{a}_1 - z_5\,\mathbf{a}_3$	=	$-\left(ax_5 + cz_5\cos\beta\right)\,\hat{\mathbf{x}} - cz_5\sin\beta\,\hat{\mathbf{z}}$	(2m)	B I
$\mathbf{B_7}$	=	$x_6\,\mathbf{a}_1 + z_6\,\mathbf{a}_3$	=	$\left(ax_6 + cz_6\cos\beta\right)\,\hat{\mathbf{x}} + cz_6\sin\beta\,\hat{\mathbf{z}}$	(2m)	O I
$\mathbf{B_8}$	=	$-x_6\,\mathbf{a}_1 - z_6\,\mathbf{a}_3$	=	$-\left(ax_6 + cz_6\cos\beta\right)\,\hat{\mathbf{x}} - cz_6\sin\beta\,\hat{\mathbf{z}}$	(2m)	O I
$\mathbf{B_9}$	=	$x_7\,\mathbf{a}_1 + z_7\,\mathbf{a}_3$	=	$\left(ax_7 + cz_7\cos\beta\right)\,\hat{\mathbf{x}} + cz_7\sin\beta\,\hat{\mathbf{z}}$	(2m)	O II
$\mathbf{B_{10}}$	=	$-x_7\,\mathbf{a}_1 - z_7\,\mathbf{a}_3$	=	$-\left(ax_7 + cz_7\cos\beta\right)\,\hat{\mathbf{x}} - cz_7\sin\beta\,\hat{\mathbf{z}}$	(2m)	O II
$\mathbf{B_{11}}$	=	$x_8\,\mathbf{a}_1 + z_8\,\mathbf{a}_3$	=	$\left(ax_8 + cz_8\cos\beta\right)\,\hat{\mathbf{x}} + cz_8\sin\beta\,\hat{\mathbf{z}}$	(2m)	O III
$\mathbf{B_{12}}$	=	$-x_8\,\mathbf{a}_1 - z_8\,\mathbf{a}_3$	=	$-\left(ax_8 + cz_8\cos\beta\right)\,\hat{\mathbf{x}} - cz_8\sin\beta\,\hat{\mathbf{z}}$	(2m)	O III
$\mathbf{B_{13}}$	=	$x_9\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + z_9\,\mathbf{a}_3$	=	$\left(ax_9 + cz_9\cos\beta\right)\,\hat{\mathbf{x}} + \frac{1}{2}b\,\hat{\mathbf{y}} + cz_9\sin\beta\,\hat{\mathbf{z}}$	(2n)	Mg II
$\mathbf{B_{14}}$	=	$-x_9\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 - z_9\,\mathbf{a}_3$	=	$-\left(ax_9 + cz_9\cos\beta\right)\,\hat{\mathbf{x}} + \frac{1}{2}b\,\hat{\mathbf{y}} - cz_9\sin\beta\,\hat{\mathbf{z}}$	(2n)	Mg II
$\mathbf{B_{15}}$	=	$x_{10}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + z_{10}\,\mathbf{a}_3$	=	$\left(ax_{10} + cz_{10}\cos\beta\right)\,\hat{\mathbf{x}} + \frac{1}{2}b\,\hat{\mathbf{y}} + cz_{10}\sin\beta\,\hat{\mathbf{z}}$	(2n)	O IV
$\mathbf{B_{16}}$	=	$-x_{10}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 - z_{10}\,\mathbf{a}_3$	=	$-\left(ax_{10} + cz_{10}\cos\beta\right)\,\hat{\mathbf{x}} + \frac{1}{2}b\,\hat{\mathbf{y}} - cz_{10}\sin\beta\,\hat{\mathbf{z}}$	(2n)	O IV
$\mathbf{B_{17}}$	=	$x_{11}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + z_{11}\,\mathbf{a}_3$	=	$\left(ax_{11} + cz_{11}\cos\beta\right)\,\hat{\mathbf{x}} + \frac{1}{2}b\,\hat{\mathbf{y}} + cz_{11}\sin\beta\,\hat{\mathbf{z}}$	(2n)	O V
$\mathbf{B_{18}}$	=	$-x_{11}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 - z_{11}\,\mathbf{a}_3$	=	$-\left(ax_{11} + cz_{11}\cos\beta\right)\,\hat{\mathbf{x}} + \frac{1}{2}b\,\hat{\mathbf{y}} - cz_{11}\sin\beta\,\hat{\mathbf{z}}$	(2n)	O V

References

[1] J. A. Konnert, D. E. Appleman, J. R. Clark, L. W. Finger, T. Kato, and Y. Miura, *Crystal structure and cation distribution of hulsite, a tin-iron borate*, Am. Mineral. **61**, 116–122 (1976).

Found in

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