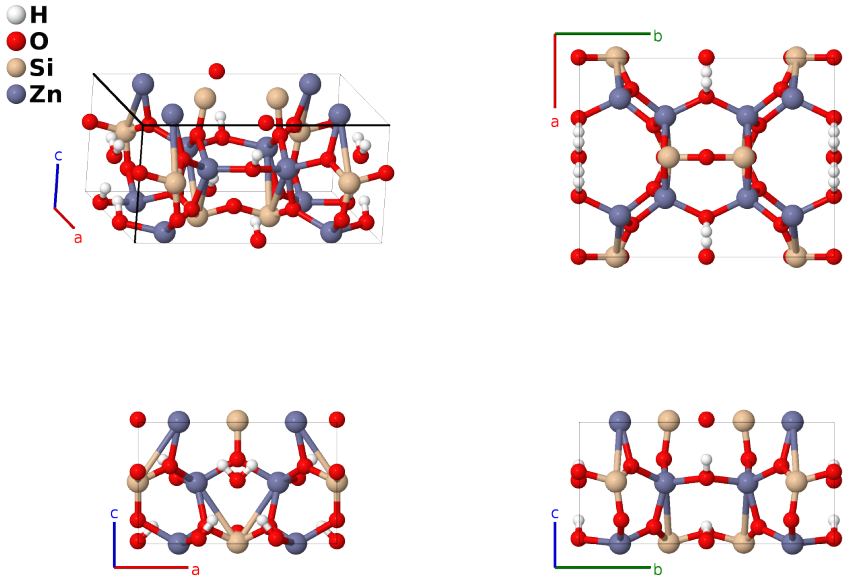
Hemimorphite ($Zn_4Si_2O_7(OH)_2{\cdot}H_2O$, $S2_2$) Structure: A2B5CD2_oI40_44_2c_abcde_d_e-001

This structure originally had the label `A2B5CD2_oI40_44_2c_abcde_d_e`. Calls to that address will be redirected here.

Cite this page as: D. Hicks, M. J. Mehl, M. Esters, C. Oses, O. Levy, G. L. W. Hart, C. Toher, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 3*, Comput. Mater. Sci. **199**, 110450 (2021), doi: 10.1016/j.commatsci.2021.110450.

https://aflow.org/p/W7BE

https://aflow.org/p/A2B5CD2_oI40_44_2c_abcde_d_e-001

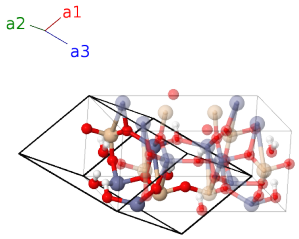


Prototype	$H_2O_{10}Si_2Zn_4$
AFLOW prototype label	A2B5CD2_oI40_44_2c_abcde_d_e-001
***Strukturbericht* designation**	$S2_2$
Mineral name	hemimorphite
ICSD	100201
Pearson symbol	oI40
Space group number	44
Space group symbol	$Imm2$
AFLOW prototype command	`aflow --proto=A2B5CD2_oI40_44_2c_abcde_d_e-001 --params=`$a, b/a, c/a, z_1, z_2, x_3, z_3, x_4, z_4, x_5, z_5, y_6, z_6, y_7, z_7, x_8, y_8, z_8, x_9, y_9, z_9$

- The original (Ito, 1932) determination of this structure did not locate the positions of the hydrogen atoms. (Hill, 1977) were able to do this, so we use the updated structure as the prototype.
- (Hill, 1977) gives the z coordinates of the atoms on the (2c) sites as 0.0190, 0.0643, and 0.0410, respectively, but this gives unrealistic H-O distances. Examination of the figures and distance tables shows that we should take $z_2 = 0.190$, $z_3 = 0.643$, and $z_4 = 0.041$, a conclusion also reached by (Downs, 2003) and the ICSD.

Body-centered Orthorhombic primitive vectors

$$
\begin{aligned}
\mathbf{a_1} &= -\tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}b\,\hat{\mathbf{y}} + \tfrac{1}{2}c\,\hat{\mathbf{z}} \\
\mathbf{a_2} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{1}{2}b\,\hat{\mathbf{y}} + \tfrac{1}{2}c\,\hat{\mathbf{z}} \\
\mathbf{a_3} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}b\,\hat{\mathbf{y}} - \tfrac{1}{2}c\,\hat{\mathbf{z}}
\end{aligned}
$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$z_1\,\mathbf{a}_1 + z_1\,\mathbf{a}_2$	=	$cz_1\,\hat{\mathbf{z}}$	(2a)	O I
$\mathbf{B_2}$	=	$\left(z_2 + \frac{1}{2}\right)\,\mathbf{a}_1 + z_2\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}b\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(2b)	O II
$\mathbf{B_3}$	=	$z_3\,\mathbf{a}_1 + (x_3 + z_3)\,\mathbf{a}_2 + x_3\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} + cz_3\,\hat{\mathbf{z}}$	(4c)	H I
$\mathbf{B_4}$	=	$z_3\,\mathbf{a}_1 - (x_3 - z_3)\,\mathbf{a}_2 - x_3\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} + cz_3\,\hat{\mathbf{z}}$	(4c)	H I
$\mathbf{B_5}$	=	$z_4\,\mathbf{a}_1 + (x_4 + z_4)\,\mathbf{a}_2 + x_4\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}} + cz_4\,\hat{\mathbf{z}}$	(4c)	H II
$\mathbf{B_6}$	=	$z_4\,\mathbf{a}_1 - (x_4 - z_4)\,\mathbf{a}_2 - x_4\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}} + cz_4\,\hat{\mathbf{z}}$	(4c)	H II
$\mathbf{B_7}$	=	$z_5\,\mathbf{a}_1 + (x_5 + z_5)\,\mathbf{a}_2 + x_5\,\mathbf{a}_3$	=	$ax_5\,\hat{\mathbf{x}} + cz_5\,\hat{\mathbf{z}}$	(4c)	O III
$\mathbf{B_8}$	=	$z_5\,\mathbf{a}_1 - (x_5 - z_5)\,\mathbf{a}_2 - x_5\,\mathbf{a}_3$	=	$-ax_5\,\hat{\mathbf{x}} + cz_5\,\hat{\mathbf{z}}$	(4c)	O III
$\mathbf{B_9}$	=	$(y_6 + z_6)\,\mathbf{a}_1 + z_6\,\mathbf{a}_2 + y_6\,\mathbf{a}_3$	=	$by_6\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(4d)	O IV
$\mathbf{B_{10}}$	=	$-(y_6 - z_6)\,\mathbf{a}_1 + z_6\,\mathbf{a}_2 - y_6\,\mathbf{a}_3$	=	$-by_6\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(4d)	O IV
$\mathbf{B_{11}}$	=	$(y_7 + z_7)\,\mathbf{a}_1 + z_7\,\mathbf{a}_2 + y_7\,\mathbf{a}_3$	=	$by_7\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}}$	(4d)	Si I
$\mathbf{B_{12}}$	=	$-(y_7 - z_7)\,\mathbf{a}_1 + z_7\,\mathbf{a}_2 - y_7\,\mathbf{a}_3$	=	$-by_7\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}}$	(4d)	Si I
$\mathbf{B_{13}}$	=	$(y_8 + z_8)\,\mathbf{a}_1 + (x_8 + z_8)\,\mathbf{a}_2 + (x_8 + y_8)\,\mathbf{a}_3$	=	$ax_8\,\hat{\mathbf{x}} + by_8\,\hat{\mathbf{y}} + cz_8\,\hat{\mathbf{z}}$	(8e)	O V
$\mathbf{B_{14}}$	=	$-(y_8 - z_8)\,\mathbf{a}_1 - (x_8 - z_8)\,\mathbf{a}_2 - (x_8 + y_8)\,\mathbf{a}_3$	=	$-ax_8\,\hat{\mathbf{x}} - by_8\,\hat{\mathbf{y}} + cz_8\,\hat{\mathbf{z}}$	(8e)	O V
$\mathbf{B_{15}}$	=	$-(y_8 - z_8)\,\mathbf{a}_1 + (x_8 + z_8)\,\mathbf{a}_2 + (x_8 - y_8)\,\mathbf{a}_3$	=	$ax_8\,\hat{\mathbf{x}} - by_8\,\hat{\mathbf{y}} + cz_8\,\hat{\mathbf{z}}$	(8e)	O V
$\mathbf{B_{16}}$	=	$(y_8 + z_8)\,\mathbf{a}_1 - (x_8 - z_8)\,\mathbf{a}_2 - (x_8 - y_8)\,\mathbf{a}_3$	=	$-ax_8\,\hat{\mathbf{x}} + by_8\,\hat{\mathbf{y}} + cz_8\,\hat{\mathbf{z}}$	(8e)	O V
$\mathbf{B_{17}}$	=	$(y_9 + z_9)\,\mathbf{a}_1 + (x_9 + z_9)\,\mathbf{a}_2 + (x_9 + y_9)\,\mathbf{a}_3$	=	$ax_9\,\hat{\mathbf{x}} + by_9\,\hat{\mathbf{y}} + cz_9\,\hat{\mathbf{z}}$	(8e)	Zn I
$\mathbf{B_{18}}$	=	$-(y_9 - z_9)\,\mathbf{a}_1 - (x_9 - z_9)\,\mathbf{a}_2 - (x_9 + y_9)\,\mathbf{a}_3$	=	$-ax_9\,\hat{\mathbf{x}} - by_9\,\hat{\mathbf{y}} + cz_9\,\hat{\mathbf{z}}$	(8e)	Zn I
$\mathbf{B_{19}}$	=	$-(y_9 - z_9)\,\mathbf{a}_1 + (x_9 + z_9)\,\mathbf{a}_2 + (x_9 - y_9)\,\mathbf{a}_3$	=	$ax_9\,\hat{\mathbf{x}} - by_9\,\hat{\mathbf{y}} + cz_9\,\hat{\mathbf{z}}$	(8e)	Zn I
$\mathbf{B_{20}}$	=	$(y_9 + z_9)\,\mathbf{a}_1 - (x_9 - z_9)\,\mathbf{a}_2 - (x_9 - y_9)\,\mathbf{a}_3$	=	$-ax_9\,\hat{\mathbf{x}} + by_9\,\hat{\mathbf{y}} + cz_9\,\hat{\mathbf{z}}$	(8e)	Zn I

References

[1] R. J. Hill, G. V. Gibbs, J. R. Craig, F. K. Ross, and J. M. Williams, *A neutron-diffraction study of hemimorphite*, Z. Kristallogr. **146**, 241–259 (1977), doi:10.1524/zkri.1978.146.16.241.

[2] T. Ito and J. West, *The Structure of Hemimorphite ($H_2Zn_2SiO_5$)*, Z. Kristallogr. **83**, 1–8 (1932), doi:10.1524/zkri.1932.83.1.1.

Found in

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