Wülfingite (ϵ-Zn(OH)$_2$, C31) Structure: A2B2C_oP20_19_2a_2a_a-001
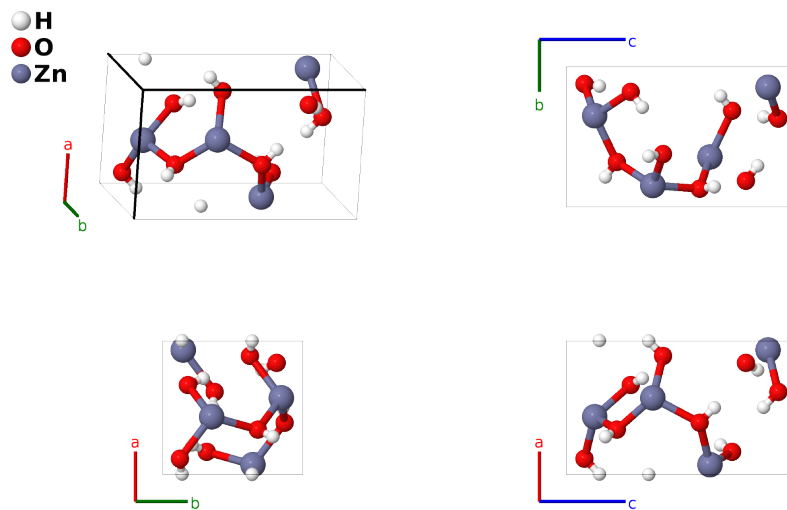
This structure originally had the label A2B2C_oP20_19_2a_2a_a. Calls to that address will be redirected here.

https://aflow.org/p/HY2J

https://aflow.org/p/A2B2C_oP20_19_2a_2a_a-001

|	
Prototype	H$_2$O$_2$Zn
AFLOW prototype label	A2B2C_oP20_19_2a_2a_a-001
Strukturbericht **designation**	$C31$
Mineral name	wülfingite
ICSD	50447
Pearson symbol	oP20
Space group number	19
Space group symbol	$P2_12_12_1$
AFLOW prototype command	aflow --proto=A2B2C_oP20_19_2a_2a_a-001
	--params=$a, b/a, c/a, x_1, y_1, z_1, x_2, y_2, z_2, x_3, y_3, z_3, x_4, y_4, z_4, x_5, y_5, z_5$

Other compounds with this structure

β-Be(OH)$_2$

- (Corey, 1933) originally determined the structure of ϵ-Zn(OH)$_2$, but they were unable to locate the hydrogen atoms. This structure was given the *Strukturbericht* designation $C31$ by (Gottfried, 1937).

- (Stahl, 1998) located the hydrogen atoms, and found that they did not change the space group, so we use the updated structure as our $C31$ prototype.

Simple Orthorhombic primitive vectors

$$\mathbf{a_1} = a\,\hat{\mathbf{x}}$$
$$\mathbf{a_2} = b\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$
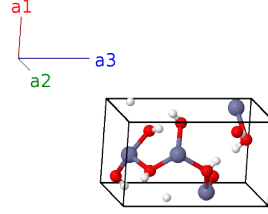
Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	$=$	$x_1\,\mathbf{a_1} + y_1\,\mathbf{a_2} + z_1\,\mathbf{a_3}$	$=$	$ax_1\,\hat{\mathbf{x}} + by_1\,\hat{\mathbf{y}} + cz_1\,\hat{\mathbf{z}}$	(4a)	H I
$\mathbf{B_2}$	$=$	$-\left(x_1 - \frac{1}{2}\right)\mathbf{a_1} - y_1\,\mathbf{a_2} + \left(z_1 + \frac{1}{2}\right)\mathbf{a_3}$	$=$	$-a\left(x_1 - \frac{1}{2}\right)\hat{\mathbf{x}} - by_1\,\hat{\mathbf{y}} + c\left(z_1 + \frac{1}{2}\right)\hat{\mathbf{z}}$	(4a)	H I
$\mathbf{B_3}$	$=$	$-x_1\,\mathbf{a_1} + \left(y_1 + \frac{1}{2}\right)\mathbf{a_2} - \left(z_1 - \frac{1}{2}\right)\mathbf{a_3}$	$=$	$-ax_1\,\hat{\mathbf{x}} + b\left(y_1 + \frac{1}{2}\right)\hat{\mathbf{y}} - c\left(z_1 - \frac{1}{2}\right)\hat{\mathbf{z}}$	(4a)	H I
$\mathbf{B_4}$	$=$	$\left(x_1 + \frac{1}{2}\right)\mathbf{a_1} - \left(y_1 - \frac{1}{2}\right)\mathbf{a_2} - z_1\,\mathbf{a_3}$	$=$	$a\left(x_1 + \frac{1}{2}\right)\hat{\mathbf{x}} - b\left(y_1 - \frac{1}{2}\right)\hat{\mathbf{y}} - cz_1\,\hat{\mathbf{z}}$	(4a)	H I
$\mathbf{B_5}$	$=$	$x_2\,\mathbf{a_1} + y_2\,\mathbf{a_2} + z_2\,\mathbf{a_3}$	$=$	$ax_2\,\hat{\mathbf{x}} + by_2\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(4a)	H II
$\mathbf{B_6}$	$=$	$-\left(x_2 - \frac{1}{2}\right)\mathbf{a_1} - y_2\,\mathbf{a_2} + \left(z_2 + \frac{1}{2}\right)\mathbf{a_3}$	$=$	$-a\left(x_2 - \frac{1}{2}\right)\hat{\mathbf{x}} - by_2\,\hat{\mathbf{y}} + c\left(z_2 + \frac{1}{2}\right)\hat{\mathbf{z}}$	(4a)	H II
$\mathbf{B_7}$	$=$	$-x_2\,\mathbf{a_1} + \left(y_2 + \frac{1}{2}\right)\mathbf{a_2} - \left(z_2 - \frac{1}{2}\right)\mathbf{a_3}$	$=$	$-ax_2\,\hat{\mathbf{x}} + b\left(y_2 + \frac{1}{2}\right)\hat{\mathbf{y}} - c\left(z_2 - \frac{1}{2}\right)\hat{\mathbf{z}}$	(4a)	H II
$\mathbf{B_8}$	$=$	$\left(x_2 + \frac{1}{2}\right)\mathbf{a_1} - \left(y_2 - \frac{1}{2}\right)\mathbf{a_2} - z_2\,\mathbf{a_3}$	$=$	$a\left(x_2 + \frac{1}{2}\right)\hat{\mathbf{x}} - b\left(y_2 - \frac{1}{2}\right)\hat{\mathbf{y}} - cz_2\,\hat{\mathbf{z}}$	(4a)	H II
$\mathbf{B_9}$	$=$	$x_3\,\mathbf{a_1} + y_3\,\mathbf{a_2} + z_3\,\mathbf{a_3}$	$=$	$ax_3\,\hat{\mathbf{x}} + by_3\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(4a)	O I
$\mathbf{B_{10}}$	$=$	$-\left(x_3 - \frac{1}{2}\right)\mathbf{a_1} - y_3\,\mathbf{a_2} + \left(z_3 + \frac{1}{2}\right)\mathbf{a_3}$	$=$	$-a\left(x_3 - \frac{1}{2}\right)\hat{\mathbf{x}} - by_3\,\hat{\mathbf{y}} + c\left(z_3 + \frac{1}{2}\right)\hat{\mathbf{z}}$	(4a)	O I
$\mathbf{B_{11}}$	$=$	$-x_3\,\mathbf{a_1} + \left(y_3 + \frac{1}{2}\right)\mathbf{a_2} - \left(z_3 - \frac{1}{2}\right)\mathbf{a_3}$	$=$	$-ax_3\,\hat{\mathbf{x}} + b\left(y_3 + \frac{1}{2}\right)\hat{\mathbf{y}} - c\left(z_3 - \frac{1}{2}\right)\hat{\mathbf{z}}$	(4a)	O I
$\mathbf{B_{12}}$	$=$	$\left(x_3 + \frac{1}{2}\right)\mathbf{a_1} - \left(y_3 - \frac{1}{2}\right)\mathbf{a_2} - z_3\,\mathbf{a_3}$	$=$	$a\left(x_3 + \frac{1}{2}\right)\hat{\mathbf{x}} - b\left(y_3 - \frac{1}{2}\right)\hat{\mathbf{y}} - cz_3\,\hat{\mathbf{z}}$	(4a)	O I
$\mathbf{B_{13}}$	$=$	$x_4\,\mathbf{a_1} + y_4\,\mathbf{a_2} + z_4\,\mathbf{a_3}$	$=$	$ax_4\,\hat{\mathbf{x}} + by_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(4a)	O II
$\mathbf{B_{14}}$	$=$	$-\left(x_4 - \frac{1}{2}\right)\mathbf{a_1} - y_4\,\mathbf{a_2} + \left(z_4 + \frac{1}{2}\right)\mathbf{a_3}$	$=$	$-a\left(x_4 - \frac{1}{2}\right)\hat{\mathbf{x}} - by_4\,\hat{\mathbf{y}} + c\left(z_4 + \frac{1}{2}\right)\hat{\mathbf{z}}$	(4a)	O II
$\mathbf{B_{15}}$	$=$	$-x_4\,\mathbf{a_1} + \left(y_4 + \frac{1}{2}\right)\mathbf{a_2} - \left(z_4 - \frac{1}{2}\right)\mathbf{a_3}$	$=$	$-ax_4\,\hat{\mathbf{x}} + b\left(y_4 + \frac{1}{2}\right)\hat{\mathbf{y}} - c\left(z_4 - \frac{1}{2}\right)\hat{\mathbf{z}}$	(4a)	O II
$\mathbf{B_{16}}$	$=$	$\left(x_4 + \frac{1}{2}\right)\mathbf{a_1} - \left(y_4 - \frac{1}{2}\right)\mathbf{a_2} - z_4\,\mathbf{a_3}$	$=$	$a\left(x_4 + \frac{1}{2}\right)\hat{\mathbf{x}} - b\left(y_4 - \frac{1}{2}\right)\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$	(4a)	O II
$\mathbf{B_{17}}$	$=$	$x_5\,\mathbf{a_1} + y_5\,\mathbf{a_2} + z_5\,\mathbf{a_3}$	$=$	$ax_5\,\hat{\mathbf{x}} + by_5\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(4a)	Zn I
$\mathbf{B_{18}}$	$=$	$-\left(x_5 - \frac{1}{2}\right)\mathbf{a_1} - y_5\,\mathbf{a_2} + \left(z_5 + \frac{1}{2}\right)\mathbf{a_3}$	$=$	$-a\left(x_5 - \frac{1}{2}\right)\hat{\mathbf{x}} - by_5\,\hat{\mathbf{y}} + c\left(z_5 + \frac{1}{2}\right)\hat{\mathbf{z}}$	(4a)	Zn I
$\mathbf{B_{19}}$	$=$	$-x_5\,\mathbf{a_1} + \left(y_5 + \frac{1}{2}\right)\mathbf{a_2} - \left(z_5 - \frac{1}{2}\right)\mathbf{a_3}$	$=$	$-ax_5\,\hat{\mathbf{x}} + b\left(y_5 + \frac{1}{2}\right)\hat{\mathbf{y}} - c\left(z_5 - \frac{1}{2}\right)\hat{\mathbf{z}}$	(4a)	Zn I
$\mathbf{B_{20}}$	$=$	$\left(x_5 + \frac{1}{2}\right)\mathbf{a_1} - \left(y_5 - \frac{1}{2}\right)\mathbf{a_2} - z_5\,\mathbf{a_3}$	$=$	$a\left(x_5 + \frac{1}{2}\right)\hat{\mathbf{x}} - b\left(y_5 - \frac{1}{2}\right)\hat{\mathbf{y}} - cz_5\,\hat{\mathbf{z}}$	(4a)	Zn I

References

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[2] R. B. Corey and R. W. G. Wyckoff, *The crystal structure of Zinc Hydroxide*, Z. Kristallogr. **86**, 3–18 (1933), doi:10.1524/zkri.1933.86.1.8.

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