Th_2Zn_{17} Structure: A2B17_hR19_166_c_cdfh-001

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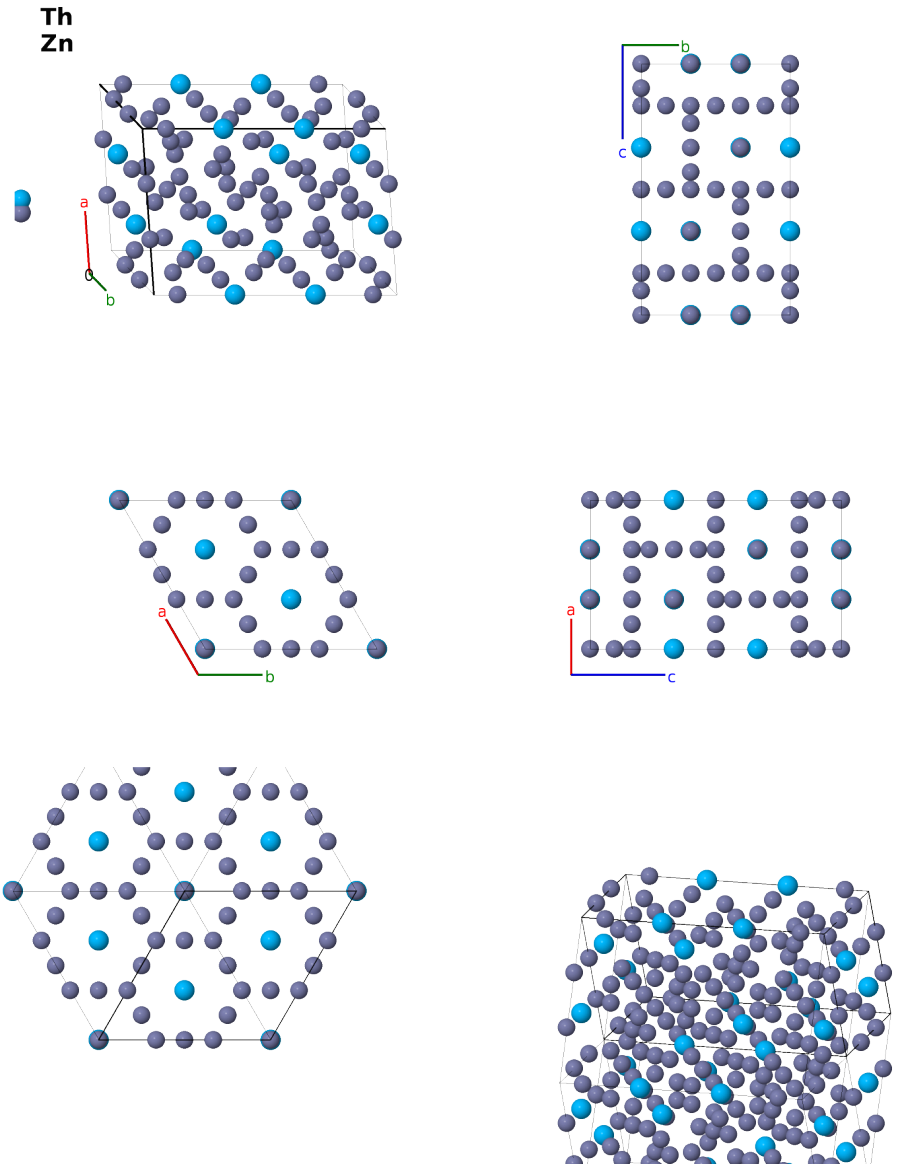
https://aflow.org/prototype-encyclopedia/PZ2T

https://aflow.org/prototype-encyclopedia/A2B17_hR19_166_c_cdfh-001



Prototype	Th_2Zn_{17}
AFLOW prototype label	A2B17_hR19_166_c_cdfh-001
ICSD	20238

CCDC	1598060
Pearson symbol	hR19
Space group number	166
Space group symbol	$R\bar{3}m$
AFLOW prototype command	`aflow --proto=A2B17_hR19_166_c_cdfh-001 --params=`$a, c/a, x_1, x_2, x_4, x_5, z_5$

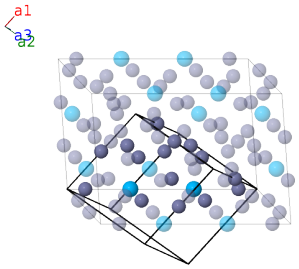
Other compounds with this structure

Ba_2Mg_{17}, Ce_2Co_{17}, Ce_2Fe_{17}, Ce_2Zn_{17}, Dy_2Co_{17}, Dy_2Fe_{17}, Dy_2Zn_{17}, Er_2Zn_{17}, Gd_2Co_{17}, Gd_2Fe_{17}, Gd_2Zn_{17}, Hf_2Be_{17}, Ho_2Co_{17}, Ho_2Zn_{17}, La_2Zn_{17}, Lu_2Zn_{17}, Nb_2Be_{17}, Nd_2Co_{17}, Nd_2Fe_{17}, Nd_2Zn_{17}, Pr_2Co_{17}, Pr_2Fe_{17}, Pr_2Zn_{17}, Pu_2Zn_{17}, Sm_2Co_{17}, Sm_2Fe_{17}, Sm_2Zn_{17}, Ta_2Be_{17}, Tb_2Co_{17}, Tb_2Fe_{17}, Tb_2Zn_{17}, Th_2Co_{17}, Th_2Fe_{17}, Th_2Zn_{17}, Ti_2Be_{17}, Tm_2Zn_{17}, U_2Zn_{17}, Y_2Co_{17}, Y_2Fe_{17}, Y_2Zn_{17}, Yb_2Zn_{17}, Zr_2Be_{17}, $Al_2Ce_2Co_{15}$, $Ce_2Mn_7Al_{10}$

- Hexagonal settings of this structure can be obtained with the option `--hex`.

Rhombohedral primitive vectors

$$\mathbf{a_1} = \frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{1}{3}c\,\hat{\mathbf{z}}$$
$$\mathbf{a_2} = \frac{1}{\sqrt{3}}a\,\hat{\mathbf{y}} + \frac{1}{3}c\,\hat{\mathbf{z}}$$
$$\mathbf{a_3} = -\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{1}{3}c\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$x_1\,\mathbf{a}_1 + x_1\,\mathbf{a}_2 + x_1\,\mathbf{a}_3$	=	$cx_1\,\hat{\mathbf{z}}$	(2c)	Th I
$\mathbf{B_2}$	=	$-x_1\,\mathbf{a}_1 - x_1\,\mathbf{a}_2 - x_1\,\mathbf{a}_3$	=	$-cx_1\,\hat{\mathbf{z}}$	(2c)	Th I
$\mathbf{B_3}$	=	$x_2\,\mathbf{a}_1 + x_2\,\mathbf{a}_2 + x_2\,\mathbf{a}_3$	=	$cx_2\,\hat{\mathbf{z}}$	(2c)	Zn I
$\mathbf{B_4}$	=	$-x_2\,\mathbf{a}_1 - x_2\,\mathbf{a}_2 - x_2\,\mathbf{a}_3$	=	$-cx_2\,\hat{\mathbf{z}}$	(2c)	Zn I
$\mathbf{B_5}$	=	$\frac{1}{2}\,\mathbf{a}_1$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{12}a\,\hat{\mathbf{y}} + \frac{1}{6}c\,\hat{\mathbf{z}}$	(3d)	Zn II
$\mathbf{B_6}$	=	$\frac{1}{2}\,\mathbf{a}_2$	=	$\frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{1}{6}c\,\hat{\mathbf{z}}$	(3d)	Zn II
$\mathbf{B_7}$	=	$\frac{1}{2}\,\mathbf{a}_3$	=	$-\frac{1}{4}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{12}a\,\hat{\mathbf{y}} + \frac{1}{6}c\,\hat{\mathbf{z}}$	(3d)	Zn II
$\mathbf{B_8}$	=	$x_4\,\mathbf{a}_1 - x_4\,\mathbf{a}_2$	=	$\frac{1}{2}ax_4\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_4\,\hat{\mathbf{y}}$	(6f)	Zn III
$\mathbf{B_9}$	=	$x_4\,\mathbf{a}_2 - x_4\,\mathbf{a}_3$	=	$\frac{1}{2}ax_4\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_4\,\hat{\mathbf{y}}$	(6f)	Zn III
$\mathbf{B_{10}}$	=	$-x_4\,\mathbf{a}_1 + x_4\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}}$	(6f)	Zn III
$\mathbf{B_{11}}$	=	$-x_4\,\mathbf{a}_1 + x_4\,\mathbf{a}_2$	=	$-\frac{1}{2}ax_4\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_4\,\hat{\mathbf{y}}$	(6f)	Zn III
$\mathbf{B_{12}}$	=	$-x_4\,\mathbf{a}_2 + x_4\,\mathbf{a}_3$	=	$-\frac{1}{2}ax_4\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_4\,\hat{\mathbf{y}}$	(6f)	Zn III
$\mathbf{B_{13}}$	=	$x_4\,\mathbf{a}_1 - x_4\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}}$	(6f)	Zn III
$\mathbf{B_{14}}$	=	$x_5\,\mathbf{a}_1 + x_5\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_5 - z_5)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(x_5 - z_5)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(2x_5 + z_5)\,\hat{\mathbf{z}}$	(6h)	Zn IV

$\mathbf{B_{15}}$	$=$	$z_5\,\mathbf{a}_1 + x_5\,\mathbf{a}_2 + x_5\,\mathbf{a}_3$	$=$	$-\frac{1}{2}a\,(x_5 - z_5)\;\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(x_5 - z_5)\;\hat{\mathbf{y}} + \frac{1}{3}c\,(2x_5 + z_5)\;\hat{\mathbf{z}}$	(6h)	Zn IV
$\mathbf{B_{16}}$	$=$	$x_5\,\mathbf{a}_1 + z_5\,\mathbf{a}_2 + x_5\,\mathbf{a}_3$	$=$	$-\frac{1}{\sqrt{3}}a\,(x_5 - z_5)\;\hat{\mathbf{y}} + \frac{1}{3}c\,(2x_5 + z_5)\;\hat{\mathbf{z}}$	(6h)	Zn IV
$\mathbf{B_{17}}$	$=$	$-z_5\,\mathbf{a}_1 - x_5\,\mathbf{a}_2 - x_5\,\mathbf{a}_3$	$=$	$\frac{1}{2}a\,(x_5 - z_5)\;\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,(x_5 - z_5)\;\hat{\mathbf{y}} - \frac{1}{3}c\,(2x_5 + z_5)\;\hat{\mathbf{z}}$	(6h)	Zn IV
$\mathbf{B_{18}}$	$=$	$-x_5\,\mathbf{a}_1 - x_5\,\mathbf{a}_2 - z_5\,\mathbf{a}_3$	$=$	$-\frac{1}{2}a\,(x_5 - z_5)\;\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,(x_5 - z_5)\;\hat{\mathbf{y}} - \frac{1}{3}c\,(2x_5 + z_5)\;\hat{\mathbf{z}}$	(6h)	Zn IV
$\mathbf{B_{19}}$	$=$	$-x_5\,\mathbf{a}_1 - z_5\,\mathbf{a}_2 - x_5\,\mathbf{a}_3$	$=$	$\frac{1}{\sqrt{3}}a\,(x_5 - z_5)\;\hat{\mathbf{y}} - \frac{1}{3}c\,(2x_5 + z_5)\;\hat{\mathbf{z}}$	(6h)	Zn IV

References

[1] E. S. Makarov and S. I. Vinogradov, *Crystal Structure of Th_2Zn_{17} and U_2Zn_{17}*, Sov. Phys. Crystallogr. **1**, 499–504 (1956). Translated from Kristallografiya 1, 634 (1956).

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