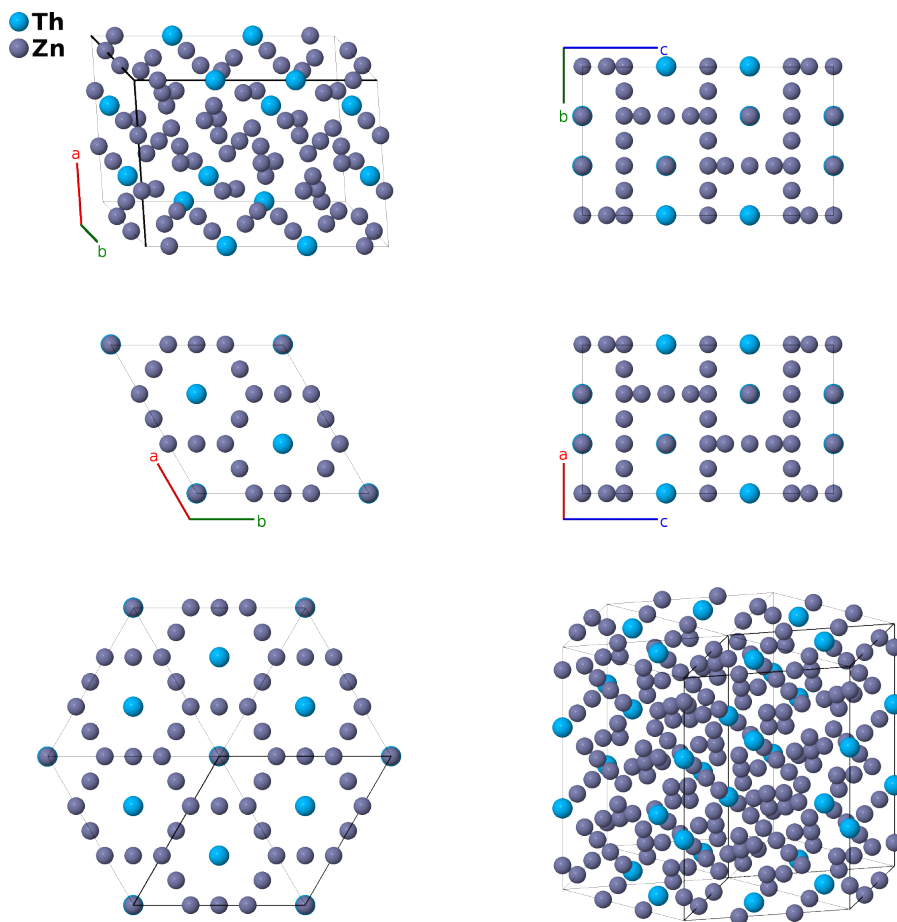


Th₂Zn₁₇ Structure: A2B17_hR19_166_c_cdfh-001

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/PZ2T>

https://aflow.org/p/A2B17_hR19_166_c_cdfh-001



| | |
|-------------------------|---|
| Prototype | Th ₂ Zn ₁₇ |
| AFLOW prototype label | A2B17_hR19_166_c_cdfh-001 |
| ICSD | 20238 |
| Pearson symbol | hR19 |
| Space group number | 166 |
| Space group symbol | $R\bar{3}m$ |
| AFLOW prototype command | <code>aflow --proto=A2B17_hR19_166_c_cdfh-001 --params=a, c/a, x₁, x₂, x₄, x₅, z₅</code> |

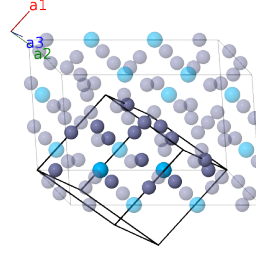
Other compounds with this structure

Ba₂Mg₁₇, Ce₂Co₁₇, Ce₂Fe₁₇, Ce₂Zn₁₇, Dy₂Zn₁₇, Er₂Zn₁₇, Gd₂Co₁₇, Gd₂Fe₁₇, Gd₂Zn₁₇, Ho₂Zn₁₇, La₂Zn₁₇, Lu₂Zn₁₇, Nd₂Co₁₇, Nd₂Fe₁₇, Nd₂Zn₁₇, Pr₂Co₁₇, Pr₂Zn₁₇, Sm₂Co₁₇, Sm₂Zn₁₇, Tb₂Co₁₇, Tb₂Zn₁₇, Th₂Co₁₇, Th₂Fe₁₇, Tm₂Zn₁₇, U₂Zn₁₇, Yb₂Zn₁₇, Al₂Ce₂Co₁₅, Ce₂Mn₇Al₁₀

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

Rhombohedral primitive vectors

$$\begin{aligned}\mathbf{a}_1 &= \frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + \frac{1}{3}c \hat{\mathbf{z}} \\ \mathbf{a}_2 &= \frac{1}{\sqrt{3}}a \hat{\mathbf{y}} + \frac{1}{3}c \hat{\mathbf{z}} \\ \mathbf{a}_3 &= -\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + \frac{1}{3}c \hat{\mathbf{z}}\end{aligned}$$



Basis vectors

| | Lattice coordinates | | Cartesian coordinates | Wyckoff position | Atom type |
|-----------------------|---|---|---|------------------|-----------|
| B₁ | $x_1 \mathbf{a}_1 + x_1 \mathbf{a}_2 + x_1 \mathbf{a}_3$ | = | $cx_1 \hat{\mathbf{z}}$ | (2c) | Th I |
| B₂ | $-x_1 \mathbf{a}_1 - x_1 \mathbf{a}_2 - x_1 \mathbf{a}_3$ | = | $-cx_1 \hat{\mathbf{z}}$ | (2c) | Th I |
| B₃ | $x_2 \mathbf{a}_1 + x_2 \mathbf{a}_2 + x_2 \mathbf{a}_3$ | = | $cx_2 \hat{\mathbf{z}}$ | (2c) | Zn I |
| B₄ | $-x_2 \mathbf{a}_1 - x_2 \mathbf{a}_2 - x_2 \mathbf{a}_3$ | = | $-cx_2 \hat{\mathbf{z}}$ | (2c) | Zn I |
| B₅ | $\frac{1}{2} \mathbf{a}_1$ | = | $\frac{1}{4}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{12}a \hat{\mathbf{y}} + \frac{1}{6}c \hat{\mathbf{z}}$ | (3d) | Zn II |
| B₆ | $\frac{1}{2} \mathbf{a}_2$ | = | $\frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + \frac{1}{6}c \hat{\mathbf{z}}$ | (3d) | Zn II |
| B₇ | $\frac{1}{2} \mathbf{a}_3$ | = | $-\frac{1}{4}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{12}a \hat{\mathbf{y}} + \frac{1}{6}c \hat{\mathbf{z}}$ | (3d) | Zn II |
| B₈ | $x_4 \mathbf{a}_1 - x_4 \mathbf{a}_2$ | = | $\frac{1}{2}ax_4 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_4 \hat{\mathbf{y}}$ | (6f) | Zn III |
| B₉ | $x_4 \mathbf{a}_2 - x_4 \mathbf{a}_3$ | = | $\frac{1}{2}ax_4 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_4 \hat{\mathbf{y}}$ | (6f) | Zn III |
| B₁₀ | $-x_4 \mathbf{a}_1 + x_4 \mathbf{a}_3$ | = | $-ax_4 \hat{\mathbf{x}}$ | (6f) | Zn III |
| B₁₁ | $-x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2$ | = | $-\frac{1}{2}ax_4 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_4 \hat{\mathbf{y}}$ | (6f) | Zn III |
| B₁₂ | $-x_4 \mathbf{a}_2 + x_4 \mathbf{a}_3$ | = | $-\frac{1}{2}ax_4 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_4 \hat{\mathbf{y}}$ | (6f) | Zn III |
| B₁₃ | $x_4 \mathbf{a}_1 - x_4 \mathbf{a}_3$ | = | $ax_4 \hat{\mathbf{x}}$ | (6f) | Zn III |
| B₁₄ | $x_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$ | = | $\frac{1}{2}a(x_5 - z_5) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(x_5 - z_5) \hat{\mathbf{y}} + \frac{1}{3}c(2x_5 + z_5) \hat{\mathbf{z}}$ | (6h) | Zn IV |
| B₁₅ | $z_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 + x_5 \mathbf{a}_3$ | = | $-\frac{1}{2}a(x_5 - z_5) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(x_5 - z_5) \hat{\mathbf{y}} + \frac{1}{3}c(2x_5 + z_5) \hat{\mathbf{z}}$ | (6h) | Zn IV |
| B₁₆ | $x_5 \mathbf{a}_1 + z_5 \mathbf{a}_2 + x_5 \mathbf{a}_3$ | = | $-\frac{1}{\sqrt{3}}a(x_5 - z_5) \hat{\mathbf{y}} + \frac{1}{3}c(2x_5 + z_5) \hat{\mathbf{z}}$ | (6h) | Zn IV |
| B₁₇ | $-z_5 \mathbf{a}_1 - x_5 \mathbf{a}_2 - x_5 \mathbf{a}_3$ | = | $\frac{1}{2}a(x_5 - z_5) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_5 - z_5) \hat{\mathbf{y}} - \frac{1}{3}c(2x_5 + z_5) \hat{\mathbf{z}}$ | (6h) | Zn IV |
| B₁₈ | $-x_5 \mathbf{a}_1 - x_5 \mathbf{a}_2 - z_5 \mathbf{a}_3$ | = | $-\frac{1}{2}a(x_5 - z_5) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_5 - z_5) \hat{\mathbf{y}} - \frac{1}{3}c(2x_5 + z_5) \hat{\mathbf{z}}$ | (6h) | Zn IV |
| B₁₉ | $-x_5 \mathbf{a}_1 - z_5 \mathbf{a}_2 - x_5 \mathbf{a}_3$ | = | $\frac{1}{\sqrt{3}}a(x_5 - z_5) \hat{\mathbf{y}} - \frac{1}{3}c(2x_5 + z_5) \hat{\mathbf{z}}$ | (6h) | Zn IV |

References

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