

CeTe₃ Structure:

AB3_oC16_40_b_3b-001

This structure previously used the label(s) **AB3_oC16_40_b_3b**. Calls to these addresses will be redirected here.

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<https://aflow.org/prototype-encyclopedia/WA7J>

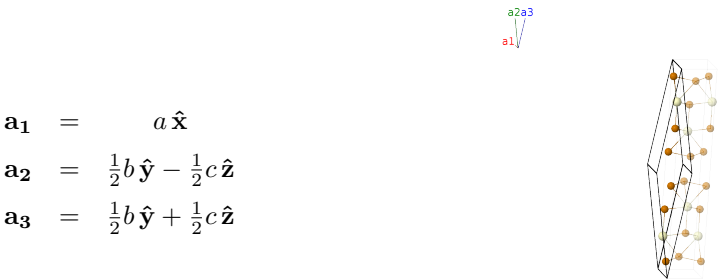
https://aflow.org/prototype-encyclopedia/AB3_oC16_40_b_3b-001

Prototype	CeTe ₃
AFLOW prototype label	AB3_oC16_40_b_3b-001
ICSD	170556
CCDC	1686028
Pearson symbol	oC16
Space group number	40
Space group symbol	<i>Ama</i> 2
AFLOW prototype command	<code>aflow --proto=AB3_oC16_40_b_3b-001</code> <code>--params=a, b/a, c/a, y₁, z₁, y₂, z₂, y₃, z₃, y₄, z₄</code>

Other compounds with this structure

NdTe₃, PrTe₃

Base-centered Orthorhombic primitive vectors



Basis vectors

	Lattice coordinates	Cartesian coordinates	Wyckoff position	Atom type
B₁	$= \frac{1}{4} \mathbf{a}_1 + (y_1 - z_1) \mathbf{a}_2 + (y_1 + z_1) \mathbf{a}_3$	$= \frac{1}{4}a \hat{\mathbf{x}} + by_1 \hat{\mathbf{y}} + cz_1 \hat{\mathbf{z}}$	(4b)	Ce I
B₂	$= \frac{3}{4} \mathbf{a}_1 - (y_1 + z_1) \mathbf{a}_2 - (y_1 - z_1) \mathbf{a}_3$	$= \frac{3}{4}a \hat{\mathbf{x}} - by_1 \hat{\mathbf{y}} + cz_1 \hat{\mathbf{z}}$	(4b)	Ce I

$$\begin{aligned}
\mathbf{B}_3 &= \frac{1}{4} \mathbf{a}_1 + (y_2 - z_2) \mathbf{a}_2 + (y_2 + z_2) \mathbf{a}_3 = \frac{1}{4} a \hat{\mathbf{x}} + by_2 \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}} & (4b) & \text{Te I} \\
\mathbf{B}_4 &= \frac{3}{4} \mathbf{a}_1 - (y_2 + z_2) \mathbf{a}_2 - (y_2 - z_2) \mathbf{a}_3 = \frac{3}{4} a \hat{\mathbf{x}} - by_2 \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}} & (4b) & \text{Te I} \\
\mathbf{B}_5 &= \frac{1}{4} \mathbf{a}_1 + (y_3 - z_3) \mathbf{a}_2 + (y_3 + z_3) \mathbf{a}_3 = \frac{1}{4} a \hat{\mathbf{x}} + by_3 \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}} & (4b) & \text{Te II} \\
\mathbf{B}_6 &= \frac{3}{4} \mathbf{a}_1 - (y_3 + z_3) \mathbf{a}_2 - (y_3 - z_3) \mathbf{a}_3 = \frac{3}{4} a \hat{\mathbf{x}} - by_3 \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}} & (4b) & \text{Te II} \\
\mathbf{B}_7 &= \frac{1}{4} \mathbf{a}_1 + (y_4 - z_4) \mathbf{a}_2 + (y_4 + z_4) \mathbf{a}_3 = \frac{1}{4} a \hat{\mathbf{x}} + by_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}} & (4b) & \text{Te III} \\
\mathbf{B}_8 &= \frac{3}{4} \mathbf{a}_1 - (y_4 + z_4) \mathbf{a}_2 - (y_4 - z_4) \mathbf{a}_3 = \frac{3}{4} a \hat{\mathbf{x}} - by_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}} & (4b) & \text{Te III}
\end{aligned}$$

References

- [1] C. Malliakas, S. J. L. Billinge, H. J. Kim, and M. G. Kanatzidis, *Square Nets of Tellurium: Rare-Earth Dependent Variation in the Charge-Density Wave of $RETe_3$ ($RE = \text{Rare-Earth Element}$)*, J. Am. Chem. Soc. **127**, 6510–6511 (2005), doi:10.1021/ja0505292.

Found in

- [1] P. Villars and K. Cenzual, *Pearson's Crystal Data – Crystal Structure Database for Inorganic Compounds* (2013). ASM International.

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- D. Hicks, M. J. Mehl, E. Gossett, C. Toher, O. Levy, R. M. Hanson, G. Hart, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 2*, Comput. Mater. Sci. **161**, S1 (2019). doi: 10.1016/j.commatsci.2018.10.043

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