

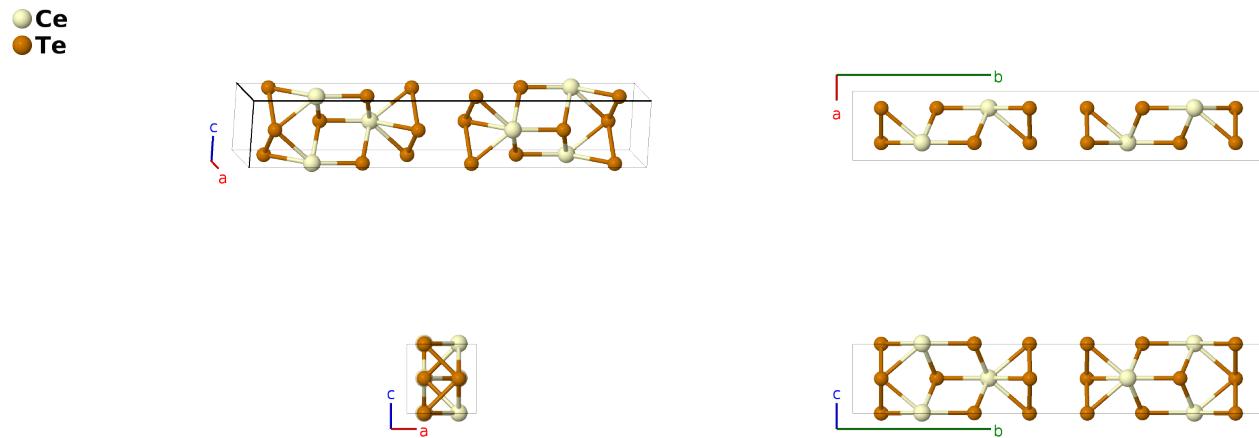
# CeTe<sub>3</sub> Structure: AB<sub>3</sub>\_oC16\_40\_b\_3b-001

This structure originally had the label AB<sub>3</sub>\_oC16\_40\_b\_3b. Calls to that address will be redirected here.

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<https://aflow.org/p/WA7J>

[https://aflow.org/p/AB3\\_oC16\\_40\\_b\\_3b-001](https://aflow.org/p/AB3_oC16_40_b_3b-001)



Prototype	CeTe <sub>3</sub>
AFLOW prototype label	AB <sub>3</sub> _oC16_40_b_3b-001
ICSD	170556
Pearson symbol	oC16
Space group number	40
Space group symbol	Ama2
AFLOW prototype command	<pre>aflow --proto=AB3_oC16_40_b_3b-001 --params=a, b/a, c/a, y1, z1, y2, z2, y3, z3, y4, z4</pre>

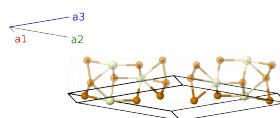
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Other compounds with this structure  
NdTe<sub>3</sub>, PrTe<sub>3</sub>

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Base-centered Orthorhombic primitive vectors

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




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Basis vectors

	Lattice coordinates	Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$\frac{1}{4} \mathbf{a}_1 + (y_1 - z_1) \mathbf{a}_2 + (y_1 + z_1) \mathbf{a}_3 =$	$\frac{1}{4}a\hat{\mathbf{x}} + by_1\hat{\mathbf{y}} + cz_1\hat{\mathbf{z}}$	(4b)	Ce I
$\mathbf{B}_2$	$\frac{3}{4} \mathbf{a}_1 - (y_1 + z_1) \mathbf{a}_2 - (y_1 - z_1) \mathbf{a}_3 =$	$\frac{3}{4}a\hat{\mathbf{x}} - by_1\hat{\mathbf{y}} + cz_1\hat{\mathbf{z}}$	(4b)	Ce I
$\mathbf{B}_3$	$\frac{1}{4} \mathbf{a}_1 + (y_2 - z_2) \mathbf{a}_2 + (y_2 + z_2) \mathbf{a}_3 =$	$\frac{1}{4}a\hat{\mathbf{x}} + by_2\hat{\mathbf{y}} + cz_2\hat{\mathbf{z}}$	(4b)	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)	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)	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)	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)	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)	Te III

## 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<sub>3</sub> (RE = 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.