

# NbCoTe<sub>2</sub> Structure:

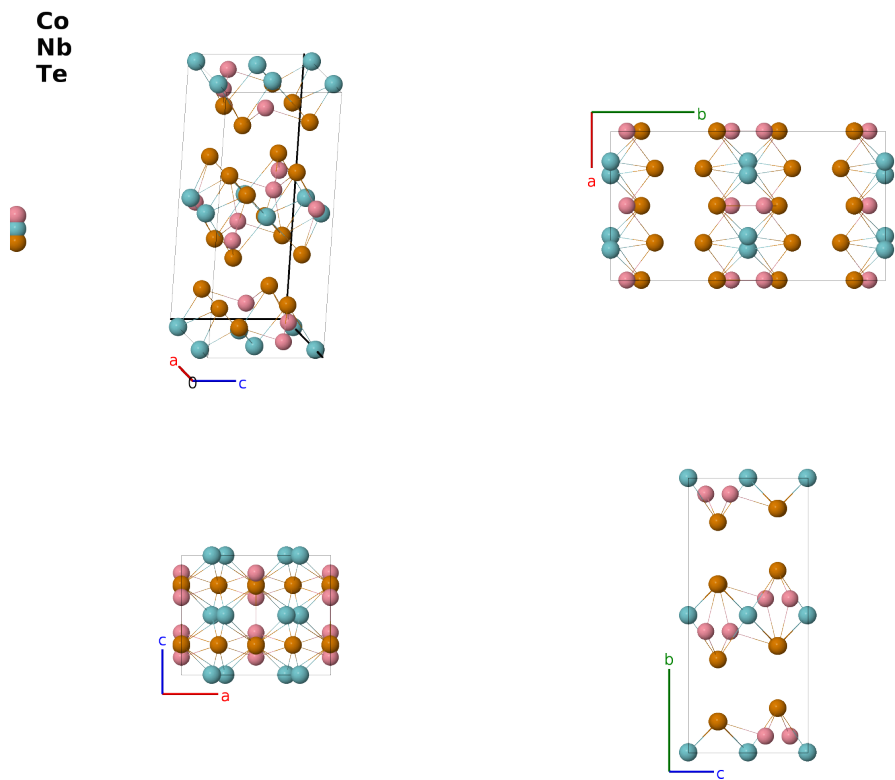
## ABC2\_oC32\_64\_f\_d\_ef-001

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<https://aflow.org/prototype-encyclopedia/15T5>

[https://aflow.org/prototype-encyclopedia/ABC2\\_oC32\\_64\\_f\\_d\\_ef-001](https://aflow.org/prototype-encyclopedia/ABC2_oC32_64_f_d_ef-001)



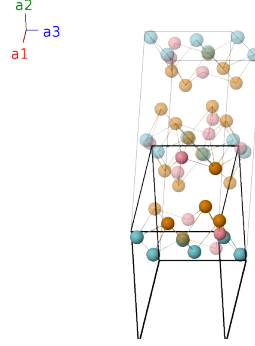
|                         |                                                                                                                                                                                   |
|-------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Prototype               | CoNbTe <sub>2</sub>                                                                                                                                                               |
| AFLOW prototype label   | ABC2_oC32_64_f_d_ef-001                                                                                                                                                           |
| ICSD                    | 71196                                                                                                                                                                             |
| CCDC                    | 1632099                                                                                                                                                                           |
| Pearson symbol          | oC32                                                                                                                                                                              |
| Space group number      | 64                                                                                                                                                                                |
| Space group symbol      | <i>Cmce</i>                                                                                                                                                                       |
| AFLOW prototype command | <code>aflow --proto=ABC2_oC32_64_f_d_ef-001</code><br><code>--params=a, b/a, c/a, x<sub>1</sub>, y<sub>2</sub>, y<sub>3</sub>, z<sub>3</sub>, y<sub>4</sub>, z<sub>4</sub></code> |

- (Tremel, 1991) does not explicitly list the atomic positions, only the distances between atoms in the crystal. Rather than converting these distances into Wyckoff coordinates we use the data from the ICSD entry.

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### Base-centered Orthorhombic primitive vectors

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




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### Basis vectors

|                   | Lattice<br>coordinates                                                                                                                         |  | Cartesian<br>coordinates                                                                                      | Wyckoff<br>position | Atom<br>type |
|-------------------|------------------------------------------------------------------------------------------------------------------------------------------------|--|---------------------------------------------------------------------------------------------------------------|---------------------|--------------|
| $\mathbf{B}_1$    | $= x_1 \mathbf{a}_1 + x_1 \mathbf{a}_2 =$                                                                                                      |  | $a x_1 \hat{\mathbf{x}}$                                                                                      | (8d)                | Nb I         |
| $\mathbf{B}_2$    | $= -\left(x_1 - \frac{1}{2}\right) \mathbf{a}_1 - \left(x_1 - \frac{1}{2}\right) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 =$                    |  | $-a \left(x_1 - \frac{1}{2}\right) \hat{\mathbf{x}} + \frac{1}{2} c \hat{\mathbf{z}}$                         | (8d)                | Nb I         |
| $\mathbf{B}_3$    | $= -x_1 \mathbf{a}_1 - x_1 \mathbf{a}_2 =$                                                                                                     |  | $-a x_1 \hat{\mathbf{x}}$                                                                                     | (8d)                | Nb I         |
| $\mathbf{B}_4$    | $= \left(x_1 + \frac{1}{2}\right) \mathbf{a}_1 + \left(x_1 + \frac{1}{2}\right) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 =$                     |  | $a \left(x_1 + \frac{1}{2}\right) \hat{\mathbf{x}} + \frac{1}{2} c \hat{\mathbf{z}}$                          | (8d)                | Nb I         |
| $\mathbf{B}_5$    | $= -\left(y_2 - \frac{1}{4}\right) \mathbf{a}_1 + \left(y_2 + \frac{1}{4}\right) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3 =$                    |  | $\frac{1}{4} a \hat{\mathbf{x}} + b y_2 \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$                    | (8e)                | Te I         |
| $\mathbf{B}_6$    | $= \left(y_2 + \frac{1}{4}\right) \mathbf{a}_1 - \left(y_2 - \frac{1}{4}\right) \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3 =$                     |  | $\frac{1}{4} a \hat{\mathbf{x}} - b y_2 \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$                    | (8e)                | Te I         |
| $\mathbf{B}_7$    | $= \left(y_2 + \frac{3}{4}\right) \mathbf{a}_1 - \left(y_2 - \frac{3}{4}\right) \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3 =$                     |  | $\frac{3}{4} a \hat{\mathbf{x}} - b y_2 \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$                    | (8e)                | Te I         |
| $\mathbf{B}_8$    | $= -\left(y_2 - \frac{3}{4}\right) \mathbf{a}_1 + \left(y_2 + \frac{3}{4}\right) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3 =$                    |  | $\frac{3}{4} a \hat{\mathbf{x}} + b y_2 \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$                    | (8e)                | Te I         |
| $\mathbf{B}_9$    | $= -y_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3 =$                                                                                  |  | $b y_3 \hat{\mathbf{y}} + c z_3 \hat{\mathbf{z}}$                                                             | (8f)                | Co I         |
| $\mathbf{B}_{10}$ | $= \left(y_3 + \frac{1}{2}\right) \mathbf{a}_1 - \left(y_3 - \frac{1}{2}\right) \mathbf{a}_2 + \left(z_3 + \frac{1}{2}\right) \mathbf{a}_3 =$  |  | $\frac{1}{2} a \hat{\mathbf{x}} - b y_3 \hat{\mathbf{y}} + c \left(z_3 + \frac{1}{2}\right) \hat{\mathbf{z}}$ | (8f)                | Co I         |
| $\mathbf{B}_{11}$ | $= -\left(y_3 - \frac{1}{2}\right) \mathbf{a}_1 + \left(y_3 + \frac{1}{2}\right) \mathbf{a}_2 - \left(z_3 - \frac{1}{2}\right) \mathbf{a}_3 =$ |  | $\frac{1}{2} a \hat{\mathbf{x}} + b y_3 \hat{\mathbf{y}} - c \left(z_3 - \frac{1}{2}\right) \hat{\mathbf{z}}$ | (8f)                | Co I         |
| $\mathbf{B}_{12}$ | $= y_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 - z_3 \mathbf{a}_3 =$                                                                                   |  | $-b y_3 \hat{\mathbf{y}} - c z_3 \hat{\mathbf{z}}$                                                            | (8f)                | Co I         |
| $\mathbf{B}_{13}$ | $= -y_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3 =$                                                                                  |  | $b y_4 \hat{\mathbf{y}} + c z_4 \hat{\mathbf{z}}$                                                             | (8f)                | Te II        |
| $\mathbf{B}_{14}$ | $= \left(y_4 + \frac{1}{2}\right) \mathbf{a}_1 - \left(y_4 - \frac{1}{2}\right) \mathbf{a}_2 + \left(z_4 + \frac{1}{2}\right) \mathbf{a}_3 =$  |  | $\frac{1}{2} a \hat{\mathbf{x}} - b y_4 \hat{\mathbf{y}} + c \left(z_4 + \frac{1}{2}\right) \hat{\mathbf{z}}$ | (8f)                | Te II        |
| $\mathbf{B}_{15}$ | $= -\left(y_4 - \frac{1}{2}\right) \mathbf{a}_1 + \left(y_4 + \frac{1}{2}\right) \mathbf{a}_2 - \left(z_4 - \frac{1}{2}\right) \mathbf{a}_3 =$ |  | $\frac{1}{2} a \hat{\mathbf{x}} + b y_4 \hat{\mathbf{y}} - c \left(z_4 - \frac{1}{2}\right) \hat{\mathbf{z}}$ | (8f)                | Te II        |
| $\mathbf{B}_{16}$ | $= y_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 - z_4 \mathbf{a}_3 =$                                                                                   |  | $-b y_4 \hat{\mathbf{y}} - c z_4 \hat{\mathbf{z}}$                                                            | (8f)                | Te II        |

### References

- [1] W. Tremel, *Isolated and condensed  $M_2\text{Co}_2$  clusters ( $M = \text{Nb}, \text{Ta}$ ) in the layered tellurides  $\text{Nb}_2\text{Co}_2\text{Te}_4$  and  $\text{TaCo}_2\text{Te}_2$* , J. Chem. Soc., Chem. Commun. pp. 1405–1407 (1991), doi:10.1039/C39910001405.

**Found in**

- [1] W. Tremel, *TaNi<sub>2</sub>Te<sub>2</sub>, A Novel Layered Telluride, and TaCo<sub>2</sub>Te<sub>2</sub>, a Structural Variant with Peierls Distortion*, Angew. Chem. Int. Ed. **31**, 217–220 (1992), doi:10.1002/anie.199202171.

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