

# K<sub>2</sub>Te<sub>3</sub> Structure:

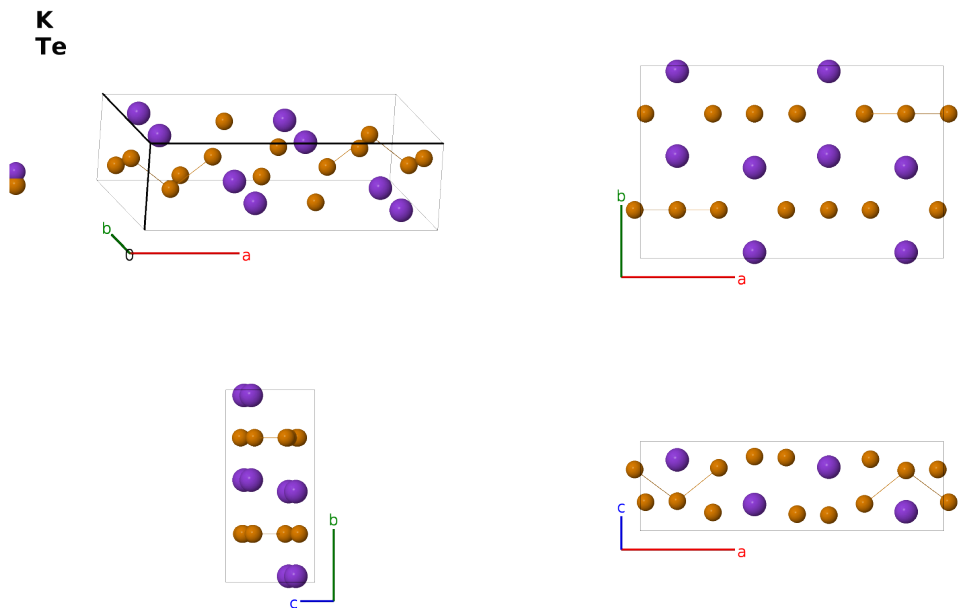
## A2B3\_oP20\_62\_d\_3c-001

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

[https://aflow.org/prototype-encyclopedia/A2B3\\_oP20\\_62\\_d\\_3c-001](https://aflow.org/prototype-encyclopedia/A2B3_oP20_62_d_3c-001)



|                         |                                                                                                                                                                                                                              |
|-------------------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Prototype               | K <sub>2</sub> Te <sub>3</sub>                                                                                                                                                                                               |
| AFLOW prototype label   | A2B3_oP20_62_d_3c-001                                                                                                                                                                                                        |
| ICSD                    | 2453                                                                                                                                                                                                                         |
| CCDC                    | 1592346                                                                                                                                                                                                                      |
| Pearson symbol          | oP20                                                                                                                                                                                                                         |
| Space group number      | 62                                                                                                                                                                                                                           |
| Space group symbol      | <i>Pnma</i>                                                                                                                                                                                                                  |
| AFLOW prototype command | <code>aflow --proto=A2B3_oP20_62_d_3c-001</code><br><code>--params=a, b/a, c/a, x<sub>1</sub>, z<sub>1</sub>, x<sub>2</sub>, z<sub>2</sub>, x<sub>3</sub>, z<sub>3</sub>, x<sub>4</sub>, y<sub>4</sub>, z<sub>4</sub></code> |

### Other compounds with this structure

Rb<sub>2</sub>Te<sub>3</sub>

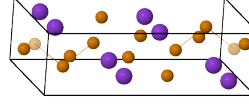
### Simple Orthorhombic primitive vectors



$$\mathbf{a}_1 = a \hat{\mathbf{x}}$$

$$\mathbf{a}_2 = b \hat{\mathbf{y}}$$

$$\mathbf{a}_3 = c \hat{\mathbf{z}}$$



## Basis vectors

|                   | Lattice<br>coordinates                                                                                                                            |     | Cartesian<br>coordinates                                                                                                                                  | Wyckoff<br>position | Atom<br>type |
|-------------------|---------------------------------------------------------------------------------------------------------------------------------------------------|-----|-----------------------------------------------------------------------------------------------------------------------------------------------------------|---------------------|--------------|
| $\mathbf{B}_1$    | $= x_1 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_1 \mathbf{a}_3$                                                                                | $=$ | $ax_1 \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} + cz_1 \hat{\mathbf{z}}$                                                                           | (4c)                | Te I         |
| $\mathbf{B}_2$    | $= -\left(x_1 - \frac{1}{2}\right) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 +$<br>$\left(z_1 + \frac{1}{2}\right) \mathbf{a}_3$                    | $=$ | $-a\left(x_1 - \frac{1}{2}\right) \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} + c\left(z_1 + \frac{1}{2}\right) \hat{\mathbf{z}}$                    | (4c)                | Te I         |
| $\mathbf{B}_3$    | $= -x_1 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_1 \mathbf{a}_3$                                                                               | $=$ | $-ax_1 \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} - cz_1 \hat{\mathbf{z}}$                                                                          | (4c)                | Te I         |
| $\mathbf{B}_4$    | $= \left(x_1 + \frac{1}{2}\right) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 - \left(z_1 - \frac{1}{2}\right) \mathbf{a}_3$                          | $=$ | $a\left(x_1 + \frac{1}{2}\right) \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} - c\left(z_1 - \frac{1}{2}\right) \hat{\mathbf{z}}$                     | (4c)                | Te I         |
| $\mathbf{B}_5$    | $= x_2 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_2 \mathbf{a}_3$                                                                                | $=$ | $ax_2 \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$                                                                           | (4c)                | Te II        |
| $\mathbf{B}_6$    | $= -\left(x_2 - \frac{1}{2}\right) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 +$<br>$\left(z_2 + \frac{1}{2}\right) \mathbf{a}_3$                    | $=$ | $-a\left(x_2 - \frac{1}{2}\right) \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} + c\left(z_2 + \frac{1}{2}\right) \hat{\mathbf{z}}$                    | (4c)                | Te II        |
| $\mathbf{B}_7$    | $= -x_2 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_2 \mathbf{a}_3$                                                                               | $=$ | $-ax_2 \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} - cz_2 \hat{\mathbf{z}}$                                                                          | (4c)                | Te II        |
| $\mathbf{B}_8$    | $= \left(x_2 + \frac{1}{2}\right) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 - \left(z_2 - \frac{1}{2}\right) \mathbf{a}_3$                          | $=$ | $a\left(x_2 + \frac{1}{2}\right) \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} - c\left(z_2 - \frac{1}{2}\right) \hat{\mathbf{z}}$                     | (4c)                | Te II        |
| $\mathbf{B}_9$    | $= x_3 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_3 \mathbf{a}_3$                                                                                | $=$ | $ax_3 \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$                                                                           | (4c)                | Te III       |
| $\mathbf{B}_{10}$ | $= -\left(x_3 - \frac{1}{2}\right) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 +$<br>$\left(z_3 + \frac{1}{2}\right) \mathbf{a}_3$                    | $=$ | $-a\left(x_3 - \frac{1}{2}\right) \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} + c\left(z_3 + \frac{1}{2}\right) \hat{\mathbf{z}}$                    | (4c)                | Te III       |
| $\mathbf{B}_{11}$ | $= -x_3 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_3 \mathbf{a}_3$                                                                               | $=$ | $-ax_3 \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} - cz_3 \hat{\mathbf{z}}$                                                                          | (4c)                | Te III       |
| $\mathbf{B}_{12}$ | $= \left(x_3 + \frac{1}{2}\right) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 - \left(z_3 - \frac{1}{2}\right) \mathbf{a}_3$                          | $=$ | $a\left(x_3 + \frac{1}{2}\right) \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} - c\left(z_3 - \frac{1}{2}\right) \hat{\mathbf{z}}$                     | (4c)                | Te III       |
| $\mathbf{B}_{13}$ | $= x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$                                                                                        | $=$ | $ax_4 \hat{\mathbf{x}} + by_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$                                                                                   | (8d)                | K I          |
| $\mathbf{B}_{14}$ | $= -\left(x_4 - \frac{1}{2}\right) \mathbf{a}_1 - y_4 \mathbf{a}_2 +$<br>$\left(z_4 + \frac{1}{2}\right) \mathbf{a}_3$                            | $=$ | $-a\left(x_4 - \frac{1}{2}\right) \hat{\mathbf{x}} - by_4 \hat{\mathbf{y}} + c\left(z_4 + \frac{1}{2}\right) \hat{\mathbf{z}}$                            | (8d)                | K I          |
| $\mathbf{B}_{15}$ | $= -x_4 \mathbf{a}_1 + \left(y_4 + \frac{1}{2}\right) \mathbf{a}_2 - z_4 \mathbf{a}_3$                                                            | $=$ | $-ax_4 \hat{\mathbf{x}} + b\left(y_4 + \frac{1}{2}\right) \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}}$                                                       | (8d)                | K I          |
| $\mathbf{B}_{16}$ | $= \left(x_4 + \frac{1}{2}\right) \mathbf{a}_1 - \left(y_4 - \frac{1}{2}\right) \mathbf{a}_2 -$<br>$\left(z_4 - \frac{1}{2}\right) \mathbf{a}_3$  | $=$ | $a\left(x_4 + \frac{1}{2}\right) \hat{\mathbf{x}} - b\left(y_4 - \frac{1}{2}\right) \hat{\mathbf{y}} - c\left(z_4 - \frac{1}{2}\right) \hat{\mathbf{z}}$  | (8d)                | K I          |
| $\mathbf{B}_{17}$ | $= -x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 - z_4 \mathbf{a}_3$                                                                                       | $=$ | $-ax_4 \hat{\mathbf{x}} - by_4 \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}}$                                                                                  | (8d)                | K I          |
| $\mathbf{B}_{18}$ | $= \left(x_4 + \frac{1}{2}\right) \mathbf{a}_1 + y_4 \mathbf{a}_2 - \left(z_4 - \frac{1}{2}\right) \mathbf{a}_3$                                  | $=$ | $a\left(x_4 + \frac{1}{2}\right) \hat{\mathbf{x}} + by_4 \hat{\mathbf{y}} - c\left(z_4 - \frac{1}{2}\right) \hat{\mathbf{z}}$                             | (8d)                | K I          |
| $\mathbf{B}_{19}$ | $= x_4 \mathbf{a}_1 - \left(y_4 - \frac{1}{2}\right) \mathbf{a}_2 + z_4 \mathbf{a}_3$                                                             | $=$ | $ax_4 \hat{\mathbf{x}} - b\left(y_4 - \frac{1}{2}\right) \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$                                                        | (8d)                | K I          |
| $\mathbf{B}_{20}$ | $= -\left(x_4 - \frac{1}{2}\right) \mathbf{a}_1 + \left(y_4 + \frac{1}{2}\right) \mathbf{a}_2 +$<br>$\left(z_4 + \frac{1}{2}\right) \mathbf{a}_3$ | $=$ | $-a\left(x_4 - \frac{1}{2}\right) \hat{\mathbf{x}} + b\left(y_4 + \frac{1}{2}\right) \hat{\mathbf{y}} + c\left(z_4 + \frac{1}{2}\right) \hat{\mathbf{z}}$ | (8d)                | K I          |

## References

- [1] B. Eisenmann and H. Schäfer, *K<sub>2</sub>Te<sub>3</sub>: The First Binary Alkali-Metal Polytelluride with Te<sub>3</sub><sup>2-</sup> Ions*, Angew. Chem. Int. Ed. **17**, 684 (1978), doi:10.1002/anie.197806841.

**Found in**

- [1] P. Böttcher, *Synthesis and crystal structure of  $Rb_2Te_3$  and  $Cs_2Te_3$* , J. Less-Common Met. **70**, 263–271 (1980), doi:10.1016/0022-5088(80)90235-0.

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