

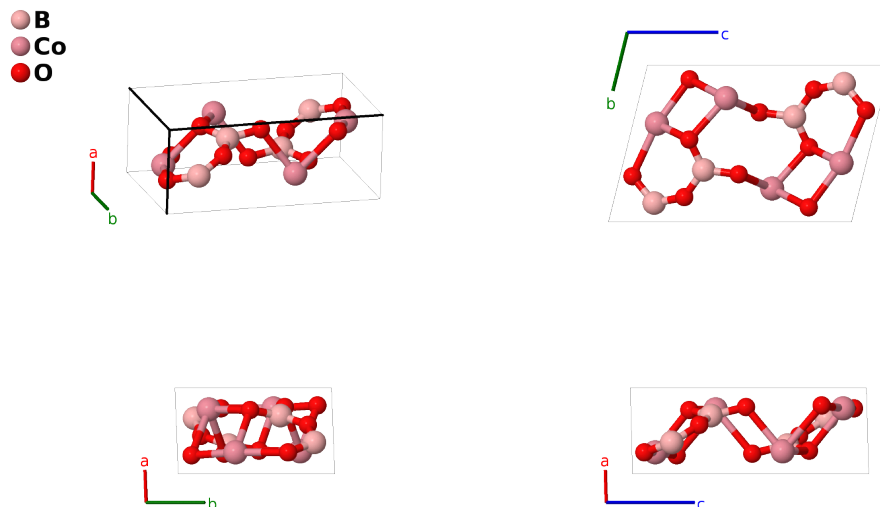
# Co<sub>2</sub>B<sub>2</sub>O<sub>5</sub> Structure: A2B2C5\_aP18\_2\_2i\_2i\_5i-001

This structure originally had the label A2B2C5\_aP18\_2\_2i\_2i\_5i. Calls to that address will be redirected here.

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

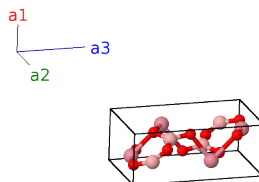
[https://aflow.org/p/A2B2C5\\_aP18\\_2\\_2i\\_2i\\_5i-001](https://aflow.org/p/A2B2C5_aP18_2_2i_2i_5i-001)



|                                |   |
|--------------------------------|---|
| <b>Prototype</b>               | B <sub>2</sub> Co <sub>2</sub> O <sub>5</sub>   |
| <b>AFLOW prototype label</b>   | A2B2C5_aP18_2_2i_2i_5i-001  |
| <b>ICSD</b>                    | 24284   |
| <b>Pearson symbol</b>          | aP18  |
| <b>Space group number</b>      | 2   |
| <b>Space group symbol</b>      | $P\bar{1}$  |
| <b>AFLOW prototype command</b> | aflow --proto=A2B2C5_aP18_2_2i_2i_5i-001<br>--params=a, b/a, c/a, $\alpha$ , $\beta$ , $\gamma$ , $x_1, y_1, z_1, x_2, y_2, z_2, x_3, y_3, z_3, x_4, y_4, z_4, x_5, y_5, z_5, x_6, y_6, z_6, x_7, y_7, z_7, x_8, y_8, z_8, x_9, y_9, z_9$ |

## Triclinic primitive vectors

$$\begin{aligned} \mathbf{a}_1 &= a \hat{\mathbf{x}} \\ \mathbf{a}_2 &= b \cos \gamma \hat{\mathbf{x}} + b \sin \gamma \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c_x \hat{\mathbf{x}} + c_y \hat{\mathbf{y}} + c_z \hat{\mathbf{z}} \\ c_x &= c \cos \beta \\ c_y &= c(\cos \alpha - \cos \beta \cos \gamma) / \sin \gamma \\ c_z &= \sqrt{c^2 - c_x^2 - c_y^2} \end{aligned}$$



## Basis vectors

|                   | Lattice<br>coordinates                                      |     | Cartesian<br>coordinates   | Wyckoff<br>position | Atom<br>type |
|-------------------|---|-----|--|---------------------|--------------|
| $\mathbf{B}_1$    | $= x_1 \mathbf{a}_1 + y_1 \mathbf{a}_2 + z_1 \mathbf{a}_3$  | $=$ | $(ax_1 + by_1 \cos \gamma + c_x z_1) \hat{\mathbf{x}} + (by_1 \sin \gamma + c_y z_1) \hat{\mathbf{y}} + c_z z_1 \hat{\mathbf{z}}$  | (2i)                | B I          |
| $\mathbf{B}_2$    | $= -x_1 \mathbf{a}_1 - y_1 \mathbf{a}_2 - z_1 \mathbf{a}_3$ | $=$ | $-(ax_1 + by_1 \cos \gamma + c_x z_1) \hat{\mathbf{x}} - (by_1 \sin \gamma + c_y z_1) \hat{\mathbf{y}} - c_z z_1 \hat{\mathbf{z}}$ | (2i)                | B I          |
| $\mathbf{B}_3$    | $= x_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$  | $=$ | $(ax_2 + by_2 \cos \gamma + c_x z_2) \hat{\mathbf{x}} + (by_2 \sin \gamma + c_y z_2) \hat{\mathbf{y}} + c_z z_2 \hat{\mathbf{z}}$  | (2i)                | B II         |
| $\mathbf{B}_4$    | $= -x_2 \mathbf{a}_1 - y_2 \mathbf{a}_2 - z_2 \mathbf{a}_3$ | $=$ | $-(ax_2 + by_2 \cos \gamma + c_x z_2) \hat{\mathbf{x}} - (by_2 \sin \gamma + c_y z_2) \hat{\mathbf{y}} - c_z z_2 \hat{\mathbf{z}}$ | (2i)                | B II         |
| $\mathbf{B}_5$    | $= x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$  | $=$ | $(ax_3 + by_3 \cos \gamma + c_x z_3) \hat{\mathbf{x}} + (by_3 \sin \gamma + c_y z_3) \hat{\mathbf{y}} + c_z z_3 \hat{\mathbf{z}}$  | (2i)                | Co I         |
| $\mathbf{B}_6$    | $= -x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 - z_3 \mathbf{a}_3$ | $=$ | $-(ax_3 + by_3 \cos \gamma + c_x z_3) \hat{\mathbf{x}} - (by_3 \sin \gamma + c_y z_3) \hat{\mathbf{y}} - c_z z_3 \hat{\mathbf{z}}$ | (2i)                | Co I         |
| $\mathbf{B}_7$    | $= x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$  | $=$ | $(ax_4 + by_4 \cos \gamma + c_x z_4) \hat{\mathbf{x}} + (by_4 \sin \gamma + c_y z_4) \hat{\mathbf{y}} + c_z z_4 \hat{\mathbf{z}}$  | (2i)                | Co II        |
| $\mathbf{B}_8$    | $= -x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 - z_4 \mathbf{a}_3$ | $=$ | $-(ax_4 + by_4 \cos \gamma + c_x z_4) \hat{\mathbf{x}} - (by_4 \sin \gamma + c_y z_4) \hat{\mathbf{y}} - c_z z_4 \hat{\mathbf{z}}$ | (2i)                | Co II        |
| $\mathbf{B}_9$    | $= x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$  | $=$ | $(ax_5 + by_5 \cos \gamma + c_x z_5) \hat{\mathbf{x}} + (by_5 \sin \gamma + c_y z_5) \hat{\mathbf{y}} + c_z z_5 \hat{\mathbf{z}}$  | (2i)                | O I          |
| $\mathbf{B}_{10}$ | $= -x_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 - z_5 \mathbf{a}_3$ | $=$ | $-(ax_5 + by_5 \cos \gamma + c_x z_5) \hat{\mathbf{x}} - (by_5 \sin \gamma + c_y z_5) \hat{\mathbf{y}} - c_z z_5 \hat{\mathbf{z}}$ | (2i)                | O I          |
| $\mathbf{B}_{11}$ | $= x_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$  | $=$ | $(ax_6 + by_6 \cos \gamma + c_x z_6) \hat{\mathbf{x}} + (by_6 \sin \gamma + c_y z_6) \hat{\mathbf{y}} + c_z z_6 \hat{\mathbf{z}}$  | (2i)                | O II         |
| $\mathbf{B}_{12}$ | $= -x_6 \mathbf{a}_1 - y_6 \mathbf{a}_2 - z_6 \mathbf{a}_3$ | $=$ | $-(ax_6 + by_6 \cos \gamma + c_x z_6) \hat{\mathbf{x}} - (by_6 \sin \gamma + c_y z_6) \hat{\mathbf{y}} - c_z z_6 \hat{\mathbf{z}}$ | (2i)                | O II         |
| $\mathbf{B}_{13}$ | $= x_7 \mathbf{a}_1 + y_7 \mathbf{a}_2 + z_7 \mathbf{a}_3$  | $=$ | $(ax_7 + by_7 \cos \gamma + c_x z_7) \hat{\mathbf{x}} + (by_7 \sin \gamma + c_y z_7) \hat{\mathbf{y}} + c_z z_7 \hat{\mathbf{z}}$  | (2i)                | O III        |
| $\mathbf{B}_{14}$ | $= -x_7 \mathbf{a}_1 - y_7 \mathbf{a}_2 - z_7 \mathbf{a}_3$ | $=$ | $-(ax_7 + by_7 \cos \gamma + c_x z_7) \hat{\mathbf{x}} - (by_7 \sin \gamma + c_y z_7) \hat{\mathbf{y}} - c_z z_7 \hat{\mathbf{z}}$ | (2i)                | O III        |
| $\mathbf{B}_{15}$ | $= x_8 \mathbf{a}_1 + y_8 \mathbf{a}_2 + z_8 \mathbf{a}_3$  | $=$ | $(ax_8 + by_8 \cos \gamma + c_x z_8) \hat{\mathbf{x}} + (by_8 \sin \gamma + c_y z_8) \hat{\mathbf{y}} + c_z z_8 \hat{\mathbf{z}}$  | (2i)                | O IV         |
| $\mathbf{B}_{16}$ | $= -x_8 \mathbf{a}_1 - y_8 \mathbf{a}_2 - z_8 \mathbf{a}_3$ | $=$ | $-(ax_8 + by_8 \cos \gamma + c_x z_8) \hat{\mathbf{x}} - (by_8 \sin \gamma + c_y z_8) \hat{\mathbf{y}} - c_z z_8 \hat{\mathbf{z}}$ | (2i)                | O IV         |
| $\mathbf{B}_{17}$ | $= x_9 \mathbf{a}_1 + y_9 \mathbf{a}_2 + z_9 \mathbf{a}_3$  | $=$ | $(ax_9 + by_9 \cos \gamma + c_x z_9) \hat{\mathbf{x}} + (by_9 \sin \gamma + c_y z_9) \hat{\mathbf{y}} + c_z z_9 \hat{\mathbf{z}}$  | (2i)                | O V          |
| $\mathbf{B}_{18}$ | $= -x_9 \mathbf{a}_1 - y_9 \mathbf{a}_2 - z_9 \mathbf{a}_3$ | $=$ | $-(ax_9 + by_9 \cos \gamma + c_x z_9) \hat{\mathbf{x}} - (by_9 \sin \gamma + c_y z_9) \hat{\mathbf{y}} - c_z z_9 \hat{\mathbf{z}}$ | (2i)                | O V          |

## References

- [1] S. V. Berger, *The Crystal Structure of Cobaltpyroborate*, Acta Chem. Scand. **4**, 1054–1065 (1950), doi:10.3891/acta.chem.scand.04-1054.