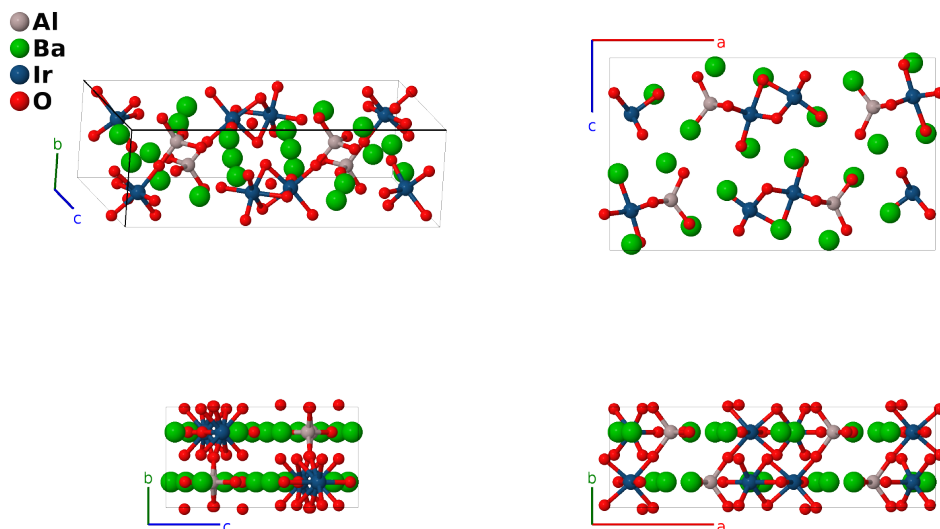


Ba₅AlIr₂O₁₁ Structure: AB5C2D11_oP76_62_c_5c_2c_5c3d-001

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<https://aflow.org/p/CZW8>

https://aflow.org/p/AB5C2D11_oP76_62_c_5c_2c_5c3d-001



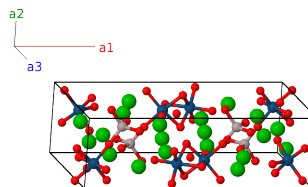
Prototype	AlBa ₅ Ir ₂ O ₁₁
AFLOW prototype label	AB5C2D11_oP76_62_c_5c_2c_5c3d-001
ICSD	67143
Pearson symbol	oP76
Space group number	62
Space group symbol	<i>Pnma</i>
AFLOW prototype command	aflow --proto=AB5C2D11_oP76_62_c_5c_2c_5c3d-001 --params= <i>a, b/a, c/a, x₁, z₁, x₂, z₂, x₃, z₃, x₄, z₄, x₅, z₅, x₆, z₆, x₇, z₇, x₈, z₈, x₉, z₉, x₁₀, z₁₀, x₁₁, z₁₁, x₁₂, z₁₂, x₁₃, z₁₃, x₁₄, y₁₄, z₁₄, x₁₅, y₁₅, z₁₅, x₁₆, y₁₆, z₁₆</i>

Simple Orthorhombic primitive vectors

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

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

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



Basis vectors

$$\begin{aligned}
\mathbf{B}_{64} &= \begin{pmatrix} (x_{15} + \frac{1}{2}) \mathbf{a}_1 - (y_{15} - \frac{1}{2}) \mathbf{a}_2 - \\ (z_{15} - \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = \begin{pmatrix} a(x_{15} + \frac{1}{2}) \hat{\mathbf{x}} - b(y_{15} - \frac{1}{2}) \hat{\mathbf{y}} - \\ c(z_{15} - \frac{1}{2}) \hat{\mathbf{z}} \end{pmatrix} & (8d) & \text{O VII} \\
\mathbf{B}_{65} &= -x_{15} \mathbf{a}_1 - y_{15} \mathbf{a}_2 - z_{15} \mathbf{a}_3 = -ax_{15} \hat{\mathbf{x}} - by_{15} \hat{\mathbf{y}} - cz_{15} \hat{\mathbf{z}} & (8d) & \text{O VII} \\
\mathbf{B}_{66} &= \begin{pmatrix} (x_{15} + \frac{1}{2}) \mathbf{a}_1 + y_{15} \mathbf{a}_2 - \\ (z_{15} - \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = \begin{pmatrix} a(x_{15} + \frac{1}{2}) \hat{\mathbf{x}} + by_{15} \hat{\mathbf{y}} - c(z_{15} - \frac{1}{2}) \hat{\mathbf{z}} \end{pmatrix} & (8d) & \text{O VII} \\
\mathbf{B}_{67} &= x_{15} \mathbf{a}_1 - (y_{15} - \frac{1}{2}) \mathbf{a}_2 + z_{15} \mathbf{a}_3 = ax_{15} \hat{\mathbf{x}} - b(y_{15} - \frac{1}{2}) \hat{\mathbf{y}} + cz_{15} \hat{\mathbf{z}} & (8d) & \text{O VII} \\
\mathbf{B}_{68} &= -\begin{pmatrix} (x_{15} - \frac{1}{2}) \mathbf{a}_1 + (y_{15} + \frac{1}{2}) \mathbf{a}_2 + \\ (z_{15} + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = -a(x_{15} - \frac{1}{2}) \hat{\mathbf{x}} + b(y_{15} + \frac{1}{2}) \hat{\mathbf{y}} + \\ & c(z_{15} + \frac{1}{2}) \hat{\mathbf{z}} & (8d) & \text{O VII} \\
\mathbf{B}_{69} &= x_{16} \mathbf{a}_1 + y_{16} \mathbf{a}_2 + z_{16} \mathbf{a}_3 = ax_{16} \hat{\mathbf{x}} + by_{16} \hat{\mathbf{y}} + cz_{16} \hat{\mathbf{z}} & (8d) & \text{O VIII} \\
\mathbf{B}_{70} &= -\begin{pmatrix} (x_{16} - \frac{1}{2}) \mathbf{a}_1 - y_{16} \mathbf{a}_2 + \\ (z_{16} + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = -a(x_{16} - \frac{1}{2}) \hat{\mathbf{x}} - by_{16} \hat{\mathbf{y}} + c(z_{16} + \frac{1}{2}) \hat{\mathbf{z}} & (8d) & \text{O VIII} \\
\mathbf{B}_{71} &= -x_{16} \mathbf{a}_1 + (y_{16} + \frac{1}{2}) \mathbf{a}_2 - z_{16} \mathbf{a}_3 = -ax_{16} \hat{\mathbf{x}} + b(y_{16} + \frac{1}{2}) \hat{\mathbf{y}} - cz_{16} \hat{\mathbf{z}} & (8d) & \text{O VIII} \\
\mathbf{B}_{72} &= \begin{pmatrix} (x_{16} + \frac{1}{2}) \mathbf{a}_1 - (y_{16} - \frac{1}{2}) \mathbf{a}_2 - \\ (z_{16} - \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = \begin{pmatrix} a(x_{16} + \frac{1}{2}) \hat{\mathbf{x}} - b(y_{16} - \frac{1}{2}) \hat{\mathbf{y}} - \\ c(z_{16} - \frac{1}{2}) \hat{\mathbf{z}} \end{pmatrix} & (8d) & \text{O VIII} \\
\mathbf{B}_{73} &= -x_{16} \mathbf{a}_1 - y_{16} \mathbf{a}_2 - z_{16} \mathbf{a}_3 = -ax_{16} \hat{\mathbf{x}} - by_{16} \hat{\mathbf{y}} - cz_{16} \hat{\mathbf{z}} & (8d) & \text{O VIII} \\
\mathbf{B}_{74} &= \begin{pmatrix} (x_{16} + \frac{1}{2}) \mathbf{a}_1 + y_{16} \mathbf{a}_2 - \\ (z_{16} - \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = \begin{pmatrix} a(x_{16} + \frac{1}{2}) \hat{\mathbf{x}} + by_{16} \hat{\mathbf{y}} - c(z_{16} - \frac{1}{2}) \hat{\mathbf{z}} \end{pmatrix} & (8d) & \text{O VIII} \\
\mathbf{B}_{75} &= x_{16} \mathbf{a}_1 - (y_{16} - \frac{1}{2}) \mathbf{a}_2 + z_{16} \mathbf{a}_3 = ax_{16} \hat{\mathbf{x}} - b(y_{16} - \frac{1}{2}) \hat{\mathbf{y}} + cz_{16} \hat{\mathbf{z}} & (8d) & \text{O VIII} \\
\mathbf{B}_{76} &= -\begin{pmatrix} (x_{16} - \frac{1}{2}) \mathbf{a}_1 + (y_{16} + \frac{1}{2}) \mathbf{a}_2 + \\ (z_{16} + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = -a(x_{16} - \frac{1}{2}) \hat{\mathbf{x}} + b(y_{16} + \frac{1}{2}) \hat{\mathbf{y}} + \\ & c(z_{16} + \frac{1}{2}) \hat{\mathbf{z}} & (8d) & \text{O VIII}
\end{aligned}$$

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