

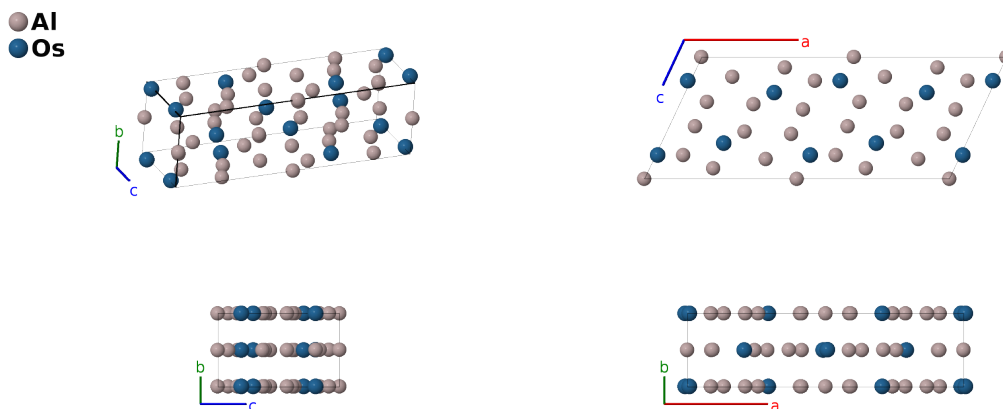
# Os<sub>4</sub>Al<sub>13</sub> Structure: A13B4\_mC34\_12\_a6i\_2i-001

This structure originally had the label A13B4\_mC34\_12\_b6i\_2i. Calls to that address will be redirected here.

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<https://aflow.org/p/XT4N>

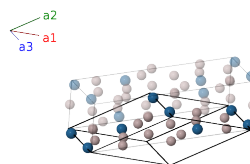
[https://aflow.org/p/A13B4\\_mC34\\_12\\_a6i\\_2i-001](https://aflow.org/p/A13B4_mC34_12_a6i_2i-001)



Prototype	Al <sub>13</sub> Os <sub>4</sub>
AFLOW prototype label	A13B4_mC34_12_a6i_2i-001
ICSD	58110
Pearson symbol	mC34
Space group number	12
Space group symbol	<i>C</i> 2/ <i>m</i>
AFLOW prototype command	aflow --proto=A13B4_mC34_12_a6i_2i-001 --params= <i>a</i> , <i>b/a</i> , <i>c/a</i> , $\beta$ , <i>x</i> <sub>2</sub> , <i>z</i> <sub>2</sub> , <i>x</i> <sub>3</sub> , <i>z</i> <sub>3</sub> , <i>x</i> <sub>4</sub> , <i>z</i> <sub>4</sub> , <i>x</i> <sub>5</sub> , <i>z</i> <sub>5</sub> , <i>x</i> <sub>6</sub> , <i>z</i> <sub>6</sub> , <i>x</i> <sub>7</sub> , <i>z</i> <sub>7</sub> , <i>x</i> <sub>8</sub> , <i>z</i> <sub>8</sub> , <i>x</i> <sub>9</sub> , <i>z</i> <sub>9</sub>

## Base-centered Monoclinic primitive vectors

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



## Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	=	0	=	0	(2a) Al I

$$\begin{aligned}
\mathbf{B}_2 &= x_2 \mathbf{a}_1 + x_2 \mathbf{a}_2 + z_2 \mathbf{a}_3 &= (ax_2 + cz_2 \cos \beta) \hat{\mathbf{x}} + cz_2 \sin \beta \hat{\mathbf{z}} &(4i) &\text{Al II} \\
\mathbf{B}_3 &= -x_2 \mathbf{a}_1 - x_2 \mathbf{a}_2 - z_2 \mathbf{a}_3 &= -(ax_2 + cz_2 \cos \beta) \hat{\mathbf{x}} - cz_2 \sin \beta \hat{\mathbf{z}} &(4i) &\text{Al II} \\
\mathbf{B}_4 &= x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + z_3 \mathbf{a}_3 &= (ax_3 + cz_3 \cos \beta) \hat{\mathbf{x}} + cz_3 \sin \beta \hat{\mathbf{z}} &(4i) &\text{Al III} \\
\mathbf{B}_5 &= -x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 - z_3 \mathbf{a}_3 &= -(ax_3 + cz_3 \cos \beta) \hat{\mathbf{x}} - cz_3 \sin \beta \hat{\mathbf{z}} &(4i) &\text{Al III} \\
\mathbf{B}_6 &= x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + z_4 \mathbf{a}_3 &= (ax_4 + cz_4 \cos \beta) \hat{\mathbf{x}} + cz_4 \sin \beta \hat{\mathbf{z}} &(4i) &\text{Al IV} \\
\mathbf{B}_7 &= -x_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 - z_4 \mathbf{a}_3 &= -(ax_4 + cz_4 \cos \beta) \hat{\mathbf{x}} - cz_4 \sin \beta \hat{\mathbf{z}} &(4i) &\text{Al IV} \\
\mathbf{B}_8 &= x_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 + z_5 \mathbf{a}_3 &= (ax_5 + cz_5 \cos \beta) \hat{\mathbf{x}} + cz_5 \sin \beta \hat{\mathbf{z}} &(4i) &\text{Al V} \\
\mathbf{B}_9 &= -x_5 \mathbf{a}_1 - x_5 \mathbf{a}_2 - z_5 \mathbf{a}_3 &= -(ax_5 + cz_5 \cos \beta) \hat{\mathbf{x}} - cz_5 \sin \beta \hat{\mathbf{z}} &(4i) &\text{Al V} \\
\mathbf{B}_{10} &= x_6 \mathbf{a}_1 + x_6 \mathbf{a}_2 + z_6 \mathbf{a}_3 &= (ax_6 + cz_6 \cos \beta) \hat{\mathbf{x}} + cz_6 \sin \beta \hat{\mathbf{z}} &(4i) &\text{Al VI} \\
\mathbf{B}_{11} &= -x_6 \mathbf{a}_1 - x_6 \mathbf{a}_2 - z_6 \mathbf{a}_3 &= -(ax_6 + cz_6 \cos \beta) \hat{\mathbf{x}} - cz_6 \sin \beta \hat{\mathbf{z}} &(4i) &\text{Al VI} \\
\mathbf{B}_{12} &= x_7 \mathbf{a}_1 + x_7 \mathbf{a}_2 + z_7 \mathbf{a}_3 &= (ax_7 + cz_7 \cos \beta) \hat{\mathbf{x}} + cz_7 \sin \beta \hat{\mathbf{z}} &(4i) &\text{Al VII} \\
\mathbf{B}_{13} &= -x_7 \mathbf{a}_1 - x_7 \mathbf{a}_2 - z_7 \mathbf{a}_3 &= -(ax_7 + cz_7 \cos \beta) \hat{\mathbf{x}} - cz_7 \sin \beta \hat{\mathbf{z}} &(4i) &\text{Al VII} \\
\mathbf{B}_{14} &= x_8 \mathbf{a}_1 + x_8 \mathbf{a}_2 + z_8 \mathbf{a}_3 &= (ax_8 + cz_8 \cos \beta) \hat{\mathbf{x}} + cz_8 \sin \beta \hat{\mathbf{z}} &(4i) &\text{Os I} \\
\mathbf{B}_{15} &= -x_8 \mathbf{a}_1 - x_8 \mathbf{a}_2 - z_8 \mathbf{a}_3 &= -(ax_8 + cz_8 \cos \beta) \hat{\mathbf{x}} - cz_8 \sin \beta \hat{\mathbf{z}} &(4i) &\text{Os I} \\
\mathbf{B}_{16} &= x_9 \mathbf{a}_1 + x_9 \mathbf{a}_2 + z_9 \mathbf{a}_3 &= (ax_9 + cz_9 \cos \beta) \hat{\mathbf{x}} + cz_9 \sin \beta \hat{\mathbf{z}} &(4i) &\text{Os II} \\
\mathbf{B}_{17} &= -x_9 \mathbf{a}_1 - x_9 \mathbf{a}_2 - z_9 \mathbf{a}_3 &= -(ax_9 + cz_9 \cos \beta) \hat{\mathbf{x}} - cz_9 \sin \beta \hat{\mathbf{z}} &(4i) &\text{Os II}
\end{aligned}$$

## References

- [1] L.-E. Edshammar, *The Crystal Structure of Os<sub>4</sub>Al<sub>13</sub>*, Acta Chem. Scand. **18**, 2294–2302 (1964), doi:10.3891/acta.chem.scand.18-2294.