

OsGe₂ Structure:

A2B_mC12_12_2i_i-007

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

https://aflow.org/prototype-encyclopedia/A2B_mC12_12_2i_i-007



Prototype	Ge ₂ Os
AFLOW prototype label	A2B_mC12_12_2i_i-007
ICSD	43690
CCDC	1613162
Pearson symbol	mC12
Space group number	12
Space group symbol	$C2/m$
AFLOW prototype command	<code>aflow --proto=A2B_mC12_12_2i_i-007</code> <code>--params=a, b/a, c/a, β, x_1, z_1, x_2, z_2, x_3, z_3</code>

Other compounds with this structure

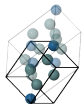
VP₂, NbP₂

- OsGe₂ shares the same AFLOW label, A2B_mC12_12_2i_i, with CaC₂-III and α -Bi₂Pd. The structures are generated by the same symmetry operations with different sets of parameters (`--params`) specified in their corresponding CIF files.

Base-centered Monoclinic primitive vectors

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

$\begin{matrix} a_2 \\ \leftarrow a_1 \\ a_3 \end{matrix}$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= x_1 \mathbf{a}_1 + x_1 \mathbf{a}_2 + z_1 \mathbf{a}_3$	$=$	$(ax_1 + cz_1 \cos \beta) \hat{\mathbf{x}} + cz_1 \sin \beta \hat{\mathbf{z}}$	(4i)	Ge I
$\mathbf{B}_2$	$= -x_1 \mathbf{a}_1 - x_1 \mathbf{a}_2 - z_1 \mathbf{a}_3$	$=$	$-(ax_1 + cz_1 \cos \beta) \hat{\mathbf{x}} - cz_1 \sin \beta \hat{\mathbf{z}}$	(4i)	Ge I
$\mathbf{B}_3$	$= x_2 \mathbf{a}_1 + x_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$(ax_2 + cz_2 \cos \beta) \hat{\mathbf{x}} + cz_2 \sin \beta \hat{\mathbf{z}}$	(4i)	Ge II
$\mathbf{B}_4$	$= -x_2 \mathbf{a}_1 - x_2 \mathbf{a}_2 - z_2 \mathbf{a}_3$	$=$	$-(ax_2 + cz_2 \cos \beta) \hat{\mathbf{x}} - cz_2 \sin \beta \hat{\mathbf{z}}$	(4i)	Ge II
$\mathbf{B}_5$	$= x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$(ax_3 + cz_3 \cos \beta) \hat{\mathbf{x}} + cz_3 \sin \beta \hat{\mathbf{z}}$	(4i)	Os I
$\mathbf{B}_6$	$= -x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$-(ax_3 + cz_3 \cos \beta) \hat{\mathbf{x}} - cz_3 \sin \beta \hat{\mathbf{z}}$	(4i)	Os I

References

- [1] G. Weitz, L. Born, and E. Hellner, *Zur Struktur des OsGe₂*, Z. Metallkd. **51**, 238–243 (1960).

Found in

- [1] M. Gölin, B. Carlsson, and S. Rundqvist, *Refinement of the Crystal Structure of VP₂*, Acta Chem. Scand. A **29**, 706–708 (1975), doi:10.3891/acta.chem.scand.29a-0706.

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