$OsGe_2$ Structure: A2B_mC12_12_2i_i-007

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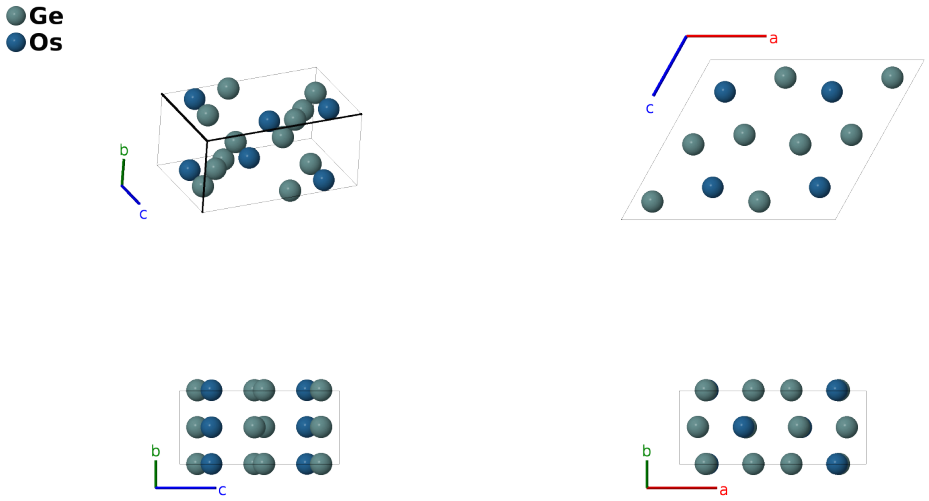
https://aflow.org/p/RQLL

https://aflow.org/p/A2B_mC12_12_2i_i-007



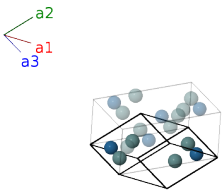
Prototype	Ge_2Os
AFLOW prototype label	A2B_mC12_12_2i_i-007
ICSD	43690
Pearson symbol	mC12
Space group number	12
Space group symbol	$C2/m$
AFLOW prototype command	`aflow --proto=A2B_mC12_12_2i_i-007 --params=`$a, b/a, c/a, \beta, x_1, z_1, x_2, z_2, x_3, z_3$

Other compounds with this structure
VP_2, NbP_2

- $OsGe_2$ shares the same AFLOW label, A2B_mC12_12_2i_i, with CaC_2-III and α-Bi_2Pd. 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

$$
\begin{aligned}
\mathbf{a_1} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{1}{2}b\,\hat{\mathbf{y}} \\
\mathbf{a_2} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}b\,\hat{\mathbf{y}} \\
\mathbf{a_3} &= c\cos\beta\,\hat{\mathbf{x}} + c\sin\beta\,\hat{\mathbf{z}}
\end{aligned}
$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$x_1\,\mathbf{a}_1 + x_1\,\mathbf{a}_2 + z_1\,\mathbf{a}_3$	=	$(ax_1 + cz_1\cos\beta)\,\hat{\mathbf{x}} + cz_1\sin\beta\,\hat{\mathbf{z}}$	(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 $OsGe_2$*, Z. Metallkd. **51**, 238–243 (1960).

Found in

[1] M. Gölin, B. Carlsson, and S. Rundqvist, *Refinement of the Crystal Structure of VP_2*, Acta Chem. Scand. A **29**, 706–708 (1975), doi:10.3891/acta.chem.scand.29a-0706.