

ZrSe₃ Structure:

A3B_mP8_11_3e_e-001

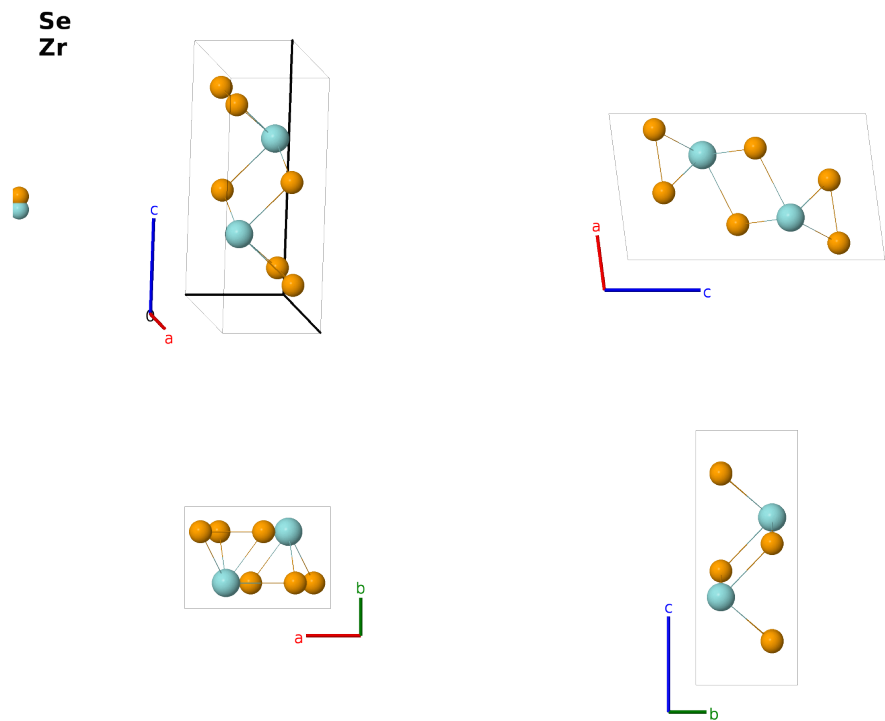
This structure previously used the label(s) **A3B_mP8_11_3e_e**. Calls to these addresses will be redirected here.

Cite this page as:

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<https://aflow.org/prototype-encyclopedia/54KB>

https://aflow.org/prototype-encyclopedia/A3B_mP8_11_3e_e-001



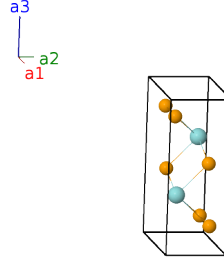
Prototype	Se ₃ Zr
AFLOW prototype label	A3B_mP8_11_3e_e-001
ICSD	652229
CCDC	1765043
Pearson symbol	mP8
Space group number	11
Space group symbol	$P2_1/m$
AFLOW prototype command	<code>aflow --proto=A3B_mP8_11_3e_e-001</code> <code>--params=a, b/a, c/a, β, x_1, z_1, x_2, z_2, x_3, z_3, x_4, z_4</code>

Other compounds with this structure

HfS₃, HfSe₃, HfTe₃, NbTe₃, TaS₂, TaSe₃, TiS₃, US₃, ZrS₃, ZrTe₃

Simple Monoclinic primitive vectors

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



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= x_1 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_1 \mathbf{a}_3$	$=$	$(ax_1 + cz_1 \cos \beta) \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} + cz_1 \sin \beta \hat{\mathbf{z}}$	(2e)	Se I
$\mathbf{B}_2$	$= -x_1 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_1 \mathbf{a}_3$	$=$	$-(ax_1 + cz_1 \cos \beta) \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} - cz_1 \sin \beta \hat{\mathbf{z}}$	(2e)	Se I
$\mathbf{B}_3$	$= x_2 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$(ax_2 + cz_2 \cos \beta) \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} + cz_2 \sin \beta \hat{\mathbf{z}}$	(2e)	Se II
$\mathbf{B}_4$	$= -x_2 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_2 \mathbf{a}_3$	$=$	$-(ax_2 + cz_2 \cos \beta) \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} - cz_2 \sin \beta \hat{\mathbf{z}}$	(2e)	Se II
$\mathbf{B}_5$	$= x_3 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$(ax_3 + cz_3 \cos \beta) \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} + cz_3 \sin \beta \hat{\mathbf{z}}$	(2e)	Se III
$\mathbf{B}_6$	$= -x_3 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$-(ax_3 + cz_3 \cos \beta) \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} - cz_3 \sin \beta \hat{\mathbf{z}}$	(2e)	Se III
$\mathbf{B}_7$	$= x_4 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$(ax_4 + cz_4 \cos \beta) \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} + cz_4 \sin \beta \hat{\mathbf{z}}$	(2e)	Zr I
$\mathbf{B}_8$	$= -x_4 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$-(ax_4 + cz_4 \cos \beta) \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} - cz_4 \sin \beta \hat{\mathbf{z}}$	(2e)	Zr I

References

- [1] S. Furuseth, L. Brattås, and A. Kjekshus, *On the Crystal Structures of TiS₃, ZrS₃, ZrSe₃, ZrTe₃, HfS₃, and HfSe₃*, Acta Chem. Scand. A **29**, 623–631 (1975), doi:10.3891/acta.chem.scand.29a-0623.

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