

Monoclinic FeTlSe₂ Structure: AB2C_mC16_12_g_2i_i-001

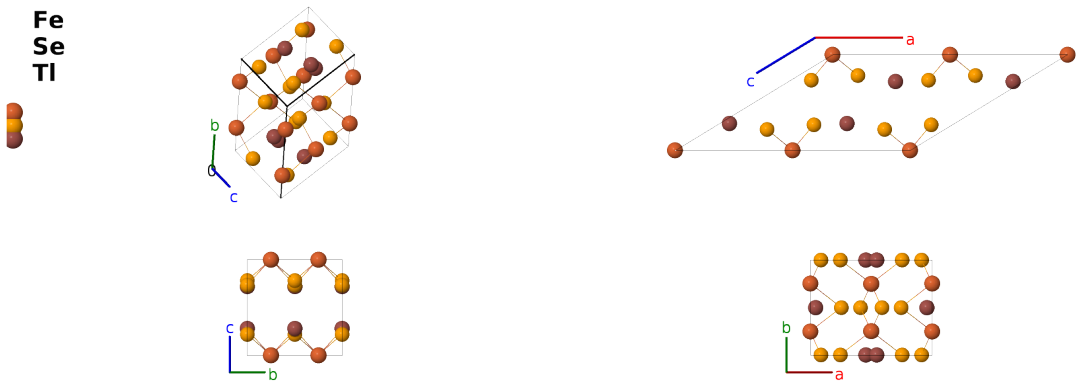
This structure previously used the label(s) **AB2C_mC16_12_g_2i_i**. Calls to these addresses will be redirected here.

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

https://aflow.org/prototype-encyclopedia/AB2C_mC16_12_g_2i_i-001



Prototype	FeSe ₂ Tl
AFLOW prototype label	AB2C_mC16_12_g_2i_i-001
ICSD	100354
CCDC	1659496
Pearson symbol	mC16
Space group number	12
Space group symbol	<i>C</i> 2/ <i>m</i>
AFLOW prototype command	<code>aflow --proto=AB2C_mC16_12_g_2i_i-001 --params=a,b/a,c/a,β,y₁,x₂,z₂,x₃,z₃,x₄,z₄</code>

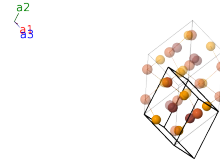
Other compounds with this structure

FeTlS₂

- This is the low temperature structure of FeTlSe₂/FeTlS₂. At high temperatures it transforms to the tetragonal FeTlS₂ structure.

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
$\mathbf{B}_1$	$= -y_1 \mathbf{a}_1 + y_1 \mathbf{a}_2$	$=$	$by_1 \hat{\mathbf{y}}$	(4g)	Fe I
$\mathbf{B}_2$	$= y_1 \mathbf{a}_1 - y_1 \mathbf{a}_2$	$=$	$-by_1 \hat{\mathbf{y}}$	(4g)	Fe 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)	Se I
$\mathbf{B}_4$	$= -x_2 \mathbf{a}_1 - x_2 \mathbf{a}_2 - z_2 \mathbf{a}_3$	$=$	$-(ax_2 + cz_2 \cos \beta) \hat{\mathbf{x}} - cz_2 \sin \beta \hat{\mathbf{z}}$	(4i)	Se I
$\mathbf{B}_5$	$= x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$(ax_3 + cz_3 \cos \beta) \hat{\mathbf{x}} + cz_3 \sin \beta \hat{\mathbf{z}}$	(4i)	Se II
$\mathbf{B}_6$	$= -x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$-(ax_3 + cz_3 \cos \beta) \hat{\mathbf{x}} - cz_3 \sin \beta \hat{\mathbf{z}}$	(4i)	Se II
$\mathbf{B}_7$	$= x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$(ax_4 + cz_4 \cos \beta) \hat{\mathbf{x}} + cz_4 \sin \beta \hat{\mathbf{z}}$	(4i)	Tl I
$\mathbf{B}_8$	$= -x_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$-(ax_4 + cz_4 \cos \beta) \hat{\mathbf{x}} - cz_4 \sin \beta \hat{\mathbf{z}}$	(4i)	Tl I

References

- [1] K. Klepp and H. Boller, *Die Kristallstruktur von TlFeSe₂ und TlFeS₂*, Mh. Chem. **110**, 1045–1055 (1979), doi:10.1007/BF00910952.

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