

Tetragonal TlFeS_2 Structure:

AB2C_tI8_119_c_e_a-001

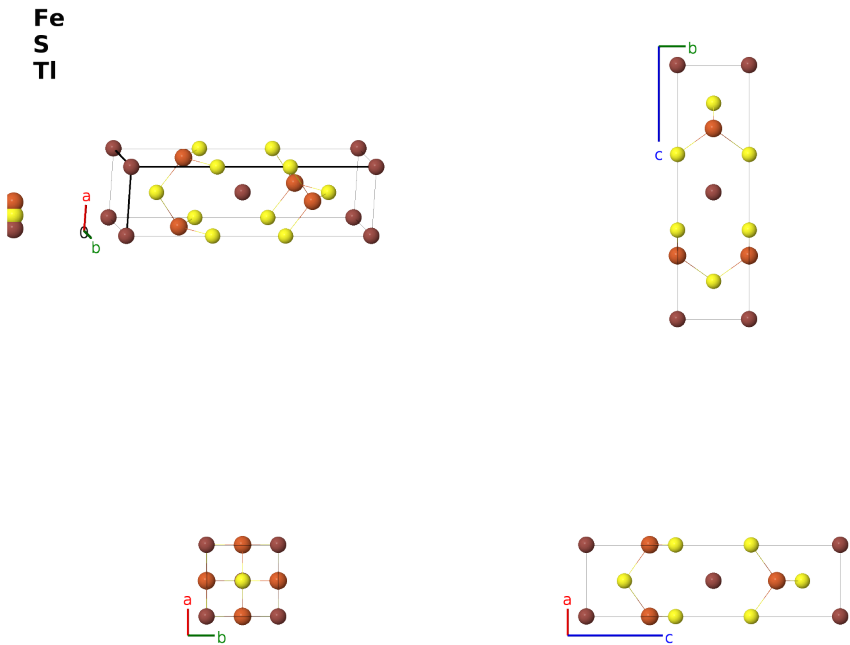
This structure previously used the label(s) **AB2C.tI8_119_c_e_a**. Calls to these addresses will be redirected here.

Cite this page as:

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<https://aflow.org/prototype-encyclopedia/J41Y>

https://aflow.org/prototype-encyclopedia/AB2C_tI8_119_c_e_a-001



Prototype	FeS_2Tl
AFLOW prototype label	AB2C.tI8_119_c_e_a-001
ICSD	150822
CCDC	1667951
Pearson symbol	tI8
Space group number	119
Space group symbol	$I\bar{4}m2$
AFLOW prototype command	<code>aflow --proto=AB2C_tI8_119_c_e_a-001 --params=a, c/a, z₃</code>

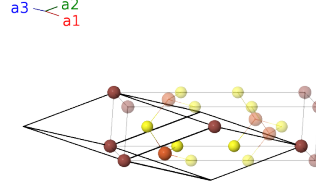
Other compounds with this structure

CsFeSe₂, KFeSe₂, RbFeSe₂, TlAgTe₂, TlFeSe₂

- This is the high-temperature form of TlFeS₂/TlFeSe₂, formed above 300°C. Below that temperature it transforms into the monoclinic TlFeSe₂ structure.
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Body-centered Tetragonal primitive vectors

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



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	=	0	=	0	(2a) Tl I
$\mathbf{B}_2$	=	$\frac{3}{4}\mathbf{a}_1 + \frac{1}{4}\mathbf{a}_2 + \frac{1}{2}\mathbf{a}_3$	=	$\frac{1}{2}a\hat{\mathbf{y}} + \frac{1}{4}c\hat{\mathbf{z}}$	(2c) Fe I
$\mathbf{B}_3$	=	$z_3\mathbf{a}_1 + z_3\mathbf{a}_2$	=	$cz_3\hat{\mathbf{z}}$	(4e) S I
$\mathbf{B}_4$	=	$-z_3\mathbf{a}_1 - z_3\mathbf{a}_2$	=	$-cz_3\hat{\mathbf{z}}$	(4e) S I

References

- [1] A. Kutoglu, *Synthese und Kristallstrukturen von TlFeS₂ und TlFeSe₂*, Naturwissenschaften **61**, 125–126 (1974), doi:10.1007/BF00606283.

Found in

- [1] E. B. Asgerov, A. I. Madadzada, A. I. Beskrovnyy, D. I. Ismayilov, R. N. Mehdieva, S. H. Jabarov, E. M. Kerimova, and D. Neov, *Neutron-Diffraction Study in TlFeS₂ and TlFeSe₂ at Low Temperatures*, J Surf. Invest. **8**, 1193–1197 (2014), doi:10.1134/S1027451014060238.

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