

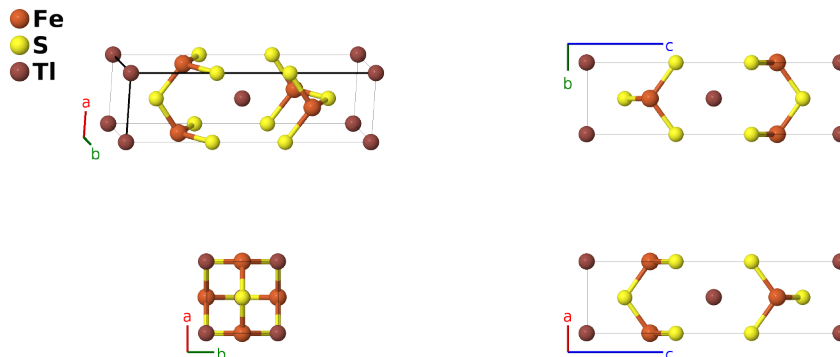
# Tetragonal TlFeS<sub>2</sub> Structure: AB2C\_tI8\_119\_c\_e\_a-001

This structure originally had the label AB2C\_tI8\_119\_c\_e\_a. Calls to that address will be redirected here.

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<https://aflow.org/p/J41Y>

[https://aflow.org/p/AB2C\\_tI8\\_119\\_c\\_e\\_a-001](https://aflow.org/p/AB2C_tI8_119_c_e_a-001)



Prototype	FeS <sub>2</sub> Tl
AFLOW prototype label	AB2C_tI8_119_c_e_a-001
ICSD	150822
Pearson symbol	tI8
Space group number	119
Space group symbol	$I\bar{4}m2$
AFLOW prototype command	aflow --proto=AB2C_tI8_119_c_e_a-001 --params=a, c/a, z <sub>3</sub>

## Other compounds with this structure

CsFeSe<sub>2</sub>, KFeSe<sub>2</sub>, RbFeSe<sub>2</sub>, TlAgTe<sub>2</sub>, TlFeSe<sub>2</sub>

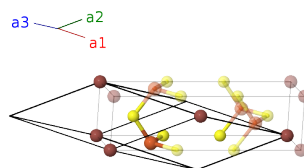
- This is the high-temperature form of TlFeS<sub>2</sub>/TlFeSe<sub>2</sub>, formed above 300°C. Below that temperature it transforms into the monoclinic TlFeSe<sub>2</sub> structure.

## Body-centered Tetragonal primitive vectors

$$\mathbf{a}_1 = -\frac{1}{2}a \hat{x} + \frac{1}{2}a \hat{y} + \frac{1}{2}c \hat{z}$$

$$\mathbf{a}_2 = \frac{1}{2}a \hat{x} - \frac{1}{2}a \hat{y} + \frac{1}{2}c \hat{z}$$

$$\mathbf{a}_3 = \frac{1}{2}a \hat{x} + \frac{1}{2}a \hat{y} - \frac{1}{2}c \hat{z}$$



## 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  $TlFeS_2$  und  $TlFeSe_2$* , 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  $TlFeS_2$  and  $TlFeSe_2$  at Low Temperatures*, J Surf. Invest. **8**, 1193–1197 (2014), doi:10.1134/S1027451014060238.