α-FeSe Structure: AB_oC8_67_a_g-001

This structure originally had the label `AB_oC8_67_a_g.FeSe`. Calls to that address will be redirected here.

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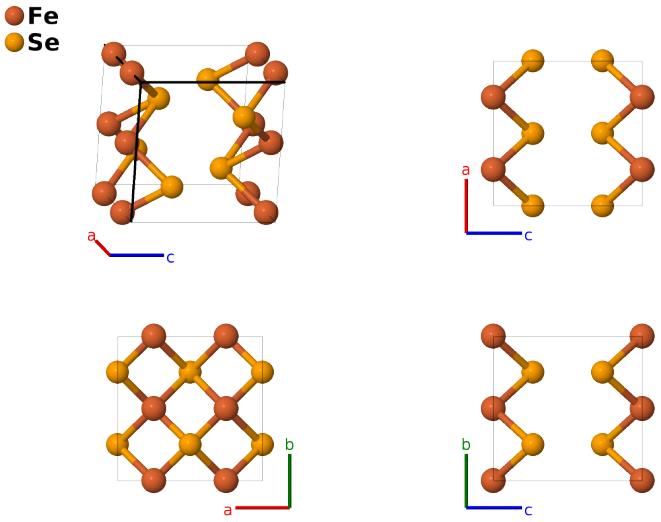
https://aflow.org/p/JFD1

https://aflow.org/p/AB_oC8_67_a_g-001



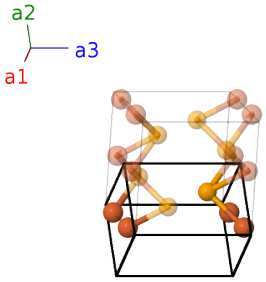
Prototype	FeSe
AFLOW prototype label	AB_oC8_67_a_g-001
ICSD	185465
Pearson symbol	oC8
Space group number	67
Space group symbol	*Cmme*
AFLOW prototype command	`aflow --proto=AB_oC8_67_a_g-001 --params=`$a, b/a, c/a, z_2$

- We follow (Louca, 2010) in calling this α-FeSe. While some authorities list this as a prototype of α-PbO, we find that the difference in structures is enough to warrant giving FeSe its own prototype.
- (Louca, 2010) note that "the Se ion concentration is close to 1."
- The data is presented for the structure at 7 K.
- The ICSD entry is from the (Lehman, 2010) conference proceedings.
- (Louca, 2010) find $a \approx b$. As with orthorhombic α-PbO and tetragonal ($B10$) PbO, this causes AFLOW to place this in the tetragonal $P4/nmm$ #129 space group if the default settings are used. The experimentally reported structure is only obtained if we use the command

- aflow --proto=AB_oC8_67_a_g --tolerance=0.001 --params=a,c/a,z_2 .
- α-FeSe and α-PbO have the same AFLOW prototype label, AB_oC8_67_a_g. They are generated by the same symmetry operations with different sets of parameters (`--params`) specified in their corresponding CIF files.

Base-centered Orthorhombic primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2$	=	$\frac{1}{4}a\,\hat{\mathbf{x}}$	(4a)	Fe I
$\mathbf{B_2}$	=	$\frac{3}{4}\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2$	=	$\frac{3}{4}a\,\hat{\mathbf{x}}$	(4a)	Fe I
$\mathbf{B_3}$	=	$\frac{3}{4}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{1}{4}b\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(4g)	Se I
$\mathbf{B_4}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 - z_2\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} - cz_2\,\hat{\mathbf{z}}$	(4g)	Se I

References

[1] D. Louca, K. Horigane, A. Llobet, R. Arita, S. Ji, N. Katayama, S. Konbu, K. Nakamura, T.-Y. Koo, P. Tong, and K. Yamada, *Local atomic structure of superconducting $FeSe_{1-x}Te_x$*, Phys. Rev. B **81**, 134524 (2010), doi:10.1103/PhysRevB.81.134524.

[2] M. C. Lehman, A. Llobet, K. Horigane, and D. Louca, *The crystal structure of superconducting $FeSe_{1-x}Te_x$ by pulsed neutron diffraction*, J. Phys: Conf. Ser. **251**, 012009 (2010), doi:10.1088/1742-6596/251/1/012009.