$CsFeS_2$ (100K) Structure: ABC2_oI16_71_e_g_fi-001

This structure originally had the label `ABC2_oI16_71_g_i_eh`. Calls to that address will be redirected here.

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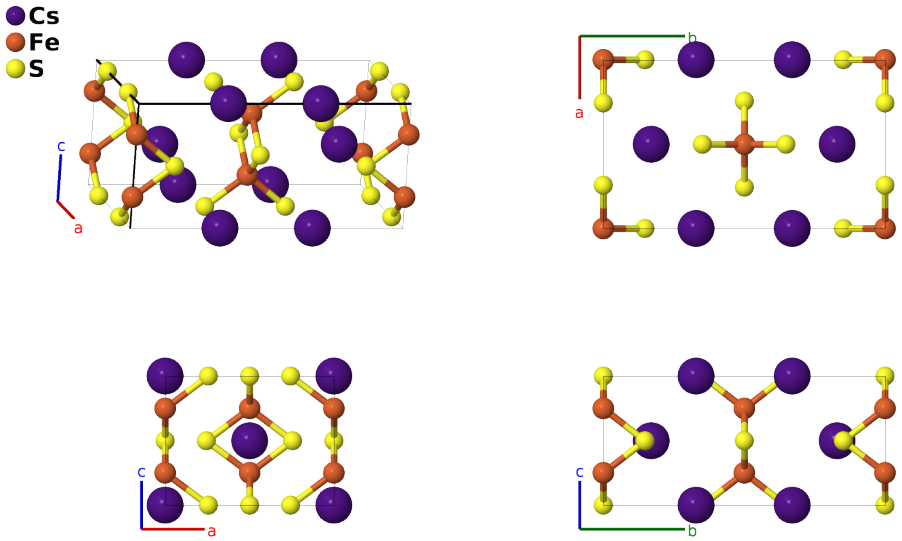
https://aflow.org/p/R5TH

https://aflow.org/p/ABC2_oI16_71_e_g_fi-001



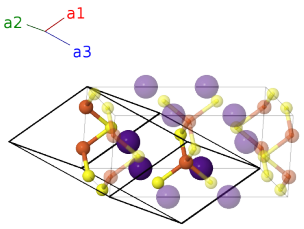
Prototype	$CsFeS_2$
AFLOW prototype label	ABC2_oI16_71_e_g_fi-001
ICSD	53234
Pearson symbol	oI16
Space group number	71
Space group symbol	$Immm$
AFLOW prototype command	`aflow --proto=ABC2_oI16_71_e_g_fi-001 --params=`$a, b/a, c/a, x_1, x_2, y_3, z_4$

Other compounds with this structure
$RbFeS_2$

- This structure is stable at 100K and above. At 40K the structure is triclinic, with as yet undetermined atomic positions. (Ito, 1985)

Body-centered Orthorhombic primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$x_1\,\mathbf{a}_2 + x_1\,\mathbf{a}_3$	=	$ax_1\,\hat{\mathbf{x}}$	(4e)	Cs I
$\mathbf{B_2}$	=	$-x_1\,\mathbf{a}_2 - x_1\,\mathbf{a}_3$	=	$-ax_1\,\hat{\mathbf{x}}$	(4e)	Cs I
$\mathbf{B_3}$	=	$\frac{1}{2}\,\mathbf{a}_1 + x_2\,\mathbf{a}_2 + \left(x_2 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$ax_2\,\hat{\mathbf{x}} + \frac{1}{2}b\,\hat{\mathbf{y}}$	(4f)	S I
$\mathbf{B_4}$	=	$\frac{1}{2}\,\mathbf{a}_1 - x_2\,\mathbf{a}_2 - \left(x_2 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_2\,\hat{\mathbf{x}} + \frac{1}{2}b\,\hat{\mathbf{y}}$	(4f)	S I
$\mathbf{B_5}$	=	$y_3\,\mathbf{a}_1 + y_3\,\mathbf{a}_3$	=	$by_3\,\hat{\mathbf{y}}$	(4g)	Fe I
$\mathbf{B_6}$	=	$-y_3\,\mathbf{a}_1 - y_3\,\mathbf{a}_3$	=	$-by_3\,\hat{\mathbf{y}}$	(4g)	Fe I
$\mathbf{B_7}$	=	$z_4\,\mathbf{a}_1 + z_4\,\mathbf{a}_2$	=	$cz_4\,\hat{\mathbf{z}}$	(4i)	S II
$\mathbf{B_8}$	=	$-z_4\,\mathbf{a}_1 - z_4\,\mathbf{a}_2$	=	$-cz_4\,\hat{\mathbf{z}}$	(4i)	S II

References

[1] Y. Ito, M. Nishi, C. F. Majkrzak, and L. Passell, *Low Temperature Powder Neutron Diffraction Studies of $CsFeS_2$*, J. Phys. Soc. Japan **54**, 348–357 (1985), doi:10.1143/JPSJ.54.348.

Found in

[1] P. Villars, *CsFeS2 (100K) Crystal Structure* (2016). PAULING FILE in: Inorganic Solid Phases, SpringerMaterials (online database), Springer, Heidelberg (ed.) SpringerMaterials.