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

This structure previously used the label(s) `ABC2_oI16_71_g_i_eh`. Calls to these addresses will be redirected here.

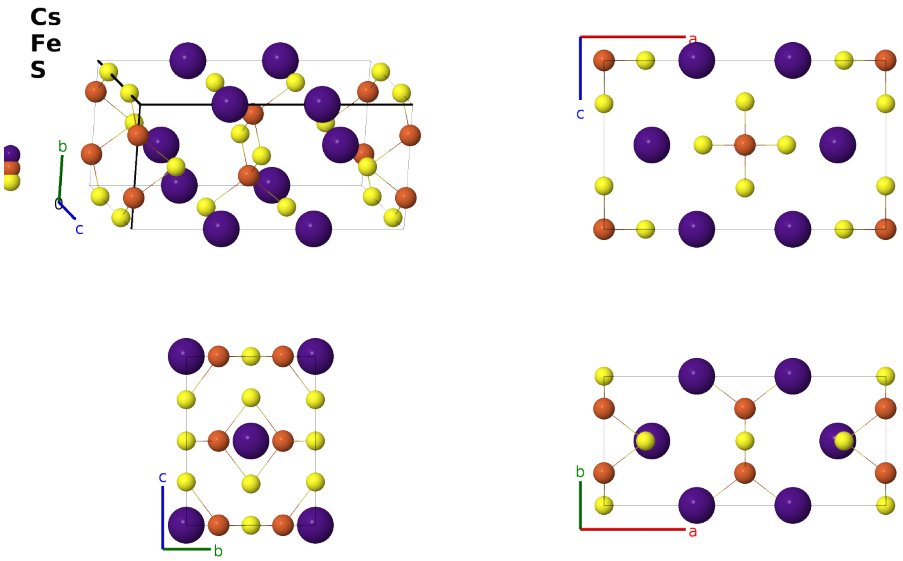
Cite this page as:

- H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettel, M. Esters, X. Campilongo, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*, Comput. Mater. Sci. **240**, 112988 (2024), doi: 10.1016/j.commatsci.2024.112988.
- D. Hicks, M. J. Mehl, M. Esters, C. Oses, O. Levy, G. L. W. Hart, C. Toher, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 3*, Comput. Mater. Sci. **199**, 110450 (2021), doi: 10.1016/j.commatsci.2021.110450.

---

https://aflow.org/prototype-encyclopedia/R5TH

https://aflow.org/prototype-encyclopedia/ABC2_oI16_71_e_g_fi-001




| | |
|---|---|
| **Prototype** | $CsFeS_2$ |
| **AFLOW prototype label** | ABC2_oI16_71_e_g_fi-001 |
| **ICSD** | 53234 |
| **CCDC** | 1617931 |
| **Pearson symbol** | oI16 |
| **Space group number** | 71 |
| **Space group symbol** | $Immm$ |
| **AFLOW prototype command** | `aflow --proto=ABC2_oI16_71_e_g_fi-001 --params=`$a, b/a, c/a, x_1, x_2, y_3, z_4$ |

---

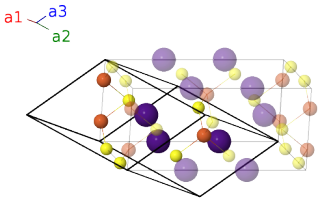
**Other compounds with this structure**
$RbFeS_2$

---

- 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

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




### 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.


### First cited in


D. Hicks, M. J. Mehl, M. Esters, C. Oses, O. Levy, G. L. W. Hart, C. Toher, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 3*, Comput. Mater. Sci. **199**, 110450 (2021), doi: 10.1016/j.commatsci.2021.110450.