# $\alpha$-$F_2$ Structure: A_mC8_15_f-001

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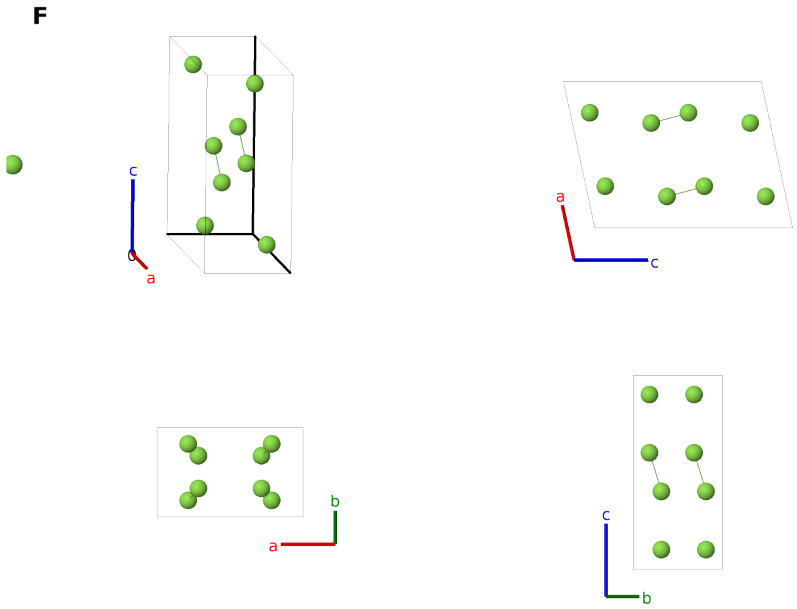
https://aflow.org/prototype-encyclopedia/6S9D

https://aflow.org/prototype-encyclopedia/A_mC8_15_f-001




| | |
|---|---|
| **Prototype** | $F_2$ |
| **AFLOW prototype label** | A_mC8_15_f-001 |
| **ICSD** | 16262 |
| **CCDC** | 1596861 |
| **Pearson symbol** | mC8 |
| **Space group number** | 15 |
| **Space group symbol** | $C2/c$ |
| **AFLOW prototype command** | `aflow --proto=A_mC8_15_f-001 --params=`$a, b/a, c/a, \beta, x_1, y_1, z_1$ |

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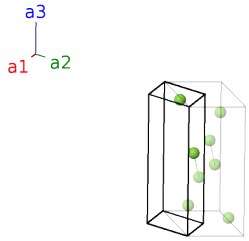
- This the ground state of fluorine. Above 45.6K it transforms into the disordered $\beta$-$F_2$ structure and melts at 53.53K (Ivlev, 2019).

## Base-centered Monoclinic primitive vectors

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




## Basis vectors

| | | Lattice coordinates | | Cartesian coordinates | Wyckoff position | Atom type |
|---|---|---|---|---|---|---|
| $\mathbf{B_1}$ | = | $(x_1 - y_1)\,\mathbf{a}_1 + (x_1 + y_1)\,\mathbf{a}_2 + z_1\,\mathbf{a}_3$ | = | $(ax_1 + cz_1\cos\beta)\,\hat{\mathbf{x}} + by_1\,\hat{\mathbf{y}} + cz_1\sin\beta\,\hat{\mathbf{z}}$ | (8f) | F I |
| $\mathbf{B_2}$ | = | $-(x_1 + y_1)\,\mathbf{a}_1 - (x_1 - y_1)\,\mathbf{a}_2 - \left(z_1 - \frac{1}{2}\right)\mathbf{a}_3$ | = | $-\left(ax_1 + c\left(z_1 - \frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} + by_1\,\hat{\mathbf{y}} - c\left(z_1 - \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$ | (8f) | F I |
| $\mathbf{B_3}$ | = | $-(x_1 - y_1)\,\mathbf{a}_1 - (x_1 + y_1)\,\mathbf{a}_2 - z_1\,\mathbf{a}_3$ | = | $-(ax_1 + cz_1\cos\beta)\,\hat{\mathbf{x}} - by_1\,\hat{\mathbf{y}} - cz_1\sin\beta\,\hat{\mathbf{z}}$ | (8f) | F I |
| $\mathbf{B_4}$ | = | $(x_1 + y_1)\,\mathbf{a}_1 + (x_1 - y_1)\,\mathbf{a}_2 + \left(z_1 + \frac{1}{2}\right)\mathbf{a}_3$ | = | $\left(ax_1 + c\left(z_1 + \frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} - by_1\,\hat{\mathbf{y}} + c\left(z_1 + \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$ | (8f) | F I |

## References


[1] L. Pauling, I. Keaveny, and A. B. Robinson, *The crystal structure of α-fluorine*, J. Solid State Chem. **2**, 225–227 (1970), doi:10.1016/0022-4596(70)90074-5.


## Found in


[1] S. I. Ivlev, A. J. Karttunen, M. Hoelzel, M. Conrad, and F. Kraus, *The Crystal Structures of α- and β-$F_2$ Revisited*, Chem. Eur. J. **25**, 3310–3317 (2019), doi:10.1002/chem.201805298.


## First cited in

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