β-F_2 Structure: A_cP8_223_ac-001

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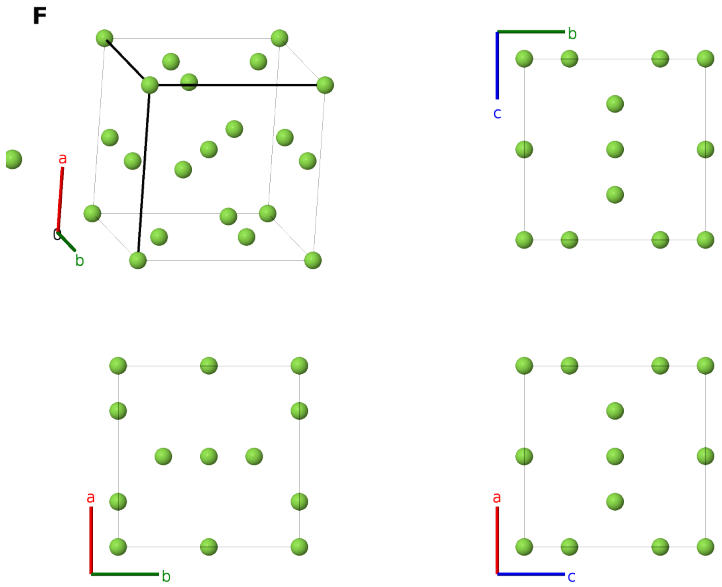
https://aflow.org/prototype-encyclopedia/57F4

https://aflow.org/prototype-encyclopedia/A_cP8_223_ac-001



Prototype	F_2
AFLOW prototype label	A_cP8_223_ac-001
ICSD	15821
CCDC	1596505
Pearson symbol	cP8
Space group number	223
Space group symbol	$Pm\bar{3}n$
AFLOW prototype command	`aflow --proto=A_cP8_223_ac-001 --params=`a

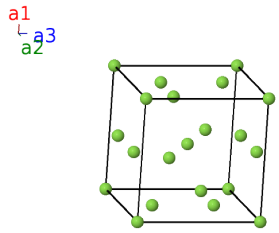
Other compounds with this structure
γ-O_2

- Below 45.6K this transforms to the ordered monoclinic α-F_2 structure (Ivlev, 2019). It melts at 53.53K.
- This is an approximate and somewhat misleading structure for β-F_2. Both fluorine sites are actually F_2 *molecules* which have random orientation. Thus there are actually 16 fluorine *atoms* in the unit cell.

- Treating the F_2 molecules as "atoms," this is isostructural with the $A15$ structure.
- (Ivlev, 2019) presents (CCDC 1874485) an alternative version of this structure, with partially occupied fixed points for all of the fluorine atoms. This structure does not add much to our understanding, so we will use the simpler version of (Jordan, 1964).

Simple Cubic primitive vectors

$$\mathbf{a_1} = a\,\hat{\mathbf{x}}$$
$$\mathbf{a_2} = a\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = a\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(2a)	F I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{2}a\,\hat{\mathbf{z}}$	(2a)	F I
$\mathbf{B_3}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{z}}$	(6c)	F II
$\mathbf{B_4}$	=	$\frac{3}{4}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{3}{4}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{z}}$	(6c)	F II
$\mathbf{B_5}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}}$	(6c)	F II
$\mathbf{B_6}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{3}{4}a\,\hat{\mathbf{y}}$	(6c)	F II
$\mathbf{B_7}$	=	$\frac{1}{2}\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{4}a\,\hat{\mathbf{z}}$	(6c)	F II
$\mathbf{B_8}$	=	$\frac{1}{2}\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{y}} + \frac{3}{4}a\,\hat{\mathbf{z}}$	(6c)	F II

References

[1] T. H. Jordan, W. D. Streib, H. W. Smith, and W. N. Lipscomb, *Single-crystal studies of β-F_2 and γ-O_2*, Acta Cryst. **17**, 777–778 (1964), doi:10.1107/S0365110X6400202X.

[2] 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.

Found in

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First cited in

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