

Fluorite (CaF₂, *C*1) Structure: AB2_cF12_225_a_c-001

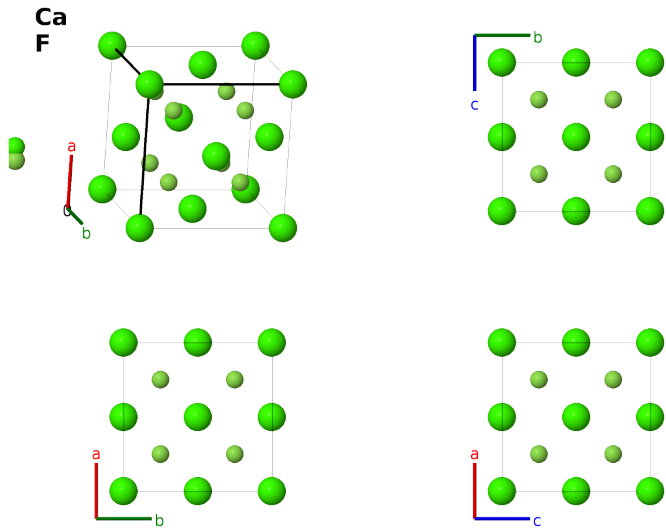
This structure previously used the label(s) **AB2_cF12_225_a_c**. Calls to these addresses will be redirected here.

Cite this page as:

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<https://aflow.org/prototype-encyclopedia/8VXQ>

https://aflow.org/prototype-encyclopedia/AB2_cF12_225_a_c-001



Prototype	CaF ₂
AFLOW prototype label	AB2_cF12_225_a_c-001
<i>Strukturbericht</i> designation	<i>C</i> 1
Mineral name	fluorite
ICSD	44937
CCDC	1614261
Pearson symbol	cF12
Space group number	225
Space group symbol	<i>Fm</i> $\bar{3}m$
AFLOW prototype command	<code>aflow --proto=AB2_cF12_225_a_c-001 --params=a</code>

Other compounds with this structure

AmO₂, AuAl₂, AuGa₂, AuIn₂, BBe₂, BaF₂, CO₂, CdF₂, CeH₂, CeO₂, CmO₂, CoSi₂, DyH₂, EuF₂, GdH₂, GeMg₂, HgF₂, IrSn₂, LaH₂, LuH₂, MgPu₂, NbH₂, NdH₂, NiSi₂, OK₂, OLi₂, ONa₂, ORb₂, PIr₂, PRh₂, PaO₂, PbMg₂, PoO₂, PrH₂, PrO₂, PtAl₂, PtGa₂, PtSn₂, PuH₂, PuO₂, RbO₂, RbS₂, SCu₂, SH₂, SK₂, SLi₂, SRb₂, ScH₂, SeH₂, SeK₂, SeLi₂, SiMg₂, SmH₂, SmO₂, β -SrBr₂, SrCl₂, SrF₂, SrMg₂, TbH₂, TbO₂, TeK₂, TeLi₂, ThH₂, ThO₂, TmH₂, UC₂, UN₂, UO₂, YH₂, ZrO₂

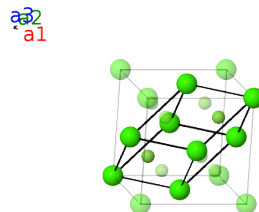
- We do not have an ICSD entry from (Speziale, 2002), so we use the one provided by (Smakula, 1955).

Face-centered Cubic primitive vectors

$$\mathbf{a}_1 = \frac{1}{2}a\hat{\mathbf{y}} + \frac{1}{2}a\hat{\mathbf{z}}$$

$$\mathbf{a}_2 = \frac{1}{2}a\hat{\mathbf{x}} + \frac{1}{2}a\hat{\mathbf{z}}$$

$$\mathbf{a}_3 = \frac{1}{2}a\hat{\mathbf{x}} + \frac{1}{2}a\hat{\mathbf{y}}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	=	0	=	0	(4a) Ca I
$\mathbf{B}_2$	=	$\frac{1}{4}\mathbf{a}_1 + \frac{1}{4}\mathbf{a}_2 + \frac{1}{4}\mathbf{a}_3$	=	$\frac{1}{4}a\hat{\mathbf{x}} + \frac{1}{4}a\hat{\mathbf{y}} + \frac{1}{4}a\hat{\mathbf{z}}$	(8c) F I
$\mathbf{B}_3$	=	$\frac{3}{4}\mathbf{a}_1 + \frac{3}{4}\mathbf{a}_2 + \frac{3}{4}\mathbf{a}_3$	=	$\frac{3}{4}a\hat{\mathbf{x}} + \frac{3}{4}a\hat{\mathbf{y}} + \frac{3}{4}a\hat{\mathbf{z}}$	(8c) F I

References

- [1] S. Speziale and T. S. Duffy, *Single-crystal elastic constants of fluorite (CaF_2) to 9.3 GPa*, Phys. Chem. Miner. **29**, 465–472 (2002), doi:10.1007/s00269-002-0250-x.
- [2] A. Smakula and J. Kalnajs, *Precision Determination of Lattice Constants with a Geiger-Counter X-Ray Diffractometer*, Phys. Rev. **99**, 1737–1743 (1955), doi:10.1103/PhysRev.99.1737.

Found in

- [1] R. T. Downs and M. Hall-Wallace, *The American Mineralogist Crystal Structure Database*, Am. Mineral. **88**, 247–250 (2003).

First cited in

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