Fluorite (CaF_2, $C1$) Structure: AB2_cF12_225_a_c-001

This structure originally had the label `AB2_cF12_225_a_c`. Calls to that address will be redirected here.

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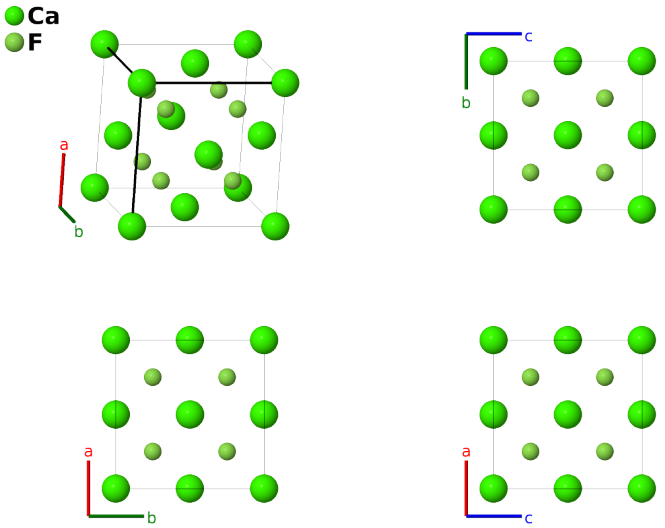
https://aflow.org/p/8VXQ

https://aflow.org/p/AB2_cF12_225_a_c-001



Prototype	CaF_2
AFLOW prototype label	AB2_cF12_225_a_c-001
***Strukturbericht* designation**	$C1$
Mineral name	fluorite
ICSD	44937
Pearson symbol	cF12
Space group number	225
Space group symbol	$Fm\bar{3}m$
AFLOW prototype command	`aflow --proto=AB2_cF12_225_a_c-001 --params=`a

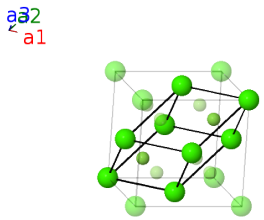
Other compounds with this structure

AmO_2, $AuAl_2$, $AuGa_2$, $AuIn_2$, BBe_2, BaF_2, CO_2, CdF_2, CeH_2, CeO_2, CmO_2, $CoSi_2$, DyH_2, EuF_2, GdH_2, $GeMg_2$, HgF_2, $IrSn_2$, LaH_2, LuH_2, $MgPu_2$, NbH_2, NdH_2, $NiSi_2$, OK_2, OLi_2, ONa_2, ORb_2, PIr_2, PRh_2, PaO_2, $PbMg_2$, PoO_2, PrH_2, PrO_2, $PtAl_2$, $PtGa_2$, $PtSn_2$, PuH_2, PuO_2, RbO_2, RbS_2, SCu_2, SH_2, SK_2, SLi_2, SRb_2, ScH_2, SeH_2, SeK_2, $SeLi_2$, $SiMg_2$, SmH_2, SmO_2, β-$SrBr_2$, $SrCl_2$, SrF_2, $SrMg_2$, TbH_2, TbO_2, TeK_2, $TeLi_2$, ThH_2, ThO_2, TmH_2, UC_2, UN_2, UO_2, YH_2, ZrO_2

- 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).