Gananite (BiF_3, $D0_3$) Structure: AB3_cF16_225_a_bc-001

This structure previously used the label(s) `AB3_cF16_225_a_bc`. Calls to these addresses will be redirected here.

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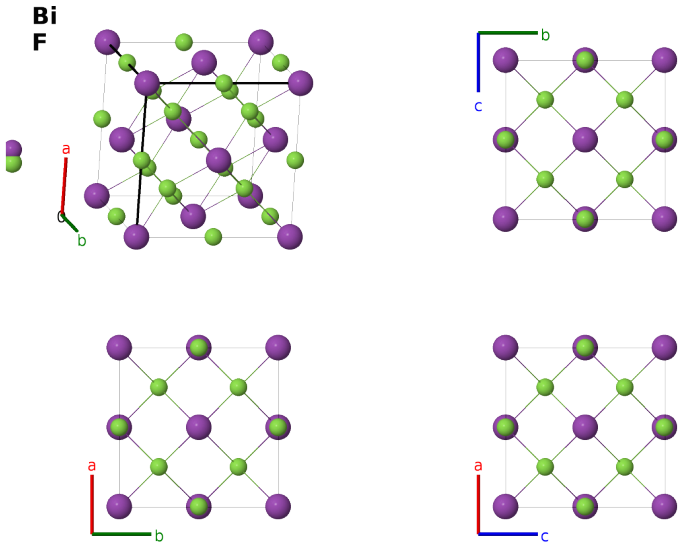
https://aflow.org/prototype-encyclopedia/KFY2

https://aflow.org/prototype-encyclopedia/AB3_cF16_225_a_bc-001



Prototype	BiF_3
AFLOW prototype label	AB3_cF16_225_a_bc-001
***Strukturbericht* designation**	$D0_3$
Mineral name	gananite
ICSD	25567
CCDC	1601221
Pearson symbol	cF16
Space group number	225
Space group symbol	$Fm\bar{3}m$
AFLOW prototype command	`aflow --proto=AB3_cF16_225_a_bc-001 --params=`a

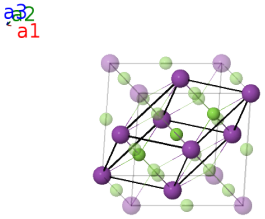
Other compounds with this structure

$AgLi_3$, $AlCu_3$, $AlFe_3$, $AmBa_3$, $AsLi_3$, $AsNa_3$, $AsPd_3$, $AuLi_3$, $BiCs_3$, $BiFe_3$, β-BiK_3 (HT), $BiLi_3$, BiO_3, $BiPd_3$, $BiRb_3$, CaH_3, $CdLi_3$, $CeCd_3$, CeH_3, CeO_3, $CeMg_3$, $DyMg_3$, ErH_3, FeH_3, $GaFe_3$, $GaMn_3$, GdH_3, $GdMg_3$, $GeCo_3$, $GeCu_3$, $GeFe_3$, $GeLi_3$, $GeMg_3$, $GeMn_3$, HoH_3, $HgLi_3$, IAg_3, $InCa_3$, $InSr_3$, LaH_3, $LaMg_3$, LaO_3, LuH_3, $MgAg_3$, $MgCe_3$, MgH_3, $MnFe_3$, NNa_3, NbO_3, $NbSr_3$, $NdCd_3$, NdH_3, $NdMg_3$, $NpBa_3$, OAl_3, OFe_3, OMo_3, PLi_3, PbF_3, $PbLi_3$, $PrCd_3$, PrH_3, $PrMg_3$, PuH_3, $RbBi_3$, RuK_3, SAg_3, SLi_3, SPd_3, β-$SbCu_3$ (HT), SbK_3, $SbLi_3$, $SbNi_3$ (HT), ScH_3, $SePd_3$, $SiCo_3$, $SiFe_3$, $SiMg_3$, $SiMn_3$, $SiNa_3$, $SmCd_3$, $SmMg_3$, SmO_3, γ-$SnCu_3$ (HT), $SnLi_3$, $SnNi_3$ (HT), $SrCl_3$, TaO_3, TbH_3, $TbMg_3$, TiH_3, $TlCa_3$, $TlLi_3$, UO_3, VH_3, YCd_3, YH_3, YMg_3, YbH_3, YbO_3

- (Villars, 1991) corrects (Hund, 1949), changing the positions of one third of the fluorine atoms so that the space group becomes $Fm\bar{3}m$ #225, as is accepted for $D0_3$, and in agreement with (Hassel, 1929). This structure is crystallographically equivalent to the Heusler ($L2_1$) structure and a derivative of the "quaternary-Heusler," LiMgAuSn.

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)	Bi I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{2}a\,\hat{\mathbf{z}}$	(4b)	F I
$\mathbf{B_3}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} + \frac{1}{4}a\,\hat{\mathbf{z}}$	(8c)	F II
$\mathbf{B_4}$	=	$\frac{3}{4}\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{3}{4}a\,\hat{\mathbf{x}} + \frac{3}{4}a\,\hat{\mathbf{y}} + \frac{3}{4}a\,\hat{\mathbf{z}}$	(8c)	F II

References

[1] O. Hassel and S. Nilssen, *Der Kristallbau des BiF_3*, Z. Anorganische und Allgemeine Chemie **181**, 172–176 (1929), doi:10.1002/zaac.19291810117.

[2] F. Hund and R. Fricke, *Der Kristallbau von α-BiF_3*, Z. Anorganische und Allgemeine Chemie **258**, 198–204 (1949), doi:10.1002/zaac.19492580310.

Found in

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First cited in

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