BiF_3 ($D0_3$) Structure: AB3_cF16_225_a_bc-001

This structure originally had the label `AB3_cF16_225_a_bc`. Calls to that address will be redirected here.

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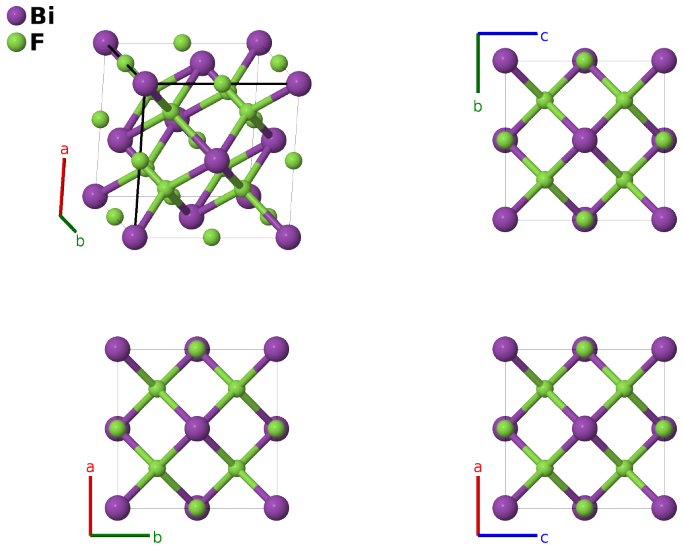
https://aflow.org/p/KFY2

https://aflow.org/p/AB3_cF16_225_a_bc-001



Prototype	BiF_3
AFLOW prototype label	AB3_cF16_225_a_bc-001
***Strukturbericht* designation**	$D0_3$
ICSD	25567
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

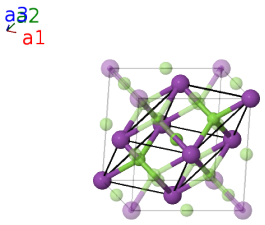
Other compounds with this structure

$AlFe_3$, $BiFe_3$, β-BiK_3 (HT), $BiLi_3$, $CeCd_3$, ErH_3, GdH_3, $GeMg_3$, HoH_3, $HgLi_3$, LaH_3, $LaMg_3$, LuH_3, $NdCd_3$, $PbLi_3$, $PrCd_3$, β-$SbCu_3$ (HT), $SbLi_3$, $SbNi_3$ (HT), $SiFe_3$, $SiMg_3$, $SmCd_3$, $SmMg_3$, γ-$SnCu_3$ (HT), $SnNi_3$ (HT)

- (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

[1] P. Villars and L. Calvert, *Pearson's Handbook of Crystallographic Data for Intermetallic Phases* (ASM International, Materials Park, OH, 1991), 2nd edn.