Galenobismutite ($PbBi_2S_4$) Structure: A2BC4_oP28_62_2c_c_4c-001

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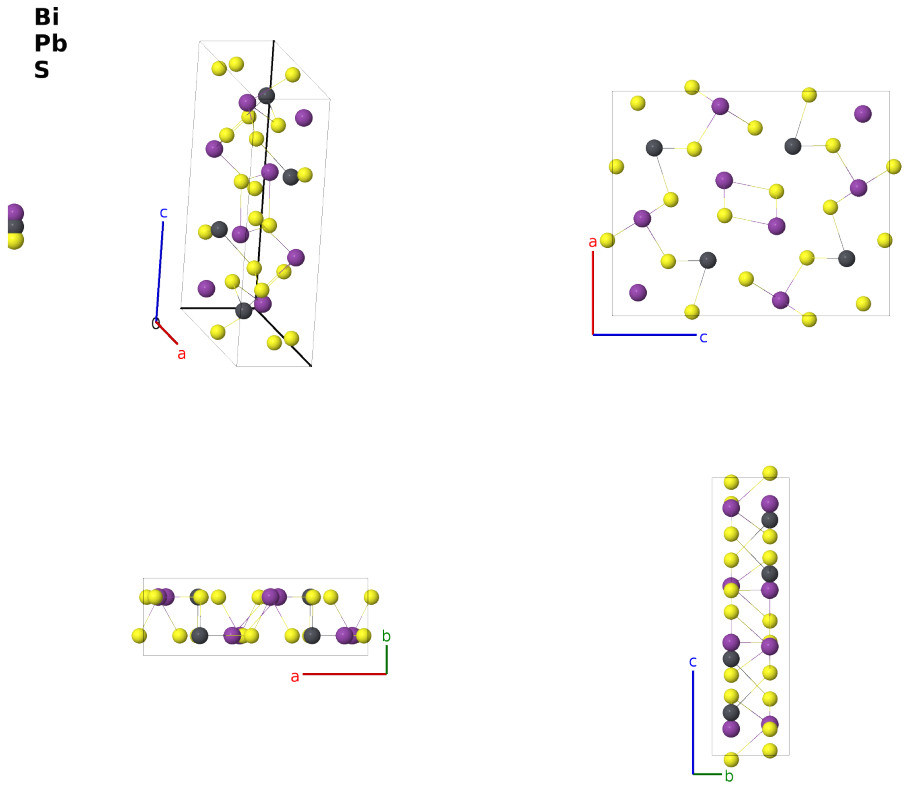
https://aflow.org/prototype-encyclopedia/PUZH

https://aflow.org/prototype-encyclopedia/A2BC4_oP28_62_2c_c_4c-001



Prototype	Bi_2PbS_4
AFLOW prototype label	A2BC4_oP28_62_2c_c_4c-001
Mineral name	galenobismutite
ICSD	158392
CCDC	1674904
Pearson symbol	oP28
Space group number	62
Space group symbol	*Pnma*
AFLOW prototype command	`aflow --proto=A2BC4_oP28_62_2c_c_4c-001 --params=`$a, b/a, c/a, x_1, z_1, x_2, z_2, x_3, z_3, x_4, z_4, x_5, z_5, x_6, z_6, x_7, z_7$

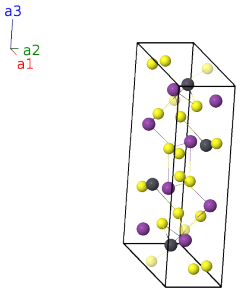
Other compounds with this structure

$(Cd_xNa_{1-x})Rh_2O_4$, Li(Fe, Ti)$_2O_4$, Na(Al, Ge)$_2O_4$, Na(Al, Si)$_2O_4$, Na(Fe$_{0.75}$, Sb$_{0.25}$)$_2O_4$, Na(Fe, Ru)$_2O_4$, Na(Fe, Sn)$_2O_4$, Na(Fe, Ti)$_2O_4$, Na(Sc, Hf)$_2O_4$, Na(Sc, Sn)$_2O_4$, Na(Sc, Ti)$_2O_4$, Na(Sc, Zr)$_2O_4$, Na(Sn, V)$_2O_4$, Sr(In, Yb)$_2O_4$, (Ba, Sr)Dy_2O_4, (Ba, Sr)Er_2O_4, (Ba, Sr)Eu_2O_4, (Ba, Sr)Gd_2O_4, (Ba, Sr)Ho_2O_4, (Ba, Sr)La_2O_4, (Ba, Sr)Lu_2O_4, (Ba, Sr)Nd_2O_4, (Ba, Sr)Sm_2O_4, (Ba, Sr)Tm_2O_4, (Ba, Sr)Y_2O_4, (Ba, Sr)Yb_2O_4, $BaCe_2O_4$, $BaDy_2S_4$, $BaDy_2Se_4$, $BaDy_2Te_4$, $BaEr_2O_4$, $BaEr_2S_4$, $BaEr_2Se_4$, $BaEr_2Te_4$, $BaEu_2O_4$, $BaGd_2O_4$, $BaGd_2S_4$, $BaGd_2Se_4$, $BaGd_2Te_4$, $BaHo_2O_4$, $BaHo_2S_4$, $BaHo_2Te_4$, $BaLa_2O_4$, $BaLu_2O_4$, $BaLu_2S_4$, $BaLu_2Se_4$, $BaLu_2Te_4$, $BaNd_2O_4$, $BaNd_2S_4$, $BaPr_2O_4$, $BaSc_2Te_4$, $BaSm_2O_4$, $BaSm_2S_4$, $BaSm_2Se_4$, $BaSm_2Te_4$, $BaTb_2O_4$, $BaTb_2S_4$, $BaTb_2Te_4$, $BaTm_2O_4$, $BaTm_2S_4$, $BaTm_2Se_4$, $BaTm_2Te_4$, BaY_2O_4, BaY_2S_4, BaY_2Se_4, BaY_2Te_4, $BaYb_2O_4$, $BaYb_2S_4$, $BaYb_2Se_4$, $BiEu_2S_4$, $CaAl_2O_4$, $CaCo_2O_4$, $CaCr_2O_4$ (Ellinaite), $CaFe_2O_4$, $CaGa_2O_4$, $CaIn_2O_4$, $CaLu_2O_4$, $CaRh_2O_4$, $CaSc_2O_4$, $CaSc_2S_4$, CaV_2O_4, $CaYb_2O_4$, $CdRh_2O_4$, $EuBi_2S_4$, $EuBi_2Se_4$, $EuDy_2S_4$, $EuDy_2Se_4$, $EuEr_2S_4$, $EuEr_2Se_4$, $EuHo_2S_4$, $EuHo_2Se_4$, $EuLu_2O_4$, $EuLu_2Se_4$, $EuSb_2S_4$, $EuSb_2Se_4$, $EuSc_2Se_4$, $EuTb_2Se_4$, $EuTm_2Se_4$, EuY_2Se_4, $EuYb_2S_4$, $EuYb_2Se_4$, $FeCr_2O_4$, $FeNb_2S_4$, $FeSb_2S_4$, $LiMn_2O_4$, $LiRu_2O_4$, $LuPb_2S_4$, $MgAl_2O_4$, $MgSc_2O_4$, $MnCr_2S_4$, $MnSb_2S_4$, $NaCr_2O_4$, $NaMn_2O_4$, $NaRh_2O_4$, $NaRu_2O_4$, $NaTi_2O_4$, NaV_2O_4, $NiNb_2S_4$, $PbEr_2S_4$, $PbEr_2Se_4$, $PbHo_2S_4$, $PbIn_2S_4$, $PbLu_2S_4$, $PbLu_2Se_4$, $PbSc_2S_4$, $PbSc_2Se_4$, $PbTm_2S_4$, $PbTm_2Se_4$, $PbYb_2S_4$, $PbYb_2Se_4$, $SmTm_2O_4$, $SnCe_2Se_4$, $SrDy_2O_4$, $SrDy_2S_4$, $SrDy_2Se_4$, $SrEr_2O_4$, $SrEr_2S_4$, $SrEr_2Se_4$, $SrGd_2O_4$, $SrHo_2O_4$, $SrHo_2S_4$, $SrIn_2O_4$, $SrLu_2O_4$, $SrLu_2S_4$, $SrLu_2Se_4$, $SrSc_2O_4$, $SrSc_2S_4$, $SrTb_2O_4$, $SrTb_2S_4$, $SrTb_2Se_4$, $SrTl_2O_4$, $SrTm_2S_4$, SrY_2O_4, SrY_2S_4, SrY_2Se_4, $SrYb_2O_4$, $SrYb_2S_4$, $SrYb_2Se_4$, $YbBi_2S_4$, $YbSb_2S_4$, $YbSb_2Se_4$

- This is the ternary form of the binary Eu_3O_4 and the quaternary $FeSbBiS_4$ structures.
- (Olson, 2007) put this structure in the *Pnam* setting of space group #62. We used FINDSYM to transform this the standard *Pnma* setting. We used the data taken at 1 atmosphere (100 kPa).
- The ICSD uses $CaFe_2O_4$ as the prototype for this structure.

Simple Orthorhombic primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$x_1\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + z_1\,\mathbf{a}_3$	=	$ax_1\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} + cz_1\,\hat{\mathbf{z}}$	(4c)	Bi I
$\mathbf{B_2}$	=	$-\left(x_1 - \frac{1}{2}\right)\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 + \left(z_1 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_1 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} + c\left(z_1 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4c)	Bi I
$\mathbf{B_3}$	=	$-x_1\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 - z_1\,\mathbf{a}_3$	=	$-ax_1\,\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} - cz_1\,\hat{\mathbf{z}}$	(4c)	Bi I
$\mathbf{B_4}$	=	$\left(x_1 + \frac{1}{2}\right)\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 - \left(z_1 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(x_1 + \frac{1}{2}\right)\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} - c\left(z_1 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4c)	Bi I
$\mathbf{B_5}$	=	$x_2\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$ax_2\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(4c)	Bi II
$\mathbf{B_6}$	=	$-\left(x_2 - \frac{1}{2}\right)\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 + \left(z_2 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_2 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} + c\left(z_2 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4c)	Bi II
$\mathbf{B_7}$	=	$-x_2\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 - z_2\,\mathbf{a}_3$	=	$-ax_2\,\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} - cz_2\,\hat{\mathbf{z}}$	(4c)	Bi II
$\mathbf{B_8}$	=	$\left(x_2 + \frac{1}{2}\right)\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 - \left(z_2 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(x_2 + \frac{1}{2}\right)\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} - c\left(z_2 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4c)	Bi II
$\mathbf{B_9}$	=	$x_3\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(4c)	Pb I

$$\mathbf{B_{10}} = -\left(x_3 - \tfrac{1}{2}\right)\mathbf{a}_1 + \tfrac{3}{4}\mathbf{a}_2 + \left(z_3 + \tfrac{1}{2}\right)\mathbf{a}_3 = -a\left(x_3 - \tfrac{1}{2}\right)\hat{\mathbf{x}} + \tfrac{3}{4}b\hat{\mathbf{y}} + c\left(z_3 + \tfrac{1}{2}\right)\hat{\mathbf{z}} \quad (4c) \quad \text{Pb I}$$

$$\mathbf{B_{11}} = -x_3\mathbf{a}_1 + \tfrac{3}{4}\mathbf{a}_2 - z_3\mathbf{a}_3 = -ax_3\hat{\mathbf{x}} + \tfrac{3}{4}b\hat{\mathbf{y}} - cz_3\hat{\mathbf{z}} \quad (4c) \quad \text{Pb I}$$

$$\mathbf{B_{12}} = \left(x_3 + \tfrac{1}{2}\right)\mathbf{a}_1 + \tfrac{1}{4}\mathbf{a}_2 - \left(z_3 - \tfrac{1}{2}\right)\mathbf{a}_3 = a\left(x_3 + \tfrac{1}{2}\right)\hat{\mathbf{x}} + \tfrac{1}{4}b\hat{\mathbf{y}} - c\left(z_3 - \tfrac{1}{2}\right)\hat{\mathbf{z}} \quad (4c) \quad \text{Pb I}$$

$$\mathbf{B_{13}} = x_4\mathbf{a}_1 + \tfrac{1}{4}\mathbf{a}_2 + z_4\mathbf{a}_3 = ax_4\hat{\mathbf{x}} + \tfrac{1}{4}b\hat{\mathbf{y}} + cz_4\hat{\mathbf{z}} \quad (4c) \quad \text{S I}$$

$$\mathbf{B_{14}} = -\left(x_4 - \tfrac{1}{2}\right)\mathbf{a}_1 + \tfrac{3}{4}\mathbf{a}_2 + \left(z_4 + \tfrac{1}{2}\right)\mathbf{a}_3 = -a\left(x_4 - \tfrac{1}{2}\right)\hat{\mathbf{x}} + \tfrac{3}{4}b\hat{\mathbf{y}} + c\left(z_4 + \tfrac{1}{2}\right)\hat{\mathbf{z}} \quad (4c) \quad \text{S I}$$

$$\mathbf{B_{15}} = -x_4\mathbf{a}_1 + \tfrac{3}{4}\mathbf{a}_2 - z_4\mathbf{a}_3 = -ax_4\hat{\mathbf{x}} + \tfrac{3}{4}b\hat{\mathbf{y}} - cz_4\hat{\mathbf{z}} \quad (4c) \quad \text{S I}$$

$$\mathbf{B_{16}} = \left(x_4 + \tfrac{1}{2}\right)\mathbf{a}_1 + \tfrac{1}{4}\mathbf{a}_2 - \left(z_4 - \tfrac{1}{2}\right)\mathbf{a}_3 = a\left(x_4 + \tfrac{1}{2}\right)\hat{\mathbf{x}} + \tfrac{1}{4}b\hat{\mathbf{y}} - c\left(z_4 - \tfrac{1}{2}\right)\hat{\mathbf{z}} \quad (4c) \quad \text{S I}$$

$$\mathbf{B_{17}} = x_5\mathbf{a}_1 + \tfrac{1}{4}\mathbf{a}_2 + z_5\mathbf{a}_3 = ax_5\hat{\mathbf{x}} + \tfrac{1}{4}b\hat{\mathbf{y}} + cz_5\hat{\mathbf{z}} \quad (4c) \quad \text{S II}$$

$$\mathbf{B_{18}} = -\left(x_5 - \tfrac{1}{2}\right)\mathbf{a}_1 + \tfrac{3}{4}\mathbf{a}_2 + \left(z_5 + \tfrac{1}{2}\right)\mathbf{a}_3 = -a\left(x_5 - \tfrac{1}{2}\right)\hat{\mathbf{x}} + \tfrac{3}{4}b\hat{\mathbf{y}} + c\left(z_5 + \tfrac{1}{2}\right)\hat{\mathbf{z}} \quad (4c) \quad \text{S II}$$

$$\mathbf{B_{19}} = -x_5\mathbf{a}_1 + \tfrac{3}{4}\mathbf{a}_2 - z_5\mathbf{a}_3 = -ax_5\hat{\mathbf{x}} + \tfrac{3}{4}b\hat{\mathbf{y}} - cz_5\hat{\mathbf{z}} \quad (4c) \quad \text{S II}$$

$$\mathbf{B_{20}} = \left(x_5 + \tfrac{1}{2}\right)\mathbf{a}_1 + \tfrac{1}{4}\mathbf{a}_2 - \left(z_5 - \tfrac{1}{2}\right)\mathbf{a}_3 = a\left(x_5 + \tfrac{1}{2}\right)\hat{\mathbf{x}} + \tfrac{1}{4}b\hat{\mathbf{y}} - c\left(z_5 - \tfrac{1}{2}\right)\hat{\mathbf{z}} \quad (4c) \quad \text{S II}$$

$$\mathbf{B_{21}} = x_6\mathbf{a}_1 + \tfrac{1}{4}\mathbf{a}_2 + z_6\mathbf{a}_3 = ax_6\hat{\mathbf{x}} + \tfrac{1}{4}b\hat{\mathbf{y}} + cz_6\hat{\mathbf{z}} \quad (4c) \quad \text{S III}$$

$$\mathbf{B_{22}} = -\left(x_6 - \tfrac{1}{2}\right)\mathbf{a}_1 + \tfrac{3}{4}\mathbf{a}_2 + \left(z_6 + \tfrac{1}{2}\right)\mathbf{a}_3 = -a\left(x_6 - \tfrac{1}{2}\right)\hat{\mathbf{x}} + \tfrac{3}{4}b\hat{\mathbf{y}} + c\left(z_6 + \tfrac{1}{2}\right)\hat{\mathbf{z}} \quad (4c) \quad \text{S III}$$

$$\mathbf{B_{23}} = -x_6\mathbf{a}_1 + \tfrac{3}{4}\mathbf{a}_2 - z_6\mathbf{a}_3 = -ax_6\hat{\mathbf{x}} + \tfrac{3}{4}b\hat{\mathbf{y}} - cz_6\hat{\mathbf{z}} \quad (4c) \quad \text{S III}$$

$$\mathbf{B_{24}} = \left(x_6 + \tfrac{1}{2}\right)\mathbf{a}_1 + \tfrac{1}{4}\mathbf{a}_2 - \left(z_6 - \tfrac{1}{2}\right)\mathbf{a}_3 = a\left(x_6 + \tfrac{1}{2}\right)\hat{\mathbf{x}} + \tfrac{1}{4}b\hat{\mathbf{y}} - c\left(z_6 - \tfrac{1}{2}\right)\hat{\mathbf{z}} \quad (4c) \quad \text{S III}$$

$$\mathbf{B_{25}} = x_7\mathbf{a}_1 + \tfrac{1}{4}\mathbf{a}_2 + z_7\mathbf{a}_3 = ax_7\hat{\mathbf{x}} + \tfrac{1}{4}b\hat{\mathbf{y}} + cz_7\hat{\mathbf{z}} \quad (4c) \quad \text{S IV}$$

$$\mathbf{B_{26}} = -\left(x_7 - \tfrac{1}{2}\right)\mathbf{a}_1 + \tfrac{3}{4}\mathbf{a}_2 + \left(z_7 + \tfrac{1}{2}\right)\mathbf{a}_3 = -a\left(x_7 - \tfrac{1}{2}\right)\hat{\mathbf{x}} + \tfrac{3}{4}b\hat{\mathbf{y}} + c\left(z_7 + \tfrac{1}{2}\right)\hat{\mathbf{z}} \quad (4c) \quad \text{S IV}$$

$$\mathbf{B_{27}} = -x_7\mathbf{a}_1 + \tfrac{3}{4}\mathbf{a}_2 - z_7\mathbf{a}_3 = -ax_7\hat{\mathbf{x}} + \tfrac{3}{4}b\hat{\mathbf{y}} - cz_7\hat{\mathbf{z}} \quad (4c) \quad \text{S IV}$$

$$\mathbf{B_{28}} = \left(x_7 + \tfrac{1}{2}\right)\mathbf{a}_1 + \tfrac{1}{4}\mathbf{a}_2 - \left(z_7 - \tfrac{1}{2}\right)\mathbf{a}_3 = a\left(x_7 + \tfrac{1}{2}\right)\hat{\mathbf{x}} + \tfrac{1}{4}b\hat{\mathbf{y}} - c\left(z_7 - \tfrac{1}{2}\right)\hat{\mathbf{z}} \quad (4c) \quad \text{S IV}$$

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First cited in

H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettel, M. Esters, X. Campilongo, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*, Comput. Mater. Sci. **240**, 112988 (2024), doi: 10.1016/j.commatsci.2024.112988.