Eulytine ($Bi_4(SiO_4)_3$, $S1_5$) Structure: A4B12C3_cI76_220_c_e_a-001

This structure previously used the label(s) `A4B12C3_cI76_220_c_e_a`. Calls to these addresses will be redirected here.

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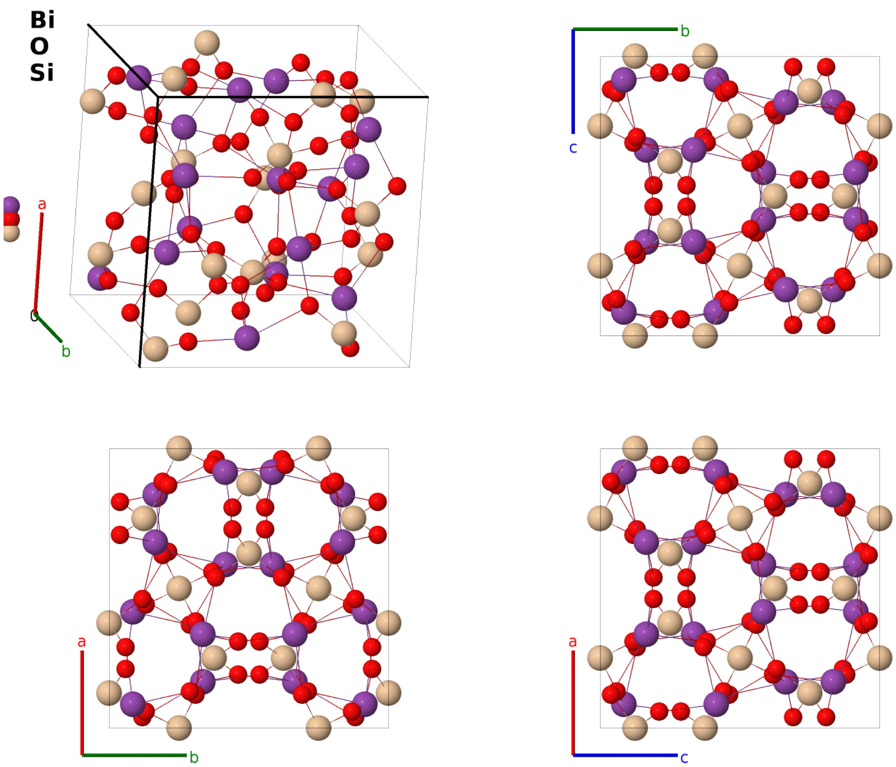
https://aflow.org/prototype-encyclopedia/VQL6

https://aflow.org/prototype-encyclopedia/A4B12C3_cI76_220_c_e_a-001



Prototype	$Bi_4O_{12}Si_3$
AFLOW prototype label	A4B12C3_cI76_220_c_e_a-001
***Strukturbericht* designation**	$S1_5$
Mineral name	eulytine
ICSD	402349
CCDC	1724849
Pearson symbol	cI76
Space group number	220
Space group symbol	$I\bar{4}3d$

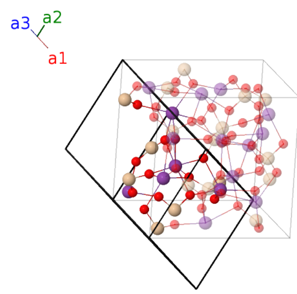
AFLOW prototype command `aflow --proto=A4B12C3_cI76_220_c_e_a-001`
`--params=`a, x_2, x_3, y_3, z_3

Other compounds with this structure

$Ba_3Bi(PO_4)_3$, $Ba_3Gd(PO_4)_3$, $Ba_3In(PO_4)_3$, $Ba_3La(PO_4)_3$, $Ba_3Lu(PO_4)_3$, $Ba_3Nd(PO_4)_3$, $Ba_3Y(PO_4)_3$, $Sr_3Bi(PO_4)_3$, $Sr_3Gd(PO_4)_3$, $Sr_3In(PO_4)_3$, $Sr_3La(PO_4)_3$, $Sr_3Lu(PO_4)_3$, $Sr_3Nd(PO_4)_3$, $Sr_3Y(PO_4)_3$, $Bi_4(GeO_4)_3$, $Ca_3Bi(PO_4)_3$

Body-centered Cubic primitive vectors

$$\mathbf{a_1} = -\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{2}a\,\hat{\mathbf{z}}$$
$$\mathbf{a_2} = \frac{1}{2}a\,\hat{\mathbf{x}} - \frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{2}a\,\hat{\mathbf{z}}$$
$$\mathbf{a_3} = \frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}} - \frac{1}{2}a\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \frac{5}{8}\,\mathbf{a}_2 + \frac{3}{8}\,\mathbf{a}_3$	=	$\frac{3}{8}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{z}}$	(12a)	Si I
$\mathbf{B_2}$	=	$\frac{3}{4}\,\mathbf{a}_1 + \frac{7}{8}\,\mathbf{a}_2 + \frac{1}{8}\,\mathbf{a}_3$	=	$\frac{1}{8}a\,\hat{\mathbf{x}} + \frac{3}{4}a\,\hat{\mathbf{z}}$	(12a)	Si I
$\mathbf{B_3}$	=	$\frac{3}{8}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + \frac{5}{8}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{3}{8}a\,\hat{\mathbf{y}}$	(12a)	Si I
$\mathbf{B_4}$	=	$\frac{1}{8}\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 + \frac{7}{8}\,\mathbf{a}_3$	=	$\frac{3}{4}a\,\hat{\mathbf{x}} + \frac{1}{8}a\,\hat{\mathbf{y}}$	(12a)	Si I
$\mathbf{B_5}$	=	$\frac{5}{8}\,\mathbf{a}_1 + \frac{3}{8}\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{y}} + \frac{3}{8}a\,\hat{\mathbf{z}}$	(12a)	Si I
$\mathbf{B_6}$	=	$\frac{7}{8}\,\mathbf{a}_1 + \frac{1}{8}\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{3}{4}a\,\hat{\mathbf{y}} + \frac{1}{8}a\,\hat{\mathbf{z}}$	(12a)	Si I
$\mathbf{B_7}$	=	$2x_2\,\mathbf{a}_1 + 2x_2\,\mathbf{a}_2 + 2x_2\,\mathbf{a}_3$	=	$ax_2\,\hat{\mathbf{x}} + ax_2\,\hat{\mathbf{y}} + ax_2\,\hat{\mathbf{z}}$	(16c)	Bi I
$\mathbf{B_8}$	=	$\frac{1}{2}\,\mathbf{a}_1 - \left(2x_2 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_2\,\hat{\mathbf{x}} - a\left(x_2 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + ax_2\,\hat{\mathbf{z}}$	(16c)	Bi I
$\mathbf{B_9}$	=	$-\left(2x_2 - \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-a\left(x_2 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + ax_2\,\hat{\mathbf{y}} - ax_2\,\hat{\mathbf{z}}$	(16c)	Bi I
$\mathbf{B_{10}}$	=	$-\left(2x_2 - \frac{1}{2}\right)\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2$	=	$ax_2\,\hat{\mathbf{x}} - ax_2\,\hat{\mathbf{y}} - a\left(x_2 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(16c)	Bi I
$\mathbf{B_{11}}$	=	$\left(2x_2 + \frac{1}{2}\right)\,\mathbf{a}_1 + \left(2x_2 + \frac{1}{2}\right)\,\mathbf{a}_2 + \left(2x_2 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(x_2 + \frac{1}{4}\right)\,\hat{\mathbf{x}} + a\left(x_2 + \frac{1}{4}\right)\,\hat{\mathbf{y}} + a\left(x_2 + \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(16c)	Bi I
$\mathbf{B_{12}}$	=	$\frac{1}{2}\,\mathbf{a}_1 - 2x_2\,\mathbf{a}_3$	=	$-a\left(x_2 + \frac{1}{4}\right)\,\hat{\mathbf{x}} - a\left(x_2 - \frac{1}{4}\right)\,\hat{\mathbf{y}} + a\left(x_2 + \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(16c)	Bi I
$\mathbf{B_{13}}$	=	$-2x_2\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2$	=	$a\left(x_2 + \frac{1}{4}\right)\,\hat{\mathbf{x}} - a\left(x_2 + \frac{1}{4}\right)\,\hat{\mathbf{y}} - a\left(x_2 - \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(16c)	Bi I
$\mathbf{B_{14}}$	=	$-2x_2\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-a\left(x_2 - \frac{1}{4}\right)\,\hat{\mathbf{x}} + a\left(x_2 + \frac{1}{4}\right)\,\hat{\mathbf{y}} - a\left(x_2 + \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(16c)	Bi I
$\mathbf{B_{15}}$	=	$(y_3 + z_3)\,\mathbf{a}_1 + (x_3 + z_3)\,\mathbf{a}_2 + (x_3 + y_3)\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} + ay_3\,\hat{\mathbf{y}} + az_3\,\hat{\mathbf{z}}$	(48e)	O I
$\mathbf{B_{16}}$	=	$\left(-y_3 + z_3 + \frac{1}{2}\right)\,\mathbf{a}_1 - (x_3 - z_3)\,\mathbf{a}_2 - \left(x_3 + y_3 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} - a\left(y_3 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + az_3\,\hat{\mathbf{z}}$	(48e)	O I
$\mathbf{B_{17}}$	=	$(y_3 - z_3)\,\mathbf{a}_1 - \left(x_3 + z_3 - \frac{1}{2}\right)\,\mathbf{a}_2 + \left(-x_3 + y_3 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_3 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + ay_3\,\hat{\mathbf{y}} - az_3\,\hat{\mathbf{z}}$	(48e)	O I
$\mathbf{B_{18}}$	=	$-\left(y_3 + z_3 - \frac{1}{2}\right)\,\mathbf{a}_1 + \left(x_3 - z_3 + \frac{1}{2}\right)\,\mathbf{a}_2 + (x_3 - y_3)\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} - ay_3\,\hat{\mathbf{y}} - a\left(z_3 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(48e)	O I

$\mathbf{B_{19}}$	$=$	$\left(x_3+y_3\right)\,\mathbf{a}_1+\left(y_3+z_3\right)\,\mathbf{a}_2+\left(x_3+z_3\right)\,\mathbf{a}_3$	$=$	$az_3\,\hat{\mathbf{x}}+ax_3\,\hat{\mathbf{y}}+ay_3\,\hat{\mathbf{z}}$	(48e)	O I
$\mathbf{B_{20}}$	$=$	$-\left(x_3+y_3-\frac{1}{2}\right)\,\mathbf{a}_1+\left(-y_3+z_3+\frac{1}{2}\right)\,\mathbf{a}_2-\left(x_3-z_3\right)\,\mathbf{a}_3$	$=$	$az_3\,\hat{\mathbf{x}}-ax_3\,\hat{\mathbf{y}}-a\left(y_3-\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(48e)	O I
$\mathbf{B_{21}}$	$=$	$\left(-x_3+y_3+\frac{1}{2}\right)\,\mathbf{a}_1+\left(y_3-z_3\right)\,\mathbf{a}_2-\left(x_3+z_3-\frac{1}{2}\right)\,\mathbf{a}_3$	$=$	$-az_3\,\hat{\mathbf{x}}-a\left(x_3-\frac{1}{2}\right)\,\hat{\mathbf{y}}+ay_3\,\hat{\mathbf{z}}$	(48e)	O I
$\mathbf{B_{22}}$	$=$	$\left(x_3-y_3\right)\,\mathbf{a}_1-\left(y_3+z_3-\frac{1}{2}\right)\,\mathbf{a}_2+\left(x_3-z_3+\frac{1}{2}\right)\,\mathbf{a}_3$	$=$	$-a\left(z_3-\frac{1}{2}\right)\,\hat{\mathbf{x}}+ax_3\,\hat{\mathbf{y}}-ay_3\,\hat{\mathbf{z}}$	(48e)	O I
$\mathbf{B_{23}}$	$=$	$\left(x_3+z_3\right)\,\mathbf{a}_1+\left(x_3+y_3\right)\,\mathbf{a}_2+\left(y_3+z_3\right)\,\mathbf{a}_3$	$=$	$ay_3\,\hat{\mathbf{x}}+az_3\,\hat{\mathbf{y}}+ax_3\,\hat{\mathbf{z}}$	(48e)	O I
$\mathbf{B_{24}}$	$=$	$-\left(x_3-z_3\right)\,\mathbf{a}_1-\left(x_3+y_3-\frac{1}{2}\right)\,\mathbf{a}_2+\left(-y_3+z_3+\frac{1}{2}\right)\,\mathbf{a}_3$	$=$	$-a\left(y_3-\frac{1}{2}\right)\,\hat{\mathbf{x}}+az_3\,\hat{\mathbf{y}}-ax_3\,\hat{\mathbf{z}}$	(48e)	O I
$\mathbf{B_{25}}$	$=$	$-\left(x_3+z_3-\frac{1}{2}\right)\,\mathbf{a}_1+\left(-x_3+y_3+\frac{1}{2}\right)\,\mathbf{a}_2+\left(y_3-z_3\right)\,\mathbf{a}_3$	$=$	$ay_3\,\hat{\mathbf{x}}-az_3\,\hat{\mathbf{y}}-a\left(x_3-\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(48e)	O I
$\mathbf{B_{26}}$	$=$	$\left(x_3-z_3+\frac{1}{2}\right)\,\mathbf{a}_1+\left(x_3-y_3\right)\,\mathbf{a}_2-\left(y_3+z_3-\frac{1}{2}\right)\,\mathbf{a}_3$	$=$	$-ay_3\,\hat{\mathbf{x}}-a\left(z_3-\frac{1}{2}\right)\,\hat{\mathbf{y}}+ax_3\,\hat{\mathbf{z}}$	(48e)	O I
$\mathbf{B_{27}}$	$=$	$\left(x_3+z_3+\frac{1}{2}\right)\,\mathbf{a}_1+\left(y_3+z_3+\frac{1}{2}\right)\,\mathbf{a}_2+\left(x_3+y_3+\frac{1}{2}\right)\,\mathbf{a}_3$	$=$	$a\left(y_3+\frac{1}{4}\right)\,\hat{\mathbf{x}}+a\left(x_3+\frac{1}{4}\right)\,\hat{\mathbf{y}}+a\left(z_3+\frac{1}{4}\right)\,\hat{\mathbf{z}}$	(48e)	O I
$\mathbf{B_{28}}$	$=$	$\left(-x_3+z_3+\frac{1}{2}\right)\,\mathbf{a}_1-\left(y_3-z_3\right)\,\mathbf{a}_2-\left(x_3+y_3\right)\,\mathbf{a}_3$	$=$	$-a\left(y_3+\frac{1}{4}\right)\,\hat{\mathbf{x}}-a\left(x_3-\frac{1}{4}\right)\,\hat{\mathbf{y}}+a\left(z_3+\frac{1}{4}\right)\,\hat{\mathbf{z}}$	(48e)	O I
$\mathbf{B_{29}}$	$=$	$-\left(x_3+z_3\right)\,\mathbf{a}_1+\left(y_3-z_3+\frac{1}{2}\right)\,\mathbf{a}_2-\left(x_3-y_3\right)\,\mathbf{a}_3$	$=$	$a\left(y_3+\frac{1}{4}\right)\,\hat{\mathbf{x}}-a\left(x_3+\frac{1}{4}\right)\,\hat{\mathbf{y}}-a\left(z_3-\frac{1}{4}\right)\,\hat{\mathbf{z}}$	(48e)	O I
$\mathbf{B_{30}}$	$=$	$\left(x_3-z_3\right)\,\mathbf{a}_1-\left(y_3+z_3\right)\,\mathbf{a}_2+\left(x_3-y_3+\frac{1}{2}\right)\,\mathbf{a}_3$	$=$	$-a\left(y_3-\frac{1}{4}\right)\,\hat{\mathbf{x}}+a\left(x_3+\frac{1}{4}\right)\,\hat{\mathbf{y}}-a\left(z_3+\frac{1}{4}\right)\,\hat{\mathbf{z}}$	(48e)	O I
$\mathbf{B_{31}}$	$=$	$\left(y_3+z_3+\frac{1}{2}\right)\,\mathbf{a}_1+\left(x_3+y_3+\frac{1}{2}\right)\,\mathbf{a}_2+\left(x_3+z_3+\frac{1}{2}\right)\,\mathbf{a}_3$	$=$	$a\left(x_3+\frac{1}{4}\right)\,\hat{\mathbf{x}}+a\left(z_3+\frac{1}{4}\right)\,\hat{\mathbf{y}}+a\left(y_3+\frac{1}{4}\right)\,\hat{\mathbf{z}}$	(48e)	O I
$\mathbf{B_{32}}$	$=$	$-\left(y_3-z_3\right)\,\mathbf{a}_1-\left(x_3+y_3\right)\,\mathbf{a}_2+\left(-x_3+z_3+\frac{1}{2}\right)\,\mathbf{a}_3$	$=$	$-a\left(x_3-\frac{1}{4}\right)\,\hat{\mathbf{x}}+a\left(z_3+\frac{1}{4}\right)\,\hat{\mathbf{y}}-a\left(y_3+\frac{1}{4}\right)\,\hat{\mathbf{z}}$	(48e)	O I
$\mathbf{B_{33}}$	$=$	$\left(y_3-z_3+\frac{1}{2}\right)\,\mathbf{a}_1-\left(x_3-y_3\right)\,\mathbf{a}_2-\left(x_3+z_3\right)\,\mathbf{a}_3$	$=$	$-a\left(x_3+\frac{1}{4}\right)\,\hat{\mathbf{x}}-a\left(z_3-\frac{1}{4}\right)\,\hat{\mathbf{y}}+a\left(y_3+\frac{1}{4}\right)\,\hat{\mathbf{z}}$	(48e)	O I
$\mathbf{B_{34}}$	$=$	$-\left(y_3+z_3\right)\,\mathbf{a}_1+\left(x_3-y_3+\frac{1}{2}\right)\,\mathbf{a}_2+\left(x_3-z_3\right)\,\mathbf{a}_3$	$=$	$a\left(x_3+\frac{1}{4}\right)\,\hat{\mathbf{x}}-a\left(z_3+\frac{1}{4}\right)\,\hat{\mathbf{y}}-a\left(y_3-\frac{1}{4}\right)\,\hat{\mathbf{z}}$	(48e)	O I
$\mathbf{B_{35}}$	$=$	$\left(x_3+y_3+\frac{1}{2}\right)\,\mathbf{a}_1+\left(x_3+z_3+\frac{1}{2}\right)\,\mathbf{a}_2+\left(y_3+z_3+\frac{1}{2}\right)\,\mathbf{a}_3$	$=$	$a\left(z_3+\frac{1}{4}\right)\,\hat{\mathbf{x}}+a\left(y_3+\frac{1}{4}\right)\,\hat{\mathbf{y}}+a\left(x_3+\frac{1}{4}\right)\,\hat{\mathbf{z}}$	(48e)	O I
$\mathbf{B_{36}}$	$=$	$-\left(x_3+y_3\right)\,\mathbf{a}_1+\left(-x_3+z_3+\frac{1}{2}\right)\,\mathbf{a}_2-\left(y_3-z_3\right)\,\mathbf{a}_3$	$=$	$a\left(z_3+\frac{1}{4}\right)\,\hat{\mathbf{x}}-a\left(y_3+\frac{1}{4}\right)\,\hat{\mathbf{y}}-a\left(x_3-\frac{1}{4}\right)\,\hat{\mathbf{z}}$	(48e)	O I
$\mathbf{B_{37}}$	$=$	$-\left(x_3-y_3\right)\,\mathbf{a}_1-\left(x_3+z_3\right)\,\mathbf{a}_2+\left(y_3-z_3+\frac{1}{2}\right)\,\mathbf{a}_3$	$=$	$-a\left(z_3-\frac{1}{4}\right)\,\hat{\mathbf{x}}+a\left(y_3+\frac{1}{4}\right)\,\hat{\mathbf{y}}-a\left(x_3+\frac{1}{4}\right)\,\hat{\mathbf{z}}$	(48e)	O I
$\mathbf{B_{38}}$	$=$	$\left(x_3-y_3+\frac{1}{2}\right)\,\mathbf{a}_1+\left(x_3-z_3\right)\,\mathbf{a}_2-\left(y_3+z_3\right)\,\mathbf{a}_3$	$=$	$-a\left(z_3+\frac{1}{4}\right)\,\hat{\mathbf{x}}-a\left(y_3-\frac{1}{4}\right)\,\hat{\mathbf{y}}+a\left(x_3+\frac{1}{4}\right)\,\hat{\mathbf{z}}$	(48e)	O I

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[1] H. Liu and C. Kuo, *Crystal structure of bismuth(III) silicate, $Bi_4SiO_4)_3$*, Z. Kristallogr. **212**, 48 (1997), doi:10.1524/zkri.1997.212.1.48.

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

D. Hicks, M. J. Mehl, M. Esters, C. Oses, O. Levy, G. L. W. Hart, C. Toher, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 3*, Comput. Mater. Sci. **199**, 110450 (2021), doi: 10.1016/j.commatsci.2021.110450.