BiTeI Structure: ABC_hP3_156_a_b_c-001

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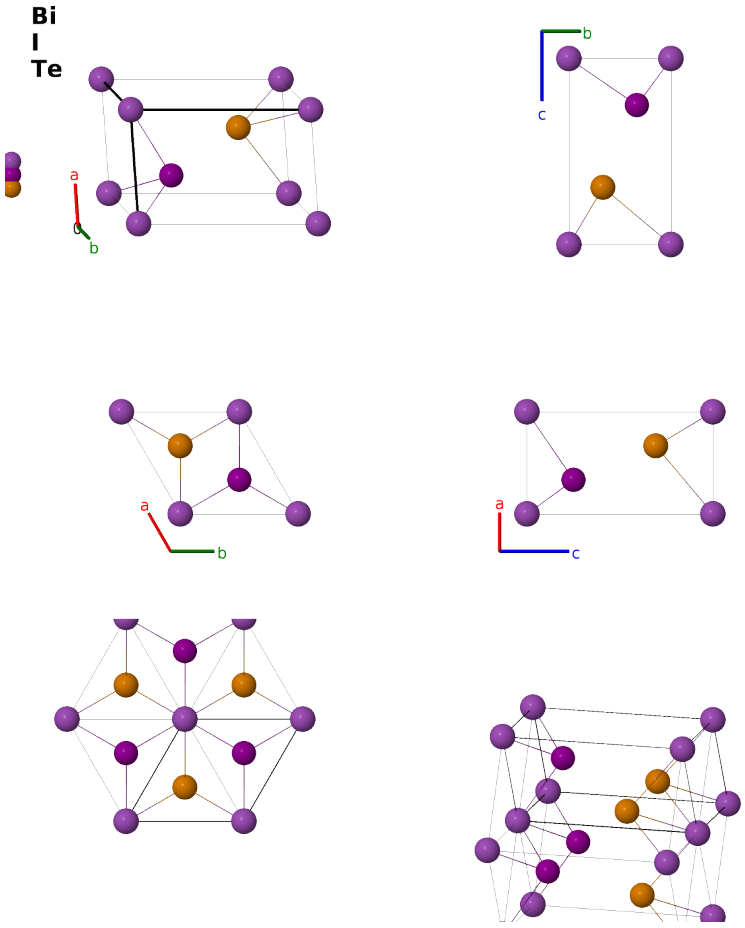
https://aflow.org/prototype-encyclopedia/Z4FL

https://aflow.org/prototype-encyclopedia/ABC_hP3_156_a_b_c-001



Prototype	BiITe
AFLOW prototype label	ABC_hP3_156_a_b_c-001
ICSD	79364
CCDC	1639613
Pearson symbol	hP3
Space group number	156
Space group symbol	$P3m1$

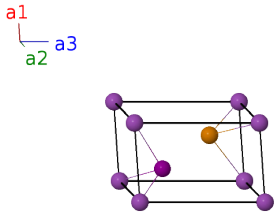
AFLOW prototype command `aflow --proto=ABC_hP3_156_a_b_c-001 --params=`$a, c/a, z_1, z_2, z_3$

Other compounds with this structure
BiBrTe, OSTi

- Space group $P3m1$ #156 allows an arbitary placement of the origin of the z-axis. We follow (Shevelkov, 1995) and set $z_1 = 0$ for the bismuth atom.

Trigonal (Hexagonal) primitive vectors

$$\mathbf{a_1} = \frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,\hat{\mathbf{y}}$$
$$\mathbf{a_2} = \frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$z_1\,\mathbf{a}_3$	=	$cz_1\,\hat{\mathbf{z}}$	(1a)	Bi I
$\mathbf{B_2}$	=	$\frac{1}{3}\,\mathbf{a}_1 + \frac{2}{3}\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(1b)	I I
$\mathbf{B_3}$	=	$\frac{2}{3}\,\mathbf{a}_1 + \frac{1}{3}\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(1c)	Te I

References

[1] A. V. Shevelkov, E. V. Dikarev, R. V. Shpanchenko, and B. A. Popovkin, *Crystal Structures of Bismuth Tellurohalides BiTeX (X = Cl, Br, I) from X-Ray Powder Diffraction Data*, J. Solid State Chem. **114**, 379–384 (1995), doi:10.1006/jssc.1995.1058.

Found in

[1] S. Güler-Kılıç and Ç. Kılıç, *Crystal and electronic structure of BiTeI, AuTeI, and PdTeI compounds: A dispersion-corrected density-functional study*, Phys. Rev. B **91**, 24524 (2015), doi:10.1103/PhysRevB.91.245204.

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