Bi_2Te_3 ($C33$) Structure: A2B3_hR5_166_c_ac-001

This structure previously used the label(s) `A2B3_hR5_166_c_ac`. Calls to these addresses will be redirected here.

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https://aflow.org/prototype-encyclopedia/NGV5

https://aflow.org/prototype-encyclopedia/A2B3_hR5_166_c_ac-001

Prototype	Bi_2Te_3
AFLOW prototype label	A2B3_hR5_166_c_ac-001
***Strukturbericht* designation**	$C33$
ICSD	15753
CCDC	1596451
Pearson symbol	hR5
Space group number	166
Space group symbol	$R\bar{3}m$
AFLOW prototype command	`aflow --proto=A2B3_hR5_166_c_ac-001 --params=`$a, c/a, x_2, x_3$

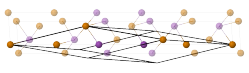
Other compounds with this structure

β-As_2Te_3, Bi_2Se_3, Ga_2Te_5, In_2Se_3, In_2Te_3, Sb_2Te_3, (Bi, Sm)Te_3, (Bi, Tb)Te_3, (Bi, Tm)Te_3, (Bi, Y)Te_3, (Dy, Sb)Te_3

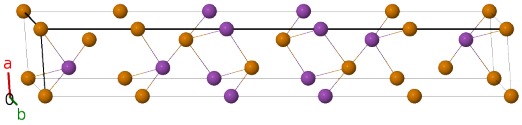
- (Gottfried, 1937) assigns tetradymite, Bi_2Te_2S as the prototype for *Strukturbericht* symbol $C33$, but (Lange, 1939) shows that this is isostructural with Bi_2Te_3, the sulfur atom being replaced by a tellurium atom. We will therefore retain our original designation.
- Hexagonal settings for rhombohedral structures can be obtained with the option `--hex`.

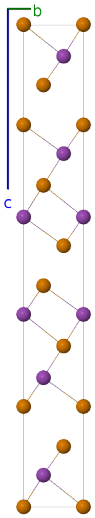
Rhombohedral primitive vectors

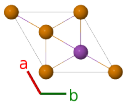
$$\mathbf{a_1} = \frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{1}{3}c\,\hat{\mathbf{z}}$$
$$\mathbf{a_2} = \frac{1}{\sqrt{3}}a\,\hat{\mathbf{y}} + \frac{1}{3}c\,\hat{\mathbf{z}}$$
$$\mathbf{a_3} = -\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{1}{3}c\,\hat{\mathbf{z}}$$

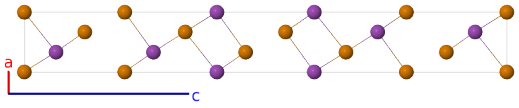


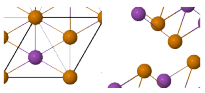
Bi
Te











Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(1a)	Te I
$\mathbf{B_2}$	=	$x_2\,\mathbf{a}_1 + x_2\,\mathbf{a}_2 + x_2\,\mathbf{a}_3$	=	$cx_2\,\hat{\mathbf{z}}$	(2c)	Bi I
$\mathbf{B_3}$	=	$-x_2\,\mathbf{a}_1 - x_2\,\mathbf{a}_2 - x_2\,\mathbf{a}_3$	=	$-cx_2\,\hat{\mathbf{z}}$	(2c)	Bi I
$\mathbf{B_4}$	=	$x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + x_3\,\mathbf{a}_3$	=	$cx_3\,\hat{\mathbf{z}}$	(2c)	Te II
$\mathbf{B_5}$	=	$-x_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 - x_3\,\mathbf{a}_3$	=	$-cx_3\,\hat{\mathbf{z}}$	(2c)	Te II

References

[1] P. W. Lange, *Ein Vergleich zwischen Bi_2Te_3 und Bi_2Te_2S*, Naturwissenschaften **27**, 133–134 (1939), doi:10.1007/BF01490284.

[2] C. Gottfried and F. Schossberger, eds., *Strukturbericht Band III 1933-1935* (Akademische Verlagsgesellschaft M. B. H., Leipzig, 1937).

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