Tetradymite (Bi_2Te_2S, $C33$) Structure: A2BC2_hR5_166_c_a_c-002

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

https://aflow.org/prototype-encyclopedia/A2BC2_hR5_166_c_a_c-002

Prototype	Bi_2STe_2
AFLOW prototype label	A2BC2_hR5_166_c_a_c-002
Mineral name	tetradymite
ICSD	26720
CCDC	1602106
Pearson symbol	hR5
Space group number	166
Space group symbol	$R\bar{3}m$
AFLOW prototype command	`aflow --proto=A2BC2_hR5_166_c_a_c-002 --params=`$a, c/a, x_2, x_3$

Other compounds with this structure

Ag_2O_2Ni, As_2Sn_2Eu, Bi_2Te_2Se, Gd_2I_2Ge, La_2I_2Ge, La_2I_2Te, Sb_2Se_2Te, Sn_2As_2Na

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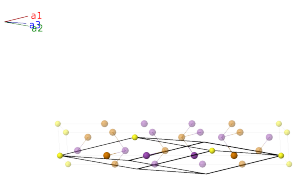
- This is the ternary form of Bi_2Te_3, *Strukturbericht* symbol $C33$. It was the original $C33$ structure assigned by (Gottfried, 1937), but we decided to use the binary form as the designated structure.
- Hexagonal settings for rhombohedral structures can be obtained with the option `--hex`.

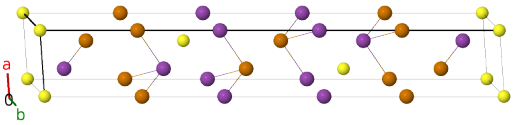
Rhombohedral primitive vectors

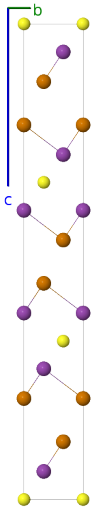
$$\mathbf{a_1} = \frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{1}{3}c\,\hat{\mathbf{z}}$$
$$\mathbf{a_2} = \frac{1}{\sqrt{3}}a\,\hat{\mathbf{y}} + \frac{1}{3}c\,\hat{\mathbf{z}}$$
$$\mathbf{a_3} = -\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}}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

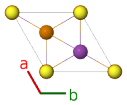


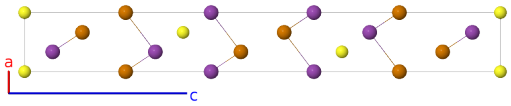
Basis vectors

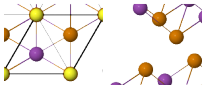
Bi
S
Te











		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(1a)	S 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 I
$\mathbf{B_5}$	=	$-x_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 - x_3\,\mathbf{a}_3$	=	$-cx_3\,\hat{\mathbf{z}}$	(2c)	Te I

References

[1] D. Harker, *The Crystal Structure of the Mineral Tetradymite, Bi_2Te_2S* **89**, 175–181 (1934), doi:10.1524/zkri.1934.89.1.175.

Found in

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

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