Ga_2Te_5 Structure: A2B5_tI14_87_d_ah-001

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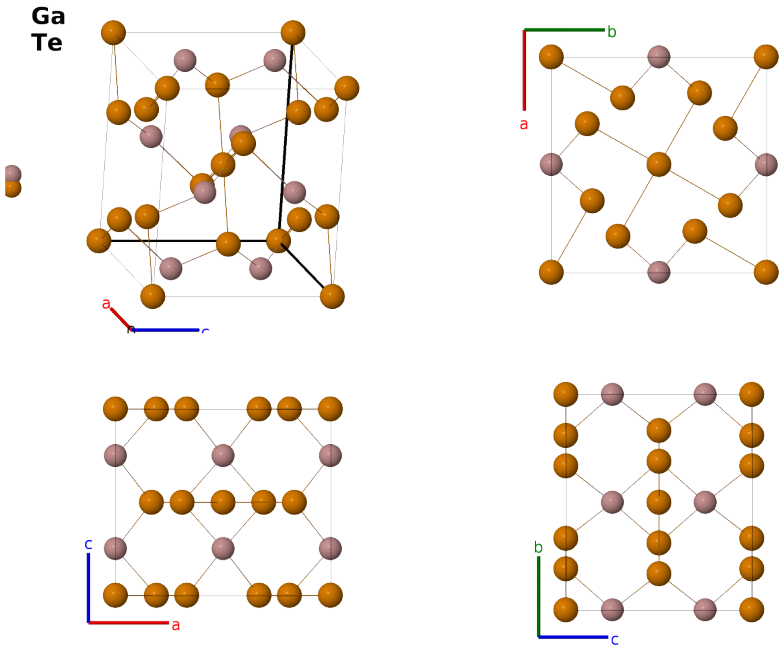
https://aflow.org/prototype-encyclopedia/4RP0

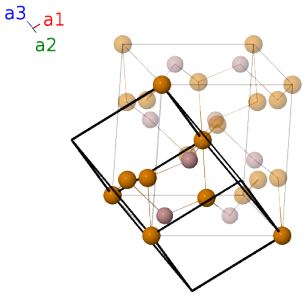
https://aflow.org/prototype-encyclopedia/A2B5_tI14_87_d_ah-001



Prototype	Ga_2Te_5
AFLOW prototype label	A2B5_tI14_87_d_ah-001
ICSD	1085
CCDC	1591275
Pearson symbol	tI14
Space group number	87
Space group symbol	$I4/m$
AFLOW prototype command	`aflow --proto=A2B5_tI14_87_d_ah-001 --params=`$a, c/a, x_3, y_3$

Body-centered Tetragonal primitive vectors

$$
\begin{aligned}
\mathbf{a_1} &= -\tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}a\,\hat{\mathbf{y}} + \tfrac{1}{2}c\,\hat{\mathbf{z}} \\
\mathbf{a_2} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{1}{2}a\,\hat{\mathbf{y}} + \tfrac{1}{2}c\,\hat{\mathbf{z}} \\
\mathbf{a_3} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}a\,\hat{\mathbf{y}} - \tfrac{1}{2}c\,\hat{\mathbf{z}}
\end{aligned}
$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(2a)	Te I
$\mathbf{B_2}$	=	$\frac{3}{4}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(4d)	Ga I
$\mathbf{B_3}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(4d)	Ga I
$\mathbf{B_4}$	=	$y_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + (x_3 + y_3)\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} + ay_3\,\hat{\mathbf{y}}$	(8h)	Te II
$\mathbf{B_5}$	=	$-y_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 - (x_3 + y_3)\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} - ay_3\,\hat{\mathbf{y}}$	(8h)	Te II
$\mathbf{B_6}$	=	$x_3\,\mathbf{a}_1 - y_3\,\mathbf{a}_2 + (x_3 - y_3)\,\mathbf{a}_3$	=	$-ay_3\,\hat{\mathbf{x}} + ax_3\,\hat{\mathbf{y}}$	(8h)	Te II
$\mathbf{B_7}$	=	$-x_3\,\mathbf{a}_1 + y_3\,\mathbf{a}_2 - (x_3 - y_3)\,\mathbf{a}_3$	=	$ay_3\,\hat{\mathbf{x}} - ax_3\,\hat{\mathbf{y}}$	(8h)	Te II

References

[1] M. Julien-Pouzol, S. Jaulmes, and F. Alapini, *Tellurure de gallium*, Acta Crystallogr. Sect. B **33**, 2270–2272 (1977), doi:10.1107/S0567740877008152.

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[1] H. J. Deiseroth, P. Amann, and H. Thurn, *Die Pentatelluride M_2Te_5 (M = Al, Ga, In): Polymorphie, Strukturbeziehungen und Homogenitätsbereiche*, Z. Anorganische und Allgemeine Chemie **622**, 985–993 (1996), doi:10.1002/zaac.19966220611.

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