Ga$_2$Te$_5$ Structure: A2B5_tI14_87_d_ah-001
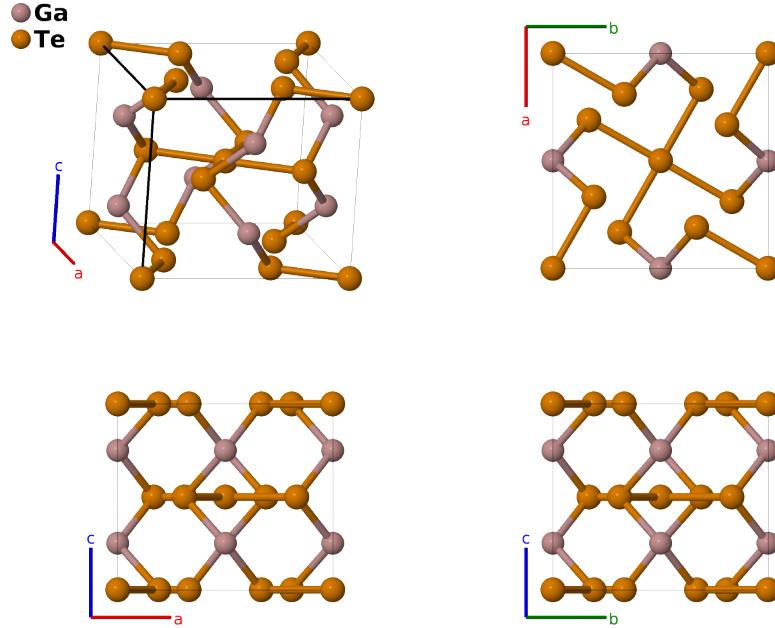
Prototype	Ga$_2$Te$_5$
AFLOW prototype label	A2B5_tI14_87_d_ah-001
ICSD	1085
Pearson symbol	tI14
Space group number	87
Space group symbol	$I4/m$
AFLOW prototype command	aflow --proto=A2B5_tI14_87_d_ah-001 --params=$a, c/a, x_3, y_3$

Body-centered Tetragonal primitive vectors

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

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

$$\mathbf{a_3} = \frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}} - \frac{1}{2}c\,\hat{\mathbf{z}}$$
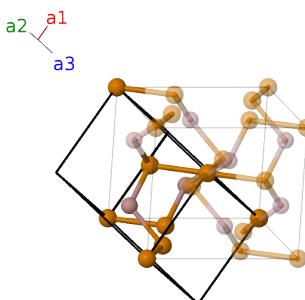
Basis vectors

		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

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