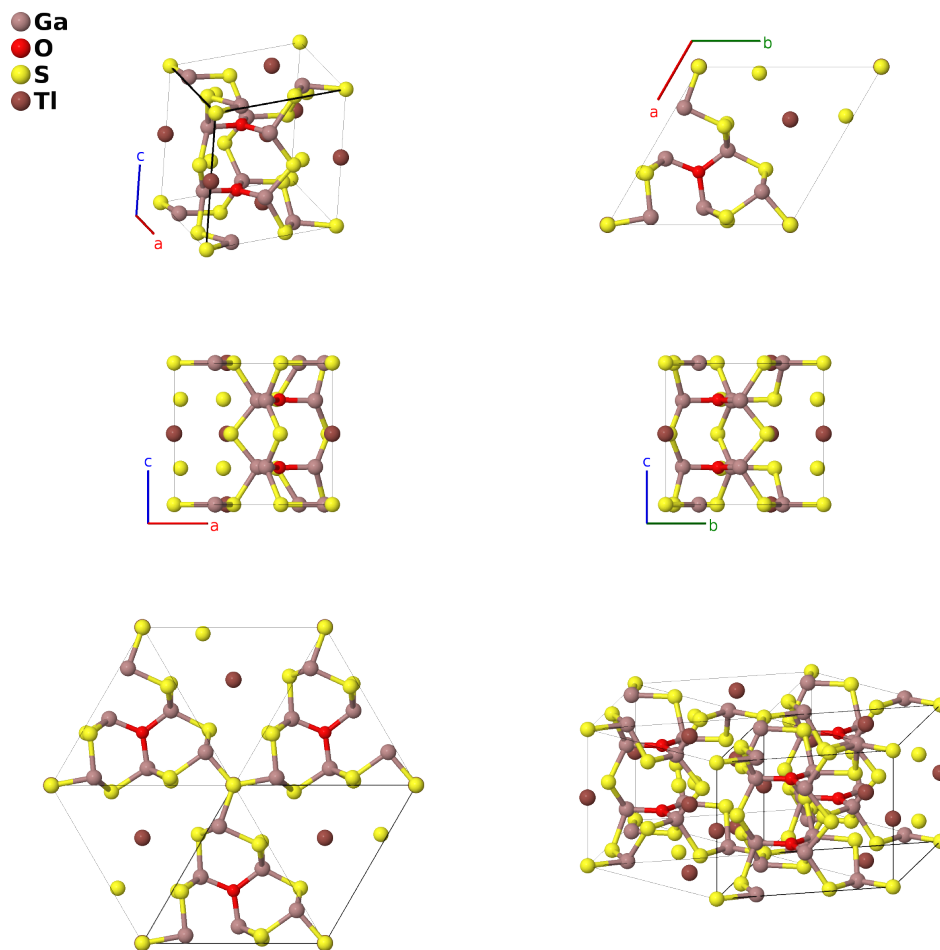


Tl₃Ga₉S₁₃O₂ Structure: A9B2C13D3_hP27_174_jl_i_ajkl_bcd-001

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<https://aflow.org/p/Q3WS>

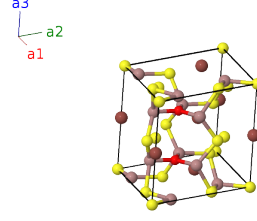
https://aflow.org/p/A9B2C13D3_hP27_174_jl_i_ajkl_bcd-001



Prototype	Ga ₉ O ₂ S ₁₃ Tl ₃
AFLOW prototype label	A9B2C13D3_hP27_174_jl_i_ajkl_bcd-001
ICSD	61256
Pearson symbol	hP27
Space group number	174
Space group symbol	$P\bar{6}$
AFLOW prototype command	<code>aflow --proto=A9B2C13D3_hP27_174_jl_i_ajkl_bcd-001 --params=a, c/a, z₅, x₆, y₆, x₇, y₇, x₈, y₈, x₉, y₉, z₉, x₁₀, y₁₀, z₁₀</code>

Hexagonal primitive vectors

$$\begin{aligned}\mathbf{a}_1 &= \frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a \hat{\mathbf{y}} \\ \mathbf{a}_2 &= \frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}}\end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
\mathbf{B}_1	0	$=$	0	(1a)	S I
\mathbf{B}_2	$\frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2}c \hat{\mathbf{z}}$	(1b)	Tl I
\mathbf{B}_3	$\frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a \hat{\mathbf{y}}$	(1c)	Tl II
\mathbf{B}_4	$\frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(1d)	Tl III
\mathbf{B}_5	$\frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(2i)	O I
\mathbf{B}_6	$\frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 - z_5 \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} - cz_5 \hat{\mathbf{z}}$	(2i)	O I
\mathbf{B}_7	$x_6 \mathbf{a}_1 + y_6 \mathbf{a}_2$	$=$	$\frac{1}{2}a(x_6 + y_6) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a(x_6 - y_6) \hat{\mathbf{y}}$	(3j)	Ga I
\mathbf{B}_8	$-y_6 \mathbf{a}_1 + (x_6 - y_6) \mathbf{a}_2$	$=$	$\frac{1}{2}a(x_6 - 2y_6) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_6 \hat{\mathbf{y}}$	(3j)	Ga I
\mathbf{B}_9	$-(x_6 - y_6) \mathbf{a}_1 - x_6 \mathbf{a}_2$	$=$	$-\frac{1}{2}a(2x_6 - y_6) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_6 \hat{\mathbf{y}}$	(3j)	Ga I
\mathbf{B}_{10}	$x_7 \mathbf{a}_1 + y_7 \mathbf{a}_2$	$=$	$\frac{1}{2}a(x_7 + y_7) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a(x_7 - y_7) \hat{\mathbf{y}}$	(3j)	S II
\mathbf{B}_{11}	$-y_7 \mathbf{a}_1 + (x_7 - y_7) \mathbf{a}_2$	$=$	$\frac{1}{2}a(x_7 - 2y_7) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_7 \hat{\mathbf{y}}$	(3j)	S II
\mathbf{B}_{12}	$-(x_7 - y_7) \mathbf{a}_1 - x_7 \mathbf{a}_2$	$=$	$-\frac{1}{2}a(2x_7 - y_7) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_7 \hat{\mathbf{y}}$	(3j)	S II
\mathbf{B}_{13}	$x_8 \mathbf{a}_1 + y_8 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_8 + y_8) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a(x_8 - y_8) \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(3k)	S III
\mathbf{B}_{14}	$-y_8 \mathbf{a}_1 + (x_8 - y_8) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_8 - 2y_8) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_8 \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(3k)	S III
\mathbf{B}_{15}	$-(x_8 - y_8) \mathbf{a}_1 - x_8 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-\frac{1}{2}a(2x_8 - y_8) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_8 \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(3k)	S III
\mathbf{B}_{16}	$x_9 \mathbf{a}_1 + y_9 \mathbf{a}_2 + z_9 \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_9 + y_9) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a(x_9 - y_9) \hat{\mathbf{y}} + cz_9 \hat{\mathbf{z}}$	(6l)	Ga II
\mathbf{B}_{17}	$-y_9 \mathbf{a}_1 + (x_9 - y_9) \mathbf{a}_2 + z_9 \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_9 - 2y_9) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_9 \hat{\mathbf{y}} + cz_9 \hat{\mathbf{z}}$	(6l)	Ga II
\mathbf{B}_{18}	$-(x_9 - y_9) \mathbf{a}_1 - x_9 \mathbf{a}_2 + z_9 \mathbf{a}_3$	$=$	$-\frac{1}{2}a(2x_9 - y_9) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_9 \hat{\mathbf{y}} + cz_9 \hat{\mathbf{z}}$	(6l)	Ga II
\mathbf{B}_{19}	$x_9 \mathbf{a}_1 + y_9 \mathbf{a}_2 - z_9 \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_9 + y_9) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a(x_9 - y_9) \hat{\mathbf{y}} - cz_9 \hat{\mathbf{z}}$	(6l)	Ga II
\mathbf{B}_{20}	$-y_9 \mathbf{a}_1 + (x_9 - y_9) \mathbf{a}_2 - z_9 \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_9 - 2y_9) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_9 \hat{\mathbf{y}} - cz_9 \hat{\mathbf{z}}$	(6l)	Ga II
\mathbf{B}_{21}	$-(x_9 - y_9) \mathbf{a}_1 - x_9 \mathbf{a}_2 - z_9 \mathbf{a}_3$	$=$	$-\frac{1}{2}a(2x_9 - y_9) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_9 \hat{\mathbf{y}} - cz_9 \hat{\mathbf{z}}$	(6l)	Ga II
\mathbf{B}_{22}	$x_{10} \mathbf{a}_1 + y_{10} \mathbf{a}_2 + z_{10} \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_{10} + y_{10}) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a(x_{10} - y_{10}) \hat{\mathbf{y}} + cz_{10} \hat{\mathbf{z}}$	(6l)	S IV
\mathbf{B}_{23}	$-y_{10} \mathbf{a}_1 + (x_{10} - y_{10}) \mathbf{a}_2 + z_{10} \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_{10} - 2y_{10}) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_{10} \hat{\mathbf{y}} + cz_{10} \hat{\mathbf{z}}$	(6l)	S IV
\mathbf{B}_{24}	$-(x_{10} - y_{10}) \mathbf{a}_1 - x_{10} \mathbf{a}_2 + z_{10} \mathbf{a}_3$	$=$	$-\frac{1}{2}a(2x_{10} - y_{10}) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_{10} \hat{\mathbf{y}} + cz_{10} \hat{\mathbf{z}}$	(6l)	S IV
\mathbf{B}_{25}	$x_{10} \mathbf{a}_1 + y_{10} \mathbf{a}_2 - z_{10} \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_{10} + y_{10}) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a(x_{10} - y_{10}) \hat{\mathbf{y}} - cz_{10} \hat{\mathbf{z}}$	(6l)	S IV
\mathbf{B}_{26}	$-y_{10} \mathbf{a}_1 + (x_{10} - y_{10}) \mathbf{a}_2 - z_{10} \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_{10} - 2y_{10}) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_{10} \hat{\mathbf{y}} - cz_{10} \hat{\mathbf{z}}$	(6l)	S IV
\mathbf{B}_{27}	$-(x_{10} - y_{10}) \mathbf{a}_1 - x_{10} \mathbf{a}_2 - z_{10} \mathbf{a}_3$	$=$	$-\frac{1}{2}a(2x_{10} - y_{10}) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_{10} \hat{\mathbf{y}} - cz_{10} \hat{\mathbf{z}}$	(6l)	S IV

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