

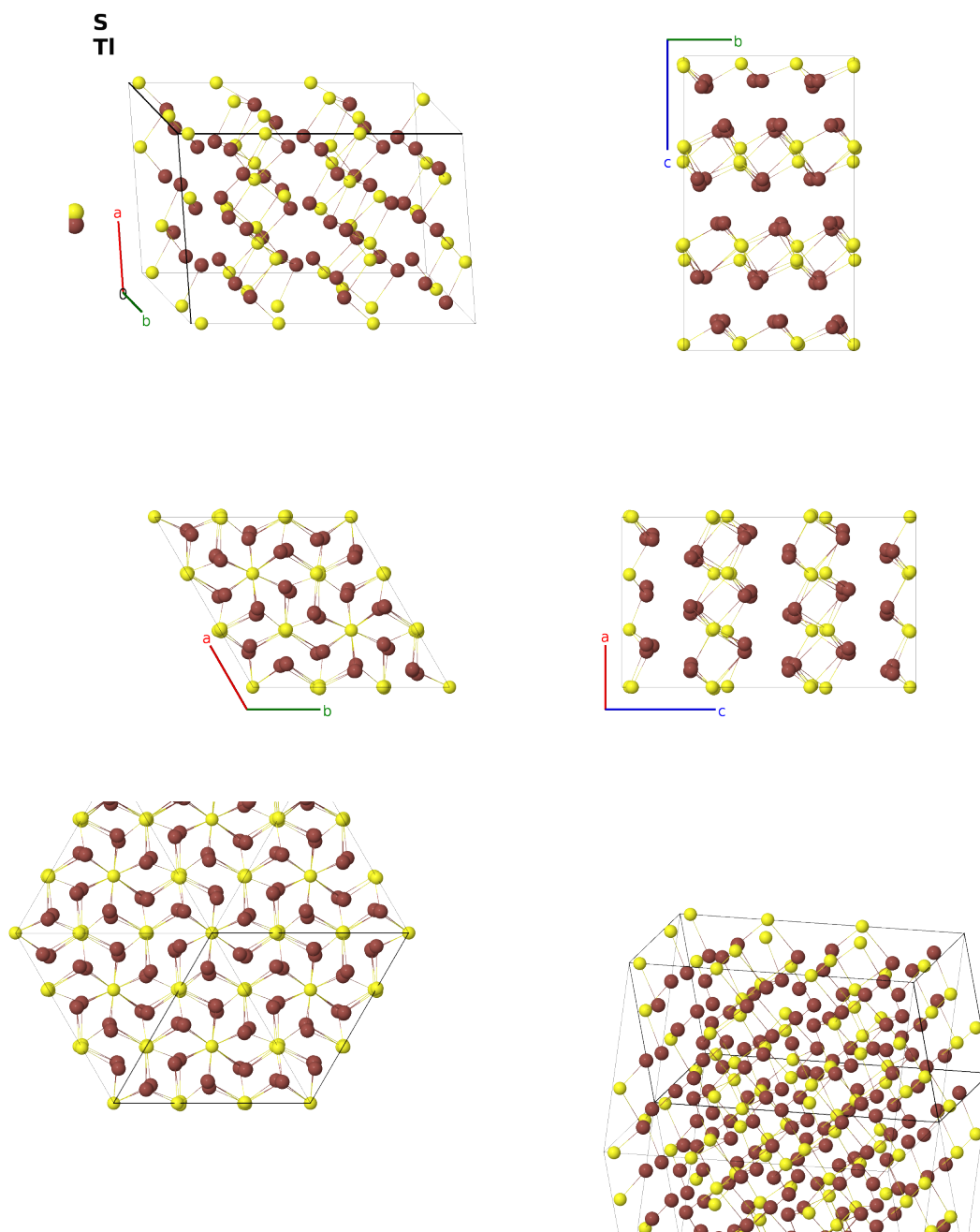
Carlinite (Tl₂S) Structure: AB2_hR27_146_3a2b_6b-001

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<https://aflow.org/prototype-encyclopedia/X2PG>

https://aflow.org/prototype-encyclopedia/AB2_hR27_146_3a2b_6b-001

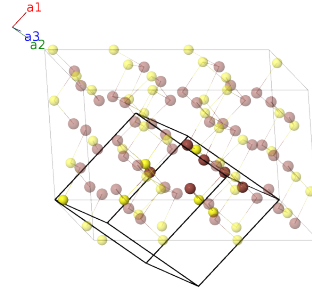


Prototype	STl ₂
AFLOW prototype label	AB2_hR27_146_3a2b_6b-001
Mineral name	carlinite
ICSD	59735
CCDC	1623535
Pearson symbol	hR27
Space group number	146
Space group symbol	<i>R</i> 3
AFLOW prototype command	<pre>aflow --proto=AB2_hR27_146_3a2b_6b-001 --params=a, c/a, x₁, x₂, x₃, x₄, y₄, z₄, x₅, y₅, z₅, x₆, y₆, z₆, x₇, y₇, z₇, x₈, y₈, z₈, x₉, y₉, z₉, x₁₀, y₁₀, z₁₀, x₁₁, y₁₁, z₁₁</pre>

- Hexagonal settings of this structure can be obtained with the option `--hex`.

Rhombohedral primitive vectors

$$\begin{aligned}
\mathbf{a}_1 &= \frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + \frac{1}{3}c \hat{\mathbf{z}} \\
\mathbf{a}_2 &= \frac{1}{\sqrt{3}}a \hat{\mathbf{y}} + \frac{1}{3}c \hat{\mathbf{z}} \\
\mathbf{a}_3 &= -\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + \frac{1}{3}c \hat{\mathbf{z}}
\end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= x_1 \mathbf{a}_1 + x_1 \mathbf{a}_2 + x_1 \mathbf{a}_3$	$=$	$cx_1 \hat{\mathbf{z}}$	(1a)	S I
$\mathbf{B}_2$	$= x_2 \mathbf{a}_1 + x_2 \mathbf{a}_2 + x_2 \mathbf{a}_3$	$=$	$cx_2 \hat{\mathbf{z}}$	(1a)	S II
$\mathbf{B}_3$	$= x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + x_3 \mathbf{a}_3$	$=$	$cx_3 \hat{\mathbf{z}}$	(1a)	S III
$\mathbf{B}_4$	$= x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_4 - z_4) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_4 - 2y_4 + z_4) \hat{\mathbf{y}} + \frac{1}{3}c(x_4 + y_4 + z_4) \hat{\mathbf{z}}$	(3b)	S IV
$\mathbf{B}_5$	$= z_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + y_4 \mathbf{a}_3$	$=$	$-\frac{1}{2}a(y_4 - z_4) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(2x_4 - y_4 - z_4) \hat{\mathbf{y}} + \frac{1}{3}c(x_4 + y_4 + z_4) \hat{\mathbf{z}}$	(3b)	S IV
$\mathbf{B}_6$	$= y_4 \mathbf{a}_1 + z_4 \mathbf{a}_2 + x_4 \mathbf{a}_3$	$=$	$-\frac{1}{2}a(x_4 - y_4) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_4 + y_4 - 2z_4) \hat{\mathbf{y}} + \frac{1}{3}c(x_4 + y_4 + z_4) \hat{\mathbf{z}}$	(3b)	S IV
$\mathbf{B}_7$	$= x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_5 - z_5) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_5 - 2y_5 + z_5) \hat{\mathbf{y}} + \frac{1}{3}c(x_5 + y_5 + z_5) \hat{\mathbf{z}}$	(3b)	S V
$\mathbf{B}_8$	$= z_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 + y_5 \mathbf{a}_3$	$=$	$-\frac{1}{2}a(y_5 - z_5) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(2x_5 - y_5 - z_5) \hat{\mathbf{y}} + \frac{1}{3}c(x_5 + y_5 + z_5) \hat{\mathbf{z}}$	(3b)	S V
$\mathbf{B}_9$	$= y_5 \mathbf{a}_1 + z_5 \mathbf{a}_2 + x_5 \mathbf{a}_3$	$=$	$-\frac{1}{2}a(x_5 - y_5) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_5 + y_5 - 2z_5) \hat{\mathbf{y}} + \frac{1}{3}c(x_5 + y_5 + z_5) \hat{\mathbf{z}}$	(3b)	S V

$\mathbf{B}_{10}$	$=$	$x_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_6 - z_6) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_6 - 2y_6 + z_6) \hat{\mathbf{y}} + \frac{1}{3}c(x_6 + y_6 + z_6) \hat{\mathbf{z}}$	(3b)	Tl I
$\mathbf{B}_{11}$	$=$	$z_6 \mathbf{a}_1 + x_6 \mathbf{a}_2 + y_6 \mathbf{a}_3$	$=$	$-\frac{1}{2}a(y_6 - z_6) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(2x_6 - y_6 - z_6) \hat{\mathbf{y}} + \frac{1}{3}c(x_6 + y_6 + z_6) \hat{\mathbf{z}}$	(3b)	Tl I
$\mathbf{B}_{12}$	$=$	$y_6 \mathbf{a}_1 + z_6 \mathbf{a}_2 + x_6 \mathbf{a}_3$	$=$	$-\frac{1}{2}a(x_6 - y_6) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_6 + y_6 - 2z_6) \hat{\mathbf{y}} + \frac{1}{3}c(x_6 + y_6 + z_6) \hat{\mathbf{z}}$	(3b)	Tl I
$\mathbf{B}_{13}$	$=$	$x_7 \mathbf{a}_1 + y_7 \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_7 - z_7) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_7 - 2y_7 + z_7) \hat{\mathbf{y}} + \frac{1}{3}c(x_7 + y_7 + z_7) \hat{\mathbf{z}}$	(3b)	Tl II
$\mathbf{B}_{14}$	$=$	$z_7 \mathbf{a}_1 + x_7 \mathbf{a}_2 + y_7 \mathbf{a}_3$	$=$	$-\frac{1}{2}a(y_7 - z_7) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(2x_7 - y_7 - z_7) \hat{\mathbf{y}} + \frac{1}{3}c(x_7 + y_7 + z_7) \hat{\mathbf{z}}$	(3b)	Tl II
$\mathbf{B}_{15}$	$=$	$y_7 \mathbf{a}_1 + z_7 \mathbf{a}_2 + x_7 \mathbf{a}_3$	$=$	$-\frac{1}{2}a(x_7 - y_7) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_7 + y_7 - 2z_7) \hat{\mathbf{y}} + \frac{1}{3}c(x_7 + y_7 + z_7) \hat{\mathbf{z}}$	(3b)	Tl II
$\mathbf{B}_{16}$	$=$	$x_8 \mathbf{a}_1 + y_8 \mathbf{a}_2 + z_8 \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_8 - z_8) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_8 - 2y_8 + z_8) \hat{\mathbf{y}} + \frac{1}{3}c(x_8 + y_8 + z_8) \hat{\mathbf{z}}$	(3b)	Tl III
$\mathbf{B}_{17}$	$=$	$z_8 \mathbf{a}_1 + x_8 \mathbf{a}_2 + y_8 \mathbf{a}_3$	$=$	$-\frac{1}{2}a(y_8 - z_8) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(2x_8 - y_8 - z_8) \hat{\mathbf{y}} + \frac{1}{3}c(x_8 + y_8 + z_8) \hat{\mathbf{z}}$	(3b)	Tl III
$\mathbf{B}_{18}$	$=$	$y_8 \mathbf{a}_1 + z_8 \mathbf{a}_2 + x_8 \mathbf{a}_3$	$=$	$-\frac{1}{2}a(x_8 - y_8) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_8 + y_8 - 2z_8) \hat{\mathbf{y}} + \frac{1}{3}c(x_8 + y_8 + z_8) \hat{\mathbf{z}}$	(3b)	Tl III
$\mathbf{B}_{19}$	$=$	$x_9 \mathbf{a}_1 + y_9 \mathbf{a}_2 + z_9 \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_9 - z_9) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_9 - 2y_9 + z_9) \hat{\mathbf{y}} + \frac{1}{3}c(x_9 + y_9 + z_9) \hat{\mathbf{z}}$	(3b)	Tl IV
$\mathbf{B}_{20}$	$=$	$z_9 \mathbf{a}_1 + x_9 \mathbf{a}_2 + y_9 \mathbf{a}_3$	$=$	$-\frac{1}{2}a(y_9 - z_9) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(2x_9 - y_9 - z_9) \hat{\mathbf{y}} + \frac{1}{3}c(x_9 + y_9 + z_9) \hat{\mathbf{z}}$	(3b)	Tl IV
$\mathbf{B}_{21}$	$=$	$y_9 \mathbf{a}_1 + z_9 \mathbf{a}_2 + x_9 \mathbf{a}_3$	$=$	$-\frac{1}{2}a(x_9 - y_9) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_9 + y_9 - 2z_9) \hat{\mathbf{y}} + \frac{1}{3}c(x_9 + y_9 + z_9) \hat{\mathbf{z}}$	(3b)	Tl IV
$\mathbf{B}_{22}$	$=$	$x_{10} \mathbf{a}_1 + y_{10} \mathbf{a}_2 + z_{10} \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_{10} - z_{10}) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_{10} - 2y_{10} + z_{10}) \hat{\mathbf{y}} + \frac{1}{3}c(x_{10} + y_{10} + z_{10}) \hat{\mathbf{z}}$	(3b)	Tl V
$\mathbf{B}_{23}$	$=$	$z_{10} \mathbf{a}_1 + x_{10} \mathbf{a}_2 + y_{10} \mathbf{a}_3$	$=$	$-\frac{1}{2}a(y_{10} - z_{10}) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(2x_{10} - y_{10} - z_{10}) \hat{\mathbf{y}} + \frac{1}{3}c(x_{10} + y_{10} + z_{10}) \hat{\mathbf{z}}$	(3b)	Tl V
$\mathbf{B}_{24}$	$=$	$y_{10} \mathbf{a}_1 + z_{10} \mathbf{a}_2 + x_{10} \mathbf{a}_3$	$=$	$-\frac{1}{2}a(x_{10} - y_{10}) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_{10} + y_{10} - 2z_{10}) \hat{\mathbf{y}} + \frac{1}{3}c(x_{10} + y_{10} + z_{10}) \hat{\mathbf{z}}$	(3b)	Tl V
$\mathbf{B}_{25}$	$=$	$x_{11} \mathbf{a}_1 + y_{11} \mathbf{a}_2 + z_{11} \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_{11} - z_{11}) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_{11} - 2y_{11} + z_{11}) \hat{\mathbf{y}} + \frac{1}{3}c(x_{11} + y_{11} + z_{11}) \hat{\mathbf{z}}$	(3b)	Tl VI
$\mathbf{B}_{26}$	$=$	$z_{11} \mathbf{a}_1 + x_{11} \mathbf{a}_2 + y_{11} \mathbf{a}_3$	$=$	$-\frac{1}{2}a(y_{11} - z_{11}) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(2x_{11} - y_{11} - z_{11}) \hat{\mathbf{y}} + \frac{1}{3}c(x_{11} + y_{11} + z_{11}) \hat{\mathbf{z}}$	(3b)	Tl VI
$\mathbf{B}_{27}$	$=$	$y_{11} \mathbf{a}_1 + z_{11} \mathbf{a}_2 + x_{11} \mathbf{a}_3$	$=$	$-\frac{1}{2}a(x_{11} - y_{11}) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_{11} + y_{11} - 2z_{11}) \hat{\mathbf{y}} + \frac{1}{3}c(x_{11} + y_{11} + z_{11}) \hat{\mathbf{z}}$	(3b)	Tl VI

References

- [1] G. Giester, C. L. Lengauer, E. Tillmanns, and J. Zemann, *Th₂S: Re-Determination of Crystal Structure and Stereochemical Discussion*, J. Solid State Chem. **168**, 322–330 (2002), doi:10.1006/jssc.2002.9711.

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