Carlinite (Tl_2S) Structure: AB2_hR27_146_3a2b_6b-001

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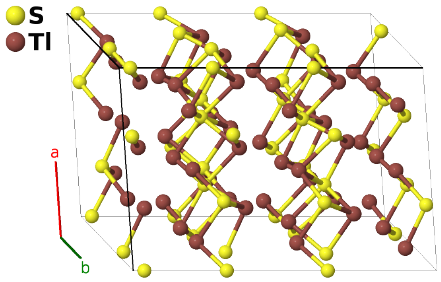
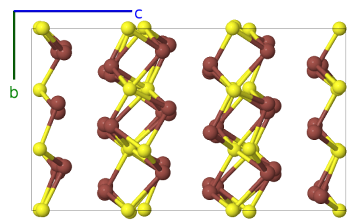
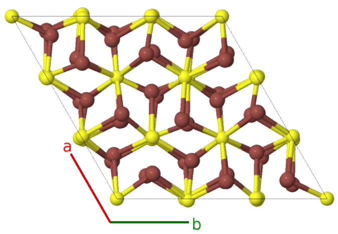
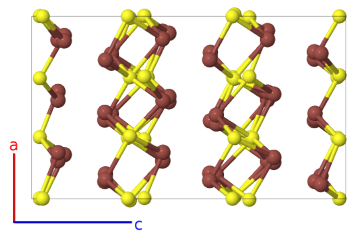
https://aflow.org/p/X2PG

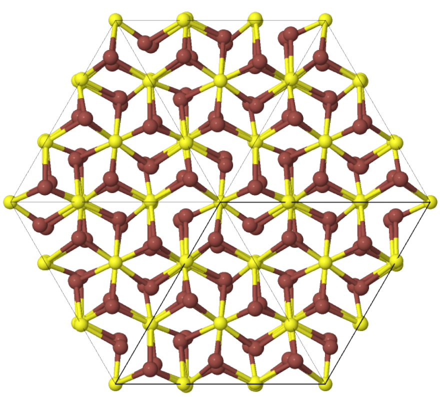
https://aflow.org/p/AB2_hR27_146_3a2b_6b-001

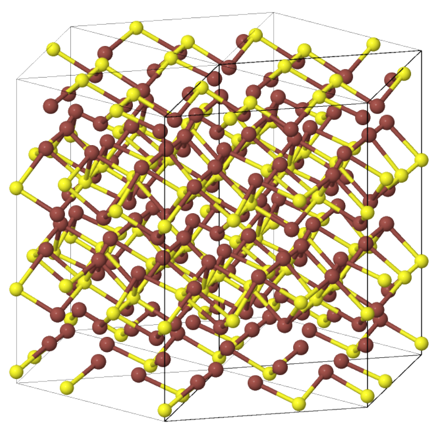












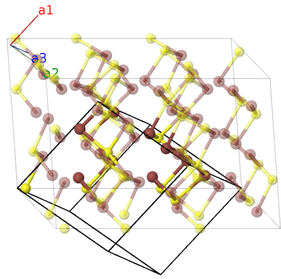
Prototype	STl_2
AFLOW prototype label	AB2_hR27_146_3a2b_6b-001
Mineral name	carlinite
ICSD	59735
Pearson symbol	hR27
Space group number	146
Space group symbol	$R3$

AFLOW prototype command `aflow --proto=AB2_hR27_146_3a2b_6b-001`
`--params=`$a, c/a, x_1, x_2, x_3, x_4, y_4, z_4, x_5, y_5, z_5, x_6, y_6, z_6, x_7, y_7, z_7, x_8, y_8, z_8, x_9, y_9, z_9, x_{10}, y_{10}, z_{10}, x_{11}, y_{11}, z_{11}$

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

Rhombohedral primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$x_1\,\mathbf{a}_1 + x_1\,\mathbf{a}_2 + x_1\,\mathbf{a}_3$	=	$cx_1\,\mathbf{\hat{z}}$	(1a)	S I
$\mathbf{B_2}$	=	$x_2\,\mathbf{a}_1 + x_2\,\mathbf{a}_2 + x_2\,\mathbf{a}_3$	=	$cx_2\,\mathbf{\hat{z}}$	(1a)	S II
$\mathbf{B_3}$	=	$x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + x_3\,\mathbf{a}_3$	=	$cx_3\,\mathbf{\hat{z}}$	(1a)	S III
$\mathbf{B_4}$	=	$x_4\,\mathbf{a}_1 + y_4\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_4 - z_4)\,\mathbf{\hat{x}} - \frac{\sqrt{3}}{6}a\,(x_4 - 2y_4 + z_4)\,\mathbf{\hat{y}} + \frac{1}{3}c\,(x_4 + y_4 + z_4)\,\mathbf{\hat{z}}$	(3b)	S IV
$\mathbf{B_5}$	=	$z_4\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 + y_4\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(y_4 - z_4)\,\mathbf{\hat{x}} + \frac{\sqrt{3}}{6}a\,(2x_4 - y_4 - z_4)\,\mathbf{\hat{y}} + \frac{1}{3}c\,(x_4 + y_4 + z_4)\,\mathbf{\hat{z}}$	(3b)	S IV
$\mathbf{B_6}$	=	$y_4\,\mathbf{a}_1 + z_4\,\mathbf{a}_2 + x_4\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(x_4 - y_4)\,\mathbf{\hat{x}} - \frac{\sqrt{3}}{6}a\,(x_4 + y_4 - 2z_4)\,\mathbf{\hat{y}} + \frac{1}{3}c\,(x_4 + y_4 + z_4)\,\mathbf{\hat{z}}$	(3b)	S IV
$\mathbf{B_7}$	=	$x_5\,\mathbf{a}_1 + y_5\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_5 - z_5)\,\mathbf{\hat{x}} - \frac{\sqrt{3}}{6}a\,(x_5 - 2y_5 + z_5)\,\mathbf{\hat{y}} + \frac{1}{3}c\,(x_5 + y_5 + z_5)\,\mathbf{\hat{z}}$	(3b)	S V
$\mathbf{B_8}$	=	$z_5\,\mathbf{a}_1 + x_5\,\mathbf{a}_2 + y_5\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(y_5 - z_5)\,\mathbf{\hat{x}} + \frac{\sqrt{3}}{6}a\,(2x_5 - y_5 - z_5)\,\mathbf{\hat{y}} + \frac{1}{3}c\,(x_5 + y_5 + z_5)\,\mathbf{\hat{z}}$	(3b)	S V
$\mathbf{B_9}$	=	$y_5\,\mathbf{a}_1 + z_5\,\mathbf{a}_2 + x_5\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(x_5 - y_5)\,\mathbf{\hat{x}} - \frac{\sqrt{3}}{6}a\,(x_5 + y_5 - 2z_5)\,\mathbf{\hat{y}} + \frac{1}{3}c\,(x_5 + y_5 + z_5)\,\mathbf{\hat{z}}$	(3b)	S V
$\mathbf{B_{10}}$	=	$x_6\,\mathbf{a}_1 + y_6\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_6 - z_6)\,\mathbf{\hat{x}} - \frac{\sqrt{3}}{6}a\,(x_6 - 2y_6 + z_6)\,\mathbf{\hat{y}} + \frac{1}{3}c\,(x_6 + y_6 + z_6)\,\mathbf{\hat{z}}$	(3b)	Tl I
$\mathbf{B_{11}}$	=	$z_6\,\mathbf{a}_1 + x_6\,\mathbf{a}_2 + y_6\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(y_6 - z_6)\,\mathbf{\hat{x}} + \frac{\sqrt{3}}{6}a\,(2x_6 - y_6 - z_6)\,\mathbf{\hat{y}} + \frac{1}{3}c\,(x_6 + y_6 + z_6)\,\mathbf{\hat{z}}$	(3b)	Tl I
$\mathbf{B_{12}}$	=	$y_6\,\mathbf{a}_1 + z_6\,\mathbf{a}_2 + x_6\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(x_6 - y_6)\,\mathbf{\hat{x}} - \frac{\sqrt{3}}{6}a\,(x_6 + y_6 - 2z_6)\,\mathbf{\hat{y}} + \frac{1}{3}c\,(x_6 + y_6 + z_6)\,\mathbf{\hat{z}}$	(3b)	Tl I
$\mathbf{B_{13}}$	=	$x_7\,\mathbf{a}_1 + y_7\,\mathbf{a}_2 + z_7\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_7 - z_7)\,\mathbf{\hat{x}} - \frac{\sqrt{3}}{6}a\,(x_7 - 2y_7 + z_7)\,\mathbf{\hat{y}} + \frac{1}{3}c\,(x_7 + y_7 + z_7)\,\mathbf{\hat{z}}$	(3b)	Tl II
$\mathbf{B_{14}}$	=	$z_7\,\mathbf{a}_1 + x_7\,\mathbf{a}_2 + y_7\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(y_7 - z_7)\,\mathbf{\hat{x}} + \frac{\sqrt{3}}{6}a\,(2x_7 - y_7 - z_7)\,\mathbf{\hat{y}} + \frac{1}{3}c\,(x_7 + y_7 + z_7)\,\mathbf{\hat{z}}$	(3b)	Tl II
$\mathbf{B_{15}}$	=	$y_7\,\mathbf{a}_1 + z_7\,\mathbf{a}_2 + x_7\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(x_7 - y_7)\,\mathbf{\hat{x}} - \frac{\sqrt{3}}{6}a\,(x_7 + y_7 - 2z_7)\,\mathbf{\hat{y}} + \frac{1}{3}c\,(x_7 + y_7 + z_7)\,\mathbf{\hat{z}}$	(3b)	Tl II
$\mathbf{B_{16}}$	=	$x_8\,\mathbf{a}_1 + y_8\,\mathbf{a}_2 + z_8\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_8 - z_8)\,\mathbf{\hat{x}} - \frac{\sqrt{3}}{6}a\,(x_8 - 2y_8 + z_8)\,\mathbf{\hat{y}} + \frac{1}{3}c\,(x_8 + y_8 + z_8)\,\mathbf{\hat{z}}$	(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, *Tl_2S: Re-Determination of Crystal Structure and Stereochemical Discussion*, J. Solid State Chem. **168**, 322–330 (2002), doi:10.1006/jssc.2002.9711.