Rosickýite (γ-monoclinic Sulfur) Structure: A_mP32_13_8g-001

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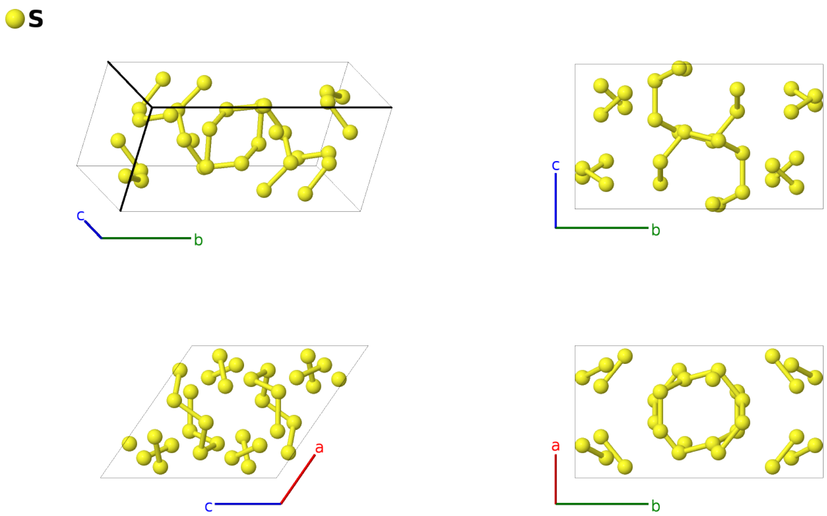
https://aflow.org/p/Y7J6

https://aflow.org/p/A_mP32_13_8g-001



Prototype S

AFLOW prototype label A_mP32_13_8g-001

Mineral name rosickýite

ICSD 66517

Pearson symbol mP32

Space group number 13

Space group symbol $P2/c$

AFLOW prototype command `aflow --proto=A_mP32_13_8g-001`
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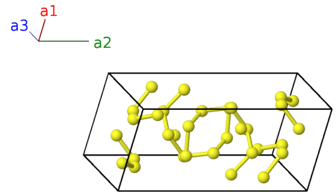
Other compounds with this structure

Se_3S_5

- We take the name of this structure from (Donohue, 1976), which occurs naturally as the mineral rosickýite. (Donohue, 1976; Downs, 2003) The sulfur atoms form eight-atom rings, just like α sulfur ($A16$) and β-monoclinic sulfur.

Simple Monoclinic primitive vectors

$$\mathbf{a_1} = a\,\mathbf{\hat{x}}$$
$$\mathbf{a_2} = b\,\mathbf{\hat{y}}$$
$$\mathbf{a_3} = c\cos\beta\,\mathbf{\hat{x}} + c\sin\beta\,\mathbf{\hat{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$x_1\,\mathbf{a}_1 + y_1\,\mathbf{a}_2 + z_1\,\mathbf{a}_3$	=	$(ax_1 + cz_1\cos\beta)\,\mathbf{\hat{x}} + by_1\,\mathbf{\hat{y}} + cz_1\sin\beta\,\mathbf{\hat{z}}$	(4g)	S I
$\mathbf{B_2}$	=	$-x_1\,\mathbf{a}_1 + y_1\,\mathbf{a}_2 - \left(z_1 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\left(ax_1 + c\left(z_1 - \frac{1}{2}\right)\cos\beta\right)\,\mathbf{\hat{x}} + by_1\,\mathbf{\hat{y}} - c\left(z_1 - \frac{1}{2}\right)\sin\beta\,\mathbf{\hat{z}}$	(4g)	S I
$\mathbf{B_3}$	=	$-x_1\,\mathbf{a}_1 - y_1\,\mathbf{a}_2 - z_1\,\mathbf{a}_3$	=	$-(ax_1 + cz_1\cos\beta)\,\mathbf{\hat{x}} - by_1\,\mathbf{\hat{y}} - cz_1\sin\beta\,\mathbf{\hat{z}}$	(4g)	S I
$\mathbf{B_4}$	=	$x_1\,\mathbf{a}_1 - y_1\,\mathbf{a}_2 + \left(z_1 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\left(ax_1 + c\left(z_1 + \frac{1}{2}\right)\cos\beta\right)\,\mathbf{\hat{x}} - by_1\,\mathbf{\hat{y}} + c\left(z_1 + \frac{1}{2}\right)\sin\beta\,\mathbf{\hat{z}}$	(4g)	S I
$\mathbf{B_5}$	=	$x_2\,\mathbf{a}_1 + y_2\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$(ax_2 + cz_2\cos\beta)\,\mathbf{\hat{x}} + by_2\,\mathbf{\hat{y}} + cz_2\sin\beta\,\mathbf{\hat{z}}$	(4g)	S II
$\mathbf{B_6}$	=	$-x_2\,\mathbf{a}_1 + y_2\,\mathbf{a}_2 - \left(z_2 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\left(ax_2 + c\left(z_2 - \frac{1}{2}\right)\cos\beta\right)\,\mathbf{\hat{x}} + by_2\,\mathbf{\hat{y}} - c\left(z_2 - \frac{1}{2}\right)\sin\beta\,\mathbf{\hat{z}}$	(4g)	S II
$\mathbf{B_7}$	=	$-x_2\,\mathbf{a}_1 - y_2\,\mathbf{a}_2 - z_2\,\mathbf{a}_3$	=	$-(ax_2 + cz_2\cos\beta)\,\mathbf{\hat{x}} - by_2\,\mathbf{\hat{y}} - cz_2\sin\beta\,\mathbf{\hat{z}}$	(4g)	S II
$\mathbf{B_8}$	=	$x_2\,\mathbf{a}_1 - y_2\,\mathbf{a}_2 + \left(z_2 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\left(ax_2 + c\left(z_2 + \frac{1}{2}\right)\cos\beta\right)\,\mathbf{\hat{x}} - by_2\,\mathbf{\hat{y}} + c\left(z_2 + \frac{1}{2}\right)\sin\beta\,\mathbf{\hat{z}}$	(4g)	S II
$\mathbf{B_9}$	=	$x_3\,\mathbf{a}_1 + y_3\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$(ax_3 + cz_3\cos\beta)\,\mathbf{\hat{x}} + by_3\,\mathbf{\hat{y}} + cz_3\sin\beta\,\mathbf{\hat{z}}$	(4g)	S III
$\mathbf{B_{10}}$	=	$-x_3\,\mathbf{a}_1 + y_3\,\mathbf{a}_2 - \left(z_3 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\left(ax_3 + c\left(z_3 - \frac{1}{2}\right)\cos\beta\right)\,\mathbf{\hat{x}} + by_3\,\mathbf{\hat{y}} - c\left(z_3 - \frac{1}{2}\right)\sin\beta\,\mathbf{\hat{z}}$	(4g)	S III
$\mathbf{B_{11}}$	=	$-x_3\,\mathbf{a}_1 - y_3\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$	=	$-(ax_3 + cz_3\cos\beta)\,\mathbf{\hat{x}} - by_3\,\mathbf{\hat{y}} - cz_3\sin\beta\,\mathbf{\hat{z}}$	(4g)	S III
$\mathbf{B_{12}}$	=	$x_3\,\mathbf{a}_1 - y_3\,\mathbf{a}_2 + \left(z_3 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\left(ax_3 + c\left(z_3 + \frac{1}{2}\right)\cos\beta\right)\,\mathbf{\hat{x}} - by_3\,\mathbf{\hat{y}} + c\left(z_3 + \frac{1}{2}\right)\sin\beta\,\mathbf{\hat{z}}$	(4g)	S III
$\mathbf{B_{13}}$	=	$x_4\,\mathbf{a}_1 + y_4\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$(ax_4 + cz_4\cos\beta)\,\mathbf{\hat{x}} + by_4\,\mathbf{\hat{y}} + cz_4\sin\beta\,\mathbf{\hat{z}}$	(4g)	S IV
$\mathbf{B_{14}}$	=	$-x_4\,\mathbf{a}_1 + y_4\,\mathbf{a}_2 - \left(z_4 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\left(ax_4 + c\left(z_4 - \frac{1}{2}\right)\cos\beta\right)\,\mathbf{\hat{x}} + by_4\,\mathbf{\hat{y}} - c\left(z_4 - \frac{1}{2}\right)\sin\beta\,\mathbf{\hat{z}}$	(4g)	S IV
$\mathbf{B_{15}}$	=	$-x_4\,\mathbf{a}_1 - y_4\,\mathbf{a}_2 - z_4\,\mathbf{a}_3$	=	$-(ax_4 + cz_4\cos\beta)\,\mathbf{\hat{x}} - by_4\,\mathbf{\hat{y}} - cz_4\sin\beta\,\mathbf{\hat{z}}$	(4g)	S IV
$\mathbf{B_{16}}$	=	$x_4\,\mathbf{a}_1 - y_4\,\mathbf{a}_2 + \left(z_4 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\left(ax_4 + c\left(z_4 + \frac{1}{2}\right)\cos\beta\right)\,\mathbf{\hat{x}} - by_4\,\mathbf{\hat{y}} + c\left(z_4 + \frac{1}{2}\right)\sin\beta\,\mathbf{\hat{z}}$	(4g)	S IV
$\mathbf{B_{17}}$	=	$x_5\,\mathbf{a}_1 + y_5\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$(ax_5 + cz_5\cos\beta)\,\mathbf{\hat{x}} + by_5\,\mathbf{\hat{y}} + cz_5\sin\beta\,\mathbf{\hat{z}}$	(4g)	S V
$\mathbf{B_{18}}$	=	$-x_5\,\mathbf{a}_1 + y_5\,\mathbf{a}_2 - \left(z_5 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\left(ax_5 + c\left(z_5 - \frac{1}{2}\right)\cos\beta\right)\,\mathbf{\hat{x}} + by_5\,\mathbf{\hat{y}} - c\left(z_5 - \frac{1}{2}\right)\sin\beta\,\mathbf{\hat{z}}$	(4g)	S V
$\mathbf{B_{19}}$	=	$-x_5\,\mathbf{a}_1 - y_5\,\mathbf{a}_2 - z_5\,\mathbf{a}_3$	=	$-(ax_5 + cz_5\cos\beta)\,\mathbf{\hat{x}} - by_5\,\mathbf{\hat{y}} - cz_5\sin\beta\,\mathbf{\hat{z}}$	(4g)	S V
$\mathbf{B_{20}}$	=	$x_5\,\mathbf{a}_1 - y_5\,\mathbf{a}_2 + \left(z_5 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\left(ax_5 + c\left(z_5 + \frac{1}{2}\right)\cos\beta\right)\,\mathbf{\hat{x}} - by_5\,\mathbf{\hat{y}} + c\left(z_5 + \frac{1}{2}\right)\sin\beta\,\mathbf{\hat{z}}$	(4g)	S V
$\mathbf{B_{21}}$	=	$x_6\,\mathbf{a}_1 + y_6\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	=	$(ax_6 + cz_6\cos\beta)\,\mathbf{\hat{x}} + by_6\,\mathbf{\hat{y}} + cz_6\sin\beta\,\mathbf{\hat{z}}$	(4g)	S VI
$\mathbf{B_{22}}$	=	$-x_6\,\mathbf{a}_1 + y_6\,\mathbf{a}_2 - \left(z_6 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\left(ax_6 + c\left(z_6 - \frac{1}{2}\right)\cos\beta\right)\,\mathbf{\hat{x}} + by_6\,\mathbf{\hat{y}} - c\left(z_6 - \frac{1}{2}\right)\sin\beta\,\mathbf{\hat{z}}$	(4g)	S VI
$\mathbf{B_{23}}$	=	$-x_6\,\mathbf{a}_1 - y_6\,\mathbf{a}_2 - z_6\,\mathbf{a}_3$	=	$-(ax_6 + cz_6\cos\beta)\,\mathbf{\hat{x}} - by_6\,\mathbf{\hat{y}} - cz_6\sin\beta\,\mathbf{\hat{z}}$	(4g)	S VI

$\mathbf{B_{24}}$	=	$x_6\,\mathbf{a}_1 - y_6\,\mathbf{a}_2 + \left(z_6 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\left(ax_6 + c\left(z_6 + \frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} - by_6\,\hat{\mathbf{y}} + c\left(z_6 + \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4g)	S VI
$\mathbf{B_{25}}$	=	$x_7\,\mathbf{a}_1 + y_7\,\mathbf{a}_2 + z_7\,\mathbf{a}_3$	=	$(ax_7 + cz_7\cos\beta)\,\hat{\mathbf{x}} + by_7\,\hat{\mathbf{y}} + cz_7\sin\beta\,\hat{\mathbf{z}}$	(4g)	S VII
$\mathbf{B_{26}}$	=	$-x_7\,\mathbf{a}_1 + y_7\,\mathbf{a}_2 - \left(z_7 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\left(ax_7 + c\left(z_7 - \frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} + by_7\,\hat{\mathbf{y}} - c\left(z_7 - \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4g)	S VII
$\mathbf{B_{27}}$	=	$-x_7\,\mathbf{a}_1 - y_7\,\mathbf{a}_2 - z_7\,\mathbf{a}_3$	=	$-(ax_7 + cz_7\cos\beta)\,\hat{\mathbf{x}} - by_7\,\hat{\mathbf{y}} - cz_7\sin\beta\,\hat{\mathbf{z}}$	(4g)	S VII
$\mathbf{B_{28}}$	=	$x_7\,\mathbf{a}_1 - y_7\,\mathbf{a}_2 + \left(z_7 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\left(ax_7 + c\left(z_7 + \frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} - by_7\,\hat{\mathbf{y}} + c\left(z_7 + \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4g)	S VII
$\mathbf{B_{29}}$	=	$x_8\,\mathbf{a}_1 + y_8\,\mathbf{a}_2 + z_8\,\mathbf{a}_3$	=	$(ax_8 + cz_8\cos\beta)\,\hat{\mathbf{x}} + by_8\,\hat{\mathbf{y}} + cz_8\sin\beta\,\hat{\mathbf{z}}$	(4g)	S VIII
$\mathbf{B_{30}}$	=	$-x_8\,\mathbf{a}_1 + y_8\,\mathbf{a}_2 - \left(z_8 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\left(ax_8 + c\left(z_8 - \frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} + by_8\,\hat{\mathbf{y}} - c\left(z_8 - \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4g)	S VIII
$\mathbf{B_{31}}$	=	$-x_8\,\mathbf{a}_1 - y_8\,\mathbf{a}_2 - z_8\,\mathbf{a}_3$	=	$-(ax_8 + cz_8\cos\beta)\,\hat{\mathbf{x}} - by_8\,\hat{\mathbf{y}} - cz_8\sin\beta\,\hat{\mathbf{z}}$	(4g)	S VIII
$\mathbf{B_{32}}$	=	$x_8\,\mathbf{a}_1 - y_8\,\mathbf{a}_2 + \left(z_8 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\left(ax_8 + c\left(z_8 + \frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} - by_8\,\hat{\mathbf{y}} + c\left(z_8 + \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4g)	S VIII

References

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