

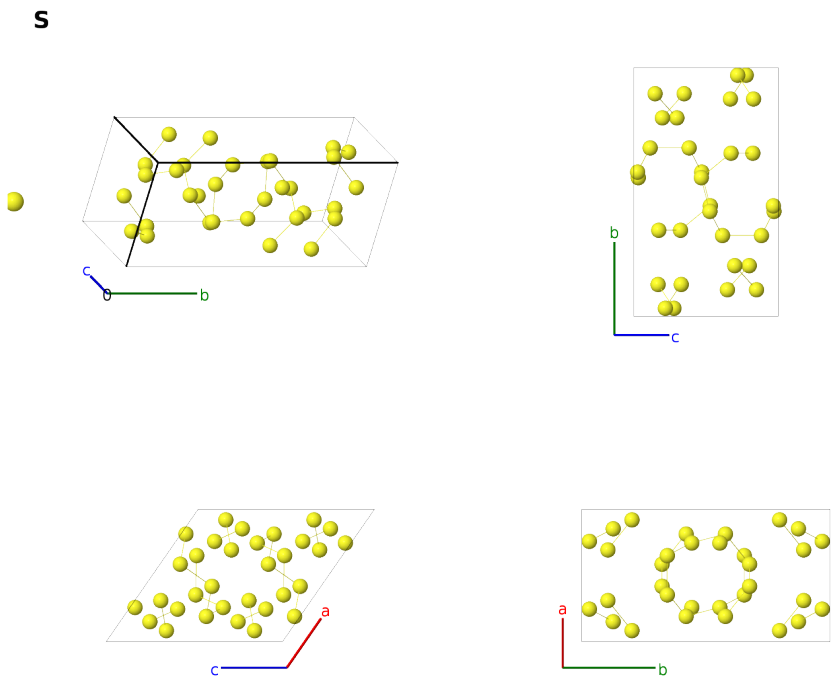
Rosickýite (γ -monoclinic Sulfur) Structure: A_mP32_13_8g-001

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<https://aflow.org/prototype-encyclopedia/Y7J6>

https://aflow.org/prototype-encyclopedia/A_mP32_13_8g-001



Prototype	S
AFLOW prototype label	A_mP32_13_8g-001
Mineral name	rosickýite
ICSD	66517
CCDC	1161501
Pearson symbol	mP32
Space group number	13
Space group symbol	$P2/c$
AFLOW prototype command	<code>aflow --proto=A_mP32_13_8g-001 --params=a, b/a, c/a, β, $x_1, y_1, z_1, x_2, y_2, z_2, x_3, y_3, z_3, x_4, y_4, z_4, x_5, y_5, z_5, x_6, y_6, z_6, x_7, y_7, z_7, x_8, y_8, z_8$</code>

Other compounds with this structure

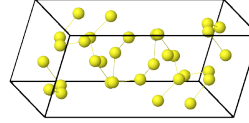
Se₃S₅

- 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

$$\begin{aligned} \mathbf{a}_1 &= a \hat{\mathbf{x}} \\ \mathbf{a}_2 &= b \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \cos \beta \hat{\mathbf{x}} + c \sin \beta \hat{\mathbf{z}} \end{aligned}$$

$\mathbf{a}_3^{\mathbf{a}_1}$
 $\mathbf{a}_2$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$x_1 \mathbf{a}_1 + y_1 \mathbf{a}_2 + z_1 \mathbf{a}_3$	=	$(ax_1 + cz_1 \cos \beta) \hat{\mathbf{x}} + by_1 \hat{\mathbf{y}} + cz_1 \sin \beta \hat{\mathbf{z}}$	(4g)	S I
$\mathbf{B}_2$	$-x_1 \mathbf{a}_1 + y_1 \mathbf{a}_2 - (z_1 - \frac{1}{2}) \mathbf{a}_3$	=	$-(ax_1 + c(z_1 - \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} + by_1 \hat{\mathbf{y}} - c(z_1 - \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(4g)	S I
$\mathbf{B}_3$	$-x_1 \mathbf{a}_1 - y_1 \mathbf{a}_2 - z_1 \mathbf{a}_3$	=	$-(ax_1 + cz_1 \cos \beta) \hat{\mathbf{x}} - by_1 \hat{\mathbf{y}} - cz_1 \sin \beta \hat{\mathbf{z}}$	(4g)	S I
$\mathbf{B}_4$	$x_1 \mathbf{a}_1 - y_1 \mathbf{a}_2 + (z_1 + \frac{1}{2}) \mathbf{a}_3$	=	$(ax_1 + c(z_1 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_1 \hat{\mathbf{y}} + c(z_1 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(4g)	S I
$\mathbf{B}_5$	$x_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	=	$(ax_2 + cz_2 \cos \beta) \hat{\mathbf{x}} + by_2 \hat{\mathbf{y}} + cz_2 \sin \beta \hat{\mathbf{z}}$	(4g)	S II
$\mathbf{B}_6$	$-x_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 - (z_2 - \frac{1}{2}) \mathbf{a}_3$	=	$-(ax_2 + c(z_2 - \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} + by_2 \hat{\mathbf{y}} - c(z_2 - \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(4g)	S II
$\mathbf{B}_7$	$-x_2 \mathbf{a}_1 - y_2 \mathbf{a}_2 - z_2 \mathbf{a}_3$	=	$-(ax_2 + cz_2 \cos \beta) \hat{\mathbf{x}} - by_2 \hat{\mathbf{y}} - cz_2 \sin \beta \hat{\mathbf{z}}$	(4g)	S II
$\mathbf{B}_8$	$x_2 \mathbf{a}_1 - y_2 \mathbf{a}_2 + (z_2 + \frac{1}{2}) \mathbf{a}_3$	=	$(ax_2 + c(z_2 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_2 \hat{\mathbf{y}} + c(z_2 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(4g)	S II
$\mathbf{B}_9$	$x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	=	$(ax_3 + cz_3 \cos \beta) \hat{\mathbf{x}} + by_3 \hat{\mathbf{y}} + cz_3 \sin \beta \hat{\mathbf{z}}$	(4g)	S III
$\mathbf{B}_{10}$	$-x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 - (z_3 - \frac{1}{2}) \mathbf{a}_3$	=	$-(ax_3 + c(z_3 - \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} + by_3 \hat{\mathbf{y}} - c(z_3 - \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(4g)	S III
$\mathbf{B}_{11}$	$-x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 - z_3 \mathbf{a}_3$	=	$-(ax_3 + cz_3 \cos \beta) \hat{\mathbf{x}} - by_3 \hat{\mathbf{y}} - cz_3 \sin \beta \hat{\mathbf{z}}$	(4g)	S III
$\mathbf{B}_{12}$	$x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$	=	$(ax_3 + c(z_3 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_3 \hat{\mathbf{y}} + c(z_3 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(4g)	S III
$\mathbf{B}_{13}$	$x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	=	$(ax_4 + cz_4 \cos \beta) \hat{\mathbf{x}} + by_4 \hat{\mathbf{y}} + cz_4 \sin \beta \hat{\mathbf{z}}$	(4g)	S IV
$\mathbf{B}_{14}$	$-x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 - (z_4 - \frac{1}{2}) \mathbf{a}_3$	=	$-(ax_4 + c(z_4 - \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} + by_4 \hat{\mathbf{y}} - c(z_4 - \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(4g)	S IV
$\mathbf{B}_{15}$	$-x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 - z_4 \mathbf{a}_3$	=	$-(ax_4 + cz_4 \cos \beta) \hat{\mathbf{x}} - by_4 \hat{\mathbf{y}} - cz_4 \sin \beta \hat{\mathbf{z}}$	(4g)	S IV
$\mathbf{B}_{16}$	$x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3$	=	$(ax_4 + c(z_4 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_4 \hat{\mathbf{y}} + c(z_4 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(4g)	S IV
$\mathbf{B}_{17}$	$x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	=	$(ax_5 + cz_5 \cos \beta) \hat{\mathbf{x}} + by_5 \hat{\mathbf{y}} + cz_5 \sin \beta \hat{\mathbf{z}}$	(4g)	S V

$$\begin{aligned}
\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) \hat{\mathbf{x}} + by_5 \hat{\mathbf{y}} - &(4g) & \text{S V} \\
&&& c\left(z_5 - \frac{1}{2}\right) \sin \beta \hat{\mathbf{z}} \\
\mathbf{B}_{19} &= -x_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 - z_5 \mathbf{a}_3 &= -(ax_5 + cz_5 \cos \beta) \hat{\mathbf{x}} - by_5 \hat{\mathbf{y}} - cz_5 \sin \beta \hat{\mathbf{z}} &(4g) & \text{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) \hat{\mathbf{x}} - by_5 \hat{\mathbf{y}} + &(4g) & \text{S V} \\
&&& c\left(z_5 + \frac{1}{2}\right) \sin \beta \hat{\mathbf{z}} \\
\mathbf{B}_{21} &= x_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3 &= (ax_6 + cz_6 \cos \beta) \hat{\mathbf{x}} + by_6 \hat{\mathbf{y}} + cz_6 \sin \beta \hat{\mathbf{z}} &(4g) & \text{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 &= -(ax_6 + c\left(z_6 - \frac{1}{2}\right) \cos \beta) \hat{\mathbf{x}} + by_6 \hat{\mathbf{y}} - &(4g) & \text{S VI} \\
&&& c\left(z_6 - \frac{1}{2}\right) \sin \beta \hat{\mathbf{z}} \\
\mathbf{B}_{23} &= -x_6 \mathbf{a}_1 - y_6 \mathbf{a}_2 - z_6 \mathbf{a}_3 &= -(ax_6 + cz_6 \cos \beta) \hat{\mathbf{x}} - by_6 \hat{\mathbf{y}} - cz_6 \sin \beta \hat{\mathbf{z}} &(4g) & \text{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}} + &(4g) & \text{S VI} \\
&&& c\left(z_6 + \frac{1}{2}\right) \sin \beta \hat{\mathbf{z}} \\
\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) & \text{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 &= -(ax_7 + c\left(z_7 - \frac{1}{2}\right) \cos \beta) \hat{\mathbf{x}} + by_7 \hat{\mathbf{y}} - &(4g) & \text{S VII} \\
&&& c\left(z_7 - \frac{1}{2}\right) \sin \beta \hat{\mathbf{z}} \\
\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) & \text{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}} + &(4g) & \text{S VII} \\
&&& c\left(z_7 + \frac{1}{2}\right) \sin \beta \hat{\mathbf{z}} \\
\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) & \text{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 &= -(ax_8 + c\left(z_8 - \frac{1}{2}\right) \cos \beta) \hat{\mathbf{x}} + by_8 \hat{\mathbf{y}} - &(4g) & \text{S VIII} \\
&&& c\left(z_8 - \frac{1}{2}\right) \sin \beta \hat{\mathbf{z}} \\
\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) & \text{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}} + &(4g) & \text{S VIII} \\
&&& c\left(z_8 + \frac{1}{2}\right) \sin \beta \hat{\mathbf{z}}
\end{aligned}$$

References

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Found in

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