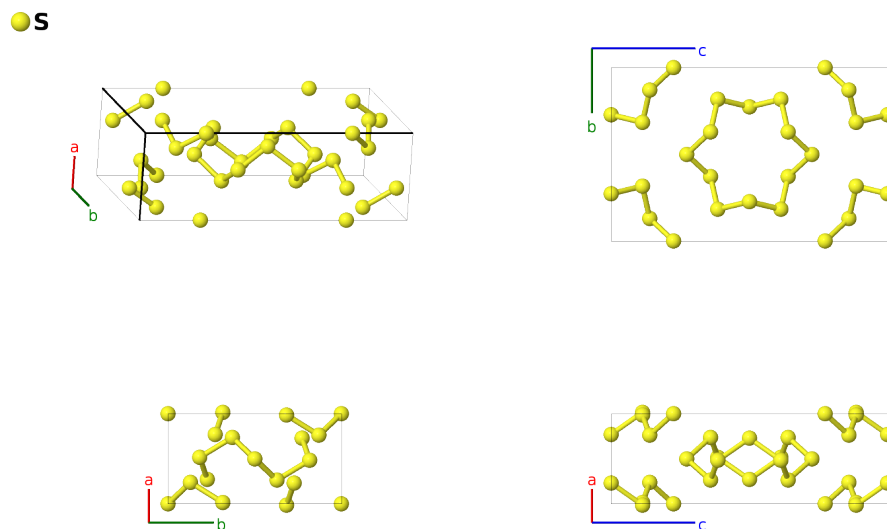


S₁₂ Sulfur Structure: A_oP24_58_eg2h-001

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<https://aflow.org/p/7TXG>

https://aflow.org/p/A_oP24_58_eg2h-001



Prototype	S
AFLOW prototype label	A_oP24_58_eg2h-001
ICSD	26463
Pearson symbol	oP24
Space group number	58
Space group symbol	<i>Pnmm</i>
AFLOW prototype command	<code>aflow --proto=A_oP24_58_eg2h-001 --params=a, b/a, c/a, z₁, x₂, y₂, x₃, y₃, z₃, x₄, y₄, z₄</code>

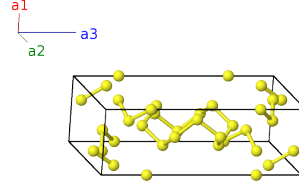
- We follow the notation of and (Donohue, 1974) and call this S₁₂ sulfur. Alternatively this can be called cyclododecasulfur. (Schmidt, 1966)
- We use the data in (Lin, 1970), but note that the Wyckoff positions given on page 30 are not consistent with space group *Pnmm* #58, found in (Kutoglu, 1966). Instead, they appear to be rotated so that $(xyz) \rightarrow (-zy - x)$, even though the lattice parameters are not similarly rotated. We rotated the coordinates to match those found in (Donohue, 1974). This gives the correct distances and angles in the 12-atom sulfur rings given by all the above authors.
- We take our data from (Lin, 1970), but this was never filed with the ICSD. Instead we use the ICSD entry from (Steidel, 1981).

Simple Orthorhombic primitive vectors

$$\mathbf{a}_1 = a \hat{\mathbf{x}}$$

$$\mathbf{a}_2 = b \hat{\mathbf{y}}$$

$$\mathbf{a}_3 = c \hat{\mathbf{z}}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
\mathbf{B}_1	$= z_1 \mathbf{a}_3$	$=$	$c z_1 \hat{\mathbf{z}}$	(4e)	S I
\mathbf{B}_2	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 - (z_1 - \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} b \hat{\mathbf{y}} - c (z_1 - \frac{1}{2}) \hat{\mathbf{z}}$	(4e)	S I
\mathbf{B}_3	$= -z_1 \mathbf{a}_3$	$=$	$-c z_1 \hat{\mathbf{z}}$	(4e)	S I
\mathbf{B}_4	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + (z_1 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} b \hat{\mathbf{y}} + c (z_1 + \frac{1}{2}) \hat{\mathbf{z}}$	(4e)	S I
\mathbf{B}_5	$= x_2 \mathbf{a}_1 + y_2 \mathbf{a}_2$	$=$	$a x_2 \hat{\mathbf{x}} + b y_2 \hat{\mathbf{y}}$	(4g)	S II
\mathbf{B}_6	$= -x_2 \mathbf{a}_1 - y_2 \mathbf{a}_2$	$=$	$-a x_2 \hat{\mathbf{x}} - b y_2 \hat{\mathbf{y}}$	(4g)	S II
\mathbf{B}_7	$= -(x_2 - \frac{1}{2}) \mathbf{a}_1 + (y_2 + \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-a (x_2 - \frac{1}{2}) \hat{\mathbf{x}} + b (y_2 + \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4g)	S II
\mathbf{B}_8	$= (x_2 + \frac{1}{2}) \mathbf{a}_1 - (y_2 - \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$a (x_2 + \frac{1}{2}) \hat{\mathbf{x}} - b (y_2 - \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4g)	S II
\mathbf{B}_9	$= x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$a x_3 \hat{\mathbf{x}} + b y_3 \hat{\mathbf{y}} + c z_3 \hat{\mathbf{z}}$	(8h)	S III
\mathbf{B}_{10}	$= -x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$-a x_3 \hat{\mathbf{x}} - b y_3 \hat{\mathbf{y}} + c z_3 \hat{\mathbf{z}}$	(8h)	S III
\mathbf{B}_{11}	$= -(x_3 - \frac{1}{2}) \mathbf{a}_1 + (y_3 + \frac{1}{2}) \mathbf{a}_2 - (z_3 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-a (x_3 - \frac{1}{2}) \hat{\mathbf{x}} + b (y_3 + \frac{1}{2}) \hat{\mathbf{y}} - c (z_3 - \frac{1}{2}) \hat{\mathbf{z}}$	(8h)	S III
\mathbf{B}_{12}	$= (x_3 + \frac{1}{2}) \mathbf{a}_1 - (y_3 - \frac{1}{2}) \mathbf{a}_2 - (z_3 - \frac{1}{2}) \mathbf{a}_3$	$=$	$a (x_3 + \frac{1}{2}) \hat{\mathbf{x}} - b (y_3 - \frac{1}{2}) \hat{\mathbf{y}} - c (z_3 - \frac{1}{2}) \hat{\mathbf{z}}$	(8h)	S III
\mathbf{B}_{13}	$= -x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$-a x_3 \hat{\mathbf{x}} - b y_3 \hat{\mathbf{y}} - c z_3 \hat{\mathbf{z}}$	(8h)	S III
\mathbf{B}_{14}	$= x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$a x_3 \hat{\mathbf{x}} + b y_3 \hat{\mathbf{y}} - c z_3 \hat{\mathbf{z}}$	(8h)	S III
\mathbf{B}_{15}	$= (x_3 + \frac{1}{2}) \mathbf{a}_1 - (y_3 - \frac{1}{2}) \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$	$=$	$a (x_3 + \frac{1}{2}) \hat{\mathbf{x}} - b (y_3 - \frac{1}{2}) \hat{\mathbf{y}} + c (z_3 + \frac{1}{2}) \hat{\mathbf{z}}$	(8h)	S III
\mathbf{B}_{16}	$= -(x_3 - \frac{1}{2}) \mathbf{a}_1 + (y_3 + \frac{1}{2}) \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a (x_3 - \frac{1}{2}) \hat{\mathbf{x}} + b (y_3 + \frac{1}{2}) \hat{\mathbf{y}} + c (z_3 + \frac{1}{2}) \hat{\mathbf{z}}$	(8h)	S III
\mathbf{B}_{17}	$= x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$a x_4 \hat{\mathbf{x}} + b y_4 \hat{\mathbf{y}} + c z_4 \hat{\mathbf{z}}$	(8h)	S IV
\mathbf{B}_{18}	$= -x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$-a x_4 \hat{\mathbf{x}} - b y_4 \hat{\mathbf{y}} + c z_4 \hat{\mathbf{z}}$	(8h)	S IV
\mathbf{B}_{19}	$= -(x_4 - \frac{1}{2}) \mathbf{a}_1 + (y_4 + \frac{1}{2}) \mathbf{a}_2 - (z_4 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-a (x_4 - \frac{1}{2}) \hat{\mathbf{x}} + b (y_4 + \frac{1}{2}) \hat{\mathbf{y}} - c (z_4 - \frac{1}{2}) \hat{\mathbf{z}}$	(8h)	S IV
\mathbf{B}_{20}	$= (x_4 + \frac{1}{2}) \mathbf{a}_1 - (y_4 - \frac{1}{2}) \mathbf{a}_2 - (z_4 - \frac{1}{2}) \mathbf{a}_3$	$=$	$a (x_4 + \frac{1}{2}) \hat{\mathbf{x}} - b (y_4 - \frac{1}{2}) \hat{\mathbf{y}} - c (z_4 - \frac{1}{2}) \hat{\mathbf{z}}$	(8h)	S IV
\mathbf{B}_{21}	$= -x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$-a x_4 \hat{\mathbf{x}} - b y_4 \hat{\mathbf{y}} - c z_4 \hat{\mathbf{z}}$	(8h)	S IV
\mathbf{B}_{22}	$= x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$a x_4 \hat{\mathbf{x}} + b y_4 \hat{\mathbf{y}} - c z_4 \hat{\mathbf{z}}$	(8h)	S IV
\mathbf{B}_{23}	$= (x_4 + \frac{1}{2}) \mathbf{a}_1 - (y_4 - \frac{1}{2}) \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3$	$=$	$a (x_4 + \frac{1}{2}) \hat{\mathbf{x}} - b (y_4 - \frac{1}{2}) \hat{\mathbf{y}} + c (z_4 + \frac{1}{2}) \hat{\mathbf{z}}$	(8h)	S IV

$$\mathbf{B}_{24} = \begin{matrix} -\left(x_4 - \frac{1}{2}\right) \mathbf{a}_1 + \left(y_4 + \frac{1}{2}\right) \mathbf{a}_2 + \\ \left(z_4 + \frac{1}{2}\right) \mathbf{a}_3 \end{matrix} = -a\left(x_4 - \frac{1}{2}\right) \hat{\mathbf{x}} + b\left(y_4 + \frac{1}{2}\right) \hat{\mathbf{y}} + c\left(z_4 + \frac{1}{2}\right) \hat{\mathbf{z}} \quad (8h) \quad \text{S IV}$$

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