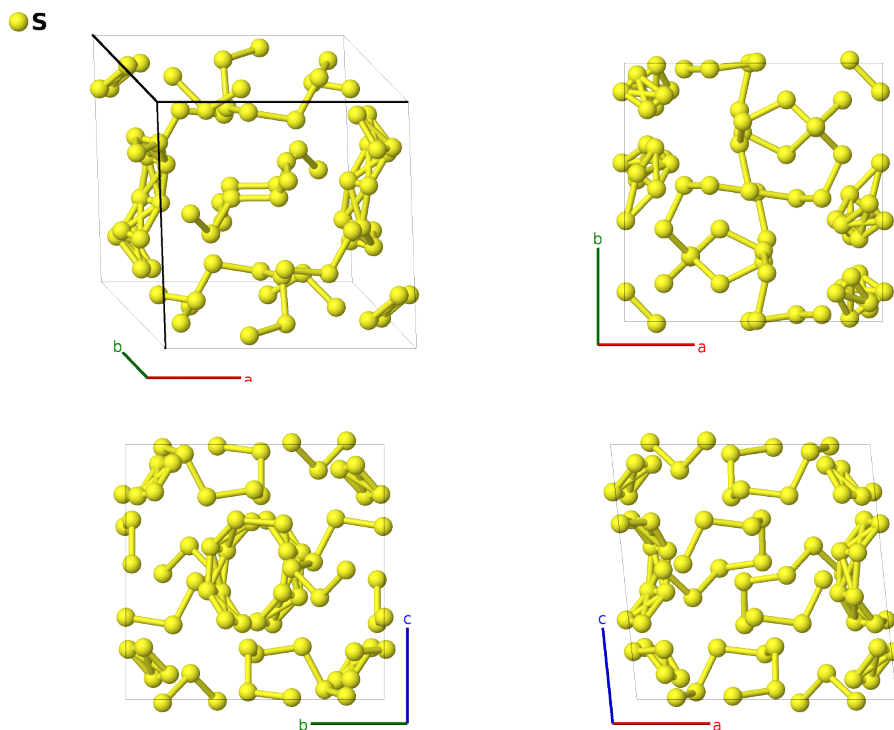


# $\beta$ -monoclinic Sulfur Structure: A\_mP64\_14\_16e-002

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<https://aflow.org/p/AYZW>

[https://aflow.org/p/A\\_mP64\\_14\\_16e-002](https://aflow.org/p/A_mP64_14_16e-002)



Prototype	S
AFLOW prototype label	A_mP64_14_16e-002
ICSD	870
Pearson symbol	mP64
Space group number	14
Space group symbol	$P2_1/c$
AFLOW prototype command	<pre>aflow --proto=A_mP64_14_16e-002       --params=a,b/a,c/a,<math>\beta</math>,x<sub>1</sub>,y<sub>1</sub>,z<sub>1</sub>,x<sub>2</sub>,y<sub>2</sub>,z<sub>2</sub>,x<sub>3</sub>,y<sub>3</sub>,z<sub>3</sub>,x<sub>4</sub>,y<sub>4</sub>,z<sub>4</sub>,x<sub>5</sub>,y<sub>5</sub>,z<sub>5</sub>,x<sub>6</sub>,y<sub>6</sub>,z<sub>6</sub>,x<sub>7</sub>, y<sub>7</sub>,z<sub>7</sub>,x<sub>8</sub>,y<sub>8</sub>,z<sub>8</sub>,x<sub>9</sub>,y<sub>9</sub>,z<sub>9</sub>,x<sub>10</sub>,y<sub>10</sub>,z<sub>10</sub>,x<sub>11</sub>,y<sub>11</sub>,z<sub>11</sub>,x<sub>12</sub>,y<sub>12</sub>,z<sub>12</sub>,x<sub>13</sub>,y<sub>13</sub>,z<sub>13</sub>,x<sub>14</sub>,y<sub>14</sub>,z<sub>14</sub>,x<sub>15</sub>, y<sub>15</sub>,z<sub>15</sub>,x<sub>16</sub>,y<sub>16</sub>,z<sub>16</sub></pre>

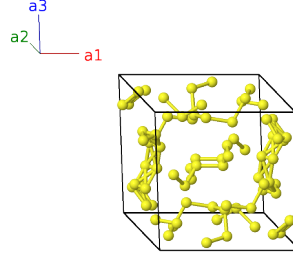
- We take the name of this structure from (Donohue, 1976). This is the high temperature phase of sulfur, stable from 95°C to the melting point at 115°C, although it can be kept at room temperatures for some time. (Templeton, 1976)
- This is a refinement of the original structure found by (Sands, 1965). There are two types of sulfur atoms in this sample:

- atoms S-I through S-VIII form stable sulfur rings with all the sites fully occupied, just as in the ground state  $\alpha$ -S (A16).
- Atoms S-IX through S-XVI form a ring with one of two orientations, randomly chosen.
- The S-IX through S-XVI sites are thus half occupied, so there are only 48 atoms and six sulfur rings in any unit cell. Contrast this with  $A_k$  selenium, which has eight complete rings in the unit cell.
- Both  $A_k$  selenium and  $\beta$ -monoclinic sulfur have the same AFLOW prototype label, A\_mP64\_14\_16e. They are generated by the same symmetry operations with different sets of parameters (`--params`) specified in their corresponding CIF files.

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### Simple Monoclinic primitive vectors

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




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### Basis vectors

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



$$\begin{aligned}
\mathbf{B}_{46} &= -x_{12} \mathbf{a}_1 + \left(y_{12} + \frac{1}{2}\right) \mathbf{a}_2 - (z_{12} - \frac{1}{2}) \mathbf{a}_3 &= -\left(ax_{12} + c\left(z_{12} - \frac{1}{2}\right) \cos \beta\right) \hat{\mathbf{x}} + b\left(y_{12} + \frac{1}{2}\right) \hat{\mathbf{y}} - c\left(z_{12} - \frac{1}{2}\right) \sin \beta \hat{\mathbf{z}} &(4e) & \text{S XII} \\
\mathbf{B}_{47} &= -x_{12} \mathbf{a}_1 - y_{12} \mathbf{a}_2 - z_{12} \mathbf{a}_3 &= -\left(ax_{12} + cz_{12} \cos \beta\right) \hat{\mathbf{x}} - by_{12} \hat{\mathbf{y}} - cz_{12} \sin \beta \hat{\mathbf{z}} &(4e) & \text{S XII} \\
\mathbf{B}_{48} &= x_{12} \mathbf{a}_1 - \left(y_{12} - \frac{1}{2}\right) \mathbf{a}_2 + \left(z_{12} + \frac{1}{2}\right) \mathbf{a}_3 &= \left(ax_{12} + c\left(z_{12} + \frac{1}{2}\right) \cos \beta\right) \hat{\mathbf{x}} - b\left(y_{12} - \frac{1}{2}\right) \hat{\mathbf{y}} + c\left(z_{12} + \frac{1}{2}\right) \sin \beta \hat{\mathbf{z}} &(4e) & \text{S XII} \\
\mathbf{B}_{49} &= x_{13} \mathbf{a}_1 + y_{13} \mathbf{a}_2 + z_{13} \mathbf{a}_3 &= \left(ax_{13} + cz_{13} \cos \beta\right) \hat{\mathbf{x}} + by_{13} \hat{\mathbf{y}} + cz_{13} \sin \beta \hat{\mathbf{z}} &(4e) & \text{S XIII} \\
\mathbf{B}_{50} &= -x_{13} \mathbf{a}_1 + \left(y_{13} + \frac{1}{2}\right) \mathbf{a}_2 - \left(z_{13} - \frac{1}{2}\right) \mathbf{a}_3 &= -\left(ax_{13} + c\left(z_{13} - \frac{1}{2}\right) \cos \beta\right) \hat{\mathbf{x}} + b\left(y_{13} + \frac{1}{2}\right) \hat{\mathbf{y}} - c\left(z_{13} - \frac{1}{2}\right) \sin \beta \hat{\mathbf{z}} &(4e) & \text{S XIII} \\
\mathbf{B}_{51} &= -x_{13} \mathbf{a}_1 - y_{13} \mathbf{a}_2 - z_{13} \mathbf{a}_3 &= -\left(ax_{13} + cz_{13} \cos \beta\right) \hat{\mathbf{x}} - by_{13} \hat{\mathbf{y}} - cz_{13} \sin \beta \hat{\mathbf{z}} &(4e) & \text{S XIII} \\
\mathbf{B}_{52} &= x_{13} \mathbf{a}_1 - \left(y_{13} - \frac{1}{2}\right) \mathbf{a}_2 + \left(z_{13} + \frac{1}{2}\right) \mathbf{a}_3 &= \left(ax_{13} + c\left(z_{13} + \frac{1}{2}\right) \cos \beta\right) \hat{\mathbf{x}} - b\left(y_{13} - \frac{1}{2}\right) \hat{\mathbf{y}} + c\left(z_{13} + \frac{1}{2}\right) \sin \beta \hat{\mathbf{z}} &(4e) & \text{S XIII} \\
\mathbf{B}_{53} &= x_{14} \mathbf{a}_1 + y_{14} \mathbf{a}_2 + z_{14} \mathbf{a}_3 &= \left(ax_{14} + cz_{14} \cos \beta\right) \hat{\mathbf{x}} + by_{14} \hat{\mathbf{y}} + cz_{14} \sin \beta \hat{\mathbf{z}} &(4e) & \text{S XIV} \\
\mathbf{B}_{54} &= -x_{14} \mathbf{a}_1 + \left(y_{14} + \frac{1}{2}\right) \mathbf{a}_2 - \left(z_{14} - \frac{1}{2}\right) \mathbf{a}_3 &= -\left(ax_{14} + c\left(z_{14} - \frac{1}{2}\right) \cos \beta\right) \hat{\mathbf{x}} + b\left(y_{14} + \frac{1}{2}\right) \hat{\mathbf{y}} - c\left(z_{14} - \frac{1}{2}\right) \sin \beta \hat{\mathbf{z}} &(4e) & \text{S XIV} \\
\mathbf{B}_{55} &= -x_{14} \mathbf{a}_1 - y_{14} \mathbf{a}_2 - z_{14} \mathbf{a}_3 &= -\left(ax_{14} + cz_{14} \cos \beta\right) \hat{\mathbf{x}} - by_{14} \hat{\mathbf{y}} - cz_{14} \sin \beta \hat{\mathbf{z}} &(4e) & \text{S XIV} \\
\mathbf{B}_{56} &= x_{14} \mathbf{a}_1 - \left(y_{14} - \frac{1}{2}\right) \mathbf{a}_2 + \left(z_{14} + \frac{1}{2}\right) \mathbf{a}_3 &= \left(ax_{14} + c\left(z_{14} + \frac{1}{2}\right) \cos \beta\right) \hat{\mathbf{x}} - b\left(y_{14} - \frac{1}{2}\right) \hat{\mathbf{y}} + c\left(z_{14} + \frac{1}{2}\right) \sin \beta \hat{\mathbf{z}} &(4e) & \text{S XIV} \\
\mathbf{B}_{57} &= x_{15} \mathbf{a}_1 + y_{15} \mathbf{a}_2 + z_{15} \mathbf{a}_3 &= \left(ax_{15} + cz_{15} \cos \beta\right) \hat{\mathbf{x}} + by_{15} \hat{\mathbf{y}} + cz_{15} \sin \beta \hat{\mathbf{z}} &(4e) & \text{S XV} \\
\mathbf{B}_{58} &= -x_{15} \mathbf{a}_1 + \left(y_{15} + \frac{1}{2}\right) \mathbf{a}_2 - \left(z_{15} - \frac{1}{2}\right) \mathbf{a}_3 &= -\left(ax_{15} + c\left(z_{15} - \frac{1}{2}\right) \cos \beta\right) \hat{\mathbf{x}} + b\left(y_{15} + \frac{1}{2}\right) \hat{\mathbf{y}} - c\left(z_{15} - \frac{1}{2}\right) \sin \beta \hat{\mathbf{z}} &(4e) & \text{S XV} \\
\mathbf{B}_{59} &= -x_{15} \mathbf{a}_1 - y_{15} \mathbf{a}_2 - z_{15} \mathbf{a}_3 &= -\left(ax_{15} + cz_{15} \cos \beta\right) \hat{\mathbf{x}} - by_{15} \hat{\mathbf{y}} - cz_{15} \sin \beta \hat{\mathbf{z}} &(4e) & \text{S XV} \\
\mathbf{B}_{60} &= x_{15} \mathbf{a}_1 - \left(y_{15} - \frac{1}{2}\right) \mathbf{a}_2 + \left(z_{15} + \frac{1}{2}\right) \mathbf{a}_3 &= \left(ax_{15} + c\left(z_{15} + \frac{1}{2}\right) \cos \beta\right) \hat{\mathbf{x}} - b\left(y_{15} - \frac{1}{2}\right) \hat{\mathbf{y}} + c\left(z_{15} + \frac{1}{2}\right) \sin \beta \hat{\mathbf{z}} &(4e) & \text{S XV} \\
\mathbf{B}_{61} &= x_{16} \mathbf{a}_1 + y_{16} \mathbf{a}_2 + z_{16} \mathbf{a}_3 &= \left(ax_{16} + cz_{16} \cos \beta\right) \hat{\mathbf{x}} + by_{16} \hat{\mathbf{y}} + cz_{16} \sin \beta \hat{\mathbf{z}} &(4e) & \text{S XVI} \\
\mathbf{B}_{62} &= -x_{16} \mathbf{a}_1 + \left(y_{16} + \frac{1}{2}\right) \mathbf{a}_2 - \left(z_{16} - \frac{1}{2}\right) \mathbf{a}_3 &= -\left(ax_{16} + c\left(z_{16} - \frac{1}{2}\right) \cos \beta\right) \hat{\mathbf{x}} + b\left(y_{16} + \frac{1}{2}\right) \hat{\mathbf{y}} - c\left(z_{16} - \frac{1}{2}\right) \sin \beta \hat{\mathbf{z}} &(4e) & \text{S XVI} \\
\mathbf{B}_{63} &= -x_{16} \mathbf{a}_1 - y_{16} \mathbf{a}_2 - z_{16} \mathbf{a}_3 &= -\left(ax_{16} + cz_{16} \cos \beta\right) \hat{\mathbf{x}} - by_{16} \hat{\mathbf{y}} - cz_{16} \sin \beta \hat{\mathbf{z}} &(4e) & \text{S XVI} \\
\mathbf{B}_{64} &= x_{16} \mathbf{a}_1 - \left(y_{16} - \frac{1}{2}\right) \mathbf{a}_2 + \left(z_{16} + \frac{1}{2}\right) \mathbf{a}_3 &= \left(ax_{16} + c\left(z_{16} + \frac{1}{2}\right) \cos \beta\right) \hat{\mathbf{x}} - b\left(y_{16} - \frac{1}{2}\right) \hat{\mathbf{y}} + c\left(z_{16} + \frac{1}{2}\right) \sin \beta \hat{\mathbf{z}} &(4e) & \text{S XVI}
\end{aligned}$$

## References

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