S_6 (ρ-S) Sulfur Structure: A_hR6_148_f-001

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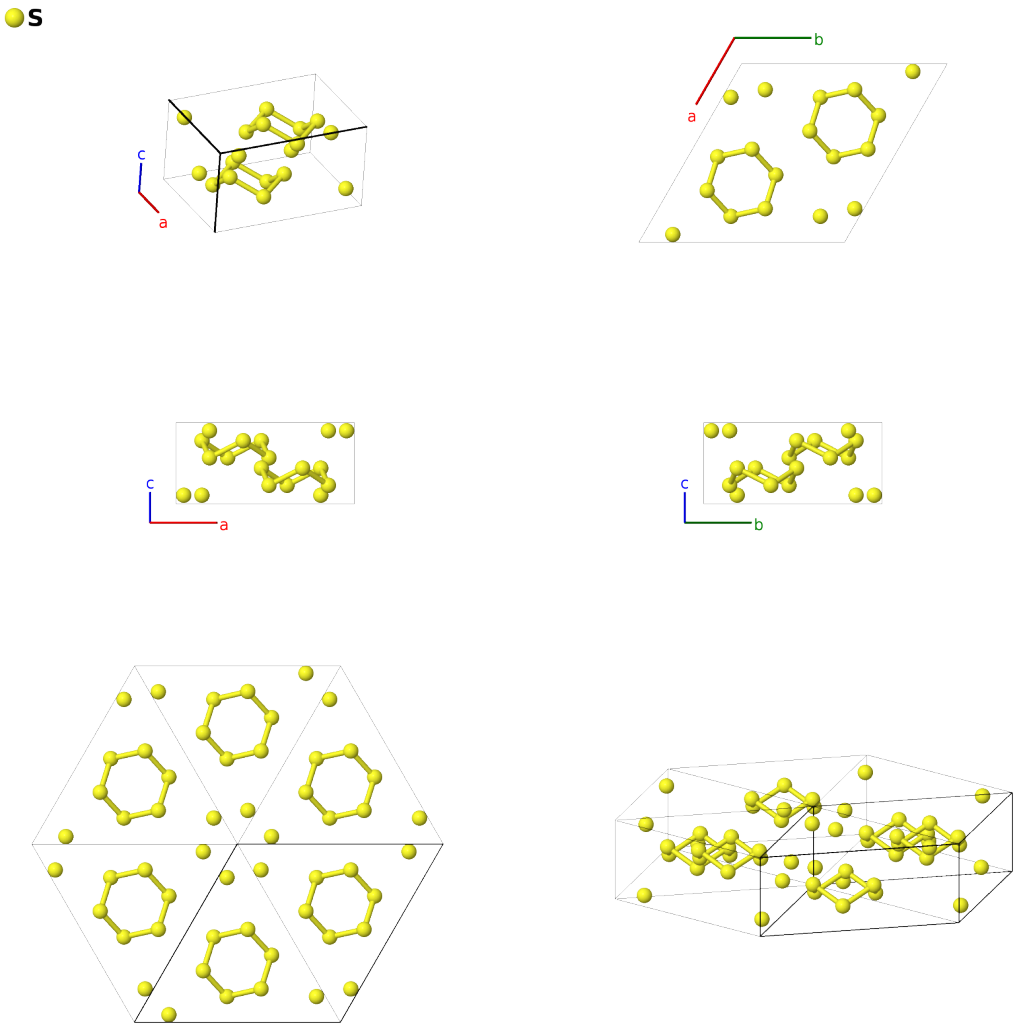
https://aflow.org/p/XW0B

https://aflow.org/p/A_hR6_148_f-001

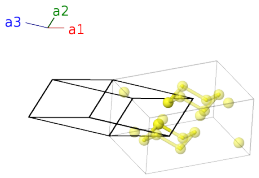


Prototype	S
AFLOW prototype label	A_hR6_148_f-001
ICSD	27495
Pearson symbol	hR6
Space group number	148
Space group symbol	$R\bar{3}$
AFLOW prototype command	`aflow --proto=A_hR6_148_f-001 --params=`$a, c/a, x_1, y_1, z_1$

- We follow the notation of (Donohue, 1961) and (Donhoue, 1974) and call this S_6 sulfur. Alternative names are: rhombohedral sulfur, trigonal sulfur, Engel's sulfur, Aten's sulfur, ϵ-sulfur, and ρ-sulfur. (Donohue, 1974)
- Hexagonal settings of this structure can be obtained with the option `--hex`.

Rhombohedral primitive vectors

$$
\begin{aligned}
\mathbf{a_1} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \tfrac{1}{3}c\,\hat{\mathbf{z}} \\
\mathbf{a_2} &= \tfrac{1}{\sqrt{3}}a\,\hat{\mathbf{y}} + \tfrac{1}{3}c\,\hat{\mathbf{z}} \\
\mathbf{a_3} &= -\tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \tfrac{1}{3}c\,\hat{\mathbf{z}}
\end{aligned}
$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$x_1\,\mathbf{a}_1 + y_1\,\mathbf{a}_2 + z_1\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_1 - z_1)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,(x_1 - 2y_1 + z_1)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(x_1 + y_1 + z_1)\,\hat{\mathbf{z}}$	(6f)	S I
$\mathbf{B_2}$	=	$z_1\,\mathbf{a}_1 + x_1\,\mathbf{a}_2 + y_1\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(y_1 - z_1)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(2x_1 - y_1 - z_1)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(x_1 + y_1 + z_1)\,\hat{\mathbf{z}}$	(6f)	S I
$\mathbf{B_3}$	=	$y_1\,\mathbf{a}_1 + z_1\,\mathbf{a}_2 + x_1\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(x_1 - y_1)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,(x_1 + y_1 - 2z_1)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(x_1 + y_1 + z_1)\,\hat{\mathbf{z}}$	(6f)	S I
$\mathbf{B_4}$	=	$-x_1\,\mathbf{a}_1 - y_1\,\mathbf{a}_2 - z_1\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(x_1 - z_1)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(x_1 - 2y_1 + z_1)\,\hat{\mathbf{y}} - \frac{1}{3}c\,(x_1 + y_1 + z_1)\,\hat{\mathbf{z}}$	(6f)	S I
$\mathbf{B_5}$	=	$-z_1\,\mathbf{a}_1 - x_1\,\mathbf{a}_2 - y_1\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(y_1 - z_1)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,(2x_1 - y_1 - z_1)\,\hat{\mathbf{y}} - \frac{1}{3}c\,(x_1 + y_1 + z_1)\,\hat{\mathbf{z}}$	(6f)	S I
$\mathbf{B_6}$	=	$-y_1\,\mathbf{a}_1 - z_1\,\mathbf{a}_2 - x_1\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_1 - y_1)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(x_1 + y_1 - 2z_1)\,\hat{\mathbf{y}} - \frac{1}{3}c\,(x_1 + y_1 + z_1)\,\hat{\mathbf{z}}$	(6f)	S I

References

[1] J. Donohue, A. Caron, and E. Goldish, *The Crystal and Molecular Structure of S_6 (Sulfur-6)*, J. Am. Chem. Soc. **83**, 3748–3751 (1961), doi:10.1021/ja01479a003.

Found in

[1] J. Donohue, *The Structures of the Elements* (Robert E. Krieger Publishing Company, New York, 1974).