

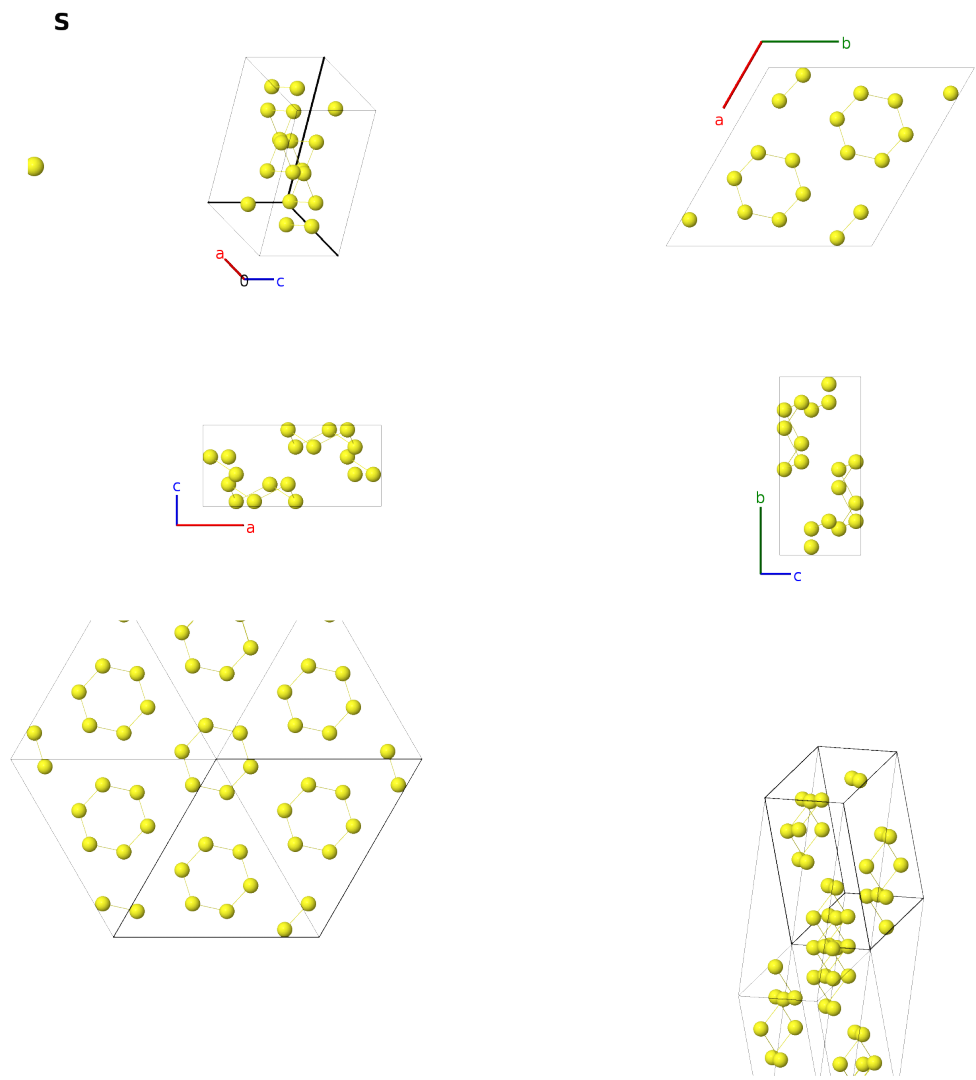
S₆ (ρ -S) Sulfur Structure: A_hR6_148_f-001

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<https://aflow.org/prototype-encyclopedia/XW0B>

https://aflow.org/prototype-encyclopedia/A_hR6_148_f-001



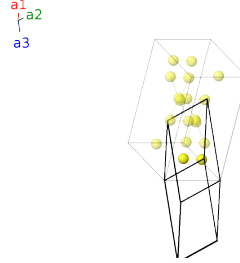
Prototype	S
AFLOW prototype label	A_hR6_148_f-001
ICSD	27495
CCDC	1602768
Pearson symbol	hR6

Space group number	148
Space group symbol	$R\bar{3}$
AFLOW prototype command	<code>aflow --proto=A_hR6_148_f-001</code> <code>--params=a, c/a, x₁, y₁, z₁</code>

- 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

$$\begin{aligned}\mathbf{a}_1 &= \frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + \frac{1}{3}c \hat{\mathbf{z}} \\ \mathbf{a}_2 &= \frac{1}{\sqrt{3}}a \hat{\mathbf{y}} + \frac{1}{3}c \hat{\mathbf{z}} \\ \mathbf{a}_3 &= -\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + \frac{1}{3}c \hat{\mathbf{z}}\end{aligned}$$



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).

First cited in

H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettel, M. Esters, X. Campilongo, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*, Comput. Mater. Sci. **240**, 112988 (2024), doi: 10.1016/j.commatsci.2024.112988.