

γ -Se (A8) Structure: A_hP3_152_a-001

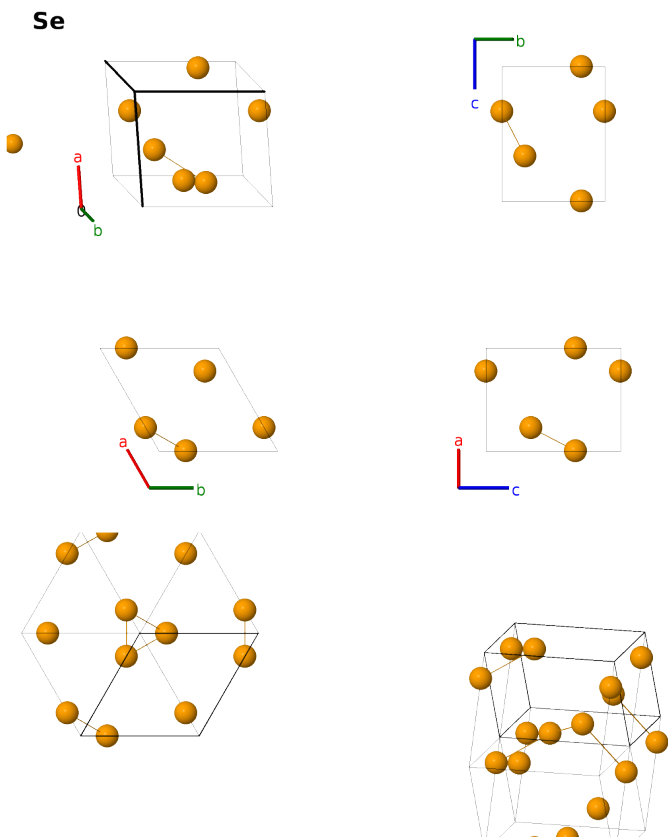
This structure previously used the label(s) **A_hP3_152_a**. Calls to these addresses will be redirected here.

Cite this page as:

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<https://aflow.org/prototype-encyclopedia/SM1V>

https://aflow.org/prototype-encyclopedia/A_hP3_152_a-001



Prototype	Se
AFLOW prototype label	A_hP3_152_a-001
<i>Strukturbericht</i> designation	A8
ICSD	22251
CCDC	1599025
Pearson symbol	hP3
Space group number	152
Space group symbol	$P3_121$

AFLOW prototype command `aflow --proto=A_hP3_152_a-001`
 `--params=a, c/a, x1`

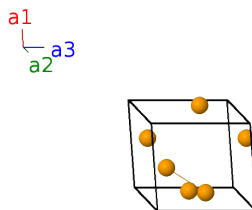
Other compounds with this structure

Te, SeTe, Se₃Te

- There are a variety of naming conventions for selenium:
- (Cherin, 1967) refers to this structure as “trigonal selenium.” (Donohue, 1982) refers to it as the α -Se structure, calling what we designate α -Se and β -Se (A_l) as “monoclinic α ” and “monoclinic β ,” respectively.
- When $x = 1/3$ this reduces to the A_i (β -Po) or $A10$ (α -Hg) structure.
 - If, in addition, $c = \sqrt{6}a$, then the structure becomes fcc ($A1$).
 - On the other hand, if $c = \sqrt{3/2}a$, then the structure becomes simple cubic (A_h).
- This structure can also be found in the enantiomorphic space group $P3_212$ #153.

Trigonal (Hexagonal) primitive vectors

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



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= x_1 \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_3$	$=$	$\frac{1}{2}ax_1\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_1\hat{\mathbf{y}} + \frac{1}{3}c\hat{\mathbf{z}}$	(3a)	Se I
$\mathbf{B}_2$	$= x_1 \mathbf{a}_2 + \frac{2}{3} \mathbf{a}_3$	$=$	$\frac{1}{2}ax_1\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_1\hat{\mathbf{y}} + \frac{2}{3}c\hat{\mathbf{z}}$	(3a)	Se I
$\mathbf{B}_3$	$= -x_1 \mathbf{a}_1 - x_1 \mathbf{a}_2$	$=$	$-ax_1\hat{\mathbf{x}}$	(3a)	Se I

References

- [1] P. Cherin and P. Unger, *The crystal structure of trigonal selenium*, Inorg. Chem. **6**, 1589–1591 (1967), doi:10.1021/ic50054a037.

Found in

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

First cited in

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