# $\gamma$-Se ($A8$) Structure: A_hP3_152_a-001

This structure originally had the label `A_hP3_152_a`. Calls to that address will be redirected here.

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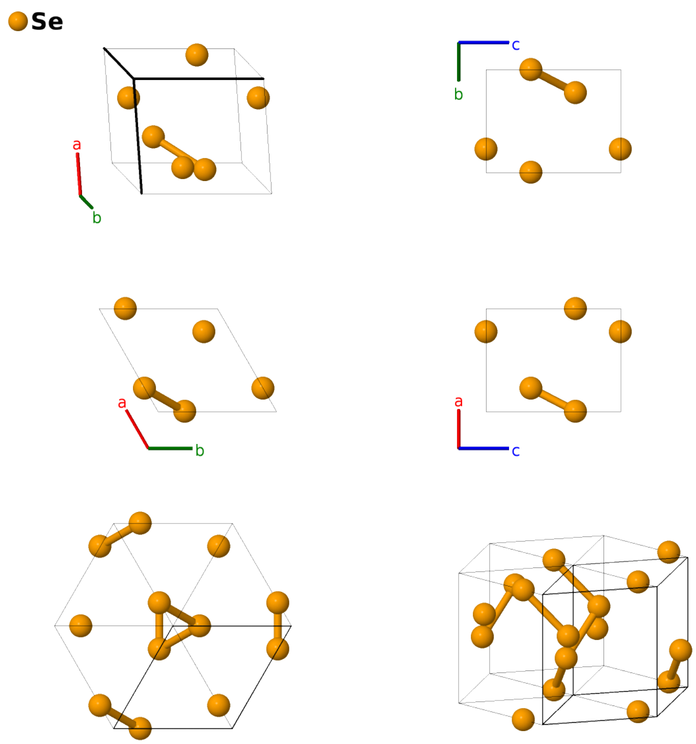
https://aflow.org/p/SM1V

https://aflow.org/p/A_hP3_152_a-001




| | |
|---|---|
| **Prototype** | Se |
| **AFLOW prototype label** | A_hP3_152_a-001 |
| ***Strukturbericht* designation** | $A8$ |
| **ICSD** | 22251 |
| **Pearson symbol** | hP3 |
| **Space group number** | 152 |
| **Space group symbol** | $P3_121$ |
| **AFLOW prototype command** | `aflow --proto=A_hP3_152_a-001`<br>`--params=`$a, c/a, x_1$ |

**Other compounds with this structure**
Te, SeTe, $Se_3Te$

- 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 $\alpha$-Se structure, calling what we designate $\alpha$-Se and $\beta$-Se ($A_l$) as "monoclinic $\alpha$" and "monoclinic $\beta$," respectively.
- When $x = 1/3$ this reduces to the $A_i$ ($\beta$-Po) or $A10$ ($\alpha$-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 $P3_2$ #153.

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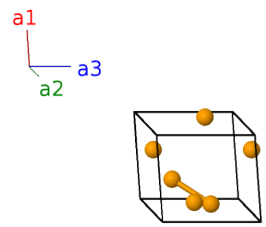
**Trigonal (Hexagonal) primitive vectors**

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

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**Basis vectors**

| | | Lattice coordinates | | Cartesian coordinates | Wyckoff position | Atom type |
|---|---|---|---|---|---|---|
| $\mathbf{B_1}$ | = | $x_1\,\mathbf{a}_1 + \frac{1}{3}\,\mathbf{a}_3$ | = | $\frac{1}{2}ax_1\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_1\,\hat{\mathbf{y}} + \frac{1}{3}c\,\hat{\mathbf{z}}$ | (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).