

# GeS<sub>2</sub> (C44) Structure: AB2\_oF72\_43\_ab\_3b-001

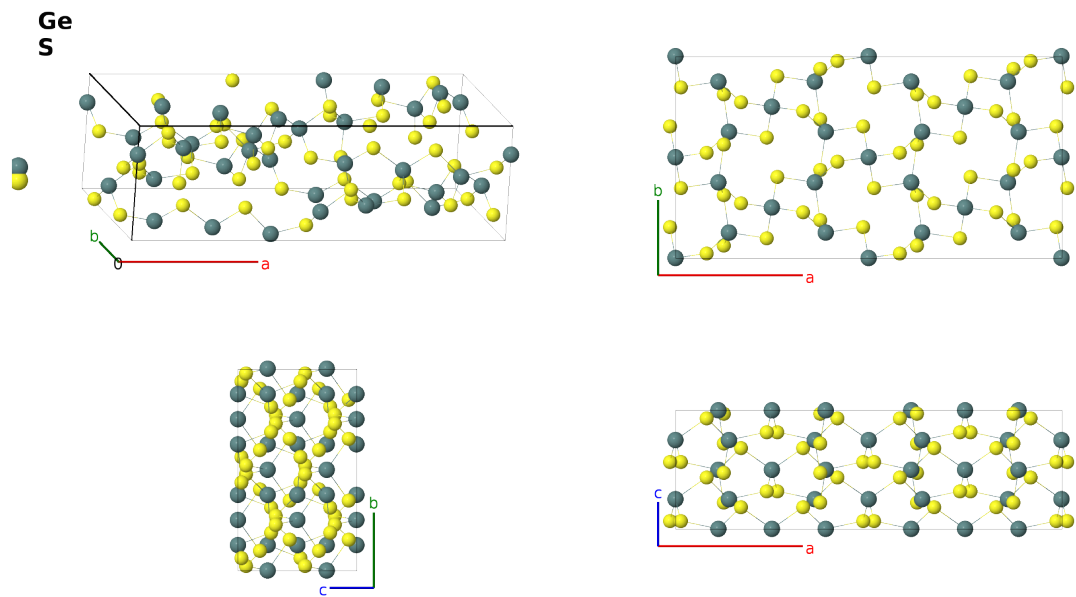
This structure previously used the label(s) **AB2\_oF72\_43\_ab\_3b**. Calls to these addresses will be redirected here.

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- D. Hicks, M. J. Mehl, M. Esters, C. Oses, O. Levy, G. L. W. Hart, C. Toher, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 3*, Comput. Mater. Sci. **199**, 110450 (2021), doi: 10.1016/j.commatsci.2021.110450.

<https://aflow.org/prototype-encyclopedia/4KUZ>

[https://aflow.org/prototype-encyclopedia/AB2\\_oF72\\_43\\_ab\\_3b-001](https://aflow.org/prototype-encyclopedia/AB2_oF72_43_ab_3b-001)



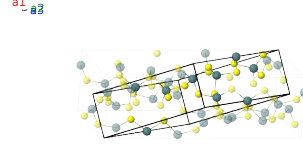
|                                    |                                                                                                                                                                                                                                                                           |
|------------------------------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Prototype                          | GeS <sub>2</sub>                                                                                                                                                                                                                                                          |
| AFLOW prototype label              | AB2_oF72_43_ab_3b-001                                                                                                                                                                                                                                                     |
| <i>Strukturbericht</i> designation | C44                                                                                                                                                                                                                                                                       |
| ICSD                               | 31685                                                                                                                                                                                                                                                                     |
| CCDC                               | 1605683                                                                                                                                                                                                                                                                   |
| Pearson symbol                     | oF72                                                                                                                                                                                                                                                                      |
| Space group number                 | 43                                                                                                                                                                                                                                                                        |
| Space group symbol                 | <i>Fdd</i> 2                                                                                                                                                                                                                                                              |
| AFLOW prototype command            | <code>aflow --proto=AB2_oF72_43_ab_3b-001</code><br><code>--params=a,b/a,c/a,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></code> |

## Other compounds with this structure

GeSe<sub>2</sub>

## Face-centered Orthorhombic primitive vectors

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



## Basis vectors

|                   | Lattice<br>coordinates                                                                                                                          |     | Cartesian<br>coordinates                                                                                              | Wyckoff<br>position | Atom<br>type |
|-------------------|-------------------------------------------------------------------------------------------------------------------------------------------------|-----|-----------------------------------------------------------------------------------------------------------------------|---------------------|--------------|
| $\mathbf{B}_1$    | $= z_1 \mathbf{a}_1 + z_1 \mathbf{a}_2 - z_1 \mathbf{a}_3$                                                                                      | $=$ | $cz_1 \hat{\mathbf{z}}$                                                                                               | (8a)                | Ge I         |
| $\mathbf{B}_2$    | $= (z_1 + \frac{1}{4}) \mathbf{a}_1 + (z_1 + \frac{1}{4}) \mathbf{a}_2 - (z_1 - \frac{1}{4}) \mathbf{a}_3$                                      | $=$ | $\frac{1}{4}a\hat{\mathbf{x}} + \frac{1}{4}b\hat{\mathbf{y}} + c(z_1 + \frac{1}{4})\hat{\mathbf{z}}$                  | (8a)                | Ge I         |
| $\mathbf{B}_3$    | $= (-x_2 + y_2 + z_2) \mathbf{a}_1 + (x_2 - y_2 + z_2) \mathbf{a}_2 + (x_2 + y_2 - z_2) \mathbf{a}_3$                                           | $=$ | $ax_2\hat{\mathbf{x}} + by_2\hat{\mathbf{y}} + cz_2\hat{\mathbf{z}}$                                                  | (16b)               | Ge II        |
| $\mathbf{B}_4$    | $= (x_2 - y_2 + z_2) \mathbf{a}_1 + (-x_2 + y_2 + z_2) \mathbf{a}_2 - (x_2 + y_2 + z_2) \mathbf{a}_3$                                           | $=$ | $-ax_2\hat{\mathbf{x}} - by_2\hat{\mathbf{y}} + cz_2\hat{\mathbf{z}}$                                                 | (16b)               | Ge II        |
| $\mathbf{B}_5$    | $= -(x_2 + y_2 - z_2 - \frac{1}{4}) \mathbf{a}_1 + (x_2 + y_2 + z_2 + \frac{1}{4}) \mathbf{a}_2 + (x_2 - y_2 - z_2 + \frac{1}{4}) \mathbf{a}_3$ | $=$ | $a(x_2 + \frac{1}{4})\hat{\mathbf{x}} - b(y_2 - \frac{1}{4})\hat{\mathbf{y}} + c(z_2 + \frac{1}{4})\hat{\mathbf{z}}$  | (16b)               | Ge II        |
| $\mathbf{B}_6$    | $= (x_2 + y_2 + z_2 + \frac{1}{4}) \mathbf{a}_1 - (x_2 + y_2 - z_2 - \frac{1}{4}) \mathbf{a}_2 - (x_2 - y_2 + z_2 - \frac{1}{4}) \mathbf{a}_3$  | $=$ | $-a(x_2 - \frac{1}{4})\hat{\mathbf{x}} + b(y_2 + \frac{1}{4})\hat{\mathbf{y}} + c(z_2 + \frac{1}{4})\hat{\mathbf{z}}$ | (16b)               | Ge II        |
| $\mathbf{B}_7$    | $= (-x_3 + y_3 + z_3) \mathbf{a}_1 + (x_3 - y_3 + z_3) \mathbf{a}_2 + (x_3 + y_3 - z_3) \mathbf{a}_3$                                           | $=$ | $ax_3\hat{\mathbf{x}} + by_3\hat{\mathbf{y}} + cz_3\hat{\mathbf{z}}$                                                  | (16b)               | S I          |
| $\mathbf{B}_8$    | $= (x_3 - y_3 + z_3) \mathbf{a}_1 + (-x_3 + y_3 + z_3) \mathbf{a}_2 - (x_3 + y_3 + z_3) \mathbf{a}_3$                                           | $=$ | $-ax_3\hat{\mathbf{x}} - by_3\hat{\mathbf{y}} + cz_3\hat{\mathbf{z}}$                                                 | (16b)               | S I          |
| $\mathbf{B}_9$    | $= -(x_3 + y_3 - z_3 - \frac{1}{4}) \mathbf{a}_1 + (x_3 + y_3 + z_3 + \frac{1}{4}) \mathbf{a}_2 + (x_3 - y_3 - z_3 + \frac{1}{4}) \mathbf{a}_3$ | $=$ | $a(x_3 + \frac{1}{4})\hat{\mathbf{x}} - b(y_3 - \frac{1}{4})\hat{\mathbf{y}} + c(z_3 + \frac{1}{4})\hat{\mathbf{z}}$  | (16b)               | S I          |
| $\mathbf{B}_{10}$ | $= (x_3 + y_3 + z_3 + \frac{1}{4}) \mathbf{a}_1 - (x_3 + y_3 - z_3 - \frac{1}{4}) \mathbf{a}_2 - (x_3 - y_3 + z_3 - \frac{1}{4}) \mathbf{a}_3$  | $=$ | $-a(x_3 - \frac{1}{4})\hat{\mathbf{x}} + b(y_3 + \frac{1}{4})\hat{\mathbf{y}} + c(z_3 + \frac{1}{4})\hat{\mathbf{z}}$ | (16b)               | S I          |
| $\mathbf{B}_{11}$ | $= (-x_4 + y_4 + z_4) \mathbf{a}_1 + (x_4 - y_4 + z_4) \mathbf{a}_2 + (x_4 + y_4 - z_4) \mathbf{a}_3$                                           | $=$ | $ax_4\hat{\mathbf{x}} + by_4\hat{\mathbf{y}} + cz_4\hat{\mathbf{z}}$                                                  | (16b)               | S II         |
| $\mathbf{B}_{12}$ | $= (x_4 - y_4 + z_4) \mathbf{a}_1 + (-x_4 + y_4 + z_4) \mathbf{a}_2 - (x_4 + y_4 + z_4) \mathbf{a}_3$                                           | $=$ | $-ax_4\hat{\mathbf{x}} - by_4\hat{\mathbf{y}} + cz_4\hat{\mathbf{z}}$                                                 | (16b)               | S II         |
| $\mathbf{B}_{13}$ | $= -(x_4 + y_4 - z_4 - \frac{1}{4}) \mathbf{a}_1 + (x_4 + y_4 + z_4 + \frac{1}{4}) \mathbf{a}_2 + (x_4 - y_4 - z_4 + \frac{1}{4}) \mathbf{a}_3$ | $=$ | $a(x_4 + \frac{1}{4})\hat{\mathbf{x}} - b(y_4 - \frac{1}{4})\hat{\mathbf{y}} + c(z_4 + \frac{1}{4})\hat{\mathbf{z}}$  | (16b)               | S II         |

$$\begin{aligned}
\mathbf{B}_{14} &= \begin{pmatrix} x_4 + y_4 + z_4 + \frac{1}{4} \\ x_4 + y_4 - z_4 - \frac{1}{4} \\ x_4 - y_4 + z_4 - \frac{1}{4} \end{pmatrix} \mathbf{a}_1 - &= -a \left( x_4 - \frac{1}{4} \right) \hat{\mathbf{x}} + b \left( y_4 + \frac{1}{4} \right) \hat{\mathbf{y}} + c \left( z_4 + \frac{1}{4} \right) \hat{\mathbf{z}} & (16b) & \text{S II} \\
\mathbf{B}_{15} &= \begin{pmatrix} -x_5 + y_5 + z_5 \\ x_5 - y_5 + z_5 \\ x_5 + y_5 - z_5 \end{pmatrix} \mathbf{a}_1 + &= ax_5 \hat{\mathbf{x}} + by_5 \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}} & (16b) & \text{S III} \\
\mathbf{B}_{16} &= \begin{pmatrix} x_5 - y_5 + z_5 \\ -x_5 + y_5 + z_5 \\ x_5 + y_5 - z_5 \end{pmatrix} \mathbf{a}_1 + &= -ax_5 \hat{\mathbf{x}} - by_5 \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}} & (16b) & \text{S III} \\
\mathbf{B}_{17} &= \begin{pmatrix} -(x_5 + y_5 - z_5 - \frac{1}{4}) \\ x_5 + y_5 + z_5 + \frac{1}{4} \\ x_5 - y_5 - z_5 + \frac{1}{4} \end{pmatrix} \mathbf{a}_1 + &= a \left( x_5 + \frac{1}{4} \right) \hat{\mathbf{x}} - b \left( y_5 - \frac{1}{4} \right) \hat{\mathbf{y}} + c \left( z_5 + \frac{1}{4} \right) \hat{\mathbf{z}} & (16b) & \text{S III} \\
\mathbf{B}_{18} &= \begin{pmatrix} x_5 + y_5 + z_5 + \frac{1}{4} \\ x_5 + y_5 - z_5 - \frac{1}{4} \\ x_5 - y_5 + z_5 - \frac{1}{4} \end{pmatrix} \mathbf{a}_1 - &= -a \left( x_5 - \frac{1}{4} \right) \hat{\mathbf{x}} + b \left( y_5 + \frac{1}{4} \right) \hat{\mathbf{y}} + c \left( z_5 + \frac{1}{4} \right) \hat{\mathbf{z}} & (16b) & \text{S III}
\end{aligned}$$

## References

- [1] W. H. Zachariasen, *The Crystal Structure of Germanium Disulphide*, J. Chem. Phys. **4**, 618–619 (1936), doi:10.1063/1.1749915.

## Found in

- [1] R. T. Downs and M. Hall-Wallace, *The American Mineralogist Crystal Structure Database*, Am. Mineral. **88**, 247–250 (2003).

## First cited in

- M. J. Mehl, D. Hicks, C. Toher, O. Levy, R. M. Hanson, G. L. W. Hart, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 1*, Comput. Mater. Sci. **136**, S1-828 (2017). doi: 10.1016/j.commatsci.2017.01.017