

# Co<sub>9</sub>S<sub>8</sub> (*D*8<sub>9</sub>) Structure: A9B8\_cF68\_225\_af\_ce-001

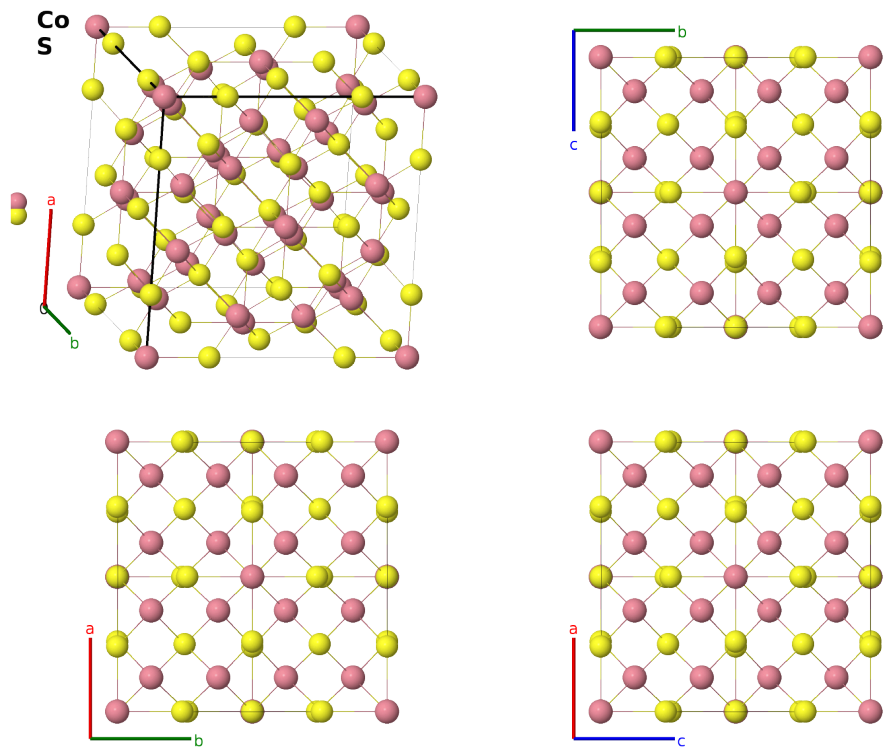
This structure previously used the label(s) **A9B8\_cF68\_225\_af\_ce**. Calls to these addresses will be redirected here.

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<https://aflow.org/prototype-encyclopedia/X1EM>

[https://aflow.org/prototype-encyclopedia/A9B8\\_cF68\\_225\\_af\\_ce-001](https://aflow.org/prototype-encyclopedia/A9B8_cF68_225_af_ce-001)



|                                    |                                                                                                                                  |
|------------------------------------|----------------------------------------------------------------------------------------------------------------------------------|
| Prototype                          | Co <sub>9</sub> S <sub>8</sub>                                                                                                   |
| AFLOW prototype label              | A9B8_cF68_225_af_ce-001                                                                                                          |
| <i>Strukturbericht</i> designation | <i>D</i> 8 <sub>9</sub>                                                                                                          |
| ICSD                               | 23929                                                                                                                            |
| CCDC                               | 1599989                                                                                                                          |
| Pearson symbol                     | cF68                                                                                                                             |
| Space group number                 | 225                                                                                                                              |
| Space group symbol                 | <i>Fm</i> $\bar{3}$ <i>m</i>                                                                                                     |
| AFLOW prototype command            | <code>aflow --proto=A9B8_cF68_225_af_ce-001</code><br><code>--params=<i>a</i>, <i>x</i><sub>3</sub>, <i>x</i><sub>4</sub></code> |

## Other compounds with this structure

(Fe, Ni)<sub>9</sub>S<sub>8</sub> (pentlandite), Co<sub>9</sub>Se<sub>8</sub>, Co<sub>8</sub>FeS<sub>8</sub>, Co<sub>8</sub>NiS<sub>8</sub>, Co<sub>8</sub>PdS<sub>8</sub>, Co<sub>8</sub>RhS<sub>8</sub>, Co<sub>8</sub>RuS<sub>8</sub>, Fe<sub>4</sub>Ni<sub>4</sub>PdS<sub>8</sub>, Fe<sub>4</sub>Ni<sub>4</sub>RhS<sub>8</sub>, Fe<sub>4</sub>Ni<sub>4</sub>RuS<sub>8</sub>

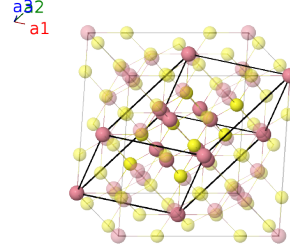
- (Geller,1962) placed the first Co atom at the (4b) Wyckoff position. We have shifted this to the origin, the (4a) Wyckoff position.

## Face-centered Cubic primitive vectors

$$\mathbf{a}_1 = \frac{1}{2}a \hat{\mathbf{y}} + \frac{1}{2}a \hat{\mathbf{z}}$$

$$\mathbf{a}_2 = \frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{2}a \hat{\mathbf{z}}$$

$$\mathbf{a}_3 = \frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{2}a \hat{\mathbf{y}}$$



## Basis vectors

|                   | Lattice<br>coordinates |                                                                                  | Cartesian<br>coordinates | Wyckoff<br>position                                                                             | Atom<br>type |
|-------------------|------------------------|----------------------------------------------------------------------------------|--------------------------|-------------------------------------------------------------------------------------------------|--------------|
| $\mathbf{B}_1$    | =                      | 0                                                                                | =                        | 0                                                                                               | (4a) Co I    |
| $\mathbf{B}_2$    | =                      | $\frac{1}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$ | =                        | $\frac{1}{4}a \hat{\mathbf{x}} + \frac{1}{4}a \hat{\mathbf{y}} + \frac{1}{4}a \hat{\mathbf{z}}$ | (8c) S I     |
| $\mathbf{B}_3$    | =                      | $\frac{3}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$ | =                        | $\frac{3}{4}a \hat{\mathbf{x}} + \frac{3}{4}a \hat{\mathbf{y}} + \frac{3}{4}a \hat{\mathbf{z}}$ | (8c) S I     |
| $\mathbf{B}_4$    | =                      | $-x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + x_3 \mathbf{a}_3$                        | =                        | $ax_3 \hat{\mathbf{x}}$                                                                         | (24e) S II   |
| $\mathbf{B}_5$    | =                      | $x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 - x_3 \mathbf{a}_3$                         | =                        | $-ax_3 \hat{\mathbf{x}}$                                                                        | (24e) S II   |
| $\mathbf{B}_6$    | =                      | $x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 + x_3 \mathbf{a}_3$                         | =                        | $ax_3 \hat{\mathbf{y}}$                                                                         | (24e) S II   |
| $\mathbf{B}_7$    | =                      | $-x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 - x_3 \mathbf{a}_3$                        | =                        | $-ax_3 \hat{\mathbf{y}}$                                                                        | (24e) S II   |
| $\mathbf{B}_8$    | =                      | $x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 - x_3 \mathbf{a}_3$                         | =                        | $ax_3 \hat{\mathbf{z}}$                                                                         | (24e) S II   |
| $\mathbf{B}_9$    | =                      | $-x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 + x_3 \mathbf{a}_3$                        | =                        | $-ax_3 \hat{\mathbf{z}}$                                                                        | (24e) S II   |
| $\mathbf{B}_{10}$ | =                      | $x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + x_4 \mathbf{a}_3$                         | =                        | $ax_4 \hat{\mathbf{x}} + ax_4 \hat{\mathbf{y}} + ax_4 \hat{\mathbf{z}}$                         | (32f) Co II  |
| $\mathbf{B}_{11}$ | =                      | $x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 - 3x_4 \mathbf{a}_3$                        | =                        | $-ax_4 \hat{\mathbf{x}} - ax_4 \hat{\mathbf{y}} + ax_4 \hat{\mathbf{z}}$                        | (32f) Co II  |
| $\mathbf{B}_{12}$ | =                      | $x_4 \mathbf{a}_1 - 3x_4 \mathbf{a}_2 + x_4 \mathbf{a}_3$                        | =                        | $-ax_4 \hat{\mathbf{x}} + ax_4 \hat{\mathbf{y}} - ax_4 \hat{\mathbf{z}}$                        | (32f) Co II  |
| $\mathbf{B}_{13}$ | =                      | $-3x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + x_4 \mathbf{a}_3$                       | =                        | $ax_4 \hat{\mathbf{x}} - ax_4 \hat{\mathbf{y}} - ax_4 \hat{\mathbf{z}}$                         | (32f) Co II  |
| $\mathbf{B}_{14}$ | =                      | $-x_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 + 3x_4 \mathbf{a}_3$                       | =                        | $ax_4 \hat{\mathbf{x}} + ax_4 \hat{\mathbf{y}} - ax_4 \hat{\mathbf{z}}$                         | (32f) Co II  |
| $\mathbf{B}_{15}$ | =                      | $-x_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 - x_4 \mathbf{a}_3$                        | =                        | $-ax_4 \hat{\mathbf{x}} - ax_4 \hat{\mathbf{y}} - ax_4 \hat{\mathbf{z}}$                        | (32f) Co II  |
| $\mathbf{B}_{16}$ | =                      | $-x_4 \mathbf{a}_1 + 3x_4 \mathbf{a}_2 - x_4 \mathbf{a}_3$                       | =                        | $ax_4 \hat{\mathbf{x}} - ax_4 \hat{\mathbf{y}} + ax_4 \hat{\mathbf{z}}$                         | (32f) Co II  |
| $\mathbf{B}_{17}$ | =                      | $3x_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 - x_4 \mathbf{a}_3$                        | =                        | $-ax_4 \hat{\mathbf{x}} + ax_4 \hat{\mathbf{y}} + ax_4 \hat{\mathbf{z}}$                        | (32f) Co II  |

## References

- [1] S. Geller, *Refinement of the crystal structure of Co<sub>9</sub>S<sub>8</sub>*, Acta Cryst. **15**, 1195–1198 (1962), doi:10.1107/S0365110X62003187.

## First cited in

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