

GeCd₄S₆ Structure:

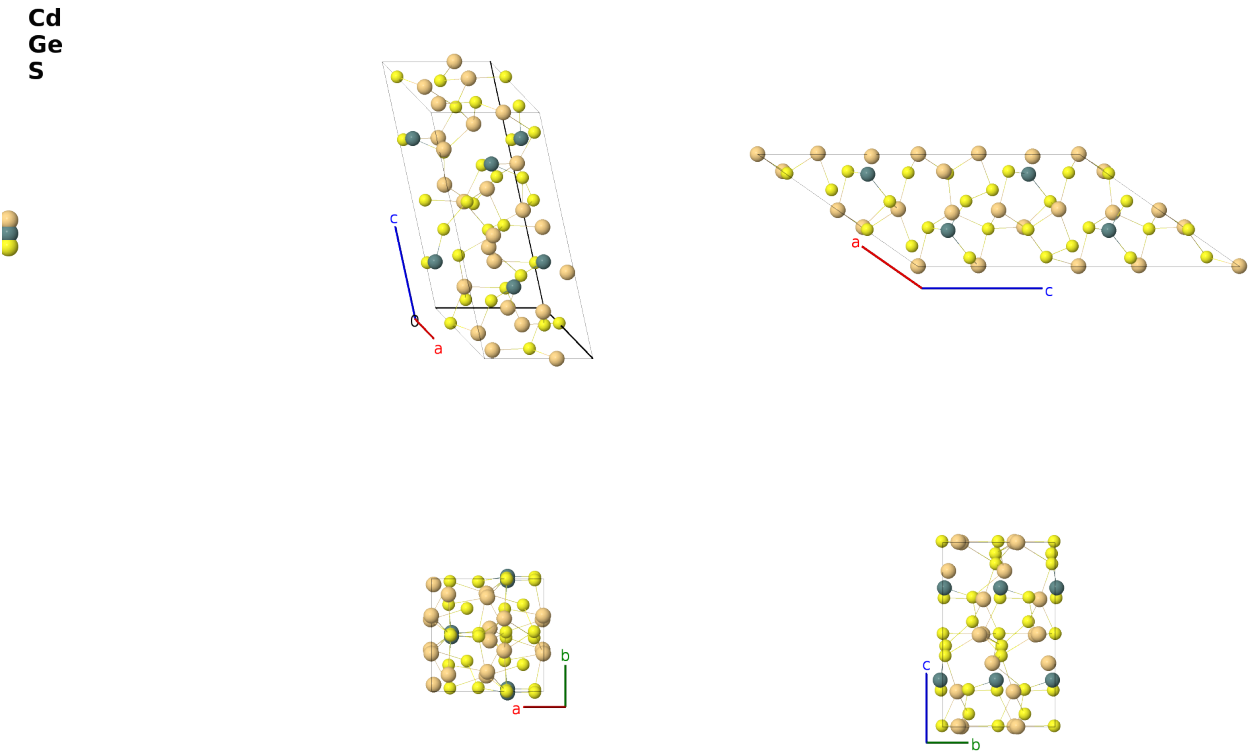
A4BC6_mC44_9_4a_a_6a-001

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<https://aflow.org/prototype-encyclopedia/ZP3W>

https://aflow.org/prototype-encyclopedia/A4BC6_mC44_9_4a_a_6a-001



Prototype	Cd ₄ GeS ₆
AFLOW prototype label	A4BC6_mC44_9_4a_a_6a-001
ICSD	26214
CCDC	1601643
Pearson symbol	mC44
Space group number	9
Space group symbol	Cc
AFLOW prototype command	<pre>aflow --proto=A4BC6_mC44_9_4a_a_6a-001 --params=a,b/a,c/a,β,x₁,y₁,z₁,x₂,y₂,z₂,x₃,y₃,z₃,x₄,y₄,z₄,x₅,y₅,z₅,x₆,y₆,z₆,x₇, y₇,z₇,x₈,y₈,z₈,x₉,y₉,z₉,x₁₀,y₁₀,z₁₀,x₁₁,y₁₁,z₁₁</pre>

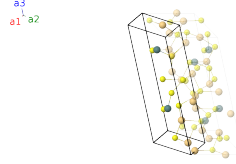
Other compounds with this structure

GeCd₄Se₆

- The is apparently the GeCd₄S₅ found in (Pearson, 1967). See the discussion in (Susa, 1971).

Base-centered Monoclinic primitive vectors

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



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$(x_1 - y_1) \mathbf{a}_1 + (x_1 + y_1) \mathbf{a}_2 + z_1 \mathbf{a}_3$	=	$(ax_1 + cz_1 \cos \beta) \hat{\mathbf{x}} + by_1 \hat{\mathbf{y}} + cz_1 \sin \beta \hat{\mathbf{z}}$	(4a)	Cd I
$\mathbf{B}_2$	$(x_1 + y_1) \mathbf{a}_1 + (x_1 - y_1) \mathbf{a}_2 + (z_1 + \frac{1}{2}) \mathbf{a}_3$	=	$(ax_1 + c(z_1 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_1 \hat{\mathbf{y}} + c(z_1 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(4a)	Cd I
$\mathbf{B}_3$	$(x_2 - y_2) \mathbf{a}_1 + (x_2 + y_2) \mathbf{a}_2 + z_2 \mathbf{a}_3$	=	$(ax_2 + cz_2 \cos \beta) \hat{\mathbf{x}} + by_2 \hat{\mathbf{y}} + cz_2 \sin \beta \hat{\mathbf{z}}$	(4a)	Cd II
$\mathbf{B}_4$	$(x_2 + y_2) \mathbf{a}_1 + (x_2 - y_2) \mathbf{a}_2 + (z_2 + \frac{1}{2}) \mathbf{a}_3$	=	$(ax_2 + c(z_2 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_2 \hat{\mathbf{y}} + c(z_2 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(4a)	Cd II
$\mathbf{B}_5$	$(x_3 - y_3) \mathbf{a}_1 + (x_3 + y_3) \mathbf{a}_2 + z_3 \mathbf{a}_3$	=	$(ax_3 + cz_3 \cos \beta) \hat{\mathbf{x}} + by_3 \hat{\mathbf{y}} + cz_3 \sin \beta \hat{\mathbf{z}}$	(4a)	Cd III
$\mathbf{B}_6$	$(x_3 + y_3) \mathbf{a}_1 + (x_3 - y_3) \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$	=	$(ax_3 + c(z_3 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_3 \hat{\mathbf{y}} + c(z_3 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(4a)	Cd III
$\mathbf{B}_7$	$(x_4 - y_4) \mathbf{a}_1 + (x_4 + y_4) \mathbf{a}_2 + z_4 \mathbf{a}_3$	=	$(ax_4 + cz_4 \cos \beta) \hat{\mathbf{x}} + by_4 \hat{\mathbf{y}} + cz_4 \sin \beta \hat{\mathbf{z}}$	(4a)	Cd IV
$\mathbf{B}_8$	$(x_4 + y_4) \mathbf{a}_1 + (x_4 - y_4) \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3$	=	$(ax_4 + c(z_4 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_4 \hat{\mathbf{y}} + c(z_4 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(4a)	Cd IV
$\mathbf{B}_9$	$(x_5 - y_5) \mathbf{a}_1 + (x_5 + y_5) \mathbf{a}_2 + z_5 \mathbf{a}_3$	=	$(ax_5 + cz_5 \cos \beta) \hat{\mathbf{x}} + by_5 \hat{\mathbf{y}} + cz_5 \sin \beta \hat{\mathbf{z}}$	(4a)	Ge I
$\mathbf{B}_{10}$	$(x_5 + y_5) \mathbf{a}_1 + (x_5 - y_5) \mathbf{a}_2 + (z_5 + \frac{1}{2}) \mathbf{a}_3$	=	$(ax_5 + c(z_5 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_5 \hat{\mathbf{y}} + c(z_5 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(4a)	Ge I
$\mathbf{B}_{11}$	$(x_6 - y_6) \mathbf{a}_1 + (x_6 + y_6) \mathbf{a}_2 + z_6 \mathbf{a}_3$	=	$(ax_6 + cz_6 \cos \beta) \hat{\mathbf{x}} + by_6 \hat{\mathbf{y}} + cz_6 \sin \beta \hat{\mathbf{z}}$	(4a)	S I
$\mathbf{B}_{12}$	$(x_6 + y_6) \mathbf{a}_1 + (x_6 - y_6) \mathbf{a}_2 + (z_6 + \frac{1}{2}) \mathbf{a}_3$	=	$(ax_6 + c(z_6 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_6 \hat{\mathbf{y}} + c(z_6 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(4a)	S I
$\mathbf{B}_{13}$	$(x_7 - y_7) \mathbf{a}_1 + (x_7 + y_7) \mathbf{a}_2 + z_7 \mathbf{a}_3$	=	$(ax_7 + cz_7 \cos \beta) \hat{\mathbf{x}} + by_7 \hat{\mathbf{y}} + cz_7 \sin \beta \hat{\mathbf{z}}$	(4a)	S II
$\mathbf{B}_{14}$	$(x_7 + y_7) \mathbf{a}_1 + (x_7 - y_7) \mathbf{a}_2 + (z_7 + \frac{1}{2}) \mathbf{a}_3$	=	$(ax_7 + c(z_7 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_7 \hat{\mathbf{y}} + c(z_7 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(4a)	S II
$\mathbf{B}_{15}$	$(x_8 - y_8) \mathbf{a}_1 + (x_8 + y_8) \mathbf{a}_2 + z_8 \mathbf{a}_3$	=	$(ax_8 + cz_8 \cos \beta) \hat{\mathbf{x}} + by_8 \hat{\mathbf{y}} + cz_8 \sin \beta \hat{\mathbf{z}}$	(4a)	S III

$$\begin{aligned}
\mathbf{B}_{16} &= \begin{pmatrix} (x_8 + y_8) \mathbf{a}_1 + (x_8 - y_8) \mathbf{a}_2 + \\ (z_8 + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = \begin{pmatrix} (ax_8 + c(z_8 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_8 \hat{\mathbf{y}} + \\ c(z_8 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}} \end{pmatrix} & (4a) & \text{S III} \\
\mathbf{B}_{17} &= \begin{pmatrix} (x_9 - y_9) \mathbf{a}_1 + (x_9 + y_9) \mathbf{a}_2 + \\ z_9 \mathbf{a}_3 \end{pmatrix} = \begin{pmatrix} (ax_9 + cz_9 \cos \beta) \hat{\mathbf{x}} + by_9 \hat{\mathbf{y}} + cz_9 \sin \beta \hat{\mathbf{z}} \end{pmatrix} & (4a) & \text{S IV} \\
\mathbf{B}_{18} &= \begin{pmatrix} (x_9 + y_9) \mathbf{a}_1 + (x_9 - y_9) \mathbf{a}_2 + \\ (z_9 + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = \begin{pmatrix} (ax_9 + c(z_9 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_9 \hat{\mathbf{y}} + \\ c(z_9 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}} \end{pmatrix} & (4a) & \text{S IV} \\
\mathbf{B}_{19} &= \begin{pmatrix} (x_{10} - y_{10}) \mathbf{a}_1 + \\ (x_{10} + y_{10}) \mathbf{a}_2 + z_{10} \mathbf{a}_3 \end{pmatrix} = \begin{pmatrix} (ax_{10} + cz_{10} \cos \beta) \hat{\mathbf{x}} + by_{10} \hat{\mathbf{y}} + cz_{10} \sin \beta \hat{\mathbf{z}} \end{pmatrix} & (4a) & \text{S V} \\
\mathbf{B}_{20} &= \begin{pmatrix} (x_{10} + y_{10}) \mathbf{a}_1 + \\ (x_{10} - y_{10}) \mathbf{a}_2 + (z_{10} + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = \begin{pmatrix} (ax_{10} + c(z_{10} + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_{10} \hat{\mathbf{y}} + \\ c(z_{10} + \frac{1}{2}) \sin \beta \hat{\mathbf{z}} \end{pmatrix} & (4a) & \text{S V} \\
\mathbf{B}_{21} &= \begin{pmatrix} (x_{11} - y_{11}) \mathbf{a}_1 + \\ (x_{11} + y_{11}) \mathbf{a}_2 + z_{11} \mathbf{a}_3 \end{pmatrix} = \begin{pmatrix} (ax_{11} + cz_{11} \cos \beta) \hat{\mathbf{x}} + by_{11} \hat{\mathbf{y}} + cz_{11} \sin \beta \hat{\mathbf{z}} \end{pmatrix} & (4a) & \text{S VI} \\
\mathbf{B}_{22} &= \begin{pmatrix} (x_{11} + y_{11}) \mathbf{a}_1 + \\ (x_{11} - y_{11}) \mathbf{a}_2 + (z_{11} + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = \begin{pmatrix} (ax_{11} + c(z_{11} + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_{11} \hat{\mathbf{y}} + \\ c(z_{11} + \frac{1}{2}) \sin \beta \hat{\mathbf{z}} \end{pmatrix} & (4a) & \text{S VI}
\end{aligned}$$

References

- [1] K. Susa and H. Steinfink, *GeCd₄S₆, a new defect tetrahedral structure type*, Inorg. Chem. **10**, 1754–1756 (1971), doi:10.1021/ic50102a044.
- [2] W. B. Pearson, *A Handbook of Lattice Spacings and Structures of Metals and Alloys, Volume 2, International Series of Monographs on Metal Physics and Physical Metallurgy*, vol. 8 (Pergamon Press, Oxford, London, Edinburgh, New York, Toronto, Sydney, Paris, Braunschweig, 1967).

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