GeS_2 ($C44$) Structure: AB2_oF72_43_ab_3b-001

This structure originally had the label `AB2_oF72_43_ab_3b`. Calls to that address will be redirected here.

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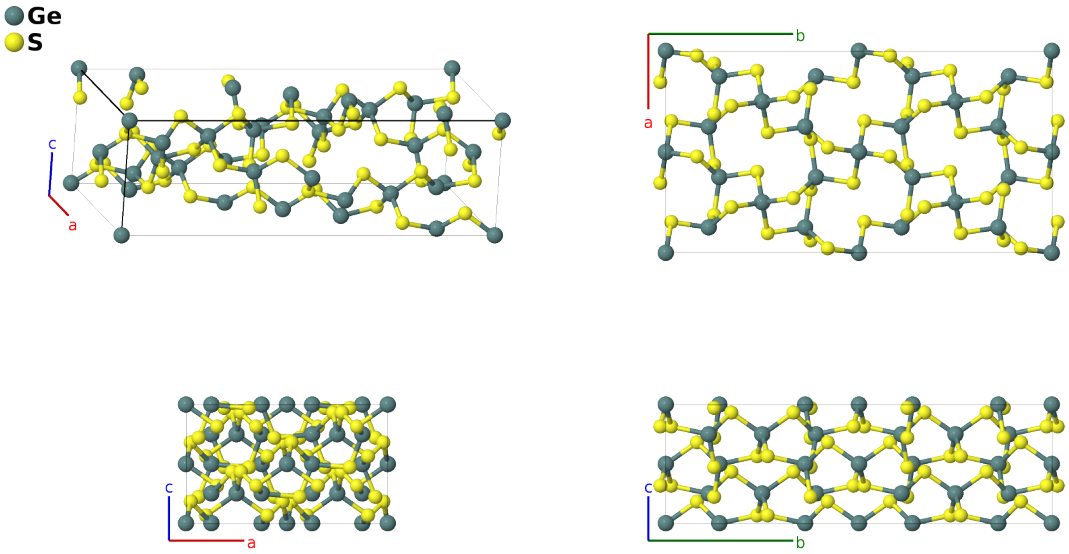
https://aflow.org/p/4KUZ

https://aflow.org/p/AB2_oF72_43_ab_3b-001

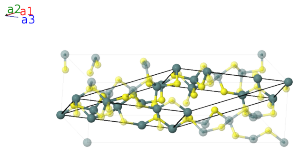


Prototype	GeS_2
AFLOW prototype label	AB2_oF72_43_ab_3b-001
***Strukturbericht* designation**	$C44$
ICSD	31685
Pearson symbol	oF72
Space group number	43
Space group symbol	$Fdd2$
AFLOW prototype command	`aflow --proto=AB2_oF72_43_ab_3b-001 --params=`$a, b/a, c/a, z_1, x_2, y_2, z_2, x_3, y_3, z_3, x_4, y_4, z_4, x_5, y_5, z_5$

Other compounds with this structure
$GeSe_2$

Face-centered Orthorhombic primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$z_1\,\mathbf{a}_1 + z_1\,\mathbf{a}_2 - z_1\,\mathbf{a}_3$	=	$c z_1\,\hat{\mathbf{z}}$	(8a)	Ge I
$\mathbf{B_2}$	=	$\left(z_1+\frac{1}{4}\right)\mathbf{a}_1 + \left(z_1+\frac{1}{4}\right)\mathbf{a}_2 - \left(z_1-\frac{1}{4}\right)\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} + c\left(z_1+\frac{1}{4}\right)\hat{\mathbf{z}}$	(8a)	Ge I
$\mathbf{B_3}$	=	$(-x_2+y_2+z_2)\,\mathbf{a}_1 + (x_2-y_2+z_2)\,\mathbf{a}_2 + (x_2+y_2-z_2)\,\mathbf{a}_3$	=	$a x_2\,\hat{\mathbf{x}} + b y_2\,\hat{\mathbf{y}} + c z_2\,\hat{\mathbf{z}}$	(16b)	Ge II
$\mathbf{B_4}$	=	$(x_2-y_2+z_2)\,\mathbf{a}_1 + (-x_2+y_2+z_2)\,\mathbf{a}_2 - (x_2+y_2+z_2)\,\mathbf{a}_3$	=	$-a x_2\,\hat{\mathbf{x}} - b y_2\,\hat{\mathbf{y}} + c z_2\,\hat{\mathbf{z}}$	(16b)	Ge II
$\mathbf{B_5}$	=	$-\left(x_2+y_2-z_2-\frac{1}{4}\right)\mathbf{a}_1 + \left(x_2+y_2+z_2+\frac{1}{4}\right)\mathbf{a}_2 + \left(x_2-y_2-z_2+\frac{1}{4}\right)\mathbf{a}_3$	=	$a\left(x_2+\frac{1}{4}\right)\hat{\mathbf{x}} - b\left(y_2-\frac{1}{4}\right)\hat{\mathbf{y}} + c\left(z_2+\frac{1}{4}\right)\hat{\mathbf{z}}$	(16b)	Ge II
$\mathbf{B_6}$	=	$\left(x_2+y_2+z_2+\frac{1}{4}\right)\mathbf{a}_1 - \left(x_2+y_2-z_2-\frac{1}{4}\right)\mathbf{a}_2 - \left(x_2-y_2+z_2-\frac{1}{4}\right)\mathbf{a}_3$	=	$-a\left(x_2-\frac{1}{4}\right)\hat{\mathbf{x}} + b\left(y_2+\frac{1}{4}\right)\hat{\mathbf{y}} + c\left(z_2+\frac{1}{4}\right)\hat{\mathbf{z}}$	(16b)	Ge II
$\mathbf{B_7}$	=	$(-x_3+y_3+z_3)\,\mathbf{a}_1 + (x_3-y_3+z_3)\,\mathbf{a}_2 + (x_3+y_3-z_3)\,\mathbf{a}_3$	=	$a x_3\,\hat{\mathbf{x}} + b y_3\,\hat{\mathbf{y}} + c z_3\,\hat{\mathbf{z}}$	(16b)	S I
$\mathbf{B_8}$	=	$(x_3-y_3+z_3)\,\mathbf{a}_1 + (-x_3+y_3+z_3)\,\mathbf{a}_2 - (x_3+y_3+z_3)\,\mathbf{a}_3$	=	$-a x_3\,\hat{\mathbf{x}} - b y_3\,\hat{\mathbf{y}} + c z_3\,\hat{\mathbf{z}}$	(16b)	S I
$\mathbf{B_9}$	=	$-\left(x_3+y_3-z_3-\frac{1}{4}\right)\mathbf{a}_1 + \left(x_3+y_3+z_3+\frac{1}{4}\right)\mathbf{a}_2 + \left(x_3-y_3-z_3+\frac{1}{4}\right)\mathbf{a}_3$	=	$a\left(x_3+\frac{1}{4}\right)\hat{\mathbf{x}} - b\left(y_3-\frac{1}{4}\right)\hat{\mathbf{y}} + c\left(z_3+\frac{1}{4}\right)\hat{\mathbf{z}}$	(16b)	S I
$\mathbf{B_{10}}$	=	$\left(x_3+y_3+z_3+\frac{1}{4}\right)\mathbf{a}_1 - \left(x_3+y_3-z_3-\frac{1}{4}\right)\mathbf{a}_2 - \left(x_3-y_3+z_3-\frac{1}{4}\right)\mathbf{a}_3$	=	$-a\left(x_3-\frac{1}{4}\right)\hat{\mathbf{x}} + b\left(y_3+\frac{1}{4}\right)\hat{\mathbf{y}} + c\left(z_3+\frac{1}{4}\right)\hat{\mathbf{z}}$	(16b)	S I
$\mathbf{B_{11}}$	=	$(-x_4+y_4+z_4)\,\mathbf{a}_1 + (x_4-y_4+z_4)\,\mathbf{a}_2 + (x_4+y_4-z_4)\,\mathbf{a}_3$	=	$a x_4\,\hat{\mathbf{x}} + b y_4\,\hat{\mathbf{y}} + c z_4\,\hat{\mathbf{z}}$	(16b)	S II
$\mathbf{B_{12}}$	=	$(x_4-y_4+z_4)\,\mathbf{a}_1 + (-x_4+y_4+z_4)\,\mathbf{a}_2 - (x_4+y_4+z_4)\,\mathbf{a}_3$	=	$-a x_4\,\hat{\mathbf{x}} - b y_4\,\hat{\mathbf{y}} + c z_4\,\hat{\mathbf{z}}$	(16b)	S II
$\mathbf{B_{13}}$	=	$-\left(x_4+y_4-z_4-\frac{1}{4}\right)\mathbf{a}_1 + \left(x_4+y_4+z_4+\frac{1}{4}\right)\mathbf{a}_2 + \left(x_4-y_4-z_4+\frac{1}{4}\right)\mathbf{a}_3$	=	$a\left(x_4+\frac{1}{4}\right)\hat{\mathbf{x}} - b\left(y_4-\frac{1}{4}\right)\hat{\mathbf{y}} + c\left(z_4+\frac{1}{4}\right)\hat{\mathbf{z}}$	(16b)	S II

$\mathbf{B_{14}}$	=	$\left(x_4+y_4+z_4+\frac{1}{4}\right)\,\mathbf{a}_1 - \left(x_4+y_4-z_4-\frac{1}{4}\right)\,\mathbf{a}_2 - \left(x_4-y_4+z_4-\frac{1}{4}\right)\,\mathbf{a}_3$	=	$-a\left(x_4-\frac{1}{4}\right)\,\hat{\mathbf{x}}+b\left(y_4+\frac{1}{4}\right)\,\hat{\mathbf{y}}+c\left(z_4+\frac{1}{4}\right)\,\hat{\mathbf{z}}$	(16b)	S II
$\mathbf{B_{15}}$	=	$(-x_5+y_5+z_5)\,\mathbf{a}_1 + (x_5-y_5+z_5)\,\mathbf{a}_2 + (x_5+y_5-z_5)\,\mathbf{a}_3$	=	$ax_5\,\hat{\mathbf{x}} + by_5\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(16b)	S III
$\mathbf{B_{16}}$	=	$(x_5-y_5+z_5)\,\mathbf{a}_1 + (-x_5+y_5+z_5)\,\mathbf{a}_2 - (x_5+y_5+z_5)\,\mathbf{a}_3$	=	$-ax_5\,\hat{\mathbf{x}} - by_5\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(16b)	S III
$\mathbf{B_{17}}$	=	$-\left(x_5+y_5-z_5-\frac{1}{4}\right)\,\mathbf{a}_1 + \left(x_5+y_5+z_5+\frac{1}{4}\right)\,\mathbf{a}_2 + \left(x_5-y_5-z_5+\frac{1}{4}\right)\,\mathbf{a}_3$	=	$a\left(x_5+\frac{1}{4}\right)\,\hat{\mathbf{x}} - b\left(y_5-\frac{1}{4}\right)\,\hat{\mathbf{y}} + c\left(z_5+\frac{1}{4}\right)\,\hat{\mathbf{z}}$	(16b)	S III
$\mathbf{B_{18}}$	=	$\left(x_5+y_5+z_5+\frac{1}{4}\right)\,\mathbf{a}_1 - \left(x_5+y_5-z_5-\frac{1}{4}\right)\,\mathbf{a}_2 - \left(x_5-y_5+z_5-\frac{1}{4}\right)\,\mathbf{a}_3$	=	$-a\left(x_5-\frac{1}{4}\right)\,\hat{\mathbf{x}}+b\left(y_5+\frac{1}{4}\right)\,\hat{\mathbf{y}}+c\left(z_5+\frac{1}{4}\right)\,\hat{\mathbf{z}}$	(16b)	S III

References

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Found in

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