$GdSi_2$ Structure: AB2_oI12_74_e_2e-001

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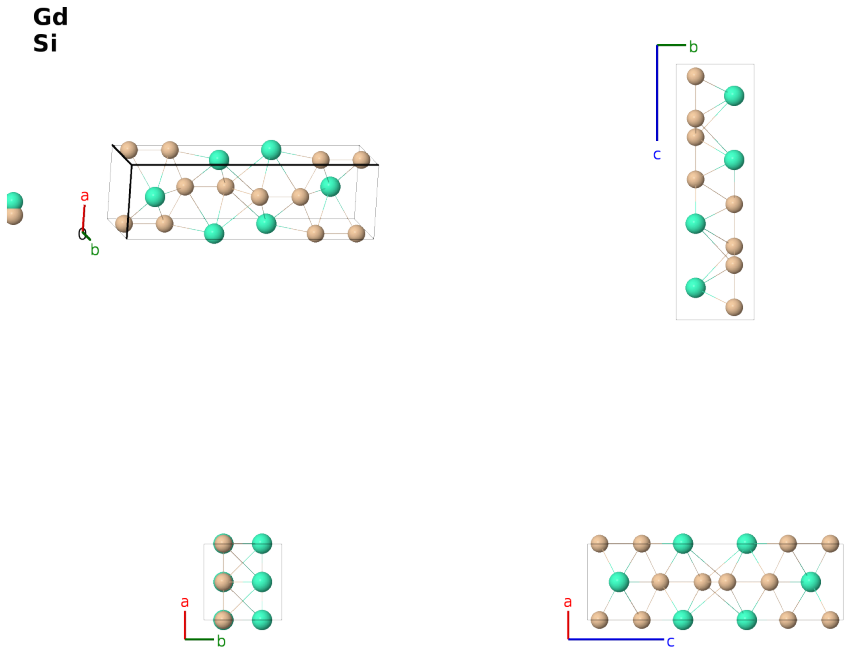
https://aflow.org/prototype-encyclopedia/EQ3C

https://aflow.org/prototype-encyclopedia/AB2_oI12_74_e_2e-001



Prototype	$GdSi_2$
AFLOW prototype label	AB2_oI12_74_e_2e-001
ICSD	291182
CCDC	1723312
Pearson symbol	oI12
Space group number	74
Space group symbol	*Imma*
AFLOW prototype command	`aflow --proto=AB2_oI12_74_e_2e-001 --params=`$a, b/a, c/a, z_1, z_2, z_3$

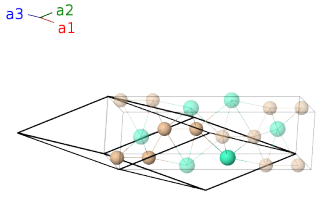
Other compounds with this structure

$GeSi_2$, $HoSi_2$, $LaGe_2$, $TbSi_2$, $DySi_{1.4}$, $GdSi_{1.4}$, $NdSi_{1.4}$, $PrSi_{1.4}$, $SmSi_{1.4}$, $YSi_{1.4}$

- (Zou, 2015) find that the Si-I site has 96.8% occupancy and the Si-II site has 81.2% occupancy, so the actual stoichiometry of their sample is $GdSi_{1.78}$.

Body-centered Orthorhombic primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$\left(z_1 + \frac{1}{4}\right)\,\mathbf{a}_1 + z_1\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{4}b\,\hat{\mathbf{y}} + cz_1\,\hat{\mathbf{z}}$	(4e)	Gd I
$\mathbf{B_2}$	=	$-\left(z_1 - \frac{3}{4}\right)\,\mathbf{a}_1 - z_1\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{3}{4}b\,\hat{\mathbf{y}} - cz_1\,\hat{\mathbf{z}}$	(4e)	Gd I
$\mathbf{B_3}$	=	$\left(z_2 + \frac{1}{4}\right)\,\mathbf{a}_1 + z_2\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{4}b\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(4e)	Si I
$\mathbf{B_4}$	=	$-\left(z_2 - \frac{3}{4}\right)\,\mathbf{a}_1 - z_2\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{3}{4}b\,\hat{\mathbf{y}} - cz_2\,\hat{\mathbf{z}}$	(4e)	Si I
$\mathbf{B_5}$	=	$\left(z_3 + \frac{1}{4}\right)\,\mathbf{a}_1 + z_3\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{4}b\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(4e)	Si II
$\mathbf{B_6}$	=	$-\left(z_3 - \frac{3}{4}\right)\,\mathbf{a}_1 - z_3\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{3}{4}b\,\hat{\mathbf{y}} - cz_3\,\hat{\mathbf{z}}$	(4e)	Si II

References

[1] J. D. Zou, J. Liu, and M. Yan, *Crystal structure and magnetic properties of $GdSi_{1.78}$, $Gd(Si_{0.684}Ge_{0.316})_{1.78}$, $GdGe_{1.57}$, and $GdSn_2$ compounds*, J. Magn. Magn. Mater. **385**, 77–82 (2015), doi:10.1016/j.jmmm.2015.02.057.

[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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