

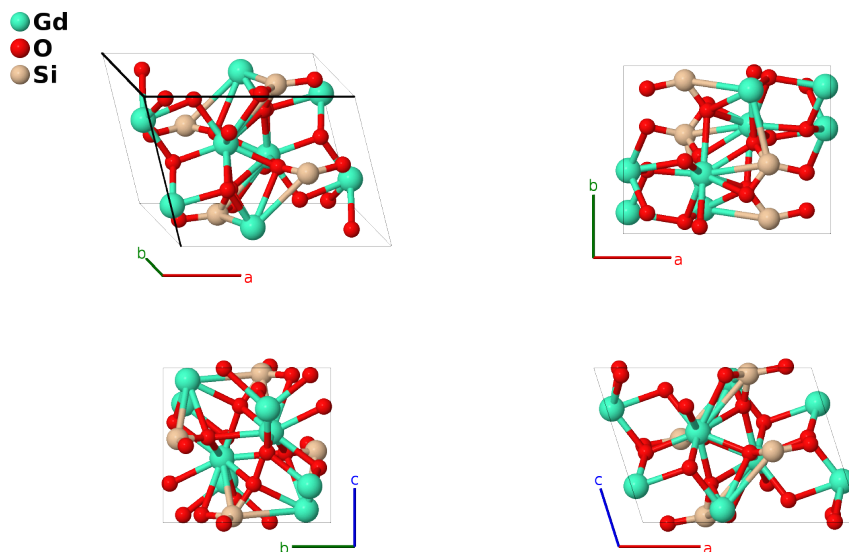
# Gd<sub>2</sub>SiO<sub>5</sub> (RE<sub>2</sub>SiO<sub>5</sub> X1) Structure: A2B5C\_mP32\_14\_2e\_5e\_e-001

This structure originally had the label `A2B5C_mP32_14_2e_5e_e`. Calls to that address will be redirected here.

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<https://afLOW.org/p/HBLG>

[https://afLOW.org/p/A2B5C\\_mP32\\_14\\_2e\\_5e\\_e-001](https://afLOW.org/p/A2B5C_mP32_14_2e_5e_e-001)



Prototype	Gd <sub>2</sub> O <sub>5</sub> Si
AFLOW prototype label	A2B5C_mP32_14_2e_5e_e-001
ICSD	154796
Pearson symbol	mP32
Space group number	14
Space group symbol	<i>P2</i> <sub>1</sub> / <i>c</i>
AFLOW prototype command	<pre>afLOW --proto=A2B5C_mP32_14_2e_5e_e-001       --params=a, b/a, c/a, β, x<sub>1</sub>, y<sub>1</sub>, 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>, x<sub>6</sub>, y<sub>6</sub>, z<sub>6</sub>, x<sub>7</sub>,       y<sub>7</sub>, z<sub>7</sub>, x<sub>8</sub>, y<sub>8</sub>, z<sub>8</sub></pre>

## Other compounds with this structure

Dy<sub>2</sub>SiO<sub>5</sub>, La<sub>2</sub>SiO<sub>5</sub>, Tb<sub>2</sub>SiO<sub>5</sub>, Y<sub>2</sub>SiO<sub>5</sub>

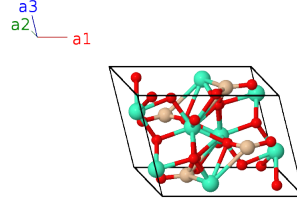
- Compounds of the form RE<sub>2</sub>SiO<sub>5</sub> (RE = Rare Earth and related elements) crystallize in one of two forms (Wang, 2001 and Tian, 2016):
- X1, shown here, for rare earths between lanthanum and gadolinium, and
- X2, space group *C2/c* #15 for the later rare earths, with the dysprosium, yttrium and ytterbium compounds existing in both structures.

- The ICSD entry is from the later work of (Dramićanin, 2006).

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### Simple Monoclinic primitive vectors

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




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### Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$x_1 \mathbf{a}_1 + y_1 \mathbf{a}_2 + z_1 \mathbf{a}_3$	=	$(ax_1 + cz_1 \cos \beta) \hat{\mathbf{x}} + by_1 \hat{\mathbf{y}} + cz_1 \sin \beta \hat{\mathbf{z}}$	(4e)	Gd I
$\mathbf{B}_2$	$-x_1 \mathbf{a}_1 + (y_1 + \frac{1}{2}) \mathbf{a}_2 - (z_1 - \frac{1}{2}) \mathbf{a}_3$	=	$-(ax_1 + c(z_1 - \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} + b(y_1 + \frac{1}{2}) \hat{\mathbf{y}} - c(z_1 - \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(4e)	Gd I
$\mathbf{B}_3$	$-x_1 \mathbf{a}_1 - y_1 \mathbf{a}_2 - z_1 \mathbf{a}_3$	=	$-(ax_1 + cz_1 \cos \beta) \hat{\mathbf{x}} - by_1 \hat{\mathbf{y}} - cz_1 \sin \beta \hat{\mathbf{z}}$	(4e)	Gd I
$\mathbf{B}_4$	$x_1 \mathbf{a}_1 - (y_1 - \frac{1}{2}) \mathbf{a}_2 + (z_1 + \frac{1}{2}) \mathbf{a}_3$	=	$(ax_1 + c(z_1 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - b(y_1 - \frac{1}{2}) \hat{\mathbf{y}} + c(z_1 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(4e)	Gd I
$\mathbf{B}_5$	$x_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	=	$(ax_2 + cz_2 \cos \beta) \hat{\mathbf{x}} + by_2 \hat{\mathbf{y}} + cz_2 \sin \beta \hat{\mathbf{z}}$	(4e)	Gd II
$\mathbf{B}_6$	$-x_2 \mathbf{a}_1 + (y_2 + \frac{1}{2}) \mathbf{a}_2 - (z_2 - \frac{1}{2}) \mathbf{a}_3$	=	$-(ax_2 + c(z_2 - \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} + b(y_2 + \frac{1}{2}) \hat{\mathbf{y}} - c(z_2 - \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(4e)	Gd II
$\mathbf{B}_7$	$-x_2 \mathbf{a}_1 - y_2 \mathbf{a}_2 - z_2 \mathbf{a}_3$	=	$-(ax_2 + cz_2 \cos \beta) \hat{\mathbf{x}} - by_2 \hat{\mathbf{y}} - cz_2 \sin \beta \hat{\mathbf{z}}$	(4e)	Gd II
$\mathbf{B}_8$	$x_2 \mathbf{a}_1 - (y_2 - \frac{1}{2}) \mathbf{a}_2 + (z_2 + \frac{1}{2}) \mathbf{a}_3$	=	$(ax_2 + c(z_2 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - b(y_2 - \frac{1}{2}) \hat{\mathbf{y}} + c(z_2 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(4e)	Gd II
$\mathbf{B}_9$	$x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	=	$(ax_3 + cz_3 \cos \beta) \hat{\mathbf{x}} + by_3 \hat{\mathbf{y}} + cz_3 \sin \beta \hat{\mathbf{z}}$	(4e)	O I
$\mathbf{B}_{10}$	$-x_3 \mathbf{a}_1 + (y_3 + \frac{1}{2}) \mathbf{a}_2 - (z_3 - \frac{1}{2}) \mathbf{a}_3$	=	$-(ax_3 + c(z_3 - \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} + b(y_3 + \frac{1}{2}) \hat{\mathbf{y}} - c(z_3 - \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(4e)	O I
$\mathbf{B}_{11}$	$-x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 - z_3 \mathbf{a}_3$	=	$-(ax_3 + cz_3 \cos \beta) \hat{\mathbf{x}} - by_3 \hat{\mathbf{y}} - cz_3 \sin \beta \hat{\mathbf{z}}$	(4e)	O I
$\mathbf{B}_{12}$	$x_3 \mathbf{a}_1 - (y_3 - \frac{1}{2}) \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$	=	$(ax_3 + c(z_3 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - b(y_3 - \frac{1}{2}) \hat{\mathbf{y}} + c(z_3 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(4e)	O I
$\mathbf{B}_{13}$	$x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	=	$(ax_4 + cz_4 \cos \beta) \hat{\mathbf{x}} + by_4 \hat{\mathbf{y}} + cz_4 \sin \beta \hat{\mathbf{z}}$	(4e)	O II
$\mathbf{B}_{14}$	$-x_4 \mathbf{a}_1 + (y_4 + \frac{1}{2}) \mathbf{a}_2 - (z_4 - \frac{1}{2}) \mathbf{a}_3$	=	$-(ax_4 + c(z_4 - \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} + b(y_4 + \frac{1}{2}) \hat{\mathbf{y}} - c(z_4 - \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(4e)	O II
$\mathbf{B}_{15}$	$-x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 - z_4 \mathbf{a}_3$	=	$-(ax_4 + cz_4 \cos \beta) \hat{\mathbf{x}} - by_4 \hat{\mathbf{y}} - cz_4 \sin \beta \hat{\mathbf{z}}$	(4e)	O II
$\mathbf{B}_{16}$	$x_4 \mathbf{a}_1 - (y_4 - \frac{1}{2}) \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3$	=	$(ax_4 + c(z_4 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - b(y_4 - \frac{1}{2}) \hat{\mathbf{y}} + c(z_4 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(4e)	O II
$\mathbf{B}_{17}$	$x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	=	$(ax_5 + cz_5 \cos \beta) \hat{\mathbf{x}} + by_5 \hat{\mathbf{y}} + cz_5 \sin \beta \hat{\mathbf{z}}$	(4e)	O III
$\mathbf{B}_{18}$	$-x_5 \mathbf{a}_1 + (y_5 + \frac{1}{2}) \mathbf{a}_2 - (z_5 - \frac{1}{2}) \mathbf{a}_3$	=	$-(ax_5 + c(z_5 - \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} + b(y_5 + \frac{1}{2}) \hat{\mathbf{y}} - c(z_5 - \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(4e)	O III
$\mathbf{B}_{19}$	$-x_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 - z_5 \mathbf{a}_3$	=	$-(ax_5 + cz_5 \cos \beta) \hat{\mathbf{x}} - by_5 \hat{\mathbf{y}} - cz_5 \sin \beta \hat{\mathbf{z}}$	(4e)	O III
$\mathbf{B}_{20}$	$x_5 \mathbf{a}_1 - (y_5 - \frac{1}{2}) \mathbf{a}_2 + (z_5 + \frac{1}{2}) \mathbf{a}_3$	=	$(ax_5 + c(z_5 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - b(y_5 - \frac{1}{2}) \hat{\mathbf{y}} + c(z_5 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(4e)	O III
$\mathbf{B}_{21}$	$x_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	=	$(ax_6 + cz_6 \cos \beta) \hat{\mathbf{x}} + by_6 \hat{\mathbf{y}} + cz_6 \sin \beta \hat{\mathbf{z}}$	(4e)	O IV

$$\begin{aligned}
\mathbf{B}_{22} &= -x_6 \mathbf{a}_1 + \left(y_6 + \frac{1}{2}\right) \mathbf{a}_2 - \left(z_6 - \frac{1}{2}\right) \mathbf{a}_3 &= -\left(ax_6 + c\left(z_6 - \frac{1}{2}\right) \cos \beta\right) \hat{\mathbf{x}} + b\left(y_6 + \frac{1}{2}\right) \hat{\mathbf{y}} - c\left(z_6 - \frac{1}{2}\right) \sin \beta \hat{\mathbf{z}} &(4e) & \text{O IV} \\
\mathbf{B}_{23} &= -x_6 \mathbf{a}_1 - y_6 \mathbf{a}_2 - z_6 \mathbf{a}_3 &= -\left(ax_6 + cz_6 \cos \beta\right) \hat{\mathbf{x}} - by_6 \hat{\mathbf{y}} - cz_6 \sin \beta \hat{\mathbf{z}} &(4e) & \text{O IV} \\
\mathbf{B}_{24} &= x_6 \mathbf{a}_1 - \left(y_6 - \frac{1}{2}\right) \mathbf{a}_2 + \left(z_6 + \frac{1}{2}\right) \mathbf{a}_3 &= \left(ax_6 + c\left(z_6 + \frac{1}{2}\right) \cos \beta\right) \hat{\mathbf{x}} - b\left(y_6 - \frac{1}{2}\right) \hat{\mathbf{y}} + c\left(z_6 + \frac{1}{2}\right) \sin \beta \hat{\mathbf{z}} &(4e) & \text{O IV} \\
\mathbf{B}_{25} &= x_7 \mathbf{a}_1 + y_7 \mathbf{a}_2 + z_7 \mathbf{a}_3 &= \left(ax_7 + cz_7 \cos \beta\right) \hat{\mathbf{x}} + by_7 \hat{\mathbf{y}} + cz_7 \sin \beta \hat{\mathbf{z}} &(4e) & \text{O V} \\
\mathbf{B}_{26} &= -x_7 \mathbf{a}_1 + \left(y_7 + \frac{1}{2}\right) \mathbf{a}_2 - \left(z_7 - \frac{1}{2}\right) \mathbf{a}_3 &= -\left(ax_7 + c\left(z_7 - \frac{1}{2}\right) \cos \beta\right) \hat{\mathbf{x}} + b\left(y_7 + \frac{1}{2}\right) \hat{\mathbf{y}} - c\left(z_7 - \frac{1}{2}\right) \sin \beta \hat{\mathbf{z}} &(4e) & \text{O V} \\
\mathbf{B}_{27} &= -x_7 \mathbf{a}_1 - y_7 \mathbf{a}_2 - z_7 \mathbf{a}_3 &= -\left(ax_7 + cz_7 \cos \beta\right) \hat{\mathbf{x}} - by_7 \hat{\mathbf{y}} - cz_7 \sin \beta \hat{\mathbf{z}} &(4e) & \text{O V} \\
\mathbf{B}_{28} &= x_7 \mathbf{a}_1 - \left(y_7 - \frac{1}{2}\right) \mathbf{a}_2 + \left(z_7 + \frac{1}{2}\right) \mathbf{a}_3 &= \left(ax_7 + c\left(z_7 + \frac{1}{2}\right) \cos \beta\right) \hat{\mathbf{x}} - b\left(y_7 - \frac{1}{2}\right) \hat{\mathbf{y}} + c\left(z_7 + \frac{1}{2}\right) \sin \beta \hat{\mathbf{z}} &(4e) & \text{O V} \\
\mathbf{B}_{29} &= x_8 \mathbf{a}_1 + y_8 \mathbf{a}_2 + z_8 \mathbf{a}_3 &= \left(ax_8 + cz_8 \cos \beta\right) \hat{\mathbf{x}} + by_8 \hat{\mathbf{y}} + cz_8 \sin \beta \hat{\mathbf{z}} &(4e) & \text{Si I} \\
\mathbf{B}_{30} &= -x_8 \mathbf{a}_1 + \left(y_8 + \frac{1}{2}\right) \mathbf{a}_2 - \left(z_8 - \frac{1}{2}\right) \mathbf{a}_3 &= -\left(ax_8 + c\left(z_8 - \frac{1}{2}\right) \cos \beta\right) \hat{\mathbf{x}} + b\left(y_8 + \frac{1}{2}\right) \hat{\mathbf{y}} - c\left(z_8 - \frac{1}{2}\right) \sin \beta \hat{\mathbf{z}} &(4e) & \text{Si I} \\
\mathbf{B}_{31} &= -x_8 \mathbf{a}_1 - y_8 \mathbf{a}_2 - z_8 \mathbf{a}_3 &= -\left(ax_8 + cz_8 \cos \beta\right) \hat{\mathbf{x}} - by_8 \hat{\mathbf{y}} - cz_8 \sin \beta \hat{\mathbf{z}} &(4e) & \text{Si I} \\
\mathbf{B}_{32} &= x_8 \mathbf{a}_1 - \left(y_8 - \frac{1}{2}\right) \mathbf{a}_2 + \left(z_8 + \frac{1}{2}\right) \mathbf{a}_3 &= \left(ax_8 + c\left(z_8 + \frac{1}{2}\right) \cos \beta\right) \hat{\mathbf{x}} - b\left(y_8 - \frac{1}{2}\right) \hat{\mathbf{y}} + c\left(z_8 + \frac{1}{2}\right) \sin \beta \hat{\mathbf{z}} &(4e) & \text{Si I}
\end{aligned}$$

## References

- [1] G. V. Anan'eva, A. M. Korovkin, T. I. Merkulyaeva, A. M. Morozova, M. V. Petrov, I. R. Savinova, V. R. Startsev, and P. P. Feofilov, *Growth of lanthanide oxyorthosilicate single crystals, and their structural and optical characteristics*, Inorg. Mater. **17**, 754–758 (1981). Translated from *Neorganicheskie Materialy*.
- [2] J. Wang, S. Tian, G. Li, F. Liao, and X. Jing, *Preparation and X-ray characterization of low-temperature phases of  $R_2SiO_5$  ( $R = \text{rare earth elements}$ )*, Mater. Res. Bull. **36**, 1855–1861 (2001), doi:10.1016/S0025-5408(01)00664-X.
- [3] Z. Tian, L. Zheng, J. Wang, P. Wan, J. Li, and J. Wang, *Theoretical and experimental determination of the major thermo-mechanical properties of  $RE_2SiO_5$  ( $RE = Tb, Dy, Ho, Er, Tm, Yb, Lu, \text{ and } Y$ ) for environmental and thermal barrier coating applications*, J. Am. Ceram. Soc. **36**, 189–202 (2016), doi:10.1016/j.jeurceramsoc.2015.09.013.
- [4] C. Michel, G. Buisson, and E. F. Bertaut, *Structure de  $Y_2SiO_5$* , Compt. Rend. B: Sci. Phys. **264**, 397–399 (1967).
- [5] M. D. Dramićanin, V. Jokanović, B. Viana, E. Antic-Fidancev, M. Mitrić, and ž. Andrić, *Luminescence and structural properties of  $Gd_2SiO_5:Eu^{3+}$  nanophosphors synthesized from the hydrothermal obtained silica sol*, Journal of Alloys and Compounds **424**, 213–217 (2006), doi:10.1016/j.jallcom.2005.10.086.

## Found in

- [1] P. Villars, *Gd<sub>2</sub>SiO<sub>5</sub> (Gd<sub>2</sub>[SiO<sub>4</sub>]O) Crystal Structure* (2016). PAULING FILE in: Inorganic Solid Phases, SpringerMaterials (online database), Springer, Heidelberg (ed.) SpringerMaterials.