

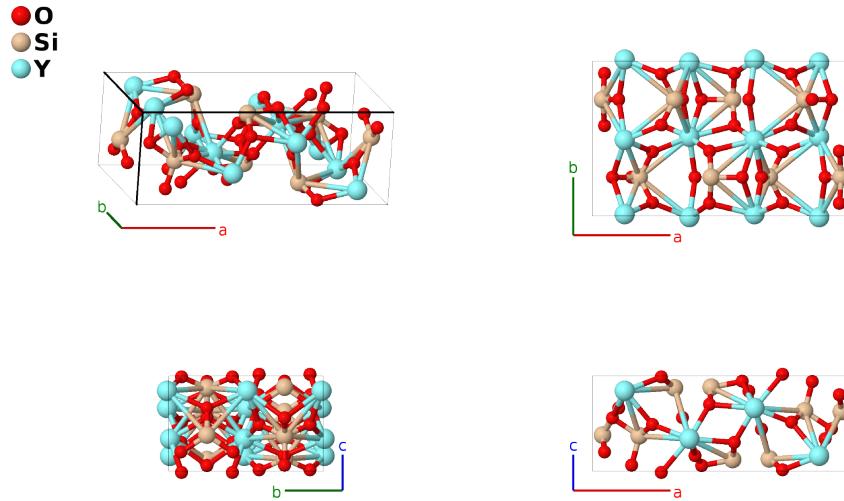
# Possible $\delta$ - $\text{Y}_2\text{Si}_2\text{O}_7$ Structure: A7B2C2\_oP44\_62\_3c2d\_2c\_d-001

This structure originally had the label A7B2C2\_oP44\_62\_3c2d\_2c\_d. Calls to that address will be redirected here.

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<https://aflow.org/p/Y82X>

[https://aflow.org/p/A7B2C2\\_oP44\\_62\\_3c2d\\_2c\\_d-001](https://aflow.org/p/A7B2C2_oP44_62_3c2d_2c_d-001)



<b>Prototype</b>	$\text{O}_7\text{Si}_2\text{Y}_2$
<b>AFLOW prototype label</b>	A7B2C2_oP44_62_3c2d_2c_d-001
<b>ICSD</b>	33721
<b>Pearson symbol</b>	oP44
<b>Space group number</b>	62
<b>Space group symbol</b>	$Pnma$
<b>AFLOW prototype command</b>	<code>aflow --proto=A7B2C2_oP44_62_3c2d_2c_d-001 --params=a, b/a, c/a, x1, z1, x2, z2, x3, z3, x4, z4, x5, z5, x6, y6, z6, x7, y7, z7, x8, y8, z8</code>

## Other compounds with this structure

$\delta$ - $\text{Ho}_2\text{O}_7\text{Si}_2$ ,  $\delta$ - $\text{Dy}_2\text{O}_7\text{Si}_2$ ,  $\delta$ - $\text{Y}_2\text{O}_7\text{Si}_2$ ,  $\text{Li}_2\text{S}_2\text{O}_7$

- (Diaz, 1990) found that some structures of  $\text{RE}_2\text{O}_7\text{Si}_2$  ( $\text{RE} = \text{Ho}, \text{Dy}, \text{Gd}, \text{Y}$ ) were in the centro-symmetric orthorhombic  $Pnma$  #62 space group, in which case this would be the prototype of  $\delta$ - $\text{RE}_2\text{O}_7\text{Si}_2$  (Becerro, 2004).
- (Smolin, 1970) found  $\delta$ - $\text{Gd}_2\text{O}_7\text{Si}_2$  to be in the non-centro-symmetric  $Pna2_1$  #33 space group.
- (Becerro, 2004) found only one yttrium site in the  $\delta$ -structure, supporting (Diaz, 1990).
- In addition if we allow a small amount of uncertainty (0.2 Å) in the atomic positions in the  $Pna2_1$  structure findsym places this structure in the  $Pnma$  group.

- Nevertheless we have found no work explicitly stating that the structure of (Smolin, 1970) is in error, and indeed (Christensen, 1994) found  $\delta$ - $\text{Y}_2\text{O}_7\text{Si}_2$  in space group  $Pna2_1$ . Given this ambiguity, we list  $\text{Y}_2\text{O}_7\text{Si}_2$  only as a possible prototype for the  $\delta$ -phase pyrosilicates.

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### Simple Orthorhombic primitive vectors




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### Basis vectors

	Lattice coordinates	Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$x_1 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_1 \mathbf{a}_3$	$a x_1 \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} + c z_1 \hat{\mathbf{z}}$	(4c)	O I
$\mathbf{B}_2$	$-(x_1 - \frac{1}{2}) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + (z_1 + \frac{1}{2}) \mathbf{a}_3$	$-a(x_1 - \frac{1}{2}) \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} + c(z_1 + \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	O I
$\mathbf{B}_3$	$-x_1 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_1 \mathbf{a}_3$	$-a x_1 \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} - c z_1 \hat{\mathbf{z}}$	(4c)	O I
$\mathbf{B}_4$	$(x_1 + \frac{1}{2}) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 - (z_1 - \frac{1}{2}) \mathbf{a}_3$	$a(x_1 + \frac{1}{2}) \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} - c(z_1 - \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	O I
$\mathbf{B}_5$	$x_2 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_2 \mathbf{a}_3$	$a x_2 \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} + c z_2 \hat{\mathbf{z}}$	(4c)	O II
$\mathbf{B}_6$	$-(x_2 - \frac{1}{2}) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + (z_2 + \frac{1}{2}) \mathbf{a}_3$	$-a(x_2 - \frac{1}{2}) \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} + c(z_2 + \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	O II
$\mathbf{B}_7$	$-x_2 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_2 \mathbf{a}_3$	$-a x_2 \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} - c z_2 \hat{\mathbf{z}}$	(4c)	O II
$\mathbf{B}_8$	$(x_2 + \frac{1}{2}) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 - (z_2 - \frac{1}{2}) \mathbf{a}_3$	$a(x_2 + \frac{1}{2}) \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} - c(z_2 - \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	O II
$\mathbf{B}_9$	$x_3 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_3 \mathbf{a}_3$	$a x_3 \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} + c z_3 \hat{\mathbf{z}}$	(4c)	O III
$\mathbf{B}_{10}$	$-(x_3 - \frac{1}{2}) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$	$-a(x_3 - \frac{1}{2}) \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} + c(z_3 + \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	O III
$\mathbf{B}_{11}$	$-x_3 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_3 \mathbf{a}_3$	$-a x_3 \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} - c z_3 \hat{\mathbf{z}}$	(4c)	O III
$\mathbf{B}_{12}$	$(x_3 + \frac{1}{2}) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 - (z_3 - \frac{1}{2}) \mathbf{a}_3$	$a(x_3 + \frac{1}{2}) \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} - c(z_3 - \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	O III
$\mathbf{B}_{13}$	$x_4 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_4 \mathbf{a}_3$	$a x_4 \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} + c z_4 \hat{\mathbf{z}}$	(4c)	Si I
$\mathbf{B}_{14}$	$-(x_4 - \frac{1}{2}) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3$	$-a(x_4 - \frac{1}{2}) \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} + c(z_4 + \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	Si I
$\mathbf{B}_{15}$	$-x_4 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_4 \mathbf{a}_3$	$-a x_4 \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} - c z_4 \hat{\mathbf{z}}$	(4c)	Si I
$\mathbf{B}_{16}$	$(x_4 + \frac{1}{2}) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 - (z_4 - \frac{1}{2}) \mathbf{a}_3$	$a(x_4 + \frac{1}{2}) \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} - c(z_4 - \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	Si I
$\mathbf{B}_{17}$	$x_5 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_5 \mathbf{a}_3$	$a x_5 \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} + c z_5 \hat{\mathbf{z}}$	(4c)	Si II
$\mathbf{B}_{18}$	$-(x_5 - \frac{1}{2}) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + (z_5 + \frac{1}{2}) \mathbf{a}_3$	$-a(x_5 - \frac{1}{2}) \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} + c(z_5 + \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	Si II
$\mathbf{B}_{19}$	$-x_5 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_5 \mathbf{a}_3$	$-a x_5 \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} - c z_5 \hat{\mathbf{z}}$	(4c)	Si II
$\mathbf{B}_{20}$	$(x_5 + \frac{1}{2}) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 - (z_5 - \frac{1}{2}) \mathbf{a}_3$	$a(x_5 + \frac{1}{2}) \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} - c(z_5 - \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	Si II
$\mathbf{B}_{21}$	$x_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	$a x_6 \hat{\mathbf{x}} + b y_6 \hat{\mathbf{y}} + c z_6 \hat{\mathbf{z}}$	(8d)	O IV
$\mathbf{B}_{22}$	$-(x_6 - \frac{1}{2}) \mathbf{a}_1 - y_6 \mathbf{a}_2 + (z_6 + \frac{1}{2}) \mathbf{a}_3$	$-a(x_6 - \frac{1}{2}) \hat{\mathbf{x}} - b y_6 \hat{\mathbf{y}} + c(z_6 + \frac{1}{2}) \hat{\mathbf{z}}$	(8d)	O IV
$\mathbf{B}_{23}$	$-x_6 \mathbf{a}_1 + (y_6 + \frac{1}{2}) \mathbf{a}_2 - z_6 \mathbf{a}_3$	$-a x_6 \hat{\mathbf{x}} + b(y_6 + \frac{1}{2}) \hat{\mathbf{y}} - c z_6 \hat{\mathbf{z}}$	(8d)	O IV

$\mathbf{B}_{24}$	$=$	$(x_6 + \frac{1}{2}) \mathbf{a}_1 - (y_6 - \frac{1}{2}) \mathbf{a}_2 - (z_6 - \frac{1}{2}) \mathbf{a}_3$	$=$	$a(x_6 + \frac{1}{2}) \hat{\mathbf{x}} - b(y_6 - \frac{1}{2}) \hat{\mathbf{y}} - c(z_6 - \frac{1}{2}) \hat{\mathbf{z}}$	(8d)	O IV
$\mathbf{B}_{25}$	$=$	$-x_6 \mathbf{a}_1 - y_6 \mathbf{a}_2 - z_6 \mathbf{a}_3$	$=$	$-ax_6 \hat{\mathbf{x}} - by_6 \hat{\mathbf{y}} - cz_6 \hat{\mathbf{z}}$	(8d)	O IV
$\mathbf{B}_{26}$	$=$	$(x_6 + \frac{1}{2}) \mathbf{a}_1 + y_6 \mathbf{a}_2 - (z_6 - \frac{1}{2}) \mathbf{a}_3$	$=$	$a(x_6 + \frac{1}{2}) \hat{\mathbf{x}} + by_6 \hat{\mathbf{y}} - c(z_6 - \frac{1}{2}) \hat{\mathbf{z}}$	(8d)	O IV
$\mathbf{B}_{27}$	$=$	$x_6 \mathbf{a}_1 - (y_6 - \frac{1}{2}) \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$ax_6 \hat{\mathbf{x}} - b(y_6 - \frac{1}{2}) \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}}$	(8d)	O IV
$\mathbf{B}_{28}$	$=$	$-(x_6 - \frac{1}{2}) \mathbf{a}_1 + (y_6 + \frac{1}{2}) \mathbf{a}_2 + (z_6 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_6 - \frac{1}{2}) \hat{\mathbf{x}} + b(y_6 + \frac{1}{2}) \hat{\mathbf{y}} + c(z_6 + \frac{1}{2}) \hat{\mathbf{z}}$	(8d)	O IV
$\mathbf{B}_{29}$	$=$	$x_7 \mathbf{a}_1 + y_7 \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$ax_7 \hat{\mathbf{x}} + by_7 \hat{\mathbf{y}} + cz_7 \hat{\mathbf{z}}$	(8d)	O V
$\mathbf{B}_{30}$	$=$	$-(x_7 - \frac{1}{2}) \mathbf{a}_1 - y_7 \mathbf{a}_2 + (z_7 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_7 - \frac{1}{2}) \hat{\mathbf{x}} - by_7 \hat{\mathbf{y}} + c(z_7 + \frac{1}{2}) \hat{\mathbf{z}}$	(8d)	O V
$\mathbf{B}_{31}$	$=$	$-x_7 \mathbf{a}_1 + (y_7 + \frac{1}{2}) \mathbf{a}_2 - z_7 \mathbf{a}_3$	$=$	$-ax_7 \hat{\mathbf{x}} + b(y_7 + \frac{1}{2}) \hat{\mathbf{y}} - cz_7 \hat{\mathbf{z}}$	(8d)	O V
$\mathbf{B}_{32}$	$=$	$(x_7 + \frac{1}{2}) \mathbf{a}_1 - (y_7 - \frac{1}{2}) \mathbf{a}_2 - (z_7 - \frac{1}{2}) \mathbf{a}_3$	$=$	$a(x_7 + \frac{1}{2}) \hat{\mathbf{x}} - b(y_7 - \frac{1}{2}) \hat{\mathbf{y}} - c(z_7 - \frac{1}{2}) \hat{\mathbf{z}}$	(8d)	O V
$\mathbf{B}_{33}$	$=$	$-x_7 \mathbf{a}_1 - y_7 \mathbf{a}_2 - z_7 \mathbf{a}_3$	$=$	$-ax_7 \hat{\mathbf{x}} - by_7 \hat{\mathbf{y}} - cz_7 \hat{\mathbf{z}}$	(8d)	O V
$\mathbf{B}_{34}$	$=$	$(x_7 + \frac{1}{2}) \mathbf{a}_1 + y_7 \mathbf{a}_2 - (z_7 - \frac{1}{2}) \mathbf{a}_3$	$=$	$a(x_7 + \frac{1}{2}) \hat{\mathbf{x}} + by_7 \hat{\mathbf{y}} - c(z_7 - \frac{1}{2}) \hat{\mathbf{z}}$	(8d)	O V
$\mathbf{B}_{35}$	$=$	$x_7 \mathbf{a}_1 - (y_7 - \frac{1}{2}) \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$ax_7 \hat{\mathbf{x}} - b(y_7 - \frac{1}{2}) \hat{\mathbf{y}} + cz_7 \hat{\mathbf{z}}$	(8d)	O V
$\mathbf{B}_{36}$	$=$	$-(x_7 - \frac{1}{2}) \mathbf{a}_1 + (y_7 + \frac{1}{2}) \mathbf{a}_2 + (z_7 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_7 - \frac{1}{2}) \hat{\mathbf{x}} + b(y_7 + \frac{1}{2}) \hat{\mathbf{y}} + c(z_7 + \frac{1}{2}) \hat{\mathbf{z}}$	(8d)	O V
$\mathbf{B}_{37}$	$=$	$x_8 \mathbf{a}_1 + y_8 \mathbf{a}_2 + z_8 \mathbf{a}_3$	$=$	$ax_8 \hat{\mathbf{x}} + by_8 \hat{\mathbf{y}} + cz_8 \hat{\mathbf{z}}$	(8d)	Y I
$\mathbf{B}_{38}$	$=$	$-(x_8 - \frac{1}{2}) \mathbf{a}_1 - y_8 \mathbf{a}_2 + (z_8 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_8 - \frac{1}{2}) \hat{\mathbf{x}} - by_8 \hat{\mathbf{y}} + c(z_8 + \frac{1}{2}) \hat{\mathbf{z}}$	(8d)	Y I
$\mathbf{B}_{39}$	$=$	$-x_8 \mathbf{a}_1 + (y_8 + \frac{1}{2}) \mathbf{a}_2 - z_8 \mathbf{a}_3$	$=$	$-ax_8 \hat{\mathbf{x}} + b(y_8 + \frac{1}{2}) \hat{\mathbf{y}} - cz_8 \hat{\mathbf{z}}$	(8d)	Y I
$\mathbf{B}_{40}$	$=$	$(x_8 + \frac{1}{2}) \mathbf{a}_1 - (y_8 - \frac{1}{2}) \mathbf{a}_2 - (z_8 - \frac{1}{2}) \mathbf{a}_3$	$=$	$a(x_8 + \frac{1}{2}) \hat{\mathbf{x}} - b(y_8 - \frac{1}{2}) \hat{\mathbf{y}} - c(z_8 - \frac{1}{2}) \hat{\mathbf{z}}$	(8d)	Y I
$\mathbf{B}_{41}$	$=$	$-x_8 \mathbf{a}_1 - y_8 \mathbf{a}_2 - z_8 \mathbf{a}_3$	$=$	$-ax_8 \hat{\mathbf{x}} - by_8 \hat{\mathbf{y}} - cz_8 \hat{\mathbf{z}}$	(8d)	Y I
$\mathbf{B}_{42}$	$=$	$(x_8 + \frac{1}{2}) \mathbf{a}_1 + y_8 \mathbf{a}_2 - (z_8 - \frac{1}{2}) \mathbf{a}_3$	$=$	$a(x_8 + \frac{1}{2}) \hat{\mathbf{x}} + by_8 \hat{\mathbf{y}} - c(z_8 - \frac{1}{2}) \hat{\mathbf{z}}$	(8d)	Y I
$\mathbf{B}_{43}$	$=$	$x_8 \mathbf{a}_1 - (y_8 - \frac{1}{2}) \mathbf{a}_2 + z_8 \mathbf{a}_3$	$=$	$ax_8 \hat{\mathbf{x}} - b(y_8 - \frac{1}{2}) \hat{\mathbf{y}} + cz_8 \hat{\mathbf{z}}$	(8d)	Y I
$\mathbf{B}_{44}$	$=$	$-(x_8 - \frac{1}{2}) \mathbf{a}_1 + (y_8 + \frac{1}{2}) \mathbf{a}_2 + (z_8 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_8 - \frac{1}{2}) \hat{\mathbf{x}} + b(y_8 + \frac{1}{2}) \hat{\mathbf{y}} + c(z_8 + \frac{1}{2}) \hat{\mathbf{z}}$	(8d)	Y I

## References

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