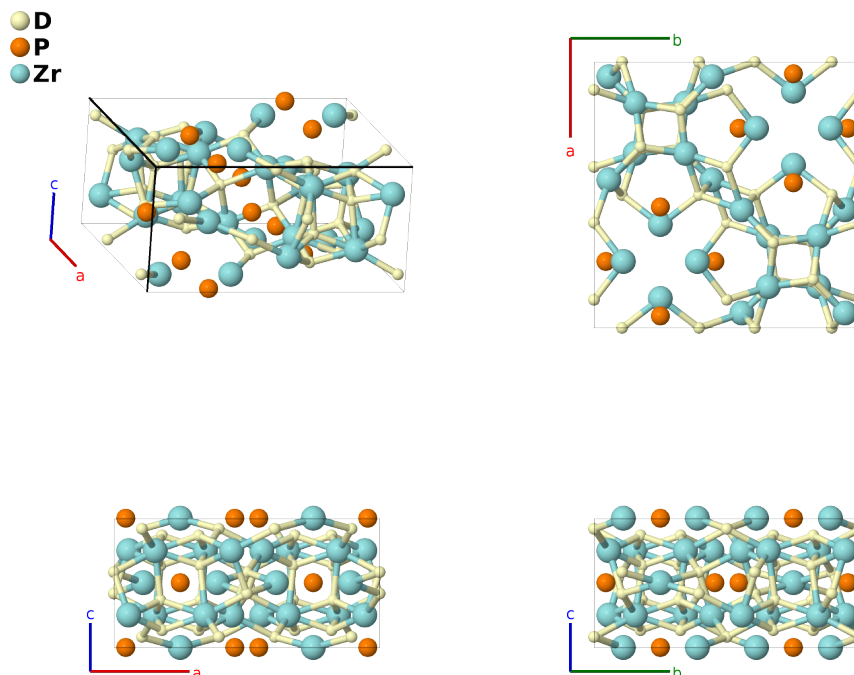


# Zr<sub>3</sub>PD<sub>3</sub> Structure: A4BC3\_tP64\_133\_2k\_h\_i2j-001

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

[https://aflow.org/p/A4BC3\\_tP64\\_133\\_2k\\_h\\_i2j-001](https://aflow.org/p/A4BC3_tP64_133_2k_h_i2j-001)



Prototype	H <sub>3</sub> PZr <sub>3</sub>
AFLOW prototype label	A4BC3_tP64_133_2k_h_i2j-001
ICSD	68531
Pearson symbol	tP64
Space group number	133
Space group symbol	<i>P4<sub>2</sub>/nbc</i>
AFLOW prototype command	<code>aflow --proto=A4BC3_tP64_133_2k_h_i2j-001 --params=a, c/a, x<sub>1</sub>, x<sub>2</sub>, x<sub>3</sub>, x<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></code>

## Other compounds with this structure

Ti<sub>3</sub>PD<sub>3</sub>

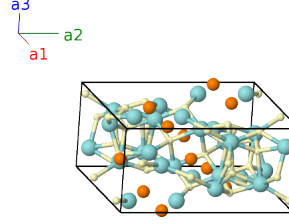
- The D-I (16k) site has a small number of vacancies (0.4%).
- The D-II (16k) site is 44.7% occupied.

- Removing all of the deuterium atoms makes this isostructural with  $\beta$ -V<sub>3</sub>S.

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### Simple Tetragonal primitive vectors

$$\begin{aligned}\mathbf{a}_1 &= a \hat{\mathbf{x}} \\ \mathbf{a}_2 &= a \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}}\end{aligned}$$




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### Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= x_1 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2$	$=$	$ax_1 \hat{\mathbf{x}} + \frac{1}{4}a \hat{\mathbf{y}}$	(8h)	P I
$\mathbf{B}_2$	$= -\left(x_1 - \frac{1}{2}\right) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2$	$=$	$-a\left(x_1 - \frac{1}{2}\right) \hat{\mathbf{x}} + \frac{1}{4}a \hat{\mathbf{y}}$	(8h)	P I
$\mathbf{B}_3$	$= \frac{1}{4} \mathbf{a}_1 + x_1 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} + ax_1 \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(8h)	P I
$\mathbf{B}_4$	$= \frac{1}{4} \mathbf{a}_1 - \left(x_1 - \frac{1}{2}\right) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} - a\left(x_1 - \frac{1}{2}\right) \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(8h)	P I
$\mathbf{B}_5$	$= -x_1 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2$	$=$	$-ax_1 \hat{\mathbf{x}} + \frac{3}{4}a \hat{\mathbf{y}}$	(8h)	P I
$\mathbf{B}_6$	$= \left(x_1 + \frac{1}{2}\right) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2$	$=$	$a\left(x_1 + \frac{1}{2}\right) \hat{\mathbf{x}} + \frac{3}{4}a \hat{\mathbf{y}}$	(8h)	P I
$\mathbf{B}_7$	$= \frac{3}{4} \mathbf{a}_1 - x_1 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{3}{4}a \hat{\mathbf{x}} - ax_1 \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(8h)	P I
$\mathbf{B}_8$	$= \frac{3}{4} \mathbf{a}_1 + \left(x_1 + \frac{1}{2}\right) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{3}{4}a \hat{\mathbf{x}} + a\left(x_1 + \frac{1}{2}\right) \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(8h)	P I
$\mathbf{B}_9$	$= x_2 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$ax_2 \hat{\mathbf{x}} + \frac{1}{4}a \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(8i)	Zr I
$\mathbf{B}_{10}$	$= -\left(x_2 - \frac{1}{2}\right) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-a\left(x_2 - \frac{1}{2}\right) \hat{\mathbf{x}} + \frac{1}{4}a \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(8i)	Zr I
$\mathbf{B}_{11}$	$= \frac{1}{4} \mathbf{a}_1 + x_2 \mathbf{a}_2$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} + ax_2 \hat{\mathbf{y}}$	(8i)	Zr I
$\mathbf{B}_{12}$	$= \frac{1}{4} \mathbf{a}_1 - \left(x_2 - \frac{1}{2}\right) \mathbf{a}_2$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} - a\left(x_2 - \frac{1}{2}\right) \hat{\mathbf{y}}$	(8i)	Zr I
$\mathbf{B}_{13}$	$= -x_2 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-ax_2 \hat{\mathbf{x}} + \frac{3}{4}a \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(8i)	Zr I
$\mathbf{B}_{14}$	$= \left(x_2 + \frac{1}{2}\right) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$a\left(x_2 + \frac{1}{2}\right) \hat{\mathbf{x}} + \frac{3}{4}a \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(8i)	Zr I
$\mathbf{B}_{15}$	$= \frac{3}{4} \mathbf{a}_1 - x_2 \mathbf{a}_2$	$=$	$\frac{3}{4}a \hat{\mathbf{x}} - ax_2 \hat{\mathbf{y}}$	(8i)	Zr I
$\mathbf{B}_{16}$	$= \frac{3}{4} \mathbf{a}_1 + \left(x_2 + \frac{1}{2}\right) \mathbf{a}_2$	$=$	$\frac{3}{4}a \hat{\mathbf{x}} + a\left(x_2 + \frac{1}{2}\right) \hat{\mathbf{y}}$	(8i)	Zr I
$\mathbf{B}_{17}$	$= x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$ax_3 \hat{\mathbf{x}} + ax_3 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(8j)	Zr II
$\mathbf{B}_{18}$	$= -\left(x_3 - \frac{1}{2}\right) \mathbf{a}_1 - \left(x_3 - \frac{1}{2}\right) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$-a\left(x_3 - \frac{1}{2}\right) \hat{\mathbf{x}} - a\left(x_3 - \frac{1}{2}\right) \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(8j)	Zr II
$\mathbf{B}_{19}$	$= -\left(x_3 - \frac{1}{2}\right) \mathbf{a}_1 + x_3 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$-a\left(x_3 - \frac{1}{2}\right) \hat{\mathbf{x}} + ax_3 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(8j)	Zr II
$\mathbf{B}_{20}$	$= x_3 \mathbf{a}_1 - \left(x_3 - \frac{1}{2}\right) \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$ax_3 \hat{\mathbf{x}} - a\left(x_3 - \frac{1}{2}\right) \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(8j)	Zr II
$\mathbf{B}_{21}$	$= -x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$-ax_3 \hat{\mathbf{x}} - ax_3 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(8j)	Zr II
$\mathbf{B}_{22}$	$= \left(x_3 + \frac{1}{2}\right) \mathbf{a}_1 + \left(x_3 + \frac{1}{2}\right) \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$a\left(x_3 + \frac{1}{2}\right) \hat{\mathbf{x}} + a\left(x_3 + \frac{1}{2}\right) \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(8j)	Zr II
$\mathbf{B}_{23}$	$= \left(x_3 + \frac{1}{2}\right) \mathbf{a}_1 - x_3 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$a\left(x_3 + \frac{1}{2}\right) \hat{\mathbf{x}} - ax_3 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(8j)	Zr II
$\mathbf{B}_{24}$	$= -x_3 \mathbf{a}_1 + \left(x_3 + \frac{1}{2}\right) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$-ax_3 \hat{\mathbf{x}} + a\left(x_3 + \frac{1}{2}\right) \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(8j)	Zr II
$\mathbf{B}_{25}$	$= x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$ax_4 \hat{\mathbf{x}} + ax_4 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(8j)	Zr III
$\mathbf{B}_{26}$	$= -\left(x_4 - \frac{1}{2}\right) \mathbf{a}_1 - \left(x_4 - \frac{1}{2}\right) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$-a\left(x_4 - \frac{1}{2}\right) \hat{\mathbf{x}} - a\left(x_4 - \frac{1}{2}\right) \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(8j)	Zr III



$$\mathbf{B}_{61} = (x_6 + \frac{1}{2}) \mathbf{a}_1 - y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3 = a(x_6 + \frac{1}{2}) \hat{\mathbf{x}} - ay_6 \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}} \quad (16k) \quad \text{D II}$$

$$\mathbf{B}_{62} = -x_6 \mathbf{a}_1 + (y_6 + \frac{1}{2}) \mathbf{a}_2 + z_6 \mathbf{a}_3 = -ax_6 \hat{\mathbf{x}} + a(y_6 + \frac{1}{2}) \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}} \quad (16k) \quad \text{D II}$$

$$\mathbf{B}_{63} = -y_6 \mathbf{a}_1 - x_6 \mathbf{a}_2 + (z_6 + \frac{1}{2}) \mathbf{a}_3 = -ay_6 \hat{\mathbf{x}} - ax_6 \hat{\mathbf{y}} + c(z_6 + \frac{1}{2}) \hat{\mathbf{z}} \quad (16k) \quad \text{D II}$$

$$\mathbf{B}_{64} = (y_6 + \frac{1}{2}) \mathbf{a}_1 + (x_6 + \frac{1}{2}) \mathbf{a}_2 + (z_6 + \frac{1}{2}) \mathbf{a}_3 = a(y_6 + \frac{1}{2}) \hat{\mathbf{x}} + a(x_6 + \frac{1}{2}) \hat{\mathbf{y}} + c(z_6 + \frac{1}{2}) \hat{\mathbf{z}} \quad (16k) \quad \text{D II}$$

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