

ZrP₂O₇ (*K*6₁) High-Temperature Structure: A7B2C_cP40_205_ad_c_b-001

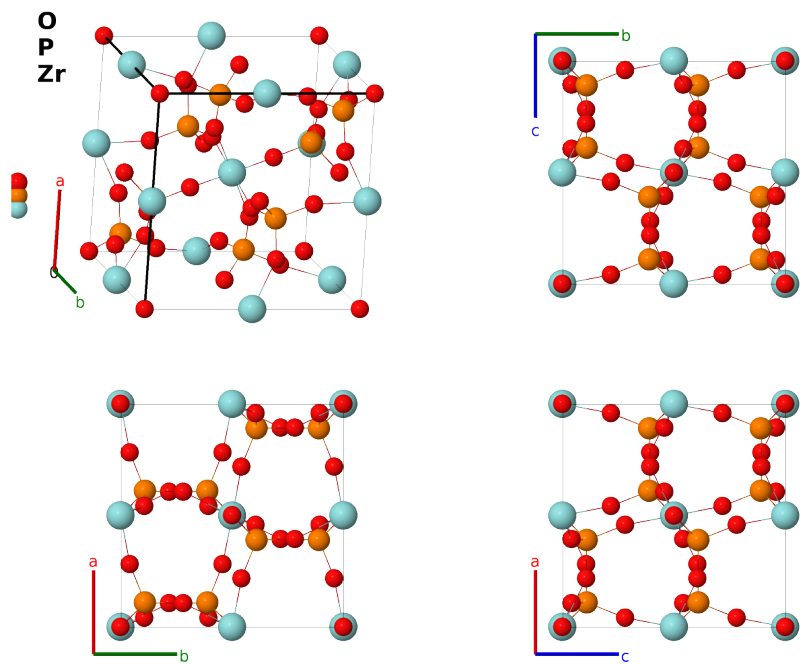
This structure previously used the label(s) **A7B2C_cP40_205_bd_c_a**. Calls to these addresses will be redirected here.

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<https://aflow.org/prototype-encyclopedia/NTUQ>

https://aflow.org/prototype-encyclopedia/A7B2C_cP40_205_ad_c_b-001



Prototype	P ₂ O ₇ Zr
AFLOW prototype label	A7B2C_cP40_205_ad_c_b-001
Strukturbericht designation	K6 ₁
ICSD	30272
CCDC	1604640
Pearson symbol	cP40
Space group number	205
Space group symbol	$P\bar{a}3$
AFLOW prototype command	<pre>aflow --proto=A7B2C_cP40_205_ad_c_b-001 --params=a, x₃, x₄, y₄, z₄</pre>

Other compounds with this structure

CeAs₂O₇, CeP₂O₇, CeV₂O₇, GeAs₂O₇, GeP₂O₇, GeV₂O₇, HfAs₂O₇, HfP₂O₇, HfV₂O₇, MoAs₂O₇, MoP₂O₇, MoV₂O₇, PbAs₂O₇, PbP₂O₇, PbV₂O₇, ReAs₂O₇, ReP₂O₇, ReV₂O₇, SiAs₂O₇, SiP₂O₇, SiV₂O₇, SnAs₂O₇, SnP₂O₇, SnV₂O₇, TiAs₂O₇, TiP₂O₇, TiV₂O₇, UAs₂O₇, UP₂O₇, UV₂O₇, WAs₂O₇, WP₂O₇, WV₂O₇, ZrAs₂O₇, ZrP₂O₇, ZrV₂O₇

- This is the high temperature form of all the structures listed. The low temperature structure depends on the composition. Below 290°C ZrP₂O₇ transforms to an orthorhombic structure, space group *Pbca* #61, with 136 unique crystallographic positions and 1080 atomic sites. See (Birkedal, 2006) and (Stinton, 2006) for more details.

Simple Cubic primitive vectors



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	0	$=$	0	(4a)	O I
$\mathbf{B}_2$	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{z}}$	(4a)	O I
$\mathbf{B}_3$	$\frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{y}} + \frac{1}{2} a \hat{\mathbf{z}}$	(4a)	O I
$\mathbf{B}_4$	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}}$	(4a)	O I
$\mathbf{B}_5$	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} + \frac{1}{2} a \hat{\mathbf{z}}$	(4b)	Zr I
$\mathbf{B}_6$	$\frac{1}{2} \mathbf{a}_2$	$=$	$\frac{1}{2} a \hat{\mathbf{y}}$	(4b)	Zr I
$\mathbf{B}_7$	$\frac{1}{2} \mathbf{a}_1$	$=$	$\frac{1}{2} a \hat{\mathbf{x}}$	(4b)	Zr I
$\mathbf{B}_8$	$\frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{z}}$	(4b)	Zr I
$\mathbf{B}_9$	$x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + x_3 \mathbf{a}_3$	$=$	$ax_3 \hat{\mathbf{x}} + ax_3 \hat{\mathbf{y}} + ax_3 \hat{\mathbf{z}}$	(8c)	P I
$\mathbf{B}_{10}$	$-\left(x_3 - \frac{1}{2}\right) \mathbf{a}_1 - x_3 \mathbf{a}_2 + \left(x_3 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a\left(x_3 - \frac{1}{2}\right) \hat{\mathbf{x}} - ax_3 \hat{\mathbf{y}} + a\left(x_3 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(8c)	P I
$\mathbf{B}_{11}$	$-x_3 \mathbf{a}_1 + \left(x_3 + \frac{1}{2}\right) \mathbf{a}_2 - \left(x_3 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-ax_3 \hat{\mathbf{x}} + a\left(x_3 + \frac{1}{2}\right) \hat{\mathbf{y}} - a\left(x_3 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(8c)	P I
$\mathbf{B}_{12}$	$\left(x_3 + \frac{1}{2}\right) \mathbf{a}_1 - \left(x_3 - \frac{1}{2}\right) \mathbf{a}_2 - x_3 \mathbf{a}_3$	$=$	$a\left(x_3 + \frac{1}{2}\right) \hat{\mathbf{x}} - a\left(x_3 - \frac{1}{2}\right) \hat{\mathbf{y}} - ax_3 \hat{\mathbf{z}}$	(8c)	P I
$\mathbf{B}_{13}$	$-x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 - x_3 \mathbf{a}_3$	$=$	$-ax_3 \hat{\mathbf{x}} - ax_3 \hat{\mathbf{y}} - ax_3 \hat{\mathbf{z}}$	(8c)	P I
$\mathbf{B}_{14}$	$\left(x_3 + \frac{1}{2}\right) \mathbf{a}_1 + x_3 \mathbf{a}_2 - \left(x_3 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$a\left(x_3 + \frac{1}{2}\right) \hat{\mathbf{x}} + ax_3 \hat{\mathbf{y}} - a\left(x_3 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(8c)	P I
$\mathbf{B}_{15}$	$x_3 \mathbf{a}_1 - \left(x_3 - \frac{1}{2}\right) \mathbf{a}_2 + \left(x_3 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$ax_3 \hat{\mathbf{x}} - a\left(x_3 - \frac{1}{2}\right) \hat{\mathbf{y}} + a\left(x_3 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(8c)	P I
$\mathbf{B}_{16}$	$-\left(x_3 - \frac{1}{2}\right) \mathbf{a}_1 + \left(x_3 + \frac{1}{2}\right) \mathbf{a}_2 + x_3 \mathbf{a}_3$	$=$	$-a\left(x_3 - \frac{1}{2}\right) \hat{\mathbf{x}} + a\left(x_3 + \frac{1}{2}\right) \hat{\mathbf{y}} + ax_3 \hat{\mathbf{z}}$	(8c)	P I
$\mathbf{B}_{17}$	$x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$ax_4 \hat{\mathbf{x}} + ay_4 \hat{\mathbf{y}} + az_4 \hat{\mathbf{z}}$	(24d)	O II
$\mathbf{B}_{18}$	$-\left(x_4 - \frac{1}{2}\right) \mathbf{a}_1 - y_4 \mathbf{a}_2 + \left(z_4 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a\left(x_4 - \frac{1}{2}\right) \hat{\mathbf{x}} - ay_4 \hat{\mathbf{y}} + a\left(z_4 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(24d)	O II

$$\begin{aligned}
\mathbf{B}_{19} &= -x_4 \mathbf{a}_1 + \left(y_4 + \frac{1}{2}\right) \mathbf{a}_2 - \left(z_4 - \frac{1}{2}\right) \mathbf{a}_3 = -ax_4 \hat{\mathbf{x}} + a \left(y_4 + \frac{1}{2}\right) \hat{\mathbf{y}} - a \left(z_4 - \frac{1}{2}\right) \hat{\mathbf{z}} & (24d) & \text{O II} \\
\mathbf{B}_{20} &= \left(x_4 + \frac{1}{2}\right) \mathbf{a}_1 - \left(y_4 - \frac{1}{2}\right) \mathbf{a}_2 - z_4 \mathbf{a}_3 = a \left(x_4 + \frac{1}{2}\right) \hat{\mathbf{x}} - a \left(y_4 - \frac{1}{2}\right) \hat{\mathbf{y}} - az_4 \hat{\mathbf{z}} & (24d) & \text{O II} \\
\mathbf{B}_{21} &= z_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + y_4 \mathbf{a}_3 = az_4 \hat{\mathbf{x}} + ax_4 \hat{\mathbf{y}} + ay_4 \hat{\mathbf{z}} & (24d) & \text{O II} \\
\mathbf{B}_{22} &= \left(z_4 + \frac{1}{2}\right) \mathbf{a}_1 - \left(x_4 - \frac{1}{2}\right) \mathbf{a}_2 - y_4 \mathbf{a}_3 = a \left(z_4 + \frac{1}{2}\right) \hat{\mathbf{x}} - a \left(x_4 - \frac{1}{2}\right) \hat{\mathbf{y}} - ay_4 \hat{\mathbf{z}} & (24d) & \text{O II} \\
\mathbf{B}_{23} &= -\left(z_4 - \frac{1}{2}\right) \mathbf{a}_1 - x_4 \mathbf{a}_2 + \left(y_4 + \frac{1}{2}\right) \mathbf{a}_3 = -a \left(z_4 - \frac{1}{2}\right) \hat{\mathbf{x}} - ax_4 \hat{\mathbf{y}} + a \left(y_4 + \frac{1}{2}\right) \hat{\mathbf{z}} & (24d) & \text{O II} \\
\mathbf{B}_{24} &= -z_4 \mathbf{a}_1 + \left(x_4 + \frac{1}{2}\right) \mathbf{a}_2 - \left(y_4 - \frac{1}{2}\right) \mathbf{a}_3 = -az_4 \hat{\mathbf{x}} + a \left(x_4 + \frac{1}{2}\right) \hat{\mathbf{y}} - a \left(y_4 - \frac{1}{2}\right) \hat{\mathbf{z}} & (24d) & \text{O II} \\
\mathbf{B}_{25} &= y_4 \mathbf{a}_1 + z_4 \mathbf{a}_2 + x_4 \mathbf{a}_3 = ay_4 \hat{\mathbf{x}} + az_4 \hat{\mathbf{y}} + ax_4 \hat{\mathbf{z}} & (24d) & \text{O II} \\
\mathbf{B}_{26} &= -y_4 \mathbf{a}_1 + \left(z_4 + \frac{1}{2}\right) \mathbf{a}_2 - \left(x_4 - \frac{1}{2}\right) \mathbf{a}_3 = -ay_4 \hat{\mathbf{x}} + a \left(z_4 + \frac{1}{2}\right) \hat{\mathbf{y}} - a \left(x_4 - \frac{1}{2}\right) \hat{\mathbf{z}} & (24d) & \text{O II} \\
\mathbf{B}_{27} &= \left(y_4 + \frac{1}{2}\right) \mathbf{a}_1 - \left(z_4 - \frac{1}{2}\right) \mathbf{a}_2 - x_4 \mathbf{a}_3 = a \left(y_4 + \frac{1}{2}\right) \hat{\mathbf{x}} - a \left(z_4 - \frac{1}{2}\right) \hat{\mathbf{y}} - ax_4 \hat{\mathbf{z}} & (24d) & \text{O II} \\
\mathbf{B}_{28} &= -\left(y_4 - \frac{1}{2}\right) \mathbf{a}_1 - z_4 \mathbf{a}_2 + \left(x_4 + \frac{1}{2}\right) \mathbf{a}_3 = -a \left(y_4 - \frac{1}{2}\right) \hat{\mathbf{x}} - az_4 \hat{\mathbf{y}} + a \left(x_4 + \frac{1}{2}\right) \hat{\mathbf{z}} & (24d) & \text{O II} \\
\mathbf{B}_{29} &= -x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 - z_4 \mathbf{a}_3 = -ax_4 \hat{\mathbf{x}} - ay_4 \hat{\mathbf{y}} - az_4 \hat{\mathbf{z}} & (24d) & \text{O II} \\
\mathbf{B}_{30} &= \left(x_4 + \frac{1}{2}\right) \mathbf{a}_1 + y_4 \mathbf{a}_2 - \left(z_4 - \frac{1}{2}\right) \mathbf{a}_3 = a \left(x_4 + \frac{1}{2}\right) \hat{\mathbf{x}} + ay_4 \hat{\mathbf{y}} - a \left(z_4 - \frac{1}{2}\right) \hat{\mathbf{z}} & (24d) & \text{O II} \\
\mathbf{B}_{31} &= x_4 \mathbf{a}_1 - \left(y_4 - \frac{1}{2}\right) \mathbf{a}_2 + \left(z_4 + \frac{1}{2}\right) \mathbf{a}_3 = ax_4 \hat{\mathbf{x}} - a \left(y_4 - \frac{1}{2}\right) \hat{\mathbf{y}} + a \left(z_4 + \frac{1}{2}\right) \hat{\mathbf{z}} & (24d) & \text{O II} \\
\mathbf{B}_{32} &= -\left(x_4 - \frac{1}{2}\right) \mathbf{a}_1 + \left(y_4 + \frac{1}{2}\right) \mathbf{a}_2 + z_4 \mathbf{a}_3 = -a \left(x_4 - \frac{1}{2}\right) \hat{\mathbf{x}} + a \left(y_4 + \frac{1}{2}\right) \hat{\mathbf{y}} + az_4 \hat{\mathbf{z}} & (24d) & \text{O II} \\
\mathbf{B}_{33} &= -z_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 - y_4 \mathbf{a}_3 = -az_4 \hat{\mathbf{x}} - ax_4 \hat{\mathbf{y}} - ay_4 \hat{\mathbf{z}} & (24d) & \text{O II} \\
\mathbf{B}_{34} &= -\left(z_4 - \frac{1}{2}\right) \mathbf{a}_1 + \left(x_4 + \frac{1}{2}\right) \mathbf{a}_2 + y_4 \mathbf{a}_3 = -a \left(z_4 - \frac{1}{2}\right) \hat{\mathbf{x}} + a \left(x_4 + \frac{1}{2}\right) \hat{\mathbf{y}} + ay_4 \hat{\mathbf{z}} & (24d) & \text{O II} \\
\mathbf{B}_{35} &= \left(z_4 + \frac{1}{2}\right) \mathbf{a}_1 + x_4 \mathbf{a}_2 - \left(y_4 - \frac{1}{2}\right) \mathbf{a}_3 = a \left(z_4 + \frac{1}{2}\right) \hat{\mathbf{x}} + ax_4 \hat{\mathbf{y}} - a \left(y_4 - \frac{1}{2}\right) \hat{\mathbf{z}} & (24d) & \text{O II} \\
\mathbf{B}_{36} &= z_4 \mathbf{a}_1 - \left(x_4 - \frac{1}{2}\right) \mathbf{a}_2 + \left(y_4 + \frac{1}{2}\right) \mathbf{a}_3 = az_4 \hat{\mathbf{x}} - a \left(x_4 - \frac{1}{2}\right) \hat{\mathbf{y}} + a \left(y_4 + \frac{1}{2}\right) \hat{\mathbf{z}} & (24d) & \text{O II} \\
\mathbf{B}_{37} &= -y_4 \mathbf{a}_1 - z_4 \mathbf{a}_2 - x_4 \mathbf{a}_3 = -ay_4 \hat{\mathbf{x}} - az_4 \hat{\mathbf{y}} - ax_4 \hat{\mathbf{z}} & (24d) & \text{O II} \\
\mathbf{B}_{38} &= y_4 \mathbf{a}_1 - \left(z_4 - \frac{1}{2}\right) \mathbf{a}_2 + \left(x_4 + \frac{1}{2}\right) \mathbf{a}_3 = ay_4 \hat{\mathbf{x}} - a \left(z_4 - \frac{1}{2}\right) \hat{\mathbf{y}} + a \left(x_4 + \frac{1}{2}\right) \hat{\mathbf{z}} & (24d) & \text{O II} \\
\mathbf{B}_{39} &= -\left(y_4 - \frac{1}{2}\right) \mathbf{a}_1 + \left(z_4 + \frac{1}{2}\right) \mathbf{a}_2 + x_4 \mathbf{a}_3 = -a \left(y_4 - \frac{1}{2}\right) \hat{\mathbf{x}} + a \left(z_4 + \frac{1}{2}\right) \hat{\mathbf{y}} + ax_4 \hat{\mathbf{z}} & (24d) & \text{O II} \\
\mathbf{B}_{40} &= \left(y_4 + \frac{1}{2}\right) \mathbf{a}_1 + z_4 \mathbf{a}_2 - \left(x_4 - \frac{1}{2}\right) \mathbf{a}_3 = a \left(y_4 + \frac{1}{2}\right) \hat{\mathbf{x}} + az_4 \hat{\mathbf{y}} - a \left(x_4 - \frac{1}{2}\right) \hat{\mathbf{z}} & (24d) & \text{O II}
\end{aligned}$$

References

- [1] G. R. Levi and G. Peyronel, *Struttura Cristallografica del Gruppo Isomorfo (Si^{4+} , Ti^{4+} , Zr^{4+} , Sn^{4+} , Hf^{4+}) P_2O_7* , Z. Kristallogr. **92**, 190–209 (1935), doi:10.1524/zkri.1935.92.1.210.
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First cited in

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