ZrP$_2$O$_7$ ($K6_1$) High-Temperature Structure: A7B2C_cP40_205_ad_c_b-001
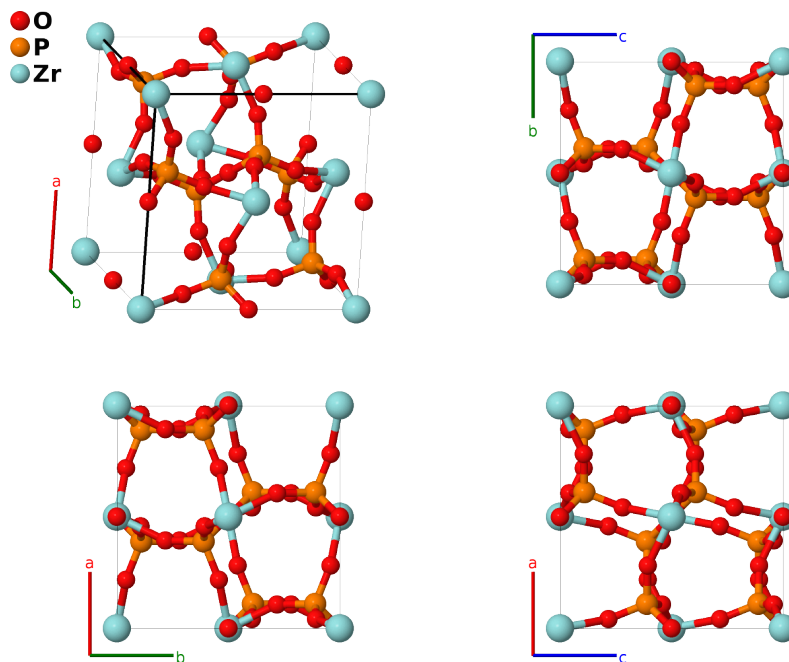
This structure originally had the label `A7B2C_cP40_205_bd_c_a`. Calls to that address will be redirected here.

https://aflow.org/p/NTUQ

https://aflow.org/p/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
Pearson symbol	cP40
Space group number	205
Space group symbol	$Pa\overline{3}$
AFLOW prototype command	aflow --proto=A7B2C_cP40_205_ad_c_b-001
	--params=a, x_3, x_4, y_4, z_4

Other compounds with this structure

CeAs$_2$O$_7$, CeP$_2$O$_7$, CeV$_2$O$_7$, GeAs$_2$O$_7$, GeP$_2$O$_7$, GeV$_2$O$_7$, HfAs$_2$O$_7$, HfP$_2$O$_7$, HfV$_2$O$_7$, MoAs$_2$O$_7$, MoP$_2$O$_7$, MoV$_2$O$_7$, PbAs$_2$O$_7$, PbP$_2$O$_7$, PbV$_2$O$_7$, ReAs$_2$O$_7$, ReP$_2$O$_7$, ReV$_2$O$_7$, SiAs$_2$O$_7$, SiP$_2$O$_7$, SiV$_2$O$_7$, SnAs$_2$O$_7$, SnP$_2$O$_7$, SnV$_2$O$_7$, TiAs$_2$O$_7$, TiP$_2$O$_7$, TiV$_2$O$_7$, UAs$_2$O$_7$, UP$_2$O$_7$, UV$_2$O$_7$, WAs$_2$O$_7$, WP$_2$O$_7$, WV$_2$O$_7$, ZrAs$_2$O$_7$, ZrP$_2$O$_7$, ZrV$_2$O$_7$

- This is the high temperature form of all the structures listed. The low temperature structure depends on the composition. Below 290°C ZrP_2O_7 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

$$\mathbf{a_1} = a\,\hat{\mathbf{x}}$$
$$\mathbf{a_2} = a\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = a\,\hat{\mathbf{z}}$$
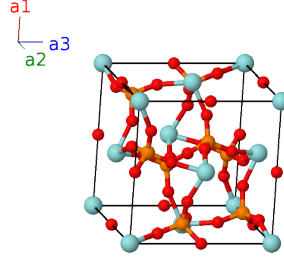
Basis vectors

		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
$\mathbf{B_{19}}$	$=$	$-x_4\,\mathbf{a_1} + \left(y_4 + \frac{1}{2}\right)\mathbf{a_2} - \left(z_4 - \frac{1}{2}\right)\mathbf{a_3}$	$=$	$-ax_4\,\hat{\mathbf{x}} + a\left(y_4 + \frac{1}{2}\right)\hat{\mathbf{y}} - a\left(z_4 - \frac{1}{2}\right)\hat{\mathbf{z}}$	(24d)	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)	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)	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)	O II

$\mathbf{B_{23}}$	$=$	$-\left(z_4-\tfrac{1}{2}\right)\mathbf{a}_1-x_4\,\mathbf{a}_2+\left(y_4+\tfrac{1}{2}\right)\mathbf{a}_3$	$=$	$-a\left(z_4-\tfrac{1}{2}\right)\hat{\mathbf{x}}-ax_4\,\hat{\mathbf{y}}+a\left(y_4+\tfrac{1}{2}\right)\hat{\mathbf{z}}$	(24d)	O II
$\mathbf{B_{24}}$	$=$	$-z_4\,\mathbf{a}_1+\left(x_4+\tfrac{1}{2}\right)\mathbf{a}_2-\left(y_4-\tfrac{1}{2}\right)\mathbf{a}_3$	$=$	$-az_4\,\hat{\mathbf{x}}+a\left(x_4+\tfrac{1}{2}\right)\hat{\mathbf{y}}-a\left(y_4-\tfrac{1}{2}\right)\hat{\mathbf{z}}$	(24d)	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)	O II
$\mathbf{B_{26}}$	$=$	$-y_4\,\mathbf{a}_1+\left(z_4+\tfrac{1}{2}\right)\mathbf{a}_2-\left(x_4-\tfrac{1}{2}\right)\mathbf{a}_3$	$=$	$-ay_4\,\hat{\mathbf{x}}+a\left(z_4+\tfrac{1}{2}\right)\hat{\mathbf{y}}-a\left(x_4-\tfrac{1}{2}\right)\hat{\mathbf{z}}$	(24d)	O II
$\mathbf{B_{27}}$	$=$	$\left(y_4+\tfrac{1}{2}\right)\mathbf{a}_1-\left(z_4-\tfrac{1}{2}\right)\mathbf{a}_2-x_4\,\mathbf{a}_3$	$=$	$a\left(y_4+\tfrac{1}{2}\right)\hat{\mathbf{x}}-a\left(z_4-\tfrac{1}{2}\right)\hat{\mathbf{y}}-ax_4\,\hat{\mathbf{z}}$	(24d)	O II
$\mathbf{B_{28}}$	$=$	$-\left(y_4-\tfrac{1}{2}\right)\mathbf{a}_1-z_4\,\mathbf{a}_2+\left(x_4+\tfrac{1}{2}\right)\mathbf{a}_3$	$=$	$-a\left(y_4-\tfrac{1}{2}\right)\hat{\mathbf{x}}-az_4\,\hat{\mathbf{y}}+a\left(x_4+\tfrac{1}{2}\right)\hat{\mathbf{z}}$	(24d)	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)	O II
$\mathbf{B_{30}}$	$=$	$\left(x_4+\tfrac{1}{2}\right)\mathbf{a}_1+y_4\,\mathbf{a}_2-\left(z_4-\tfrac{1}{2}\right)\mathbf{a}_3$	$=$	$a\left(x_4+\tfrac{1}{2}\right)\hat{\mathbf{x}}+ay_4\,\hat{\mathbf{y}}-a\left(z_4-\tfrac{1}{2}\right)\hat{\mathbf{z}}$	(24d)	O II
$\mathbf{B_{31}}$	$=$	$x_4\,\mathbf{a}_1-\left(y_4-\tfrac{1}{2}\right)\mathbf{a}_2+\left(z_4+\tfrac{1}{2}\right)\mathbf{a}_3$	$=$	$ax_4\,\hat{\mathbf{x}}-a\left(y_4-\tfrac{1}{2}\right)\hat{\mathbf{y}}+a\left(z_4+\tfrac{1}{2}\right)\hat{\mathbf{z}}$	(24d)	O II
$\mathbf{B_{32}}$	$=$	$-\left(x_4-\tfrac{1}{2}\right)\mathbf{a}_1+\left(y_4+\tfrac{1}{2}\right)\mathbf{a}_2+z_4\,\mathbf{a}_3$	$=$	$-a\left(x_4-\tfrac{1}{2}\right)\hat{\mathbf{x}}+a\left(y_4+\tfrac{1}{2}\right)\hat{\mathbf{y}}+az_4\,\hat{\mathbf{z}}$	(24d)	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)	O II
$\mathbf{B_{34}}$	$=$	$-\left(z_4-\tfrac{1}{2}\right)\mathbf{a}_1+\left(x_4+\tfrac{1}{2}\right)\mathbf{a}_2+y_4\,\mathbf{a}_3$	$=$	$-a\left(z_4-\tfrac{1}{2}\right)\hat{\mathbf{x}}+a\left(x_4+\tfrac{1}{2}\right)\hat{\mathbf{y}}+ay_4\,\hat{\mathbf{z}}$	(24d)	O II
$\mathbf{B_{35}}$	$=$	$\left(z_4+\tfrac{1}{2}\right)\mathbf{a}_1+x_4\,\mathbf{a}_2-\left(y_4-\tfrac{1}{2}\right)\mathbf{a}_3$	$=$	$a\left(z_4+\tfrac{1}{2}\right)\hat{\mathbf{x}}+ax_4\,\hat{\mathbf{y}}-a\left(y_4-\tfrac{1}{2}\right)\hat{\mathbf{z}}$	(24d)	O II
$\mathbf{B_{36}}$	$=$	$z_4\,\mathbf{a}_1-\left(x_4-\tfrac{1}{2}\right)\mathbf{a}_2+\left(y_4+\tfrac{1}{2}\right)\mathbf{a}_3$	$=$	$az_4\,\hat{\mathbf{x}}-a\left(x_4-\tfrac{1}{2}\right)\hat{\mathbf{y}}+a\left(y_4+\tfrac{1}{2}\right)\hat{\mathbf{z}}$	(24d)	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)	O II
$\mathbf{B_{38}}$	$=$	$y_4\,\mathbf{a}_1-\left(z_4-\tfrac{1}{2}\right)\mathbf{a}_2+\left(x_4+\tfrac{1}{2}\right)\mathbf{a}_3$	$=$	$ay_4\,\hat{\mathbf{x}}-a\left(z_4-\tfrac{1}{2}\right)\hat{\mathbf{y}}+a\left(x_4+\tfrac{1}{2}\right)\hat{\mathbf{z}}$	(24d)	O II
$\mathbf{B_{39}}$	$=$	$-\left(y_4-\tfrac{1}{2}\right)\mathbf{a}_1+\left(z_4+\tfrac{1}{2}\right)\mathbf{a}_2+x_4\,\mathbf{a}_3$	$=$	$-a\left(y_4-\tfrac{1}{2}\right)\hat{\mathbf{x}}+a\left(z_4+\tfrac{1}{2}\right)\hat{\mathbf{y}}+ax_4\,\hat{\mathbf{z}}$	(24d)	O II
$\mathbf{B_{40}}$	$=$	$\left(y_4+\tfrac{1}{2}\right)\mathbf{a}_1+z_4\,\mathbf{a}_2-\left(x_4-\tfrac{1}{2}\right)\mathbf{a}_3$	$=$	$a\left(y_4+\tfrac{1}{2}\right)\hat{\mathbf{x}}+az_4\,\hat{\mathbf{y}}-a\left(x_4-\tfrac{1}{2}\right)\hat{\mathbf{z}}$	(24d)	O II

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.

[2] H. Birkedal, A. M. K. Andersen, A. Arakcheeva, G. Chapuis, P. Norby, and P. Pattison, *The Room-Temperature Superstructure of ZrP_2O_7 Is Orthorhombic: There Are No Unusual 180° P-O-P Bond Angles*, Inorg. Chem. **45**, 4346–4351 (2006), doi:10.1021/ic0600174.

[3] G. W. Stinton, M. R. Hampson, and J. S. O. Evans, *The 136-Atom Structure of ZrP_2O_7 and HfP_2O_7 from Powder Diffraction Data*, Inorg. Chem. **45**, 4352–4358 (2006), doi:10.1021/ic060016b.

Found in

[1] R. T. Downs and M. Hall-Wallace, *The American Mineralogist Crystal Structure Database*, Am. Mineral. **88**, 247–250 (2003).