

Zircon (ZrSiO_4 , $S1_1$) Structure: A4BC_tI24_141_h_a_b-001

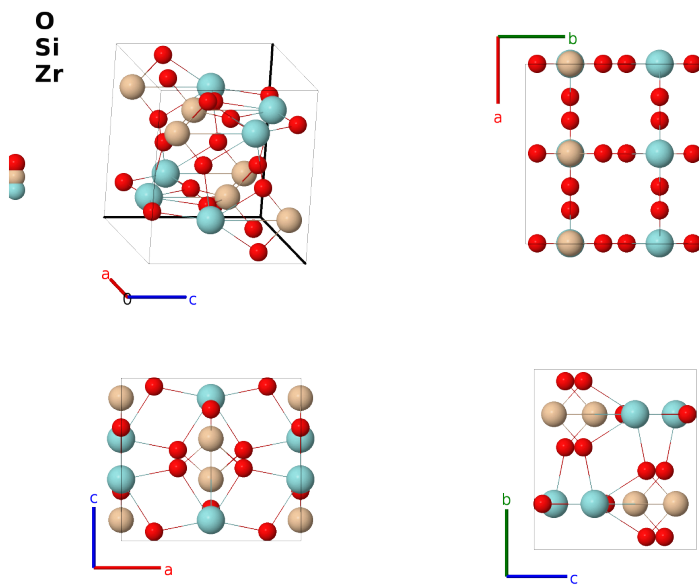
This structure previously used the label(s) **A4BC_tI24_141_h.b.a**. Calls to these addresses will be redirected here.

Cite this page as:

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<https://aflow.org/prototype-encyclopedia/0FQT>

https://aflow.org/prototype-encyclopedia/A4BC_tI24_141_h_a_b-001



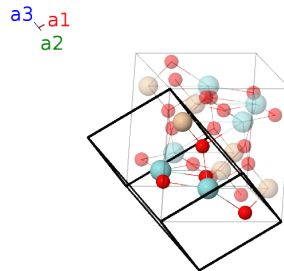
Prototype	O_4SiZr
AFLOW prototype label	A4BC.tI24_141_h_a_b-001
<i>Strukturbericht</i> designation	$S1_1$
Mineral name	zircon
ICSD	100239
CCDC	1659387
Pearson symbol	tI24
Space group number	141
Space group symbol	$I4_1/amd$
AFLOW prototype command	<pre>aflow --proto=A4BC_tI24_141_h_a_b-001 --params=a,c/a,y3,z3</pre>

Other compounds with this structure

BiVO₄, CeSiO₄, CeVO₄, DyPO₄, ErPO₄, ErVO₄, HfSO₄, HoPO₄, HoVO₄, LuPO₄, LuVO₄, NdVO₄, PrVO₄, ScPO₄, ScVO₄, TbPO₄, TbVO₄, ThSiO₄, TmPO₄, TmVO₄, YPO₄, YVO₄, YbAsO₄, YbPO₄, YbVO₄

Body-centered Tetragonal primitive vectors

$$\begin{aligned}\mathbf{a}_1 &= -\frac{1}{2}a\hat{\mathbf{x}} + \frac{1}{2}a\hat{\mathbf{y}} + \frac{1}{2}c\hat{\mathbf{z}} \\ \mathbf{a}_2 &= \frac{1}{2}a\hat{\mathbf{x}} - \frac{1}{2}a\hat{\mathbf{y}} + \frac{1}{2}c\hat{\mathbf{z}} \\ \mathbf{a}_3 &= \frac{1}{2}a\hat{\mathbf{x}} + \frac{1}{2}a\hat{\mathbf{y}} - \frac{1}{2}c\hat{\mathbf{z}}\end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates		Wyckoff position	Atom type
$\mathbf{B}_1$	$= \frac{7}{8}\mathbf{a}_1 + \frac{1}{8}\mathbf{a}_2 + \frac{3}{4}\mathbf{a}_3$	$=$	$\frac{3}{4}a\hat{\mathbf{y}} + \frac{1}{8}c\hat{\mathbf{z}}$		(4a)	Si I
$\mathbf{B}_2$	$= \frac{1}{8}\mathbf{a}_1 + \frac{7}{8}\mathbf{a}_2 + \frac{1}{4}\mathbf{a}_3$	$=$	$\frac{1}{2}a\hat{\mathbf{x}} - \frac{1}{4}a\hat{\mathbf{y}} + \frac{3}{8}c\hat{\mathbf{z}}$		(4a)	Si I
$\mathbf{B}_3$	$= \frac{5}{8}\mathbf{a}_1 + \frac{3}{8}\mathbf{a}_2 + \frac{1}{4}\mathbf{a}_3$	$=$	$\frac{1}{4}a\hat{\mathbf{y}} + \frac{3}{8}c\hat{\mathbf{z}}$		(4b)	Zr I
$\mathbf{B}_4$	$= \frac{3}{8}\mathbf{a}_1 + \frac{5}{8}\mathbf{a}_2 + \frac{3}{4}\mathbf{a}_3$	$=$	$\frac{1}{2}a\hat{\mathbf{x}} + \frac{1}{4}a\hat{\mathbf{y}} + \frac{1}{8}c\hat{\mathbf{z}}$		(4b)	Zr I
$\mathbf{B}_5$	$= (y_3 + z_3)\mathbf{a}_1 + z_3\mathbf{a}_2 + y_3\mathbf{a}_3$	$=$	$ay_3\hat{\mathbf{y}} + cz_3\hat{\mathbf{z}}$		(16h)	O I
$\mathbf{B}_6$	$= \left(-y_3 + z_3 + \frac{1}{2}\right)\mathbf{a}_1 + z_3\mathbf{a}_2 - \left(y_3 - \frac{1}{2}\right)\mathbf{a}_3$	$=$	$-a\left(y_3 - \frac{1}{2}\right)\hat{\mathbf{y}} + cz_3\hat{\mathbf{z}}$		(16h)	O I
$\mathbf{B}_7$	$= z_3\mathbf{a}_1 + \left(-y_3 + z_3 + \frac{1}{2}\right)\mathbf{a}_2 - y_3\mathbf{a}_3$	$=$	$-a\left(y_3 - \frac{1}{4}\right)\hat{\mathbf{x}} - \frac{1}{4}a\hat{\mathbf{y}} + c\left(z_3 + \frac{1}{4}\right)\hat{\mathbf{z}}$		(16h)	O I
$\mathbf{B}_8$	$= z_3\mathbf{a}_1 + (y_3 + z_3)\mathbf{a}_2 + \left(y_3 + \frac{1}{2}\right)\mathbf{a}_3$	$=$	$a\left(y_3 + \frac{1}{4}\right)\hat{\mathbf{x}} + \frac{1}{4}a\hat{\mathbf{y}} + c\left(z_3 - \frac{1}{4}\right)\hat{\mathbf{z}}$		(16h)	O I
$\mathbf{B}_9$	$= \left(y_3 - z_3 + \frac{1}{2}\right)\mathbf{a}_1 - z_3\mathbf{a}_2 + \left(y_3 + \frac{1}{2}\right)\mathbf{a}_3$	$=$	$a\left(y_3 + \frac{1}{2}\right)\hat{\mathbf{y}} - cz_3\hat{\mathbf{z}}$		(16h)	O I
$\mathbf{B}_{10}$	$= -(y_3 + z_3)\mathbf{a}_1 - z_3\mathbf{a}_2 - y_3\mathbf{a}_3$	$=$	$-ay_3\hat{\mathbf{y}} - cz_3\hat{\mathbf{z}}$		(16h)	O I
$\mathbf{B}_{11}$	$= -z_3\mathbf{a}_1 + \left(y_3 - z_3 + \frac{1}{2}\right)\mathbf{a}_2 + y_3\mathbf{a}_3$	$=$	$a\left(y_3 + \frac{1}{4}\right)\hat{\mathbf{x}} - \frac{1}{4}a\hat{\mathbf{y}} - c\left(z_3 - \frac{1}{4}\right)\hat{\mathbf{z}}$		(16h)	O I
$\mathbf{B}_{12}$	$= -z_3\mathbf{a}_1 - (y_3 + z_3)\mathbf{a}_2 - \left(y_3 - \frac{1}{2}\right)\mathbf{a}_3$	$=$	$-a\left(y_3 - \frac{1}{4}\right)\hat{\mathbf{x}} + \frac{1}{4}a\hat{\mathbf{y}} - c\left(z_3 + \frac{1}{4}\right)\hat{\mathbf{z}}$		(16h)	O I

References

- [1] R. M. Hazen and L. W. Finger, *Crystal structure and compressibility of zircon at high pressure*, Am. Mineral. **64**, 196–201 (1979).

Found in

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

First cited in

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