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

This structure originally had the label `A4BC_tI24_141_h_b_a`. Calls to that address will be redirected here.

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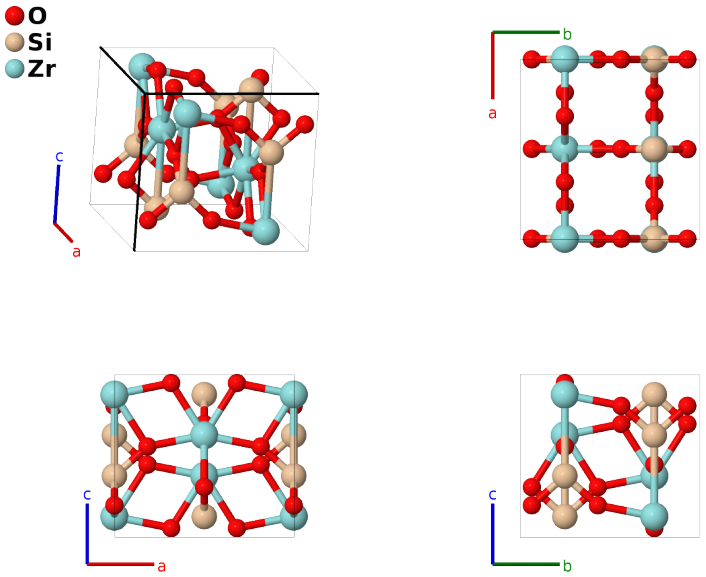
https://aflow.org/p/0FQT

https://aflow.org/p/A4BC_tI24_141_h_a_b-001



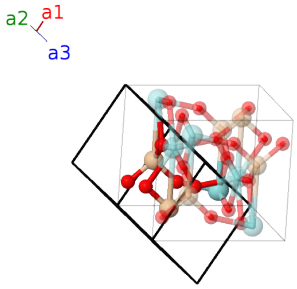
Prototype	O_4SiZr
AFLOW prototype label	A4BC_tI24_141_h_a_b-001
***Strukturbericht* designation**	$S1_1$
Mineral name	zircon
ICSD	100239
Pearson symbol	tI24
Space group number	141
Space group symbol	$I4_1/amd$
AFLOW prototype command	`aflow --proto=A4BC_tI24_141_h_a_b-001 --params=`$a, c/a, y_3, z_3$

Other compounds with this structure

$BiVO_4$, $CeSiO_4$, $CeVO_4$, $DyPO_4$, $ErPO_4$, $ErVO_4$, $HfSO_4$, $HoPO_4$, $HoVO_4$, $LuPO_4$, $LuVO_4$, $NdVO_4$, $PrVO_4$, $ScPO_4$, $ScVO_4$, $TbPO_4$, $TbVO_4$, $ThSiO_4$, $TmPO_4$, $TmVO_4$, YPO_4, YVO_4, $YbAsO_4$, $YbPO_4$, $YbVO_4$

Body-centered Tetragonal primitive vectors

$$
\begin{aligned}
\mathbf{a_1} &= -\tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}a\,\hat{\mathbf{y}} + \tfrac{1}{2}c\,\hat{\mathbf{z}} \\
\mathbf{a_2} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{1}{2}a\,\hat{\mathbf{y}} + \tfrac{1}{2}c\,\hat{\mathbf{z}} \\
\mathbf{a_3} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}a\,\hat{\mathbf{y}} - \tfrac{1}{2}c\,\hat{\mathbf{z}}
\end{aligned}
$$



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
$\mathbf{B_{10}}$	=	$-\left(y_3 + z_3\right)\,\mathbf{a}_1 - z_3\,\mathbf{a}_2 - y_3\,\mathbf{a}_3$	=	$-ay_3\,\hat{\mathbf{y}} - cz_3\,\hat{\mathbf{z}}$	(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).