Baddeleyite (ZrO$_2$, $C43$) Structure: A2B_mP12_14_2e_e-001
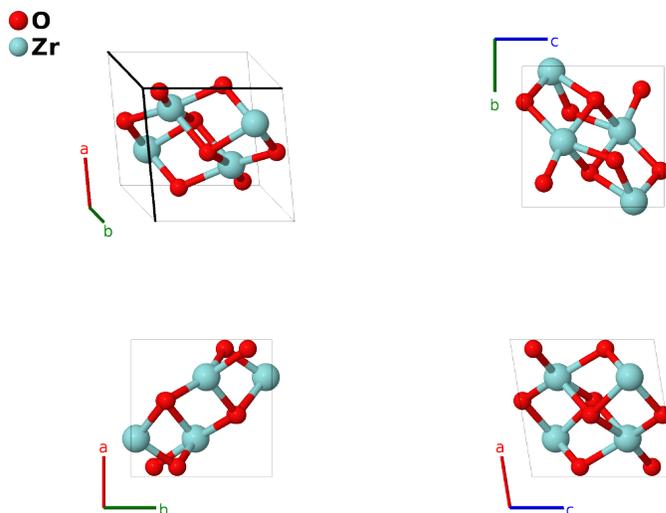
This structure originally had the label `A2B_mP12_14_2e_e`. Calls to that address will be redirected here.

https://aflow.org/p/5CSN

https://aflow.org/p/A2B_mP12_14_2e_e-001

|	
Prototype	O$_2$Zr
AFLOW prototype label	A2B_mP12_14_2e_e-001
***Strukturbericht* designation**	$C43$
Mineral name	baddeleyite
ICSD	62993
Pearson symbol	mP12
Space group number	14
Space group symbol	$P2_1/c$
AFLOW prototype command	aflow --proto=A2B_mP12_14_2e_e-001
	--params=$a, b/a, c/a, \beta, x_1, y_1, z_1, x_2, y_2, z_2, x_3, y_3, z_3$

Other compounds with this structure

CoSb$_2$, HfO$_2$, TeAg$_2$, VO$_2$

- Acanthite (Ag$_2$S), baddeleyite (ZrO$_2$, $C43$), and NdAs$_2$ all have the same AFLOW prototype label, A2B_mP12_14_2e_e. They are generated by the same symmetry operations with different sets of parameters (`--params`) specified in their corresponding CIF files.

Simple Monoclinic primitive vectors

$$\mathbf{a_1} = a\,\hat{\mathbf{x}}$$

$$\mathbf{a_2} = b\,\hat{\mathbf{y}}$$

$$\mathbf{a_3} = c\cos\beta\,\hat{\mathbf{x}} + c\sin\beta\,\hat{\mathbf{z}}$$
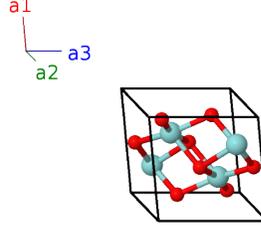
Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	$=$	$x_1\,\mathbf{a_1} + y_1\,\mathbf{a_2} + z_1\,\mathbf{a_3}$	$=$	$(ax_1 + cz_1\cos\beta)\,\hat{\mathbf{x}} + by_1\,\hat{\mathbf{y}} + cz_1\sin\beta\,\hat{\mathbf{z}}$	(4e)	O I
$\mathbf{B_2}$	$=$	$-x_1\,\mathbf{a_1} + \left(y_1+\frac{1}{2}\right)\,\mathbf{a_2} - \left(z_1-\frac{1}{2}\right)\,\mathbf{a_3}$	$=$	$-\left(ax_1 + c\left(z_1-\frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} + b\left(y_1+\frac{1}{2}\right)\,\hat{\mathbf{y}} - c\left(z_1-\frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4e)	O I
$\mathbf{B_3}$	$=$	$-x_1\,\mathbf{a_1} - y_1\,\mathbf{a_2} - z_1\,\mathbf{a_3}$	$=$	$-(ax_1 + cz_1\cos\beta)\,\hat{\mathbf{x}} - by_1\,\hat{\mathbf{y}} - cz_1\sin\beta\,\hat{\mathbf{z}}$	(4e)	O I
$\mathbf{B_4}$	$=$	$x_1\,\mathbf{a_1} - \left(y_1-\frac{1}{2}\right)\,\mathbf{a_2} + \left(z_1+\frac{1}{2}\right)\,\mathbf{a_3}$	$=$	$\left(ax_1 + c\left(z_1+\frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} - b\left(y_1-\frac{1}{2}\right)\,\hat{\mathbf{y}} + c\left(z_1+\frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4e)	O I
$\mathbf{B_5}$	$=$	$x_2\,\mathbf{a_1} + y_2\,\mathbf{a_2} + z_2\,\mathbf{a_3}$	$=$	$(ax_2 + cz_2\cos\beta)\,\hat{\mathbf{x}} + by_2\,\hat{\mathbf{y}} + cz_2\sin\beta\,\hat{\mathbf{z}}$	(4e)	O II
$\mathbf{B_6}$	$=$	$-x_2\,\mathbf{a_1} + \left(y_2+\frac{1}{2}\right)\,\mathbf{a_2} - \left(z_2-\frac{1}{2}\right)\,\mathbf{a_3}$	$=$	$-\left(ax_2 + c\left(z_2-\frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} + b\left(y_2+\frac{1}{2}\right)\,\hat{\mathbf{y}} - c\left(z_2-\frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4e)	O II
$\mathbf{B_7}$	$=$	$-x_2\,\mathbf{a_1} - y_2\,\mathbf{a_2} - z_2\,\mathbf{a_3}$	$=$	$-(ax_2 + cz_2\cos\beta)\,\hat{\mathbf{x}} - by_2\,\hat{\mathbf{y}} - cz_2\sin\beta\,\hat{\mathbf{z}}$	(4e)	O II
$\mathbf{B_8}$	$=$	$x_2\,\mathbf{a_1} - \left(y_2-\frac{1}{2}\right)\,\mathbf{a_2} + \left(z_2+\frac{1}{2}\right)\,\mathbf{a_3}$	$=$	$\left(ax_2 + c\left(z_2+\frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} - b\left(y_2-\frac{1}{2}\right)\,\hat{\mathbf{y}} + c\left(z_2+\frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4e)	O II
$\mathbf{B_9}$	$=$	$x_3\,\mathbf{a_1} + y_3\,\mathbf{a_2} + z_3\,\mathbf{a_3}$	$=$	$(ax_3 + cz_3\cos\beta)\,\hat{\mathbf{x}} + by_3\,\hat{\mathbf{y}} + cz_3\sin\beta\,\hat{\mathbf{z}}$	(4e)	Zr I
$\mathbf{B_{10}}$	$=$	$-x_3\,\mathbf{a_1} + \left(y_3+\frac{1}{2}\right)\,\mathbf{a_2} - \left(z_3-\frac{1}{2}\right)\,\mathbf{a_3}$	$=$	$-\left(ax_3 + c\left(z_3-\frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} + b\left(y_3+\frac{1}{2}\right)\,\hat{\mathbf{y}} - c\left(z_3-\frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4e)	Zr I
$\mathbf{B_{11}}$	$=$	$-x_3\,\mathbf{a_1} - y_3\,\mathbf{a_2} - z_3\,\mathbf{a_3}$	$=$	$-(ax_3 + cz_3\cos\beta)\,\hat{\mathbf{x}} - by_3\,\hat{\mathbf{y}} - cz_3\sin\beta\,\hat{\mathbf{z}}$	(4e)	Zr I
$\mathbf{B_{12}}$	$=$	$x_3\,\mathbf{a_1} - \left(y_3-\frac{1}{2}\right)\,\mathbf{a_2} + \left(z_3+\frac{1}{2}\right)\,\mathbf{a_3}$	$=$	$\left(ax_3 + c\left(z_3+\frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} - b\left(y_3-\frac{1}{2}\right)\,\hat{\mathbf{y}} + c\left(z_3+\frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4e)	Zr I

References

[1] C. J. Howard, R. J. Hill, and B. E. Reichert, *Structures of ZrO$_2$ polymorphs at room temperature by high-resolution neutron powder diffraction*, Acta Crystallogr. Sect. B **44**, 116–120 (1988), doi:10.1107/S0108768187010279.