β-BeO Structure: AB_tP8_136_f_g-001

This structure originally had the label `AB_tP8_136_g_f`. Calls to that address will be redirected here.

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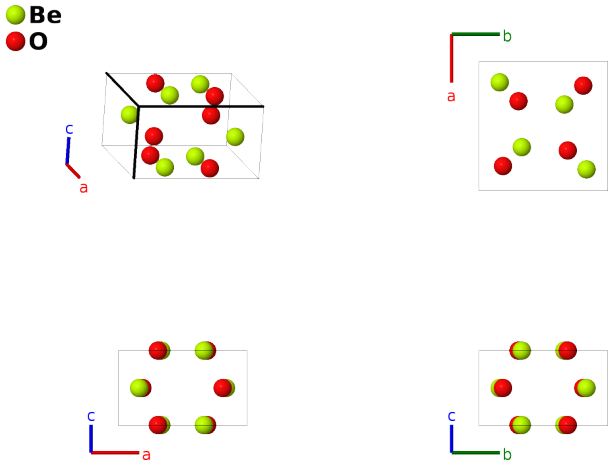
https://aflow.org/p/FJT4

https://aflow.org/p/AB_tP8_136_f_g-001

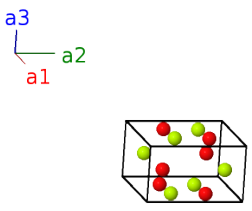


Prototype	BeO
AFLOW prototype label	AB_tP8_136_f_g-001
ICSD	18147
Pearson symbol	tP8
Space group number	136
Space group symbol	$P4_2/mnm$
AFLOW prototype command	`aflow --proto=AB_tP8_136_f_g-001 --params=`$a, c/a, x_1, x_2$

Other compounds with this structure
ZnO

Simple Tetragonal primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$x_1\,\mathbf{a}_1 + x_1\,\mathbf{a}_2$	=	$ax_1\,\hat{\mathbf{x}} + ax_1\,\hat{\mathbf{y}}$	(4f)	Be I
$\mathbf{B_2}$	=	$-x_1\,\mathbf{a}_1 - x_1\,\mathbf{a}_2$	=	$-ax_1\,\hat{\mathbf{x}} - ax_1\,\hat{\mathbf{y}}$	(4f)	Be I
$\mathbf{B_3}$	=	$-\left(x_1 - \frac{1}{2}\right)\,\mathbf{a}_1 + \left(x_1 + \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-a\left(x_1 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + a\left(x_1 + \frac{1}{2}\right)\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4f)	Be I
$\mathbf{B_4}$	=	$\left(x_1 + \frac{1}{2}\right)\,\mathbf{a}_1 - \left(x_1 - \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$a\left(x_1 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - a\left(x_1 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4f)	Be I
$\mathbf{B_5}$	=	$x_2\,\mathbf{a}_1 - x_2\,\mathbf{a}_2$	=	$ax_2\,\hat{\mathbf{x}} - ax_2\,\hat{\mathbf{y}}$	(4g)	O I
$\mathbf{B_6}$	=	$-x_2\,\mathbf{a}_1 + x_2\,\mathbf{a}_2$	=	$-ax_2\,\hat{\mathbf{x}} + ax_2\,\hat{\mathbf{y}}$	(4g)	O I
$\mathbf{B_7}$	=	$\left(x_2 + \frac{1}{2}\right)\,\mathbf{a}_1 + \left(x_2 + \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$a\left(x_2 + \frac{1}{2}\right)\,\hat{\mathbf{x}} + a\left(x_2 + \frac{1}{2}\right)\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4g)	O I
$\mathbf{B_8}$	=	$-\left(x_2 - \frac{1}{2}\right)\,\mathbf{a}_1 - \left(x_2 - \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-a\left(x_2 - \frac{1}{2}\right)\,\hat{\mathbf{x}} - a\left(x_2 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4g)	O I

References

[1] D. K. Smith, C. F. Cline, and S. B. Austerman, *The Crystal Structure of β-Beryllia*, Acta Cryst. **18**, 393–397 (1965), doi:10.1107/S0365110X65000877.