

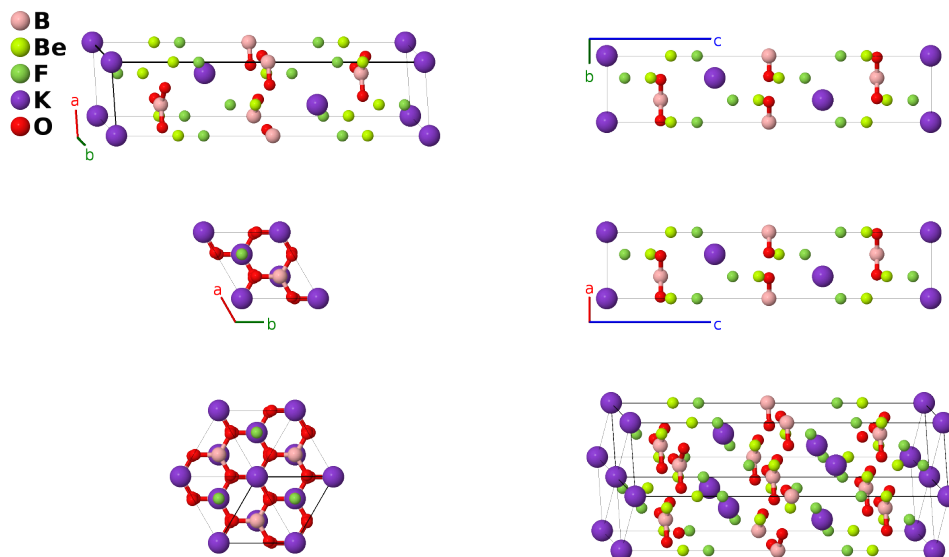
KBe₂BO₃F₂ Structure: AB2C2DE3_hR9_155_a_c_c_b_d-001

This structure originally had the label AB2C2DE3_hR9_155_b_c_c_a_e. Calls to that address will be redirected here.

Cite this page as: D. Hicks, M. J. Mehl, M. Esters, C. Oses, O. Levy, G. L. W. Hart, C. Toher, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 3*, Comput. Mater. Sci. **199**, 110450 (2021), doi: 10.1016/j.commatsci.2021.110450.

<https://aflow.org/p/Q3TB>

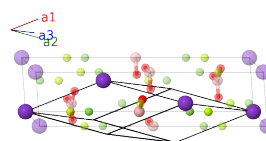
https://aflow.org/p/AB2C2DE3_hR9_155_a_c_c_b_d-001



Prototype	BB _e ₂ F ₂ KO ₃
AFLOW prototype label	AB2C2DE3_hR9_155_a_c_c_b_d-001
ICSD	77277
Pearson symbol	hR9
Space group number	155
Space group symbol	<i>R</i> 32
AFLOW prototype command	<code>aflow --proto=AB2C2DE3_hR9_155_a_c_c_b_d-001 --params=a, c/a, x₃, x₄, y₅</code>

Rhombohedral primitive vectors

$$\begin{aligned} \mathbf{a}_1 &= \frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + \frac{1}{3}c \hat{\mathbf{z}} \\ \mathbf{a}_2 &= \frac{1}{\sqrt{3}}a \hat{\mathbf{y}} + \frac{1}{3}c \hat{\mathbf{z}} \\ \mathbf{a}_3 &= -\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + \frac{1}{3}c \hat{\mathbf{z}} \end{aligned}$$



Basis vectors

	Lattice coordinates	=	Cartesian coordinates	Wyckoff position	Atom type
\mathbf{B}_1	=	0	=	0	(1a) B I
\mathbf{B}_2	=	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	=	$\frac{1}{2} c \hat{\mathbf{z}}$	(1b) K I
\mathbf{B}_3	=	$x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + x_3 \mathbf{a}_3$	=	$cx_3 \hat{\mathbf{z}}$	(2c) Be I
\mathbf{B}_4	=	$-x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 - x_3 \mathbf{a}_3$	=	$-cx_3 \hat{\mathbf{z}}$	(2c) Be I
\mathbf{B}_5	=	$x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + x_4 \mathbf{a}_3$	=	$cx_4 \hat{\mathbf{z}}$	(2c) F I
\mathbf{B}_6	=	$-x_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 - x_4 \mathbf{a}_3$	=	$-cx_4 \hat{\mathbf{z}}$	(2c) F I
\mathbf{B}_7	=	$y_5 \mathbf{a}_2 - y_5 \mathbf{a}_3$	=	$\frac{1}{2} ay_5 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} ay_5 \hat{\mathbf{y}}$	(3d) O I
\mathbf{B}_8	=	$-y_5 \mathbf{a}_1 + y_5 \mathbf{a}_3$	=	$-ay_5 \hat{\mathbf{x}}$	(3d) O I
\mathbf{B}_9	=	$y_5 \mathbf{a}_1 - y_5 \mathbf{a}_2$	=	$\frac{1}{2} ay_5 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} ay_5 \hat{\mathbf{y}}$	(3d) O I

References

- [1] L. Mei, X. Huang, Y. Want, Q. Wu, and C. Chen, *Crystal Structure of $KBe_2BO_3F_2$* , *Z. Kristallogr.* **210**, 93–95 (1995), doi:10.1524/zkri.1995.210.2.93.