KBO_2 ($F5_{13}$) Structure: ABC2_hR24_167_e_e_2e-001

This structure previously used the label(s) `ABC2_hR24_167_e_e_2e`. Calls to these addresses will be redirected here.

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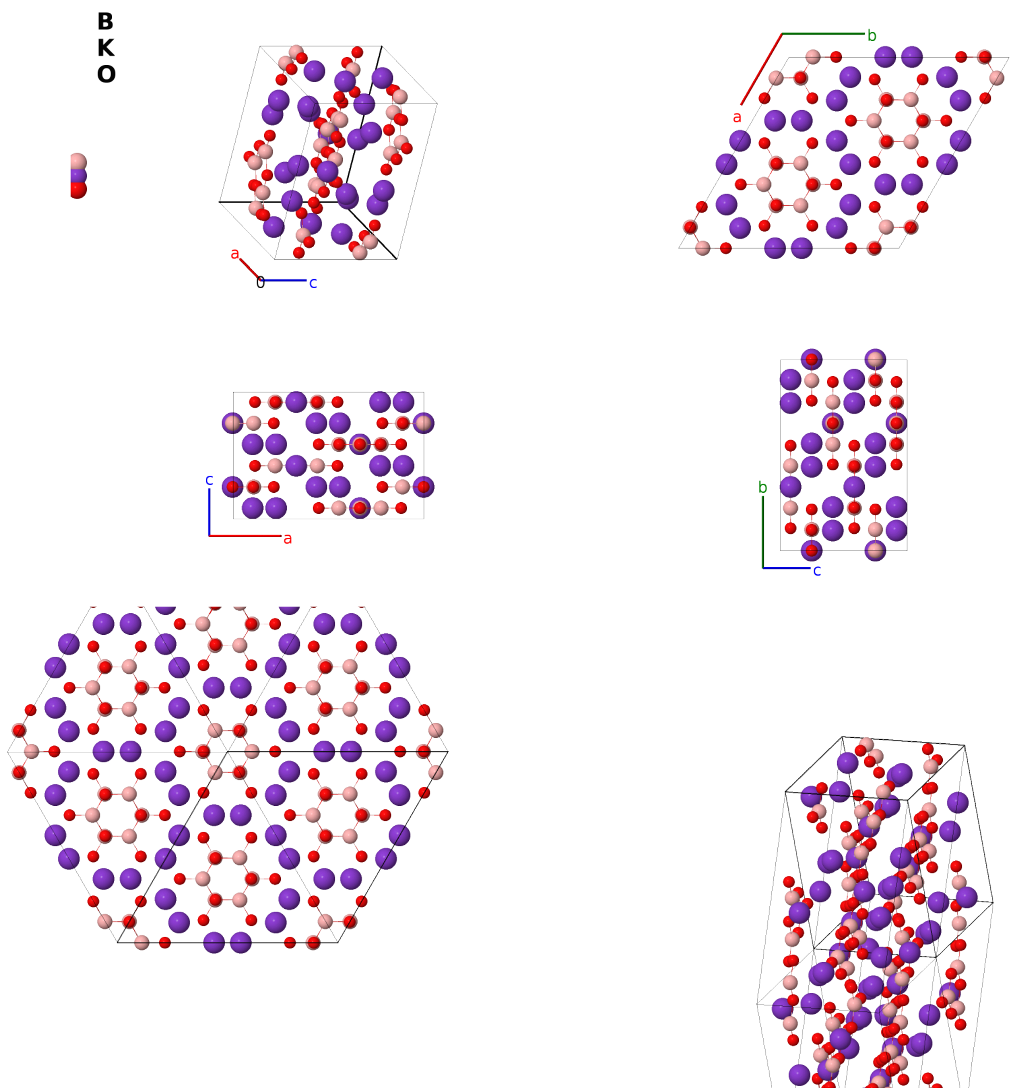
https://aflow.org/prototype-encyclopedia/L33F

https://aflow.org/prototype-encyclopedia/ABC2_hR24_167_e_e_2e-001



Prototype	BKO_2
AFLOW prototype label	ABC2_hR24_167_e_e_2e-001
***Strukturbericht* designation**	$F5_{13}$

ICSD	16005
CCDC	1596666
Pearson symbol	hR24
Space group number	167
Space group symbol	$R\bar{3}c$
AFLOW prototype command	`aflow --proto=ABC2_hR24_167_e_e_2e-001` `--params=`$a, c/a, x_1, x_2, x_3, x_4$

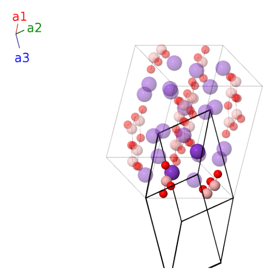
Other compounds with this structure

$NaBO_2$, $NaBS_2$

- Hexagonal settings of this structure can be obtained with the option `--hex`.

Rhombohedral primitive vectors

$$
\begin{aligned}
\mathbf{a_1} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \tfrac{1}{3}c\,\hat{\mathbf{z}} \\
\mathbf{a_2} &= \tfrac{1}{\sqrt{3}}a\,\hat{\mathbf{y}} + \tfrac{1}{3}c\,\hat{\mathbf{z}} \\
\mathbf{a_3} &= -\tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \tfrac{1}{3}c\,\hat{\mathbf{z}}
\end{aligned}
$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$x_1\,\mathbf{a}_1 - \left(x_1 - \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{8}a\,(4x_1-1)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{8}a\,(4x_1-1)\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(6e)	B I
$\mathbf{B_2}$	=	$\frac{1}{4}\,\mathbf{a}_1 + x_1\,\mathbf{a}_2 - \left(x_1 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{8}a\,(4x_1-1)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{8}a\,(4x_1-1)\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(6e)	B I
$\mathbf{B_3}$	=	$-\left(x_1 - \frac{1}{2}\right)\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + x_1\,\mathbf{a}_3$	=	$-a\left(x_1 - \frac{1}{4}\right)\,\hat{\mathbf{x}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(6e)	B I
$\mathbf{B_4}$	=	$-x_1\,\mathbf{a}_1 + \left(x_1 + \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$-\frac{1}{8}a\,(4x_1+3)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{24}a\,(12x_1+1)\,\hat{\mathbf{y}} + \frac{5}{12}c\,\hat{\mathbf{z}}$	(6e)	B I
$\mathbf{B_5}$	=	$\frac{3}{4}\,\mathbf{a}_1 - x_1\,\mathbf{a}_2 + \left(x_1 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\frac{1}{8}a\,(4x_1-1)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{24}a\,(12x_1+5)\,\hat{\mathbf{y}} + \frac{5}{12}c\,\hat{\mathbf{z}}$	(6e)	B I
$\mathbf{B_6}$	=	$\left(x_1 + \frac{1}{2}\right)\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 - x_1\,\mathbf{a}_3$	=	$a\left(x_1 + \frac{1}{4}\right)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{5}{12}c\,\hat{\mathbf{z}}$	(6e)	B I
$\mathbf{B_7}$	=	$x_2\,\mathbf{a}_1 - \left(x_2 - \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{8}a\,(4x_2-1)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{8}a\,(4x_2-1)\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(6e)	K I
$\mathbf{B_8}$	=	$\frac{1}{4}\,\mathbf{a}_1 + x_2\,\mathbf{a}_2 - \left(x_2 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{8}a\,(4x_2-1)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{8}a\,(4x_2-1)\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(6e)	K I
$\mathbf{B_9}$	=	$-\left(x_2 - \frac{1}{2}\right)\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + x_2\,\mathbf{a}_3$	=	$-a\left(x_2 - \frac{1}{4}\right)\,\hat{\mathbf{x}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(6e)	K I
$\mathbf{B_{10}}$	=	$-x_2\,\mathbf{a}_1 + \left(x_2 + \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$-\frac{1}{8}a\,(4x_2+3)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{24}a\,(12x_2+1)\,\hat{\mathbf{y}} + \frac{5}{12}c\,\hat{\mathbf{z}}$	(6e)	K I
$\mathbf{B_{11}}$	=	$\frac{3}{4}\,\mathbf{a}_1 - x_2\,\mathbf{a}_2 + \left(x_2 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\frac{1}{8}a\,(4x_2-1)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{24}a\,(12x_2+5)\,\hat{\mathbf{y}} + \frac{5}{12}c\,\hat{\mathbf{z}}$	(6e)	K I
$\mathbf{B_{12}}$	=	$\left(x_2 + \frac{1}{2}\right)\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 - x_2\,\mathbf{a}_3$	=	$a\left(x_2 + \frac{1}{4}\right)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{5}{12}c\,\hat{\mathbf{z}}$	(6e)	K I
$\mathbf{B_{13}}$	=	$x_3\,\mathbf{a}_1 - \left(x_3 - \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{8}a\,(4x_3-1)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{8}a\,(4x_3-1)\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(6e)	O I
$\mathbf{B_{14}}$	=	$\frac{1}{4}\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 - \left(x_3 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{8}a\,(4x_3-1)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{8}a\,(4x_3-1)\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(6e)	O I
$\mathbf{B_{15}}$	=	$-\left(x_3 - \frac{1}{2}\right)\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + x_3\,\mathbf{a}_3$	=	$-a\left(x_3 - \frac{1}{4}\right)\,\hat{\mathbf{x}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(6e)	O I
$\mathbf{B_{16}}$	=	$-x_3\,\mathbf{a}_1 + \left(x_3 + \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$-\frac{1}{8}a\,(4x_3+3)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{24}a\,(12x_3+1)\,\hat{\mathbf{y}} + \frac{5}{12}c\,\hat{\mathbf{z}}$	(6e)	O I
$\mathbf{B_{17}}$	=	$\frac{3}{4}\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 + \left(x_3 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\frac{1}{8}a\,(4x_3-1)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{24}a\,(12x_3+5)\,\hat{\mathbf{y}} + \frac{5}{12}c\,\hat{\mathbf{z}}$	(6e)	O I

$\mathbf{B_{18}}$	$=$	$\left(x_3+\frac{1}{2}\right)\,\mathbf{a}_1+\frac{3}{4}\,\mathbf{a}_2-x_3\,\mathbf{a}_3$	$=$	$a\left(x_3+\frac{1}{4}\right)\,\hat{\mathbf{x}}+\frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}}+\frac{5}{12}c\,\hat{\mathbf{z}}$	(6e)	O I
$\mathbf{B_{19}}$	$=$	$x_4\,\mathbf{a}_1-\left(x_4-\frac{1}{2}\right)\,\mathbf{a}_2+\frac{1}{4}\,\mathbf{a}_3$	$=$	$\frac{1}{8}a\,(4x_4-1)\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{8}a\,(4x_4-1)\,\hat{\mathbf{y}}+\frac{1}{4}c\,\hat{\mathbf{z}}$	(6e)	O II
$\mathbf{B_{20}}$	$=$	$\frac{1}{4}\,\mathbf{a}_1+x_4\,\mathbf{a}_2-\left(x_4-\frac{1}{2}\right)\,\mathbf{a}_3$	$=$	$\frac{1}{8}a\,(4x_4-1)\,\hat{\mathbf{x}}+\frac{\sqrt{3}}{8}a\,(4x_4-1)\,\hat{\mathbf{y}}+\frac{1}{4}c\,\hat{\mathbf{z}}$	(6e)	O II
$\mathbf{B_{21}}$	$=$	$-\left(x_4-\frac{1}{2}\right)\,\mathbf{a}_1+\frac{1}{4}\,\mathbf{a}_2+x_4\,\mathbf{a}_3$	$=$	$-a\left(x_4-\frac{1}{4}\right)\,\hat{\mathbf{x}}+\frac{1}{4}c\,\hat{\mathbf{z}}$	(6e)	O II
$\mathbf{B_{22}}$	$=$	$-x_4\,\mathbf{a}_1+\left(x_4+\frac{1}{2}\right)\,\mathbf{a}_2+\frac{3}{4}\,\mathbf{a}_3$	$=$	$-\frac{1}{8}a\,(4x_4+3)\,\hat{\mathbf{x}}+\frac{\sqrt{3}}{24}a\,(12x_4+1)\,\hat{\mathbf{y}}+\frac{5}{12}c\,\hat{\mathbf{z}}$	(6e)	O II
$\mathbf{B_{23}}$	$=$	$\frac{3}{4}\,\mathbf{a}_1-x_4\,\mathbf{a}_2+\left(x_4+\frac{1}{2}\right)\,\mathbf{a}_3$	$=$	$-\frac{1}{8}a\,(4x_4-1)\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{24}a\,(12x_4+5)\,\hat{\mathbf{y}}+\frac{5}{12}c\,\hat{\mathbf{z}}$	(6e)	O II
$\mathbf{B_{24}}$	$=$	$\left(x_4+\frac{1}{2}\right)\,\mathbf{a}_1+\frac{3}{4}\,\mathbf{a}_2-x_4\,\mathbf{a}_3$	$=$	$a\left(x_4+\frac{1}{4}\right)\,\hat{\mathbf{x}}+\frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}}+\frac{5}{12}c\,\hat{\mathbf{z}}$	(6e)	O II

References

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