KO Structure: AB_oC16_64_e_f-002

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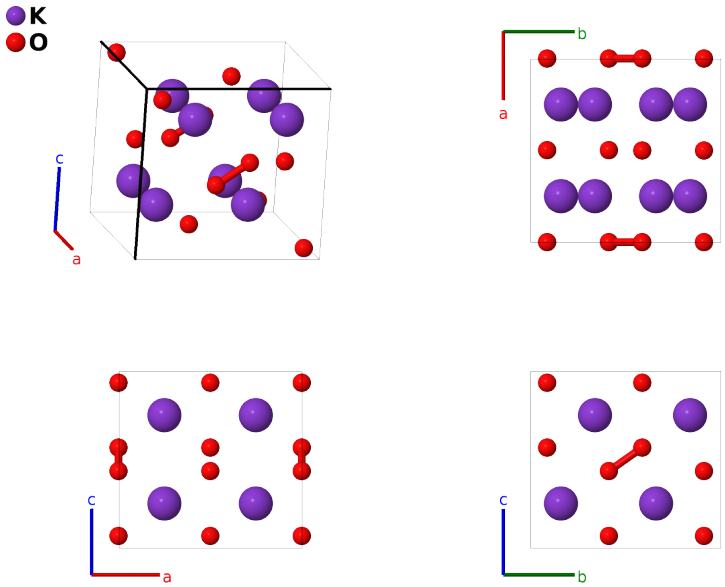
https://aflow.org/p/HZUD

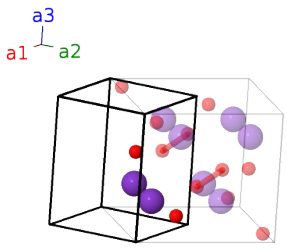
https://aflow.org/p/AB_oC16_64_e_f-002



Prototype	KO
AFLOW prototype label	AB_oC16_64_e_f-002
ICSD	25527
Pearson symbol	oC16
Space group number	64
Space group symbol	*Cmce*
AFLOW prototype command	`aflow --proto=AB_oC16_64_e_f-002 --params=`$a, b/a, c/a, y_1, y_2, z_2$

Base-centered Orthorhombic primitive vectors

$$\mathbf{a_1} = \frac{1}{2}a\,\hat{\mathbf{x}} - \frac{1}{2}b\,\hat{\mathbf{y}}$$
$$\mathbf{a_2} = \frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}b\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$-\left(y_1-\frac{1}{4}\right)\,\mathbf{a}_1+\left(y_1+\frac{1}{4}\right)\,\mathbf{a}_2+\frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}}+by_1\,\hat{\mathbf{y}}+\frac{1}{4}c\,\hat{\mathbf{z}}$	(8e)	K I
$\mathbf{B_2}$	=	$\left(y_1+\frac{1}{4}\right)\,\mathbf{a}_1-\left(y_1-\frac{1}{4}\right)\,\mathbf{a}_2+\frac{3}{4}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}}-by_1\,\hat{\mathbf{y}}+\frac{3}{4}c\,\hat{\mathbf{z}}$	(8e)	K I
$\mathbf{B_3}$	=	$\left(y_1+\frac{3}{4}\right)\,\mathbf{a}_1-\left(y_1-\frac{3}{4}\right)\,\mathbf{a}_2+\frac{3}{4}\,\mathbf{a}_3$	=	$\frac{3}{4}a\,\hat{\mathbf{x}}-by_1\,\hat{\mathbf{y}}+\frac{3}{4}c\,\hat{\mathbf{z}}$	(8e)	K I
$\mathbf{B_4}$	=	$-\left(y_1-\frac{3}{4}\right)\,\mathbf{a}_1+\left(y_1+\frac{3}{4}\right)\,\mathbf{a}_2+\frac{1}{4}\,\mathbf{a}_3$	=	$\frac{3}{4}a\,\hat{\mathbf{x}}+by_1\,\hat{\mathbf{y}}+\frac{1}{4}c\,\hat{\mathbf{z}}$	(8e)	K I
$\mathbf{B_5}$	=	$-y_2\,\mathbf{a}_1+y_2\,\mathbf{a}_2+z_2\,\mathbf{a}_3$	=	$by_2\,\hat{\mathbf{y}}+cz_2\,\hat{\mathbf{z}}$	(8f)	O I
$\mathbf{B_6}$	=	$\left(y_2+\frac{1}{2}\right)\,\mathbf{a}_1-\left(y_2-\frac{1}{2}\right)\,\mathbf{a}_2+\left(z_2+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}}-by_2\,\hat{\mathbf{y}}+c\left(z_2+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8f)	O I
$\mathbf{B_7}$	=	$-\left(y_2-\frac{1}{2}\right)\,\mathbf{a}_1+\left(y_2+\frac{1}{2}\right)\,\mathbf{a}_2-\left(z_2-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}}+by_2\,\hat{\mathbf{y}}-c\left(z_2-\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8f)	O I
$\mathbf{B_8}$	=	$y_2\,\mathbf{a}_1-y_2\,\mathbf{a}_2-z_2\,\mathbf{a}_3$	=	$-by_2\,\hat{\mathbf{y}}-cz_2\,\hat{\mathbf{z}}$	(8f)	O I

References

[1] H. Föppl, *Die Kristallstrukturen der Alkaliperoxyde*, Z. Anorganische und Allgemeine Chemie **291**, 12–50 (1957), doi:10.1002/zaac.19572910104.