KO Structure: AB_oC16_64_e_f-002

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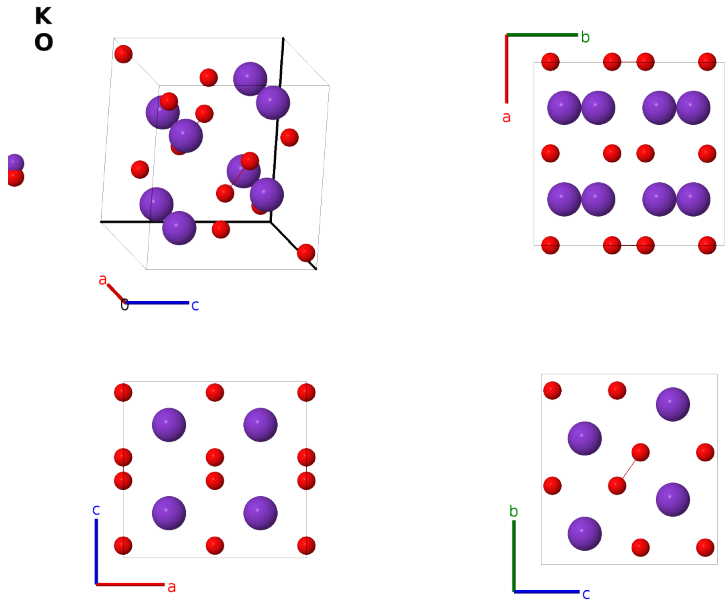
https://aflow.org/prototype-encyclopedia/HZUD

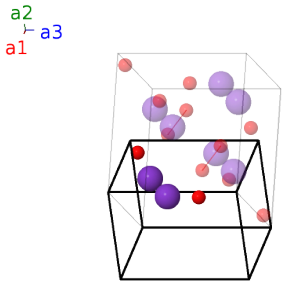
https://aflow.org/prototype-encyclopedia/AB_oC16_64_e_f-002



Prototype	KO
AFLOW prototype label	AB_oC16_64_e_f-002
ICSD	25527
CCDC	1601181
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

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



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.

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