$KClO_3$ ($G0_6$) Structure: ABC3_mP10_11_e_e_ef-001

This structure previously used the label(s) `ABC3_mP10_11_e_e_ef`. Calls to these addresses will be redirected here.

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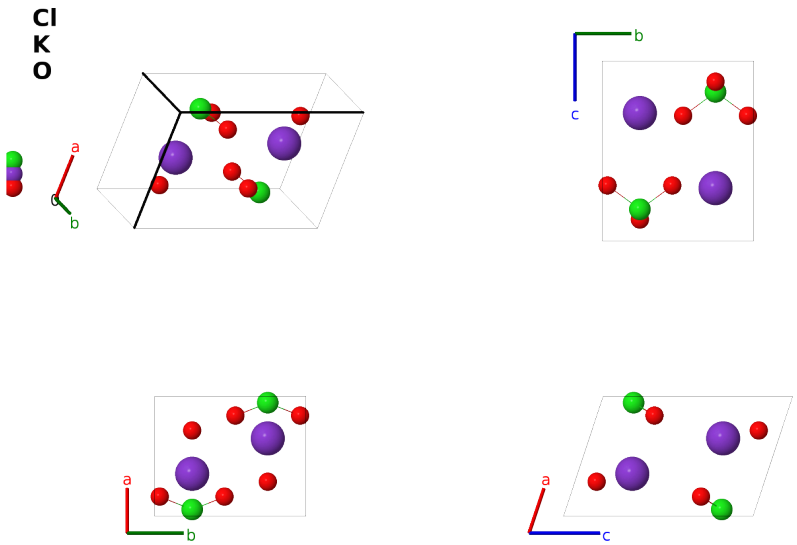
https://aflow.org/prototype-encyclopedia/RT35

https://aflow.org/prototype-encyclopedia/ABC3_mP10_11_e_e_ef-001

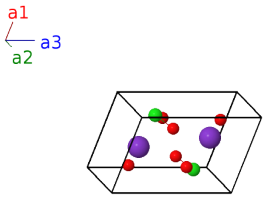


Prototype	$ClKO_3$
AFLOW prototype label	ABC3_mP10_11_e_e_ef-001
***Strukturbericht* designation**	$G0_6$
ICSD	26408
CCDC	1601816
Pearson symbol	mP10
Space group number	11
Space group symbol	$P2_1/m$
AFLOW prototype command	`aflow --proto=ABC3_mP10_11_e_e_ef-001 --params=`$a, b/a, c/a, \beta, x_1, z_1, x_2, z_2, x_3, z_3, x_4, y_4, z_4$

Other compounds with this structure
$BaSeO_3$, $BaTeO_3$, $CeAsO_3$, $LaAsO_3$, $PbSO_3$, $PbSeO_3$, $RbGeCl_3$, $SrSeO_3$

Simple Monoclinic primitive vectors

$$\mathbf{a_1} = a\,\hat{\mathbf{x}}$$
$$\mathbf{a_2} = b\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\cos\beta\,\hat{\mathbf{x}} + c\sin\beta\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$x_1\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + z_1\,\mathbf{a}_3$	=	$(ax_1 + cz_1\cos\beta)\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} + cz_1\sin\beta\,\hat{\mathbf{z}}$	(2e)	Cl I
$\mathbf{B_2}$	=	$-x_1\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 - z_1\,\mathbf{a}_3$	=	$-(ax_1 + cz_1\cos\beta)\,\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} - cz_1\sin\beta\,\hat{\mathbf{z}}$	(2e)	Cl I
$\mathbf{B_3}$	=	$x_2\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$(ax_2 + cz_2\cos\beta)\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} + cz_2\sin\beta\,\hat{\mathbf{z}}$	(2e)	K I
$\mathbf{B_4}$	=	$-x_2\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 - z_2\,\mathbf{a}_3$	=	$-(ax_2 + cz_2\cos\beta)\,\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} - cz_2\sin\beta\,\hat{\mathbf{z}}$	(2e)	K I
$\mathbf{B_5}$	=	$x_3\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$(ax_3 + cz_3\cos\beta)\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} + cz_3\sin\beta\,\hat{\mathbf{z}}$	(2e)	O I
$\mathbf{B_6}$	=	$-x_3\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$	=	$-(ax_3 + cz_3\cos\beta)\,\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} - cz_3\sin\beta\,\hat{\mathbf{z}}$	(2e)	O I
$\mathbf{B_7}$	=	$x_4\,\mathbf{a}_1 + y_4\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$(ax_4 + cz_4\cos\beta)\,\hat{\mathbf{x}} + by_4\,\hat{\mathbf{y}} + cz_4\sin\beta\,\hat{\mathbf{z}}$	(4f)	O II
$\mathbf{B_8}$	=	$-x_4\,\mathbf{a}_1 + \left(y_4 + \frac{1}{2}\right)\,\mathbf{a}_2 - z_4\,\mathbf{a}_3$	=	$-(ax_4 + cz_4\cos\beta)\,\hat{\mathbf{x}} + b\left(y_4 + \frac{1}{2}\right)\,\hat{\mathbf{y}} - cz_4\sin\beta\,\hat{\mathbf{z}}$	(4f)	O II
$\mathbf{B_9}$	=	$-x_4\,\mathbf{a}_1 - y_4\,\mathbf{a}_2 - z_4\,\mathbf{a}_3$	=	$-(ax_4 + cz_4\cos\beta)\,\hat{\mathbf{x}} - by_4\,\hat{\mathbf{y}} - cz_4\sin\beta\,\hat{\mathbf{z}}$	(4f)	O II
$\mathbf{B_{10}}$	=	$x_4\,\mathbf{a}_1 - \left(y_4 - \frac{1}{2}\right)\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$(ax_4 + cz_4\cos\beta)\,\hat{\mathbf{x}} - b\left(y_4 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_4\sin\beta\,\hat{\mathbf{z}}$	(4f)	O II

References

[1] J. Danielsen, A. Hazell, and F. K. Larsen, *The Structure of Potassium Chlorate at 77 and 298 K*, Acta Crystallogr. Sect. B **37**, 913–915 (1981), doi:10.1107/S0567740881004573.

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