

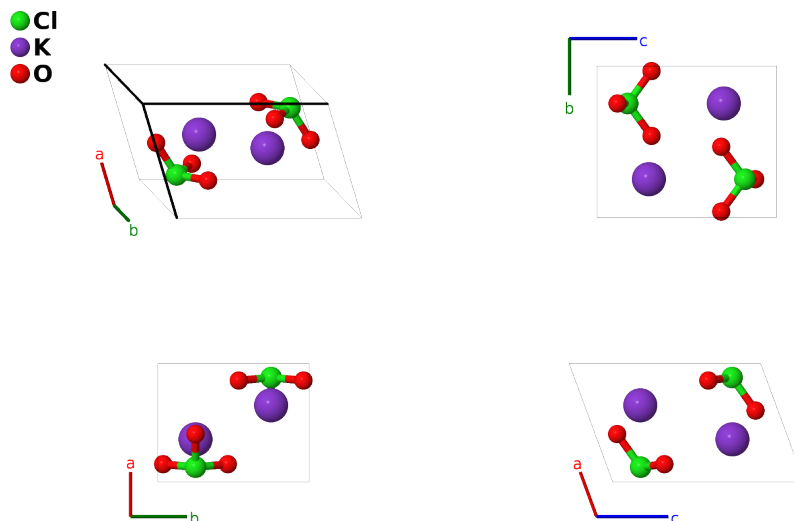
KClO₃ (*G*₀₆) Structure: ABC3_mP10_11_e_e_ef-001

This structure originally had the label ABC3_mP10_11_e_e_ef. Calls to that address will be redirected here.

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<https://afLOW.org/p/RT35>

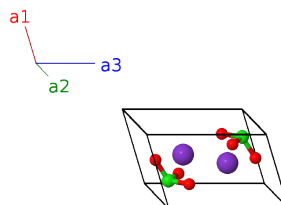
https://afLOW.org/p/ABC3_mP10_11_e_e_ef-001



Prototype	ClKO ₃
AFLOW prototype label	ABC3_mP10_11_e_e_ef-001
<i>Strukturbericht</i> designation	<i>G</i> ₀₆
ICSD	26408
Pearson symbol	mP10
Space group number	11
Space group symbol	<i>P</i> 2 ₁ / <i>m</i>
AFLOW prototype command	afLOW --proto=ABC3_mP10_11_e_e_ef-001 --params= <i>a</i> , <i>b/a</i> , <i>c/a</i> , β , <i>x</i> ₁ , <i>z</i> ₁ , <i>x</i> ₂ , <i>z</i> ₂ , <i>x</i> ₃ , <i>z</i> ₃ , <i>x</i> ₄ , <i>y</i> ₄ , <i>z</i> ₄

Simple Monoclinic primitive vectors

$$\begin{aligned} \mathbf{a}_1 &= a \hat{\mathbf{x}} \\ \mathbf{a}_2 &= b \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \cos \beta \hat{\mathbf{x}} + c \sin \beta \hat{\mathbf{z}} \end{aligned}$$



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	$= -x_4 \mathbf{a}_1 + (y_4 + \frac{1}{2}) \mathbf{a}_2 - z_4 \mathbf{a}_3$	=	$-(ax_4 + cz_4 \cos \beta) \hat{\mathbf{x}} + b(y_4 + \frac{1}{2}) \hat{\mathbf{y}} - cz_4 \sin \beta \hat{\mathbf{z}}$	=	(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}	$= x_4 \mathbf{a}_1 - (y_4 - \frac{1}{2}) \mathbf{a}_2 + z_4 \mathbf{a}_3$	=	$(ax_4 + cz_4 \cos \beta) \hat{\mathbf{x}} - b(y_4 - \frac{1}{2}) \hat{\mathbf{y}} + cz_4 \sin \beta \hat{\mathbf{z}}$	=	(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.