High-Temperature Cubic $KClO_4$ ($H0_5$) Structure: ABC4_cF24_216_a_b_e-001

This structure originally had the label `ABC4_cF24_216_b_a_e`. Calls to that address will be redirected here.

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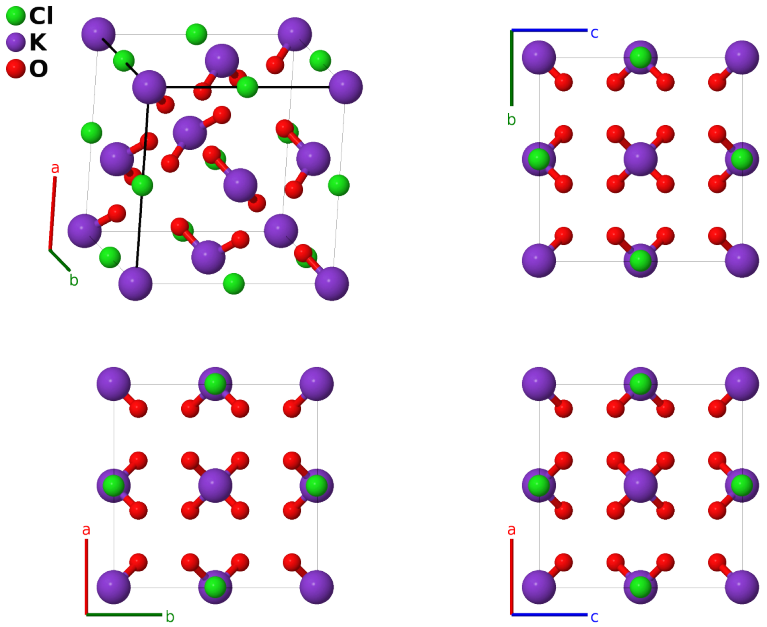
https://aflow.org/p/Q1UZ

https://aflow.org/p/ABC4_cF24_216_a_b_e-001



Prototype	$ClKO_4$
AFLOW prototype label	ABC4_cF24_216_a_b_e-001
***Strukturbericht* designation**	$H0_5$
ICSD	33562
Pearson symbol	cF24
Space group number	216
Space group symbol	$F\bar{4}3m$
AFLOW prototype command	`aflow --proto=ABC4_cF24_216_a_b_e-001 --params=`a, x_3

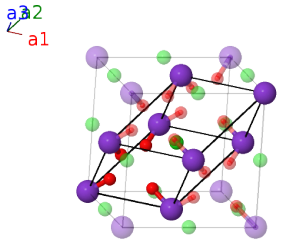
Other compounds with this structure
$ClCsO_4$, $ClKO_4$, $EuPtIn_4$, $MgSnCu_4$, $NaClO_4$, $RbClO_4$, NH_4ClO_4, $AgClO_4$, $TlClO_4$

- This is the high-temperature phase of the listed perchlorate structures. $KClO_4$ transforms from its ground-state orthorhombic structure, $H0_2$ into this structure at 299.5°C. The transition temperature for the other compounds range from 155°C ($AgClO_4$) to 308°C ($NaClO_4$).

- The lattice constant for $KClO_4$ was measured at 310°C.

Face-centered Cubic primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(4a)	Cl I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{2}a\,\hat{\mathbf{z}}$	(4b)	K I
$\mathbf{B_3}$	=	$x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + x_3\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} + ax_3\,\hat{\mathbf{y}} + ax_3\,\hat{\mathbf{z}}$	(16e)	O I
$\mathbf{B_4}$	=	$x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 - 3x_3\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} - ax_3\,\hat{\mathbf{y}} + ax_3\,\hat{\mathbf{z}}$	(16e)	O I
$\mathbf{B_5}$	=	$x_3\,\mathbf{a}_1 - 3x_3\,\mathbf{a}_2 + x_3\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} + ax_3\,\hat{\mathbf{y}} - ax_3\,\hat{\mathbf{z}}$	(16e)	O I
$\mathbf{B_6}$	=	$-3x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + x_3\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} - ax_3\,\hat{\mathbf{y}} - ax_3\,\hat{\mathbf{z}}$	(16e)	O I

References

[1] K. Hermann and W. Ilge, *Röntgenographische Strukturerforschung der kubischen Modifikation der Perchlorate*, Z. Kristallogr. **71**, 41–66 (1930), doi:10.1515/zkri-1930-0105.

Found in

[1] C. Hermann, O. Lohrmann, and H. Philipp, eds., *Strukturbericht Band II 1928-1932* (Akademische Verlagsgesellschaft M. B. H., Leipzig, 1937).