Sodium Chlorate ($NaClO_3$, $G0_3$) Structure: ABC3_cP20_198_a_a_b-001

This structure previously used the label(s) `ABC3_cP20_198_a_a_b`. Calls to these addresses will be redirected here.

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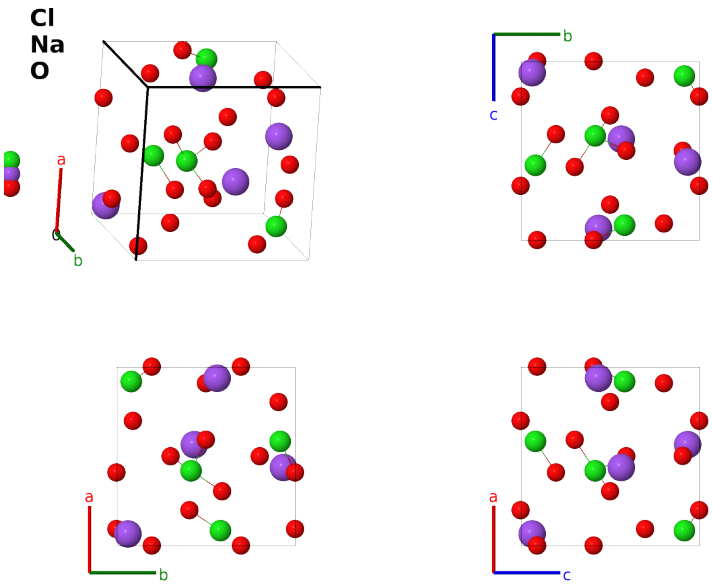
https://aflow.org/prototype-encyclopedia/QEXW

https://aflow.org/prototype-encyclopedia/ABC3_cP20_198_a_a_b-001

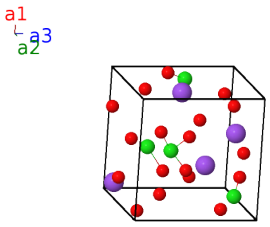


Prototype	$NaClO_3$
AFLOW prototype label	ABC3_cP20_198_a_a_b-001
***Strukturbericht* designation**	$G0_3$
Mineral name	sodium chlorate
ICSD	16714
CCDC	1597266
Pearson symbol	cP20
Space group number	198
Space group symbol	$P2_13$
AFLOW prototype command	`aflow --proto=ABC3_cP20_198_a_a_b-001 --params=`$a, x_1, x_2, x_3, y_3, z_3$

Other compounds with this structure
$NaBrO_3$

Simple Cubic primitive vectors

$$\mathbf{a_1} = a\,\hat{\mathbf{x}}$$
$$\mathbf{a_2} = a\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = a\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$x_1\,\mathbf{a}_1 + x_1\,\mathbf{a}_2 + x_1\,\mathbf{a}_3$	=	$ax_1\,\hat{\mathbf{x}} + ax_1\,\hat{\mathbf{y}} + ax_1\,\hat{\mathbf{z}}$	(4a)	Cl I
$\mathbf{B_2}$	=	$-\left(x_1 - \frac{1}{2}\right)\,\mathbf{a}_1 - x_1\,\mathbf{a}_2 + \left(x_1 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_1 - \frac{1}{2}\right)\,\hat{\mathbf{x}} - ax_1\,\hat{\mathbf{y}} + a\left(x_1 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4a)	Cl I
$\mathbf{B_3}$	=	$-x_1\,\mathbf{a}_1 + \left(x_1 + \frac{1}{2}\right)\,\mathbf{a}_2 - \left(x_1 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_1\,\hat{\mathbf{x}} + a\left(x_1 + \frac{1}{2}\right)\,\hat{\mathbf{y}} - a\left(x_1 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4a)	Cl I
$\mathbf{B_4}$	=	$\left(x_1 + \frac{1}{2}\right)\,\mathbf{a}_1 - \left(x_1 - \frac{1}{2}\right)\,\mathbf{a}_2 - x_1\,\mathbf{a}_3$	=	$a\left(x_1 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - a\left(x_1 - \frac{1}{2}\right)\,\hat{\mathbf{y}} - ax_1\,\hat{\mathbf{z}}$	(4a)	Cl I
$\mathbf{B_5}$	=	$x_2\,\mathbf{a}_1 + x_2\,\mathbf{a}_2 + x_2\,\mathbf{a}_3$	=	$ax_2\,\hat{\mathbf{x}} + ax_2\,\hat{\mathbf{y}} + ax_2\,\hat{\mathbf{z}}$	(4a)	Na I
$\mathbf{B_6}$	=	$-\left(x_2 - \frac{1}{2}\right)\,\mathbf{a}_1 - x_2\,\mathbf{a}_2 + \left(x_2 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_2 - \frac{1}{2}\right)\,\hat{\mathbf{x}} - ax_2\,\hat{\mathbf{y}} + a\left(x_2 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4a)	Na I
$\mathbf{B_7}$	=	$-x_2\,\mathbf{a}_1 + \left(x_2 + \frac{1}{2}\right)\,\mathbf{a}_2 - \left(x_2 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_2\,\hat{\mathbf{x}} + a\left(x_2 + \frac{1}{2}\right)\,\hat{\mathbf{y}} - a\left(x_2 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4a)	Na I
$\mathbf{B_8}$	=	$\left(x_2 + \frac{1}{2}\right)\,\mathbf{a}_1 - \left(x_2 - \frac{1}{2}\right)\,\mathbf{a}_2 - x_2\,\mathbf{a}_3$	=	$a\left(x_2 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - a\left(x_2 - \frac{1}{2}\right)\,\hat{\mathbf{y}} - ax_2\,\hat{\mathbf{z}}$	(4a)	Na I
$\mathbf{B_9}$	=	$x_3\,\mathbf{a}_1 + y_3\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} + ay_3\,\hat{\mathbf{y}} + az_3\,\hat{\mathbf{z}}$	(12b)	O I
$\mathbf{B_{10}}$	=	$-\left(x_3 - \frac{1}{2}\right)\,\mathbf{a}_1 - y_3\,\mathbf{a}_2 + \left(z_3 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_3 - \frac{1}{2}\right)\,\hat{\mathbf{x}} - ay_3\,\hat{\mathbf{y}} + a\left(z_3 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(12b)	O I
$\mathbf{B_{11}}$	=	$-x_3\,\mathbf{a}_1 + \left(y_3 + \frac{1}{2}\right)\,\mathbf{a}_2 - \left(z_3 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} + a\left(y_3 + \frac{1}{2}\right)\,\hat{\mathbf{y}} - a\left(z_3 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(12b)	O I
$\mathbf{B_{12}}$	=	$\left(x_3 + \frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_3 - \frac{1}{2}\right)\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$	=	$a\left(x_3 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - a\left(y_3 - \frac{1}{2}\right)\,\hat{\mathbf{y}} - az_3\,\hat{\mathbf{z}}$	(12b)	O I
$\mathbf{B_{13}}$	=	$z_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + y_3\,\mathbf{a}_3$	=	$az_3\,\hat{\mathbf{x}} + ax_3\,\hat{\mathbf{y}} + ay_3\,\hat{\mathbf{z}}$	(12b)	O I
$\mathbf{B_{14}}$	=	$\left(z_3 + \frac{1}{2}\right)\,\mathbf{a}_1 - \left(x_3 - \frac{1}{2}\right)\,\mathbf{a}_2 - y_3\,\mathbf{a}_3$	=	$a\left(z_3 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - a\left(x_3 - \frac{1}{2}\right)\,\hat{\mathbf{y}} - ay_3\,\hat{\mathbf{z}}$	(12b)	O I
$\mathbf{B_{15}}$	=	$-\left(z_3 - \frac{1}{2}\right)\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 + \left(y_3 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(z_3 - \frac{1}{2}\right)\,\hat{\mathbf{x}} - ax_3\,\hat{\mathbf{y}} + a\left(y_3 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(12b)	O I
$\mathbf{B_{16}}$	=	$-z_3\,\mathbf{a}_1 + \left(x_3 + \frac{1}{2}\right)\,\mathbf{a}_2 - \left(y_3 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-az_3\,\hat{\mathbf{x}} + a\left(x_3 + \frac{1}{2}\right)\,\hat{\mathbf{y}} - a\left(y_3 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(12b)	O I
$\mathbf{B_{17}}$	=	$y_3\,\mathbf{a}_1 + z_3\,\mathbf{a}_2 + x_3\,\mathbf{a}_3$	=	$ay_3\,\hat{\mathbf{x}} + az_3\,\hat{\mathbf{y}} + ax_3\,\hat{\mathbf{z}}$	(12b)	O I
$\mathbf{B_{18}}$	=	$-y_3\,\mathbf{a}_1 + \left(z_3 + \frac{1}{2}\right)\,\mathbf{a}_2 - \left(x_3 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ay_3\,\hat{\mathbf{x}} + a\left(z_3 + \frac{1}{2}\right)\,\hat{\mathbf{y}} - a\left(x_3 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(12b)	O I
$\mathbf{B_{19}}$	=	$\left(y_3 + \frac{1}{2}\right)\,\mathbf{a}_1 - \left(z_3 - \frac{1}{2}\right)\,\mathbf{a}_2 - x_3\,\mathbf{a}_3$	=	$a\left(y_3 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - a\left(z_3 - \frac{1}{2}\right)\,\hat{\mathbf{y}} - ax_3\,\hat{\mathbf{z}}$	(12b)	O I

$$\mathbf{B_{20}} = -\left(y_3 - \tfrac{1}{2}\right)\mathbf{a}_1 - z_3\,\mathbf{a}_2 + \left(x_3 + \tfrac{1}{2}\right)\mathbf{a}_3 = -a\left(y_3 - \tfrac{1}{2}\right)\hat{\mathbf{x}} - az_3\,\hat{\mathbf{y}} + a\left(x_3 + \tfrac{1}{2}\right)\hat{\mathbf{z}} \quad (12b) \quad \text{O I}$$

References

[1] G. N. Ramachandran and K. S. Chandrasekaran, *The absolute configuration of sodium chlorate* **10**, 671–675 (1957), doi:10.1107/S0365110X57002327.

Found in

[1] A. A. Kaminskii, S. N. Bagayev, J. Hulliger, H. Eichler, J. Findeisen, and R. Macdonald, *Acentric cubic $NaClO_3$–a new crystal for Raman lasers*, Applied Physics B **67**, 157–162 (1998), doi:10.1007/s003400050487.

First cited in

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