

K₃CrO₈ Structure:

AB3C8_tI24_121_a_bd_2i-001

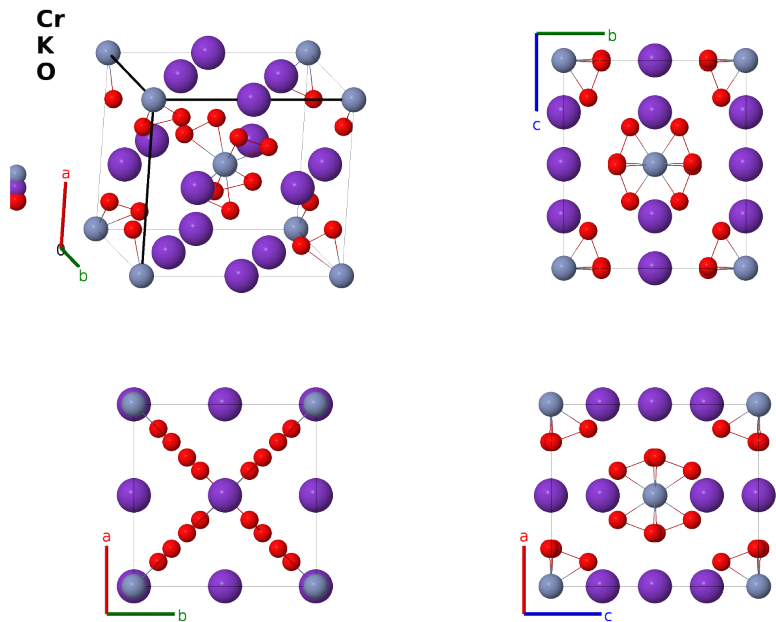
This structure previously used the label(s) **AB3C8_tI24_121_a_bd_2i**. Calls to these addresses will be redirected here.

Cite this page as:

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<https://aflow.org/prototype-encyclopedia/FR9M>

https://aflow.org/prototype-encyclopedia/AB3C8_tI24_121_a_bd_2i-001



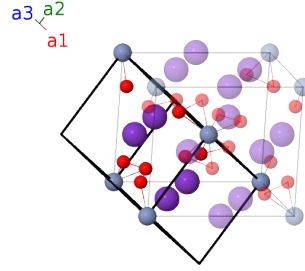
Prototype	CrK ₃ O ₈
AFLOW prototype label	AB3C8_tI24_121_a_bd_2i-001
ICSD	9356
CCDC	1594365
Pearson symbol	tI24
Space group number	121
Space group symbol	$I\bar{4}2m$
AFLOW prototype command	<code>aflow --proto=AB3C8_tI24_121_a_bd_2i-001</code> <code>--params=a, c/a, x₄, z₄, x₅, z₅</code>

Other compounds with this structure

Zr₃GeO₈

Body-centered Tetragonal primitive vectors

$$\begin{aligned}\mathbf{a}_1 &= -\frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{2}a \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}} \\ \mathbf{a}_2 &= \frac{1}{2}a \hat{\mathbf{x}} - \frac{1}{2}a \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}} \\ \mathbf{a}_3 &= \frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{2}a \hat{\mathbf{y}} - \frac{1}{2}c \hat{\mathbf{z}}\end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$=$	0	$=$	0	Cr I
$\mathbf{B}_2$	$=$	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2$	$=$	$\frac{1}{2} c \hat{\mathbf{z}}$	K I
$\mathbf{B}_3$	$=$	$\frac{3}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	K II
$\mathbf{B}_4$	$=$	$\frac{1}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{4} c \hat{\mathbf{z}}$	K II
$\mathbf{B}_5$	$=$	$(x_4 + z_4) \mathbf{a}_1 + (x_4 + z_4) \mathbf{a}_2 + 2x_4 \mathbf{a}_3$	$=$	$ax_4 \hat{\mathbf{x}} + ax_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	O I
$\mathbf{B}_6$	$=$	$-(x_4 - z_4) \mathbf{a}_1 - (x_4 - z_4) \mathbf{a}_2 - 2x_4 \mathbf{a}_3$	$=$	$-ax_4 \hat{\mathbf{x}} - ax_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	O I
$\mathbf{B}_7$	$=$	$-(x_4 + z_4) \mathbf{a}_1 + (x_4 - z_4) \mathbf{a}_2$	$=$	$ax_4 \hat{\mathbf{x}} - ax_4 \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}}$	O I
$\mathbf{B}_8$	$=$	$(x_4 - z_4) \mathbf{a}_1 - (x_4 + z_4) \mathbf{a}_2$	$=$	$-ax_4 \hat{\mathbf{x}} + ax_4 \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}}$	O I
$\mathbf{B}_9$	$=$	$(x_5 + z_5) \mathbf{a}_1 + (x_5 + z_5) \mathbf{a}_2 + 2x_5 \mathbf{a}_3$	$=$	$ax_5 \hat{\mathbf{x}} + ax_5 \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	O II
$\mathbf{B}_{10}$	$=$	$-(x_5 - z_5) \mathbf{a}_1 - (x_5 - z_5) \mathbf{a}_2 - 2x_5 \mathbf{a}_3$	$=$	$-ax_5 \hat{\mathbf{x}} - ax_5 \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	O II
$\mathbf{B}_{11}$	$=$	$-(x_5 + z_5) \mathbf{a}_1 + (x_5 - z_5) \mathbf{a}_2$	$=$	$ax_5 \hat{\mathbf{x}} - ax_5 \hat{\mathbf{y}} - cz_5 \hat{\mathbf{z}}$	O II
$\mathbf{B}_{12}$	$=$	$(x_5 - z_5) \mathbf{a}_1 - (x_5 + z_5) \mathbf{a}_2$	$=$	$-ax_5 \hat{\mathbf{x}} + ax_5 \hat{\mathbf{y}} - cz_5 \hat{\mathbf{z}}$	O II

References

- [1] R. Stomberg, *Least-Squares Refinement of the Crystal Structure of Potassium Peroxochromate*, Acta Chem. Scand. **17**, 1563–1566 (1963), doi:10.3891/acta.chem.scand.17-1563.

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