

Orthorhombic CrO₃ Structure: AB3_oC16_40_b_a2b-002

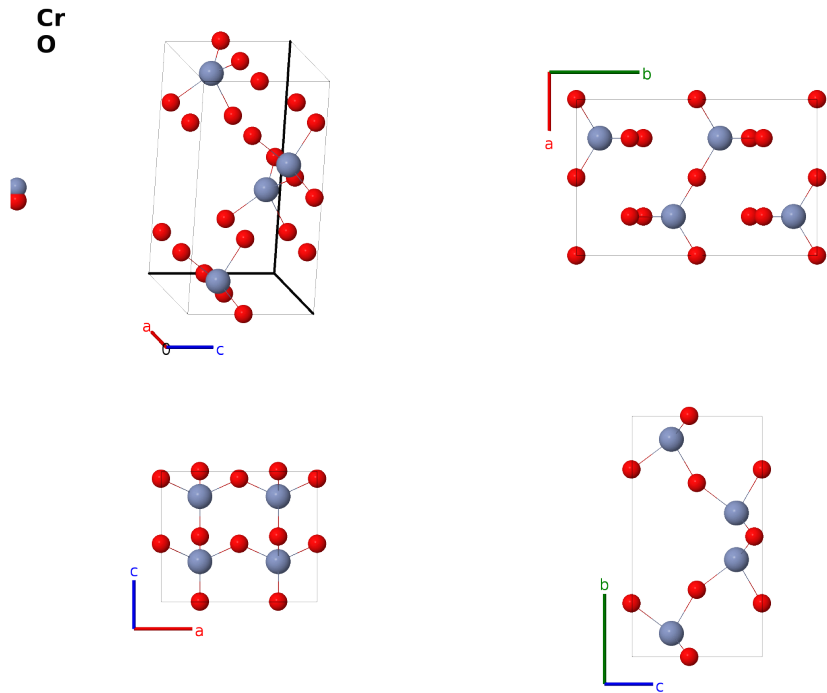
This structure previously used the label(s) **AB3_oC16_40_b_a2b**. Calls to these addresses will be redirected here.

Cite this page as:

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<https://aflow.org/prototype-encyclopedia/8E60>

https://aflow.org/prototype-encyclopedia/AB3_oC16_40_b_a2b-002



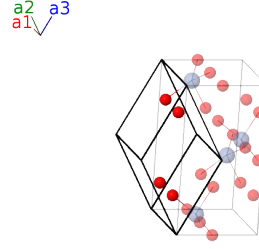
Prototype	CrO ₃
AFLOW prototype label	AB3_oC16_40_b_a2b-002
ICSD	24043
CCDC	1600098
Pearson symbol	oC16
Space group number	40
Space group symbol	<i>Ama</i> 2
AFLOW prototype command	<code>aflow --proto=AB3_oC16_40_b_a2b-002</code> <code>--params=a, b/a, c/a, z₁, y₂, z₂, y₃, z₃, y₄, z₄</code>

- This is an updated version of the D0₇ CrO₃ structure.

- (Byström, 1950) give this structure in the $C2cm$ setting of space group #40. We have shifted it to the standard $Ama2$ setting.

Base-centered Orthorhombic primitive vectors

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



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= -z_1 \mathbf{a}_2 + z_1 \mathbf{a}_3$	$=$	$cz_1 \hat{\mathbf{z}}$	(4a)	O I
$\mathbf{B}_2$	$= \frac{1}{2} \mathbf{a}_1 - z_1 \mathbf{a}_2 + z_1 \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + cz_1 \hat{\mathbf{z}}$	(4a)	O I
$\mathbf{B}_3$	$= \frac{1}{4} \mathbf{a}_1 + (y_2 - z_2) \mathbf{a}_2 + (y_2 + z_2) \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} + by_2 \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$	(4b)	Cr I
$\mathbf{B}_4$	$= \frac{3}{4} \mathbf{a}_1 - (y_2 + z_2) \mathbf{a}_2 - (y_2 - z_2) \mathbf{a}_3$	$=$	$\frac{3}{4}a \hat{\mathbf{x}} - by_2 \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$	(4b)	Cr I
$\mathbf{B}_5$	$= \frac{1}{4} \mathbf{a}_1 + (y_3 - z_3) \mathbf{a}_2 + (y_3 + z_3) \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} + by_3 \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(4b)	O II
$\mathbf{B}_6$	$= \frac{3}{4} \mathbf{a}_1 - (y_3 + z_3) \mathbf{a}_2 - (y_3 - z_3) \mathbf{a}_3$	$=$	$\frac{3}{4}a \hat{\mathbf{x}} - by_3 \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(4b)	O II
$\mathbf{B}_7$	$= \frac{1}{4} \mathbf{a}_1 + (y_4 - z_4) \mathbf{a}_2 + (y_4 + z_4) \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} + by_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(4b)	O III
$\mathbf{B}_8$	$= \frac{3}{4} \mathbf{a}_1 - (y_4 + z_4) \mathbf{a}_2 - (y_4 - z_4) \mathbf{a}_3$	$=$	$\frac{3}{4}a \hat{\mathbf{x}} - by_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(4b)	O III

References

- [1] A. Byström and K.-A. Wilhelmi, *The Crystal Structure of Chromium Trioxide*, Acta Chem. Scand. **4**, 1131–1141 (1950), doi:10.3891/acta.chem.scand.04-1131.
- [2] C. Hermann, O. Lohrmann, and H. Philipp, eds., *Strukturebericht Band II, 1928-1932* (Akademische Verlagsgesellschaft M. B. H, Leipzig, 1937).

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