

$D0_7$ (CrO_3) Structure (*Obsolete*): AB3_oC16_20_a_bc-001

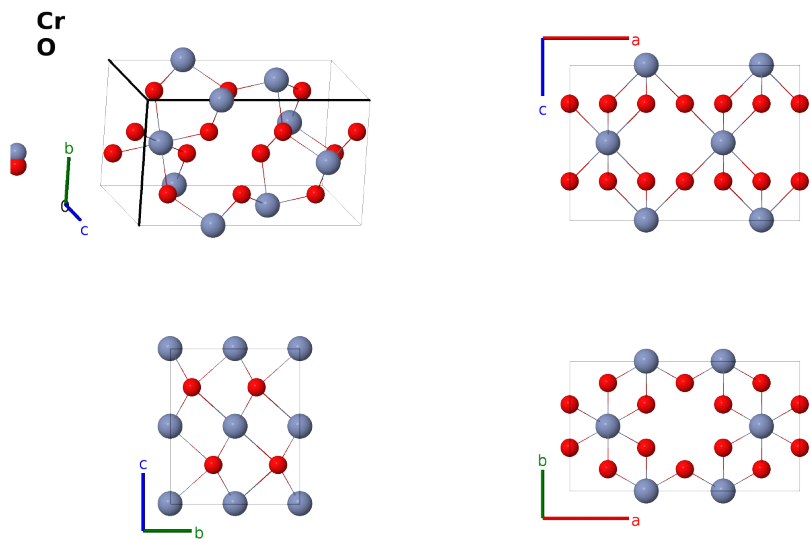
This structure previously used the label(s) **AB3_oC16_20_a_bc**. Calls to these addresses will be redirected here.

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

https://aflow.org/prototype-encyclopedia/AB3_oC16_20_a_bc-001

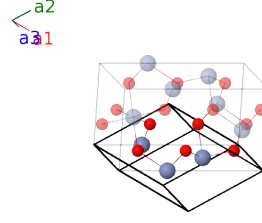


Prototype	CrO_3
AFLOW prototype label	AB3_oC16_20_a_bc-001
<i>Strukturbericht</i> designation	$D0_7$
Pearson symbol	oC16
Space group number	20
Space group symbol	$C222_1$
AFLOW prototype command	<code>aflow --proto=AB3_oC16_20_a_bc-001</code> <code>--params=a, b/a, c/a, x₁, y₂, x₃, y₃, z₃</code>

- This is the determination of the orthorhombic structure of CrO_3 given the $D0_7$ symbol by (Hermann, 1937). This structure is superceded by the one found by (Byström, 1950), which we call the “orthorhombic CrO_3 phase.” The current structure has the Cr atom at the center of a distorted oxygen octahedron, while the newer structure as the Cr atom at center of a distorted tetrahedron.

Base-centered Orthorhombic primitive vectors

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



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= x_1 \mathbf{a}_1 + x_1 \mathbf{a}_2$	$=$	$ax_1 \hat{\mathbf{x}}$	(4a)	Cr I
$\mathbf{B}_2$	$= -x_1 \mathbf{a}_1 - x_1 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-ax_1 \hat{\mathbf{x}} + \frac{1}{2}c \hat{\mathbf{z}}$	(4a)	Cr I
$\mathbf{B}_3$	$= -y_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$by_2 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(4b)	O I
$\mathbf{B}_4$	$= y_2 \mathbf{a}_1 - y_2 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$-by_2 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(4b)	O I
$\mathbf{B}_5$	$= (x_3 - y_3) \mathbf{a}_1 + (x_3 + y_3) \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$ax_3 \hat{\mathbf{x}} + by_3 \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(8c)	O II
$\mathbf{B}_6$	$= -(x_3 - y_3) \mathbf{a}_1 - (x_3 + y_3) \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_3 \hat{\mathbf{x}} - by_3 \hat{\mathbf{y}} + c(z_3 + \frac{1}{2}) \hat{\mathbf{z}}$	(8c)	O II
$\mathbf{B}_7$	$= -(x_3 + y_3) \mathbf{a}_1 - (x_3 - y_3) \mathbf{a}_2 - (z_3 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_3 \hat{\mathbf{x}} + by_3 \hat{\mathbf{y}} - c(z_3 - \frac{1}{2}) \hat{\mathbf{z}}$	(8c)	O II
$\mathbf{B}_8$	$= (x_3 + y_3) \mathbf{a}_1 + (x_3 - y_3) \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$ax_3 \hat{\mathbf{x}} - by_3 \hat{\mathbf{y}} - cz_3 \hat{\mathbf{z}}$	(8c)	O II

References

- [1] H. Bräkken, *Die Kristallstrukturen der Trioxyde von Chrom, Molybdän und Wolfram*, Z. Kristallgr. **78**, 484–488 (1931), doi:10.1524/zkri.1931.78.1.484.
- [2] C. Hermann, O. Lohrmann, and H. Philipp, eds., *Strukturebericht Band II, 1928-1932* (Akademische Verlagsgesellschaft M. B. H, Leipzig, 1937).

Found in

- [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.

First cited in

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