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

This structure originally had the label `AB3_oC16_20_a_bc`. Calls to that address will be redirected here.

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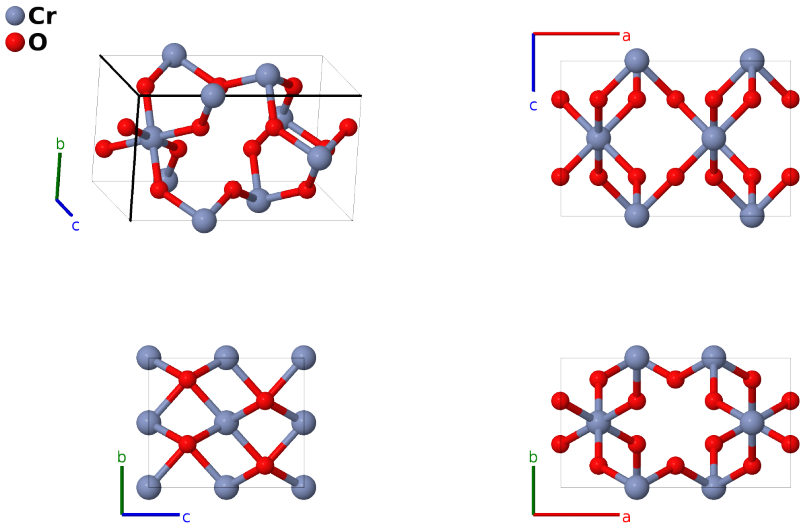
https://aflow.org/p/KCMH

https://aflow.org/p/AB3_oC16_20_a_bc-001

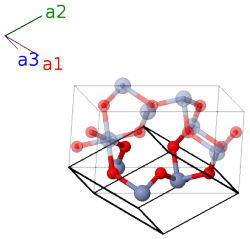


Prototype	CrO_3
AFLOW prototype label	AB3_oC16_20_a_bc-001
***Strukturbericht* designation**	$D0_7$
ICSD	none
Pearson symbol	oC16
Space group number	20
Space group symbol	$C222_1$
AFLOW prototype command	`aflow --proto=AB3_oC16_20_a_bc-001 --params=`$a, b/a, c/a, x_1, y_2, x_3, y_3, z_3$

- This is the determination of the orthorhombic structure of CrO_3 given the $D0_7$ structure 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 This structure is superceded by the one found by (Byström, 1950), which we call the "orthorhombic CrO_3 phase."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

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



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
$\mathbf{B_6}$	=	$-(x_3 - y_3)\,\mathbf{a}_1 - (x_3 + y_3)\,\mathbf{a}_2 + \left(z_3 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} - by_3\,\hat{\mathbf{y}} + c\left(z_3 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8c)	O II
$\mathbf{B_7}$	=	$-(x_3 + y_3)\,\mathbf{a}_1 - (x_3 - y_3)\,\mathbf{a}_2 - \left(z_3 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} + by_3\,\hat{\mathbf{y}} - c\left(z_3 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(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* (Akademsiche 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.