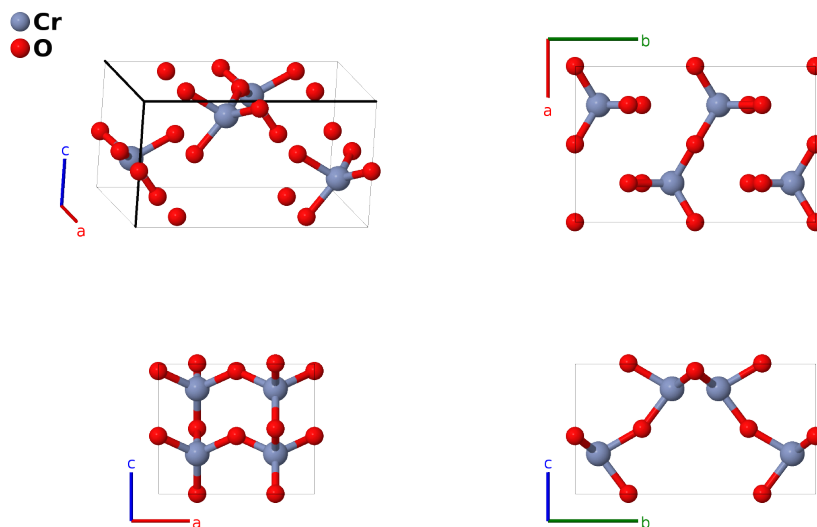# Orthorhombic CrO$_3$ Structure: AB3_oC16_40_b_a2b-002

This structure originally had the label `AB3_oC16_40_b_a2b`. Calls to that address will be redirected here.

https://aflow.org/p/8E60

https://aflow.org/p/AB3_oC16_40_b_a2b-002

Prototype	CrO$_3$
AFLOW prototype label	AB3_oC16_40_b_a2b-002
ICSD	24043
Pearson symbol	oC16
Space group number	40
Space group symbol	$Ama2$
AFLOW prototype command	aflow --proto=AB3_oC16_40_b_a2b-002 --params=$a, b/a, c/a, z_1, y_2, z_2, y_3, z_3, y_4, z_4$

- This is an updated version of the D0$_7$ CrO$_3$ 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

$$\mathbf{a_1} = a\,\hat{\mathbf{x}}$$

$$\mathbf{a_2} = \tfrac{1}{2}b\,\hat{\mathbf{y}} - \tfrac{1}{2}c\,\hat{\mathbf{z}}$$

$$\mathbf{a_3} = \tfrac{1}{2}b\,\hat{\mathbf{y}} + \tfrac{1}{2}c\,\hat{\mathbf{z}}$$
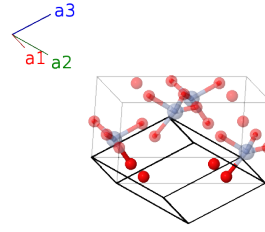
Basis vectors

		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
$\mathbf{B_2}$	$=$	$\tfrac{1}{2}\,\mathbf{a_1} - z_1\,\mathbf{a_2} + z_1\,\mathbf{a_3}$	$=$	$\tfrac{1}{2}a\,\hat{\mathbf{x}} + cz_1\,\hat{\mathbf{z}}$	(4a)	O I
$\mathbf{B_3}$	$=$	$\tfrac{1}{4}\,\mathbf{a_1} + (y_2 - z_2)\,\mathbf{a_2} + (y_2 + z_2)\,\mathbf{a_3}$	$=$	$\tfrac{1}{4}a\,\hat{\mathbf{x}} + by_2\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(4b)	Cr I
$\mathbf{B_4}$	$=$	$\tfrac{3}{4}\,\mathbf{a_1} - (y_2 + z_2)\,\mathbf{a_2} - (y_2 - z_2)\,\mathbf{a_3}$	$=$	$\tfrac{3}{4}a\,\hat{\mathbf{x}} - by_2\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(4b)	Cr I
$\mathbf{B_5}$	$=$	$\tfrac{1}{4}\,\mathbf{a_1} + (y_3 - z_3)\,\mathbf{a_2} + (y_3 + z_3)\,\mathbf{a_3}$	$=$	$\tfrac{1}{4}a\,\hat{\mathbf{x}} + by_3\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(4b)	O II
$\mathbf{B_6}$	$=$	$\tfrac{3}{4}\,\mathbf{a_1} - (y_3 + z_3)\,\mathbf{a_2} - (y_3 - z_3)\,\mathbf{a_3}$	$=$	$\tfrac{3}{4}a\,\hat{\mathbf{x}} - by_3\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(4b)	O II
$\mathbf{B_7}$	$=$	$\tfrac{1}{4}\,\mathbf{a_1} + (y_4 - z_4)\,\mathbf{a_2} + (y_4 + z_4)\,\mathbf{a_3}$	$=$	$\tfrac{1}{4}a\,\hat{\mathbf{x}} + by_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(4b)	O III
$\mathbf{B_8}$	$=$	$\tfrac{3}{4}\,\mathbf{a_1} - (y_4 + z_4)\,\mathbf{a_2} - (y_4 - z_4)\,\mathbf{a_3}$	$=$	$\tfrac{3}{4}a\,\hat{\mathbf{x}} - by_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(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., *Strukturbericht Band II, 1928-1932* (Akademsiche Verlagsgesellschaft M. B. H, Leipzig, 1937).