

Cr₅O₁₂ Structure:

A5B12_oP68_60_c2d_6d-001

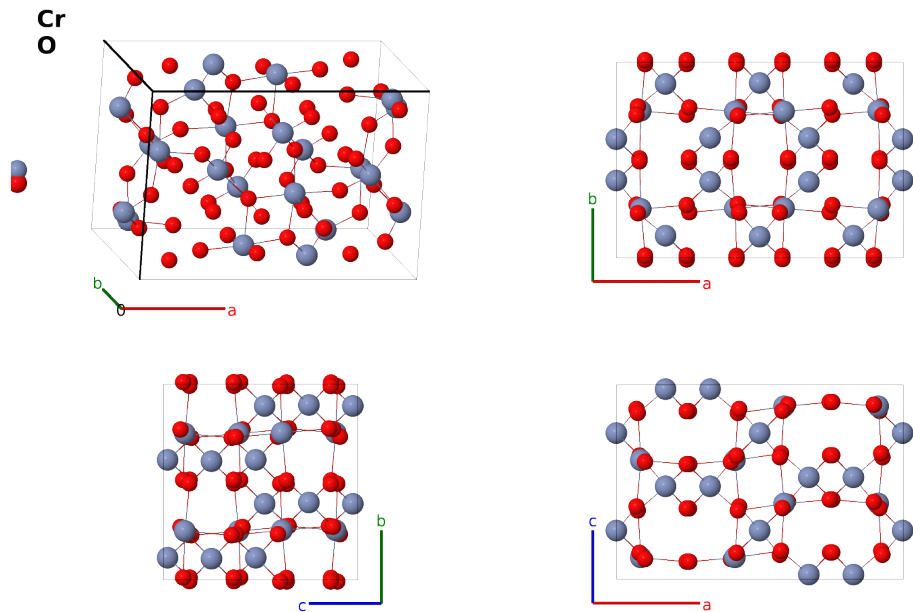
This structure previously used the label(s) **A5B12_oP68_60_c2d_6d**. Calls to these addresses will be redirected here.

Cite this page as:

- H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettl, M. Esters, X. Campilongo, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*, Comput. Mater. Sci. **240**, 112988 (2024), doi: 10.1016/j.commatsci.2024.112988.
- D. Hicks, M. J. Mehl, M. Esters, C. Oses, O. Levy, G. L. W. Hart, C. Toher, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 3*, Comput. Mater. Sci. **199**, 110450 (2021), doi: 10.1016/j.commatsci.2021.110450.

<https://aflow.org/prototype-encyclopedia/NF0B>

https://aflow.org/prototype-encyclopedia/A5B12_oP68_60_c2d_6d-001

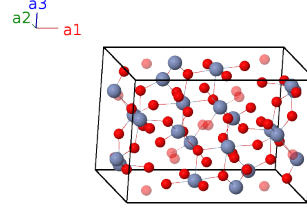


Prototype	Cr ₅ O ₁₂
AFLOW prototype label	A5B12_oP68_60_c2d_6d-001
ICSD	24299
CCDC	1600344
Pearson symbol	oP68
Space group number	60
Space group symbol	<i>Pbcn</i>
AFLOW prototype command	<pre>aflow --proto=A5B12_oP68_60_c2d_6d-001 --params=a,b/a,c/a,y1,x2,y2,z2,x3,y3,z3,x4,y4,z4,x5,y5,z5,x6,y6,z6,x7,y7,z7, x8,y8,z8,x9,y9,z9</pre>

- (Wilhelmi, 1965) describes this as a distorted face-centered cubic lattice of oxygen atoms with the chromium atoms in interstitial sites. One can very clearly see the CrO₄ tetrahedra and CrO₆ octahedra, indicating the presence of both Cr⁺² and Cr⁺³ ions.

Simple Orthorhombic primitive vectors

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



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= y_1 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$by_1 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(4c)	Cr I
$\mathbf{B}_2$	$= \frac{1}{2} \mathbf{a}_1 - (y_1 - \frac{1}{2}) \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - b(y_1 - \frac{1}{2}) \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(4c)	Cr I
$\mathbf{B}_3$	$= -y_1 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$-by_1 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(4c)	Cr I
$\mathbf{B}_4$	$= \frac{1}{2} \mathbf{a}_1 + (y_1 + \frac{1}{2}) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + b(y_1 + \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(4c)	Cr I
$\mathbf{B}_5$	$= x_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$ax_2 \hat{\mathbf{x}} + by_2 \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$	(8d)	Cr II
$\mathbf{B}_6$	$= -(x_2 - \frac{1}{2}) \mathbf{a}_1 - (y_2 - \frac{1}{2}) \mathbf{a}_2 + (z_2 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_2 - \frac{1}{2}) \hat{\mathbf{x}} - b(y_2 - \frac{1}{2}) \hat{\mathbf{y}} + c(z_2 + \frac{1}{2}) \hat{\mathbf{z}}$	(8d)	Cr II
$\mathbf{B}_7$	$= -x_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 - (z_2 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_2 \hat{\mathbf{x}} + by_2 \hat{\mathbf{y}} - c(z_2 - \frac{1}{2}) \hat{\mathbf{z}}$	(8d)	Cr II
$\mathbf{B}_8$	$= (x_2 + \frac{1}{2}) \mathbf{a}_1 - (y_2 - \frac{1}{2}) \mathbf{a}_2 - z_2 \mathbf{a}_3$	$=$	$a(x_2 + \frac{1}{2}) \hat{\mathbf{x}} - b(y_2 - \frac{1}{2}) \hat{\mathbf{y}} - cz_2 \hat{\mathbf{z}}$	(8d)	Cr II
$\mathbf{B}_9$	$= -x_2 \mathbf{a}_1 - y_2 \mathbf{a}_2 - z_2 \mathbf{a}_3$	$=$	$-ax_2 \hat{\mathbf{x}} - by_2 \hat{\mathbf{y}} - cz_2 \hat{\mathbf{z}}$	(8d)	Cr II
$\mathbf{B}_{10}$	$= (x_2 + \frac{1}{2}) \mathbf{a}_1 + (y_2 + \frac{1}{2}) \mathbf{a}_2 - (z_2 - \frac{1}{2}) \mathbf{a}_3$	$=$	$a(x_2 + \frac{1}{2}) \hat{\mathbf{x}} + b(y_2 + \frac{1}{2}) \hat{\mathbf{y}} - c(z_2 - \frac{1}{2}) \hat{\mathbf{z}}$	(8d)	Cr II
$\mathbf{B}_{11}$	$= x_2 \mathbf{a}_1 - y_2 \mathbf{a}_2 + (z_2 + \frac{1}{2}) \mathbf{a}_3$	$=$	$ax_2 \hat{\mathbf{x}} - by_2 \hat{\mathbf{y}} + c(z_2 + \frac{1}{2}) \hat{\mathbf{z}}$	(8d)	Cr II
$\mathbf{B}_{12}$	$= -(x_2 - \frac{1}{2}) \mathbf{a}_1 + (y_2 + \frac{1}{2}) \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$-a(x_2 - \frac{1}{2}) \hat{\mathbf{x}} + b(y_2 + \frac{1}{2}) \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$	(8d)	Cr II
$\mathbf{B}_{13}$	$= x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$ax_3 \hat{\mathbf{x}} + by_3 \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(8d)	Cr III
$\mathbf{B}_{14}$	$= -(x_3 - \frac{1}{2}) \mathbf{a}_1 - (y_3 - \frac{1}{2}) \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_3 - \frac{1}{2}) \hat{\mathbf{x}} - b(y_3 - \frac{1}{2}) \hat{\mathbf{y}} + c(z_3 + \frac{1}{2}) \hat{\mathbf{z}}$	(8d)	Cr III
$\mathbf{B}_{15}$	$= -x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 - (z_3 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_3 \hat{\mathbf{x}} + by_3 \hat{\mathbf{y}} - c(z_3 - \frac{1}{2}) \hat{\mathbf{z}}$	(8d)	Cr III
$\mathbf{B}_{16}$	$= (x_3 + \frac{1}{2}) \mathbf{a}_1 - (y_3 - \frac{1}{2}) \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$a(x_3 + \frac{1}{2}) \hat{\mathbf{x}} - b(y_3 - \frac{1}{2}) \hat{\mathbf{y}} - cz_3 \hat{\mathbf{z}}$	(8d)	Cr III
$\mathbf{B}_{17}$	$= -x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$-ax_3 \hat{\mathbf{x}} - by_3 \hat{\mathbf{y}} - cz_3 \hat{\mathbf{z}}$	(8d)	Cr III
$\mathbf{B}_{18}$	$= (x_3 + \frac{1}{2}) \mathbf{a}_1 + (y_3 + \frac{1}{2}) \mathbf{a}_2 - (z_3 - \frac{1}{2}) \mathbf{a}_3$	$=$	$a(x_3 + \frac{1}{2}) \hat{\mathbf{x}} + b(y_3 + \frac{1}{2}) \hat{\mathbf{y}} - c(z_3 - \frac{1}{2}) \hat{\mathbf{z}}$	(8d)	Cr III
$\mathbf{B}_{19}$	$= x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$	$=$	$ax_3 \hat{\mathbf{x}} - by_3 \hat{\mathbf{y}} + c(z_3 + \frac{1}{2}) \hat{\mathbf{z}}$	(8d)	Cr III
$\mathbf{B}_{20}$	$= -(x_3 - \frac{1}{2}) \mathbf{a}_1 + (y_3 + \frac{1}{2}) \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$-a(x_3 - \frac{1}{2}) \hat{\mathbf{x}} + b(y_3 + \frac{1}{2}) \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(8d)	Cr III
$\mathbf{B}_{21}$	$= x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$ax_4 \hat{\mathbf{x}} + by_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(8d)	O I
$\mathbf{B}_{22}$	$= -(x_4 - \frac{1}{2}) \mathbf{a}_1 - (y_4 - \frac{1}{2}) \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_4 - \frac{1}{2}) \hat{\mathbf{x}} - b(y_4 - \frac{1}{2}) \hat{\mathbf{y}} + c(z_4 + \frac{1}{2}) \hat{\mathbf{z}}$	(8d)	O I
$\mathbf{B}_{23}$	$= -x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 - (z_4 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_4 \hat{\mathbf{x}} + by_4 \hat{\mathbf{y}} - c(z_4 - \frac{1}{2}) \hat{\mathbf{z}}$	(8d)	O I
$\mathbf{B}_{24}$	$= (x_4 + \frac{1}{2}) \mathbf{a}_1 - (y_4 - \frac{1}{2}) \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$a(x_4 + \frac{1}{2}) \hat{\mathbf{x}} - b(y_4 - \frac{1}{2}) \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}}$	(8d)	O I

$\mathbf{B}_{25} =$	$-x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$-ax_4 \hat{\mathbf{x}} - by_4 \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}}$	(8d)	O I
$\mathbf{B}_{26} =$	$(x_4 + \frac{1}{2}) \mathbf{a}_1 + (y_4 + \frac{1}{2}) \mathbf{a}_2 -$ $(z_4 - \frac{1}{2}) \mathbf{a}_3$	$=$	$a(x_4 + \frac{1}{2}) \hat{\mathbf{x}} + b(y_4 + \frac{1}{2}) \hat{\mathbf{y}} - c(z_4 - \frac{1}{2}) \hat{\mathbf{z}}$	(8d)	O I
$\mathbf{B}_{27} =$	$x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3$	$=$	$ax_4 \hat{\mathbf{x}} - by_4 \hat{\mathbf{y}} + c(z_4 + \frac{1}{2}) \hat{\mathbf{z}}$	(8d)	O I
$\mathbf{B}_{28} =$	$-(x_4 - \frac{1}{2}) \mathbf{a}_1 + (y_4 + \frac{1}{2}) \mathbf{a}_2 +$ $z_4 \mathbf{a}_3$	$=$	$-a(x_4 - \frac{1}{2}) \hat{\mathbf{x}} + b(y_4 + \frac{1}{2}) \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(8d)	O I
$\mathbf{B}_{29} =$	$x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$ax_5 \hat{\mathbf{x}} + by_5 \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(8d)	O II
$\mathbf{B}_{30} =$	$-(x_5 - \frac{1}{2}) \mathbf{a}_1 - (y_5 - \frac{1}{2}) \mathbf{a}_2 +$ $(z_5 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_5 - \frac{1}{2}) \hat{\mathbf{x}} - b(y_5 - \frac{1}{2}) \hat{\mathbf{y}} + c(z_5 + \frac{1}{2}) \hat{\mathbf{z}}$	(8d)	O II
$\mathbf{B}_{31} =$	$-x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 - (z_5 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_5 \hat{\mathbf{x}} + by_5 \hat{\mathbf{y}} - c(z_5 - \frac{1}{2}) \hat{\mathbf{z}}$	(8d)	O II
$\mathbf{B}_{32} =$	$(x_5 + \frac{1}{2}) \mathbf{a}_1 - (y_5 - \frac{1}{2}) \mathbf{a}_2 - z_5 \mathbf{a}_3$	$=$	$a(x_5 + \frac{1}{2}) \hat{\mathbf{x}} - b(y_5 - \frac{1}{2}) \hat{\mathbf{y}} - cz_5 \hat{\mathbf{z}}$	(8d)	O II
$\mathbf{B}_{33} =$	$-x_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 - z_5 \mathbf{a}_3$	$=$	$-ax_5 \hat{\mathbf{x}} - by_5 \hat{\mathbf{y}} - cz_5 \hat{\mathbf{z}}$	(8d)	O II
$\mathbf{B}_{34} =$	$(x_5 + \frac{1}{2}) \mathbf{a}_1 + (y_5 + \frac{1}{2}) \mathbf{a}_2 -$ $(z_5 - \frac{1}{2}) \mathbf{a}_3$	$=$	$a(x_5 + \frac{1}{2}) \hat{\mathbf{x}} + b(y_5 + \frac{1}{2}) \hat{\mathbf{y}} - c(z_5 - \frac{1}{2}) \hat{\mathbf{z}}$	(8d)	O II
$\mathbf{B}_{35} =$	$x_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 + (z_5 + \frac{1}{2}) \mathbf{a}_3$	$=$	$ax_5 \hat{\mathbf{x}} - by_5 \hat{\mathbf{y}} + c(z_5 + \frac{1}{2}) \hat{\mathbf{z}}$	(8d)	O II
$\mathbf{B}_{36} =$	$-(x_5 - \frac{1}{2}) \mathbf{a}_1 + (y_5 + \frac{1}{2}) \mathbf{a}_2 +$ $z_5 \mathbf{a}_3$	$=$	$-a(x_5 - \frac{1}{2}) \hat{\mathbf{x}} + b(y_5 + \frac{1}{2}) \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(8d)	O II
$\mathbf{B}_{37} =$	$x_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$ax_6 \hat{\mathbf{x}} + by_6 \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}}$	(8d)	O III
$\mathbf{B}_{38} =$	$-(x_6 - \frac{1}{2}) \mathbf{a}_1 - (y_6 - \frac{1}{2}) \mathbf{a}_2 +$ $(z_6 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_6 - \frac{1}{2}) \hat{\mathbf{x}} - b(y_6 - \frac{1}{2}) \hat{\mathbf{y}} + c(z_6 + \frac{1}{2}) \hat{\mathbf{z}}$	(8d)	O III
$\mathbf{B}_{39} =$	$-x_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 - (z_6 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_6 \hat{\mathbf{x}} + by_6 \hat{\mathbf{y}} - c(z_6 - \frac{1}{2}) \hat{\mathbf{z}}$	(8d)	O III
$\mathbf{B}_{40} =$	$(x_6 + \frac{1}{2}) \mathbf{a}_1 - (y_6 - \frac{1}{2}) \mathbf{a}_2 - z_6 \mathbf{a}_3$	$=$	$a(x_6 + \frac{1}{2}) \hat{\mathbf{x}} - b(y_6 - \frac{1}{2}) \hat{\mathbf{y}} - cz_6 \hat{\mathbf{z}}$	(8d)	O III
$\mathbf{B}_{41} =$	$-x_6 \mathbf{a}_1 - y_6 \mathbf{a}_2 - z_6 \mathbf{a}_3$	$=$	$-ax_6 \hat{\mathbf{x}} - by_6 \hat{\mathbf{y}} - cz_6 \hat{\mathbf{z}}$	(8d)	O III
$\mathbf{B}_{42} =$	$(x_6 + \frac{1}{2}) \mathbf{a}_1 + (y_6 + \frac{1}{2}) \mathbf{a}_2 -$ $(z_6 - \frac{1}{2}) \mathbf{a}_3$	$=$	$a(x_6 + \frac{1}{2}) \hat{\mathbf{x}} + b(y_6 + \frac{1}{2}) \hat{\mathbf{y}} - c(z_6 - \frac{1}{2}) \hat{\mathbf{z}}$	(8d)	O III
$\mathbf{B}_{43} =$	$x_6 \mathbf{a}_1 - y_6 \mathbf{a}_2 + (z_6 + \frac{1}{2}) \mathbf{a}_3$	$=$	$ax_6 \hat{\mathbf{x}} - by_6 \hat{\mathbf{y}} + c(z_6 + \frac{1}{2}) \hat{\mathbf{z}}$	(8d)	O III
$\mathbf{B}_{44} =$	$-(x_6 - \frac{1}{2}) \mathbf{a}_1 + (y_6 + \frac{1}{2}) \mathbf{a}_2 +$ $z_6 \mathbf{a}_3$	$=$	$-a(x_6 - \frac{1}{2}) \hat{\mathbf{x}} + b(y_6 + \frac{1}{2}) \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}}$	(8d)	O III
$\mathbf{B}_{45} =$	$x_7 \mathbf{a}_1 + y_7 \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$ax_7 \hat{\mathbf{x}} + by_7 \hat{\mathbf{y}} + cz_7 \hat{\mathbf{z}}$	(8d)	O IV
$\mathbf{B}_{46} =$	$-(x_7 - \frac{1}{2}) \mathbf{a}_1 - (y_7 - \frac{1}{2}) \mathbf{a}_2 +$ $(z_7 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_7 - \frac{1}{2}) \hat{\mathbf{x}} - b(y_7 - \frac{1}{2}) \hat{\mathbf{y}} + c(z_7 + \frac{1}{2}) \hat{\mathbf{z}}$	(8d)	O IV
$\mathbf{B}_{47} =$	$-x_7 \mathbf{a}_1 + y_7 \mathbf{a}_2 - (z_7 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_7 \hat{\mathbf{x}} + by_7 \hat{\mathbf{y}} - c(z_7 - \frac{1}{2}) \hat{\mathbf{z}}$	(8d)	O IV
$\mathbf{B}_{48} =$	$(x_7 + \frac{1}{2}) \mathbf{a}_1 - (y_7 - \frac{1}{2}) \mathbf{a}_2 - z_7 \mathbf{a}_3$	$=$	$a(x_7 + \frac{1}{2}) \hat{\mathbf{x}} - b(y_7 - \frac{1}{2}) \hat{\mathbf{y}} - cz_7 \hat{\mathbf{z}}$	(8d)	O IV
$\mathbf{B}_{49} =$	$-x_7 \mathbf{a}_1 - y_7 \mathbf{a}_2 - z_7 \mathbf{a}_3$	$=$	$-ax_7 \hat{\mathbf{x}} - by_7 \hat{\mathbf{y}} - cz_7 \hat{\mathbf{z}}$	(8d)	O IV
$\mathbf{B}_{50} =$	$(x_7 + \frac{1}{2}) \mathbf{a}_1 + (y_7 + \frac{1}{2}) \mathbf{a}_2 -$ $(z_7 - \frac{1}{2}) \mathbf{a}_3$	$=$	$a(x_7 + \frac{1}{2}) \hat{\mathbf{x}} + b(y_7 + \frac{1}{2}) \hat{\mathbf{y}} - c(z_7 - \frac{1}{2}) \hat{\mathbf{z}}$	(8d)	O IV
$\mathbf{B}_{51} =$	$x_7 \mathbf{a}_1 - y_7 \mathbf{a}_2 + (z_7 + \frac{1}{2}) \mathbf{a}_3$	$=$	$ax_7 \hat{\mathbf{x}} - by_7 \hat{\mathbf{y}} + c(z_7 + \frac{1}{2}) \hat{\mathbf{z}}$	(8d)	O IV
$\mathbf{B}_{52} =$	$-(x_7 - \frac{1}{2}) \mathbf{a}_1 + (y_7 + \frac{1}{2}) \mathbf{a}_2 +$ $z_7 \mathbf{a}_3$	$=$	$-a(x_7 - \frac{1}{2}) \hat{\mathbf{x}} + b(y_7 + \frac{1}{2}) \hat{\mathbf{y}} + cz_7 \hat{\mathbf{z}}$	(8d)	O IV
$\mathbf{B}_{53} =$	$x_8 \mathbf{a}_1 + y_8 \mathbf{a}_2 + z_8 \mathbf{a}_3$	$=$	$ax_8 \hat{\mathbf{x}} + by_8 \hat{\mathbf{y}} + cz_8 \hat{\mathbf{z}}$	(8d)	O V
$\mathbf{B}_{54} =$	$-(x_8 - \frac{1}{2}) \mathbf{a}_1 - (y_8 - \frac{1}{2}) \mathbf{a}_2 +$ $(z_8 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_8 - \frac{1}{2}) \hat{\mathbf{x}} - b(y_8 - \frac{1}{2}) \hat{\mathbf{y}} + c(z_8 + \frac{1}{2}) \hat{\mathbf{z}}$	(8d)	O V
$\mathbf{B}_{55} =$	$-x_8 \mathbf{a}_1 + y_8 \mathbf{a}_2 - (z_8 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_8 \hat{\mathbf{x}} + by_8 \hat{\mathbf{y}} - c(z_8 - \frac{1}{2}) \hat{\mathbf{z}}$	(8d)	O V
$\mathbf{B}_{56} =$	$(x_8 + \frac{1}{2}) \mathbf{a}_1 - (y_8 - \frac{1}{2}) \mathbf{a}_2 - z_8 \mathbf{a}_3$	$=$	$a(x_8 + \frac{1}{2}) \hat{\mathbf{x}} - b(y_8 - \frac{1}{2}) \hat{\mathbf{y}} - cz_8 \hat{\mathbf{z}}$	(8d)	O V

$$\begin{aligned}
\mathbf{B}_{57} &= -x_8 \mathbf{a}_1 - y_8 \mathbf{a}_2 - z_8 \mathbf{a}_3 &= -ax_8 \hat{\mathbf{x}} - by_8 \hat{\mathbf{y}} - cz_8 \hat{\mathbf{z}} &(8d) &\text{O V} \\
\mathbf{B}_{58} &= \begin{pmatrix} x_8 + \frac{1}{2} \\ z_8 - \frac{1}{2} \end{pmatrix} \mathbf{a}_1 + \begin{pmatrix} y_8 + \frac{1}{2} \\ z_8 - \frac{1}{2} \end{pmatrix} \mathbf{a}_2 - &= a \begin{pmatrix} x_8 + \frac{1}{2} \\ z_8 - \frac{1}{2} \end{pmatrix} \hat{\mathbf{x}} + b \begin{pmatrix} y_8 + \frac{1}{2} \\ z_8 - \frac{1}{2} \end{pmatrix} \hat{\mathbf{y}} - c \begin{pmatrix} z_8 - \frac{1}{2} \end{pmatrix} \hat{\mathbf{z}} &(8d) &\text{O V} \\
\mathbf{B}_{59} &= x_8 \mathbf{a}_1 - y_8 \mathbf{a}_2 + \begin{pmatrix} z_8 + \frac{1}{2} \\ z_8 \end{pmatrix} \mathbf{a}_3 &= ax_8 \hat{\mathbf{x}} - by_8 \hat{\mathbf{y}} + c \begin{pmatrix} z_8 + \frac{1}{2} \\ z_8 \end{pmatrix} \hat{\mathbf{z}} &(8d) &\text{O V} \\
\mathbf{B}_{60} &= -\begin{pmatrix} x_8 - \frac{1}{2} \\ z_8 \end{pmatrix} \mathbf{a}_1 + \begin{pmatrix} y_8 + \frac{1}{2} \\ z_8 \end{pmatrix} \mathbf{a}_2 + &= -a \begin{pmatrix} x_8 - \frac{1}{2} \\ z_8 \end{pmatrix} \hat{\mathbf{x}} + b \begin{pmatrix} y_8 + \frac{1}{2} \\ z_8 \end{pmatrix} \hat{\mathbf{y}} + cz_8 \hat{\mathbf{z}} &(8d) &\text{O V} \\
\mathbf{B}_{61} &= x_9 \mathbf{a}_1 + y_9 \mathbf{a}_2 + z_9 \mathbf{a}_3 &= ax_9 \hat{\mathbf{x}} + by_9 \hat{\mathbf{y}} + cz_9 \hat{\mathbf{z}} &(8d) &\text{O VI} \\
\mathbf{B}_{62} &= -\begin{pmatrix} x_9 - \frac{1}{2} \\ z_9 + \frac{1}{2} \end{pmatrix} \mathbf{a}_1 - \begin{pmatrix} y_9 - \frac{1}{2} \\ z_9 + \frac{1}{2} \end{pmatrix} \mathbf{a}_2 + &= -a \begin{pmatrix} x_9 - \frac{1}{2} \\ z_9 + \frac{1}{2} \end{pmatrix} \hat{\mathbf{x}} - b \begin{pmatrix} y_9 - \frac{1}{2} \\ z_9 + \frac{1}{2} \end{pmatrix} \hat{\mathbf{y}} + c \begin{pmatrix} z_9 + \frac{1}{2} \end{pmatrix} \hat{\mathbf{z}} &(8d) &\text{O VI} \\
\mathbf{B}_{63} &= -x_9 \mathbf{a}_1 + y_9 \mathbf{a}_2 - \begin{pmatrix} z_9 - \frac{1}{2} \\ z_9 \end{pmatrix} \mathbf{a}_3 &= -ax_9 \hat{\mathbf{x}} + by_9 \hat{\mathbf{y}} - c \begin{pmatrix} z_9 - \frac{1}{2} \\ z_9 \end{pmatrix} \hat{\mathbf{z}} &(8d) &\text{O VI} \\
\mathbf{B}_{64} &= \begin{pmatrix} x_9 + \frac{1}{2} \\ z_9 - \frac{1}{2} \end{pmatrix} \mathbf{a}_1 - \begin{pmatrix} y_9 - \frac{1}{2} \\ z_9 - \frac{1}{2} \end{pmatrix} \mathbf{a}_2 - z_9 \mathbf{a}_3 &= a \begin{pmatrix} x_9 + \frac{1}{2} \\ z_9 - \frac{1}{2} \end{pmatrix} \hat{\mathbf{x}} - b \begin{pmatrix} y_9 - \frac{1}{2} \\ z_9 - \frac{1}{2} \end{pmatrix} \hat{\mathbf{y}} - cz_9 \hat{\mathbf{z}} &(8d) &\text{O VI} \\
\mathbf{B}_{65} &= -x_9 \mathbf{a}_1 - y_9 \mathbf{a}_2 - z_9 \mathbf{a}_3 &= -ax_9 \hat{\mathbf{x}} - by_9 \hat{\mathbf{y}} - cz_9 \hat{\mathbf{z}} &(8d) &\text{O VI} \\
\mathbf{B}_{66} &= \begin{pmatrix} x_9 + \frac{1}{2} \\ z_9 - \frac{1}{2} \end{pmatrix} \mathbf{a}_1 + \begin{pmatrix} y_9 + \frac{1}{2} \\ z_9 - \frac{1}{2} \end{pmatrix} \mathbf{a}_2 - &= a \begin{pmatrix} x_9 + \frac{1}{2} \\ z_9 - \frac{1}{2} \end{pmatrix} \hat{\mathbf{x}} + b \begin{pmatrix} y_9 + \frac{1}{2} \\ z_9 - \frac{1}{2} \end{pmatrix} \hat{\mathbf{y}} - c \begin{pmatrix} z_9 - \frac{1}{2} \end{pmatrix} \hat{\mathbf{z}} &(8d) &\text{O VI} \\
\mathbf{B}_{67} &= x_9 \mathbf{a}_1 - y_9 \mathbf{a}_2 + \begin{pmatrix} z_9 + \frac{1}{2} \\ z_9 \end{pmatrix} \mathbf{a}_3 &= ax_9 \hat{\mathbf{x}} - by_9 \hat{\mathbf{y}} + c \begin{pmatrix} z_9 + \frac{1}{2} \\ z_9 \end{pmatrix} \hat{\mathbf{z}} &(8d) &\text{O VI} \\
\mathbf{B}_{68} &= -\begin{pmatrix} x_9 - \frac{1}{2} \\ z_9 \end{pmatrix} \mathbf{a}_1 + \begin{pmatrix} y_9 + \frac{1}{2} \\ z_9 \end{pmatrix} \mathbf{a}_2 + &= -a \begin{pmatrix} x_9 - \frac{1}{2} \\ z_9 \end{pmatrix} \hat{\mathbf{x}} + b \begin{pmatrix} y_9 + \frac{1}{2} \\ z_9 \end{pmatrix} \hat{\mathbf{y}} + cz_9 \hat{\mathbf{z}} &(8d) &\text{O VI}
\end{aligned}$$

References

- [1] K.-A. Wilhelmi, *The Crystal Structure of Cr_5O_{12}* , Acta Chem. Scand. **19**, 165–176 (1965), doi:10.3891/acta.chem.scand.19-0165.

First cited in

D. Hicks, M. J. Mehl, M. Esters, C. Oses, O. Levy, G. L. W. Hart, C. Toher, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 3*, Comput. Mater. Sci. **199**, 110450 (2021), doi: 10.1016/j.commatsci.2021.110450.