

C₃Cr₇ (*D*10₁) Structure: A3B7_oP40_62_cd_3c2d-001

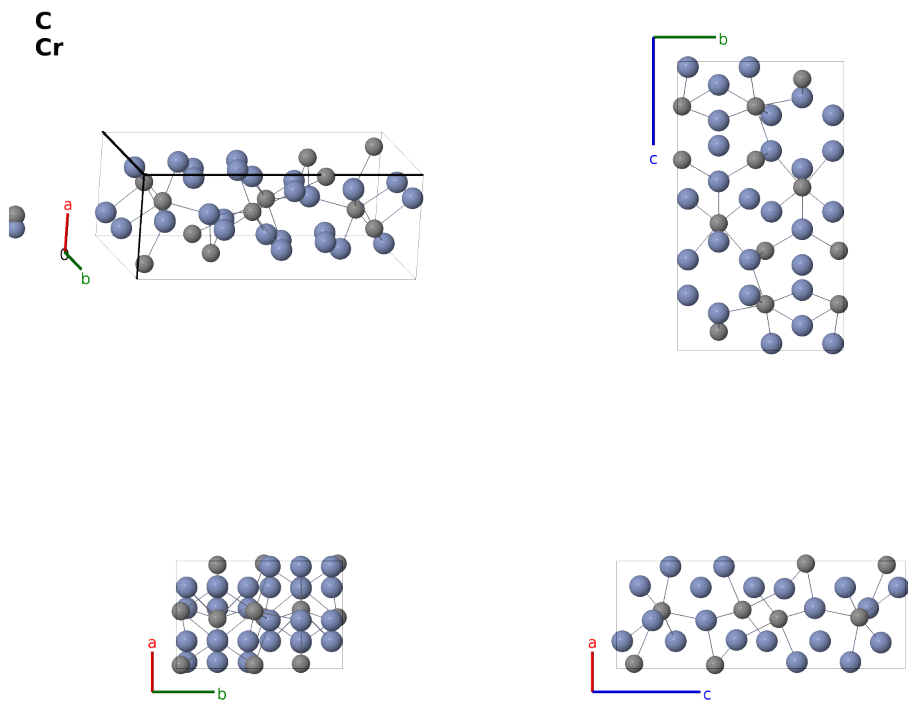
This structure previously used the label(s) A3B7_oP40_62_cd_3c2d. Calls to these addresses will be redirected here.

Cite this page as:

- H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettel, 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/9Z5M>

https://aflow.org/prototype-encyclopedia/A3B7_oP40_62_cd_3c2d-001



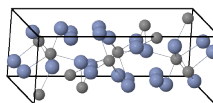
Prototype	C ₃ Cr ₇
AFLOW prototype label	A3B7_oP40_62_cd_3c2d-001
<i>Strukturbericht</i> designation	<i>D</i> 10 ₁
ICSD	76799
CCDC	1637324
Pearson symbol	oP40
Space group number	62
Space group symbol	<i>Pnma</i>

AFLOW prototype command `aflow --proto=A3B7_oP40_62_cd_3c2d-001`
 `--params=a,b/a,c/a,x1,z1,x2,z2,x3,z3,x4,z4,x5,y5,z5,x6,y6,z6,x7,y7,z7`

Other compounds with this structure

 $\text{C}_3\text{Fe}_7, \text{C}_3\text{Mn}_7$

Simple Orthorhombic primitive vectors



$$\mathbf{a}_1 = a \hat{\mathbf{x}}$$

$$\mathbf{a}_2 = b \hat{\mathbf{y}}$$

$$\mathbf{a}_3 = c \hat{\mathbf{z}}$$

Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= x_1 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_1 \mathbf{a}_3$	$=$	$ax_1 \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} + cz_1 \hat{\mathbf{z}}$	(4c)	C I
$\mathbf{B}_2$	$= -\left(x_1 - \frac{1}{2}\right) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 +$ $\left(z_1 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a\left(x_1 - \frac{1}{2}\right) \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} + c\left(z_1 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(4c)	C I
$\mathbf{B}_3$	$= -x_1 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_1 \mathbf{a}_3$	$=$	$-ax_1 \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} - cz_1 \hat{\mathbf{z}}$	(4c)	C I
$\mathbf{B}_4$	$= \left(x_1 + \frac{1}{2}\right) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 - \left(z_1 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$a\left(x_1 + \frac{1}{2}\right) \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} - c\left(z_1 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(4c)	C I
$\mathbf{B}_5$	$= x_2 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$ax_2 \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$	(4c)	Cr I
$\mathbf{B}_6$	$= -\left(x_2 - \frac{1}{2}\right) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 +$ $\left(z_2 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a\left(x_2 - \frac{1}{2}\right) \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} + c\left(z_2 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(4c)	Cr I
$\mathbf{B}_7$	$= -x_2 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_2 \mathbf{a}_3$	$=$	$-ax_2 \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} - cz_2 \hat{\mathbf{z}}$	(4c)	Cr I
$\mathbf{B}_8$	$= \left(x_2 + \frac{1}{2}\right) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 - \left(z_2 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$a\left(x_2 + \frac{1}{2}\right) \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} - c\left(z_2 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(4c)	Cr I
$\mathbf{B}_9$	$= x_3 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$ax_3 \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(4c)	Cr II
$\mathbf{B}_{10}$	$= -\left(x_3 - \frac{1}{2}\right) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 +$ $\left(z_3 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a\left(x_3 - \frac{1}{2}\right) \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} + c\left(z_3 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(4c)	Cr II
$\mathbf{B}_{11}$	$= -x_3 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$-ax_3 \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} - cz_3 \hat{\mathbf{z}}$	(4c)	Cr II
$\mathbf{B}_{12}$	$= \left(x_3 + \frac{1}{2}\right) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 - \left(z_3 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$a\left(x_3 + \frac{1}{2}\right) \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} - c\left(z_3 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(4c)	Cr II
$\mathbf{B}_{13}$	$= x_4 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$ax_4 \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(4c)	Cr III
$\mathbf{B}_{14}$	$= -\left(x_4 - \frac{1}{2}\right) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 +$ $\left(z_4 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a\left(x_4 - \frac{1}{2}\right) \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} + c\left(z_4 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(4c)	Cr III
$\mathbf{B}_{15}$	$= -x_4 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$-ax_4 \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}}$	(4c)	Cr III
$\mathbf{B}_{16}$	$= \left(x_4 + \frac{1}{2}\right) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 - \left(z_4 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$a\left(x_4 + \frac{1}{2}\right) \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} - c\left(z_4 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(4c)	Cr III
$\mathbf{B}_{17}$	$= x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$ax_5 \hat{\mathbf{x}} + by_5 \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(8d)	C II
$\mathbf{B}_{18}$	$= -\left(x_5 - \frac{1}{2}\right) \mathbf{a}_1 - y_5 \mathbf{a}_2 +$ $\left(z_5 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a\left(x_5 - \frac{1}{2}\right) \hat{\mathbf{x}} - by_5 \hat{\mathbf{y}} + c\left(z_5 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(8d)	C II
$\mathbf{B}_{19}$	$= -x_5 \mathbf{a}_1 + \left(y_5 + \frac{1}{2}\right) \mathbf{a}_2 - z_5 \mathbf{a}_3$	$=$	$-ax_5 \hat{\mathbf{x}} + b\left(y_5 + \frac{1}{2}\right) \hat{\mathbf{y}} - cz_5 \hat{\mathbf{z}}$	(8d)	C II

$$\begin{aligned}
\mathbf{B}_{20} &= \begin{pmatrix} x_5 + \frac{1}{2} \\ z_5 - \frac{1}{2} \end{pmatrix} \mathbf{a}_1 - \begin{pmatrix} y_5 - \frac{1}{2} \\ z_5 - \frac{1}{2} \end{pmatrix} \mathbf{a}_2 - \mathbf{a}_3 &= a \begin{pmatrix} x_5 + \frac{1}{2} \\ z_5 - \frac{1}{2} \end{pmatrix} \hat{\mathbf{x}} - b \begin{pmatrix} y_5 - \frac{1}{2} \\ z_5 - \frac{1}{2} \end{pmatrix} \hat{\mathbf{y}} - c \begin{pmatrix} z_5 - \frac{1}{2} \\ z_5 - \frac{1}{2} \end{pmatrix} \hat{\mathbf{z}} &(8d) & \text{C II} \\
\mathbf{B}_{21} &= -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) & \text{C II} \\
\mathbf{B}_{22} &= \begin{pmatrix} x_5 + \frac{1}{2} \\ z_5 - \frac{1}{2} \end{pmatrix} \mathbf{a}_1 + y_5 \mathbf{a}_2 - \begin{pmatrix} z_5 - \frac{1}{2} \\ z_5 - \frac{1}{2} \end{pmatrix} \mathbf{a}_3 &= a \begin{pmatrix} x_5 + \frac{1}{2} \\ z_5 - \frac{1}{2} \end{pmatrix} \hat{\mathbf{x}} + by_5 \hat{\mathbf{y}} - c \begin{pmatrix} z_5 - \frac{1}{2} \\ z_5 - \frac{1}{2} \end{pmatrix} \hat{\mathbf{z}} &(8d) & \text{C II} \\
\mathbf{B}_{23} &= x_5 \mathbf{a}_1 - \begin{pmatrix} y_5 - \frac{1}{2} \\ z_5 - \frac{1}{2} \end{pmatrix} \mathbf{a}_2 + z_5 \mathbf{a}_3 &= ax_5 \hat{\mathbf{x}} - b \begin{pmatrix} y_5 - \frac{1}{2} \\ z_5 - \frac{1}{2} \end{pmatrix} \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}} &(8d) & \text{C II} \\
\mathbf{B}_{24} &= -\begin{pmatrix} x_5 - \frac{1}{2} \\ z_5 + \frac{1}{2} \end{pmatrix} \mathbf{a}_1 + \begin{pmatrix} y_5 + \frac{1}{2} \\ z_5 + \frac{1}{2} \end{pmatrix} \mathbf{a}_2 + \mathbf{a}_3 &= -a \begin{pmatrix} x_5 - \frac{1}{2} \\ z_5 + \frac{1}{2} \end{pmatrix} \hat{\mathbf{x}} + b \begin{pmatrix} y_5 + \frac{1}{2} \\ z_5 + \frac{1}{2} \end{pmatrix} \hat{\mathbf{y}} + c \begin{pmatrix} z_5 + \frac{1}{2} \\ z_5 + \frac{1}{2} \end{pmatrix} \hat{\mathbf{z}} &(8d) & \text{C II} \\
\mathbf{B}_{25} &= 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) & \text{Cr IV} \\
\mathbf{B}_{26} &= -\begin{pmatrix} x_6 - \frac{1}{2} \\ z_6 + \frac{1}{2} \end{pmatrix} \mathbf{a}_1 - y_6 \mathbf{a}_2 + \mathbf{a}_3 &= -a \begin{pmatrix} x_6 - \frac{1}{2} \\ z_6 + \frac{1}{2} \end{pmatrix} \hat{\mathbf{x}} - by_6 \hat{\mathbf{y}} + c \begin{pmatrix} z_6 + \frac{1}{2} \\ z_6 + \frac{1}{2} \end{pmatrix} \hat{\mathbf{z}} &(8d) & \text{Cr IV} \\
\mathbf{B}_{27} &= -x_6 \mathbf{a}_1 + \begin{pmatrix} y_6 + \frac{1}{2} \\ z_6 - \frac{1}{2} \end{pmatrix} \mathbf{a}_2 - z_6 \mathbf{a}_3 &= -ax_6 \hat{\mathbf{x}} + b \begin{pmatrix} y_6 + \frac{1}{2} \\ z_6 - \frac{1}{2} \end{pmatrix} \hat{\mathbf{y}} - cz_6 \hat{\mathbf{z}} &(8d) & \text{Cr IV} \\
\mathbf{B}_{28} &= \begin{pmatrix} x_6 + \frac{1}{2} \\ z_6 - \frac{1}{2} \end{pmatrix} \mathbf{a}_1 - \begin{pmatrix} y_6 - \frac{1}{2} \\ z_6 - \frac{1}{2} \end{pmatrix} \mathbf{a}_2 - \mathbf{a}_3 &= a \begin{pmatrix} x_6 + \frac{1}{2} \\ z_6 - \frac{1}{2} \end{pmatrix} \hat{\mathbf{x}} - b \begin{pmatrix} y_6 - \frac{1}{2} \\ z_6 - \frac{1}{2} \end{pmatrix} \hat{\mathbf{y}} - c \begin{pmatrix} z_6 - \frac{1}{2} \\ z_6 - \frac{1}{2} \end{pmatrix} \hat{\mathbf{z}} &(8d) & \text{Cr IV} \\
\mathbf{B}_{29} &= -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) & \text{Cr IV} \\
\mathbf{B}_{30} &= \begin{pmatrix} x_6 + \frac{1}{2} \\ z_6 - \frac{1}{2} \end{pmatrix} \mathbf{a}_1 + y_6 \mathbf{a}_2 - \begin{pmatrix} z_6 - \frac{1}{2} \\ z_6 - \frac{1}{2} \end{pmatrix} \mathbf{a}_3 &= a \begin{pmatrix} x_6 + \frac{1}{2} \\ z_6 - \frac{1}{2} \end{pmatrix} \hat{\mathbf{x}} + by_6 \hat{\mathbf{y}} - c \begin{pmatrix} z_6 - \frac{1}{2} \\ z_6 - \frac{1}{2} \end{pmatrix} \hat{\mathbf{z}} &(8d) & \text{Cr IV} \\
\mathbf{B}_{31} &= x_6 \mathbf{a}_1 - \begin{pmatrix} y_6 - \frac{1}{2} \\ z_6 - \frac{1}{2} \end{pmatrix} \mathbf{a}_2 + z_6 \mathbf{a}_3 &= ax_6 \hat{\mathbf{x}} - b \begin{pmatrix} y_6 - \frac{1}{2} \\ z_6 - \frac{1}{2} \end{pmatrix} \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}} &(8d) & \text{Cr IV} \\
\mathbf{B}_{32} &= -\begin{pmatrix} x_6 - \frac{1}{2} \\ z_6 + \frac{1}{2} \end{pmatrix} \mathbf{a}_1 + \begin{pmatrix} y_6 + \frac{1}{2} \\ z_6 + \frac{1}{2} \end{pmatrix} \mathbf{a}_2 + \mathbf{a}_3 &= -a \begin{pmatrix} x_6 - \frac{1}{2} \\ z_6 + \frac{1}{2} \end{pmatrix} \hat{\mathbf{x}} + b \begin{pmatrix} y_6 + \frac{1}{2} \\ z_6 + \frac{1}{2} \end{pmatrix} \hat{\mathbf{y}} + c \begin{pmatrix} z_6 + \frac{1}{2} \\ z_6 + \frac{1}{2} \end{pmatrix} \hat{\mathbf{z}} &(8d) & \text{Cr IV} \\
\mathbf{B}_{33} &= 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) & \text{Cr V} \\
\mathbf{B}_{34} &= -\begin{pmatrix} x_7 - \frac{1}{2} \\ z_7 + \frac{1}{2} \end{pmatrix} \mathbf{a}_1 - y_7 \mathbf{a}_2 + \mathbf{a}_3 &= -a \begin{pmatrix} x_7 - \frac{1}{2} \\ z_7 + \frac{1}{2} \end{pmatrix} \hat{\mathbf{x}} - by_7 \hat{\mathbf{y}} + c \begin{pmatrix} z_7 + \frac{1}{2} \\ z_7 + \frac{1}{2} \end{pmatrix} \hat{\mathbf{z}} &(8d) & \text{Cr V} \\
\mathbf{B}_{35} &= -x_7 \mathbf{a}_1 + \begin{pmatrix} y_7 + \frac{1}{2} \\ z_7 - \frac{1}{2} \end{pmatrix} \mathbf{a}_2 - z_7 \mathbf{a}_3 &= -ax_7 \hat{\mathbf{x}} + b \begin{pmatrix} y_7 + \frac{1}{2} \\ z_7 - \frac{1}{2} \end{pmatrix} \hat{\mathbf{y}} - cz_7 \hat{\mathbf{z}} &(8d) & \text{Cr V} \\
\mathbf{B}_{36} &= \begin{pmatrix} x_7 + \frac{1}{2} \\ z_7 - \frac{1}{2} \end{pmatrix} \mathbf{a}_1 - \begin{pmatrix} y_7 - \frac{1}{2} \\ z_7 - \frac{1}{2} \end{pmatrix} \mathbf{a}_2 - \mathbf{a}_3 &= a \begin{pmatrix} x_7 + \frac{1}{2} \\ z_7 - \frac{1}{2} \end{pmatrix} \hat{\mathbf{x}} - b \begin{pmatrix} y_7 - \frac{1}{2} \\ z_7 - \frac{1}{2} \end{pmatrix} \hat{\mathbf{y}} - c \begin{pmatrix} z_7 - \frac{1}{2} \\ z_7 - \frac{1}{2} \end{pmatrix} \hat{\mathbf{z}} &(8d) & \text{Cr V} \\
\mathbf{B}_{37} &= -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) & \text{Cr V} \\
\mathbf{B}_{38} &= \begin{pmatrix} x_7 + \frac{1}{2} \\ z_7 - \frac{1}{2} \end{pmatrix} \mathbf{a}_1 + y_7 \mathbf{a}_2 - \begin{pmatrix} z_7 - \frac{1}{2} \\ z_7 - \frac{1}{2} \end{pmatrix} \mathbf{a}_3 &= a \begin{pmatrix} x_7 + \frac{1}{2} \\ z_7 - \frac{1}{2} \end{pmatrix} \hat{\mathbf{x}} + by_7 \hat{\mathbf{y}} - c \begin{pmatrix} z_7 - \frac{1}{2} \\ z_7 - \frac{1}{2} \end{pmatrix} \hat{\mathbf{z}} &(8d) & \text{Cr V} \\
\mathbf{B}_{39} &= x_7 \mathbf{a}_1 - \begin{pmatrix} y_7 - \frac{1}{2} \\ z_7 - \frac{1}{2} \end{pmatrix} \mathbf{a}_2 + z_7 \mathbf{a}_3 &= ax_7 \hat{\mathbf{x}} - b \begin{pmatrix} y_7 - \frac{1}{2} \\ z_7 - \frac{1}{2} \end{pmatrix} \hat{\mathbf{y}} + cz_7 \hat{\mathbf{z}} &(8d) & \text{Cr V} \\
\mathbf{B}_{40} &= -\begin{pmatrix} x_7 - \frac{1}{2} \\ z_7 + \frac{1}{2} \end{pmatrix} \mathbf{a}_1 + \begin{pmatrix} y_7 + \frac{1}{2} \\ z_7 + \frac{1}{2} \end{pmatrix} \mathbf{a}_2 + \mathbf{a}_3 &= -a \begin{pmatrix} x_7 - \frac{1}{2} \\ z_7 + \frac{1}{2} \end{pmatrix} \hat{\mathbf{x}} + b \begin{pmatrix} y_7 + \frac{1}{2} \\ z_7 + \frac{1}{2} \end{pmatrix} \hat{\mathbf{y}} + c \begin{pmatrix} z_7 + \frac{1}{2} \\ z_7 + \frac{1}{2} \end{pmatrix} \hat{\mathbf{z}} &(8d) & \text{Cr V}
\end{aligned}$$

References

- [1] M. A. Rouault, P. Herpin, and M. R. Fruchart, *Etude Cristallographique des Carbures Cr_7C_3 et Mn_7C_3* , Annales de Chimie (Paris) **5**, 461–470 (1970).

Found in

- [1] P. Villars and L. Calvert, *Pearson's Handbook of Crystallographic Data for Intermetallic Phases* (ASM International, Materials Park, OH, 1991), 2nd edn.

First cited in

M. J. Mehl, D. Hicks, C. Toher, O. Levy, R. M. Hanson, G. L. W. Hart, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 1*, Comput. Mater. Sci. **136**, S1-828 (2017). doi: 10.1016/j.commatsci.2017.01.017