

Cr₅Al₈ (*D*8₁₀) Structure: A8B5_hR26_160_a3bc_a3b-001

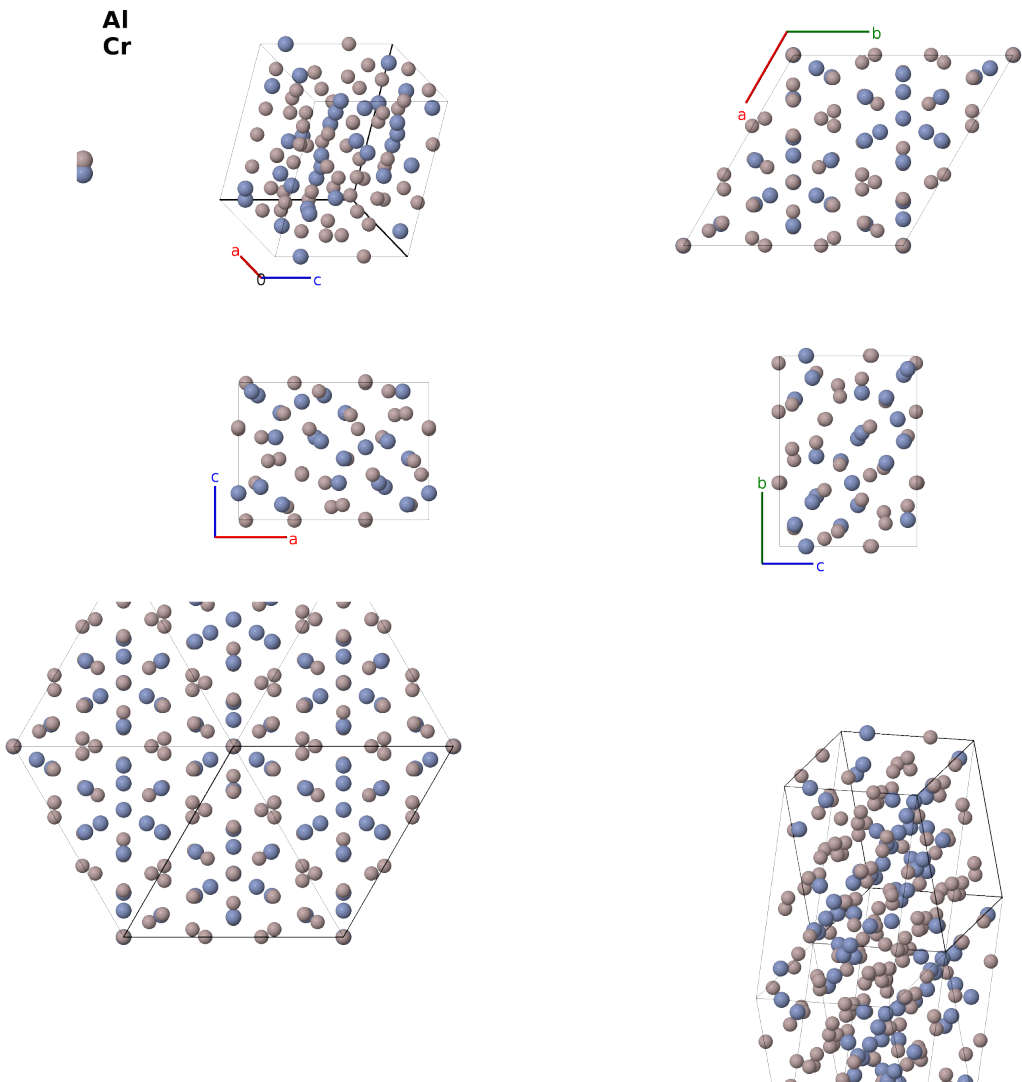
This structure previously used the label(s) A8B5_hR26_160_a3bc_a3b. Calls to these addresses will be redirected here.

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- 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/X9QA>

https://aflow.org/prototype-encyclopedia/A8B5_hR26_160_a3bc_a3b-001



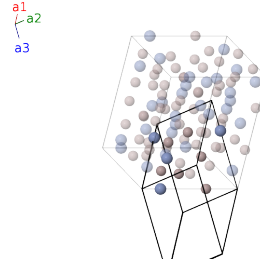
Prototype	Al ₈ Cr ₅
AFLOW prototype label	A8B5_hR26_160_a3bc_a3b-001
Strukturbericht designation	D8 ₁₀
ICSD	606753

CCDC	1742187
Pearson symbol	hR26
Space group number	160
Space group symbol	$R\bar{3}m$
AFLOW prototype command	aflow --proto=A8B5_hR26_160_a3bc_a3b-001 --params= $a, c/a, x_1, x_2, x_3, z_3, x_4, z_4, x_5, z_5, x_6, z_6, x_7, z_7, x_8, z_8, x_9, y_9, z_9$

- (Bradley, 1937) notes that the positions here are very close to the positions of the atoms in the γ -brass (Cu_5Zn_8 , $D8_2$) structure.
- (Mizutani, 2010) classifies this as an “R-cell” γ -brass.

Rhombohedral primitive vectors

$$\begin{aligned}
\mathbf{a}_1 &= \frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + \frac{1}{3}c \hat{\mathbf{z}} \\
\mathbf{a}_2 &= \frac{1}{\sqrt{3}}a \hat{\mathbf{y}} + \frac{1}{3}c \hat{\mathbf{z}} \\
\mathbf{a}_3 &= -\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + \frac{1}{3}c \hat{\mathbf{z}}
\end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= x_1 \mathbf{a}_1 + x_1 \mathbf{a}_2 + x_1 \mathbf{a}_3$	$=$	$cx_1 \hat{\mathbf{z}}$	(1a)	Al I
$\mathbf{B}_2$	$= x_2 \mathbf{a}_1 + x_2 \mathbf{a}_2 + x_2 \mathbf{a}_3$	$=$	$cx_2 \hat{\mathbf{z}}$	(1a)	Cr I
$\mathbf{B}_3$	$= x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + x_3 \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_3 - z_3) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(x_3 - z_3) \hat{\mathbf{y}} + \frac{1}{3}c(2x_3 + z_3) \hat{\mathbf{z}}$	(3b)	Al II
$\mathbf{B}_4$	$= z_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + x_3 \mathbf{a}_3$	$=$	$-\frac{1}{2}a(x_3 - z_3) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(x_3 - z_3) \hat{\mathbf{y}} + \frac{1}{3}c(2x_3 + z_3) \hat{\mathbf{z}}$	(3b)	Al II
$\mathbf{B}_5$	$= x_3 \mathbf{a}_1 + z_3 \mathbf{a}_2 + x_3 \mathbf{a}_3$	$=$	$-\frac{1}{\sqrt{3}}a(x_3 - z_3) \hat{\mathbf{y}} + \frac{1}{3}c(2x_3 + z_3) \hat{\mathbf{z}}$	(3b)	Al II
$\mathbf{B}_6$	$= x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_4 - z_4) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(x_4 - z_4) \hat{\mathbf{y}} + \frac{1}{3}c(2x_4 + z_4) \hat{\mathbf{z}}$	(3b)	Al III
$\mathbf{B}_7$	$= z_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + x_4 \mathbf{a}_3$	$=$	$-\frac{1}{2}a(x_4 - z_4) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(x_4 - z_4) \hat{\mathbf{y}} + \frac{1}{3}c(2x_4 + z_4) \hat{\mathbf{z}}$	(3b)	Al III
$\mathbf{B}_8$	$= x_4 \mathbf{a}_1 + z_4 \mathbf{a}_2 + x_4 \mathbf{a}_3$	$=$	$-\frac{1}{\sqrt{3}}a(x_4 - z_4) \hat{\mathbf{y}} + \frac{1}{3}c(2x_4 + z_4) \hat{\mathbf{z}}$	(3b)	Al III
$\mathbf{B}_9$	$= x_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_5 - z_5) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(x_5 - z_5) \hat{\mathbf{y}} + \frac{1}{3}c(2x_5 + z_5) \hat{\mathbf{z}}$	(3b)	Al IV
$\mathbf{B}_{10}$	$= z_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 + x_5 \mathbf{a}_3$	$=$	$-\frac{1}{2}a(x_5 - z_5) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(x_5 - z_5) \hat{\mathbf{y}} + \frac{1}{3}c(2x_5 + z_5) \hat{\mathbf{z}}$	(3b)	Al IV
$\mathbf{B}_{11}$	$= x_5 \mathbf{a}_1 + z_5 \mathbf{a}_2 + x_5 \mathbf{a}_3$	$=$	$-\frac{1}{\sqrt{3}}a(x_5 - z_5) \hat{\mathbf{y}} + \frac{1}{3}c(2x_5 + z_5) \hat{\mathbf{z}}$	(3b)	Al IV
$\mathbf{B}_{12}$	$= x_6 \mathbf{a}_1 + x_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_6 - z_6) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(x_6 - z_6) \hat{\mathbf{y}} + \frac{1}{3}c(2x_6 + z_6) \hat{\mathbf{z}}$	(3b)	Cr II
$\mathbf{B}_{13}$	$= z_6 \mathbf{a}_1 + x_6 \mathbf{a}_2 + x_6 \mathbf{a}_3$	$=$	$-\frac{1}{2}a(x_6 - z_6) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(x_6 - z_6) \hat{\mathbf{y}} + \frac{1}{3}c(2x_6 + z_6) \hat{\mathbf{z}}$	(3b)	Cr II

$\mathbf{B}_{14}$	$=$	$x_6 \mathbf{a}_1 + z_6 \mathbf{a}_2 + x_6 \mathbf{a}_3$	$=$	$-\frac{1}{\sqrt{3}}a(x_6 - z_6) \hat{\mathbf{y}} + \frac{1}{3}c(2x_6 + z_6) \hat{\mathbf{z}}$	(3b)	Cr II
$\mathbf{B}_{15}$	$=$	$x_7 \mathbf{a}_1 + x_7 \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_7 - z_7) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(x_7 - z_7) \hat{\mathbf{y}} + \frac{1}{3}c(2x_7 + z_7) \hat{\mathbf{z}}$	(3b)	Cr III
$\mathbf{B}_{16}$	$=$	$z_7 \mathbf{a}_1 + x_7 \mathbf{a}_2 + x_7 \mathbf{a}_3$	$=$	$-\frac{1}{2}a(x_7 - z_7) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(x_7 - z_7) \hat{\mathbf{y}} + \frac{1}{3}c(2x_7 + z_7) \hat{\mathbf{z}}$	(3b)	Cr III
$\mathbf{B}_{17}$	$=$	$x_7 \mathbf{a}_1 + z_7 \mathbf{a}_2 + x_7 \mathbf{a}_3$	$=$	$-\frac{1}{\sqrt{3}}a(x_7 - z_7) \hat{\mathbf{y}} + \frac{1}{3}c(2x_7 + z_7) \hat{\mathbf{z}}$	(3b)	Cr III
$\mathbf{B}_{18}$	$=$	$x_8 \mathbf{a}_1 + x_8 \mathbf{a}_2 + z_8 \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_8 - z_8) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(x_8 - z_8) \hat{\mathbf{y}} + \frac{1}{3}c(2x_8 + z_8) \hat{\mathbf{z}}$	(3b)	Cr IV
$\mathbf{B}_{19}$	$=$	$z_8 \mathbf{a}_1 + x_8 \mathbf{a}_2 + x_8 \mathbf{a}_3$	$=$	$-\frac{1}{2}a(x_8 - z_8) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(x_8 - z_8) \hat{\mathbf{y}} + \frac{1}{3}c(2x_8 + z_8) \hat{\mathbf{z}}$	(3b)	Cr IV
$\mathbf{B}_{20}$	$=$	$x_8 \mathbf{a}_1 + z_8 \mathbf{a}_2 + x_8 \mathbf{a}_3$	$=$	$-\frac{1}{\sqrt{3}}a(x_8 - z_8) \hat{\mathbf{y}} + \frac{1}{3}c(2x_8 + z_8) \hat{\mathbf{z}}$	(3b)	Cr IV
$\mathbf{B}_{21}$	$=$	$x_9 \mathbf{a}_1 + y_9 \mathbf{a}_2 + z_9 \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_9 - z_9) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_9 - 2y_9 + z_9) \hat{\mathbf{y}} + \frac{1}{3}c(x_9 + y_9 + z_9) \hat{\mathbf{z}}$	(6c)	Al V
$\mathbf{B}_{22}$	$=$	$z_9 \mathbf{a}_1 + x_9 \mathbf{a}_2 + y_9 \mathbf{a}_3$	$=$	$-\frac{1}{2}a(y_9 - z_9) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(2x_9 - y_9 - z_9) \hat{\mathbf{y}} + \frac{1}{3}c(x_9 + y_9 + z_9) \hat{\mathbf{z}}$	(6c)	Al V
$\mathbf{B}_{23}$	$=$	$y_9 \mathbf{a}_1 + z_9 \mathbf{a}_2 + x_9 \mathbf{a}_3$	$=$	$-\frac{1}{2}a(x_9 - y_9) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_9 + y_9 - 2z_9) \hat{\mathbf{y}} + \frac{1}{3}c(x_9 + y_9 + z_9) \hat{\mathbf{z}}$	(6c)	Al V
$\mathbf{B}_{24}$	$=$	$z_9 \mathbf{a}_1 + y_9 \mathbf{a}_2 + x_9 \mathbf{a}_3$	$=$	$-\frac{1}{2}a(x_9 - z_9) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_9 - 2y_9 + z_9) \hat{\mathbf{y}} + \frac{1}{3}c(x_9 + y_9 + z_9) \hat{\mathbf{z}}$	(6c)	Al V
$\mathbf{B}_{25}$	$=$	$y_9 \mathbf{a}_1 + x_9 \mathbf{a}_2 + z_9 \mathbf{a}_3$	$=$	$\frac{1}{2}a(y_9 - z_9) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(2x_9 - y_9 - z_9) \hat{\mathbf{y}} + \frac{1}{3}c(x_9 + y_9 + z_9) \hat{\mathbf{z}}$	(6c)	Al V
$\mathbf{B}_{26}$	$=$	$x_9 \mathbf{a}_1 + z_9 \mathbf{a}_2 + y_9 \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_9 - y_9) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_9 + y_9 - 2z_9) \hat{\mathbf{y}} + \frac{1}{3}c(x_9 + y_9 + z_9) \hat{\mathbf{z}}$	(6c)	Al V

References

- [1] A. J. Bradley and S. S. Lu, *The Crystal Structures of Cr_2Al and Cr_5Al_8* , Z. Kristallgr. **96**, 20–37 (1937), doi:10.1524/zkri.1937.96.1.20.
- [2] U. Mizutani, *Hume-Rothery Rules for Structurally Complex Alloy Phases* (CRC Press, Boca Raton, London, New York, 2010).

Found in

- [1] S. Grazulis, *Crystal Data* (2014). Crystallography-online.com.

First cited in

D. Hicks, M. J. Mehl, E. Gossett, C. Toher, O. Levy, R. M. Hanson, G. Hart, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 2*, Comput. Mater. Sci. **161**, S1 (2019). doi: 10.1016/j.commatsci.2018.10.043