

CrB₄ Structure:

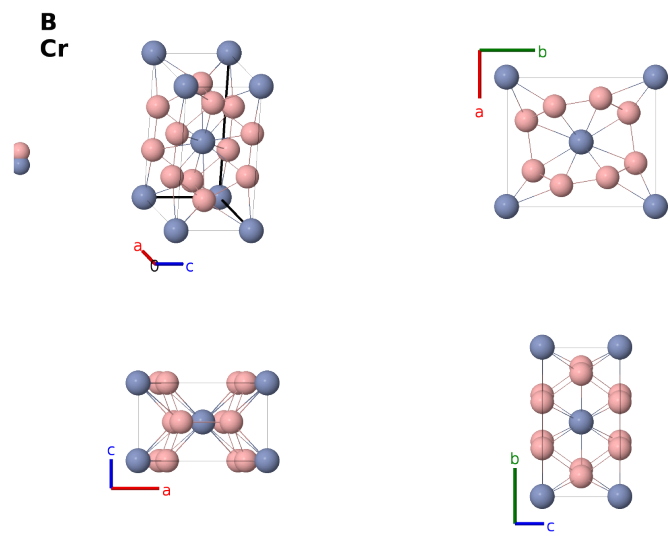
A4B_oP10_58_2g_a-001

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<https://aflow.org/prototype-encyclopedia/F5HF>

https://aflow.org/prototype-encyclopedia/A4B_oP10_58_2g_a-001



Prototype	B ₄ Cr
AFLOW prototype label	A4B_oP10_58_2g_a-001
ICSD	144116
CCDC	2199348
Pearson symbol	oP10
Space group number	58
Space group symbol	<i>Pnnm</i>
AFLOW prototype command	<code>aflow --proto=A4B_oP10_58_2g_a-001</code> <code>--params=a, b/a, c/a, x₂, y₂, x₃, y₃</code>

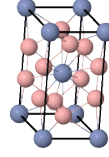
Other compounds with this structure

FeB₄, MnB₄

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
$\mathbf{B}_1$	=	0	=	0	(2a) Cr I
$\mathbf{B}_2$	=	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	=	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} b \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(2a) Cr I
$\mathbf{B}_3$	=	$x_2 \mathbf{a}_1 + y_2 \mathbf{a}_2$	=	$ax_2 \hat{\mathbf{x}} + by_2 \hat{\mathbf{y}}$	(4g) B I
$\mathbf{B}_4$	=	$-x_2 \mathbf{a}_1 - y_2 \mathbf{a}_2$	=	$-ax_2 \hat{\mathbf{x}} - by_2 \hat{\mathbf{y}}$	(4g) B I
$\mathbf{B}_5$	=	$-(x_2 - \frac{1}{2}) \mathbf{a}_1 + (y_2 + \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	=	$-a(x_2 - \frac{1}{2}) \hat{\mathbf{x}} + b(y_2 + \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4g) B I
$\mathbf{B}_6$	=	$(x_2 + \frac{1}{2}) \mathbf{a}_1 - (y_2 - \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	=	$a(x_2 + \frac{1}{2}) \hat{\mathbf{x}} - b(y_2 - \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4g) B I
$\mathbf{B}_7$	=	$x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2$	=	$ax_3 \hat{\mathbf{x}} + by_3 \hat{\mathbf{y}}$	(4g) B II
$\mathbf{B}_8$	=	$-x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2$	=	$-ax_3 \hat{\mathbf{x}} - by_3 \hat{\mathbf{y}}$	(4g) B II
$\mathbf{B}_9$	=	$-(x_3 - \frac{1}{2}) \mathbf{a}_1 + (y_3 + \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	=	$-a(x_3 - \frac{1}{2}) \hat{\mathbf{x}} + b(y_3 + \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4g) B II
$\mathbf{B}_{10}$	=	$(x_3 + \frac{1}{2}) \mathbf{a}_1 - (y_3 - \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	=	$a(x_3 + \frac{1}{2}) \hat{\mathbf{x}} - b(y_3 - \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4g) B II

References

- [1] H. Niu, J. Wang, X.-Q. Chen, D. Li, Y. Li, P. Lazar, R. Podloucky, and A. N. Kolmogorov, *Structure, bonding, and possible superhardness of CrB₄*, Phys. Rev. B **85**, 144116 (2012), doi:10.1103/PhysRevB.85.144116.

Found in

- [1] *AFLOW Database*. CrB₄, ICSD entry 186851.

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