

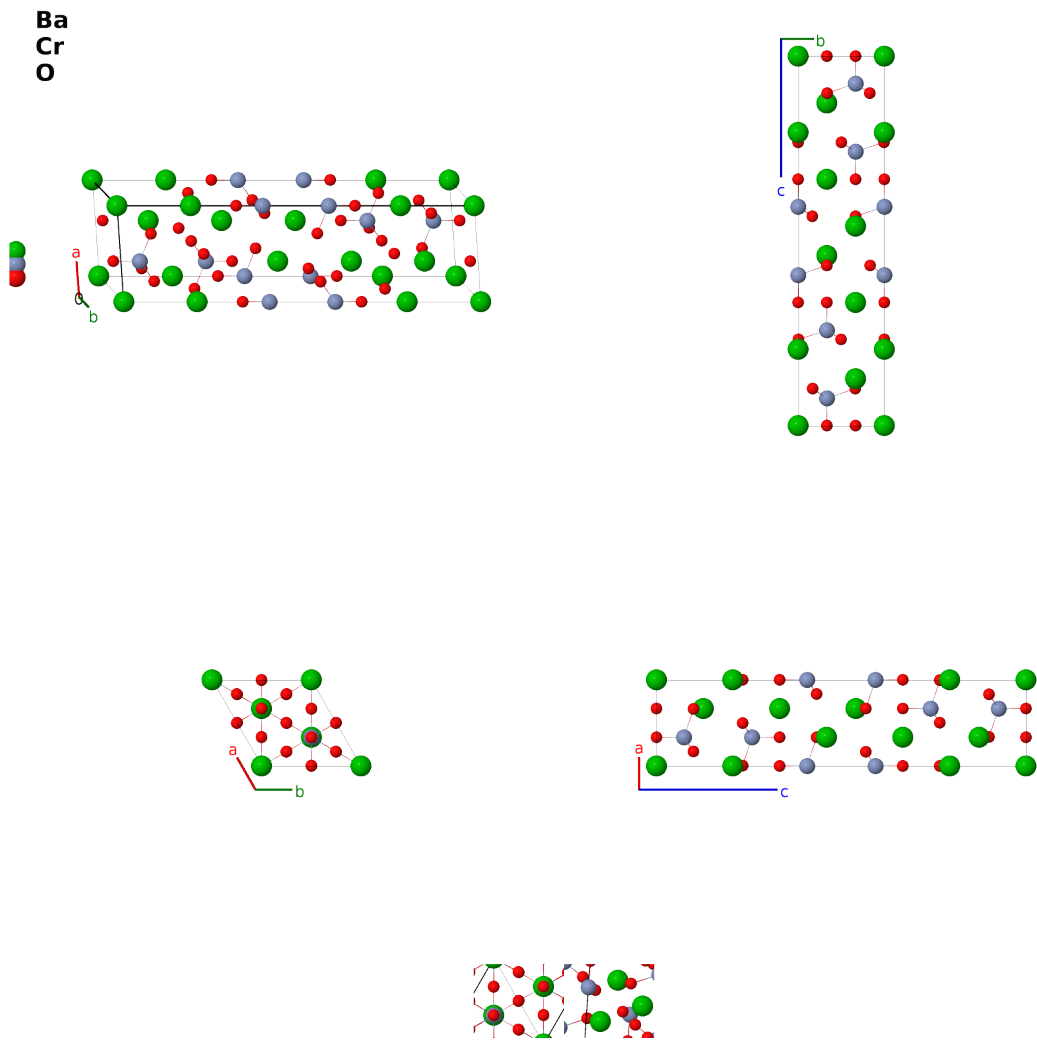
Ba₃Cr₂O₈ Structure: A3B2C8_hR13_166_ac_c_ch-002

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<https://aflow.org/prototype-encyclopedia/7UDV>

https://aflow.org/prototype-encyclopedia/A3B2C8_hR13_166_ac_c_ch-002



Prototype	Ba ₃ Cr ₂ O ₈
AFLOW prototype label	A3B2C8_hR13_166_ac_c_ch-002
ICSD	159409
CCDC	1675881
Pearson symbol	hR13
Space group number	166

Space group symbol $R\bar{3}m$

AFLOW prototype command `aflow --proto=A3B2C8_hR13_166_ac_c_ch-002`
`--params=a, c/a, x2, x3, x4, x5, z5`

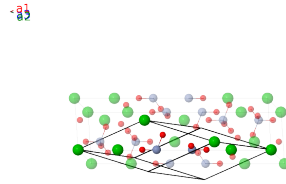
Other compounds with this structure

Sr₃Cr₂O₈

- This is the ternary version of the $D8_5$ (Fe₇W₆) structure. The structure given by (Nakajima, 2008) does not appear in the ICSD. We give the ICSD entry for the structure determined by (Aczel, 2008).
- Hexagonal settings of this structure can be obtained with the option `--hex`.

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
$\mathbf{B}_1$	0	$=$	0	(1a)	Ba I
$\mathbf{B}_2$	$x_2 \mathbf{a}_1 + x_2 \mathbf{a}_2 + x_2 \mathbf{a}_3$	$=$	$cx_2 \hat{\mathbf{z}}$	(2c)	Ba II
$\mathbf{B}_3$	$-x_2 \mathbf{a}_1 - x_2 \mathbf{a}_2 - x_2 \mathbf{a}_3$	$=$	$-cx_2 \hat{\mathbf{z}}$	(2c)	Ba II
$\mathbf{B}_4$	$x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + x_3 \mathbf{a}_3$	$=$	$cx_3 \hat{\mathbf{z}}$	(2c)	Cr I
$\mathbf{B}_5$	$-x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 - x_3 \mathbf{a}_3$	$=$	$-cx_3 \hat{\mathbf{z}}$	(2c)	Cr I
$\mathbf{B}_6$	$x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + x_4 \mathbf{a}_3$	$=$	$cx_4 \hat{\mathbf{z}}$	(2c)	O I
$\mathbf{B}_7$	$-x_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 - x_4 \mathbf{a}_3$	$=$	$-cx_4 \hat{\mathbf{z}}$	(2c)	O I
$\mathbf{B}_8$	$x_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_5 - z_5) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(x_5 - z_5) \hat{\mathbf{y}} + \frac{1}{3}c(2x_5 + z_5) \hat{\mathbf{z}}$	(6h)	O II
$\mathbf{B}_9$	$z_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 + x_5 \mathbf{a}_3$	$=$	$-\frac{1}{2}a(x_5 - z_5) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(x_5 - z_5) \hat{\mathbf{y}} + \frac{1}{3}c(2x_5 + z_5) \hat{\mathbf{z}}$	(6h)	O II
$\mathbf{B}_{10}$	$x_5 \mathbf{a}_1 + z_5 \mathbf{a}_2 + x_5 \mathbf{a}_3$	$=$	$-\frac{1}{\sqrt{3}}a(x_5 - z_5) \hat{\mathbf{y}} + \frac{1}{3}c(2x_5 + z_5) \hat{\mathbf{z}}$	(6h)	O II
$\mathbf{B}_{11}$	$-z_5 \mathbf{a}_1 - x_5 \mathbf{a}_2 - x_5 \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_5 - z_5) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_5 - z_5) \hat{\mathbf{y}} - \frac{1}{3}c(2x_5 + z_5) \hat{\mathbf{z}}$	(6h)	O II
$\mathbf{B}_{12}$	$-x_5 \mathbf{a}_1 - x_5 \mathbf{a}_2 - z_5 \mathbf{a}_3$	$=$	$-\frac{1}{2}a(x_5 - z_5) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_5 - z_5) \hat{\mathbf{y}} - \frac{1}{3}c(2x_5 + z_5) \hat{\mathbf{z}}$	(6h)	O II
$\mathbf{B}_{13}$	$-x_5 \mathbf{a}_1 - z_5 \mathbf{a}_2 - x_5 \mathbf{a}_3$	$=$	$\frac{1}{\sqrt{3}}a(x_5 - z_5) \hat{\mathbf{y}} - \frac{1}{3}c(2x_5 + z_5) \hat{\mathbf{z}}$	(6h)	O II

References

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Found in

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First cited in

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