

Rhombohedral Cr₂S₃ Structure:

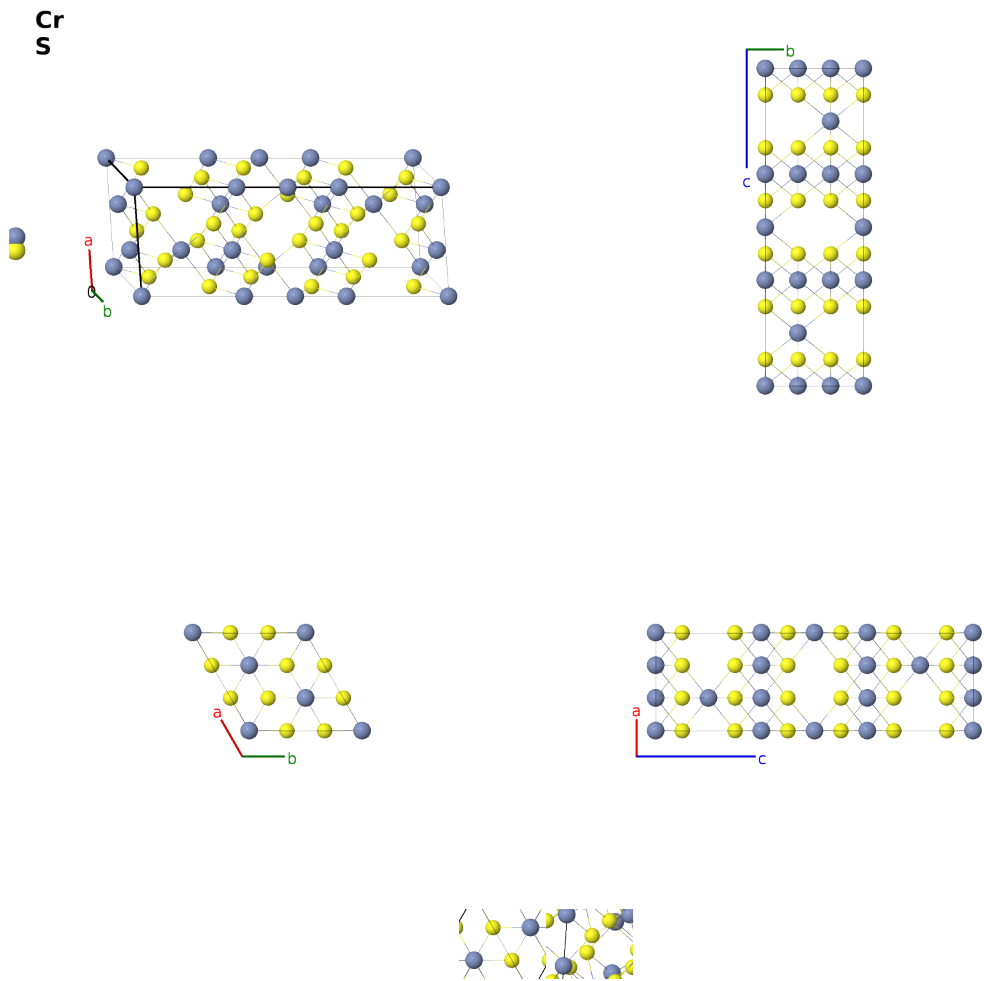
A2B3_hR10_148_abc_f-001

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

https://aflow.org/prototype-encyclopedia/A2B3_hR10_148_abc_f-001



Prototype	Cr ₂ S ₃
AFLOW prototype label	A2B3_hR10_148_abc_f-001
ICSD	16721
CCDC	1597272
Pearson symbol	hR10
Space group number	148
Space group symbol	$R\bar{3}$

AFLOW prototype command `aflow --proto=A2B3_hR10_148_abc_f-001`
 `--params=a,c/a,x3,x4,y4,z4`

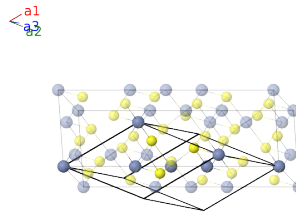
Other compounds with this structure

Cr_2Se_3 , Cr_2Te_3

- (Jellinek, 1957) lists two structures for Cr_2S_3 : this rhombohedral structure, and a trigonal structure. (Venkatraman, 1990) list this second structure as $\text{Cr}_2\text{S}_3\text{Cr}$. It is likely that this structure is Jellinek's Cr_5S_6 structure. Jellinek notes that the two structures are identical except for the atoms on the (2a) Wyckoff site. Presumably the Venkatraman structure is the Cr_5S_6 structure with the (2a) site partly filled.
 - Hexagonal settings of this structure can be obtained with the option `--hex`.
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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)	Cr I
$\mathbf{B}_2$	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2}c \hat{\mathbf{z}}$	(1b)	Cr II
$\mathbf{B}_3$	$x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + x_3 \mathbf{a}_3$	$=$	$cx_3 \hat{\mathbf{z}}$	(2c)	Cr III
$\mathbf{B}_4$	$-x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 - x_3 \mathbf{a}_3$	$=$	$-cx_3 \hat{\mathbf{z}}$	(2c)	Cr III
$\mathbf{B}_5$	$x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_4 - z_4) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_4 - 2y_4 + z_4) \hat{\mathbf{y}} + \frac{1}{3}c(x_4 + y_4 + z_4) \hat{\mathbf{z}}$	(6f)	S I
$\mathbf{B}_6$	$z_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + y_4 \mathbf{a}_3$	$=$	$-\frac{1}{2}a(y_4 - z_4) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(2x_4 - y_4 - z_4) \hat{\mathbf{y}} + \frac{1}{3}c(x_4 + y_4 + z_4) \hat{\mathbf{z}}$	(6f)	S I
$\mathbf{B}_7$	$y_4 \mathbf{a}_1 + z_4 \mathbf{a}_2 + x_4 \mathbf{a}_3$	$=$	$-\frac{1}{2}a(x_4 - y_4) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_4 + y_4 - 2z_4) \hat{\mathbf{y}} + \frac{1}{3}c(x_4 + y_4 + z_4) \hat{\mathbf{z}}$	(6f)	S I
$\mathbf{B}_8$	$-x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$-\frac{1}{2}a(x_4 - z_4) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(x_4 - 2y_4 + z_4) \hat{\mathbf{y}} - \frac{1}{3}c(x_4 + y_4 + z_4) \hat{\mathbf{z}}$	(6f)	S I
$\mathbf{B}_9$	$-z_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 - y_4 \mathbf{a}_3$	$=$	$\frac{1}{2}a(y_4 - z_4) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(2x_4 - y_4 - z_4) \hat{\mathbf{y}} - \frac{1}{3}c(x_4 + y_4 + z_4) \hat{\mathbf{z}}$	(6f)	S I
$\mathbf{B}_{10}$	$-y_4 \mathbf{a}_1 - z_4 \mathbf{a}_2 - x_4 \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_4 - y_4) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(x_4 + y_4 - 2z_4) \hat{\mathbf{y}} - \frac{1}{3}c(x_4 + y_4 + z_4) \hat{\mathbf{z}}$	(6f)	S I

References

- [1] F. Jellinek, *The Structures of the Chromium Sulphides*, Acta Cryst. **10**, 620–628 (1957), doi:10.1107/S0365110X57002200.
- [2] M. Venkatraman and J. P. Neumann, *Binary Alloy Phase Diagrams* (ASM International, 1990), vol. 2, chap. Cr-S (Chromium-Sulfur), ii edn. T. B. Massalski, Ed.

Found in

[1] R. T. Downs and M. Hall-Wallace, *The American Mineralogist Crystal Structure Database*, Am. Mineral. **88**, 247–250 (2003).

First cited in

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