$AlCCr_2$ Structure: ABC2_hP8_194_c_a_f-007

This structure previously used the label(s) `ABC2_hP8_194_d_a_f`. Calls to these addresses will be redirected here.

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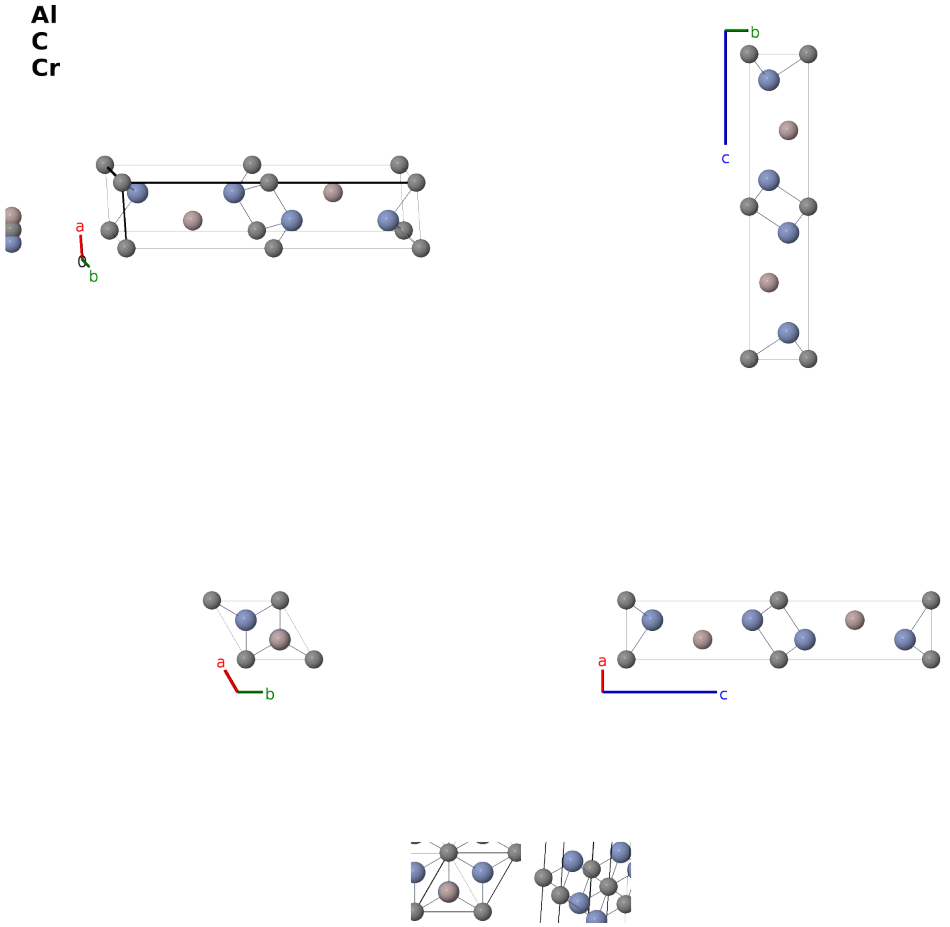
https://aflow.org/prototype-encyclopedia/NEW2

https://aflow.org/prototype-encyclopedia/ABC2_hP8_194_c_a_f-007



Prototype	$AlCCr_2$
AFLOW prototype label	ABC2_hP8_194_c_a_f-007
ICSD	42918
CCDC	1612531
Pearson symbol	hP8
Space group number	194

Space group symbol $P6_3/mmc$

AFLOW prototype command `aflow --proto=ABC2_hP8_194_c_a_f-007 --params=`$a, c/a, z_3$

Other compounds with this structure

$AlCCr_2$, $AlCCrV$, $AlCNb_2$, $AlCNbTi$, $AlCNbV$, $AlCTa_2$, $AlCTaTi$, $AlCTi_2$, $AlCTiV$, $AlCV_2$, $AlCuO_2$, $AlNTi_2$, $AsCV_2$, $CGeV_2$, $CSnTi_2$, $CdCTi_2$, CrC_2Ga, CrC_2Ge, $CuCNb_2$, $GaCCr_2$, $GaCMo_2$, $GaCNb_2$, $GaCTa_2$, $GaCTi_2$, $GaCV_2$, $GaCY_2$, $GaNCr_2$, $GaNTi_2$, $GeCCr_2$, $GeCTi_2$, $GeCV_2$, HfC_2In, HfC_2Pb, HfC_2Sn, HfC_2Tl, $InCHf_2$, $InCNb_2$, $InCTi_2$, $InCZr_2$, $InNTi_2$, $InNZr_2$, $PCNb_2$, PCV_2, $PbCHf_2$, $PbCTi_2$, $PbCZr_2$, $SCTi_2$, $SCZr_2$, $SnCHf_2$, $SnCNb_2$, $SnCSc_2$, $SnCTi_2$, $SnCZr_2$, $TlCHf_2$, $TlCTi_2$, $TlCZr_2$, $ZnCTi_2$, $ZnCV_2$, $ZnNTi_2$

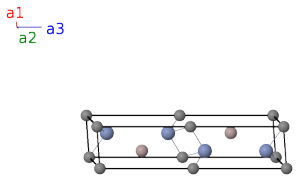
- This is a MAX phase (layered $M_{n+1}AX_n$ hexagonal structure).
- Note that all of the atoms sit on close-packed <0001> planes. The stacking sequence may be written

Atom	Cr	C	Cr	Al	Cr	C	Cr	Al
Position	B	A	C	B	C	A	B	C

- AFLOW shifts the origin by (0 0 c/2), moving the aluminum atoms from the published (2d) Wyckoff position to the (2c) position.

Hexagonal primitive vectors

$$\mathbf{a_1} = \frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,\hat{\mathbf{y}}$$
$$\mathbf{a_2} = \frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(2a)	C I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}c\,\hat{\mathbf{z}}$	(2a)	C I
$\mathbf{B_3}$	=	$\frac{1}{3}\,\mathbf{a}_1 + \frac{2}{3}\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(2c)	Al I
$\mathbf{B_4}$	=	$\frac{2}{3}\,\mathbf{a}_1 + \frac{1}{3}\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(2c)	Al I
$\mathbf{B_5}$	=	$\frac{1}{3}\,\mathbf{a}_1 + \frac{2}{3}\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(4f)	Cr I
$\mathbf{B_6}$	=	$\frac{2}{3}\,\mathbf{a}_1 + \frac{1}{3}\,\mathbf{a}_2 + \left(z_3 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + c\left(z_3 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4f)	Cr I
$\mathbf{B_7}$	=	$\frac{2}{3}\,\mathbf{a}_1 + \frac{1}{3}\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} - cz_3\,\hat{\mathbf{z}}$	(4f)	Cr I
$\mathbf{B_8}$	=	$\frac{1}{3}\,\mathbf{a}_1 + \frac{2}{3}\,\mathbf{a}_2 - \left(z_3 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} - c\left(z_3 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4f)	Cr I

References

[1] W. Jeitschko, H. Nowotny, and F. Benesovsky, *Kohlenstoffhaltige ternäre Verbindungen (H-Phase)*, Monatsh. Chem. Verw. Tl. **94**, 672–676 (1963), doi:10.1007/BF00913068.

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.

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