$AlCCr_2$ Structure: ABC2_hP8_194_c_a_f-007

This structure originally had the label `ABC2_hP8_194_d_a_f`. Calls to that address will be redirected here.

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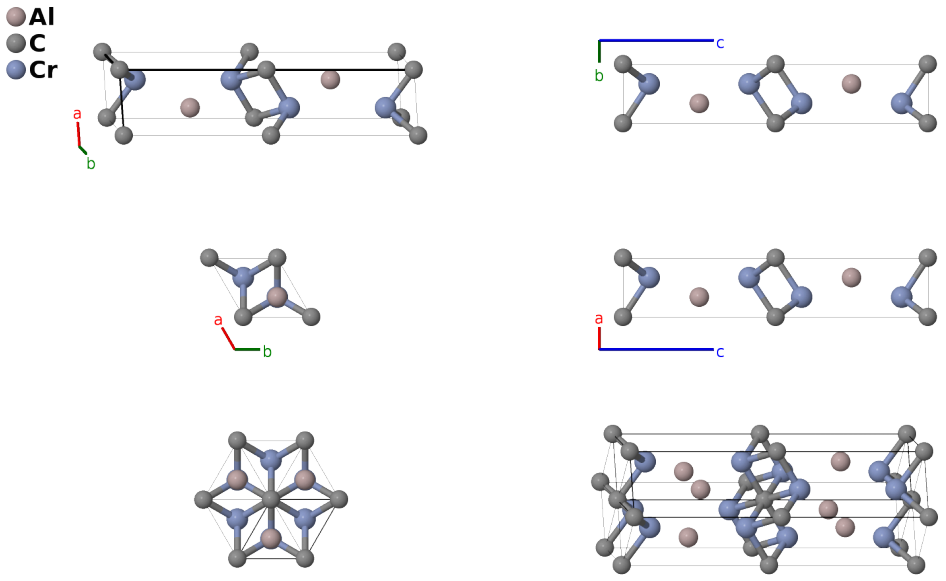
https://aflow.org/p/NEW2

https://aflow.org/p/ABC2_hP8_194_c_a_f-007



Prototype	$AlCCr_2$
AFLOW prototype label	ABC2_hP8_194_c_a_f-007
ICSD	42918
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

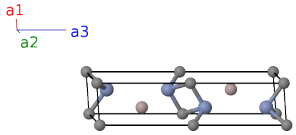
$AlCNb_2$, $AlCTa_2$, $AlCTi_2$, $AlCV_2$, $AlCuO_2$, $AlNTi_2$, $AsCV_2$, $CCdTi_2$, $CGaCr_2$, $CGaMo_2$, $CGaNb_2$, $CGaTi_2$, $CGaY_2$, $CGeCr_2$, $CGeTi_2$, $CGeV_2$, $CInHf_2$, $CInNb_2$, $CInTi_2$, $CInZr_2$, $CPNb_2$, CPV_2, $CPbHf_2$, $CPbTi_2$, $CPbZr_2$, $CSTi_2$, $CSZr_2$, $CSnHf_2$, $CSnNb_2$, $CSnTi_2$, $CSnZr_2$, $CTlHf_2$, $CTlTi_2$, $GaNCr_2$

- 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

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.