Cr_5Al_8 ($D8_{10}$) Structure: A8B5_hR26_160_a3bc_a3b-001

This structure originally had the label `A8B5_hR26_160_a3bc_a3b`. Calls to that address will be redirected here.

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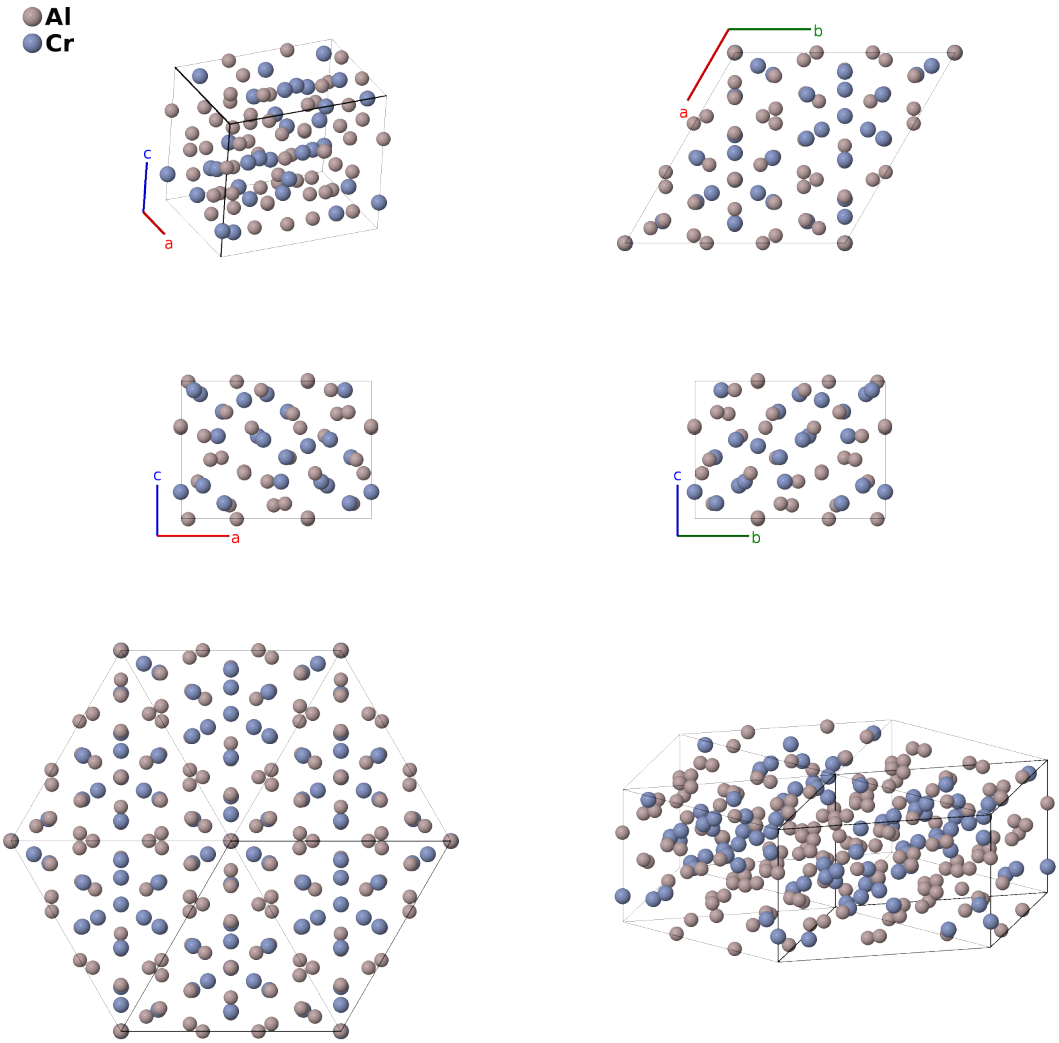
https://aflow.org/p/X9QA

https://aflow.org/p/A8B5_hR26_160_a3bc_a3b-001



Prototype	Al_8Cr_5
AFLOW prototype label	A8B5_hR26_160_a3bc_a3b-001
***Strukturbericht* designation**	$D8_{10}$
ICSD	606753
Pearson symbol	hR26
Space group number	160

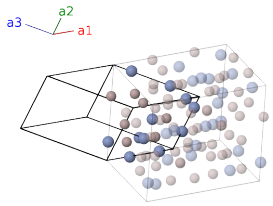
Space group symbol $R3m$

AFLOW prototype command `aflow --proto=A8B5_hR26_160_a3bc_a3b-001 --params=`$a, c/a, x_1, x_2, x_3, z_3, x_4, z_4, x_5, z_5, x_6, z_6, x_7, z_7, x_8, z_8, x_9, y_9, z_9$

- (Bradley, 1937) notes that the positions here are very close to the positions of the atoms in the γ-brass (Cu_5Zn_8, $D8_2$) structure.
- (Mizutani, 2010) classifies this as an "R-cell" γ-brass.

Rhombohedral primitive vectors

$$\mathbf{a_1} = \frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{1}{3}c\,\hat{\mathbf{z}}$$
$$\mathbf{a_2} = \frac{1}{\sqrt{3}}a\,\hat{\mathbf{y}} + \frac{1}{3}c\,\hat{\mathbf{z}}$$
$$\mathbf{a_3} = -\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{1}{3}c\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$x_1\,\mathbf{a}_1 + x_1\,\mathbf{a}_2 + x_1\,\mathbf{a}_3$	=	$cx_1\,\hat{\mathbf{z}}$	(1a)	Al I
$\mathbf{B_2}$	=	$x_2\,\mathbf{a}_1 + x_2\,\mathbf{a}_2 + x_2\,\mathbf{a}_3$	=	$cx_2\,\hat{\mathbf{z}}$	(1a)	Cr I
$\mathbf{B_3}$	=	$x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_3 - z_3)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(x_3 - z_3)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(2x_3 + z_3)\,\hat{\mathbf{z}}$	(3b)	Al II
$\mathbf{B_4}$	=	$z_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + x_3\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(x_3 - z_3)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(x_3 - z_3)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(2x_3 + z_3)\,\hat{\mathbf{z}}$	(3b)	Al II
$\mathbf{B_5}$	=	$x_3\,\mathbf{a}_1 + z_3\,\mathbf{a}_2 + x_3\,\mathbf{a}_3$	=	$-\frac{1}{\sqrt{3}}a\,(x_3 - z_3)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(2x_3 + z_3)\,\hat{\mathbf{z}}$	(3b)	Al II
$\mathbf{B_6}$	=	$x_4\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_4 - z_4)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(x_4 - z_4)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(2x_4 + z_4)\,\hat{\mathbf{z}}$	(3b)	Al III
$\mathbf{B_7}$	=	$z_4\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 + x_4\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(x_4 - z_4)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(x_4 - z_4)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(2x_4 + z_4)\,\hat{\mathbf{z}}$	(3b)	Al III
$\mathbf{B_8}$	=	$x_4\,\mathbf{a}_1 + z_4\,\mathbf{a}_2 + x_4\,\mathbf{a}_3$	=	$-\frac{1}{\sqrt{3}}a\,(x_4 - z_4)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(2x_4 + z_4)\,\hat{\mathbf{z}}$	(3b)	Al III
$\mathbf{B_9}$	=	$x_5\,\mathbf{a}_1 + x_5\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_5 - z_5)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(x_5 - z_5)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(2x_5 + z_5)\,\hat{\mathbf{z}}$	(3b)	Al IV
$\mathbf{B_{10}}$	=	$z_5\,\mathbf{a}_1 + x_5\,\mathbf{a}_2 + x_5\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(x_5 - z_5)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(x_5 - z_5)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(2x_5 + z_5)\,\hat{\mathbf{z}}$	(3b)	Al IV
$\mathbf{B_{11}}$	=	$x_5\,\mathbf{a}_1 + z_5\,\mathbf{a}_2 + x_5\,\mathbf{a}_3$	=	$-\frac{1}{\sqrt{3}}a\,(x_5 - z_5)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(2x_5 + z_5)\,\hat{\mathbf{z}}$	(3b)	Al IV
$\mathbf{B_{12}}$	=	$x_6\,\mathbf{a}_1 + x_6\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_6 - z_6)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(x_6 - z_6)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(2x_6 + z_6)\,\hat{\mathbf{z}}$	(3b)	Cr II
$\mathbf{B_{13}}$	=	$z_6\,\mathbf{a}_1 + x_6\,\mathbf{a}_2 + x_6\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(x_6 - z_6)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(x_6 - z_6)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(2x_6 + z_6)\,\hat{\mathbf{z}}$	(3b)	Cr II
$\mathbf{B_{14}}$	=	$x_6\,\mathbf{a}_1 + z_6\,\mathbf{a}_2 + x_6\,\mathbf{a}_3$	=	$-\frac{1}{\sqrt{3}}a\,(x_6 - z_6)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(2x_6 + z_6)\,\hat{\mathbf{z}}$	(3b)	Cr II
$\mathbf{B_{15}}$	=	$x_7\,\mathbf{a}_1 + x_7\,\mathbf{a}_2 + z_7\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_7 - z_7)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(x_7 - z_7)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(2x_7 + z_7)\,\hat{\mathbf{z}}$	(3b)	Cr III
$\mathbf{B_{16}}$	=	$z_7\,\mathbf{a}_1 + x_7\,\mathbf{a}_2 + x_7\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(x_7 - z_7)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(x_7 - z_7)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(2x_7 + z_7)\,\hat{\mathbf{z}}$	(3b)	Cr III

$\mathbf{B_{17}}$	$=$	$x_7\,\mathbf{a}_1 + z_7\,\mathbf{a}_2 + x_7\,\mathbf{a}_3$	$=$	$-\frac{1}{\sqrt{3}}a\,(x_7 - z_7)\;\hat{\mathbf{y}} + \frac{1}{3}c\,(2x_7 + z_7)\;\hat{\mathbf{z}}$	(3b)	Cr III
$\mathbf{B_{18}}$	$=$	$x_8\,\mathbf{a}_1 + x_8\,\mathbf{a}_2 + z_8\,\mathbf{a}_3$	$=$	$\frac{1}{2}a\,(x_8 - z_8)\;\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(x_8 - z_8)\;\hat{\mathbf{y}} + \frac{1}{3}c\,(2x_8 + z_8)\;\hat{\mathbf{z}}$	(3b)	Cr IV
$\mathbf{B_{19}}$	$=$	$z_8\,\mathbf{a}_1 + x_8\,\mathbf{a}_2 + x_8\,\mathbf{a}_3$	$=$	$-\frac{1}{2}a\,(x_8 - z_8)\;\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(x_8 - z_8)\;\hat{\mathbf{y}} + \frac{1}{3}c\,(2x_8 + z_8)\;\hat{\mathbf{z}}$	(3b)	Cr IV
$\mathbf{B_{20}}$	$=$	$x_8\,\mathbf{a}_1 + z_8\,\mathbf{a}_2 + x_8\,\mathbf{a}_3$	$=$	$-\frac{1}{\sqrt{3}}a\,(x_8 - z_8)\;\hat{\mathbf{y}} + \frac{1}{3}c\,(2x_8 + z_8)\;\hat{\mathbf{z}}$	(3b)	Cr IV
$\mathbf{B_{21}}$	$=$	$x_9\,\mathbf{a}_1 + y_9\,\mathbf{a}_2 + z_9\,\mathbf{a}_3$	$=$	$\frac{1}{2}a\,(x_9 - z_9)\;\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,(x_9 - 2y_9 + z_9)\;\hat{\mathbf{y}} + \frac{1}{3}c\,(x_9 + y_9 + z_9)\;\hat{\mathbf{z}}$	(6c)	Al V
$\mathbf{B_{22}}$	$=$	$z_9\,\mathbf{a}_1 + x_9\,\mathbf{a}_2 + y_9\,\mathbf{a}_3$	$=$	$-\frac{1}{2}a\,(y_9 - z_9)\;\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(2x_9 - y_9 - z_9)\;\hat{\mathbf{y}} + \frac{1}{3}c\,(x_9 + y_9 + z_9)\;\hat{\mathbf{z}}$	(6c)	Al V
$\mathbf{B_{23}}$	$=$	$y_9\,\mathbf{a}_1 + z_9\,\mathbf{a}_2 + x_9\,\mathbf{a}_3$	$=$	$-\frac{1}{2}a\,(x_9 - y_9)\;\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,(x_9 + y_9 - 2z_9)\;\hat{\mathbf{y}} + \frac{1}{3}c\,(x_9 + y_9 + z_9)\;\hat{\mathbf{z}}$	(6c)	Al V
$\mathbf{B_{24}}$	$=$	$z_9\,\mathbf{a}_1 + y_9\,\mathbf{a}_2 + x_9\,\mathbf{a}_3$	$=$	$-\frac{1}{2}a\,(x_9 - z_9)\;\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,(x_9 - 2y_9 + z_9)\;\hat{\mathbf{y}} + \frac{1}{3}c\,(x_9 + y_9 + z_9)\;\hat{\mathbf{z}}$	(6c)	Al V
$\mathbf{B_{25}}$	$=$	$y_9\,\mathbf{a}_1 + x_9\,\mathbf{a}_2 + z_9\,\mathbf{a}_3$	$=$	$\frac{1}{2}a\,(y_9 - z_9)\;\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(2x_9 - y_9 - z_9)\;\hat{\mathbf{y}} + \frac{1}{3}c\,(x_9 + y_9 + z_9)\;\hat{\mathbf{z}}$	(6c)	Al V
$\mathbf{B_{26}}$	$=$	$x_9\,\mathbf{a}_1 + z_9\,\mathbf{a}_2 + y_9\,\mathbf{a}_3$	$=$	$\frac{1}{2}a\,(x_9 - y_9)\;\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,(x_9 + y_9 - 2z_9)\;\hat{\mathbf{y}} + \frac{1}{3}c\,(x_9 + y_9 + z_9)\;\hat{\mathbf{z}}$	(6c)	Al V

References

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