

HoAl₃ Structure:

A3B_hR20_166_d2h_b2c-001

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<https://aflow.org/prototype-encyclopedia/4SER>

https://aflow.org/prototype-encyclopedia/A3B_hR20_166_d2h_b2c-001

Prototype	Al ₃ Ho
AFLOW prototype label	A3B_hR20_166_d2h_b2c-001
ICSD	57912
CCDC	1621951
Pearson symbol	hR20
Space group number	166
Space group symbol	$R\bar{3}m$
AFLOW prototype command	<code>aflow --proto=A3B_hR20_166_d2h_b2c-001</code> <code>--params=a, c/a, x₂, x₃, x₅, z₅, x₆, z₆</code>

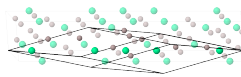
Other compounds with this structure

DyAl₃, ErAl₃, TbAl₃, YAl₃

Rhombohedral primitive vectors

$$\begin{aligned}\mathbf{a}_1 &= \frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + \frac{1}{3}c \hat{\mathbf{z}} \\ \mathbf{a}_2 &= \frac{1}{\sqrt{3}}a \hat{\mathbf{y}} + \frac{1}{3}c \hat{\mathbf{z}} \\ \mathbf{a}_3 &= -\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + \frac{1}{3}c \hat{\mathbf{z}}\end{aligned}$$

-45



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2}c \hat{\mathbf{z}}$	(1b)	Ho 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)	Ho 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)	Ho 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)	Ho III

$\mathbf{B}_5$	$=$	$-x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 - x_3 \mathbf{a}_3$	$=$	$-cx_3 \hat{\mathbf{z}}$	(2c)	Ho III
$\mathbf{B}_6$	$=$	$\frac{1}{2} \mathbf{a}_1$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{12}a \hat{\mathbf{y}} + \frac{1}{6}c \hat{\mathbf{z}}$	(3d)	Al I
$\mathbf{B}_7$	$=$	$\frac{1}{2} \mathbf{a}_2$	$=$	$\frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + \frac{1}{6}c \hat{\mathbf{z}}$	(3d)	Al I
$\mathbf{B}_8$	$=$	$\frac{1}{2} \mathbf{a}_3$	$=$	$-\frac{1}{4}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{12}a \hat{\mathbf{y}} + \frac{1}{6}c \hat{\mathbf{z}}$	(3d)	Al I
$\mathbf{B}_9$	$=$	$x_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_5 - z_5) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(x_5 - z_5) \hat{\mathbf{y}} + \frac{1}{3}c(2x_5 + z_5) \hat{\mathbf{z}}$	(6h)	Al II
$\mathbf{B}_{10}$	$=$	$z_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 + x_5 \mathbf{a}_3$	$=$	$-\frac{1}{2}a(x_5 - z_5) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(x_5 - z_5) \hat{\mathbf{y}} + \frac{1}{3}c(2x_5 + z_5) \hat{\mathbf{z}}$	(6h)	Al II
$\mathbf{B}_{11}$	$=$	$x_5 \mathbf{a}_1 + z_5 \mathbf{a}_2 + x_5 \mathbf{a}_3$	$=$	$-\frac{1}{\sqrt{3}}a(x_5 - z_5) \hat{\mathbf{y}} + \frac{1}{3}c(2x_5 + z_5) \hat{\mathbf{z}}$	(6h)	Al II
$\mathbf{B}_{12}$	$=$	$-z_5 \mathbf{a}_1 - x_5 \mathbf{a}_2 - x_5 \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_5 - z_5) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_5 - z_5) \hat{\mathbf{y}} - \frac{1}{3}c(2x_5 + z_5) \hat{\mathbf{z}}$	(6h)	Al II
$\mathbf{B}_{13}$	$=$	$-x_5 \mathbf{a}_1 - x_5 \mathbf{a}_2 - z_5 \mathbf{a}_3$	$=$	$-\frac{1}{2}a(x_5 - z_5) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_5 - z_5) \hat{\mathbf{y}} - \frac{1}{3}c(2x_5 + z_5) \hat{\mathbf{z}}$	(6h)	Al II
$\mathbf{B}_{14}$	$=$	$-x_5 \mathbf{a}_1 - z_5 \mathbf{a}_2 - x_5 \mathbf{a}_3$	$=$	$\frac{1}{\sqrt{3}}a(x_5 - z_5) \hat{\mathbf{y}} - \frac{1}{3}c(2x_5 + z_5) \hat{\mathbf{z}}$	(6h)	Al II
$\mathbf{B}_{15}$	$=$	$x_6 \mathbf{a}_1 + x_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_6 - z_6) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(x_6 - z_6) \hat{\mathbf{y}} + \frac{1}{3}c(2x_6 + z_6) \hat{\mathbf{z}}$	(6h)	Al III
$\mathbf{B}_{16}$	$=$	$z_6 \mathbf{a}_1 + x_6 \mathbf{a}_2 + x_6 \mathbf{a}_3$	$=$	$-\frac{1}{2}a(x_6 - z_6) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(x_6 - z_6) \hat{\mathbf{y}} + \frac{1}{3}c(2x_6 + z_6) \hat{\mathbf{z}}$	(6h)	Al III
$\mathbf{B}_{17}$	$=$	$x_6 \mathbf{a}_1 + z_6 \mathbf{a}_2 + x_6 \mathbf{a}_3$	$=$	$-\frac{1}{\sqrt{3}}a(x_6 - z_6) \hat{\mathbf{y}} + \frac{1}{3}c(2x_6 + z_6) \hat{\mathbf{z}}$	(6h)	Al III
$\mathbf{B}_{18}$	$=$	$-z_6 \mathbf{a}_1 - x_6 \mathbf{a}_2 - x_6 \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_6 - z_6) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_6 - z_6) \hat{\mathbf{y}} - \frac{1}{3}c(2x_6 + z_6) \hat{\mathbf{z}}$	(6h)	Al III
$\mathbf{B}_{19}$	$=$	$-x_6 \mathbf{a}_1 - x_6 \mathbf{a}_2 - z_6 \mathbf{a}_3$	$=$	$-\frac{1}{2}a(x_6 - z_6) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_6 - z_6) \hat{\mathbf{y}} - \frac{1}{3}c(2x_6 + z_6) \hat{\mathbf{z}}$	(6h)	Al III
$\mathbf{B}_{20}$	$=$	$-x_6 \mathbf{a}_1 - z_6 \mathbf{a}_2 - x_6 \mathbf{a}_3$	$=$	$\frac{1}{\sqrt{3}}a(x_6 - z_6) \hat{\mathbf{y}} - \frac{1}{3}c(2x_6 + z_6) \hat{\mathbf{z}}$	(6h)	Al III

References

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Al
Ho

