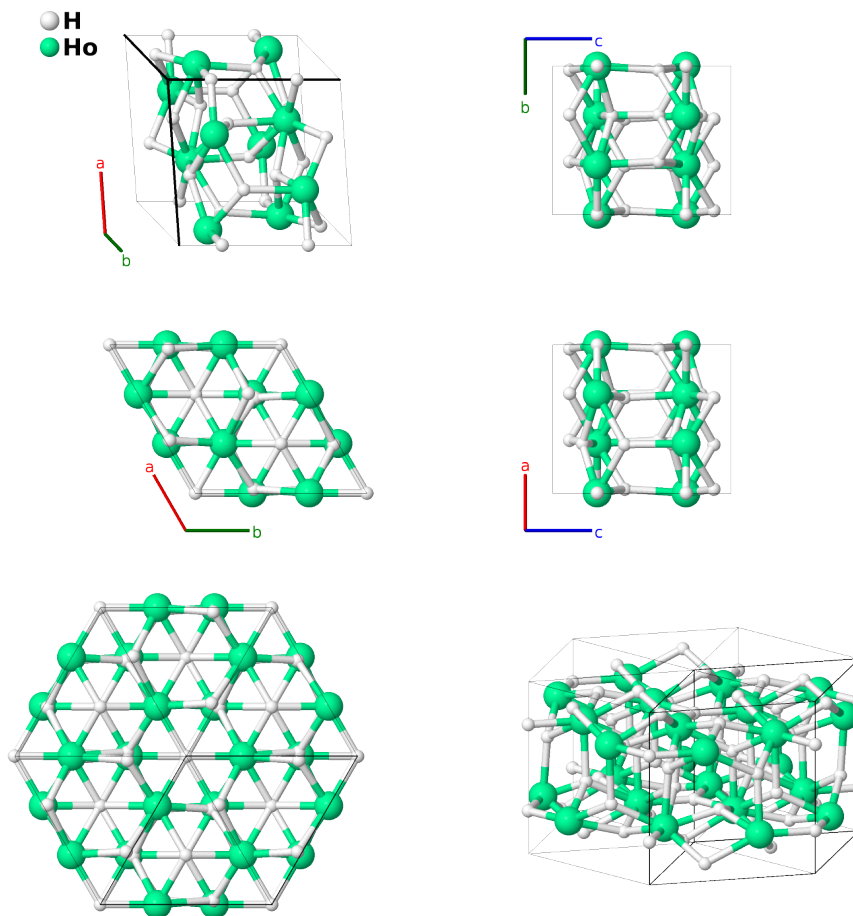# H₃Ho Structure:
A3B_hP24_165_adg_f-001

This structure originally had the label `A3B_hP24_165_adg_f`. Calls to that address will be redirected here.

https://aflow.org/p/V86P

https://aflow.org/p/A3B_hP24_165_adg_f-001

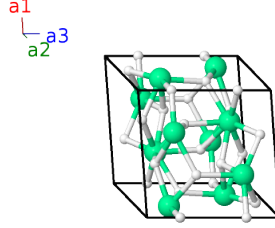|	
Prototype	H₃Ho
AFLOW prototype label	A3B_hP24_165_adg_f-001
ICSD	16880
Pearson symbol	hP24
Space group number	165
Space group symbol	$P\bar{3}c1$
AFLOW prototype command	aflow --proto=A3B_hP24_165_adg_f-001 --params=$a, c/a, z_2, x_3, x_4, y_4, z_4$

Other compounds with this structure

H_3Dy, H_3Er, H_3Gd, H_3Lu, H_3Sm, H_3Tb, H_3Tm, H_3Y, F_3La

- This structure is crystallographically equivalent to Cu_3P ($D0_{21}$). We retain it as the prototype for the subclass of this prototype containing hydrogen.

- The data was taken for the deuteride, D_3Ho.

Trigonal (Hexagonal) primitive vectors

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

Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$\tfrac{1}{4}\mathbf{a_3}$	=	$\tfrac{1}{4}c\,\hat{\mathbf{z}}$	(2a)	H I
$\mathbf{B_2}$	=	$\tfrac{3}{4}\mathbf{a_3}$	=	$\tfrac{3}{4}c\,\hat{\mathbf{z}}$	(2a)	H I
$\mathbf{B_3}$	=	$\tfrac{1}{3}\mathbf{a_1} + \tfrac{2}{3}\mathbf{a_2} + z_2\,\mathbf{a_3}$	=	$\tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(4d)	H II
$\mathbf{B_4}$	=	$\tfrac{2}{3}\mathbf{a_1} + \tfrac{1}{3}\mathbf{a_2} - \left(z_2 - \tfrac{1}{2}\right)\mathbf{a_3}$	=	$\tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} - c\left(z_2 - \tfrac{1}{2}\right)\hat{\mathbf{z}}$	(4d)	H II
$\mathbf{B_5}$	=	$\tfrac{2}{3}\mathbf{a_1} + \tfrac{1}{3}\mathbf{a_2} - z_2\,\mathbf{a_3}$	=	$\tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} - cz_2\,\hat{\mathbf{z}}$	(4d)	H II
$\mathbf{B_6}$	=	$\tfrac{1}{3}\mathbf{a_1} + \tfrac{2}{3}\mathbf{a_2} + \left(z_2 + \tfrac{1}{2}\right)\mathbf{a_3}$	=	$\tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + c\left(z_2 + \tfrac{1}{2}\right)\hat{\mathbf{z}}$	(4d)	H II
$\mathbf{B_7}$	=	$x_3\,\mathbf{a_1} + \tfrac{1}{4}\mathbf{a_3}$	=	$\tfrac{1}{2}ax_3\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}ax_3\,\hat{\mathbf{y}} + \tfrac{1}{4}c\,\hat{\mathbf{z}}$	(6f)	Ho I
$\mathbf{B_8}$	=	$x_3\,\mathbf{a_2} + \tfrac{1}{4}\mathbf{a_3}$	=	$\tfrac{1}{2}ax_3\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}ax_3\,\hat{\mathbf{y}} + \tfrac{1}{4}c\,\hat{\mathbf{z}}$	(6f)	Ho I
$\mathbf{B_9}$	=	$-x_3\,\mathbf{a_1} - x_3\,\mathbf{a_2} + \tfrac{1}{4}\mathbf{a_3}$	=	$-ax_3\,\hat{\mathbf{x}} + \tfrac{1}{4}c\,\hat{\mathbf{z}}$	(6f)	Ho I
$\mathbf{B_{10}}$	=	$-x_3\,\mathbf{a_1} + \tfrac{3}{4}\mathbf{a_3}$	=	$-\tfrac{1}{2}ax_3\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}ax_3\,\hat{\mathbf{y}} + \tfrac{3}{4}c\,\hat{\mathbf{z}}$	(6f)	Ho I
$\mathbf{B_{11}}$	=	$-x_3\,\mathbf{a_2} + \tfrac{3}{4}\mathbf{a_3}$	=	$-\tfrac{1}{2}ax_3\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}ax_3\,\hat{\mathbf{y}} + \tfrac{3}{4}c\,\hat{\mathbf{z}}$	(6f)	Ho I
$\mathbf{B_{12}}$	=	$x_3\,\mathbf{a_1} + x_3\,\mathbf{a_2} + \tfrac{3}{4}\mathbf{a_3}$	=	$ax_3\,\hat{\mathbf{x}} + \tfrac{3}{4}c\,\hat{\mathbf{z}}$	(6f)	Ho I
$\mathbf{B_{13}}$	=	$x_4\,\mathbf{a_1} + y_4\,\mathbf{a_2} + z_4\,\mathbf{a_3}$	=	$\tfrac{1}{2}a\left(x_4 + y_4\right)\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}a\left(x_4 - y_4\right)\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(12g)	H III
$\mathbf{B_{14}}$	=	$-y_4\,\mathbf{a_1} + \left(x_4 - y_4\right)\mathbf{a_2} + z_4\,\mathbf{a_3}$	=	$\tfrac{1}{2}a\left(x_4 - 2y_4\right)\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}ax_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(12g)	H III
$\mathbf{B_{15}}$	=	$-\left(x_4 - y_4\right)\mathbf{a_1} - x_4\,\mathbf{a_2} + z_4\,\mathbf{a_3}$	=	$-\tfrac{1}{2}a\left(2x_4 - y_4\right)\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}ay_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(12g)	H III
$\mathbf{B_{16}}$	=	$y_4\,\mathbf{a_1} + x_4\,\mathbf{a_2} - \left(z_4 - \tfrac{1}{2}\right)\mathbf{a_3}$	=	$\tfrac{1}{2}a\left(x_4 + y_4\right)\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}a\left(x_4 - y_4\right)\hat{\mathbf{y}} - c\left(z_4 - \tfrac{1}{2}\right)\hat{\mathbf{z}}$	(12g)	H III
$\mathbf{B_{17}}$	=	$\left(x_4 - y_4\right)\mathbf{a_1} - y_4\,\mathbf{a_2} - \left(z_4 - \tfrac{1}{2}\right)\mathbf{a_3}$	=	$\tfrac{1}{2}a\left(x_4 - 2y_4\right)\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}ax_4\,\hat{\mathbf{y}} - c\left(z_4 - \tfrac{1}{2}\right)\hat{\mathbf{z}}$	(12g)	H III
$\mathbf{B_{18}}$	=	$-x_4\,\mathbf{a_1} - \left(x_4 - y_4\right)\mathbf{a_2} - \left(z_4 - \tfrac{1}{2}\right)\mathbf{a_3}$	=	$-\tfrac{1}{2}a\left(2x_4 - y_4\right)\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}ay_4\,\hat{\mathbf{y}} - c\left(z_4 - \tfrac{1}{2}\right)\hat{\mathbf{z}}$	(12g)	H III
$\mathbf{B_{19}}$	=	$-x_4\,\mathbf{a_1} - y_4\,\mathbf{a_2} - z_4\,\mathbf{a_3}$	=	$-\tfrac{1}{2}a\left(x_4 + y_4\right)\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}a\left(x_4 - y_4\right)\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$	(12g)	H III
$\mathbf{B_{20}}$	=	$y_4\,\mathbf{a_1} - \left(x_4 - y_4\right)\mathbf{a_2} - z_4\,\mathbf{a_3}$	=	$\tfrac{1}{2}a\left(-x_4 + 2y_4\right)\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}ax_4\,\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$	(12g)	H III
$\mathbf{B_{21}}$	=	$\left(x_4 - y_4\right)\mathbf{a_1} + x_4\,\mathbf{a_2} - z_4\,\mathbf{a_3}$	=	$\tfrac{1}{2}a\left(2x_4 - y_4\right)\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}ay_4\,\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$	(12g)	H III

$$\mathbf{B_{22}} = -y_4\,\mathbf{a_1} - x_4\,\mathbf{a_2} + \left(z_4 + \tfrac{1}{2}\right)\mathbf{a_3} = -\tfrac{1}{2}a\left(x_4 + y_4\right)\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}a\left(x_4 - y_4\right)\hat{\mathbf{y}} + c\left(z_4 + \tfrac{1}{2}\right)\hat{\mathbf{z}} \quad (12\text{g}) \qquad \text{H III}$$

$$\mathbf{B_{23}} = -\left(x_4 - y_4\right)\mathbf{a_1} + y_4\,\mathbf{a_2} + \left(z_4 + \tfrac{1}{2}\right)\mathbf{a_3} = \tfrac{1}{2}a\left(-x_4 + 2y_4\right)\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}ax_4\,\hat{\mathbf{y}} + c\left(z_4 + \tfrac{1}{2}\right)\hat{\mathbf{z}} \quad (12\text{g}) \qquad \text{H III}$$

$$\mathbf{B_{24}} = x_4\,\mathbf{a_1} + \left(x_4 - y_4\right)\mathbf{a_2} + \left(z_4 + \tfrac{1}{2}\right)\mathbf{a_3} = \tfrac{1}{2}a\left(2x_4 - y_4\right)\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}ay_4\,\hat{\mathbf{y}} + c\left(z_4 + \tfrac{1}{2}\right)\hat{\mathbf{z}} \quad (12\text{g}) \qquad \text{H III}$$

References

[1] M. Mansmann and W. E. Wallace, *The Structure of HoD₃*, Le Journal de Physique **25**, 454–459 (1964), doi:10.1051/jphys:01964002505045400.

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.